

ESC384: Partial Differential Equations

Lecture Notes

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Part I

Introduction

Lecture 1

Introduction to PDEs

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1.1 Introduction

Our goal in this lecture is to introduce some of the key concepts that we will visit throughout this course. We provide a definition of partial differential equations (PDEs) and a few model (and carefully chosen) PDEs. We then discuss several ways to classify PDEs with a particular emphasis on second-order PDEs, which are ubiquitous in science and engineering. We conclude the lecture with examples of PDEs in science and engineering.

1.2 Partial differential equations

We first provide a definition of PDEs:

Definition 1.1 (partial differential equation (PDE)). A PDE is an equation that relates an unknown function u and some of its partial derivatives, where the function is defined over a n -dimensional spatial domain $\Omega \subset \mathbb{R}^n$ and time interval $I \subset \mathbb{R}$. In general, a PDE can be expressed as

$$G\left(x_1, \dots, x_n, t, u, \frac{\partial u}{\partial x_1}, \dots, \frac{\partial u}{\partial x_n}, \frac{\partial u}{\partial t}, \frac{\partial^2 u}{\partial x_1^2}, \frac{\partial^2 u}{\partial x_1 x_2}, \dots\right) = 0,$$

where x_1, \dots, x_n are the spatial coordinates, t is the time, and $\frac{\partial u}{\partial x_1}, \dots$ denote the partial derivatives.

We provide a few concrete examples of model PDEs that we will study throughout this course:

- **Laplace's equation.** Laplace's equation is given by

$$-\Delta u = 0,$$

where $\Delta = \nabla \cdot \nabla = \frac{\partial^2}{\partial x_1^2} + \dots + \frac{\partial^2}{\partial x_n^2}$ is the Laplacian. Laplace's equation describes various physical phenomena including (but not limited to) the following: steady heat transfer (without a heat source), where u is the temperature; electrostatics, where u is the electrostatic potential; and steady, inviscid, incompressible, irrotational flow, where u is the velocity potential.

- **Poisson's equation.** Poisson's equation is given by

$$-\Delta u = f,$$

where f is a source function. Poisson's equation describes the following: steady heat transfer in the presence of a heat source; and electrostatic potential in the presence of charge. Laplace's equation is a special case of Poisson's equation for $f = 0$.

- **Heat equation.** The heat equation is given by

$$\frac{\partial u}{\partial t} - \nabla \cdot a \nabla u = f,$$

where a is the diffusivity constant, and f is the source term. The heat equation describes the following: unsteady heat transfer; and the diffusion of chemical species.

- **Transport equation.** The transport equation is given by

$$\frac{\partial u}{\partial t} + b \cdot \nabla u = 0,$$

where b is an advection field. The transport equation describes the transport of conserved quantity (e.g., concentration of chemical species) in the presence of an advection field.

- **Wave equation.** The wave equation is given by

$$\frac{\partial^2 u}{\partial t^2} - c^2 \Delta u = 0,$$

where c is the wave propagation speed. The wave equation describes the propagation of waves through a medium, including the following: the propagation of the acoustic pressure wave in the air; electromagnetic fields through space; and the vibration of taut strings and membranes.

- **Burgers' equation.** The (inviscid) Burgers' equation is given by

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = 0.$$

The Burgers' equation describes the propagation of a nonlinear wave, in which the speed of propagation depends on the solution value. The equation models features such as shocks and rarefaction waves that are encountered in compressible flows.

1.3 Classification of PDEs

To facilitate our study of PDEs, we now classify PDEs by a few of their attributes. For each definition we introduce, we provide a few concrete examples.

Definition 1.2 (order of a PDE). The order of a PDE is the order of the highest-order derivative that appears in the PDE.

Example 1.3. Laplace's equation $-\Delta u = 0$ is a second-order PDE, and the transport equation $\frac{\partial u}{\partial t} + a \frac{\partial u}{\partial x} = 0$ is a first-order PDE.

Example 1.4. The heat equation $\frac{\partial u}{\partial t} - \Delta u = 0$ is a second-order PDE. More precisely, it is first-order in time and second-order in space. Note that time-dependent PDEs admit a more precise characterization.

Definition 1.5 (linear operator). An operator \mathcal{L} is a linear operator if

$$\mathcal{L}(\alpha w + \beta v) = \alpha \mathcal{L}w + \beta \mathcal{L}v$$

for any functions w and v and any scalars α and β .

Definition 1.6 (linear PDEs). A PDE is said to be linear if the PDE can be expressed as

$$\mathcal{L}u = f,$$

where \mathcal{L} is a linear operator and f is a function independent of u . If a PDE is not linear, then it is called a nonlinear PDE.

Definition 1.7 (linear homogeneous PDEs). A linear homogeneous PDE is a PDE of the form

$$\mathcal{L}u = 0,$$

where \mathcal{L} is a linear operator; i.e., the term that does not depend on u vanishes. If a linear PDE is not homogeneous, then it is nonhomogeneous (or inhomogeneous).

Example 1.8. Laplace's equation $-\Delta u = 0$ is a linear homogeneous PDE; the Laplacian $\mathcal{L} \equiv \Delta$ is a linear operator, and the right hand side is zero. Poisson's equation $-\Delta u = f$ is a linear nonhomogeneous PDE for $f \neq 0$. The heat equation $\frac{\partial u}{\partial t} - \nabla \cdot a \nabla u = f$ is a linear homogeneous PDE if $f = 0$ and is a linear nonhomogeneous PDE if $f \neq 0$. The Burgers' equation $\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = 0$ is a nonlinear PDE, as there is no way to express $u \frac{\partial u}{\partial x}$ as a linear operator on u .

The superposition principle. Linear homogeneous PDEs, just like linear homogeneous ODEs, are particularly nice to study because we can appeal to the superposition principle to seek a solution. Specifically, if u_1 and u_2 satisfy $\mathcal{L}u_1 = 0$ and $\mathcal{L}u_2 = 0$, then $u_1 + u_2$ satisfies $\mathcal{L}(u_1 + u_2) = 0$. If we in addition find a solution u_0 to a nonhomogeneous PDE $\mathcal{L}u_0 = f$, then $u_0 + u_1 + u_2$ also satisfies the nonhomogeneous PDE $\mathcal{L}(u_0 + u_1 + u_2) = f$. We will exploit these properties in many solution techniques throughout this course.

Due to the superposition principle, in general there are an infinite number of functions that satisfy a given PDE. We must supply additional conditions to find a unique solution. In the context of PDEs, these conditions are provided by *boundary conditions*, if the problem is posed in a bounded domain, and by *initial conditions*, if the problem is time dependent. (Initial conditions can be thought of as "boundary conditions" in the space-time domain.) We will study various boundary and initial conditions for each model PDE in later lectures.

1.4 Classification of second-order PDEs

We have introduced a few second-order linear PDEs including Laplace's equation, the heat equation, and the wave equation. In fact second-order PDEs are ubiquitous in sciences and engineering, which justifies a finer classification of these PDEs.

Definition 1.9 (classification of second-order linear PDEs). Consider a second-order linear PDE with a differential operator on \mathbb{R}^n :

$$\mathcal{L}u = \sum_{i,j=1}^n a_{ij} \frac{\partial^2 u}{\partial x_i \partial x_j} + \sum_{i=1}^n b_i \frac{\partial u}{\partial x_i} + cu \quad (1.1)$$

for some coefficients a_{ij} , b_i and c . Let $A \in \mathbb{R}^{n \times n}$ be a symmetric matrix such that $A_{ij} = a_{ij}$, $i, j = 1, \dots, n$. (Note that A can be always symmetrized without loss of generality since the mixed partials are the same.) Let $\lambda_1, \dots, \lambda_n$ be the eigenvalues of A . Then we have the following classification of PDEs:

- *elliptic*: all eigenvalues are nonzero and have the same sign (i.e., all positive or all negative).
- *hyperbolic*: all eigenvalues are nonzero, and one of them has the opposite sign from the $n - 1$ others.
- *ultrahyperbolic*: all eigenvalues are nonzero, and at least two of them are positive and at least two of them are negative.
- *parabolic*: exactly one eigenvalue is zero and all other eigenvalues have the same sign.

If the PDE is time-dependent, then we treat time as the zero-th coordinate and run the summations from 0 to n in (1.1).

Example 1.10 (classification: Laplace's equation). The differential operator for Laplace's equation in \mathbb{R}^n is

$$\mathcal{L} = -\Delta = -\frac{\partial^2}{\partial x_1^2} - \dots - \frac{\partial^2}{\partial x_n^2}.$$

We recognize the associated A matrix is $A = -I$. All eigenvalues are equal to -1 , and hence Laplace's equation is elliptic.

Example 1.11 (classification: Poisson's equation). Poisson's equation is also elliptic because its differential operator is the Laplacian.

Example 1.12 (classification: wave equation). The differential operator for the wave equation in \mathbb{R}^n is

$$\mathcal{L} = \frac{\partial^2}{\partial t^2} - \Delta = \frac{\partial^2}{\partial t^2} - \frac{\partial^2}{\partial x_1^2} - \dots - \frac{\partial^2}{\partial x_n^2}.$$

We treat the temporal coordinate as the zero-th coordinate and recognize the associated A matrix is $A = \text{diag}(1, -1, -1, \dots, -1) \in \mathbb{R}^{(n+1) \times (n+1)}$. We have one positive eigenvalue and $n - 1$ negative eigenvalues. The wave equation is hence hyperbolic.

Example 1.13 (classification: heat equation). The differential operator for the heat equation in \mathbb{R}^n is

$$\mathcal{L} = \frac{\partial}{\partial t} - \Delta = \frac{\partial}{\partial t} - \frac{\partial^2}{\partial x_1^2} - \cdots - \frac{\partial^2}{\partial x_n^2}$$

We treat the temporal coordinate as the zero-th coordinate and recognize the associated A matrix is $A = \text{diag}(0, -1, -1, \dots, -1) \in \mathbb{R}^{(n+1) \times (n+1)}$. Note that the entry of A associated with the temporal coordinate is 0 because the differential operator does not contain a second derivative with respect to time. We have one zero eigenvalue and $n - 1$ negative eigenvalues. The heat equation is hence parabolic.

Example 1.14 (classification: finding the A matrix). Consider a second-order PDE

$$\frac{\partial^2 u}{\partial x_1^2} - 2 \frac{\partial^2 u}{\partial x_1 \partial x_2} + 2 \frac{\partial^2 u}{\partial x_2^2} = f$$

for some f . We note that the linear differential operator can be rearranged into the form (1.1):

$$\mathcal{L}u = 1 \frac{\partial^2 u}{\partial x_1^2} - 1 \frac{\partial^2 u}{\partial x_1 \partial x_2} - 1 \frac{\partial^2 u}{\partial x_2 \partial x_1} + 2 \frac{\partial^2 u}{\partial x_2^2},$$

where we have split the mixed partial term into two so that the coefficients in front of the terms are the same. We recognize that $a_{11} = 1$, $a_{12} = a_{21} = -1$, and $a_{22} = 2$, and hence

$$A = \begin{pmatrix} 1 & -1 \\ -1 & 2 \end{pmatrix}.$$

Note that the matrix is symmetric (as required for classification) thanks to the splitting of the mixed partial term. To find the eigenvalues, we form the characteristic equation $p_A(\lambda) \equiv \det(\lambda I - A) = \lambda^2 - 3\lambda + 1$ and find its roots are $\lambda = \frac{3}{2} \pm \frac{\sqrt{5}}{2}$. Since both eigenvalues are positive and the eigenvalues have the same sign, the equation is elliptic.

Example 1.15 (classification: PDE with variable coefficient). The classification of the PDE may vary over the domain for PDEs with variable coefficients. For instance, consider the second-order PDE

$$y \frac{\partial^2 u}{\partial x^2} + \frac{\partial^2 u}{\partial y^2} = 0.$$

The matrix A associated with the PDE is $A = \text{diag}(y, 1)$, and its eigenvalues are $\lambda_1 = 1$ and $\lambda_2 = y$. Hence, the PDE is parabolic on the line $y = 0$, elliptic in the region $y > 0$, and hyperbolic in the region $y < 0$.

The classification of PDEs into elliptic, hyperbolic, and parabolic equations is useful because equations in a given class exhibit similar behaviors. For instance, the only difference between the wave equation (in the space-time space with the time as the zero-th coordinate) and Laplace's equation is that one of the eigenvalues is positive in the wave equation; however, the wave equation is hyperbolic and Laplace's equation is elliptic, and they describe different physical processes and exhibit different solution behaviors. On the other hand, while Laplace's equation and the Navier-Cauchy equation of linear elasticity might look quite different, they are both elliptic and exhibit similar behaviors. Similarly, while the wave equation and Maxwell's equations might look quite different, they are both hyperbolic and exhibit similar behaviors.

1.5 PDEs in physics and engineering

Before we conclude this lecture, we provide some examples of more complex PDEs that are encountered in science and engineering. While we will not study these PDEs in detail, we will see that much of the behaviors of these more complex PDEs are captured by our model PDEs.

- **Navier-Cauchy equations.** The Navier-Cauchy equations are a system of PDEs of the form

$$\mu \sum_{j=1}^d \frac{\partial u_i}{\partial x_j^2} + (\mu + \lambda) \sum_{j=1}^d \frac{\partial u_j}{\partial x_i \partial x_j} = f_i, \quad i = 1, \dots, d,$$

where u is the (vector-valued) displacement field, f is the body force, and λ and μ are the first and second Lamé parameters, respectively. The Navier-Cauchy equations, also known as the equations of linear elasticity, are a system of linear PDEs. The equations describe the deformation of a material under load (under the assumption of small displacement and strain), and hence the behavior of engineering structures.

- **Maxwell's equations.** Maxwell's equations in free space are given by

$$\begin{aligned} \nabla \times E &= -\frac{\partial B}{\partial t}, \\ \nabla \cdot E &= 0, \\ \nabla \times B &= \frac{1}{c^2} \frac{\partial E}{\partial t}, \\ \nabla \cdot B &= 0, \end{aligned}$$

where E is the electric field, B is the magnetic field, and c is the speed of light. Maxwell's equations are a system of linear, homogeneous PDEs. Maxwell's equations describe the propagation of electromagnetic waves in free space, and hence the behavior of electric circuits, electric motors, wireless communication, and power generation, among others.

- **Incompressible Navier-Stokes equations.** The incompressible Navier-Stokes equations are given by

$$\begin{aligned} \frac{\partial u}{\partial t} + \sum_{j=1}^d \nabla \cdot (u \otimes u) + \nabla p - \frac{1}{\text{Re}} \Delta u &= f, \\ \nabla \cdot u &= 0, \end{aligned}$$

where u is the (vector-valued) velocity field, p is the (scalar-valued) pressure field, and Re is the Reynolds number. The incompressible Navier-Stokes equations comprise a system of nonlinear PDEs that describes the velocity and pressure of an incompressible (Newtonian) flow.

- **Compressible Euler equations.** The compressible Euler equations are given by

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \nabla \cdot \rho u &= 0 \\ \frac{\partial \rho u}{\partial t} + \nabla \cdot (\rho u \otimes u) + \nabla p &= 0 \\ \frac{\partial \rho e}{\partial t} + \nabla \cdot (\rho h) &= 0, \end{aligned}$$

where ρ is the density field, u is the (vector-valued) velocity field, e is the specific internal energy field, p is the pressure field, and h is the specific enthalpy field. The compressible Euler equations is a system of nonlinear PDEs that describes the behavior of inviscid compressible flows.

- **Schrödinger equation.** The Schrödinger equation for a single particle is given by

$$i\hbar \frac{\partial \Psi}{\partial t} = \left(-\frac{\hbar^2}{2m} \Delta + V \right) \Psi,$$

where $\Psi : \mathbb{R}^n \times t \rightarrow \mathbb{C}$ is the wave function in position space, \hbar is the reduced Planck constant, m is the particle mass, and $V : \mathbb{R}^n \times t \rightarrow \mathbb{C}$ is the potential function. The Schrödinger equation describes the quantum state of an isolated non-relativistic quantum system.

- **Black-Scholes equation.** The Black-Scholes equation is given by

$$\frac{\partial V}{\partial t} + \frac{1}{2} \sigma^2 S^2 \frac{\partial^2 V}{\partial S^2} + rS \frac{\partial V}{\partial S} - rV = 0,$$

where V is the price of the option as a function of the stock price S and time t , r is the risk-free interest rate, and σ is the volatility of the stock.

1.6 Summary

We summarize key points of this lecture:

1. A PDE is an equation that relates an unknown function u and some of its partial derivatives.
2. PDEs can be classified in terms of the order, linearity, and homogeneity.
3. PDEs are augmented by initial and/or boundary conditions to provide a well-posed problem.
4. Second-order PDEs can be further classified as elliptic, hyperbolic, ultrahyperbolic, or parabolic. The classification is based on the eigenvalues of the coefficient matrix of the second derivative.
5. Laplace's equation, Poisson's equation, the heat equation, the transport equation, the wave equation, and Burgers' equation each serves as a model PDE of a given classification and will be closely studied throughout this course.

1.A Well-posedness problem

Throughout this course, we will introduce different techniques to solve PDEs. However, it only makes sense to seek a solution if the problem is *well-posed*. We study this notion in this appendix.

Definition 1.16 (well-posedness in the sense of Hadamard). A mathematical problem is said to be well-posed if (i) a solution exists, (ii) the solution is unique, and (iii) the solution depends continuously on the data. If the problem is not well-posed, it is said to be ill-posed.

As we are not yet equipped to study the well-posedness of PDEs, we consider a few examples of well-posedness in the context of linear algebra and ODEs.

Example 1.17 (linear algebra). Consider the solution of a linear system associated with a matrix $A \in \mathbb{R}^{n \times n}$: find $x \in \mathbb{R}^n$ such that

$$Ax = b$$

for some data $b \in \mathbb{R}^n$. We recall that the problem has a unique solution for any data b if A is nonsingular. In addition, we can readily show that if $Ax_1 = b_1$ and $Ax_2 = b_2$, then $\|x_1 - x_2\| \leq (1/\sigma_{\min}(A))\|b_1 - b_2\|$, where $\sigma_{\min}(A)$ is the minimum singular value of A which is nonzero for a nonsingular A . A small perturbation in the data b results in a small perturbation in the solution x . Hence the problem is well-posed if A is nonsingular.

On the other hand, if A is singular and $b \notin \text{Img}(A)$, then the solution does not exist. If A is singular and $b \in \text{Img}(A)$, then there are infinitely many solutions; if $Ax = b$, then $x + y$ is also a solution for any $y \in \text{Ker}(A)$. (Recall that $\text{Ker}(A) = \{0\}$ for a nonsingular A , but $\text{Ker}(A)$ includes other elements for a singular A .) Hence, if A is singular, then the problem is ill-posed.

Example 1.18 (initial value problem). Consider an initial value problem on $I \equiv (0, T]$ for the final time $T \in \mathbb{R}_{>0}$:

$$\begin{aligned} \frac{du}{dt} &= f(t, u) \quad \text{in } I, \\ u(t=0) &= g, \end{aligned}$$

where $u : I \rightarrow \mathbb{R}$ is the solution, $f : I \times \mathbb{R} \rightarrow \mathbb{R}$ defines the ODE, and $g \in \mathbb{R}$ is the initial condition. Suppose f is continuous in t and uniformly Lipschitz continuous in u ; i.e., there exists $\gamma < \infty$ such that for any (t, u_1) and (t, u_2) we have $|f(t, u_1) - f(t, u_2)| \leq \gamma|u_1 - u_2|$. Then the Picard-Lindelöf theorem states that a unique solution to the initial value problem exists. In addition, the energy estimate states that $|u_1(t) - u_2(t)| \leq |g_1 - g_2| \exp(\gamma t)$, which means that the solution depends continuously on data. Hence the problem is well-posed if the assumptions of the Picard-Lindelöf theorem holds.

It is also relatively simple to find f for which the problem is ill-posed. A classical example is

$$\begin{aligned} \frac{du}{dt} &= u^{1/3} \\ u(t=0) &= 0; \end{aligned}$$

this initial value problem admits infinitely many solutions of the form

$$u(t) = \begin{cases} 0, & t \in (0, \tau), \\ (\frac{2}{3}(t - \tau))^{3/2}, & t \in (\tau, T], \end{cases}$$

for any $\tau \in I$. We readily verify that $f(t, u) = u^{1/3}$ does not satisfy the uniform Lipschitz continuity condition of the Picard-Lindelöf theorem.

Lecture 2

Fourier series: formulation

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2.1 Introduction

In order to solve a PDE, we must be able to represent its solution, which is a function in space (and time). We could attempt to describe the function in terms of the value that it takes at each point in space (and time), but this representation is not convenient to solve or to analyze PDEs. A much more convenient approach is to represent the function as a linear combination of known functions, so that the function can be identified by a set of coefficients. Namely, we represent the solution $u : \Omega \rightarrow \mathbb{R}$ as $u(x) = \sum_{n=1}^{\infty} \hat{u}_n \phi_n(x)$, where ϕ_n , $n = 1, 2, \dots$, are the known functions and \hat{u}_n , $n = 1, 2, \dots$, are the coefficients to be determined. One class of infinite series that is particularly useful to represent the solution of PDEs is *Fourier series*. In this lecture we introduce Fourier series so that we can use them to solve PDEs in the following lectures. In this lecture we focus on the construction of Fourier series; we will analyze its theoretical properties in the next lecture.

2.2 Periodic, even, and odd functions

As periodic functions play an important role in the construction of Fourier series, we first provide a few definitions related to the periodicity of functions.

Definition 2.1 (periodic function). A function $f : \mathbb{R} \rightarrow \mathbb{R}$ is said to be z -*periodic* if

$$f(x + z) = f(x) \quad \forall x \in \mathbb{R}.$$

The real number z is called a *period*. The smallest real number z such that the relationship holds is called the *fundamental period*.

Example 2.2 (periodicity of sine functions). Perhaps one of the most common periodic functions is the sine function. The function $f(x) = \sin(x)$ is 2π -periodic because

$$\sin(x + 2\pi) = \sin(x) \quad \forall x \in \mathbb{R}.$$

Its fundamental period is 2π , because the relationship does not hold for any shorter period. Note that any integer multiple of the fundamental period is also a period of the function; e.g., $z = 2\pi, 4\pi, 6\pi$.

Example 2.3 (periodicity of sum of sine function). Consider $f(x) = \cos(x) + \sin(2x)$. The function $\cos(x)$ and $\sin(2x)$ are periodic functions with the fundamental period of 2π and π , respectively. The fundamental period of the sum of the functions is 2π , the larger of the two fundamental periods.

We also recall the definition of even and odd functions.

Definition 2.4 (even function). A function $f : (-a, a) \rightarrow \mathbb{R}$ is an even function if for all $x \in (-a, a)$,

$$f(-x) = f(x).$$

Definition 2.5 (odd function). A function $f : (-a, a) \rightarrow \mathbb{R}$ is an odd function if for all $x \in (-a, a)$,

$$f(-x) = -f(x).$$

If f is even, then the graph $y = f(x)$ is symmetric about the y axis; the left hand side is the mirror image of the right hand side. If f is odd, then the graph $y = f(x)$ is symmetric about the origin. We provide a few examples.

Example 2.6. For any $\lambda \geq 0$, the function $f(x) = \cos(\lambda x)$ is an even function because $f(-x) = \cos(-\lambda x) = \cos(\lambda x) = f(x)$. For any $\lambda \geq 0$, the function $f(x) = \sin(\lambda x)$ is an odd function because $f(-x) = \sin(-\lambda x) = -\sin(\lambda x) = -f(x)$.

Example 2.7. A monomial x^k is an even function if k is even and an odd function if k is odd.

We also note few properties of even and odd functions under some operations; each result can be readily proven from the definition of even and odd functions:

- *Summation.* The sum of two even functions is even. The sum of two odd functions is odd. However, the sum of an even function and an odd function is in general neither even nor odd.
- *Multiplication.* The product of two even functions or two odd functions is even. The product of an even function and an odd function is odd.
- *Differentiation.* The derivative of an odd function is even, and the derivative of an even function is odd. The result follows from the chain rule.
- *Integration.* If f is an even function, then the integral $g(x) = \int_{\xi=0}^x f(\xi)d\xi$ is odd. If f is an odd function, then the integral $g(x) = \int_{\xi=0}^x f(\xi)d\xi$ is even.
- *Integrals.* If f is odd, then $\int_{-a}^a f(x)dx = 0$. If f is even, then $\int_{-a}^a f(x)dx = 2 \int_0^a f(x)dx$.
- *Behavior at origin.* If f is even and is differentiable at $x = 0$, then its derivative must vanish: i.e., $f'(x = 0) = 0$. If f is odd and is continuous at $x = 0$, then its value must vanish: i.e., $f(x = 0) = 0$.

Given a function defined on a finite interval, we may also “extend” the function to the entire real line \mathbb{R} to construct a periodic function on \mathbb{R} . We introduce a few different extensions.

Definition 2.8 (periodic extension). Given a function $f : (0, a) \rightarrow \mathbb{R}$, its periodic extension to \mathbb{R} is the function $f^{\text{P}} : \mathbb{R} \rightarrow \mathbb{R}$ such that

$$f^{\text{P}}(x) = f(x), \quad x \in (0, a),$$

and has a period a (i.e., $f^{\text{P}}(x + a) = f^{\text{P}}(x)$, $\forall x \in \mathbb{R}$, or equivalently $f^{\text{P}}(x + na) = f(x)$, $\forall x \in (0, a)$ and $\forall n \in \mathbb{Z}$).

Definition 2.9 (even periodic extension). Given a function $f : (0, a) \rightarrow \mathbb{R}$, its even periodic extension is the function $f^{\text{e,P}} : \mathbb{R} \rightarrow \mathbb{R}$ such that

$$\begin{aligned} f^{\text{e,P}}(x) &= f(x), & x \in (0, a), \\ f^{\text{e,P}}(x) &= f(-x), & x \in (-a, 0), \end{aligned}$$

and has a period of $2a$ (i.e., $f^{\text{e,P}}(x + 2a) = f^{\text{e,P}}(x)$, $\forall x \in \mathbb{R}$).

Definition 2.10 (odd periodic extension). Given a function $f : (0, a) \rightarrow \mathbb{R}$, its odd periodic extension is the function $f^{\text{o,P}} : \mathbb{R} \rightarrow \mathbb{R}$ such that

$$\begin{aligned} f^{\text{o,P}}(x) &= f(x), & x \in (0, a), \\ f^{\text{o,P}}(x) &= -f(-x), & x \in (-a, 0), \end{aligned}$$

and has a period of $2a$ (i.e., $f^{\text{o,P}}(x + 2a) = f^{\text{o,P}}(x)$, $\forall x \in \mathbb{R}$).

In the above definitions of periodic, even-periodic, and odd-periodic extensions, we do not specify the values of the extensions at the end points $x = na$, $n \in \mathbb{Z}$. As we will see shortly, the lack of the specification does not cause a problem in our discussion of Fourier series.

We demonstrate these three periodic extensions using a concrete example.

Example 2.11 (periodic extensions). Let $f(x) = x$, $x \in (0, 1)$. Figure 2.1 shows the periodic extension, even periodic extension, and the odd periodic extension for the function. To construct the periodic extension, we simply repeat the function, with a period of 1. We construct the even periodic extension in two steps: we first mirror the function about the y -axis to construct the even extension; we then construct the periodic extension of the even extension with a period of 2. By definition the even (or odd) extension of a function is defined on a symmetric interval (e.g., $[-1, 1]$). We also note that the period of the even periodic extension is twice the domain length of the original function to match the domain length of the even extension. Similarly, we construct the odd periodic extension in two steps: we first mirror the function about the origin to construct the odd extension; we then construct the periodic extension of the odd extension with a period of 2.

2.3 Fourier series

We now introduce Fourier series, which provide a representation of a periodic function as a linear combination of sinusoidal functions. For simplicity, we consider 2-periodic functions; we will later generalize the formulation to an arbitrary period in Section 2.5.

Definition 2.12 (Fourier series). Let $f : \mathbb{R} \rightarrow \mathbb{R}$ be a 2-periodic function. The Fourier series of the function is

$$f(x) \sim \frac{1}{2}a_0 + \sum_{n=1}^{\infty} (a_n \cos(n\pi x) + b_n \sin(n\pi x)), \quad (2.1)$$

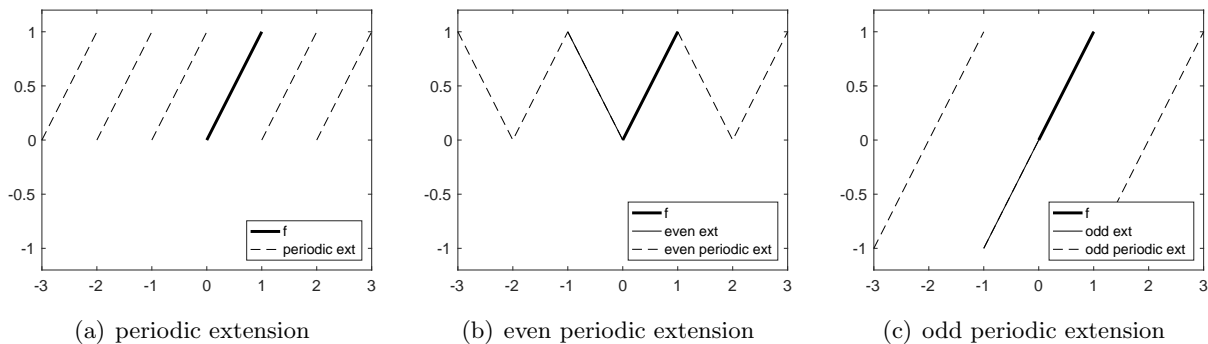


Figure 2.1: Periodic extensions of $f(x) = x$ for $x \in [0, 1]$.

with Fourier coefficients

$$\begin{aligned}
 a_n &= \int_{-1}^1 \cos(n\pi x) f(x) dx, \quad n = 0, 1, 2, \dots, \\
 b_n &= \int_{-1}^1 \sin(n\pi x) f(x) dx, \quad n = 1, 2, \dots
 \end{aligned}
 \tag{2.2}$$

Definition 2.13 (truncated Fourier series). Let $f : \mathbb{R} \rightarrow \mathbb{R}$ be a 2-periodic function. The N -term truncated Fourier series of the function is

$$s_N(x) \equiv \frac{1}{2} a_0 + \sum_{n=1}^N (a_n \cos(n\pi x) + b_n \sin(n\pi x)),$$

with coefficients given by (2.2).

We make some observations about Fourier series.

1. Because we have not verified, and in general will not be able to verify, that the Fourier series of f is the same as f , we use the notation “ \sim ” instead of “ $=$ ” in (2.1). In the next lecture we will answer various questions on the convergence of Fourier series including the following: does the series converge? In what sense does the series converge? How smooth does the function f have to be for the series to converge?
2. The set of functions

$$\left\{ \frac{1}{2}, \sin(\pi x), \cos(\pi x), \sin(2\pi x), \cos(2\pi x), \dots \right\}$$

is *orthonormal* with respect to the L^2 inner product, $(w, v) \equiv \int_{-1}^1 wv dx$. For all $n, m \in \mathbb{N}_{>0}$,

$$\begin{aligned}\int_{-1}^1 \frac{1}{2} \cos(m\pi x) dx &= \int_{-1}^1 \frac{1}{2} \sin(m\pi x) dx = 0, \\ \int_{-1}^1 \cos(n\pi x) \cos(m\pi x) dx &= \delta_{mn}, \\ \int_{-1}^1 \sin(n\pi x) \sin(m\pi x) dx &= \delta_{mn}, \\ \int_{-1}^1 \sin(n\pi x) \cos(m\pi x) dx &= 0,\end{aligned}$$

where δ_{mn} is the Kronecker delta; i.e., $\delta_{mn} = 1$ if $m = n$ and $\delta_{mn} = 0$ if $m \neq n$.

3. The expression for the coefficients (2.2) is a consequence of the orthonormality of the sinusoidal functions. For instance, to obtain the expression for a_2 , we multiply the Fourier series (2.1) by $\cos(2\pi x)$, integrate the expression over $(-1, 1)$, and appeal to the orthonormality: i.e.,

$$\begin{aligned}\int_{-1}^1 \cos(2\pi x) f(x) dx &= \int_{-1}^1 \cos(2\pi x) \left(\frac{1}{2} a_0 + \sum_{n=1}^{\infty} (a_n \cos(n\pi x) + b_n \sin(n\pi x)) \right) dx \\ &= a_0 \int_{-1}^1 \frac{1}{2} \cos(2\pi x) dx + \sum_{n=1}^{\infty} a_n \int_{-1}^1 \cos(2\pi x) \cos(n\pi x) dx + \sum_{n=1}^{\infty} b_n \int_{-1}^1 \cos(2\pi x) \sin(n\pi x) dx \\ &= \sum_{n=1}^{\infty} a_n \delta_{2n} = a_2.\end{aligned}$$

All integrals with exception of the one multiplied by a_2 vanish due to the mutual orthogonality of the sine and cosine functions. We obtain the expression for all other a_n and b_n using the same orthogonality argument.

4. We can also find the Fourier series of a function f defined on $(-1, 1)$ (instead of a 2-periodic function on \mathbb{R}). The Fourier series of $f : (-1, 1) \rightarrow \mathbb{R}$ is given by (2.1) and it converges to (i) f on $(-1, 1)$ and (ii) its periodic extension f^p on \mathbb{R} .
5. The truncated Fourier series s_N of f is the N -term partial sum of the Fourier series of f .

We now consider an example:

Example 2.14 (The Fourier series of $f(x) = x$ on $(-1, 1)$). We consider the 2-periodic extension of the function $f(x) = x$ for $x \in [-1, 1]$. We wish to find the Fourier series representation of the function. The coefficient a_n , $n \in \mathbb{N}_{\geq 0}$, is given by

$$a_n = \int_{-1}^1 \cos(n\pi x) f(x) dx = \int_{-1}^1 \cos(n\pi x) x dx = 0;$$

the integral evaluates to 0 because the integrand is an odd function, and the domain of integration

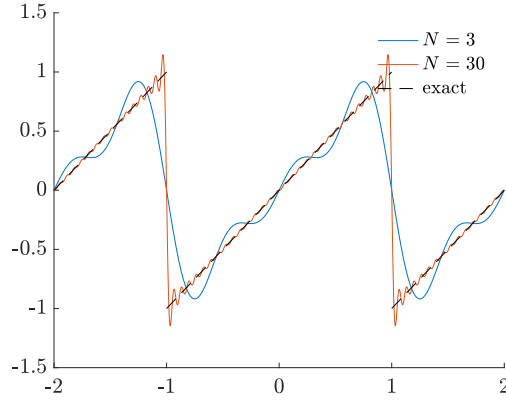


Figure 2.2: Truncated Fourier series of $f(x) = x$ for $x \in [-1, 1]$.

is symmetric. The Fourier coefficient b_n is given by

$$\begin{aligned}
 b_n &= \int_{-1}^1 \sin(n\pi x) f(x) dx = \int_{-1}^1 \sin(n\pi x) x dx = \left[-\frac{1}{n\pi} \cos(n\pi x) x \right]_{x=-1}^1 + \int_{-1}^1 \frac{1}{n\pi} \cos(n\pi x) dx \\
 &= -\frac{1}{n\pi} (\cos(n\pi) + \cos(-n\pi)) + \frac{1}{n^2\pi^2} \sin(n\pi x) \Big|_{x=-1}^1 = -\frac{2}{n\pi} \cos(n\pi) = -\frac{2}{n\pi} (-1)^n \\
 &= \frac{2}{n\pi} (-1)^{n+1};
 \end{aligned}$$

here, the third equality follows from integration by parts, and the second to last equality follows from $\cos(n\pi) = (-1)^n$, $\forall n \in \mathbb{Z}$. It follows that

$$\begin{aligned}
 f(x) &\sim \sum_{n=1}^{\infty} b_n \sin(n\pi x) = \sum_{n=1}^{\infty} \frac{2(-1)^{n+1}}{n\pi} \sin(n\pi x) \\
 &= \frac{2}{\pi} \left(\sin(\pi x) - \frac{1}{2} \sin(2\pi x) + \frac{1}{3} \sin(3\pi x) - \dots \right).
 \end{aligned}$$

The series contains only sine terms (and not cosine terms) because the function $f(x) = x$ is an odd function. Figure 2.2 illustrates the Fourier series approximation of the function. We observe that the weighted sum of the sine functions at least visually converges to f . (As noted earlier, we will analyze the convergence of Fourier series in the next lecture.)

2.4 Fourier sine and cosine series

The Fourier series provides a representation for any periodic function. It is often also useful to construct a representation specialized to odd or even periodic functions. A Fourier sine series is the Fourier series associated with odd periodic functions, and a Fourier cosine series is the Fourier series associated with even periodic functions.

Definition 2.15 (Fourier cosine series). Let $f : \mathbb{R} \rightarrow \mathbb{R}$ be an even 2-periodic function. The Fourier cosine series of f is given by

$$f(x) \sim \frac{1}{2} \hat{f}_0 + \sum_{n=1}^{\infty} \hat{f}_n \cos(n\pi x) \tag{2.3}$$

where

$$\hat{f}_n = \int_{-1}^1 \cos(n\pi x) f(x) dx = 2 \int_0^1 \cos(n\pi x) f(x) dx, \quad n \in \mathbb{N}_{\geq 0}.$$

Definition 2.16 (Fourier sine series). Let $f : \mathbb{R} \rightarrow \mathbb{R}$ be an odd 2-periodic function. The Fourier sine series of f is given by

$$f(x) \sim \sum_{n=1}^{\infty} \hat{f}_n \sin(n\pi x) \quad (2.4)$$

where

$$\hat{f}_n = \int_{-1}^1 \sin(n\pi x) f(x) dx = 2 \int_0^1 \sin(n\pi x) f(x) dx, \quad n \in \mathbb{N}_{> 0}.$$

We make some observations:

1. The domain of integration for the coefficients can be reduced from $[-1, 1]$ to $[0, 1]$ due to the symmetry of even functions for the Fourier cosine series (and due to the antisymmetry of odd functions for the Fourier sine series).
2. Similar to the (full) Fourier series, we can also find the Fourier cosine series of a function f defined on $(0, 1)$ (instead of an even 2-periodic function on the entire \mathbb{R}). The Fourier cosine series of $f : (0, 1) \rightarrow \mathbb{R}$ is given by (2.3) and it converges to (i) f on $(0, 1)$ and (ii) its even periodic extension $f^{e,p}$ on the entire \mathbb{R} .
3. Similarly, we can find the Fourier sine series of a function f defined on $(0, 1)$ (instead of an odd 2-periodic function on the entire \mathbb{R}). The Fourier sine series of $f : (0, 1) \rightarrow \mathbb{R}$ is given by (2.4) and it converges to (i) f on $(0, 1)$ and (ii) its odd periodic extension $f^{o,p}$ on the entire \mathbb{R} .
4. We use the notation $(\hat{f}_n)_{n=0}^{\infty}$ to denote the Fourier sine/cosine coefficients of f . The notation makes the connection between the function and its Fourier coefficients more explicit, which will be helpful when we work with Fourier series associated with multiple functions. (Unfortunately this notation cannot be used for the (full) Fourier series, as we require two sets of coefficients for sine and cosine.)

We now consider an example of Fourier cosine and sine series.

Example 2.17 (Fourier cosine series of $f(x) = x$ on $(0, 1)$). We consider the Fourier cosine series representation of $f(x) = x$ for $x \in (0, 1)$. The coefficient \hat{f}_0 of the Fourier cosine series is given by

$$\hat{f}_0 = 2 \int_0^1 x dx = 1.$$

For $n > 0$, we obtain

$$\begin{aligned} \hat{f}_n &= 2 \int_0^1 x \cos(n\pi x) dx = 2 \left[\frac{\cos(n\pi x)}{n^2 \pi^2} + \frac{x \sin(n\pi x)}{n\pi} \right]_{x=0}^1 = \frac{2}{n^2 \pi^2} (\cos(n\pi) - 1) \\ &= \frac{2}{n^2 \pi^2} ((-1)^n - 1) = \begin{cases} -\frac{4}{n^2 \pi^2} & n \in \text{odd}, \\ 0 & n \in \text{even}. \end{cases} \end{aligned}$$

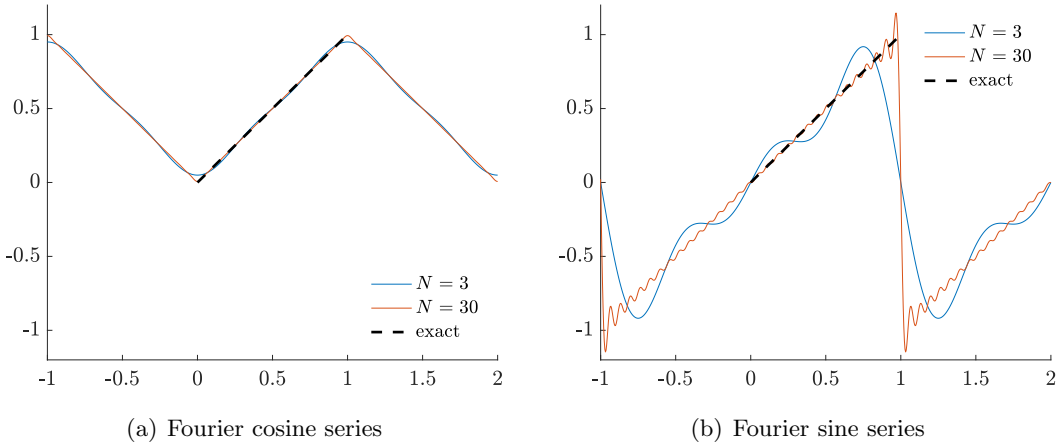


Figure 2.3: Truncated Fourier cosine and sine series of $f(x) = x$ for $x \in [0, 1]$.

The Fourier cosine series of f is hence

$$\begin{aligned}
 f(x) &\sim \frac{1}{2}\hat{f}_0 + \sum_{n=1}^{\infty} \hat{f}_n \cos(n\pi x) = \frac{1}{2} + \sum_{k=1}^{\infty} \hat{f}_{2k-1} \cos((2k-1)\pi x) \\
 &= \frac{1}{2} - \sum_{k=1}^{\infty} \frac{4}{(2k-1)^2\pi^2} \cos((2k-1)\pi x) \\
 &= \frac{1}{2} - \frac{4}{\pi^2} \left(\cos(\pi x) + \frac{1}{9} \cos(3\pi x) + \frac{1}{25} \cos(5\pi x) + \dots \right).
 \end{aligned}$$

Figure 2.3(a) illustrates the Fourier cosine series representation of the function. We observe that the series (at least visually) approximates the function $f(x) = x$ on $(0, 1)$. Note that the Fourier cosine series approximates the even periodic extension of f .

Example 2.18 (Fourier sine series approximation of $f(x) = x$ on $(0, 1)$). We consider the Fourier sine series representation of $f(x) = x$ for $x \in (0, 1)$. The coefficients of the Fourier sine series are given by

$$\hat{f}_n = 2 \int_0^1 x \sin(n\pi x) dx = 2 \left[\frac{\sin(n\pi x)}{n^2\pi^2} - \frac{x \cos(n\pi x)}{n\pi} \right]_{x=0}^1 = -\frac{2}{n\pi} \cos(n\pi) = \frac{2}{n\pi} (-1)^{n+1}.$$

The Fourier sine series of f is hence

$$f(x) \sim \sum_{n=1}^{\infty} \hat{f}_n \sin(n\pi x) = \sum_{n=1}^{\infty} \frac{2(-1)^{n+1}}{n\pi} \sin(n\pi x) = \frac{2}{\pi} \left(\sin(\pi x) - \frac{1}{2} \sin(2\pi x) + \frac{1}{3} \sin(3\pi x) - \dots \right).$$

Not surprisingly, the Fourier sine series of $f(x) = x$ on $(0, 1)$ considered here is the same as the Fourier series of $g(x) = x$ on $(-1, 1)$ considered in Example 2.14 because the odd periodic extension of f is the same as the periodic extension of g . Figure 2.3(b) illustrates the Fourier sine series representation of the function. Note that the Fourier sine series approximates the odd periodic extension of f .

2.5 Fourier series on arbitrary intervals

We now consider Fourier series for periodic functions of arbitrary periods. Given a $2L$ -periodic function $f : \mathbb{R} \rightarrow \mathbb{R}$, the Fourier series of f results from simple adjustments of the arguments of the sine and cosine functions to the period of $2L$:

$$f(x) \sim \frac{1}{2}a_0 + \sum_{n=1}^{\infty} \left(a_n \cos\left(\frac{n\pi x}{L}\right) + b_n \sin\left(\frac{n\pi x}{L}\right) \right),$$

with coefficients

$$a_n = \frac{1}{L} \int_{-L}^L \cos\left(\frac{n\pi x}{L}\right) f(x) dx, \quad n = 0, 1, 2, \dots,$$

$$b_n = \frac{1}{L} \int_{-L}^L \sin\left(\frac{n\pi x}{L}\right) f(x) dx, \quad n = 1, 2, \dots$$

The normalization factor of the coefficients for the Fourier series on $(-L, L)$ is scaled by $1/L$ relative to the Fourier series on $(-1, 1)$ because the orthogonality relations are

$$\frac{1}{L} \int_{-L}^L \sin\left(\frac{n\pi x}{L}\right) \cos\left(\frac{m\pi x}{L}\right) dx = 0,$$

$$\frac{1}{L} \int_{-L}^L \sin\left(\frac{n\pi x}{L}\right) \sin\left(\frac{m\pi x}{L}\right) dx = \delta_{mn},$$

$$\frac{1}{L} \int_{-L}^L \cos\left(\frac{n\pi x}{L}\right) \cos\left(\frac{m\pi x}{L}\right) dx = \delta_{mn}.$$

The Fourier series of a function $f : (-L, L) \rightarrow \mathbb{R}$ is also given by the same expression, and the series converges to the $2L$ -periodic extension of f on the entire \mathbb{R} .

Similarly, the Fourier cosine series of an even $2L$ -periodic function $f : \mathbb{R} \rightarrow \mathbb{R}$ is given by

$$f(x) \sim \frac{1}{2}\hat{f}_0 + \sum_{n=1}^{\infty} \hat{f}_n \cos\left(\frac{n\pi x}{L}\right)$$

with Fourier cosine coefficients

$$\hat{f}_n = \frac{2}{L} \int_0^L \cos\left(\frac{n\pi x}{L}\right) f(x) dx, \quad n = 0, 1, 2, \dots$$

The Fourier cosine series of a function $f : (0, L) \rightarrow \mathbb{R}$ is also given by the same expression, and the even $2L$ -periodic extension of f on the entire \mathbb{R} .

The Fourier sine series of an odd $2L$ -periodic function $f : \mathbb{R} \rightarrow \mathbb{R}$ is given by

$$f(x) \sim \sum_{n=1}^{\infty} \hat{f}_n \sin\left(\frac{n\pi x}{L}\right)$$

with Fourier sine coefficients

$$\hat{f}_n = \frac{2}{a} \int_0^a \sin\left(\frac{n\pi x}{L}\right) f(x) dx, \quad n = 1, 2, \dots$$

The Fourier sine series of a function $f : (0, L) \rightarrow \mathbb{R}$ is also given by the same expression, and the series converges to the odd $2L$ -periodic extension of f on the entire \mathbb{R} .

2.6 Summary

We summarize key points of this lecture:

1. Fourier series provide series representations (of approximations) of periodic functions $f : \mathbb{R} \rightarrow \mathbb{R}$ in terms of sinusoidal functions. To find the coefficients of the series, we multiply f by the sinusoidal functions and integrate over the period; this is a consequence of the orthonormality of the sinusoidal functions.
2. Fourier cosine and sine series provide series representations (of approximations) of even and odd periodic functions, respectively.
3. Given $f : (-L, L) \rightarrow \mathbb{R}$, its (full) Fourier series approximates the periodic extension of f . Given $f : (0, L) \rightarrow \mathbb{R}$, its cosine and sine Fourier series approximates the even periodic and odd periodic extensions, respectively, of f .
4. Fourier series can be applied to periodic functions of an arbitrary period by adjusting the period of the sinusoidal functions and the associated coefficients accordingly.

2.A Complex form of Fourier series

The Fourier series can be written in a more compact form using complex exponentials. To begin, we recall the DeMoivre formulas

$$\sin(x) = \frac{1}{2i}(\exp(ix) - \exp(-ix)) \quad \text{and} \quad \cos(x) = \frac{1}{2}(\exp(ix) + \exp(-ix)).$$

It follows that the set of sinusoidal functions

$$\{1, \cos(\pi x), \sin(\pi x), \cos(2\pi x), \sin(2\pi x), \dots\}$$

can be replaced by the complex exponentials

$$\{1, \exp(-i\pi x), \exp(i\pi x), \exp(-i2\pi x), \exp(i2\pi x), \dots\} = \{\exp(nx)\}_{n=-\infty}^{\infty}.$$

The complex form of the Fourier series is as follows:

Definition 2.19 (complex form of Fourier series). Let $f : \mathbb{R} \rightarrow \mathbb{R}$ be a 2-periodic function. The complex form of the Fourier series of f is

$$f(x) \sim \sum_{n=-\infty}^{\infty} \hat{f}_n \exp(in\pi x), \quad (2.5)$$

with coefficients

$$\hat{f}_n = \frac{1}{2} \int_{-1}^1 \exp(-in\pi x) f(x) dx.$$

Similar to the (real) Fourier series of f , the expression for the coefficients follows from the orthogonality relationship. Specifically, the orthogonality relationship for the complex exponentials $\exp(-im\pi x)$ and $\exp(in\pi x)$ for $m \neq n$ is

$$\begin{aligned} \int_{-1}^1 \exp(-im\pi x) \exp(in\pi x) dx &= \int_{-1}^1 \exp(i(n-m)\pi x) dx \\ &= \frac{1}{i\pi(n-m)} (\exp(i(n-m)\pi) - \exp(-i(n-m)\pi)) = \frac{2}{\pi(n-m)} \sin((n-m)\pi) = 0, \end{aligned}$$

and for $m = n$ is

$$\int_{-1}^1 \exp(i(n-m)x) dx = \int_{-1}^1 dx = 2.$$

The complex form of Fourier series (2.5) immediately follows from the orthogonality relationship.

For a $2L$ -periodic function $f : \mathbb{R} \rightarrow \mathbb{R}$, the complex form of the Fourier series is given by

$$f(x) \sim \sum_{n=-\infty}^{\infty} \hat{f}_n \exp\left(\frac{in\pi x}{L}\right),$$

with complex Fourier coefficients

$$\hat{f}_n = \frac{1}{2L} \int_{-L}^L \exp\left(\frac{-in\pi x}{L}\right) f(x) dx.$$

The Fourier series of a function $f : (-L, L) \rightarrow \mathbb{R}$ is also given by the same expression, and the series converges to the $2L$ -periodic extension of f on the entire \mathbb{R} .

The complex form of Fourier series is more concise and arguably more elegant than the real form of Fourier series, which requires separate coefficients for the sine and cosine modes. However, in this course we mostly use the real form of Fourier series; this is mainly because Fourier sine and cosine series are far more frequently encountered than the (full) Fourier series in the analysis of PDEs, and the sine/cosine series also admit a compact representation.

2.B List of useful integrals

We list a few indefinite integrals that are useful for the evaluation of Fourier series.

1. $\int \sin(\alpha x) dx = -\frac{\cos(\alpha x)}{\alpha}$
2. $\int \cos(\alpha x) dx = \frac{\sin(\alpha x)}{\alpha}$
3. $\int x \sin(\alpha x) dx = \frac{\sin(\alpha x)}{\alpha^2} - \frac{x \cos(\alpha x)}{\alpha}$
4. $\int x \cos(\alpha x) dx = \frac{\cos(\alpha x)}{\alpha^2} + \frac{x \sin(\alpha x)}{\alpha}$
5. $\int x^2 \sin(\alpha x) dx = \frac{2x \sin(\alpha x)}{\alpha^2} + \frac{(2 - \alpha^2 x^2) \cos(\alpha x)}{\alpha^3}$
6. $\int x^2 \cos(\alpha x) dx = \frac{2x \cos(\alpha x)}{\alpha^2} + \frac{(\alpha^2 x^2 - 2) \sin(\alpha x)}{\alpha^3}$
7. $\int \sin(\alpha x) \sin(\beta x) dx = \frac{\sin((\alpha - \beta)x)}{2(\alpha - \beta)} - \frac{\sin((\alpha + \beta)x)}{2(\alpha + \beta)}, \quad \alpha \neq \beta$
8. $\int \cos(\alpha x) \sin(\beta x) dx = \frac{\cos((\alpha - \beta)x)}{2(\alpha - \beta)} - \frac{\cos((\alpha + \beta)x)}{2(\alpha + \beta)}, \quad \alpha \neq \beta$
9. $\int \cos(\alpha x) \cos(\beta x) dx = \frac{\sin((\alpha - \beta)x)}{2(\alpha - \beta)} + \frac{\sin((\alpha + \beta)x)}{2(\alpha + \beta)}, \quad \alpha \neq \beta$
10. $\int \sin^2(\alpha x) dx = \frac{x}{2} - \frac{\sin(2\alpha x)}{4\alpha}$
11. $\int \cos(\alpha x) \sin(\alpha x) dx = \frac{\sin^2(\alpha x)}{2\alpha}$
12. $\int \cos^2(\alpha x) dx = \frac{x}{2} + \frac{\sin(2\alpha x)}{4\alpha}$
13. $\cos(n\pi) = (-1)^n, n \in \mathbb{Z}$
14. $\sin(n\pi) = 0, n \in \mathbb{Z}$

Lecture 3

Fourier series: analysis

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3.1 Introduction

In the previous lecture we introduced Fourier series as a means to represent (i) periodic functions on \mathbb{R} or (ii) a periodic extension of functions defined on an interval. We have yet to answer the all important question: do Fourier series converge and, if so, for what classes of functions and in what sense? In this lecture we introduce a few different types of convergence for a sequence of functions and then discuss the regularity that the underlying function must possess to achieve each type of convergence.

3.2 Regularity of functions

We first review a few different characterizations of the regularity of functions. We will use these characterizations in the subsequent discussion of Fourier series.

Definition 3.1 (continuous functions). A function $f : (a, b) \rightarrow \mathbb{R}$ defined on an open interval (a, b) is continuous on (a, b) if $\lim_{x \rightarrow c} f(x) = f(c)$ for all $c \in (a, b)$. A function $g : [a, b] \rightarrow \mathbb{R}$ defined on a closed interval $[a, b]$ is continuous on $[a, b]$ if (i) $\lim_{x \rightarrow c} f(x) = f(c)$ for all $c \in (a, b)$, (ii) $\lim_{x \rightarrow a+} f(x) = f(a)$, and (iii) $\lim_{x \rightarrow b-} f(x) = f(b)$. The space of continuous functions on an interval I is denoted $C^0(I)$.

Definition 3.2 (continuously differentiable functions). Let $I \subset \mathbb{R}$ be an open or closed interval. A function $f : I \rightarrow \mathbb{R}$ is continuously differentiable on I if its derivative f' is continuous on I . The space of continuous differentiable functions is denoted $C^1(I)$.

Definition 3.3 (piecewise continuous functions). Let $(a, b) \subset \mathbb{R}$. A function $f : (a, b) \rightarrow \mathbb{R}$ is piecewise continuous on (a, b) if there exists a set of points $a \equiv x_1 < x_2 < \cdots < x_N \equiv b$ such that f is continuous on each interval (x_i, x_{i+1}) and one-sided limits $\lim_{x \rightarrow x_i+} f(x)$ and $\lim_{x \rightarrow x_{i+1}-} f(x)$ exist for $i = 1, \dots, N - 1$.

Definition 3.4 (piecewise continuously differentiable functions). Let $(a, b) \subset \mathbb{R}$. A function $f : (a, b) \rightarrow \mathbb{R}$ is piecewise continuously differentiable on (a, b) if there exists a set of points $a \equiv x_1 <$

$x_2 < \cdots < x_N \equiv b$ such that f is continuously differentiable on each interval (x_i, x_{i+1}) and one-sided limits $\lim_{x \rightarrow x_i^+} f'(x)$ and $\lim_{x \rightarrow x_{i+1}^-} f'(x)$ exist for $i = 1, \dots, N - 1$.

A function f is continuous on (a, b) if there are no discontinuities in the function. A function f is piecewise continuous on (a, b) if we can construct a finite number of open subintervals such that f is continuous on each of the open subintervals and limits exist at the endpoints; in other words, the function may have a finite number of discontinuities as long as it is bounded everywhere. Note that if f is continuous on (a, b) , then it is also piecewise continuous on (a, b) ; however, the converse is not true in general. We now consider a few concrete examples.

Example 3.5 (continuous function). Let $f(x) = 1/x$ for $x \in [0, 1]$. The function is not continuous on the closed interval $[0, 1]$ as the function is not defined at $x = 0$. The function is however continuous on the open interval $(0, 1)$.

Example 3.6 (continuously differentiable function). Let $f(x) = \sqrt{x}$ for $x \in [0, 1]$. The function is continuous on the interval $[0, 1]$ but is not continuously differentiable on the interval; the derivative $f'(x) = 1/(2\sqrt{x})$ is not defined at $x = 0$. (The function is similarly piecewise continuous but not piecewise continuously differentiable.)

Example 3.7 (piecewise continuous function). Let

$$f(x) = \begin{cases} 0, & x \in [-1, 0], \\ 1, & x \in (0, 1]. \end{cases}$$

The function is not continuous on $[-1, 1]$ because $\lim_{x \rightarrow 0^-} f(x) = 0 \neq 1 = \lim_{x \rightarrow 0^+} f(x)$. However, the function is piecewise continuous on $[-1, 1]$ because it is continuous on $(-1, 0)$ and $(0, 1)$ and the limits at the endpoints exist.

Example 3.8. Let $f(x) = \tan(x)$ for $x \in \mathbb{R}$, and consider subintervals $I_n \equiv (n\pi - \pi/2, n\pi + \pi/2)$, $n \in \mathbb{Z}$. While the function is continuous on each open subinterval I_n , the function is not piecewise continuous because the one-sided limits do not exist at the endpoints of the subintervals.

3.3 Convergence of Fourier series

We have so far discussed the representation of various functions as Fourier series but have not discussed two important questions: does the series converge, and, if yes, in what sense do they converge? To facilitate the discussion of convergence, we recall the truncated Fourier series defined in Definition 2.13,

$$s_N(x) \equiv \frac{1}{2}a_0 + \sum_{n=1}^N (a_n \cos(n\pi x) + b_n \sin(n\pi x)),$$

which is the N -term partial sum of the Fourier series. We now provide definitions for *pointwise convergence*, *uniform convergence*, and *L^2 convergence* of Fourier series.

Theorem 3.9 (Pointwise convergence of Fourier series). Let f be a piecewise continuously differentiable function with a period 2, and s_N be the associated truncated Fourier series. Then for any fixed $x \in \mathbb{R}$,

$$s_N(x) \rightarrow \frac{1}{2}[f(x^-) + f(x^+)] \quad \text{as } N \rightarrow \infty.$$

The result also holds for the Fourier cosine (resp. sine) series if f is a piecewise continuously differentiable, even (resp. odd) function with a period 2.

Proof. See Appendix 3.A. (Optional) □

Corollary 3.10. Consider the setting of Theorem 3.9. If f is continuous at x , then $s_N(x) \rightarrow f(x)$ as $N \rightarrow \infty$. If f is not continuous at x , then $s_N(x)$ converges to the average of the two one-sided limits $f(x^-)$ and $f(x^+)$ as $N \rightarrow \infty$.

Theorem 3.11 (Uniform convergence of Fourier series). Let f be a continuous and piecewise continuously differentiable function with a period 2, and s_N be the associated truncated Fourier series. Then s_N converges uniformly to f ; i.e.,

$$\max_{x \in \mathbb{R}} |f(x) - s_N(x)| \rightarrow 0 \quad \text{as } N \rightarrow \infty.$$

The result also holds for the Fourier cosine (resp. sine) series if f is a continuous, piecewise continuously differentiable, even (resp. odd) function with a period 2.

Proof. See Appendix 3.B. (Optional) □

Theorem 3.12 (L^2 convergence of Fourier series). Let f be a square-integrable function with a period 2; i.e., f is 2-periodic and

$$\int_{-1}^1 f(x)^2 dx < \infty.$$

Then s_N converges in L^2 to f ; i.e.,

$$\int_{-1}^1 (f(x) - s_N(x))^2 dx \rightarrow 0 \quad \text{as } N \rightarrow \infty.$$

The result also holds for the Fourier cosine (resp. sine) series if f is a square-integrable, even (resp. odd) function with a period 2.

Proof. See Appendix 3.C. (Optional) □

Example 3.13 (pointwise, uniform, and L^2 convergence). In this example we illustrate pointwise, uniform, and L^2 convergence using a simple sequence of functions (which is not a truncated Fourier series). Consider a sequence of functions $f_N : [0, 1] \rightarrow \mathbb{R}$, $N = 1, 2, \dots$, given by

$$f_N(x) = x^N.$$

For any fixed $x \in [0, 1)$, this function converges to

$$f_N(x) \rightarrow 0 \quad \text{as } N \rightarrow \infty$$

because $x < 1$. For $x = 1$, the function evaluates to

$$f_N(x = 1) = 1^N = 1 \quad \forall N.$$

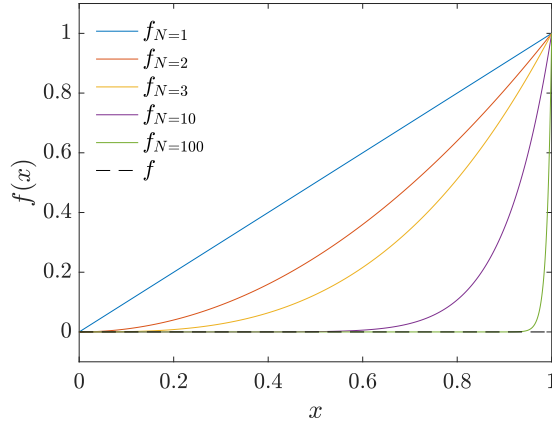


Figure 3.1: Convergence of $f_N(x) = x^N$.

Hence, the functions f_N converge to $f : [0, 1] \rightarrow \mathbb{R}$ given by

$$f(x) = \begin{cases} 0, & x \in [0, 1) \\ 1, & x = 1. \end{cases}$$

This convergence is pointwise, since we considered the convergence $f_N(x) \rightarrow f(x)$ for each fixed x .

While $f_N \rightarrow f$ pointwise, the sequence does not converge uniformly. To see this, we observe that, for any N ,

$$\max_{x \in [0, 1]} |f(x) - f_N(x)| = \max_{x \in (0, 1)} |f(x) - f_N(x)| = \max_{x \in (0, 1)} |0 - x^N| = \max_{x \in (0, 1)} |x^N| = 1 \neq 0,$$

where the first equality follows from $|f(x) - f_N(x)| = 0$ at $x = 0$ and 1 . (Technically, the “max” should be replaced by “sup”, the least upper bound.) The maximum error is equal to 1 for all N and does not converge to 0 as $N \rightarrow \infty$; hence the convergence is not uniform.

While the sequence does not converge uniformly, it does converge in L^2 because

$$\int_0^1 (f(x) - f_N(x))^2 dx = \int_0^1 (0 - x^N)^2 dx = \frac{1}{2N+1} x^{2N+1} \Big|_{x=0}^1 = \frac{1}{2N+1},$$

which converges to 0 as $N \rightarrow \infty$.

In summary, $f_N \rightarrow f$ pointwise and in L^2 , but not uniformly. In general, uniform convergence is a stronger condition than pointwise or L^2 convergence; i.e., if $f_N \rightarrow f$ uniformly, then the sequence also converges pointwise and in L^2 , but the converse is not true.

Example 3.14 (pointwise vs uniform convergence of Fourier series). We now consider uniform and pointwise convergence for Fourier series for a 2-periodic square-wave function

$$f(x) = \operatorname{sgn}(\sin(\pi x));$$

here $\operatorname{sgn}(z)$ evaluates to 1 if $z > 0$, 0 if $z = 0$, and -1 if $z < 0$. Since this is an odd function, we approximate the function using the Fourier sine series of the form $\sum_{n=1}^{\infty} \hat{f}_n \sin(n\pi x)$. We find that

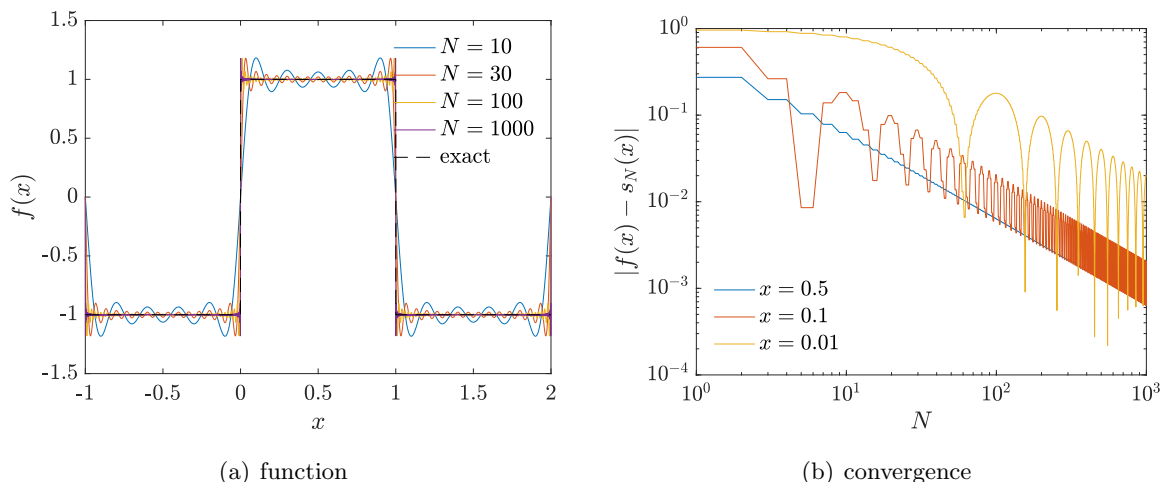


Figure 3.2: Convergence of the Fourier series for a square wave.

the coefficients must satisfy

$$\hat{f}_n = 2 \int_{x=0}^1 \sin(n\pi x) dx = \begin{cases} \frac{4}{n\pi}, & n \text{ odd,} \\ 0, & n \text{ even.} \end{cases}$$

Hence our Fourier sine series representation of the square wave is

$$f(x) \sim \sum_{k=1}^{\infty} \frac{4}{(2k-1)\pi} \sin((2k-1)\pi x).$$

Note that the square wave function is piecewise continuously differentiable but is not (globally) continuous. Hence, it satisfies the condition for pointwise convergence but not uniform convergence.

Figure 3.2(a) shows the truncated Fourier series for the square wave for $N = 10, 30, 100,$ and 1000 . We observe that (i) the truncated Fourier series at least visually gets “closer” to the exact square wave almost everywhere as N increases, but (ii) the magnitude of the oscillations near the discontinuities does not decrease. (It can be shown that peak value is approximately 1.18 as $N \rightarrow \infty$.) In particular, for *any given fixed* x (e.g., $x = 0.5$), we (at least visually) observe that the truncated Fourier series converges to the exact square wave as $N \rightarrow \infty$; this suggests pointwise convergence. However, regardless of how large N may be, we can always find some x for which the error is large (i.e., the peak of the oscillation); this suggests the series is not uniformly convergent.

We study the behavior in more detail in Figure 3.2(b), which shows the error in the truncated Fourier series as a function of the number of terms N for three different points of the square wave. To observe convergence, we fix the value of x to (say) $x = 0.5$ and observe that the error $|f(x = 0.5) - s_N(x = 0.5)|$ decreases as N increases; i.e., $s_N(x = 0.5) \rightarrow f(x = 0.5)$ as N increases. This convergence for a fixed x is also shown for $x = 0.1$ and $x = 0.01$ and in fact is observed for any x ; i.e., for any fixed x , there exists N sufficiently large such $|f(x) - s_N(x)| < \delta$ for any δ . *However, this value of N depends on x .* In particular, as $x \rightarrow 0$, the number of terms N required to achieve a given error grows in an unbounded manner. This is a manifestation of the fact that the truncated

Fourier series $s_N(x)$ is a continuous function that evaluates to $s_N(x = 0) = 0$, and hence a large number of terms is required for $s_N(x = \epsilon)$ to evaluate to 1 as $\epsilon \rightarrow 0$. Hence, the Fourier series does not converge uniformly for this discontinuous function.

We note that the key difference between the conditions for pointwise convergence and uniform convergence is the (global) continuity of the function. Namely, if $f : \mathbb{R} \rightarrow \mathbb{R}$ is discontinuous anywhere, we cannot expect the Fourier series to converge uniformly; the condition for uniform convergence is more stringent than for pointwise convergence. The condition for L^2 convergence is even weaker than the condition for pointwise convergence; all piecewise continuously differentiable functions are square integrable since the function is necessarily bounded, but square integrable functions need not be piecewise continuously differentiable. (In fact, the square integrability condition is even weaker than the piecewise continuity condition by the same argument.)

3.4 Convergence of Fourier series on finite intervals

While the convergence theorems, Theorems 3.9, 3.11, and 3.12, are provided for periodic functions on the entire \mathbb{R} , we can readily apply the theorems to a function defined on a finite interval by considering an appropriate periodic extension of the function. For instance, the (full) Fourier series of $f : (-L, L) \rightarrow \mathbb{R}$ is pointwise convergent if f is piecewise continuously differentiable; it converges to f on $(-L, L)$ in the pointwise sense (and to the periodic extension of f on the entire \mathbb{R}). Similarly, the Fourier cosine and sine series of $f : (0, L) \rightarrow \mathbb{R}$ is each pointwise convergent if f is piecewise continuously differentiable; they each converge to f on $(0, L)$ in the pointwise sense (and to the even and odd periodic extensions, respectively, of f on the entire \mathbb{R}).

The same extension also applies to uniform convergence; however, it is important to note that the (global) continuity condition for uniform convergence applies to the periodic, even periodic, and odd periodic extensions for the Fourier, Fourier cosine, and Fourier sine series, respectively. We illustrate this in a concrete example:

Example 3.15 (uniform convergence on a finite interval). Let $f(x) = x$ on $(0, 1)$. The Fourier cosine series of the function converges uniformly on $(0, 1)$ as the even periodic extension of f is a continuous and piecewise continuously differentiable function on \mathbb{R} . On the other hand, the Fourier sine series of the function does not converge uniformly on $(0, 1)$ as the odd periodic extension of f is not a continuous function on \mathbb{R} ; see Figure 2.1. (The Fourier sine series is nevertheless pointwise convergent because the odd periodic extension of f is piecewise continuously differentiable.)

The continuity requirement for each type of periodic extension, which is required for uniform convergence, can be summarized via the following conditions for the endpoints:

- (Full) Fourier series. For $f : (-L, L) \rightarrow \mathbb{R}$, the values at the endpoints should match: i.e., $f(-L^+) = f(L^-)$.
- Fourier sine series. For $f : (0, L) \rightarrow \mathbb{R}$, the function must vanish at the endpoints: i.e., $f(0^+) = f(L^-) = 0$.
- Fourier cosine series. For $f : (0, L) \rightarrow \mathbb{R}$, there are no additional endpoint conditions.

We readily arrive at these results by considering appropriate periodic extensions of f .

3.5 Uniform and absolute convergence

Theorem 3.11 provides conditions that a function f must satisfy for its Fourier series to be uniformly convergent. We now provide an alternative condition for uniform convergence in terms of the coefficients of the Fourier series.

Theorem 3.16 (absolute convergence). Let $f : \mathbb{R} \rightarrow \mathbb{R}$ be a periodic function with the Fourier series

$$f(x) \sim \frac{1}{2}a_0 + \sum_{n=1}^{\infty} (a_n \cos(n\pi x) + b_n \sin(n\pi x)),$$

where the coefficients are given by (2.1). The Fourier series converges uniformly to f if

$$\sum_{n=1}^{\infty} (|a_n| + |b_n|) < \infty.$$

Proof. See Appendix 3.B. (Optional) □

This theorem is useful because it allows us to assess the uniform convergence of an arbitrary series based solely on the decay of its Fourier coefficients, as illustrated in the following examples.

Example 3.17. Consider a Fourier cosine series

$$f(x) \sim \sum_{n=1}^{\infty} \frac{2}{n^2\pi^2} ((-1)^n - 1) \cos(n\pi x).$$

We recognize that the Fourier cosine coefficients are $\hat{f}_n = \frac{2}{n^2\pi^2} ((-1)^n - 1)$. To check if the series is uniformly convergent, we check the absolute convergence of the coefficients and observe that

$$\sum_{n=1}^{\infty} |\hat{f}_n| \leq \sum_{n=1}^{\infty} \frac{4}{n^2\pi^2} < \infty.$$

Because the coefficients are absolutely convergent, the Fourier series converges uniformly. (Note that this Fourier cosine series is associated with $f(x) = x$, $x \in (0, 1)$, considered in Example 2.17. Because the even periodic extension of the function is continuous and piecewise continuously differentiable, Theorem 3.11 also states the Fourier series is uniformly convergent. However, Theorem 3.16, unlike Theorem 3.11, does not require us to know an explicit form of f .)

Example 3.18. Consider a Fourier sine series

$$f(x) \sim \sum_{n=1}^{\infty} (-1)^{n+1} \frac{2}{n\pi} \sin(n\pi x).$$

We recognize that the Fourier sine coefficients are $\hat{f}_n = (-1)^{n+1} \frac{2}{n\pi}$. To check if the series is uniformly convergent, we check the absolute convergence of the coefficients and observe that

$$\sum_{n=1}^{\infty} |\hat{f}_n| = \sum_{n=1}^{\infty} \frac{2}{n\pi},$$

which diverges. Because the coefficients are not absolutely convergent, the Fourier series does not necessarily converge uniformly. (Note that this Fourier sine series is associated with $f(x) = x$, $x \in (0, 1)$, considered in Example 2.18. Because the odd periodic extension of the function is not continuous, Theorem 3.11 states the Fourier series is not uniformly convergent.)

3.6 Differentiation of Fourier series

We now summarize the properties of Fourier series under differentiation. These properties will play a crucial role as we use Fourier series to represent solutions to (partial) differential equations.

Theorem 3.19 (differentiation of Fourier series). Let f be a continuous periodic function with piecewise continuously differentiable derivative f' . Then the Fourier series of f' can be obtained by term-by-term differentiation of the Fourier series of f ; i.e., if

$$f(x) \sim \frac{1}{2}a_0 + \sum_{n=1}^{\infty} (a_n \cos(n\pi x) + b_n \sin(n\pi x)),$$

then

$$f'(x) \sim \sum_{n=1}^{\infty} (-a_n n\pi \sin(n\pi x) + b_n n\pi \cos(n\pi x)).$$

For any fixed $x \in \mathbb{R}$, the differentiated series converge to $\frac{1}{2}(f'(x^-) + f'(x^+))$.

Theorem 3.20 (uniform convergence of derivatives). Let f be a periodic function with Fourier coefficients a_n and b_n . Suppose

$$\sum_{n=1}^{\infty} (|n^k a_n| + |n^k b_n|) < \infty$$

for some $k \in \mathbb{N}_{>0}$. Then f has a continuous derivatives $f', \dots, f^{(k)}$, whose Fourier series are obtained by term-by-term differentiation of the Fourier series of f .

Proof. Proof follows from Theorems 3.19 and 3.16. □

Example 3.21 (C^∞ or smooth functions). One particular form of Fourier series that we encounter in the analysis of heat equation is

$$f(x) = \sum_{n=1}^{\infty} \exp(-\lambda n) \sin(n\pi x)$$

for $\lambda > 0$. We recognize that $a_n = 0$ and $b_n = \exp(-\lambda n)$. To verify if the derivative of order k exists, we consider the series

$$\sum_{n=1}^{\infty} n^k \exp(-\lambda n),$$

and observe that this series converges for any $k \in \mathbb{N}_{>0}$. Hence f is infinitely differentiable; an infinitely differentiable function is said to be *smooth* and belongs to C^∞ . (To prove the series converges, use, for instance, the comparison test with $\sum_{n=1}^{\infty} c_n = \sum_{n=1}^{\infty} 1/n^2$ and note that (i) $a_n/c_n = n^{k+2} \exp(-\lambda n) < 1$ for n sufficiently large, and (ii) $\sum_{n=1}^{\infty} c_n$ converges.)

3.7 Summary

We summarize key points of this lecture:

1. Uniform, pointwise, and L^2 convergences are three different ways to characterize the convergence of a sequence of functions $(f_n)_n$ to f . Uniform convergence is more stringent than pointwise convergence, and pointwise convergence is more stringent than L^2 convergence.
2. The Fourier series of $f : \mathbb{R} \rightarrow \mathbb{R}$ converges in L^2 for any periodic function f that is square integrable.
3. The Fourier series of $f : \mathbb{R} \rightarrow \mathbb{R}$ converges pointwise, except at discontinuities, for any periodic function f that is piecewise continuously differentiable. At the discontinuities the Fourier series converges to the average of the left and right limits.
4. The Fourier series of $f : \mathbb{R} \rightarrow \mathbb{R}$ converges uniformly for any periodic function f that is continuous and piecewise continuously differentiable.
5. A Fourier series is uniformly convergent if its coefficients are absolutely convergent.
6. The conditions for pointwise, uniform, and L^2 convergence readily extend to functions defined on a bounded domain as long as the appropriate periodic extension of the function satisfies the required continuity and differentiability conditions.
7. The term-by-term differentiation of a Fourier series is well defined only if the function is continuous and piecewise continuously differentiable.

3.A Proof of pointwise convergence

We prove the pointwise convergence of Fourier series, Theorem 3.9. We prove the result for $f : \mathbb{R} \rightarrow \mathbb{R}$ with a period 2, but the result readily generalizes for functions with any periodic function through the transformation considered in Section 2.5. The presentations in this and subsequent Appendices closely follow Strauss, *Partial Differential Equations: An Introduction*.

For simplicity, we prove the result for a continuous f . To begin, we recall that the Fourier series and the associated partial sum are given by

$$f(x) \sim \frac{1}{2}a_0 + \sum_{n=1}^{\infty} (a_n \cos(n\pi x) + b_n \sin(n\pi x)),$$

$$s_N(x) = \frac{1}{2}a_0 + \sum_{n=1}^N (a_n \cos(n\pi x) + b_n \sin(n\pi x)),$$

for coefficients

$$a_n = \int_{-1}^1 \cos(n\pi y) f(y) dy \quad \text{and} \quad b_n = \int_{-1}^1 \sin(n\pi y) f(y) dy.$$

We now substitute the expression for the coefficients to the partial sum to obtain

$$s_N(x) = \int_{y=-1}^1 \left[\frac{1}{2} + \sum_{n=1}^N (\cos(n\pi y) \cos(n\pi x) + \sin(n\pi y) \sin(n\pi x)) \right] f(y) dy$$

$$= \int_{y=-1}^1 \left[\frac{1}{2} + \sum_{n=1}^N \cos(n\pi(y-x)) \right] f(y) dy.$$

We now introduce the *Dirichlet kernel*

$$K_N(\xi) \equiv \frac{1}{2} + \sum_{n=1}^N \cos(n\pi\xi)$$

so that

$$s_N(x) = \int_{y=-1}^1 K_N(y-x) f(y) dy.$$

The Dirichlet kernel has two important properties. The first is that the sum can be expressed in a simple form:

$$K_N(\xi) = \frac{\sin((N+1/2)\pi\xi)}{2 \sin(\pi\xi/2)};$$

this result can be readily shown using the De Moivre's formula and rearranging the exponentials. The second property is that

$$\int_{-1}^1 K_N(\xi) d\xi = 1,$$

since only the leading term, $1/2$, contributes to the integral. We now set $\xi = y - x$ to obtain

$$s_N(x) = \int_{y=-1}^1 K_N(y-x) f(y) dy = \int_{\xi=x-1}^{x+1} K_N(\xi) f(x+\xi) d\xi = \int_{\xi=-1}^1 K_N(\xi) f(x+\xi) d\xi,$$

where the last equality follows since K_N and f are both 2-periodic. We now appeal to $\int_{-1}^1 K_N(\xi)d\xi = 1$ to obtain

$$f(x) - s_N(x) = \int_{\xi=-1}^1 K_N(\xi)(f(x) - f(x + \xi))d\xi.$$

We now rearrange the expression as follows:

$$f(x) - s_N(x) = \int_{\xi=-1}^1 \frac{\sin((N + 1/2)\pi\xi)}{2 \sin(\pi\xi/2)}(f(x) - f(x + \xi))d\xi = \int_{\xi=-1}^1 g(\xi; x)\phi_N(\xi)d\xi,$$

where

$$g(\xi; x) \equiv \frac{f(x) - f(x + \xi)}{2 \sin(\pi\xi/2)},$$

$$\phi(\xi) \equiv \sin((N + 1/2)\pi\xi), \quad N = 1, 2, \dots$$

We note that $\{\phi_N\}_{N=1}^\infty$ is an orthonormal set on $(-1, 1)$ because

$$\int_{-1}^1 \sin((N + 1/2)\pi\xi) \sin((M + 1/2)\pi\xi)d\xi = \int_{-1}^1 \sin(N\pi\xi) \sin(M\pi\xi)d\xi = \delta_{MN},$$

where the first equality follows from the periodicity of the sine functions. Hence by Bessel's inequality

$$\sum_{N=1}^{\infty} (g(\cdot; x), \phi_N)^2 \leq \|g(\cdot; x)\|^2.$$

It follows that if $\|g(\cdot; x)\| < \infty$ then the series converges, which implies that $(g(\cdot; x), \phi_N) = f(x) - s_N(x) \rightarrow 0$ as $N \rightarrow \infty$.

We finally verify that $\|g(\cdot; x)\| < \infty$. We have

$$\|g(\cdot; x)\|^2 = \int_{\xi=-1}^1 \left(\frac{f(x) - f(x + \xi)}{2 \sin(\pi\xi/2)} \right)^2 d\xi.$$

Since f is continuous, the numerator is bounded. The only potential difficulty arises when the denominator goes to 0 at $\xi = 0$. However we find that

$$\lim_{\xi \rightarrow 0} g(\xi) = \lim_{\xi \rightarrow 0} \frac{f(x) - f(x + \xi)}{2 \sin(\pi\xi/2)} = \lim_{\xi \rightarrow 0} \frac{-f'(x + \xi)}{\pi \cos(\pi\xi/2)} = -f'(x)/\pi < \infty$$

by L'Hopital's rule since f is differentiable at x (by assumption). Hence g is bounded everywhere and the integral $\|g\|$ is finite.

3.B Proof of uniform convergence

We prove two theorems regarding the uniform convergence of Fourier series: Theorems 3.11 and 3.16. We first prove Theorem 3.16, which states that the Fourier series converges uniformly to f if its coefficients are absolutely convergent. For a given $x \in [-1, 1]$, we take the difference between $f(x)$ and the truncated Fourier series $s_N(x)$ to obtain

$$\begin{aligned} f(x) - s_N(x) &= \frac{1}{2}a_0 + \sum_{n=1}^{\infty} (a_n \cos(n\pi x) + b_n \sin(n\pi x)) - \frac{1}{2}a_0 - \sum_{n=1}^N (a_n \cos(n\pi x) + b_n \sin(n\pi x)) \\ &= \sum_{n=N+1}^{\infty} (a_n \cos(n\pi x) + b_n \sin(n\pi x)). \end{aligned}$$

It follows that

$$\max_{x \in [-1, 1]} |f(x) - s_N(x)| = \max_{x \in [-1, 1]} \left| \sum_{n=N+1}^{\infty} (a_n \cos(n\pi x) + b_n \sin(n\pi x)) \right| \leq \sum_{n=N+1}^{\infty} (|a_n| + |b_n|).$$

Because (by assumption) the series is a tail of the absolutely convergent series $\sum_{n=1}^{\infty} (|a_n| + |b_n|) < \infty$, it must vanish as $N \rightarrow \infty$. It follows that

$$\max_{x \in [-1, 1]} |f(x) - s_N(x)| \leq \sum_{n=N+1}^{\infty} (|a_n| + |b_n|) \rightarrow 0 \quad \text{as } N \rightarrow \infty,$$

if the coefficients are absolutely convergent.

We next prove Theorem 3.11, which states that the Fourier series converges uniformly to $f : \mathbb{R} \rightarrow \mathbb{R}$ if f is continuously differentiable and has a period of 2. To begin, let a_n and b_n denote the Fourier coefficients of f and a'_n and b'_n denote the Fourier coefficients of f' . We observe that

$$\begin{aligned} a_n &= \int_{-1}^1 \cos(n\pi x) f(x) dx = \frac{1}{n\pi} f(x) \sin(n\pi x) \Big|_{x=-1}^1 - \frac{1}{n\pi} \int_{-1}^1 \sin(n\pi x) f'(x) dx = -\frac{1}{n\pi} b'_n, \\ b_n &= \int_{-1}^1 \sin(n\pi x) f(x) dx = -\frac{1}{n\pi} f(x) \cos(n\pi x) \Big|_{x=-1}^1 + \frac{1}{n\pi} \int_{-1}^1 \cos(n\pi x) f'(x) dx = \frac{1}{n\pi} a'_n, \end{aligned}$$

where the first equality follows because f is continuously differentiable, and the last equality follows from periodicity for each case. It follows that

$$\sum_{n=1}^{\infty} (|a_n| + |b_n|) = \sum_{n=1}^{\infty} \frac{1}{n\pi} (|b'_n| + |a'_n|) \leq \left(\sum_{n=1}^{\infty} \frac{1}{n^2} \right)^{1/2} \left(\sum_{n=1}^{\infty} 2(|a'_n|^2 + |b'_n|^2) \right)^{1/2} < \infty,$$

where the last inequality follows from the convergence of the p -series for $p = 2$, which implies $\sum_{n=1}^{\infty} \frac{1}{n^2} < \infty$, and Bessel's inequality for the derivative f' , which implies $\sum_{n=1}^{\infty} (|a'_n|^2 + |b'_n|^2) \leq \|f'\|^2 < \infty$. Since the Fourier coefficients for f is absolutely convergent, the Fourier series converges uniformly to f by Theorem 3.16, which we just proved.

3.C L^2 convergence and optimality of Fourier series

We now introduce some properties of Fourier series related to its convergence in L^2 . In fact, all properties we will consider apply to any series representation of functions based on a (complete) set of orthonormal functions $(\phi_n)_{n=1}^\infty$. We hence abstract our Fourier series in the following form:

$$f(x) \sim \sum_{n=1}^{\infty} \hat{f}_n \phi_n(x)$$

for coefficients

$$\hat{f}_n = \int_{-1}^1 \phi_n(x) f(x) dx.$$

The associated truncated Fourier series is defined by

$$s_N(x) \equiv \sum_{n=1}^N \hat{f}_n \phi_n(x).$$

(If the functions $(\phi_n)_{n=1}^\infty$ are orthogonal (but not orthonormal), then the coefficients are normalized by the norm of ϕ_n : i.e., $\hat{f}_n = \frac{\int_{-1}^1 \phi_n(x) f(x) dx}{\int_{-1}^1 \phi_n(x)^2 dx}$.)

Proposition 3.22 (optimality of Fourier series). Consider functions of the form

$$g_N(x) \equiv \sum_{n=1}^N \hat{g}_n \phi_n(x),$$

where \hat{g}_n , $n = 1, 2, \dots$, are some arbitrary coefficients. The truncated Fourier series s_N of f is the best N -term approximation associated with the basis (ϕ_n) in the sense that

$$\|f - s_N\| \leq \|f - g_N\| \quad \forall g_N.$$

Proof. We find

$$\begin{aligned} E_N &\equiv \|f - g_N\|^2 = \|f\|^2 - 2(f, g_N) + (g_N, g_N) = \|f\|^2 - 2(f, \sum_{n=1}^N \hat{g}_n \phi_n) + (\sum_{n=1}^N \hat{g}_n \phi_n, \sum_{m=1}^N \hat{g}_m \phi_m) \\ &= \|f\|^2 - 2 \sum_{n=1}^N \hat{g}_n (f, \phi_n) + \sum_{n,m=1}^N \hat{g}_n \hat{g}_m (\phi_n, \phi_m) = \|f\|^2 - 2 \sum_{n=1}^N \hat{g}_n \hat{f}_n + \sum_{n=1}^N \hat{g}_n^2, \end{aligned} \quad (3.1)$$

where the last equality follows from the definition of the (generalized) Fourier coefficients ($\hat{f}_n = (f, \phi_n)$) and the orthonormality of functions ($(\phi_m, \phi_n) = \delta_{mn}$).

We recall that E_N is minimized if (i) all first derivative of E_N with respect to the coefficients vanish and (ii) the Hessian (i.e., second derivative) of E_N with respect to the coefficients is positive definite. To this end, we evaluate the first derivative of E_N with respect to the coefficients:

$$\frac{\partial E_N}{\partial \hat{g}_n} = x - 2 \sum_{n=1}^N \hat{f}_n + 2 \sum_{n=1}^N \hat{g}_n = 0 \quad \Rightarrow \quad \hat{g}_n = \hat{f}_n.$$

In addition, the second derivative is

$$\frac{\partial^2 E_N}{\partial \hat{g}_n^2} = 2,$$

and all mixed partial derivatives vanish; hence the Hessian is positive definite. It follows that the set of coefficients that minimizes the square-integral error E_N is given by $\hat{g}_n = \hat{f}_n = (f, \phi_n)$, which are the generalized Fourier coefficients. \square

Theorem 3.23 (Bessel's inequality). Let $f : (-1, 1) \rightarrow \mathbb{R}$ be a square-integrable function, $(\phi_n)_{n=1}^{\infty}$ be an orthonormal set of functions, and $\hat{f}_n = (f, \phi_n)$ be the associated coefficients. Then,

$$\sum_{n=1}^{\infty} \hat{f}_n^2 \leq \int_{-1}^1 f(x)^2 dx.$$

Proof. We substitute $\hat{g}_n = \hat{f}_n$ in (3.1) to obtain, for all $N \in \mathbb{N}$,

$$E_N \equiv \|f - g_N\|^2 = \|f\|^2 - \sum_{n=1}^N \hat{f}_n^2 \geq 0.$$

We rearrange the inequality to obtain

$$\sum_{n=1}^N \hat{f}_n^2 \leq \|f\|^2.$$

Since the relationship holds for any N , we take $N \rightarrow \infty$ to obtain the desired inequality. \square

Theorem 3.24 (Parseval's identity). The Fourier series of $f : (-1, 1) \rightarrow \mathbb{R}$ converges to f in the mean-square sense if and only if

$$\sum_{n=1}^{\infty} \hat{f}_n^2 = \int_{-1}^1 f^2 dx.$$

Proof. Parseval's identity is a consequence of the L^2 convergence of Fourier series. Namely,

$$\lim_{N \rightarrow \infty} E_N \equiv \lim_{N \rightarrow \infty} \|f - g_N\|^2 = \lim_{N \rightarrow \infty} (\|f\|^2 - \sum_{n=1}^N \hat{f}_n^2) = \|f\|^2 - \sum_{n=1}^{\infty} \hat{f}_n^2 = 0,$$

which is the desired equality. \square

Remark 3.25 (decay of Fourier coefficients). Let $f : (-1, 1) \rightarrow \mathbb{R}$ be a square-integrable function, $(\phi_n)_{n=1}^{\infty}$ be an orthonormal set of functions, and $\hat{f}_n = (f, \phi_n)$ be the associated coefficients. Then

$$\hat{f}_n = (f, \phi_n) \rightarrow 0 \quad \text{as } n \rightarrow \infty.$$

This is a direct consequence of Bessel's inequality. Since the series $\sum_{n=1}^{\infty} \hat{f}_n^2 < \infty$, the coefficients must converge to 0.

Lecture 4

Sturm-Liouville theory

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4.1 Introduction

We have so far formulated and analyzed Fourier series based on sinusoidal functions. In our formulation, we have found that orthogonal functions provide a particularly simple expression for the coefficients; in our analysis, we found that many of the convergence properties derive from the orthogonality and completeness of the sinusoidal functions. In this lecture we study an important class of ordinary differential equations (ODEs): the Sturm-Liouville problem. The solution to the problem is a complete set of orthogonal functions, which can be used to form a generalized Fourier series, which shares many of the convergence properties of the “classical” Fourier series.

4.2 Motivation: Fourier series and eigenproblem

We first explore the connection between Fourier series and some select eigenproblems. To this end, consider an ODE eigenproblem: find eigenpairs (ϕ_n, λ_n) (i.e., eigenfunction ϕ_n and the associated eigenvalue λ_n) such that

$$\begin{aligned} -\phi_n'' &= \lambda_n \phi_n \quad \text{in } (0, 1), \\ \phi_n(0) &= \phi_n(1) = 0. \end{aligned} \tag{4.1}$$

To find the solution, we consider three different cases for the eigenvalue:

- *Case 1:* $\lambda_n < 0$. Let $\mu_n = -\lambda_n$ so that $\mu_n > 0$. The general solution to (4.1) is of the form

$$\phi_n(x) = A_n \cosh(\sqrt{\mu_n}x) + B_n \sinh(\sqrt{\mu_n}x).$$

The boundary condition at $x = 0$ requires

$$\phi_n(x = 0) = A_n = 0.$$

The boundary condition at $x = 1$ requires

$$\phi_n(x = 1) = B_n \sinh(\sqrt{\mu_n}) = 0 \quad \Rightarrow \quad B_n = 0,$$

since $\sinh(x) = 0$ only if $x = 0$. The only solution to the eigenproblem (4.1) is the trivial solution $\phi_n = 0$. Hence $\lambda_n < 0$ does not yield a desired family of nontrivial functions.

- *Case 2:* $\lambda_n = 0$. If $\lambda_n = 0$, the general solution to (4.1) is of the form

$$\phi_n(x) = A_n x + B_n.$$

The boundary condition at $x = 0$ requires

$$\phi_n(x = 0) = B_n = 0.$$

The boundary condition at $x = 1$ requires

$$\phi_n(x = 1) = A_n = 0.$$

Again, if $\lambda_n = 0$, the only solution to the eigenproblem (4.1) is the trivial solution $\phi_n = 0$.

- *Case 3:* $\lambda_n > 0$. The general solution to (4.1) is of the form

$$\phi_n(x) = A_n \cos(\sqrt{\lambda_n}x) + B_n \sin(\sqrt{\lambda_n}x).$$

The boundary condition at $x = 0$ requires

$$\phi_n(x = 0) = A_n = 0.$$

The boundary condition at $x = 1$ requires

$$\phi_n(x = 1) = B_n \sin(\sqrt{\lambda_n}) = 0.$$

Since we seek a nontrivial solution, we require $B_n \neq 0$. It hence follows that

$$\sin(\sqrt{\lambda_n}) = 0 \quad \Rightarrow \quad \lambda_n = n^2\pi^2, \quad n = 1, 2, \dots$$

Hence $\phi_n(x) = \sin(n\pi x)$ and $\lambda_n = n^2\pi^2$ for $n = 1, 2, \dots$ are the nontrivial solutions to the eigenproblem (4.1).

The solution to the eigenproblem (4.1) is hence

$$\phi_n(x) = \sin(n\pi x) \quad \text{and} \quad \lambda_n = n^2\pi^2 \quad \text{for} \quad n = 1, 2, \dots$$

We make a few observations:

1. The eigenfunctions are the basis of Fourier sine series, and hence the linear combination of the eigenfunctions can approximate any square integrable function.
2. The eigenfunctions are orthogonal.
3. The eigenvalues are real and nonnegative.

We now ask an important question:

Could we have known all of the above properties just by looking at the eigenproblem *without having to find the explicit expressions for the solution?*

It turns out the answer is *yes*. All of the above properties are consequences of the Sturm-Liouville theory.

4.3 Sturm-Liouville theory

We introduce the *regular Sturm-Liouville problem*.

Definition 4.1 (regular Sturm-Liouville problem). The regular Sturm-Liouville problem is given by

$$\begin{aligned} -(p\phi)' + q\phi &= \lambda w\phi \quad \text{in } (a, b), \\ \alpha_1\phi(a) - \alpha_2\phi'(a) &= 0, \\ \beta_1\phi(b) + \beta_2\phi'(b) &= 0, \end{aligned}$$

where $p : [a, b] \rightarrow \mathbb{R}$, $p' : [a, b] \rightarrow \mathbb{R}$, $q : [a, b] \rightarrow \mathbb{R}$ and $w : [a, b] \rightarrow \mathbb{R}$ are continuous on $[a, b]$, $p > 0$ and $w > 0$ on $[a, b]$, and $\alpha_1^2 + \alpha_2^2 > 0$ and $\beta_1^2 + \beta_2^2 > 0$.

While the particular form of the Sturm-Liouville equation might appear rather restrictive at the first glance, the equation is quite general; specifically, second-order ODEs of the form

$$-\gamma_2\phi'' + \gamma_1\phi' + \gamma_0\phi = \lambda\phi \quad \text{in } (a, b)$$

can be recast as the Sturm-Liouville equation through the change of variables

$$p(x) = \exp\left(\int^x -\frac{\gamma_1(\xi)}{\gamma_2(\xi)} d\xi\right), \quad q(x) = \frac{\gamma_0(x)}{\gamma_2(x)}p(x), \quad w(x) = \frac{1}{\gamma_2(x)}p(x).$$

We now introduce important properties of the Sturm-Liouville problem and its solutions. (*Note:* proofs are provided for completeness, but they should be considered optional reading items.)

Theorem 4.2 (self-adjointness of Sturm-Liouville operator). The Sturm-Liouville operator $L \equiv -\frac{d}{dx}(p\frac{d}{dx}) + q$ is self-adjoint in the sense that

$$(Lw, v) = (w, Lv)$$

for any complex-valued functions $w, v \in C^2([a, b])$ that satisfy the boundary conditions. Here $(\cdot, \cdot) : \mathbb{C} \times \mathbb{C} \rightarrow \mathbb{C}$ is the L^2 inner product on complex-valued functions given by $(f, g) \equiv \int_a^b f\bar{g}dx$, where \bar{g} denotes the complex conjugate of g .

Proof. We use integration by parts to obtain

$$(Lw, v) - (w, Lv) = \int_a^b (-(pw')' + qw)\bar{v} - (-(p\bar{v}')' + q\bar{v})w dx = [p(-w'\bar{v} + \bar{v}'w)]_{x=a}^b.$$

We now appeal to the boundary condition at $x = a$ to find that

$$\begin{aligned} \alpha_1 w(a) - \alpha_2 w'(a) &= 0, \\ \alpha_1 \bar{v}(a) - \alpha_2 \bar{v}'(a) &= 0, \end{aligned}$$

which may be written as

$$\begin{pmatrix} w(a) & -w'(a) \\ \bar{v}(a) & -\bar{v}'(a) \end{pmatrix} \begin{pmatrix} \alpha_1 \\ \alpha_2 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \end{pmatrix}.$$

Since $\alpha_1^2 + \alpha_2^2 > 0$, the linear system has a nontrivial solution and the matrix must be singular. It follows that

$$w(a)\bar{v}'(a) - w'(a)\bar{v}(a) = 0.$$

We also invoke the same argument on the boundary $x = b$ to find that

$$w(b)\bar{v}'(b) - w'(b)\bar{v}(b) = 0.$$

Hence

$$(Lw, v) - (w, Lv) = [p(-w'\bar{v} + \bar{v}'w)]_{x=a}^b = 0,$$

which is the desired equality. \square

Theorem 4.3 (realness of Sturm-Liouville eigenvalues). All eigenvalues of the regular Sturm-Liouville problem are real.

Proof. Let ϕ and λ be an eigenfunction and eigenvalue, respectively, of a regular Sturm-Liouville problem. Then $L\phi = \lambda w\phi$, and hence

$$0 = (L\phi, \phi) - (\phi, L\phi) = (\lambda - \bar{\lambda}) \int_a^b w\phi^2 dx.$$

Since $\int_a^b w\phi^2 dx \neq 0$, $\lambda - \bar{\lambda} = 2\text{Im}(\lambda) = 0$, and λ is real. \square

Theorem 4.4 (orthogonality of Sturm-Liouville eigenfunctions). The eigenfunctions of the regular Sturm-Liouville problem associated with two distinct eigenvalues λ_n and λ_m are orthogonal with respect to the weight $w : [a, b] \rightarrow \mathbb{R}_{>0}$ in the sense that

$$\int_a^b w\phi_m\phi_n dx = 0, \quad n \neq m.$$

Proof. Suppose ϕ_m and ϕ_n are eigenfunctions associated with distinct eigenvalues λ_m and λ_n so that

$$\begin{aligned} -(p\phi_n')' + q\phi_n - \lambda_n w\phi_n &= L\phi_n - \lambda_n w\phi_n = 0 \\ -(p\phi_m')' + q\phi_m - \lambda_m w\phi_m &= L\phi_m - \lambda_m w\phi_m = 0. \end{aligned}$$

We multiply the first and second equations by ϕ_m and ϕ_n , respectively, integrate over (a, b) , and take the difference of the two equations to find that

$$\begin{aligned} 0 &= (L\phi_n, \phi_m) - \lambda_n(w\phi_n, \phi_m) - (\phi_n, L\phi_m) + \lambda_m(w\phi_n, \phi_m) \\ &= [(L\phi_n, \phi_m) - (\phi_n, L\phi_m)] - (\lambda_n - \lambda_m)(w\phi_n, \phi_m). \end{aligned}$$

Because the Sturm-Liouville operator L is self-adjoint, the term in the bracket vanishes. It follows that

$$(\lambda_n - \lambda_m)(w\phi_n, \phi_m) = (\lambda_n - \lambda_m) \int_a^b w\phi_n\phi_m dx = 0.$$

Hence if $\lambda_m \neq \lambda_n$, the eigenfunctions are orthogonal with respect to the weight function w . \square

Theorem 4.5. The regular Sturm-Liouville problem has an infinite number of eigenvalues and $\lambda_n \rightarrow \infty$ as $n \rightarrow \infty$. Moreover, if $q \geq 0$ on $[a, b]$ and $\alpha_1 \geq 0$, $\alpha_2 \geq 0$, $\beta_1 \geq 0$, and $\beta_2 \geq 0$, then $\lambda_n \geq 0$ for all n .

Proof. The proof that $\lambda_n \rightarrow \infty$ as $n \rightarrow \infty$ is beyond the scope of this course. We however will show that $\lambda_n \geq 0$. Suppose ϕ_n and λ_n are an eigenfunction and the associated eigenvalue. We multiply the ODE of the Sturm-Liouville by ϕ_n and integrate over (a, b) to obtain

$$\int_a^b \phi_n (-(p\phi_n')' + q\phi_n) dx = \lambda_n \int_a^b \phi_n \phi_n w dx.$$

We integrate by parts the first term to obtain

$$\int_a^b (p(\phi_n')^2 + q\phi_n^2) dx - p(b)\phi_n(b)\phi_n'(b) + p(a)\phi_n(a)\phi_n'(a) = \lambda_n \int_a^b \phi_n^2 w dx.$$

To proceed further, we first consider the case where $\alpha_2 \neq 0$ and $\beta_2 \neq 0$. Then, the boundary conditions $\alpha_1\phi(a) - \alpha_2\phi'(a) = 0$ and $\beta_1\phi(b) + \beta_2\phi'(b) = 0$ require that $\phi'(a) = \frac{\alpha_1}{\alpha_2}\phi(a)$ and $\phi'(b) = -\frac{\beta_1}{\beta_2}\phi(b)$, respectively. Hence

$$\int_a^b (p(\phi_n')^2 + q\phi_n^2) dx + p(b)\frac{\beta_1}{\beta_2}\phi_n(b)^2 + p(a)\frac{\alpha_1}{\alpha_2}\phi_n(a)^2 = \lambda_n \int_a^b \phi_n^2 w dx. \quad (4.2)$$

We note that (i) the integral in the left-hand side is non-negative since $p \geq 0$ and $q \geq 0$, (ii) both boundary terms are non-negative since $\alpha_1 \geq 0$, $\alpha_2 \geq 0$, $\beta_1 \geq 0$, and $\beta_2 \geq 0$, and (iii) the integral in the right-hand side is (strictly) positive. We hence conclude that $\lambda_n \geq 0$.

We next consider the cases where either or both of α_2 and β_2 are zero. If $\alpha_2 = 0$ and $\beta_2 \neq 0$, then the boundary condition requires $\phi(a) = 0$ and hence the second boundary term of (4.2) vanishes; however, all remaining terms in the left-hand side are non-negative and hence $\lambda_n \geq 0$. We make analogous arguments for the case where $\alpha_2 \neq 0$ and $\beta_2 = 0$ and the case where $\alpha_2 = \beta_2 = 0$ to conclude that $\lambda_n \geq 0$. \square

These properties may look rather abstract at the first glance. However, given the Sturm-Liouville operator is a linear operator, we can relate the above properties to the familiar properties of linear operators in \mathbb{R}^n : symmetric matrices (or Hermitian matrices if complex). First, self-adjointness $(Lw, v) = (w, Lv)$ is analogous to the condition that $v^H Aw = v^H A^T w$ for real symmetric matrices, where \cdot^H denotes the conjugate transpose. Second, all eigenvalues of the Sturm-Liouville problem are real, just like real symmetric matrices have all real eigenvalues. Third, the eigenfunctions of the Sturm-Liouville problem are orthogonal, just like the eigenvectors of real symmetric matrices are orthogonal. Finally, under certain conditions all eigenvalues of the Sturm-Liouville problem are nonnegative, just like all eigenvalues of symmetric positive semi-definite matrices are nonnegative.

4.4 Examples of the Sturm-Liouville problem

We now provide some examples of orthogonal functions that arise as solutions of the regular Sturm-Liouville problem.

Example 4.6 (sine functions). Consider an eigenproblem

$$\begin{aligned} -\phi_n'' &= \lambda_n \phi_n \quad \text{in } (0, 1), \\ \phi_n(0) &= \phi_n(1) = 0. \end{aligned}$$

We readily verify that this is a regular Sturm-Liouville problem with $p = 1$, $q = 0$, $w = 1$, $\alpha_1 = \beta_1 = 1$, and $\alpha_2 = \beta_2 = 0$. It follows that the eigenfunctions $\{\phi_n\}$ are orthogonal. Moreover, because $w, \alpha_1, \alpha_2, \beta_1$, and β_2 are all nonnegative, the eigenvalues are nonnegative. The power of the Sturm-Liouville theory is that we arrive at these conclusions without necessarily knowing the explicit expressions for the eigenvalues and eigenfunctions.

(Of course, we have seen in Section 4.2 that the explicit form of the solution is $\phi_n(x) = \sin(n\pi x)$ and $\lambda_n = n^2\pi^2$ for $n = 1, 2, \dots$. We readily verify that the solution satisfies all of the above properties.)

Example 4.7 (cosine functions). Consider an eigenproblem

$$\begin{aligned} -\phi_n'' &= \lambda_n \phi_n \quad \text{in } (0, 1), \\ \phi_n'(0) &= \phi_n'(1) = 0. \end{aligned}$$

We readily verify that this is a regular Sturm-Liouville problem with $p = 1$, $q = 0$, $w = 1$, $\alpha_1 = \beta_1 = 0$, and $\alpha_2 = \beta_2 = 1$. It follows that the eigenfunctions $\{\phi_n\}$ are orthogonal. Moreover, because $w, \alpha_1, \alpha_2, \beta_1$, and β_2 are all nonnegative, the eigenvalues are nonnegative.

We can again find explicit expressions for the solutions to verify the above claims. We consider three cases:

- *Case 1:* $\lambda_n < 0$. Let $\mu_n = -\lambda_n$ so that $\mu_n > 0$. The general solution to the eigenproblem is of the form $\phi_n(x) = a_n \cosh(\sqrt{\mu_n}x) + b_n \sinh(\sqrt{\mu_n}x)$. The derivative of the function is $\phi_n'(x) = a_n \sqrt{\mu_n} \sinh(\sqrt{\mu_n}x) + b_n \sqrt{\mu_n} \cosh(\sqrt{\mu_n}x)$. The boundary condition at $x = 0$ requires that $\phi_n'(x = 0) = b_n = 0$. The boundary condition at $x = 1$ requires that $\phi_n'(x = 1) = a_n \sqrt{\mu_n} \sinh(\sqrt{\mu_n}) = 0$; as \sinh is zero only at $x = 0$, the condition requires that $a_n = 0$. Hence there is no nontrivial solution to the boundary value eigenproblem for $\mu_n > 0$.
- *Case 2:* $\lambda_n = 0$. If $\lambda_n = 0$, the general solution to the eigenproblem is $\phi_n(x) = a_n + b_n x$. The derivative of the function is $\phi_n'(x) = b_n$. The boundary conditions at $x = 0$ and $x = 1$ require that $\phi_n'(x = 0) = \phi_n'(x = 1) = b_n = 0$. We hence find that the one nontrivial solution is $\phi_n(x) = 1$.
- *Case 3:* $\lambda_n > 0$. The general solution to the eigenproblem is of the form $\phi_n(x) = a_n \cos(\sqrt{\lambda_n}x) + b_n \sin(\sqrt{\lambda_n}x)$. The derivative of the function is $\phi_n'(x) = -a_n \sqrt{\lambda_n} \sin(\sqrt{\lambda_n}x) + b_n \sqrt{\lambda_n} \cos(\sqrt{\lambda_n}x)$. The boundary condition at $x = 0$ requires $\phi_n'(x = 0) = b_n \sqrt{\lambda_n} = 0$. The boundary condition at $x = 1$ requires $\phi_n'(x = 1) = -a_n \sqrt{\lambda_n} \sin(\sqrt{\lambda_n}) = 0$; the nontrivial solution is given by $\lambda_n = n^2\pi^2$, $n = 1, 2, \dots$. We hence nontrivial solutions are of the form $\phi_n(x) = \cos(n\pi x)$, $n = 1, 2, \dots$. In fact, we can include the constant solution found in Case 2 in this general family of solutions by starting from $n = 0$.

As expected from the Sturm-Liouville theory, the problem has eigenvalues which are real and nonnegative: $\lambda_n = n^2\pi^2 \geq 0$, $n = 0, 1, 2, \dots$. In addition, the eigenfunctions $\phi_n(x) = \cos(n\pi x)$ are orthogonal on $(0, 1)$, as we have already verified in the context of classical Fourier series.

Example 4.8 (sinusoidal functions). Consider an eigenproblem

$$\begin{aligned} -\phi_n'' &= \lambda_n \phi_n \quad \text{in } (-1, 1), \\ \phi_n(-1) &= \phi_n(1), \\ \phi_n'(-1) &= \phi_n'(1). \end{aligned}$$

This is an Sturm-Liouville equation with periodic boundary condition. This is not a regular Sturm-Liouville problem, but a *periodic Sturm-Liouville problem*. The solution to this periodic Sturm-Liouville problem is given by

$$\lambda_n = m^2 \pi^2 \quad \text{and} \quad \phi_n(x) = \begin{cases} \cos(m\pi x), & n \text{ even}, \\ \sin(m\pi x), & n \text{ odd} \end{cases}$$

for $m \equiv \lceil n/2 \rceil$, $n = 0, 1, 2, \dots$. We recognize that the eigenfunctions are the basis for the full Fourier series. All eigenvalues are nonnegative and the eigenfunctions are orthogonal, as we have already verified in the context of classical Fourier series. (The orthogonality proof holds for the periodic boundary condition with little modification.)

Example 4.9 (Legendre polynomials). Consider an eigenproblem

$$-((1-x^2)\phi_n')' = \lambda_n \phi_n \quad \text{in } (-1, 1).$$

This is a Sturm-Liouville equation, with coefficients $p(x) = (1-x^2)$, $q = 0$, and $w = 1$. Because $p(x = -1) = p(x = 1) = 0$, the differential operator vanishes at the boundary; the problem hence does not require a boundary condition. A problem associated with a Sturm-Liouville equation with p that vanishes at either or both boundaries is called a *singular Sturm-Liouville problem*. The solutions to this singular Sturm-Liouville problem are the *Legendre polynomials*, which form an orthogonal set of polynomials. (The orthogonality proof holds without any boundary conditions because p vanishes at both boundaries.)

4.5 Generalized Fourier series by eigenfunctions

We now use the orthogonality and completeness of eigenfunctions of the Sturm-Liouville problem to form generalized Fourier series.

Definition 4.10 (generalized Fourier series). Let $(\phi_n)_{n=1}^{\infty}$ be eigenfunctions of a regular Sturm-Liouville problem with $q \geq 0$ on $[a, b]$, $\alpha_1 \geq 0$, $\alpha_2 \geq 0$, $\beta_1 \geq 0$, and $\beta_2 \geq 0$. We can then approximate any $f : (a, b) \rightarrow \mathbb{R}$ by a generalized Fourier series

$$f(x) \sim \sum_{n=1}^{\infty} \hat{f}_n \phi_n(x) \tag{4.3}$$

for coefficients

$$\hat{f}_n = \frac{\int_a^b f \phi_n w dx}{\int_a^b \phi_n^2 w dx}.$$

Similarly to the classical Fourier series, the expression for the coefficients is a consequence of the orthogonality of the functions $(\phi_n)_{n=1}^{\infty}$. Our expression for the coefficient has (the square of) the norm of the function as the denominator, as we did not assume the functions are orthonormal (i.e., functions in general do not have a unit norm); the expression could be simplified if we had normalized the functions.

We conclude this section by stating without proof the pointwise, uniform, and L^2 convergence of generalized Fourier series.

Theorem 4.11 (pointwise convergence of generalized Fourier series). Let $f : [a, b] \rightarrow \mathbb{R}$ be a piecewise continuously differentiable function that satisfies the boundary conditions of the regular Sturm-Liouville problem. Then the generalized Fourier series (4.3) converges for any $x \in (a, b)$ to $\frac{1}{2}(f(x^+) + f(x^-))$.

Theorem 4.12 (uniform convergence of generalized Fourier series). Let $f : [a, b] \rightarrow \mathbb{R}$ be a twice continuously differentiable function that satisfies the boundary conditions of the regular Sturm-Liouville problem. Then the generalized Fourier series (4.3) converges uniformly to f .

Theorem 4.13 (L^2 convergence of generalized Fourier series). Let $f : (a, b) \rightarrow \mathbb{R}$ be a function that is square integrable with respect to the weight function w and satisfies the boundary conditions of the regular Sturm-Liouville problem. Then the generalized Fourier series (4.3) converges with respect to the w -weighted norm $\int_a^b (\cdot)^2 w dx$.

4.6 Summary

We summarize key points of this lecture:

1. Sturm-Liouville operator is self-adjoint. As a result, all eigenvalues of a regular Sturm-Liouville problem are real, and its eigenfunctions are orthogonal.
2. The family of sine, cosine, and sine-cosine functions used in Fourier series arise as solutions to Sturm-Liouville problems. As a result, the functions are orthogonal.
3. Solutions of a Sturm-Liouville problem can be used to construct a generalized Fourier series. The coefficients of the series can be found using the relevant orthogonality relation. The series converges as a result of the completeness of the eigenfunctions.

4.A L^2 properties of generalized Fourier series

We now state some relationships between the coefficients of a generalized Fourier series and the function it approximates.

Theorem 4.14 (generalized Parseval's identity). Let $f : (a, b) \rightarrow \mathbb{R}$ be a function that is square integrable with respect to the weight function w and satisfies the boundary conditions of the regular Sturm-Liouville problem. Then

$$\sum_{n=1}^{\infty} \hat{f}_n^2 \int_a^b \phi_n^2 w dx = \int_a^b f^2 w dx.$$

In other words, the eigenfunctions of the regular Sturm-Liouville problem are complete with respect to the w -weighted L^2 norm $\int_a^b (\cdot)^2 w dx$.

Corollary 4.15 (generalized Bessel's inequality). As a consequence of the Parseval's identity, a weaker condition, *Bessel's inequality*,

$$\sum_{n=1}^{\infty} \hat{f}_n^2 \int_a^b \phi_n^2 w dx \leq \int_a^b f^2 w dx,$$

also holds.

Part II

Heat equation

Lecture 5

Heat equation: introduction

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5.1 Introduction

The heat equation describes heat conduction in media and plays an important role in the thermal analysis of many engineering systems. The heat equation is also of mathematical interest, as it is an archetype of parabolic PDEs. In this lecture we derive the heat equation and the associated boundary conditions. We then explore various properties of the equation and the solution — such as the maximum principle, energy stability, and the uniqueness of the solution — *without finding a closed form expression for the solution*. We will introduce a few different approaches to find a solution representation to the heat equation in the subsequent lectures.

5.2 Derivation of the heat equation

We derive the heat equation based on three principles of heat transfer:

1. The thermal energy density e is given by $e = \rho cu$, where $\rho > 0$ is the density, $c > 0$ is the specific heat capacity, and u is the temperature.
2. Fourier's law. The rate of heat transfer is proportional to the temperature gradient: $q = -k\nabla u$, where q is the heat flux and $k > 0$ is the thermal conductivity.
3. Conservation of energy. The change in the thermal energy in a volume over a time interval Δt is equal to the net heat entering the volume over Δt .

From these three principles, we can readily derive the heat equation.

To begin, we introduce a domain $\Omega \subset \mathbb{R}^n$ and the associated fixed subdomain $\omega \subset \Omega$. We denote the boundary of the subdomain by $\partial\omega$. (In general, the boundary of any domain $D \subset \mathbb{R}^n$ is denoted by ∂D .) We next note that the total energy in the subdomain ω is $E = \int_{\omega} \rho c u dx$. We then note that by the conservation of energy

$$\underbrace{\frac{d}{dt} \int_{\omega} \rho c u dx}_{\text{change in thermal energy}} = \underbrace{- \int_{\partial\omega} q \cdot \nu ds}_{\text{net heat entering } \omega} ,$$

where ν is the outward-pointing unit normal vector on $\partial\omega$. We make two observations: (i) the subdomain ω is independent of time and hence the time derivative can be brought inside the integral; (ii) the integral over $\partial\omega$ can be converted to an integral over ω using the divergence theorem. We hence obtain

$$\int_{\omega} \rho c \frac{\partial u}{\partial t} dx = - \int_{\omega} \nabla \cdot q dx.$$

We next note that, since the relationship above should hold for *any* $\omega \subset \Omega$, the integrands must be equal to each other:

$$\rho c \frac{\partial u}{\partial t} = -\nabla \cdot q \quad \text{in } \Omega \times \mathbb{R}_{>0}.$$

We then appeal to Fourier's law, $q = -k\nabla u$, to obtain

$$\rho c \frac{\partial u}{\partial t} = \nabla \cdot (k\nabla u) \quad \text{in } \Omega \times \mathbb{R}_{>0}.$$

This is the general form of the heat equation that can treat spatially varying density, specific heat capacity, and thermal conductivity.

If we assume that the density, specific heat capacity, and thermal conductivity are constant in space and time, we can further simplify the equation. Namely, we introduce the thermal diffusivity $\kappa \equiv \frac{k}{\rho c}$ (and appeal to our constant coefficient assumption) to obtain

$$\frac{\partial u}{\partial t} = \kappa \Delta u \quad \text{in } \Omega \times \mathbb{R}_{>0}. \tag{5.1}$$

This form of the equation is often referred to as the heat equation in the mathematics community; in this course we will follow the same convention.

5.3 Boundary and initial conditions

To define a complete initial-boundary value problem, we now complement the heat equation (5.1) with boundary and initial conditions. There are three different types of boundary conditions for the heat equation:

1. Dirichlet (first-type) boundary conditions; i.e., prescribed temperature. If the temperature at the boundary is prescribed, we obtain a boundary condition of the form

$$u = u^b \quad \text{on } \Gamma_D \times \mathbb{R}_{>0},$$

where u^b is the prescribed boundary temperature and $\Gamma_D \subset \partial\Omega$ is the Dirichlet boundary. The Dirichlet boundary condition only depends on the value (and not the derivative) of the state u . If $u^b = 0$, then the condition is called a *homogeneous* Dirichlet boundary condition; otherwise it is a *nonhomogeneous* Dirichlet boundary condition.

2. Neumann (second-type) boundary conditions; i.e., prescribed heat flux. If the heat flux at the boundary is prescribed, we obtain a boundary condition of the form

$$\nu \cdot (k\nabla u) = q^b \quad \text{on } \Gamma_N \times \mathbb{R}_{>0},$$

where q^b is the prescribed boundary heat flux into the domain and $\Gamma_N \subset \partial\Omega$ is the Neumann boundary. Note $q^b > 0$ indicates heat transfers into the domain (i.e., the boundary is heated)

and $q^b < 0$ indicates heat transfers out from the domain (i.e., the boundary is cooled). (Note that the signs are “flipped” from Fourier’s law because Fourier’s law characterizes the heat transfer from the domain into the boundary, whereas in the above q^b characterizes the heat transfer from the boundary into the domain.) The Neumann boundary condition only depends on the derivative (and not the value) of the state u . If $q^b = 0$, then the condition is called a *homogeneous* Neumann boundary condition (i.e., insulated boundary); otherwise it is a *nonhomogeneous* Neumann boundary condition.

3. Robin (third-type) boundary conditions; i.e., Newton’s law of cooling. If a boundary is exposed to a different medium (e.g., fluid), then the heat is transferred from/to the surrounding medium. Newton’s law state that the rate of this heat transfer is proportional to the difference in the temperate of the material and the surrounding. The associated boundary condition is of the form

$$\nu \cdot (k\nabla u) = h(u^{\text{env}} - u) \quad \text{on } \Gamma_R \times \mathbb{R}_{>0},$$

where $h > 0$ is the heat transfer coefficient, u^{env} is the temperature of the environment, and $\Gamma_R \subset \partial\Omega$ is the Robin boundary. The Robin boundary condition depends on both the value and derivative of the state u . If u^{env} is 0, then the condition is called a *homogeneous* Robin boundary condition; otherwise it is a *nonhomogeneous* Robin boundary condition.

As the heat equation (5.1) is second-order in space, one (and only one) boundary condition must be specified at each point on the boundary. In other words, we partition the domain boundary into non-overlapping sets so that

$$\partial\Omega = \bar{\Gamma}_D \cup \bar{\Gamma}_N \cup \bar{\Gamma}_R, \tag{5.2}$$

$$\Gamma_D \cap \Gamma_N = \Gamma_D \cap \Gamma_R = \Gamma_N \cap \Gamma_R = \emptyset, \tag{5.3}$$

and impose the appropriate boundary condition on each part of the boundary. (Some of sets Γ_D , Γ_N , and Γ_R may be empty. *Optional note:* \bar{D} denotes the closure of D ; we need to close each set in the first equality because Γ_D , Γ_N , and Γ_R are open.)

To completely specify the initial-boundary value problem, we must also specify the initial condition. As the heat equation is first order in time, we need need to specify the value of the state at the initial time:

$$u = g \quad \text{on } \bar{\Omega} \times \{t = 0\},$$

where g is the prescribed initial temperature.

Example 5.1 (heat equation initial-boundary value problem). A one-dimensional heat equation over the domain $\Omega \equiv (0, L)$ with homogeneous Dirichlet boundary conditions is given by

$$\begin{aligned} \frac{\partial u}{\partial t} &= \kappa \frac{\partial^2 u}{\partial x^2} & \text{in } (0, L) \times \mathbb{R}_{>0}, \\ u &= 0 & \text{on } \{0, L\} \times \mathbb{R}_{>0}, \\ u &= g & \text{on } [0, L] \times \{t = 0\}. \end{aligned} \tag{5.4}$$

It can be shown that this initial-boundary value problem is well-posed assuming the initial condition g is sufficiently regular.

5.4 Nonhomogeneous heat equation

In Section 5.2, we derived the heat equation assuming that there is no “volume heating”. In the presence of volume heating, the change in the thermal energy in the volume ω depends on not only on the net heat entering through the surface $\partial\omega$ but also the volume heating from inside the domain:

$$\underbrace{\frac{d}{dt} \int_{\omega} \rho c u dx}_{\text{change in thermal energy}} = \underbrace{- \int_{\partial\omega} q \cdot \nu ds}_{\text{net heat entering } \omega} + \underbrace{\int_{\omega} \tilde{f} dx}_{\text{volume heating}}.$$

After the application of the divergence theorem we obtain a PDE

$$\frac{\partial u}{\partial t} = \kappa \Delta u + f \quad \text{in } \Omega \times \mathbb{R}_{>0}$$

for $\tilde{f} \equiv f/(\rho c)$. Note that this is a nonhomogeneous equation, because the PDE cannot be expressed as $\mathcal{L}u = 0$ for any linear operator \mathcal{L} due to the presence of the source term f that is independent of u .

5.5 Nondimensionalization

In studying any PDE, it is often convenient to nondimensionalize the equations. To provide a concrete example, we consider the one-dimensional heat equation (5.4). To nondimensionalize the equation, we introduce the following scales:

1. Length scale. We choose for our length scale the domain length L . The nondimensionalized spatial coordinate is $\tilde{x} = x/L$ and the nondimensionalized domain is $\tilde{\Omega} = (0, 1)$.
2. Time scale. We choose for our time scale $T \equiv L^2/\kappa$. The nondimensionalized time is $\tilde{t} = t/(L^2/\kappa)$.
3. Temperature scale. We choose for our temperature scale $U \equiv \max(g)$. The nondimensionalized temperature is $\tilde{u} = u/\max(g)$. The nondimensional initial temperature is bounded by 1.

While the choice of the length and temperature scales may be rather obvious, the choice of the time scale is perhaps not. The choice is motivated by the following simplification of the heat equation. Namely, since

$$\frac{\partial u}{\partial t} = \frac{U}{T} \frac{\partial \tilde{u}}{\partial \tilde{t}} = \frac{U\kappa}{L^2} \frac{\partial \tilde{u}}{\partial \tilde{t}} \quad \text{and} \quad \frac{\partial^2 u}{\partial x^2} = \frac{U}{L^2} \frac{\partial^2 \tilde{u}}{\partial \tilde{x}^2},$$

we obtain

$$\frac{\partial u}{\partial t} = \kappa \frac{\partial^2 u}{\partial x^2} \quad \Rightarrow \quad \frac{U\kappa}{T} \frac{\partial \tilde{u}}{\partial \tilde{t}} = \kappa \frac{U}{L^2} \frac{\partial^2 \tilde{u}}{\partial \tilde{x}^2} \quad \Rightarrow \quad \frac{\partial \tilde{u}}{\partial \tilde{t}} = \frac{\partial^2 \tilde{u}}{\partial \tilde{x}^2};$$

in other words, the nondimensionalized diffusion coefficient is unity. The nondimensionalized initial-boundary value problem is hence

$$\begin{aligned} \frac{\partial \tilde{u}}{\partial \tilde{t}} &= \frac{\partial^2 \tilde{u}}{\partial \tilde{x}^2} \quad \text{in } (0, 1) \times \mathbb{R}_{>0}, \\ \tilde{u} &= 0 \quad \text{on } \{0, 1\} \times \mathbb{R}_{>0}, \\ \tilde{u} &= \tilde{g} \quad \text{on } [0, 1] \times \{t = 0\}, \end{aligned}$$

where $\tilde{g} \equiv g/\max(g)$.

The nondimensionalization offers simplicity without any loss of generality. Specifically, we can always recover the solution to the dimensional equation as

$$u(x, t) = \tilde{u}(x/L, t/T)\tilde{g} = \tilde{u}(x/L, \kappa t/L^2)\tilde{g}.$$

For this reason, we will focus on nondimensionalized form of the heat equation (or any other equations) in this course.

Example 5.2 (nondimensionalization). Suppose the solution to nondimensionalized heat equation is given by

$$\tilde{u}(\tilde{x}, \tilde{t}) = \sin(\pi\tilde{x}) \exp(-\pi^2\tilde{t}).$$

(This is in fact the solution to the one-dimensional heat equation above for $\tilde{g}(x) = \sin(\pi\tilde{x})$.) The solution to the non-dimensionalized equation is then given by

$$u(x, t) = \max(g)\tilde{u}(x/L, \kappa t/L^2) = \max(g) \sin\left(\frac{\pi x}{L}\right) \exp\left(-\frac{\pi^2 \kappa t}{L^2}\right).$$

5.6 Maximum principle

We now introduce a property of the heat equation that is important both in theory and in practice: *the maximum principle*. The maximum principle facilitates the verification of two of the three conditions of well-posedness — uniqueness and stability (but not existence) — of the initial and/or boundary value problems associated with the heat equation. (*Note:* proofs are provided in this and subsequent sections for completeness, but they should be considered optional reading items.)

Theorem 5.3 (maximum principle for the heat equation). Suppose we are given an open spatial domain Ω and a time interval $I \equiv (t_0, t_f]$, where Ω may be unbounded and t_f may be infinite. We define a *parabolic cylinder* $\Omega \times I$ and a *parabolic boundary*

$$\Gamma \equiv (\overline{\Omega} \times \{t = t_0\}) \cup (\partial\Omega \times I) = (\overline{\Omega \times I}) \setminus (\Omega \times I),$$

which includes the spatial boundary and initial time “boundary” (but not the final time “boundary”). If $u \in C_1^2(\Omega \times I) \cap C^0(\overline{\Omega \times I})$ satisfies the heat equation $\frac{\partial u}{\partial t} - \Delta u = 0$ in $\Omega \times I$, then

$$\max_{(x,t) \in \overline{\Omega \times I}} u(x, t) = \max_{(x,t) \in \Gamma} u(x, t).$$

In words, the solution to the heat equation attains the maximum value somewhere on the parabolic boundary Γ . (The parabolic boundary Γ in the space-time domain is shown in Figure 5.1. The space $C_1^2(\Omega \times I)$ comprises functions that are twice continuously differentiable in space and once continuously differentiable in time.)

Proof. We prove the result by contradiction: we suppose that the maximizer (x^*, t^*) of u is in $\Omega \times I$ and then show that this is not possible. We again emphasize $\Omega \times I$ is open everywhere except at the final time $t = t_f$; the maximizer (x^*, t^*) is hence either interior to $\Omega \times I$ or at the final time $t = t_f$. We first introduce an auxiliary function

$$w(x, t) = u(x, t) - \epsilon(t - t^*).$$

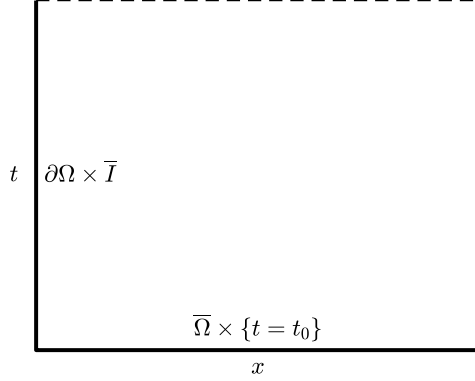


Figure 5.1: Parabolic boundary Γ in the space-time domain for the maximum principle.

We may choose $\epsilon \in \mathbb{R}_{>0}$ sufficiently small such that w also attains the maximum value in $\Omega \times I$. Suppose $(x^{**}, t^{**}) \in \Omega \times I$ is the maximizer of w . Then

$$\Delta w(x^{**}, t^{**}) \leq 0$$

because the function has to be concave at the maximizer due to the second-order optimality condition. In addition

$$\frac{\partial w}{\partial t}(x^{**}, t^{**}) \geq 0$$

because (i) $\frac{\partial u}{\partial t}(x^{**}, t^{**}) = 0$ if $t^{**} \in (t_0, t_f)$ from the first-order optimality condition and (ii) $\frac{\partial u}{\partial t}(x^{**}, t^{**}) \geq 0$ if $t^{**} = t_f$ since the function must not be decreasing with t for the point to be the maximum. It follows that

$$\begin{aligned} \Delta w(x^{**}, t^{**}) &= \Delta u(x^{**}, t^{**}) \leq 0, \\ \frac{\partial w}{\partial t}(x^{**}, t^{**}) &= \frac{\partial u}{\partial t}(x^{**}, t^{**}) - \epsilon \geq 0 \quad \Rightarrow \quad \frac{\partial u}{\partial t}(x^{**}, t^{**}) \geq \epsilon \quad \Rightarrow \quad \frac{\partial u}{\partial t}(x^{**}, t^{**}) > 0. \end{aligned}$$

However, the solution to the heat equation must satisfy $\frac{\partial u}{\partial t} = \Delta u$, which is a contradiction. We hence conclude that the maximizer must be on the parabolic boundary Γ . \square

Remark 5.4. The maximum principle (Theorem 5.3) is sometimes referred to as the *weak maximum principle*. A closely related *strong maximum principle* states that the maximum value cannot be attained anywhere in $\Omega \times I$ unless u is constant in $\Omega \times I$; i.e., if there exists a point $(x^*, t^*) \in \Omega \times I$ such that

$$u(x^*, t^*) = \max_{\Omega \times I} u(x, t),$$

then u is constant in $\Omega \times I$. (We recall that Ω is open and I is open at $t = t_0$)

Theorem 5.5 (minimum principle for the heat equation). In the same setting as Theorem 5.3, we obtain

$$\min_{(x,t) \in \Omega \times I} u(x, t) = \min_{(x,t) \in \Gamma} u(x, t).$$

Proof. Let $w = -u$. We recognize that w is also the solution to a heat equation and apply the maximum principle to obtain

$$\max_{(x,t) \in \overline{\Omega \times I}} w(x,t) = \max_{(x,t) \in \Gamma} w(x,t).$$

We expand the left hand side and the right hand side to obtain

$$\begin{aligned} \text{(LHS)} &= \max_{(x,t) \in \overline{\Omega \times I}} w(x,t) = \max_{(x,t) \in \overline{\Omega \times I}} -u(x,t) = - \min_{(x,t) \in \overline{\Omega \times I}} u(x,t), \\ \text{(RHS)} &= \max_{(x,t) \in \Gamma} w(x,t) = \max_{(x,t) \in \Gamma} -u(x,t) = - \min_{(x,t) \in \Gamma} u(x,t). \end{aligned}$$

It follows that

$$- \min_{(x,t) \in \overline{\Omega \times I}} u(x,t) = - \min_{(x,t) \in \Gamma} u(x,t) \quad \Rightarrow \quad \min_{(x,t) \in \overline{\Omega \times I}} u(x,t) = \min_{(x,t) \in \Gamma} u(x,t).$$

□

Example 5.6 (maximum principle for the heat equation). Consider the initial-boundary value problem

$$\begin{aligned} \frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} &= 0 \quad \text{in } (-1, 2) \times \mathbb{R}_{>0}, \\ u(x = -1, t) &= \exp(-t), \quad t \in \mathbb{R}_{>0}, \\ u(x = 2, t) &= |\cos(3\pi t)|, \quad t \in \mathbb{R}_{>0}, \\ u(x, t = 0) &= \frac{4}{9}(x - 1/2)^2, \quad x \in [-1, 2]. \end{aligned}$$

We observe that the value of the solution along the left and right boundaries, as well as at the initial time, are in $[0, 1]$. Hence by the maximum and minimum principles, for $u \in C_1^2(\Omega \times I) \cap C^0(\overline{\Omega \times I})$,

$$0 \leq u(x, t) \leq 1 \quad \forall (x, t) \in [-1, 2] \times \mathbb{R}_{\geq 0}.$$

We arrive at this conclusion even though we have not found the solution.

5.7 Uniqueness by the maximum principle

We now appeal to the maximum (and minimum) principle to show that the solution to the initial-boundary value problem, if it exists, is unique.

Theorem 5.7 (uniqueness of the solution to the heat equation). Let $\Omega \subset \mathbb{R}^n$ be a spatial domain and $I = (0, t_f]$ be the time interval. There is at most one solution $u \in C_1^2(\Omega \times I) \cap C^0(\overline{\Omega \times I})$ that satisfies

$$\begin{aligned} \frac{\partial u}{\partial t} - \Delta u &= f \quad \text{in } \Omega \times I, \\ u &= h \quad \text{on } \partial\Omega \times I, \\ u &= g \quad \text{on } \overline{\Omega} \times \{t = 0\}, \end{aligned}$$

where $f : \Omega \times I \rightarrow \mathbb{R}$ is a source function, $h : \partial\Omega \times I \rightarrow \mathbb{R}$ is the boundary function, and $g : \overline{\Omega} \rightarrow \mathbb{R}$ is the initial condition.

Proof. Let u_1 and u_2 be the solutions to the heat equation initial-boundary value problem. Since the equation is linear, we know by the principle of superposition that the function $w \equiv u_1 - u_2$ satisfies the initial-boundary value problem associated with the homogeneous heat equation:

$$\begin{aligned}\frac{\partial w}{\partial t} - \Delta w &= 0 & \text{in } \Omega \times I, \\ w &= 0 & \text{on } \partial\Omega \times I, \\ w &= 0 & \text{on } \overline{\Omega} \times \{t = 0\}.\end{aligned}$$

By the maximum and minimum principles, we find that

$$\begin{aligned}\max_{(x,t) \in \Omega \times I} w(x,t) &= \max_{(x,t) \in \Gamma} w(x,t) = 0 & \Rightarrow w \leq 0 & \text{in } \Omega \times I, \\ \min_{(x,t) \in \overline{\Omega \times I}} w(x,t) &= \min_{(x,t) \in \Gamma} w(x,t) = 0 & \Rightarrow w \geq 0 & \text{in } \Omega \times I,\end{aligned}$$

where $\Gamma \equiv (\overline{\Omega} \times \{t = 0\}) \cup (\partial\Omega \times I)$ is the parabolic boundary. Since $w \leq 0$ and $w \geq 0$, it follows that $w = u_1 - u_2 = 0$ in $\Omega \times I$. \square

5.8 Uniform stability by the maximum principle

We recall that the third ingredient of well-posedness is stability. In the study of PDEs, we are often interested in stability in two different senses: “uniform” and “square-integral”. In this section we study the uniform stability of the heat equation using the maximum principle.

Theorem 5.8 (uniform stability of the heat equation). Let u_1 and u_2 be solutions (in $C_1^2(\Omega \times I) \cap C^0(\overline{\Omega \times I})$) to the initial-boundary value problems associated with two different set of boundary and initial data (h_1, g_1) and (h_2, g_2) , respectively:

$$\begin{aligned}\frac{\partial u_i}{\partial t} - \Delta u_i &= 0 & \text{in } \Omega \times I, \\ u_i &= h_i & \text{on } \partial\Omega \times I, \\ u_i &= g_i & \text{on } \overline{\Omega} \times \{t = 0\}\end{aligned}$$

for $i = 1, 2$. Then the solution depends continuously on data in the sense that

$$\max_{(x,t) \in \Omega \times I} |u_1(x,t) - u_2(x,t)| = \max \left\{ \max_{(x,t) \in \partial\Omega \times I} |h_1(x,t) - h_2(x,t)|, \max_{x \in \overline{\Omega}} |g_1(x) - g_2(x)| \right\}. \quad (5.5)$$

Proof. We appeal to the linearity of the differential operators and take the difference of the two set of equations to obtain

$$\begin{aligned}\frac{\partial(u_1 - u_2)}{\partial t} - \Delta(u_1 - u_2) &= 0 & \text{in } \Omega \times I, \\ (u_1 - u_2) &= (h_1 - h_2) & \text{on } \partial\Omega \times I, \\ (u_1 - u_2) &= (g_1 - g_2) & \text{on } \overline{\Omega} \times \{t = 0\}.\end{aligned}$$

The maximum and minimum principles require, for any $(x, t) \in \Omega \times I$,

$$u_1(x, t) - u_2(x, t) \leq \max \left\{ \max_{(x,t) \in \partial\Omega \times I} (h_1(x, t) - h_2(x, t)), \max_{x \in \bar{\Omega}} (g_1(x) - g_2(x)) \right\},$$

$$u_1(x, t) - u_2(x, t) \geq \min \left\{ \min_{(x,t) \in \partial\Omega \times I} (h_1(x, t) - h_2(x, t)), \min_{x \in \bar{\Omega}} (g_1(x) - g_2(x)) \right\},$$

and each relationship holds as an equality for some point (x, t) on parabolic boundary Γ . It follows that

$$\max_{(x,t) \in \bar{\Omega} \times I} |u_1(x, t) - u_2(x, t)| = \max \left\{ \max_{(x,t) \in \partial\Omega \times I} |h_1(x, t) - h_2(x, t)|, \max_{x \in \bar{\Omega}} |g_1(x) - g_2(x)| \right\},$$

which is the desired equality. \square

The left hand side of (5.5) measures the closeness of the solutions and its right hand side measures the closeness of initial and boundary data. The equation shows that the difference in the two solutions u_1 and u_2 over any point $x \in \bar{\Omega}$ at any time $t \in \bar{I}$ is bounded by the maximum difference in the boundary data $h_1 - h_2$ and the initial data $g_1 - g_2$. Hence a small change in the data results in a small change in the solution; the problem is hence stable. As the stability statement applies to all points in the space-time domain $\Omega \times I$, this is called stability in the “uniform” sense.

5.9 Energy method: uniqueness and stability in L^2 sense

We have so far appealed to the maximum principle to show the uniqueness and stability of the solution to the heat equation initial-boundary value problem. We can also prove uniqueness and stability using the *energy method*. Unlike the results associated with the maximum principle which are in the uniform sense, the results associated with the energy methods are in the square-integral (or L^2) sense.

We first consider uniqueness. As in the proof of Theorem 5.7, suppose u_1 and u_2 are the two solutions to the heat equation initial-boundary value problem. Then their difference $w \equiv u_1 - u_2$ satisfies

$$\begin{aligned} \frac{\partial w}{\partial t} - \Delta w &= 0 \quad \text{in } \Omega \times I, \\ w &= 0 \quad \text{on } \Gamma_D \times I, \\ w &= 0 \quad \text{on } \Omega \times \{t = 0\}. \end{aligned}$$

We now define

$$E(t) \equiv \frac{1}{2} \int_{\Omega} w(x, t)^2 dx, \quad t \in I.$$

We then observe

$$\frac{d}{dt} E = \int_{\Omega} w \frac{\partial w}{\partial t} dx = \int_{\Omega} w \Delta w dx = - \int_{\Omega} \nabla w \cdot \nabla w dx + \int_{\partial\Omega} w \nu \cdot \nabla w ds = - \int_{\Omega} |\nabla w|^2 dx \leq 0;$$

in the last equality, the integral on the boundary vanishes because $w = 0$ on $\partial\Omega$. Since $\frac{dE}{dt} \leq 0$, $E(t) = \int_{\Omega} w(\cdot, t)^2 dx$ is a nonincreasing function of time and

$$\int_{\Omega} w(\cdot, t)^2 dx \leq \int_{\Omega} w(\cdot, t = 0)^2 dx = 0, \tag{5.6}$$

where the last equality follows from $w(\cdot, t = 0) = u_1(\cdot, t = 0) - u_2(\cdot, t = 0) = g - g = 0$. Consequently, $w(\cdot, t) = u_1(\cdot, t) - u_2(\cdot, t) = 0$ for each $t \in I$, and $u_1 = u_2$ in $\Omega \times I$. This energy method can be readily extended for problems that involve Neumann and Robin boundary conditions. In addition, as we will see in later lectures, the method also extends to equations that do not possess the maximum principle.

We next consider stability. To this end, we consider the same setting as Theorem 5.8, but for simplicity consider the case where only the initial data is changed and boundary data is fixed; i.e., $g_1 \neq g_2$ but $h_1 = h_2$. We appeal to energy balance (5.6) and obtain, for any $t \in I$,

$$\int_{\Omega} (u_1(\cdot, t) - u_2(\cdot, t))^2 dx \leq \int_{\Omega} (g_1 - g_2)^2 dx.$$

Again the left hand side measures the closeness of the solution and the right hand side measures the closeness of the initial data. We again observe that a small change in the data results in a small change in the solution; the problem is stable. However, the measure of “closeness” is not in the maximum (or uniform) sense but rather in the square-integral sense. We hence refer to this form of stability as stability in the square-integral (or L^2) sense.

5.10 Summary

We summarize key points of this lecture:

1. The heat equation describes the temperature distribution in a medium and is derived from the definition of thermal energy, Fourier’s law, and conservation of energy.
2. The three different types of boundary conditions that are relevant for the heat equation are associated with prescribed temperature, prescribed heat flux, and Newton’s law of cooling. The three conditions are called respectively Dirichlet, Neumann, and Robin conditions, or first-type, second-type, and third-type conditions.
3. The heat equation (just like any other equation) can be nondimensionalized. In particular, if we choose the time scale $T \equiv L^2/\kappa$, the resulting equation has the diffusivity constant of unity.
4. The maximum principle states that the value of the solution to the (homogeneous) heat equation over the entire space-time domain is bounded from above by the maximum value along the boundaries and in the initial condition. The minimum principle similarly holds.
5. The maximum principle can be used to prove the solution to the heat equation, if it exists, is unique. The principle also asserts that the solution is stable in the uniform sense.
6. The energy method can be also used to prove the uniqueness and L^2 stability of the heat equation.

Lecture 6

Heat equation: separation of variables

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6.1 Introduction

In this lecture we consider the solution of initial-boundary value problems associated with the heat equation in a bounded domain. To find a solution representation, we introduce *separation of variables*, which seeks solutions to the PDE that are separable in space and time, and then consider a linear combination of these separable solutions that satisfies the particular boundary and initial conditions. The approach builds on the Fourier series representation of various functions. We consider the treatment of various boundary conditions; we then provide physical and mathematical interpretations of the associated solutions.

6.2 Homogeneous Dirichlet boundary conditions

We consider the heat equation over the one-dimensional spatial domain $(0, 1)$ with the homogeneous Dirichlet boundary conditions:

$$\begin{aligned}\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} &= 0 && \text{in } (0, 1) \times \mathbb{R}_{>0}, \\ u &= 0 && \text{on } \{0, 1\} \times \mathbb{R}_{>0}, \\ u &= g && \text{on } [0, 1] \times \{t = 0\}.\end{aligned}$$

Our solution procedure builds on *separation of variables* and *the principle of superposition*:

1. *Separation of variables*. We seek a family of solutions to the heat equation of the form

$$u_n(x, t) = \phi_n(x)T_n(t), \quad n = 1, 2, \dots,$$

which satisfy the PDE and the boundary conditions but not necessarily the initial condition. As we will see shortly, the separable form allows us to use the standard ODE techniques to find ϕ_n and T_n .

2. *The principle of superposition.* We then consider a linear combination of the above separable functions

$$u(x, t) = \sum_{n=1}^{\infty} a_n u_n(x, t)$$

that satisfy the initial condition. Note that due to the linearity and homogeneity of the PDE and boundary conditions, any linear combination of the separable functions also satisfies the PDE and the boundary conditions. Hence if we find the coefficients (a_n) that satisfy the initial condition, then the solution will satisfy the PDE, boundary conditions, and initial condition.

This two-step procedure can be used to find a solution — and in fact a unique solution — to the heat equation. (It can be shown that any function over $(0, 1) \times \mathbb{R}_{>0}$ can be represented as a linear combination of the form $\phi_n(x)T_n(t)$.)

We first seek a family of solutions of the form $u_n(x, t) = \phi_n(x)T_n(t)$ that satisfy the heat equation and boundary conditions (but not the initial condition). To begin, we substitute the separable form $u_n(x, t) = \phi_n(x)T_n(t)$ to the heat equation to obtain

$$\phi_n T_n' = \phi_n'' T_n,$$

where $(\cdot)'$ and $(\cdot)''$ denote the first and second derivatives, respectively, of the single-variable function. We now assume that $\phi_n(x)T_n(t) \neq 0 \forall (x, t)$ and divide through the equation by $\phi_n T_n$ to obtain

$$\frac{T_n'}{T_n} = \frac{\phi_n''}{\phi_n}.$$

We make a key observation: since the left hand side T_n'/T_n is a function of t (only) and the right hand side ϕ_n''/ϕ_n is a function of x (only), each side must be independent of both x and t and hence be a constant. We denote this constant by $-\alpha_n$ to obtain

$$\frac{T_n'}{T_n} = -\alpha_n \quad \text{and} \quad \frac{\phi_n''}{\phi_n} = -\alpha_n.$$

(As we will see shortly, the choice of $-\alpha_n$ (instead of α_n) will make the presentation slightly cleaner.) Equivalently, we obtain a pair of ODEs

$$\begin{aligned} \phi_n'' &= -\alpha_n \phi_n & \text{in } (0, 1), \\ T_n' &= -\alpha_n T_n & \text{in } (0, \infty); \end{aligned}$$

note that each equation is an ODE (rather than a PDE) since each problem is associated with either x or t (but not both). In addition, the homogeneous Dirichlet boundary condition requires that

$$\begin{aligned} u_n(x=0, t) &= \phi_n(0)T_n(t) = 0, \\ u_n(x=1, t) &= \phi_n(1)T_n(t) = 0. \end{aligned}$$

As we seek a nontrivial solution (i.e., $T_n \neq 0$), we deduce that $\phi_n(0) = \phi_n(1) = 0$. Hence the spatial function ϕ_n must satisfy a boundary-value eigenproblem

$$\begin{aligned} -\phi_n'' &= \alpha_n \phi_n & \text{in } (0, 1), \\ \phi_n(0) &= \phi_n(1) = 0. \end{aligned} \tag{6.1}$$

We recognize that this is a Sturm-Liouville problem. The problem was analyzed in Section 4.4 and in particular Example 4.6; we found the solutions are $\alpha_n = \pi^2 n^2$ and $\phi_n(x) = \sin(n\pi x)$, $n = 1, 2, \dots$. (The eigenfunction ϕ_n is unique up to multiplication by a constant.)

Having found nontrivial solutions to the spatial eigenproblem, we now seek the associated solutions to the temporal ODE, $T_n' = -\alpha_n T_n$. The general solution to the ODE is of the form

$$T_n(t) = \exp(-\alpha_n t) = \exp(-n^2 \pi^2 t),$$

which again is unique up to multiplication by a constant. We combine the expressions for ϕ_n and T_n to conclude that any functions of the form

$$u_n(x, t) = \phi_n(x)T_n(t) = \exp(-n^2 \pi^2 t) \sin(n\pi x), \quad n = 1, 2, \dots,$$

satisfy the homogeneous PDE and boundary conditions (but not the initial condition).

We now appeal to the *principle of superposition* to find the solution to the initial-boundary value problem. The key observation is that if each u_n for $n = 1, 2, \dots$ satisfies the homogeneous PDE and boundary conditions, so does

$$u(x, t) = \sum_{n=1}^{\infty} a_n u_n(x, t) = \sum_{n=1}^{\infty} a_n \exp(-n^2 \pi^2 t) \sin(n\pi x),$$

for any a_n , $n = 1, 2, \dots$. The principle of superposition is a direct consequence of the linearity of the heat equation and the homogeneous boundary condition. Namely,

$$\begin{aligned} \frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} &= \frac{\partial}{\partial t} \left(\sum_{n=1}^{\infty} a_n u_n \right) - \frac{\partial^2}{\partial x^2} \left(\sum_{n=1}^{\infty} a_n u_n \right) = \sum_{n=1}^{\infty} a_n \left(\frac{\partial u_n}{\partial t} - \frac{\partial^2 u_n}{\partial x^2} \right) = 0, \\ u(x=0, t) &= \sum_{n=1}^{\infty} a_n u_n(x=0, t) = 0, \\ u(x=1, t) &= \sum_{n=1}^{\infty} a_n u_n(x=1, t) = 0, \end{aligned}$$

since each u_n satisfies the heat equation and the boundary conditions. We make one key remark: the fact that both the PDE and boundary conditions are homogeneous is crucial to apply the principle of superposition. Any linear combination of functions that satisfy a homogeneous PDE and boundary conditions satisfy the PDE and the boundary conditions (simply because sum of the multiples of 0 is always 0), but this would not be the case if the PDE or boundary condition is not homogeneous.

Having satisfied the PDE and boundary conditions, we now seek a set of coefficients a_n that satisfies the initial condition:

$$u(x, t=0) = \sum_{n=1}^{\infty} a_n \sin(n\pi x) = g(x).$$

We recognize that this is a Fourier sine series, and the coefficients are given by

$$a_n = \hat{g}_n = 2 \int_0^1 g(x) \sin(n\pi x) dx, \quad n = 1, 2, \dots$$

(Note that we denote the Fourier sine coefficients of g by \hat{g}_n , $n = 1, 2, \dots$.) Hence the solution to our initial boundary value problem is given by

$$u(x, t) = \sum_{n=1}^{\infty} \hat{g}_n \exp(-n^2 \pi^2 t) \sin(n\pi x), \quad (6.2)$$

where $\hat{g}_n = 2 \int_0^1 g(x) \sin(n\pi x) dx$. We make a few observations.

1. *Convergence.* If the initial condition g is square integrable, then the Fourier series is uniformly convergent for $u(\cdot, t)$, $t > 0$. To see this, we observe that (i) the Fourier coefficients are $b_n = \hat{g}_n \exp(-n^2 \pi^2 t)$ and (ii) the associated infinite sum $\sum_{n=1}^{\infty} b_n$ is absolutely convergent. The absolute convergence of the series follows from a comparison test with $\sum_{n=1}^{\infty} c_n = \sum_{n=1}^{\infty} 1/n^2$, which we know is convergent. We first note that $|\hat{g}_n| \rightarrow 0$ as $n \rightarrow \infty$ because the initial condition g is square integrable and then find that $b_n/c_n = |\hat{g}_n| \exp(-n^2 \pi^2 t)/(1/n^2) = |\hat{g}_n| n^2 \exp(-n^2 \pi^2 t) \rightarrow 0$ as $n \rightarrow \infty$, and hence the series converges.
2. *Smoothness.* For $t > 0$, the solution to the heat equation is smooth (i.e., infinitely differentiable and $u(\cdot, t) \in C^\infty(0, 1)$). To see this, we recall that the function has a continuous k -th order derivative if

$$\sum_{n=1}^{\infty} n^k |b_n| = \sum_{n=1}^{\infty} |\hat{g}_n| n^k \exp(-n^2 \pi^2 t) < \infty.$$

We again perform a comparison test with a convergent series $\sum_{n=1}^{\infty} c_n = \sum_{n=1}^{\infty} 1/n^2$. We find that $(n^k b_n)/c_n = |\hat{g}_n| n^k \exp(-n^2 \pi^2 t)/(1/n^2) = |\hat{g}_n| n^{k+2} \exp(-n^2 \pi^2 t) \rightarrow 0$ as $n \rightarrow \infty$ for any $k \in \mathbb{N}_{\geq 0}$ and $t > 0$, and hence the series converges. It follows that the solution to the heat equation is infinitely differentiable for any $t > 0$, even if the initial condition is only square integrable (i.e., it could be discontinuous or be unbounded).

3. *Steady state solution.* As $t \rightarrow \infty$, the solution decays and converges to $u = 0$. This agrees with our physical intuition that at steady state the temperature should be equal to the ambient temperature (i.e., the temperature on the boundary) which is 0.
4. *Mode shape and decay rate.* We observe that each mode exponentially decays with time. We also observe that higher-frequency modes decay more rapidly than lower-frequency modes. As a result, the solution gets qualitatively “smoother” as the time evolves.

Example 6.1 (heat equation with homogeneous Dirichlet boundary conditions). We consider the heat equation initial-boundary value problem

$$\begin{aligned} \frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} &= 0 \quad \text{in } (0, 1) \times \mathbb{R}_{>0}, \\ u &= 0 \quad \text{on } \{0, 1\} \times \mathbb{R}_{>0}, \\ u(x, t = 0) &= x \quad \forall x \in [0, 1]. \end{aligned}$$

We have already computed the Fourier sine series representation of the initial condition $g(x) = x$ on $(0, 1)$ in Example 2.18; the expression is

$$g(x) \sim \sum_{n=1}^{\infty} \hat{g}_n \sin(n\pi x) = \sum_{n=1}^{\infty} \frac{2(-1)^{n+1}}{n\pi} \sin(n\pi x).$$

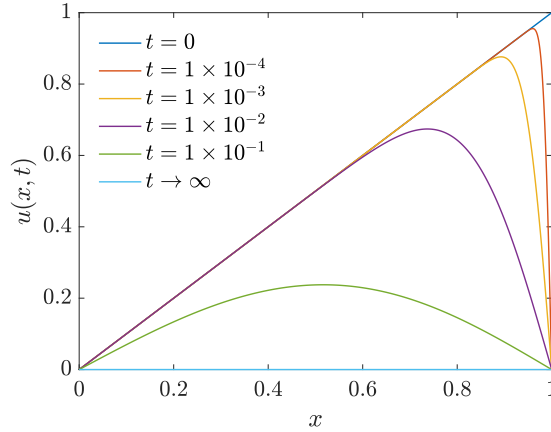


Figure 6.1: Solution to the heat equation with homogeneous Dirichlet boundary condition.

It follows that the solution to the heat equation is given by

$$u(x, t) = \sum_{n=1}^{\infty} \hat{g}_n \exp(-n^2 \pi^2 t) \sin(n\pi x) = \sum_{n=1}^{\infty} \frac{2(-1)^{n+1}}{n\pi} \exp(-n^2 \pi^2 t) \sin(n\pi x).$$

Figure 6.1 shows the solution to the heat equation at a few different time instances. We observe that the solution (i) decays in time and (ii) qualitatively becomes smoother. Both behaviors are readily predicted from our Fourier series representation of the solution. We also observe that (iii) the initial condition $g(x) = x$ does not approach 0 on the $x = 1$ boundary; however, the problem is still well-posed and the solution $u(\cdot, t)$ satisfies the boundary condition for any $t > 0$.

6.3 Homogeneous Neumann boundary conditions

We now consider a heat equation with a homogeneous Neumann boundary condition

$$\begin{aligned} \frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} &= 0 \quad \text{in } (0, 1) \times \mathbb{R}_{>0}, \\ \frac{\partial u}{\partial x} &= 0 \quad \text{on } \{0, 1\} \times \mathbb{R}_{>0}, \\ u &= g \quad \text{on } [0, 1] \times \{t = 0\}. \end{aligned}$$

We apply separation of variables and consider solutions of the form $u_n(x, t) = \phi_n(x)T_n(t)$. The substitution of the separable form of the solution yields

$$\phi_n T_n' - \phi_n'' T_n = 0 \quad \Rightarrow \quad \frac{\phi_n''}{\phi_n} = \frac{T_n'}{T_n} = -\alpha_n;$$

here we appeal to the fact that ϕ_n''/ϕ_n is a function of x only and T_n'/T_n is a function of t only, and hence each expression must be a constant.

We now focus on the solution of the spatial problem. We appeal to the boundary conditions and find that

$$\begin{aligned}\frac{\partial u_n}{\partial x}(x=0, t) &= \phi'_n(0)T_n(t) = 0, \\ \frac{\partial u_n}{\partial x}(x=1, t) &= \phi'_n(1)T_n(t) = 0;\end{aligned}$$

since we seek a nontrivial solution (i.e., $T_n \neq 0$), we require $\phi'_n(0) = \phi'_n(1) = 0$. Hence the boundary-value eigenproblem associated with the spatial function ϕ_n is

$$\begin{aligned}-\phi''_n &= \alpha_n \phi_n \quad \text{in } (0, 1), \\ \phi'_n(0) &= \phi'_n(1) = 0.\end{aligned}$$

This is again a Sturm-Liouville problem. The problem was studied in Example 4.7; the eigenvalues are $\alpha_n = n^2\pi^2$ and the eigenfunctions are $\phi_n = \cos(n\pi x)$ for $n = 1, 2, \dots$

We now seek the solution to the temporal ODE

$$T'_n(t) = -\alpha_n T_n(t)$$

for $\alpha_n = n^2\pi^2$. The solution to this ODE is of the form $T(t) = \exp(-\alpha_n t) = \exp(-n^2\pi^2 t)$ (up to multiplication by a constant). Hence the general solution is of the form

$$u(x, t) = \sum_{n=0}^{\infty} a_n T_n(t) \phi_n(x) = \sum_{n=0}^{\infty} a_n \exp(-n^2\pi^2 t) \cos(n\pi x).$$

We now impose the initial condition to find

$$u(x, t=0) = \sum_{n=0}^{\infty} a_n \cos(n\pi x) = g(x).$$

We recognize that this is almost a Fourier cosine series, with exception of the constant term having a factor of 1 instead of 1/2. We rescale the representation and find that the solution is given by

$$u(x, t) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty} a_n \exp(-n^2\pi^2 t) \cos(n\pi x),$$

where

$$a_n = \hat{g}_n = 2 \int_0^1 \cos(n\pi x) g(x) dx.$$

We make a few observations:

1. *Energy conservation.* We recall that the total thermal energy in a domain Ω at time t is $E(t) = \int_{\Omega} u(x, t) dx$ (for the nondimensionalized equation with $\rho c = 1$). We observe that, for homogeneous Neumann boundary condition, the total energy is conserved:

$$E(t) = \int_0^1 u(x, t) dx = \int_0^1 \left[\frac{1}{2} \hat{g}_0 + \sum_{n=1}^{\infty} \hat{g}_n \exp(-n^2\pi^2 t) \cos(n\pi x) \right] dx = \frac{1}{2} \hat{g}_0 = \int_0^1 g(x) dx;$$

the terms associated with $n = 1, 2, \dots$ vanish due to the orthogonality of the cosine function with the constant function. Hence the total thermal energy is conserved. Physically, the homogeneous Neumann boundary condition corresponds to an insulated boundary (i.e., a boundary without any heat transfer), and hence the observed conservation of thermal energy agrees with our physical intuition.

2. *Convergence; smoothness; mode shape and decay rate.* These observations we made for the homogeneous Dirichlet solution (6.2) also holds for the homogeneous Neumann solution.

Example 6.2 (heat equation with homogeneous Neumann boundary condition). We consider the heat equation initial boundary value problem

$$\begin{aligned} \frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} &= 0 && \text{in } (0, 1) \times \mathbb{R}_{>0}, \\ \frac{\partial u}{\partial x} &= 0 && \text{on } \{0, 1\} \times \mathbb{R}_{>0}, \\ u(x, t = 0) &= x && \text{on } [0, 1] \times \{t = 0\}. \end{aligned}$$

We have already computed the Fourier cosine series representation of the initial condition $g(x) = x$ on $(0, 1)$ in Example 2.17; the expression is

$$g(x) \sim \frac{1}{2} \hat{g}_0 + \sum_{n=1}^{\infty} \hat{g}_n \cos(n\pi x) = \frac{1}{2} - \sum_{k=1}^{\infty} \frac{4}{(2k-1)^2 \pi^2} \cos((2k-1)\pi x)$$

It follows that the solution to the heat equation is given by

$$u(x, t) = \frac{1}{2} - \sum_{n=1}^{\infty} \hat{g}_n \exp(-n^2 \pi^2 t) \cos(n\pi x) = \frac{1}{2} - \sum_{k=1}^{\infty} \frac{4}{(2k-1)^2 \pi^2} \exp(-(2k-1)^2 \pi^2 t) \cos((2k-1)\pi x).$$

Figure 6.2 shows the solution to the heat equation at a few different time instances. We observe that the solution (i) satisfies the homogeneous Neumann condition (i.e., the derivative vanishes at the endpoints) and (ii) is smooth for any time. Both behaviors are readily predicted from our Fourier series representation of the solution.

6.4 Mixed boundary conditions

We now consider a heat equation with mixed boundary conditions

$$\begin{aligned} \frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} &= 0 && \text{in } (0, 1) \times \mathbb{R}_{>0}, \\ u &= 0 && \text{on } \{x = 0\} \times \mathbb{R}_{>0}, \\ \frac{\partial u}{\partial x} &= 0 && \text{on } \{x = 1\} \times \mathbb{R}_{>0}, \\ u &= g && \text{on } [0, 1] \times \{t = 0\}. \end{aligned}$$

As the procedure is similar to the case for the homogeneous Dirichlet (or Neumann) boundary condition considered earlier, we only highlight steps that are different from the previous cases.

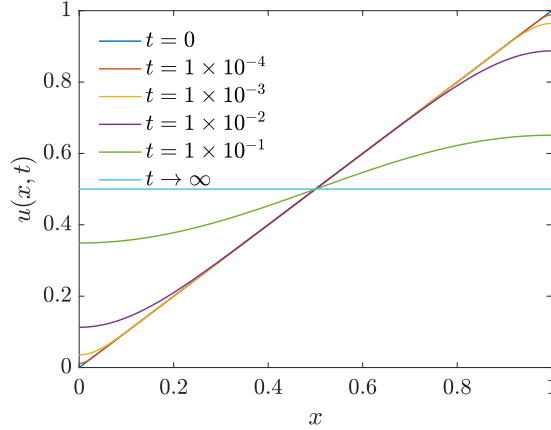


Figure 6.2: Solution to the heat equation with homogeneous Neumann boundary condition.

We apply separation of variables and arrive at the following boundary-value eigenproblem associated with the spatial function ϕ_n

$$\begin{aligned} -\phi_n'' &= \alpha_n \phi_n \quad \text{in } (0, 1), \\ \phi_n(0) &= 0, \\ \phi_n'(1) &= 0. \end{aligned}$$

This is a Sturm-Liouville problem with a mixed boundary condition; we know that the eigenvalues are real and the eigenfunctions are orthogonal. Moreover, because the conditions for Theorem 4.5 are satisfied, the eigenvalues $\alpha_n \geq 0$. We find the solutions are of the form $\phi_n(x) = a_n \cos(\sqrt{\alpha_n}x) + b_n \sin(\sqrt{\alpha_n}x)$. The boundary condition $\phi_n(x=0) = 0$ requires that $a_n = 0$. The boundary condition $\phi_n'(1) = 0$ requires that $\phi_n'(1) = b_n \sqrt{\alpha_n} \cos(\sqrt{\alpha_n}) = 0$, which implies $\sqrt{\alpha_n} = (n - 1/2)\pi$, $n = 1, 2, \dots$

The temporal ODE $T_n'(t) = -\alpha_n T_n(t)$ is the same as before, and its solution is of the form $T(t) = \exp(-\alpha_n t) = \exp(-(n - 1/2)^2 \pi^2 t)$ (up to multiplication by a constant). It follows that the solution to the mixed boundary value problem is of the form

$$u(x, t) = \sum_{n=1}^{\infty} a_n \exp(-(n - 1/2)^2 \pi^2 t) \sin((n - 1/2)\pi x). \quad (6.3)$$

We impose the initial condition to find

$$u(x, t=0) = \sum_{n=1}^{\infty} a_n \sin((n - 1/2)\pi x) = g(x).$$

We know that $\{\sin((n - 1/2)\pi x)\}_{n=1}^{\infty}$ forms an orthogonal basis because they are the eigenfunctions of a Sturm-Liouville problem. We hence multiply both sides of the equations by $\sin((m - 1/2)\pi x)$ and integrate over $(0, 1)$ to obtain

$$a_m \int_0^1 \sin((m - 1/2)\pi x)^2 dx = \int_0^1 \sin((m - 1/2)\pi x) g(x) dx, \quad m = 1, 2, \dots$$

The integral on the left hand side evaluates to

$$\int_0^1 \sin((m - 1/2)\pi x)^2 dx = \int_0^1 \frac{1}{2}(1 - \cos(2(m - 1/2)\pi x)) dx = \frac{1}{2},$$

where the last equality follows from the fact that integral of $\cos(2(m - 1/2)\pi x)$ over $(0, 1)$ is 0 for any m . Hence

$$\frac{1}{2}a_n = \int_0^1 \sin((n - 1/2)\pi x)g(x)dx$$

or equivalently

$$a_n = 2 \int_0^1 \sin((n - 1/2)\pi x)g(x)dx. \quad (6.4)$$

The series (6.3) with the coefficients (6.4) provide a solution representation to the mixed boundary value problem.

6.5 Nonhomogeneous source term

We now consider the heat equation with a nonhomogeneous source term:

$$\begin{aligned} \frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} &= f \quad \text{in } (0, 1) \times \mathbb{R}_{>0}, \\ u &= 0 \quad \text{on } \{0, 1\} \times \mathbb{R}_{>0}, \\ u &= g \quad \text{on } [0, 1] \times \{t = 0\}, \end{aligned}$$

where the source function $f : (0, 1) \times \mathbb{R}_{>0} \rightarrow \mathbb{R}$ in general depends on both space and time. This nonhomogeneous problem can also be solved using separation of variables.

To begin, we first apply separation of variables to the homogeneous PDE $\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = 0$ with the homogeneous Dirichlet boundary condition to find an appropriate spatial basis functions (ϕ_n) . This homogeneous problem, considered in Section 6.2, yields a basis functions $\phi_n(x) = \sin(n\pi x)$. We express the solution as a linear combination of these spatial basis functions to obtain a solution representation

$$u(x, t) = \sum_{n=1}^{\infty} \hat{u}_n(t) \sin(n\pi x).$$

Note that the Fourier sine series will satisfy the homogeneous Dirichlet boundary condition for any time-dependent coefficients $(\hat{u}_n(t))_{n=1}^{\infty}$ at each time. We now substitute the Fourier representation of u into the PDE to obtain

$$\sum_{n=1}^{\infty} [\hat{u}'_n(t) + n^2\pi^2\hat{u}_n(t)] \sin(n\pi x) = f(x, t).$$

We next multiply the equation by $2\sin(m\pi x)$, integrate from $x = 0$ to $x = 1$, and appeal to the orthogonality of the Fourier basis to obtain

$$\hat{u}'_m(t) + m^2\pi^2\hat{u}_m(t) = \hat{f}_m(t), \quad m = 1, 2, \dots, \quad (6.5)$$

where the Fourier coefficients of f are given by

$$\hat{f}_m(t) = 2 \int_{x=0}^1 f(x, t) \sin(m\pi x) dx, \quad m = 1, 2, \dots$$

The time-dependent coefficients $\hat{u}_n : \mathbb{R}_{\geq 0} \rightarrow \mathbb{R}$, $n = 1, 2, \dots$, must hence satisfy the ODE (6.5).

We now wish to identify the appropriate initial conditions for (6.5). To this end, we substitute the solution representation to the initial condition to obtain

$$u(x, t = 0) = \sum_{n=1}^{\infty} \hat{u}_n(t = 0) \sin(n\pi x) = g(x).$$

This is a Fourier sine series and hence we deduce that

$$\hat{u}_n(t = 0) = \hat{g}_n \equiv 2 \int_{x=0}^1 g(x) \sin(n\pi x) dx. \quad (6.6)$$

The combination of (6.5) and (6.6) yields

$$\begin{aligned} \hat{u}'_n(t) + n^2\pi^2\hat{u}_n(t) &= \hat{f}_n(t), \\ \hat{u}_n(t = 0) &= \hat{g}_n \end{aligned}$$

for $n = 1, 2, \dots$, which is a set of ODE initial value problems.

We find the solution to the ODE initial value problem using an integrating factor. To this end, we multiply each ODE by $\exp(n^2\pi^2 t)$ and note that

$$\exp(n^2\pi^2 t)\hat{u}'_n(t) + n^2\pi^2 \exp(n^2\pi^2 t)\hat{u}_n(t) = \frac{d}{dt}(\exp(n^2\pi^2 t)\hat{u}_n(t)) = \exp(n^2\pi^2 t)\hat{f}_n(t).$$

We integrate the expression from 0 to t to obtain

$$\exp(n^2\pi^2 t)\hat{u}_n(t) - \hat{u}_n(t = 0) = \int_{\tau=0}^t \exp(n^2\pi^2 \tau)\hat{f}_n(\tau) d\tau.$$

We divide through by $\exp(n^2\pi^2 t)$ and rearrange the expression to obtain

$$\hat{u}_n(t) = \hat{u}_n(t = 0) \exp(-n^2\pi^2 t) + \int_{\tau=0}^t \exp(-n^2\pi^2(t - \tau))\hat{f}_n(\tau) d\tau.$$

Since $\hat{u}_n(t = 0) = \hat{g}_n$, it follows that

$$\hat{u}_n(t) = \hat{g}_n \exp(-n^2\pi^2 t) + \int_{\tau=0}^t \exp(-n^2\pi^2(t - \tau))\hat{f}_n(\tau) d\tau. \quad (6.7)$$

Hence the solution to the nonhomogeneous heat equation is given by

$$u(x, t) = \sum_{n=1}^{\infty} \hat{u}_n(t) \sin(n\pi x),$$

where the coefficient functions are given by (6.7).

We make a few observations:

1. The solution to the nonhomogeneous heat equation is a sum of the solutions to two initial boundary value problem. The first problem is the homogeneous problem with nonzero initial condition: $\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = 0$ and $u = g$ at $t = 0$. The second problem is the nonhomogeneous problem with a zero initial condition: $\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = f$ and $u = 0$ at $t = 0$. The result is an application of the principle of superposition.
2. The term due to the nonhomogeneous source, $\int_{\tau=0}^t \exp(n^2\pi^2(\tau-t))\hat{f}_n(\tau)d\tau$, suggests that the addition of the heat source at time τ affects the solution for all $t > \tau$, which agrees with our physical intuition. However, the influence of the heat source at time τ decays exponentially in time.

Example 6.3 (heat equation with a source term). We consider a nonhomogeneous heat equation

$$\begin{aligned} \frac{\partial u}{\partial t}(x, t) - \frac{\partial^2 u}{\partial x^2}(x, t) &= x, & x \in (0, 1), t \in \mathbb{R}_{>0}, \\ u &= 0 & \text{on } \{0, 1\} \times \mathbb{R}_{>0}, \\ u &= 0 & \text{on } [0, 1] \times \{t = 0\}. \end{aligned}$$

The heat equation has a nonzero but time-independent source term.

We first recognize that our boundary conditions are homogeneous Dirichlet, and hence our spatial basis is given by $\phi_n(x) = \sin(n\pi x)$, $n = 1, 2, \dots$; the basis of Fourier sine series. To find the Fourier sine series representation of the problem, we first identify that the Fourier sine coefficients of the source term $f(x) = x$ on $x \in (0, 1)$:

$$\hat{f}_n = \frac{2(-1)^{n+1}}{n\pi} \quad n \in \mathbb{Z}_{>0}.$$

We appeal to (6.7), note that $\hat{g}_n = 0$ since the initial condition is $g = 0$, and find the Fourier sine coefficients of the solution:

$$\hat{u}_n(t) = \int_{\tau=0}^t \exp(n^2\pi^2(\tau-t))\hat{f}_n d\tau = \frac{1}{n^2\pi^2}(1 - \exp(-n^2\pi^2t))\hat{f}_n = \frac{2(-1)^{n+1}}{n^3\pi^3}(1 - \exp(-n^2\pi^2t)).$$

Hence the solution is given by

$$u(x, t) = \sum_{n=1}^{\infty} \frac{2(-1)^{n+1}}{n^3\pi^3}(1 - \exp(-n^2\pi^2t)) \sin(n\pi x).$$

Figure 6.3 shows the solution to the heat equation at a few different time instances. We make a few observations. Lastly, as $t \rightarrow \infty$ the solution converges to the non-trivial steady state solution

$$u(x, t) = \sum_{n=1}^{\infty} \frac{2(-1)^{n+1}}{n^3\pi^3} \sin(n\pi x);$$

this again agrees with our intuition that, in the presence of a steady heat source, the temperature approaches a steady nonzero distribution over time.

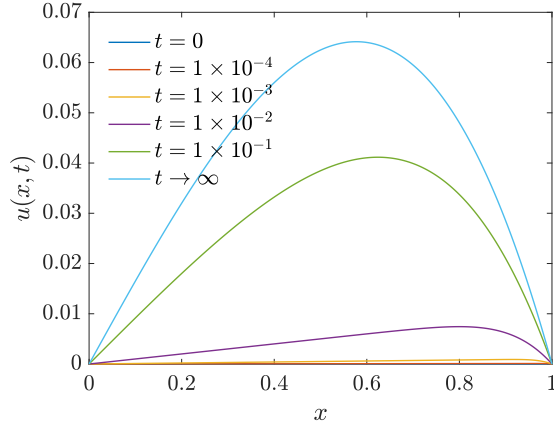


Figure 6.3: Solution to the heat equation with nonhomogeneous Dirichlet boundary condition.

6.6 Nonhomogeneous boundary conditions

We now consider the heat equation with nonhomogeneous boundary conditions:

$$\begin{aligned} \frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} &= f && \text{in } (0, 1) \times \mathbb{R}_{>0}, \\ u &= h && \text{on } \{0, 1\} \times \mathbb{R}_{>0}, \\ u &= g && \text{on } [0, 1] \times \{t = 0\}, \end{aligned}$$

where the boundary function $h : \{0, 1\} \times \mathbb{R}_{>0} \rightarrow \mathbb{R}$ in general depends on time. To solve this problem, we consider the decomposition of the solution into two parts: (i) a function u^b that satisfies the boundary condition and (ii) the remainder of the solution w such that $u = u^b + w$. We first note that the function u^b can be obtained by “extending” the boundary function h to the interior of the domain:

$$u^b(x, t) = h(0, t) + (h(1, t) - h(0, t))x;$$

this is obviously not a unique choice of a function that satisfies the boundary conditions, but it is a convenient choice because the Laplacian of the linear function vanishes. We substitute $u = u^b + w$ to our initial-boundary value problem to obtain

$$\begin{aligned} \frac{\partial u^b}{\partial t} + \frac{\partial w}{\partial t} - \frac{\partial^2 w}{\partial x^2} &= f && \text{in } (0, 1) \times \mathbb{R}_{>0}, \\ u^b + w &= h && \text{on } \{0, 1\} \times \mathbb{R}_{>0}, \\ u^b + w &= g && \text{on } [0, 1] \times \{t = 0\}, \end{aligned}$$

where we have appealed to $\frac{\partial^2 u^b}{\partial x^2} = 0$. In other words, the function w must satisfy

$$\begin{aligned} \frac{\partial w}{\partial t} - \frac{\partial^2 w}{\partial x^2} &= f - \frac{\partial u^b}{\partial t} && \text{in } (0, 1) \times \mathbb{R}_{>0}, \\ w &= 0 && \text{on } \{0, 1\} \times \mathbb{R}_{>0}, \\ w &= g - u^b && \text{on } [0, 1] \times \{t = 0\}. \end{aligned}$$

This is a heat equation with a nonhomogeneous source term but with a homogeneous boundary condition, which was considered in Section 6.5. We may hence solve for w using the procedure outlined in the section and set $u = u^b + w$. In the special case in which the boundary condition does not depend on time, the heat equation for w simplifies to $\frac{\partial w}{\partial t} - \frac{\partial^2 w}{\partial x^2} = f$.

Example 6.4 (nonhomogeneous Dirichlet boundary conditions). We consider the solution of a heat equation initial-boundary value problem

$$\begin{aligned}\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} &= 0 \quad \text{in } (0, 1) \times \mathbb{R}_{>0}, \\ u(x=0, t) &= T_L, \quad t \in \mathbb{R}_{>0}, \\ u(x=1, t) &= T_R, \quad t \in \mathbb{R}_{>0}, \\ u &= 0 \quad \text{on } [0, 1] \times \{t=0\}\end{aligned}$$

for some fixed temperatures T_L and T_R . The boundary condition is nonhomogeneous but is time-independent. We seek the solution of a form $u = u^b + w$, for some u^b that satisfies the boundary condition and w which solves the initial-boundary value problem. We choose the function

$$u^b(x, t) = T_L + (T_R - T_L)x$$

as our boundary function, which satisfies the boundary conditions. We then note that w must then satisfy

$$\begin{aligned}\frac{\partial w}{\partial t} - \frac{\partial^2 w}{\partial x^2} &= 0 \quad \text{on } (0, 1) \times \mathbb{R}_{>0}, \\ w &= 0 \quad \text{on } \{0, 1\} \times \mathbb{R}_{>0}, \\ w &= -u^b = -T_L - (T_R - T_L)x \quad \text{on } [0, 1] \times \{t=0\}.\end{aligned}$$

This is a homogeneous heat equation with homogeneous boundary conditions, the solution approach to which was discussed in Section 6.2.

The Fourier sine coefficients for the initial condition are

$$\begin{aligned}b_n &= 2 \int_0^1 \sin(n\pi x)(-T_L - (T_R - T_L)x) dx \\ &= 2T_L \left[\frac{\cos(n\pi x)}{n\pi} \right]_{x=0}^1 + 2(T_R - T_L) \left[-\frac{\sin(n\pi x)}{n^2\pi^2} + \frac{x \cos(n\pi x)}{n\pi} \right]_{x=0}^1 \\ &= 2T_L \left(\frac{\cos(n\pi) - 1}{n\pi} \right) + 2(T_R - T_L) \left(\frac{\cos(n\pi)}{n\pi} \right) = \frac{2}{n\pi} ((-1)^n T_L - T_L + (-1)^n (T_R - T_L)) \\ &= \frac{2}{n\pi} (-T_L + (-1)^n T_R).\end{aligned}$$

Hence the function w is given by

$$w(x, t) = \sum_{n=1}^{\infty} b_n \exp(-n^2\pi^2 t) \sin(n\pi x) = \sum_{n=1}^{\infty} \frac{2}{n\pi} (-T_L + (-1)^n T_R) \exp(-n^2\pi^2 t) \sin(n\pi x).$$

The solution u is

$$u(x, t) = u^b(x, t) + w(x, t) = T_L + (T_R - T_L)x + \sum_{n=1}^{\infty} \frac{2}{n\pi} (-T_L + (-1)^n T_R) \exp(-n^2\pi^2 t) \sin(n\pi x).$$

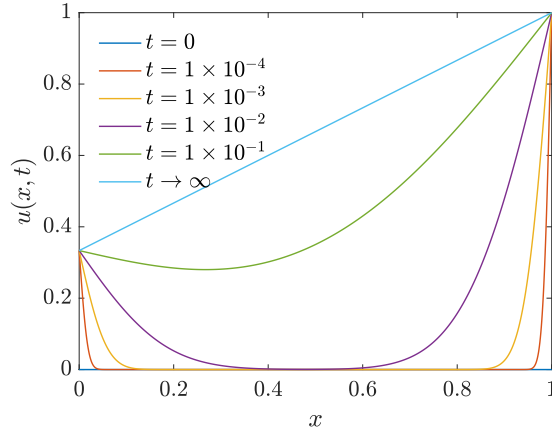


Figure 6.4: Solution to the heat equation with nonhomogeneous Dirichlet boundary condition.

Figure 6.4 shows the solution to the heat equation for $T_L = 1/3$ and $T_R = 1$ at a few different time instances. We make a few observations. First, for a small t , the series representation of w is almost equal to $-u^b$ and hence the solution u is close to zero (i.e., the initial condition). Second, as $t \rightarrow \infty$, the function $w \rightarrow 0$ and hence the solution u converges to u^b .

6.7 Summary

We summarize the key points of this lecture:

1. Using separation of variables and the principle of superposition, we can find Fourier series representations of the solution to the heat equation on a one-dimensional bounded spatial domain.
2. The application of separation of variables to the heat equation yields a Sturm-Liouville problem for the spatial modes. For homogeneous Dirichlet, Neumann, and mixed boundary conditions, the Sturm-Liouville theory can be used to deduce that all eigenvalues are non-negative and the eigenfunctions are orthogonal.
3. The solution to the heat equation is smooth (i.e., infinitely differentiable) for $t > 0$ for any boundary conditions.
4. The solution to the heat equation with homogeneous Dirichlet boundary condition is given by Fourier sine series. All modes decay in time, and higher spatial mode decay more rapidly in time.
5. The solution to the heat equation with homogeneous Neumann boundary condition is given by Fourier cosine series. The total energy is conserved in time.
6. The solutions to a heat equation with a nonhomogeneous source term or a nonhomogeneous boundary condition can be found again using separation of variables. The solution is the sum of the solutions associated with (i) a nonhomogeneous PDE (i.e., finite source) and a

homogeneous initial condition and (ii) a nonhomogeneous initial condition and a homogeneous PDE (i.e., zero source).

Lecture 7

Heat equation: fundamental solution

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7.1 Introduction

In this lecture we seek the solution of initial or initial-boundary value problems associated with the heat equation in unbounded domains. To find the solutions, we generalize Fourier series to unbounded domains to form Fourier integrals. We then identify, using Fourier integrals, the fundamental solution (or heat kernel) for heat equations in unbounded domains. We next employ the method of reflection to solve problems on the half (as opposed to entire) real line. We finally introduce the Duhamel's principle, which allows us to express the solution to nonhomogeneous problems as a linear combination of the solutions to a family of homogeneous problems.

7.2 Fourier integral representation

We have so far represented functions on bounded domains as Fourier series. For instance, the Fourier series of $f : (-L, L) \rightarrow \mathbb{R}$ is given by

$$f(x) = \frac{1}{2}a_0 + \sum_{n=1}^{\infty} (a_n \cos(n\pi x/L) + b_n \sin(n\pi x/L)),$$

where

$$a_0 \equiv \frac{1}{L} \int_{-L}^L f(x) dx, \quad a_n \equiv \frac{1}{L} \int_{-L}^L \cos(n\pi x/L) f(x) dx, \quad b_n \equiv \frac{1}{L} \int_{-L}^L \sin(n\pi x/L) f(x) dx.$$

We now introduce *Fourier integrals* which provide similar representations for functions on unbounded domains (i.e., $L \rightarrow \infty$).

Definition 7.1 (Fourier integral). Let $f : \mathbb{R} \rightarrow \mathbb{R}$ that satisfies $\int_{-\infty}^{\infty} |f(x)| dx < \infty$. The Fourier integral representation of f is given by

$$f(x) \sim \int_{\lambda=0}^{\infty} (a(\lambda) \cos(\lambda x) + b(\lambda) \sin(\lambda x)) d\lambda,$$

where the Fourier coefficients are given by

$$a(\lambda) \equiv \frac{1}{\pi} \int_{-\infty}^{\infty} \cos(\lambda x) f(x) dx, \quad b(\lambda) \equiv \frac{1}{\pi} \int_{-\infty}^{\infty} \sin(\lambda x) f(x) dx.$$

The Fourier integral, just like the Fourier series, converges for piecewise continuously differentiable functions in a point-wise sense. We here state a key result without a proof.

Theorem 7.2 (convergence of Fourier integral). Let $f : \mathbb{R} \rightarrow \mathbb{R}$ be a function that (i) is piecewise continuously differentiable on any interval and (ii) satisfies $\int_{-\infty}^{\infty} |f(x)| dx < \infty$. Then for any $x \in \mathbb{R}$,

$$\int_{\lambda=0}^{\infty} (a(\lambda) \cos(\lambda x) + b(\lambda) \sin(\lambda x)) d\lambda = \frac{1}{2}(f(x^+) + f(x^-)).$$

The Fourier integral, just like Fourier series, can be extended to odd and even functions.

Definition 7.3 (Fourier cosine integral). Let $f : \mathbb{R} \rightarrow \mathbb{R}$ be an even function that satisfies $\int_0^{\infty} |f(x)| dx < \infty$. The Fourier cosine integral representation of f is given by

$$f(x) = \int_{\lambda=0}^{\infty} \hat{f}(\lambda) \cos(\lambda x) d\lambda,$$

where the Fourier cosine coefficient is given by

$$\hat{f}(\lambda) = \frac{1}{\pi} \int_{-\infty}^{\infty} \cos(\lambda x) f(x) dx = \frac{2}{\pi} \int_0^{\infty} \cos(\lambda x) f(x) dx.$$

Definition 7.4 (Fourier sine integral). Let $f : \mathbb{R} \rightarrow \mathbb{R}$ be an odd function that satisfies $\int_0^{\infty} |f(x)| dx < \infty$. The Fourier sine integral representation of f is given by

$$f(x) = \int_{\lambda=0}^{\infty} \hat{f}(\lambda) \sin(\lambda x) d\lambda,$$

where the Fourier sine coefficient is given by

$$\hat{f}(\lambda) = \frac{1}{\pi} \int_{-\infty}^{\infty} \sin(\lambda x) f(x) dx = \frac{2}{\pi} \int_0^{\infty} \sin(\lambda x) f(x) dx.$$

The Fourier cosine and sine integrals exhibit the same convergence property as the (full) Fourier integral.

7.3 Heat equation in $\mathbb{R} \times \mathbb{R}_{\geq 0}$

We now consider the heat equation on the entire real line \mathbb{R} :

$$\begin{aligned} \frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} &= 0 \quad \text{in } \mathbb{R} \times \mathbb{R}_{>0}, \\ u &= g \quad \text{on } \mathbb{R} \times \{t = 0\}, \\ |u(x, t)| &< \infty \quad \text{as } x \rightarrow \pm\infty. \end{aligned} \tag{7.1}$$

The boundary condition is replaced by a boundedness condition which requires the solution to be finite as $x \rightarrow \pm\infty$.

As before, we apply separation of variables and express the solution as a linear combination of homogeneous solutions of the form $u(x, t) = \phi(x)T(t)$. As usual, the substitution of the separable expression to the heat equation yields a condition that

$$\frac{T'}{T} = \frac{\phi''}{\phi} = -\alpha,$$

for some constant α . The boundedness condition requires that ϕ remain finite as $x \rightarrow \infty$, and hence α must be positive so that ϕ are sinusoidal functions instead of hyperbolic sinusoidal functions which are unbounded as $x \rightarrow \infty$. Without loss of generality, we set $\alpha = \lambda^2$, and find the solutions to the eigenproblem

$$\begin{aligned} -\phi'' &= \lambda^2 \phi \quad \text{in } \mathbb{R}, \\ |\phi(x)| &< \infty \quad \text{as } x \rightarrow \pm\infty, \end{aligned}$$

are of the form

$$\phi(x) = a \cos(\lambda x) + b \sin(\lambda x);$$

the expression is bounded for any $x \in \mathbb{R}$, $\lambda \in \mathbb{R}_{>0}$. The associated temporal functions are

$$T(t) = \exp(-\lambda^2 t).$$

We consider the “linear combination” of the solutions $\phi(x)T(t)$ to obtain

$$u(x, t) = \int_{\lambda=0}^{\infty} (a(\lambda) \cos(\lambda x) + b(\lambda) \sin(\lambda x)) \exp(-\lambda^2 t) d\lambda. \quad (7.2)$$

The coefficient functions $a(\lambda)$ and $b(\lambda)$ are determined from the initial condition:

$$u(x, t = 0) = \int_{\lambda=0}^{\infty} (a(\lambda) \cos(\lambda x) + b(\lambda) \sin(\lambda x)) d\lambda = g(x).$$

We deduce that $a(\lambda)$ and $b(\lambda)$ are the Fourier coefficients of the Fourier integral of g ; i.e.,

$$a(\lambda) \equiv \frac{1}{\pi} \int_{x=-\infty}^{\infty} \cos(\lambda x) g(x) dx, \quad b(\lambda) \equiv \frac{1}{\pi} \int_{x=-\infty}^{\infty} \sin(\lambda x) g(x) dx. \quad (7.3)$$

The solution to (7.1) is hence given by (7.2) with the coefficients (7.3).

7.4 Fundamental solution of the heat equation in $\mathbb{R} \times \mathbb{R}_{>0}$

We can rearrange the Fourier integral of the solution (7.2) to gain further insight about the structure of the heat equation. To begin, we substitute the coefficients (7.3) to the Fourier integral (7.1) to obtain

$$\begin{aligned} u(x, t) &= \frac{1}{\pi} \int_{\lambda=0}^{\infty} \left(\int_{\xi=-\infty}^{\infty} \cos(\lambda \xi) g(\xi) d\xi \cos(\lambda x) + \int_{\xi=-\infty}^{\infty} \sin(\lambda \xi) g(\xi) d\xi \sin(\lambda x) \right) \exp(-\lambda^2 t) d\lambda \\ &= \frac{1}{\pi} \int_{\lambda=0}^{\infty} \int_{\xi=-\infty}^{\infty} (\cos(\lambda \xi) \cos(\lambda x) + \sin(\lambda \xi) \sin(\lambda x)) g(\xi) d\xi \exp(-\lambda^2 t) d\lambda \\ &= \frac{1}{\pi} \int_{\lambda=0}^{\infty} \int_{\xi=-\infty}^{\infty} \cos(\lambda(\xi - x)) g(\xi) d\xi \exp(-\lambda^2 t) d\lambda, \end{aligned}$$

where the last equality follows from a trigonometric identity. We now assume that the order of integration can be reversed to obtain

$$u(x, t) = \frac{1}{\pi} \int_{\xi=-\infty}^{\infty} \int_{\lambda=0}^{\infty} \cos(\lambda(\xi - x)) \exp(-\lambda^2 t) d\lambda g(\xi) d\xi.$$

The inner integral on λ over $(0, \infty)$ can be computed using an integration technique in complex analysis:

$$\int_{\lambda=0}^{\infty} \cos(\lambda(\xi - x)) \exp(-\lambda^2 t) d\lambda = \sqrt{\frac{\pi}{4t}} \exp\left(\frac{-(\xi - x)^2}{4t}\right).$$

(The evaluation is beyond the scope of this course, but those who have taken complex analysis could attempt its evaluation.) We hence find that

$$u(x, t) = \frac{1}{\sqrt{4\pi t}} \int_{\xi=-\infty}^{\infty} \exp\left(\frac{-(\xi - x)^2}{4t}\right) g(\xi) d\xi. \quad (7.4)$$

This final expression shows how the initial condition g affects the solution u .

Because the solution of the form (7.4) provides much useful information about the behavior of the PDE, we now formalize the solution representation of this form using the concept of *the fundamental solution*.

Definition 7.5 (fundamental solution of the heat equation). The fundamental solution of the heat equation $\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = 0$ in $\mathbb{R} \times \mathbb{R}_{>0}$ is

$$\Phi(x, t) \equiv \begin{cases} \frac{1}{\sqrt{4\pi t}} \exp\left(\frac{-x^2}{4t}\right), & t > 0 \\ 0, & t < 0. \end{cases}$$

The fundamental solution is also called the *heat kernel* or *diffusion kernel*.

The fundamental solution $\Phi(\cdot, t)$, $t > 0$, is the Gaussian of a variance $2t$ (or standard deviation $\sqrt{2t}$); the height of the Gaussian is $1/\sqrt{4\pi t}$. The fundamental solution for three different time instances is shown in Figure 7.1. The fundamental solution spreads and decays over time.

Using the fundamental solution, the solution to the initial value problem with $u(x, t = 0) = g(x)$ can be represented as

$$u(x, t) = \int_{-\infty}^{\infty} \Phi(x - \xi, t) g(\xi) d\xi = \int_{-\infty}^{\infty} \frac{1}{\sqrt{4\pi t}} \exp\left(\frac{-(x - \xi)^2}{4t}\right) g(\xi) d\xi.$$

We now make several observations:

1. *Isotropy.* The fundamental solution is even in x ; i.e., $\Phi(x, t) = \Phi(-x, t)$. The initial solution g spreads out to left and right in an equal manner, or more generally isotropically in higher dimensions. (This is in contrast to the transport equation, where the solution transports in a directional manner.)
2. *Conservation of thermal energy.* The spatial integral of the fundamental solution over $(-\infty, \infty)$ is given by

$$\int_{-\infty}^{\infty} \Phi(x, t) dx = 1.$$

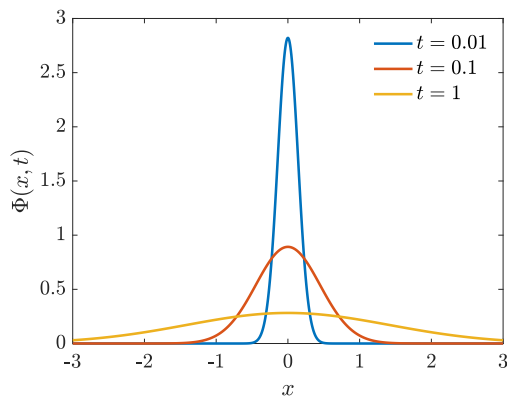


Figure 7.1: Fundamental solution of the heat equation.

Recalling that the spatial integral of the solution over $(a, b) \subset \mathbb{R}$ represents the thermal energy in the domain (a, b) , we conclude that (i) the solution spreads out over time but (ii) the thermal energy is conserved. This is consistent with our understanding of the conservation of thermal energy.

3. *Infinite propagation speed.* The expression (7.4) shows that the solution u at a (space-time) point (x, t) , $t > 0$, depends on the initial solution g everywhere because $\exp(-(x - \xi)^2/(4t))$ is nonzero for all $\xi \in \mathbb{R}$. Conversely, the initial solution g at any point ξ affects solution everywhere and immediately because the function $\exp(-(\xi - x)^2/4t)$ is nonzero everywhere in $\mathbb{R} \times \mathbb{R}_{>0}$. In other words, any change in the initial condition at some point ξ is felt for any x immediately for $t > 0$, regardless of how far apart x and ξ are; i.e., disturbances propagate at infinite speed. (This is in contrast to the finite propagation speed observed for the transport and wave equations.)
4. *Exponential decay of influence.* While any disturbance affects the solution instantaneously everywhere, their effect is quantitatively limited to a short distance over a short time. Namely, if $t \ll 1$, then the exponential in the integrand evaluates to nearly zero except for $\xi \approx x$. Hence

$$u(x, t) \approx \frac{1}{\sqrt{4\pi t}} \int_{\xi=x-a}^{x+a} \exp\left(-\frac{(\xi - x)^2}{4t}\right) g(\xi) d\xi.$$

The initial condition $g(x)$ will have a significant effect on the solution $u(\cdot, t)$ only in the vicinity of x for small t .

5. *Positivity.* If $g \geq 0$ but $g \neq 0$ (i.e., $g(x) \geq 0$ for all x and $g(x) > 0$ for some x), then the solution u is positive for *all* points $x \in \mathbb{R}$ and times $t > 0$. In words, if the initial temperature is nonnegative everywhere and positive somewhere, then the temperature is positive everywhere at any later time no matter how small.
6. *Smoothness.* It can be shown that the solution to the heat equation is smooth; the solution is infinitely differentiable in both space and time. The smoothness holds even if the initial condition g is not differentiable. This is consistent with our observation for the solution on a bounded domain obtained using the Fourier series.

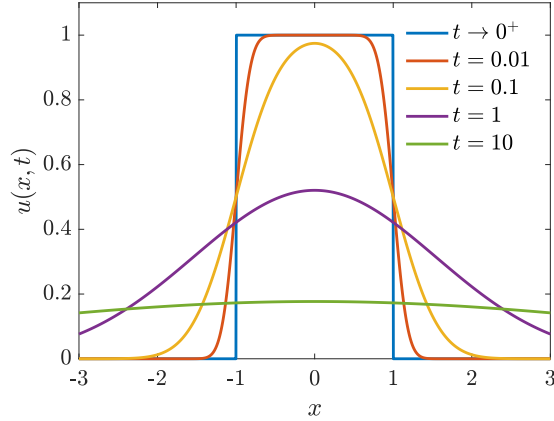


Figure 7.2: The solution to the heat equation with a square initial condition.

Example 7.6 (heat equation on $\mathbb{R} \times \mathbb{R}_{>0}$). Consider the heat equation initial value problem (7.1) with a initial condition

$$g(x) = \begin{cases} 1, & x \in (-1, 1), \\ 0, & \mathbb{R} \setminus (-1, 1). \end{cases}$$

Using the fundamental solution, we can express the solution as

$$u(x, t) = \frac{1}{\sqrt{4\pi t}} \int_{-1}^1 \exp\left(-\frac{(\xi - x)^2}{4t}\right) d\xi.$$

The integration is over $(-1, 1)$ as the initial condition g vanishes outside of this interval. Figure 7.2 shows the solution to the heat equation. We readily confirm some of the observations we made earlier. Even though the initial condition is discontinuous, the solution diffuses quickly and is smooth for $t > 0$. While the solution is formally positive everywhere for any $t > 0$ (i.e., infinite propagation speed), quantitatively the effect of the initial condition decays exponentially away from $x = \pm 1$.

Remark 7.7. Fundamental solutions also exist in $\mathbb{R}^n \times \mathbb{R}_{>0}$ for $n > 1$; see Appendix 7.B.

7.5 Heat equation in $\mathbb{R}_{>0} \times \mathbb{R}_{>0}$: homogeneous Dirichlet

We now consider heat equation on the positive half of the real line $\mathbb{R}_{>0}$:

$$\begin{aligned} \frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} &= 0 && \text{in } \mathbb{R}_{>0} \times \mathbb{R}_{>0}, \\ u &= 0 && \text{on } \{x = 0\} \times \mathbb{R}_{>0}, \\ u &= g && \text{on } \mathbb{R}_{\geq 0} \times \{t = 0\}, \\ |u(x, t)| &< \infty && \text{as } x \rightarrow \infty. \end{aligned} \tag{7.5}$$

We seek the solution using the *method of reflection*. The idea is to identify a problem on the entire real line \mathbb{R} whose solution restricted to $\mathbb{R}_{>0}$ solves the problem (7.5) on the half line. To find the

equivalent problem on \mathbb{R} , we recall a key fact: if a function is (i) continuous and (ii) odd, then the function vanishes at $x = 0$. The continuity requirement is satisfied for any solution to the heat equation because the solution is smooth (i.e., infinitely differentiable). We hence wish to find a problem on \mathbb{R} whose solution is the odd extension of the solution of (7.5). We achieve this goal by using the initial condition $\tilde{g} : \mathbb{R} \rightarrow \mathbb{R}$ that is the odd extension of $g : \mathbb{R}_{>0} \rightarrow \mathbb{R}$. The resulting problem on the entire real line \mathbb{R} is as follows:

$$\begin{aligned} \frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} &= 0 \quad \text{in } \mathbb{R} \times \mathbb{R}_{>0}, \\ u &= \tilde{g} \quad \text{on } \mathbb{R} \times \{t = 0\}, \\ |u(x, t)| &< \infty \quad \text{as } x \rightarrow \pm\infty \end{aligned}$$

where \tilde{g} is the odd extension of g ,

$$\tilde{g}(x) = \begin{cases} g(x), & x \in \mathbb{R}_{>0}, \\ -g(-x), & x \in \mathbb{R}_{<0}. \end{cases}$$

The associated solution is

$$\begin{aligned} u(x, t) &= \int_{-\infty}^{\infty} \Phi(x - \xi, t) \tilde{g}(\xi) d\xi = \int_0^{\infty} \Phi(x - \xi, t) g(\xi) d\xi - \int_{-\infty}^0 \Phi(x - \xi, t) g(-\xi) d\xi \\ &= \int_0^{\infty} (\Phi(x - \xi, t) - \Phi(x + \xi, t)) g(\xi) d\xi \\ &= \frac{1}{\sqrt{4\pi t}} \int_0^{\infty} \left(\exp\left(\frac{-(x - \xi)^2}{4t}\right) - \exp\left(\frac{-(x + \xi)^2}{4t}\right) \right) g(\xi) d\xi \end{aligned}$$

Because the method of reflection applied to the homogeneous Dirichlet boundary condition is based on the odd extension of the initial condition, the method is also called the *method of odd extensions*.

Example 7.8. We consider the heat equation initial-boundary value problem (7.5) with the initial condition $g = 1$ on $\mathbb{R}_{>0}$. The solution is

$$u(x, t) = \frac{1}{\sqrt{4\pi t}} \int_0^{\infty} \left(\exp\left(\frac{-(x - \xi)^2}{4t}\right) - \exp\left(\frac{-(x + \xi)^2}{4t}\right) \right) d\xi.$$

We substitute $z = (x - \xi)/\sqrt{4t}$ and $z = (x + \xi)/\sqrt{4t}$ to the first and second integrals, respectively, and obtain

$$\begin{aligned} u(x, t) &= \frac{1}{\sqrt{\pi}} \left(\int_{-\infty}^{x/\sqrt{4t}} \exp(-z^2) dz - \int_{x/\sqrt{4t}}^{\infty} \exp(-z^2) dz \right) \\ &= \frac{1}{\sqrt{\pi}} \int_{-x/\sqrt{4t}}^{x/\sqrt{4t}} \exp(-z^2) dz \equiv \operatorname{erf}(x/\sqrt{4t}); \end{aligned}$$

here the first equality follows from the aforementioned substitution, the second equality follows from the symmetry of the integrand and the cancellation of the integrals over $(-\infty, -x/\sqrt{4t})$ and $(x/\sqrt{4t}, \infty)$, and the last equality follows from the definition of the *error function*.

Figure 7.3 shows the odd periodic extension on the entire \mathbb{R} . We make a few observations, the latter three of which reiterate our earlier observation about the solution of the heat equation (on $\mathbb{R} \times \mathbb{R}_{>0}$).

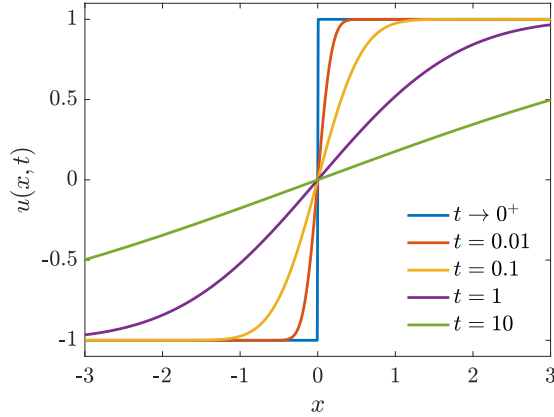


Figure 7.3: Solution of Example 7.8.

1. The solution attains $v(x = 0, t) = 0$ for all $t \in [0, \infty)$, and the homogeneous Dirichlet boundary condition is satisfied.
2. *Smoothness.* The discontinuity in the initial condition disappears immediately. The solution is infinitely differentiable for $t > 0$.
3. *Infinite propagation speed.* The discontinuity affects the solution immediately and everywhere. The disturbance propagates at infinite speed.
4. *Exponential decay of influence.* However, quantitatively, only the solution in the region $|x| \lesssim \sqrt{4t}$ sees significant deviation from the initial condition; significant impact of the diffusion process is only felt in this region, and the width of the region grows as $\sqrt{4t}$.

7.6 Heat equation in $\mathbb{R}_{>0} \times \mathbb{R}_{>0}$: homogeneous Neumann

We now consider heat equation on a half line $\mathbb{R}_{>0}$:

$$\begin{aligned}
 \frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} &= 0 && \text{in } \mathbb{R}_{>0} \times \mathbb{R}_{>0}, \\
 \frac{\partial u}{\partial x} &= 0 && \text{on } \{x = 0\} \times \mathbb{R}_{>0}, \\
 u &= g && \text{on } \mathbb{R}_{\geq 0} \times \{t = 0\}, \\
 |u(x, t)| &< \infty && \text{as } x \rightarrow \infty.
 \end{aligned} \tag{7.6}$$

We again seek the solution using the method of reflection; i.e., we seek a problem on the entire \mathbb{R} whose solution restricted to the half line $\mathbb{R}_{>0}$ is the solution to the homogeneous Neumann problem. We recall a key fact: any continuously differentiable and even function has a vanishing derivative at $x = 0$. The continuously differentiable requirement is satisfied for any solution to the heat equation because the solution is smooth (i.e., infinitely differentiable). We hence wish to find a problem on \mathbb{R} whose solution is an even extension of the solution to the homogeneous Neumann problem. To this end, we recast the problem on the entire \mathbb{R} whose initial condition is the even extension of the

initial condition g . (Note that, to ensure the derivative (instead of the value) vanishes at $x = 0$, we consider the even (instead of the odd) extension.)

The resulting problem on the entire real line \mathbb{R} is

$$\begin{aligned} \frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} &= 0 \quad \text{in } \mathbb{R} \times \mathbb{R}_{>0}, \\ u &= \tilde{g} \quad \text{on } \mathbb{R} \times \{t = 0\}, \\ |u(x, t)| &< \infty \quad \text{as } x \rightarrow \pm\infty, \end{aligned} \tag{7.7}$$

where \tilde{g} is the even extension of g ,

$$\tilde{g}(x) = \begin{cases} g(x), & x \in \mathbb{R}_{>0}, \\ g(-x), & x \in \mathbb{R}_{<0}. \end{cases}$$

The associated solution is

$$\begin{aligned} u(x, t) &= \int_0^\infty (\Phi(x - \xi, t) + \Phi(x + \xi, t))g(\xi)d\xi \\ &= \frac{1}{\sqrt{4\pi t}} \int_0^\infty \left(\exp\left(\frac{-(x - \xi)^2}{4t}\right) + \exp\left(\frac{-(x + \xi)^2}{4t}\right) \right) g(\xi)d\xi. \end{aligned}$$

The method of reflection applied to the homogeneous Neumann problem is also called the *method of even extension*. We can readily verify the earlier observations about (i) smoothness and (ii) infinite propagation speed.

7.7 Nonhomogeneous problems and Duhamel's principle

We now consider the solution of nonhomogeneous problems of the form

$$\begin{aligned} \frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} &= f \quad \text{in } \mathbb{R} \times \mathbb{R}_{>0}, \\ u &= g \quad \text{on } \mathbb{R} \times \{t = 0\}. \end{aligned} \tag{7.8}$$

We immediately note that, by the linearity of the PDE, the solution can be decomposed into $u = w + v$, where w satisfies the homogeneous heat equation with a nontrivial initial condition

$$\begin{aligned} \frac{\partial w}{\partial t} - \frac{\partial^2 w}{\partial x^2} &= 0 \quad \text{in } \mathbb{R} \times \mathbb{R}_{>0}, \\ w &= g \quad \text{on } \mathbb{R} \times \{t = 0\}. \end{aligned} \tag{7.9}$$

and v satisfies the nonhomogeneous heat equation with the trivial initial condition

$$\begin{aligned} \frac{\partial v}{\partial t} - \frac{\partial^2 v}{\partial x^2} &= f \quad \text{in } \mathbb{R} \times \mathbb{R}_{>0}, \\ v &= 0 \quad \text{on } \mathbb{R} \times \{t = 0\}. \end{aligned} \tag{7.10}$$

We have already seen how to solve (7.9) in previous sections; we hence focus on the solution of (7.10). One approach to solve the problem is to appeal to *Duhamel's principle*:

Theorem 7.9 (Duhamel's principle for the heat equation). Let $u : \mathbb{R} \times \mathbb{R}_{>0} \rightarrow \mathbb{R}$ be the solution to the initial value problem

$$\begin{aligned} \frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} &= f \quad \text{in } \mathbb{R} \times \mathbb{R}_{>0}, \\ u &= 0 \quad \text{on } \mathbb{R} \times \{t = 0\}, \end{aligned}$$

for some source function $f : \mathbb{R} \times \mathbb{R}_{>0} \rightarrow \mathbb{R}$. For any fixed $s \in \mathbb{R}_{>0}$, let $u^s : \mathbb{R} \times \mathbb{R}_{>s} \rightarrow \mathbb{R}$ be the solution to

$$\begin{aligned} \frac{\partial u^s}{\partial t} - \frac{\partial^2 u^s}{\partial x^2} &= 0 \quad \text{in } \mathbb{R} \times \mathbb{R}_{>s}, \\ u^s &= f(\cdot, s) \quad \text{on } \mathbb{R} \times \{t = s\}. \end{aligned}$$

Then, the solution $u : \mathbb{R} \times \mathbb{R}_{>0}$ is given by

$$u(x, t) = \int_{s=0}^t u^s(x, t) ds, \quad x \in \mathbb{R}, \quad t \in \mathbb{R}_{>0}. \quad (7.11)$$

Proof. We differentiate (7.11) in time to obtain

$$\frac{\partial u}{\partial t}(x, t) = \lim_{s \rightarrow t} u^s(x, t) + \int_{s=0}^t \frac{\partial u^s}{\partial t}(x, t) ds = f(x, t) + \int_{s=0}^t \frac{\partial u^s}{\partial t}(x, t) ds.$$

Similarly we apply the spatial differential operator to obtain

$$\frac{\partial^2 u}{\partial x^2}(x, t) = \int_{s=0}^t \frac{\partial^2 u^s}{\partial x^2}(x, t) ds = \int_{s=0}^t \frac{\partial u^s}{\partial t}(x, t) ds$$

It follows that

$$\frac{\partial u}{\partial t}(x, t) - \frac{\partial^2 u}{\partial x^2}(x, t) = f(x, t) + \int_{s=0}^t \frac{\partial u^s}{\partial t}(x, t) ds - \int_{s=0}^t \frac{\partial u^s}{\partial t}(x, t) ds = f(x, t),$$

and hence the solution (7.11) satisfies the PDE. We also observe that

$$u(x, t = 0) = \int_{s=0}^{t=0} u^s(x, t = 0) ds = 0, \quad x \in \mathbb{R},$$

as $u^s(\cdot, t = 0) = f(\cdot, s)$ is bounded, and hence the solution satisfies the homogeneous initial condition. \square

Intuitively, Duhamel's principle states that the solution u to nonhomogeneous heat equations can be expressed as a "linear combination" of the solutions $\{u^s\}_{s \in (0, t)}$ to homogeneous heat equations with initial conditions associated with the nonhomogeneous source term f . We note that each solution $u^s : \mathbb{R} \times \mathbb{R}_{>s} \rightarrow \mathbb{R}$ can be expressed using the fundamental solution:

$$u^s(x, t) = \int_{\mathbb{R}} \Phi(x - \xi, t - s) f(\xi, s) d\xi.$$

It follows that the solution to (7.10) with the homogeneous initial condition is

$$v(x, t) = \int_{s=0}^t u^s(x, t) ds = \int_{s=0}^t \int_{\mathbb{R}} \Phi(x - \xi, t - s) f(\xi, s) d\xi ds.$$

The complete solution to (7.8) with the initial condition $u(\cdot, t = 0) = g$ is hence

$$\begin{aligned} u(x, t) &= \int_{\mathbb{R}} \Phi(x - \xi, t) g(\xi) d\xi + \int_{s=0}^t \int_{\mathbb{R}} \Phi(x - \xi, t - s) f(\xi, s) d\xi ds \\ &= \int_{\mathbb{R}} \frac{1}{\sqrt{4\pi t}} \exp\left(-\frac{(x - \xi)^2}{4t}\right) g(\xi) d\xi + \int_{s=0}^t \int_{\mathbb{R}} \frac{1}{\sqrt{4\pi(t - s)}} \exp\left(-\frac{(x - \xi)^2}{4(t - s)}\right) f(\xi, s) d\xi ds. \end{aligned}$$

Remark 7.10. The proof of Duhamel's principle relies only on the linearity of the spatial operator (which is $\frac{\partial^2}{\partial x^2}$ for the heat equation in one dimension). Hence the principle applies to any linear nonhomogeneous PDE in any spatial dimensions.

Example 7.11 (nonhomogeneous heat equation: revisited). In Section 6.5, we considered the solution of nonhomogeneous one-dimensional heat equation using the separation of variables. For homogeneous Dirichlet problems on $\Omega \equiv (0, 1)$ with the initial condition $g = 0$, we found that the solution is given by $u(x, t) = \sum_{n=1}^{\infty} \hat{u}_n(t) \sin(n\pi x)$, where

$$\hat{u}_n(t) = \int_{\tau=0}^t \exp(-n^2\pi^2(t - \tau)) \hat{f}_n(\tau) d\tau,$$

and $\hat{f}_n(\tau)$ are the Fourier sine coefficients of the source function $f(\cdot, \tau)$.

We can derive the same relationship using the Duhamel's principle. To see this, we first recall that the solution to the homogeneous heat equation for any fixed $s \in \mathbb{R}_{>0}$,

$$\begin{aligned} \frac{\partial u^s}{\partial t} - \frac{\partial^2 u^s}{\partial x^2} &= 0 \quad \text{in } (0, 1) \times \mathbb{R}_{>s}, \\ u^s &= 0 \quad \text{on } \{0, 1\} \times \mathbb{R}_{>s}, \\ u^s &= f(\cdot, s) \quad \text{on } (0, 1) \times \{t = s\}, \end{aligned}$$

is given by

$$u^s(x, t) = \sum_{n=1}^{\infty} \hat{f}_n(s) \exp(-n^2\pi^2(t - s)) \sin(n\pi x).$$

We now appeal to Duhamel's principle to observe that

$$u(x, t) = \int_{s=0}^t u^s(x, s) ds = \sum_{n=1}^{\infty} \underbrace{\left(\int_{s=0}^t \exp(-n^2\pi^2(t - s)) \hat{f}_n(s) ds \right)}_{\hat{u}_n(t)} \sin(n\pi x),$$

which is identical to the expression obtained in Section 6.5 through an explicit manipulation of the Fourier sine series coefficients.

7.8 Nonhomogeneous boundary conditions

We now consider the solution of nonhomogeneous heat equations on a half line $\mathbb{R}_{>0}$ with nonhomogeneous boundary conditions. Our approach is similar to the approach we used to treat nonhomogeneous boundary conditions on bounded domains using separation of variables in Section 6.6.

We first consider the case with a nonhomogeneous Dirichlet boundary condition:

$$\begin{aligned}\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} &= f \quad \text{in } \mathbb{R}_{>0} \times \mathbb{R}_{>0}, \\ u &= h \quad \text{on } \{x = 0\} \times \mathbb{R}_{>0}, \\ u &= g \quad \text{on } \mathbb{R}_{\geq 0} \times \{t = 0\},\end{aligned}\tag{7.12}$$

where $f : \mathbb{R}_{>0} \times \mathbb{R}_{>0} \rightarrow \mathbb{R}$ is the source function, $h : \mathbb{R}_{>0} \rightarrow \mathbb{R}$ is the boundary function, and $g : \mathbb{R}_{>0} \rightarrow \mathbb{R}$ is the initial condition. We decompose the solution into two parts:

$$u(x, t) = v(x, t) + h(t);$$

note that the second term matches the boundary condition for all t , and hence the first term vanishes on the boundary. (Here $h(t)$ plays the role of u^b in Section 6.6.) The substitution of the decomposition into (7.12) yields another IBVP for $v : \mathbb{R}_{>0} \times \mathbb{R}_{>0} \rightarrow \mathbb{R}$:

$$\begin{aligned}\frac{\partial v}{\partial t} - \frac{\partial^2 v}{\partial x^2} &= f - \frac{dh}{dt} \quad \text{in } \mathbb{R}_{>0} \times \mathbb{R}_{>0}, \\ v &= 0 \quad \text{on } \{x = 0\} \times \mathbb{R}_{>0}, \\ v &= g - h \quad \text{on } \mathbb{R}_{\geq 0} \times \{t = 0\}.\end{aligned}$$

This is a nonhomogeneous heat equation with a homogeneous Dirichlet boundary condition, which can be solved using Duhamel's principle and fundamental solution as shown in Section 7.7.

We next consider the case with a nonhomogeneous Neumann boundary condition:

$$\begin{aligned}\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} &= f \quad \text{in } \mathbb{R}_{>0} \times \mathbb{R}_{>0}, \\ \frac{\partial u}{\partial x} &= h \quad \text{on } \{x = 0\} \times \mathbb{R}_{>0}, \\ u &= g \quad \text{on } \mathbb{R}_{\geq 0} \times \{t = 0\},\end{aligned}\tag{7.13}$$

where $f : \mathbb{R}_{>0} \times \mathbb{R}_{>0} \rightarrow \mathbb{R}$ is the source function, $h : \mathbb{R}_{>0} \times \mathbb{R}$ is the boundary derivative function, and $g : \mathbb{R}_{>0} \rightarrow \mathbb{R}$ is the initial condition. In this case, we consider the decomposition

$$u(x, t) = v(x, t) + xh(t);$$

the second term matches the nonhomogeneous Neumann boundary condition for all t , and hence the first term satisfies homogeneous Neumann boundary condition on the boundary. The substitution of the decomposition into (7.13) yields another IBVP for $v : \mathbb{R}_{>0} \times \mathbb{R}_{>0} \rightarrow \mathbb{R}$:

$$\begin{aligned}\frac{\partial v}{\partial t} - \frac{\partial^2 v}{\partial x^2} &= f - x \frac{dh}{dt} \quad \text{in } \mathbb{R}_{>0} \times \mathbb{R}_{>0}, \\ \frac{\partial v}{\partial x} &= 0 \quad \text{on } \{x = 0\} \times \mathbb{R}_{>0}, \\ v &= g - xh \quad \text{on } \mathbb{R}_{\geq 0} \times \{t = 0\},\end{aligned}$$

This is a nonhomogeneous heat equation with a homogeneous Neumann boundary condition, which again can be solved using Duhamel's principle and fundamental solution as shown in Section 7.7.

We conclude the section with an example with a nonhomogeneous Dirichlet boundary condition.

Example 7.12. Consider the heat equation on a half line,

$$\begin{aligned} \frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} &= 0 && \text{in } \mathbb{R}_{>0} \times \mathbb{R}_{>0}, \\ u &= 1 && \text{on } \{x = 0\} \times \mathbb{R}_{>0}, \\ u &= 0 && \text{on } \mathbb{R}_{\geq 0} \times \{t = 0\}, \end{aligned} \tag{7.14}$$

Our initial condition is the zero solution, and we impose the boundary condition of $u = 1$ at $x = 0$; we hence intuitively expect the temperature to increase with time, and the “warm region” to spread with time.

We recognize $h(t) = 1$ and decompose the solution u as

$$u(x, t) = v(x, t) + 1.$$

The substitution of the decomposition into (7.14) yields an IBVP for $v : \mathbb{R}_{>0} \times \mathbb{R}_{>0} \rightarrow \mathbb{R}$:

$$\begin{aligned} \frac{\partial v}{\partial t} - \frac{\partial^2 v}{\partial x^2} &= 0 && \text{in } \mathbb{R}_{>0} \times \mathbb{R}_{>0}, \\ v &= 0 && \text{on } \{x = 0\} \times \mathbb{R}_{>0}, \\ v &= -1 && \text{on } \mathbb{R}_{\geq 0} \times \{t = 0\}. \end{aligned}$$

This problem was considered in Example 7.8, and it has the solution

$$v(x, t) = -\operatorname{erf}(x/\sqrt{4t}).$$

Hence the solution to our original problem (7.14) is given by

$$u(x, t) = 1 - \operatorname{erf}(x/\sqrt{4t}) = \operatorname{erfc}(x/\sqrt{4t}).$$

We now make a few observations about the solutions v and u :

1. *Smoothness.* The inconsistency in the initial and boundary conditions at $(x, t) = (0, 0)$ disappears immediately. The solution is infinitely differentiable for $t > 0$.
2. *Infinite propagation speed.* The inconsistency affects the solution immediately and everywhere. The disturbance propagates at infinite speed.
3. *Exponential decay of influence.* However, quantitatively, only the solution in the region $x \lesssim \sqrt{4t}$ sees significant deviation from the initial condition; significant impact of the diffusion process is only felt in this region, and the width of the region grows as $\sqrt{4t}$.

7.9 Summary

We summarize key points of this lecture:

1. Fourier integral is a “generalization” of Fourier series to non-periodic functions on the entire \mathbb{R} .

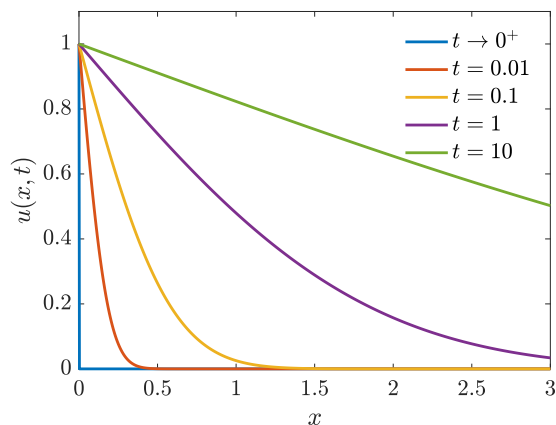


Figure 7.4: Solution to the heat equations initial-boundary value problem (7.14).

2. The solution to the heat equation on \mathbb{R} can be expressed as a convolution of the initial condition and the fundamental solution (i.e., the heat kernel).
3. Important properties of the heat kernel include isotropy, conservation of thermal energy, infinite propagation speed, exponential decay of influence, positivity, and smoothness.
4. The solution to the heat equation on $\mathbb{R}_{>0}$ with homogeneous Dirichlet boundary condition can be found using the method of odd extension, which belongs to a family of reflection methods.
5. The solution to the heat equation on $\mathbb{R}_{>0}$ with homogeneous Neumann boundary condition can be found using the method of even extension.
6. Duhamel's principle can be used to express the solution to nonhomogeneous heat equation as a linear combination of a family of solutions to homogeneous heat equations with particular initial conditions.
7. Nonhomogeneous boundary conditions can be treated by decomposing the solution into a (known) boundary function that satisfies the boundary condition and an auxiliary solution. The solution to the auxiliary problem, with homogeneous boundary conditions, can be obtained using Duhamel's principle and the fundamental solution.

7.A “Derivation” of Fourier integrals

We note that the following “derivation” of Fourier integrals is not rigorous; nevertheless it provides the correct final expression for Fourier integrals. We first analyze the constant term of the Fourier series:

$$f_0(x) \equiv a_0 \equiv \frac{1}{L} \int_{-L}^L f(x) dx \leq \frac{1}{L} \int_{-L}^L |f(x)| dx \xrightarrow{L \rightarrow \infty} 0,$$

where we have used the fact that the integral of f over \mathbb{R} is finite. (Not that if $\int_{\mathbb{R}} |f(x)| dx$ is finite, then $\frac{1}{2L} \int_{-L}^L |f(x)| dx \rightarrow 0$ as $L \rightarrow \infty$.) We next analyze the cosine terms of the Fourier series:

$$f_c(x) \equiv \sum_{n=1}^{\infty} \left(\frac{1}{L} \int_{-L}^L \cos(n\pi\xi/L) f(\xi) d\xi \right) \cos(n\pi x/L),$$

where ξ is a “dummy variable” for the integration to avoid conflation with “ x ”. We now consider the change of variables $\lambda_n \equiv n\pi/L$ and note $\Delta\lambda \equiv \lambda_{n+1} - \lambda_n = \pi/L$ to obtain

$$f_c(x) \equiv \sum_{n=1}^{\infty} \Delta\lambda \left(\frac{1}{\pi} \int_{-L}^L \cos(\lambda_n \xi) f(\xi) d\xi \right) \cos(\lambda_n x).$$

We interpret the sum as a Riemann sum and take $L \rightarrow \infty$ (and hence $\Delta\lambda \rightarrow 0$) to replace the sum with an integral and obtain

$$f_c(x) \equiv \int_{\lambda=0}^{\infty} \left(\frac{1}{\pi} \int_{-\infty}^{\infty} \cos(\lambda\xi) f(\xi) d\xi \right) \cos(\lambda x) d\lambda.$$

We can apply the same transformation to the sine terms of the Fourier series to obtain

$$f_s(x) \equiv \int_{\lambda=0}^{\infty} \left(\frac{1}{\pi} \int_{-\infty}^{\infty} \sin(\lambda\xi) f(\xi) d\xi \right) \sin(\lambda x) d\lambda.$$

We again note that the above “derivation” is not rigorous; however, it leads us to the following (correct) definition of Fourier integral.

7.B Fundamental solution in $\mathbb{R}^n \times \mathbb{R}_{>0}$

The idea of fundamental solution readily extends to higher spatial dimension. We here omit the derivation and state the key results

Definition 7.13 (fundamental solution of the heat equation in \mathbb{R}^n). The fundamental solution of the heat equation $\frac{\partial u}{\partial t} - \Delta u = 0$ in \mathbb{R}^n is

$$\Phi(x, t) \equiv \begin{cases} \frac{1}{(4\pi t)^{n/2}} \exp\left(-\frac{|x|^2}{4t}\right), & t > 0 \\ 0, & t < 0. \end{cases}$$

We verify the particular result we derived for \mathbb{R}^1 is a specialization of this general result to $n = 1$. We now consider the initial value problem

$$\begin{aligned}\frac{\partial u}{\partial t} - \Delta u &= 0 && \text{in } \mathbb{R}^n \times \mathbb{R}_{>0}, \\ u &= g && \text{on } \mathbb{R}^n \times \{t = 0\}, \\ |u| &< \infty && \text{in } \mathbb{R}^n \times \mathbb{R}_{>0}.\end{aligned}$$

Analogously to the problem on $\mathbb{R} \times \mathbb{R}_{>0}$, the solution to this problem on $\mathbb{R}^n \times \mathbb{R}_{>0}$ can be expressed using the fundamental solution:

$$u(x, t) = \int_{\mathbb{R}^n} \Phi(x - \xi, t) g(\xi) d\xi = \int_{\mathbb{R}^n} \frac{1}{(4\pi t)^{n/2}} \exp\left(-\frac{|x - \xi|^2}{4t}\right) g(\xi) d\xi. \quad (7.15)$$

We can readily show that the the four observations we have made about the solution of the heat equation in \mathbb{R}^1 — smoothness, infinite propagation speed, exponential decay of influence, and positivity — also hold for the heat equation in \mathbb{R}^n ; the observations follow from the form of the fundamental solution.

Lecture 8

Heat equation: finite difference method

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8.1 Motivation

We have so far considered analytical approaches to “solve” for — or more precisely represent — the solution to the heat equation: separation of variables and fundamental solutions. While the analytical representations are useful in understanding properties of the PDE, they cannot readily treat general heat equations involving variable coefficients and general domains, which are frequently encountered in science and engineering. In practice, these more general initial-boundary value problems are solved — or more precisely approximated — using *numerical methods*. In this lecture we consider numerical approximation of the heat equation. For simplicity, we consider a one-dimensional heat equation; we will later consider the treatment of higher-dimensional problems.

8.2 Model equation

Throughout this lecture, we consider a initial-boundary value problem defined on spatial domain $\Omega \equiv (x_L, x_R)$ and the time interval $I \equiv (0, t_f]$,

$$\begin{aligned}\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} &= f \quad \text{in } (x_L, x_R) \times (0, t_f], \\ u &= h_L \quad \text{on } \{x = x_L\} \times (0, t_f], \\ \frac{\partial u}{\partial x} &= h_R \quad \text{on } \{x = x_R\} \times (0, t_f], \\ u &= g \quad \text{on } [x_L, x_R] \times \{t = 0\},\end{aligned}$$

where the functions $f : \Omega \times I \rightarrow \mathbb{R}$, $g : \Omega \rightarrow \mathbb{R}$, $h_L : I \rightarrow \mathbb{R}$, and $h_R : I \rightarrow \mathbb{R}$ depend on space and/or time in an arbitrary manner. We consider a problem with Dirichlet and Neumann boundary conditions on the left and right boundary, respectively, to demonstrate the treatment of these two different boundary conditions.

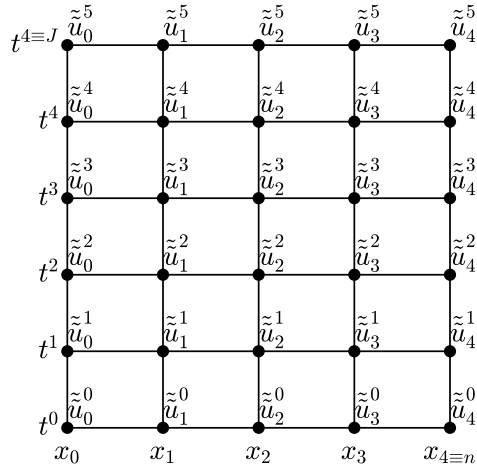


Figure 8.1: Space-time finite difference grid for one-dimensional heat equation for $n = 4$ and $J = 5$.

8.3 Discretization in space and time

To approximate the solution to the heat equation, we first *discretize* our space-time domain $(x_L, x_R) \times (0, t_f)$. To this end, we introduce the spatial computation grid comprises $n + 1$ points:

$$x_L \equiv x_0 < x_1 < \cdots < x_{n-1} < x_n \equiv x_R.$$

For simplicity we assume that the grid points are equispaced so that

$$x_i = i\Delta x, \quad i = 0, 1, \dots, n,$$

where $\Delta x \equiv (x_R - x_L)/n$. We similarly introduce a temporal computational grid comprises $J + 1$ points:

$$0 \equiv t^0 < t^1 < \cdots < t^{J-1} < t^J \equiv t_f.$$

For simplicity, we again assume that time intervals are equispaced so that

$$t^j = j\Delta t, \quad j = 0, 1, \dots, J,$$

where $\Delta t \equiv t_f/J$. Our goal is to approximate the solution at the space-time grid points $u(x_i, t^j)$ by a computational approximation \tilde{u}_i^j so that

$$u(x_i, t^j) \approx \tilde{u}_i^j, \quad i = 0, \dots, n, \quad j = 0, \dots, J.$$

Figure 8.1 shows the space-time finite difference grid. We now introduce *finite difference method* in space and time to approximate the solution at the grid points.

(While we will not consider non-equispaced grids or time intervals in this lecture, finite difference methods readily extend to these cases. In fact, adaptive and non-equispaced grids and time intervals can greatly improve the efficiency of the method for some problems.)

8.4 Finite difference in space

The numerical approximation of PDEs requires the approximation of the (spatial) derivatives that appear in the PDEs. To this end, we introduce a generic function $f : [x_L, x_R] \rightarrow \mathbb{R}$ and illustrate an approach to estimate its derivative at a set of points. Specifically, given the function values at the grid points x_0, \dots, x_n we wish to approximate the derivative at the same set of points. We first introduce an approximation of the first derivative:

Definition 8.1 (first-derivative central difference formula). The first-derivative central difference formula is

$$f'(x_i) \approx \frac{f_{i+1} - f_{i-1}}{2\Delta x}, \quad (8.1)$$

where $f_i \equiv f(x_i)$ and $\Delta x = x_{i+1} - x_i = x_i - x_{i-1}$.

This is an example of a *finite difference formula*, in which the derivative is approximated by a finite number of differences on a finite grid. Note that in the limit of $\Delta x \rightarrow 0$, the formula provides the definition of the derivative. We now formally analyze the *truncation error*.

Proposition 8.2. Given a thrice continuously differentiable function f ,

$$\left| f'(x_i) - \frac{f_{i+1} - f_{i-1}}{2\Delta x} \right| \leq \frac{1}{6} \max_{\xi \in [x_{i-1}, x_{i+1}]} |f'''(\xi)| \Delta x^2,$$

where $f_i \equiv f(x_i)$ and $\Delta x = x_{i+1} - x_i = x_i - x_{i-1}$. The formula is *second-order accurate*; i.e., the error E is bounded by $E < C\Delta x^2$ for some C independent of Δx , and in particular it depends on the *square* of the grid spacing Δx .

Proof. We consider Taylor series expansion of f_{i+1} and f_{i-1} about x_i to obtain

$$\begin{aligned} \frac{f_{i+1} - f_{i-1}}{2\Delta x} &= \frac{1}{2\Delta x} (f_i + f'_i \Delta x + \frac{1}{2} f''_i \Delta x^2 + \frac{1}{6} f'''(\xi_1) \Delta x^3 - (f_i - f'_i \Delta x + \frac{1}{2} f''_i \Delta x^2 - \frac{1}{6} f'''(\xi_2) \Delta x^3)) \\ &= \frac{1}{2\Delta x} (2f'_i \Delta x + \frac{1}{6} (f'''(\xi_1) + f'''(\xi_2)) \Delta x^3) = f'_i + \frac{1}{12} (f'''(\xi_1) + f'''(\xi_2)) \Delta x^2 \end{aligned}$$

for some $\xi_1 \in [x_{i-1}, x_i]$ and $\xi_2 \in [x_i, x_{i+1}]$. It follows that

$$\left| f'_i - \frac{f_{i+1} - f_{i-1}}{2\Delta x} \right| = \frac{1}{12} |f'''(\xi_1) + f'''(\xi_2)| \Delta x^2 \leq \frac{1}{6} \max_{\xi \in [x_{i-1}, x_{i+1}]} |f'''(\xi)| \Delta x^2,$$

which is the desired relationship. \square

We can similarly approximate the second derivative using the finite difference method.

Definition 8.3 (second-derivative central difference formula). The second-derivative central difference formula is

$$f''(x_i) \approx \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2}, \quad (8.2)$$

where $f_i \equiv f(x_i)$ and $\Delta x = x_{i+1} - x_i = x_i - x_{i-1}$.

The denominator scales with Δx^2 for the second derivative (as opposed to Δx for the first derivative); perhaps this is not too surprising if we consider the definition of the derivative and the limit. We now formally analyze the truncation error.

Proposition 8.4. Given a function f with a continuous fourth derivative,

$$\left| f_i'' - \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2} \right| \leq \frac{1}{12} \max_{\xi \in [x_{i-1}, x_{i+1}]} |f^{(4)}(\xi)| \Delta x^2,$$

where $f_i \equiv f(x_i)$ and $\Delta x = x_{i+1} - x_i = x_i - x_{i-1}$. The formula is *second-order accurate*.

Proof. We express f_{i+1} , $-2f_i$, and f_{i-1} using Taylor series expansions:

$$\begin{aligned} f_{i+1} &= f_i + f_i' \Delta x + \frac{1}{2} f_i'' \Delta x^2 + \frac{1}{6} f_i''' \Delta x^3 + \frac{1}{24} f^{(4)}(\xi_1) \Delta x^4 \\ -2f_i &= -2f_i \\ f_{i-1} &= f_i - f_i' \Delta x + \frac{1}{2} f_i'' \Delta x^2 - \frac{1}{6} f_i''' \Delta x^3 + \frac{1}{24} f^{(4)}(\xi_2) \Delta x^4 \end{aligned}$$

for some $\xi_1 \in [x_i, x_{i+1}]$ and $\xi_2 \in [x_{i-1}, x_i]$. We sum the equations to obtain

$$f_{i+1} - 2f_i + f_{i-1} = f_i'' \Delta x^2 + \frac{1}{24} [f^{(4)}(\xi_1) + f^{(4)}(\xi_2)] \Delta x^4;$$

note in particular that the odd-order terms cancel due to the symmetry. We finally note

$$\left| f_i'' - \frac{f_{i+1} - 2f_i + f_{i-1}}{\Delta x^2} \right| = \frac{1}{24} [f^{(4)}(\xi_1) + f^{(4)}(\xi_2)] \Delta x^2 \leq \frac{1}{12} \max_{s \in [x_{i-1}, x_{i+1}]} |f^{(4)}(s)| \Delta x^2,$$

which is the desired relationship. □

In general, it is possible to construct finite difference formulas for derivatives of arbitrary order. In addition, it is possible to construct finite difference formulas that are accurate to an arbitrary order, in which the error scales as Δx^p for an arbitrarily large p . Higher-order and/or higher-derivative approximations are achieved by including more points $(x_i, f(x_i))$ in the finite difference formula and choosing the associated weights so that more terms of the Taylor series expansion cancel. This can be achieved in a systematic manner using a *Taylor table*.

8.5 Semi-discrete heat equation

We now apply finite difference formulas to approximate the heat equation. In particular, we wish to approximate the value of the solution at nodes x_1, \dots, x_n at time t by

$$\tilde{u}_i(t) \approx u(x_i, t), \quad i = 1, \dots, n, \quad t \in \mathbb{R}_{>0}.$$

Note that our goal is to approximate the solution $u : \Omega \times I \rightarrow \mathbb{R}$ that depends on both space and time by a set of n functions $\tilde{u}_i : I \rightarrow \mathbb{R}$, $i = 1, \dots, n$, associated with the n fixed grid points. To this end, we start with the heat equation

$$\frac{\partial u}{\partial t}(x, t) - \frac{\partial^2 u}{\partial x^2}(x, t) = f(x, t) \quad x \in \Omega, \quad t \in I,$$

and approximate the Laplacian operator, which is the second derivative in space, using the central difference formula (8.2) to obtain the heat equation discretized in space:

$$\frac{d\tilde{u}_i}{dt}(t) - \frac{\tilde{u}_{i+1}(t) - 2\tilde{u}_i(t) + \tilde{u}_{i-1}(t)}{\Delta x^2} = \hat{f}_i(t), \quad t \in I, \quad (8.3)$$

where $\hat{f}_i(t) \equiv f(x_i, t)$. We use $\hat{f}_i(t)$ (instead of $\tilde{f}_i(t)$) to denote the evaluation of f at (x_i, t) because this evaluation is exact at x_i ; this is unlike $\tilde{u}(x_i, t)$, which in general will not equal $u(x_i, t)$ at x_i .

While (8.3) provides appropriate equations for the interior nodes $i = 2, \dots, n-1$, we need to incorporate the boundary conditions for $i = 1$ and n as follows:

1. *Left Dirichlet boundary.* On the left boundary, we wish to impose the Dirichlet boundary condition $u(x = x_L, t) = h_L(t)$. Because the solution at $i = 0$ is “known”, we replace the difference equation (8.3) for $i = 0$ with

$$\tilde{u}_{i=0}(t) = h_L(t).$$

We substitute the expression in the difference equation (8.3) for $i = 1$ to obtain

$$\frac{d\tilde{u}_1}{dt}(t) - \frac{\tilde{u}_2(t) - 2\tilde{u}_1(t) + h_L(t)}{\Delta x^2} = \hat{f}_1(t),$$

which, after some rearrangement, yields

$$\frac{d\tilde{u}_1}{dt}(t) - \frac{\tilde{u}_2(t) - 2\tilde{u}_1(t)}{\Delta x^2} = \hat{f}_1(t) + \frac{h_L(t)}{\Delta x^2}.$$

Note that we have moved the “known” value to the right hand side of the equation so that the left hand side is linear in \tilde{u} .

2. *Right Neumann boundary.* On the right boundary, we wish to impose the Neumann boundary condition $\frac{\partial u}{\partial x}(x = x_R, t) = h_R(t)$. We apply the central finite difference formula for the first derivative at $i = n$ to obtain

$$\frac{\tilde{u}_{n+1}(t) - \tilde{u}_{n-1}(t)}{2\Delta x} = h_R(t) \quad \Rightarrow \quad \tilde{u}_{n+1}(t) = \tilde{u}_{n-1}(t) + 2\Delta x h_R(t).$$

We substitute the relationship to the difference equation (8.3) for $i = n$ to obtain

$$\frac{d\tilde{u}_n}{dt}(t) - \frac{(\tilde{u}_{n-1}(t) + 2\Delta x h_R(t)) - 2\tilde{u}_n(t) + \tilde{u}_{n-1}(t)}{\Delta x^2} = \hat{f}_n(t), \quad t \in \mathbb{R}_{>0}$$

which, after some rearrangement, yields

$$\frac{d\tilde{u}_n}{dt}(t) - \frac{-2\tilde{u}_n(t) + 2\tilde{u}_{n-1}(t)}{\Delta x^2} = \hat{f}_n(t) + \frac{2h_R}{\Delta x}.$$

The finite difference approximation, which incorporates the boundary conditions, is hence given by

$$\begin{aligned} \frac{d\tilde{u}_1}{dt}(t) - \frac{\tilde{u}_2(t) - 2\tilde{u}_1(t)}{\Delta x^2} &= \hat{f}_1(t) + \frac{h_L(t)}{\Delta x^2}, \\ \frac{d\tilde{u}_i}{dt}(t) - \frac{\tilde{u}_{i+1}(t) - 2\tilde{u}_i(t) + \tilde{u}_{i-1}(t)}{\Delta x^2} &= \hat{f}_i(t), \quad i = 2, \dots, n-1, \\ \frac{d\tilde{u}_n}{dt}(t) - \frac{-2\tilde{u}_n(t) + 2\tilde{u}_{n-1}(t)}{\Delta x^2} &= \hat{f}_n(t) + \frac{2h_R(t)}{\Delta x}, \\ \tilde{u}_i(t=0) &= \hat{g}_i, \quad i = 1, \dots, n, \end{aligned} \tag{8.4}$$

where $\hat{g}_i \equiv g(x_i)$, $i = 1, \dots, n$. We make a few observations:

1. The system (8.4) is called a *semi-discrete* form of the heat equation (with appropriate boundary conditions) because the equation is discretized in space but not in time.
2. We have turned the original PDE-based initial-boundary value problem into an initial value problem based on a system of n ODEs, where the unknowns are $u(x_1), \dots, u(x_n)$ (which excludes the left boundary with the known solution).
3. Assuming the solution u is sufficiently regular, this approximation is *second-order accurate in space*; i.e.,

$$|u(x_i, t) - \tilde{u}_i(t)| \leq C\Delta x^2, \quad i = 1, \dots, n, \quad t \in \mathbb{R}_{>0}$$

for some constant $C < \infty$ independent of Δx . Decreasing the grid spacing Δx by a factor of two results in the error to decrease by a factor of four.

The system of ODEs can also be written in matrix form. We first concatenate $\tilde{u}_1(t), \dots, \tilde{u}_n(t)$ as a vector $\tilde{u}(t) \in \mathbb{R}^n$ whose i -th entry is $\tilde{u}_i(t)$. We then seek $\tilde{u} : \mathbb{R}_{>0} \rightarrow \mathbb{R}^n$ such that

$$\begin{aligned} \frac{d\tilde{u}}{dt}(t) + \hat{A}\tilde{u}(t) &= \hat{f}(t) + \hat{h}(t) \quad \text{in } \mathbb{R}^n, \quad t \in \mathbb{R}_{>0}, \\ \tilde{u}(t=0) &= \hat{g} \quad \text{in } \mathbb{R}^n, \end{aligned} \tag{8.5}$$

where $\hat{A} \in \mathbb{R}^{n \times n}$, $\hat{f}(t) \in \mathbb{R}^n$, $\hat{h}(t) \in \mathbb{R}^n$, and $\hat{g} \in \mathbb{R}^n$ are given by

$$\hat{A} = \frac{1}{\Delta x^2} \begin{pmatrix} 2 & -1 & & & & & \\ -1 & 2 & -1 & & & & \\ & & \ddots & \ddots & \ddots & & \\ & & & -1 & 2 & -1 & \\ & & & & -2 & 2 & \end{pmatrix}, \quad \hat{f} = \begin{pmatrix} \hat{f}_1 \\ \hat{f}_2 \\ \vdots \\ \hat{f}_{n-1} \\ \hat{f}_n \end{pmatrix}, \quad \hat{h} = \begin{pmatrix} h_L/\Delta x^2 \\ 0 \\ \vdots \\ 0 \\ 2h_R/\Delta x \end{pmatrix}, \quad \hat{g} = \begin{pmatrix} \hat{g}_1 \\ \hat{g}_2 \\ \vdots \\ \hat{g}_{n-1} \\ \hat{g}_n \end{pmatrix}.$$

The matrix form of the equation allows us to (i) more compactly express our finite difference approximation and (ii) efficiently implement our approximation in a computer program using a language such as MATLAB.

8.6 Temporal discretization

We next wish to apply a time discretization to the semi-discrete form (8.4). There are many time marching methods, but in this lecture we consider the *Crank-Nicolson method*. To this end, we first introduce a initial value problem associated with a system of n ODEs: find $\tilde{u} : I \rightarrow \mathbb{R}^n$ such that

$$\begin{aligned} \frac{d\tilde{u}}{dt}(t) &= F(\tilde{u}(t), t) \quad \text{in } \mathbb{R}^n, \quad t \in I, \\ \tilde{u}(t=0) &= \hat{g} \quad \text{in } \mathbb{R}^n, \end{aligned}$$

where $F : \mathbb{R}^n \times I \rightarrow \mathbb{R}^n$ describes the dynamics of the system, and $\hat{g} \in \mathbb{R}^n$ is the initial condition. We now wish to find a sequence of approximations $\tilde{u}^0, \dots, \tilde{u}^J$ such that

$$\tilde{u}(t^j) \approx \tilde{u}^j, \quad j = 0, \dots, J.$$

The Crank-Nicolson approximation is given by

$$\begin{aligned}\frac{\tilde{u}^j - \tilde{u}^{j-1}}{\Delta t} &= \frac{1}{2} (F(\tilde{u}^j, t^j) + F(\tilde{u}^{j-1}, t^{j-1})) \quad \text{in } \mathbb{R}^n, \quad j = 1, \dots, J, \\ \tilde{u}^{j=0} &= \hat{g} \quad \text{in } \mathbb{R}^n.\end{aligned}$$

As regards the accuracy of the Crank-Nicolson method, we have the following result:

Proposition 8.5. Suppose $\frac{d\tilde{u}}{dt} = F(\tilde{u}, t)$ in \mathbb{R}^n where (i) F is Lipschitz continuous in \tilde{u} and (ii) F is continuous in t . Then the Crank-Nicolson approximation of $\tilde{u}(t^j)$, \tilde{u}^j , satisfies

$$|\tilde{u}(t^j) - \tilde{u}^j| \leq C \max_{s \in [0, t^j]} |\tilde{u}'''(s)| \Delta t^2,$$

where C is independent of Δt .

We make two observations:

1. *Convergence:* $|u(t^j) - \tilde{u}^j| \rightarrow 0$ as $\Delta t \rightarrow 0$ for any t^j and hence the scheme is convergent;
2. *Order of accuracy:* $|u(t^j) - \tilde{u}^j| \leq C\Delta t^2$ and hence the scheme is second order accurate. Decreasing the time step Δt by a factor of two results in the error to decrease by a factor of four.

Remark 8.6. (This discussion is beyond the scope of this course, but we make one remark regarding the stability of time-marching schemes.) The choice of the time-marching scheme is typically governed by three factors: the order of accuracy; the cost; and the *stability* of the scheme. The stability of the scheme dictates the maximum time step Δt that can be used for the scheme to remain numerically stable (i.e., the solution to not “blow up” in time). The Crank-Nicolson method has a nice stability property and remains stable for any choice of Δt , assuming the underlying PDE is stable (which is the case for the heat equation). We just note that the order of accuracy is not the only consideration in choosing a time-marching scheme.

8.7 Fully discrete equation

We now apply the Crank-Nicolson method to the semi-discrete form of the heat equation to obtain a fully discrete equation. We denote the finite difference approximation of the state at position x_i and time t^j by

$$\tilde{u}_i^j \approx u(x_i, t^j), \quad i = 1, \dots, n, \quad j = 1, \dots, J.$$

The application of the backward Euler formula to (8.4) yields

$$\begin{aligned}\frac{\tilde{u}_1^j - \tilde{u}_1^{j-1}}{\Delta t} &= \frac{1}{2} \sum_{k \in \{j-1, j\}} \left(\frac{\tilde{u}_2^k - 2\tilde{u}_1^k}{\Delta x^2} + \hat{f}_1^k + \frac{h_L^k}{\Delta x^2} \right), \quad j = 1, \dots, J, \\ \frac{\tilde{u}_i^j - \tilde{u}_i^{j-1}}{\Delta t} &= \frac{1}{2} \sum_{k \in \{j-1, j\}} \left(\frac{\tilde{u}_{i+1}^k - 2\tilde{u}_i^k + \tilde{u}_{i-1}^k}{\Delta x^2} + \hat{f}_i^k \right), \quad i = 2, \dots, n-1, \quad j = 1, \dots, J, \\ \frac{\tilde{u}_n^j - \tilde{u}_n^{j-1}}{\Delta t} &= \frac{1}{2} \sum_{k \in \{j-1, j\}} \left(\frac{-2\tilde{u}_n^k + 2\tilde{u}_{n-1}^k}{\Delta x^2} + \hat{f}_n^k + \frac{2h_R^k}{\Delta x} \right), \quad j = 1, \dots, J, \\ \tilde{u}_i^{j=0} &= \hat{g}_i, \quad i = 1, \dots, n,\end{aligned} \tag{8.6}$$

where $\hat{f}_i^j = f(x_i, t^j)$, $h_L^j = h_L(t^j)$, and $h_R^j = h_R(t^j)$. We can also write the formulation in a more compact matrix-vector form:

$$\begin{aligned} \frac{\tilde{u}^j - \tilde{u}^{j-1}}{\Delta t} &= \frac{1}{2} \left(-\hat{A}\tilde{u}^j + \hat{f}^j + \hat{h}^j - \hat{A}\tilde{u}^{j-1} + \hat{f}^{j-1} + \hat{h}^{j-1} \right) \quad \text{in } \mathbb{R}^n, \quad j = 1, \dots, J, \\ \tilde{u}^{j=0} &= \hat{g} \quad \text{in } \mathbb{R}^n, \end{aligned}$$

where $\hat{A} \in \mathbb{R}^{n \times n}$, $\hat{f}^j = \hat{f}(t^j) \in \mathbb{R}^n$, and $\hat{h}^j = \hat{h}(t^j) \in \mathbb{R}^n$; the expressions for $\hat{f}(t)$ and $\hat{h}(t)$ are provided in the semi-discrete formulation (8.5). We make a few observations:

1. The system (8.6) is a *fully discrete* form of the heat equation because it is discretized in both space and time.
2. Assuming the solution u is sufficiently regular, the approximation is second-order accurate in both space and time; i.e.,

$$|u(x_i, t^j) - \tilde{u}_i^j| < C\Delta x^2 + D\Delta t^2, \quad i = 1, \dots, n, \quad j = 1, \dots, J,$$

for some constants $C < \infty$ and $D < \infty$. Decreasing both Δx and Δt by a factor of two results in the error to decrease by a factor of four.

3. Because the error is a *sum* of the spatial and temporal errors, it is insufficient to decrease only Δx or Δt . Both Δx and Δt must be decreased to control the error.

8.8 Solution of the fully discrete equation

We can solve the fully discrete equation by marching in time as follows:

0. Initialize the state to $\tilde{u}^{j=0} = \hat{g}$.
1. Update the state by solving a linear system

$$\left(I + \frac{1}{2}\Delta t\hat{A} \right) \tilde{u}^j = \left(I - \frac{1}{2}\Delta t\hat{A} \right) \tilde{u}^{j-1} + \frac{1}{2}\Delta t(\hat{f}^j + \hat{h}^j + \hat{f}^{j-1} + \hat{h}^{j-1}) \quad (8.7)$$

for $\tilde{u}^j \in \mathbb{R}^n$, starting with $j = 1$ and time-marching to $j = J$.

We make a few observations:

1. The matrix $I + \frac{1}{2}\Delta t\hat{A} \in \mathbb{R}^{n \times n}$ is nonsingular for all Δt and hence the linear system has a unique solution.
2. The matrices $I + \frac{1}{2}\Delta t\hat{A} \in \mathbb{R}^{n \times n}$ and $I - \frac{1}{2}\Delta t\hat{A} \in \mathbb{R}^{n \times n}$ are *tridiagonal*. The matrices have nonzero entries only on the diagonal, superdiagonal, and subdiagonal. The matrices can be efficiently stored in $\mathcal{O}(n)$ space by only storing the indices and values of the nonzero entries; this is unlike a general dense $n \times n$ matrix, which requires $\mathcal{O}(n^2)$ space to store.
3. The tridiagonal system can be solved efficiently in $\mathcal{O}(n)$ operations using the Thomas algorithm, which is a specialization of LU factorization (or Gaussian elimination) for a tridiagonal matrix. (A tridiagonal matrix is a special case of a more general *sparse matrix*, which is a matrix whose entries are mostly zero.)

4. While the matrix $I + \frac{1}{2}\Delta t \hat{A}$ is sparse, its inverse $(I + \frac{1}{2}\Delta t \hat{A})^{-1}$ is a dense matrix whose entries are nonzero everywhere. Computing $(I + \frac{1}{2}\Delta t \hat{A})^{-1}$ requires $\mathcal{O}(n^3)$ operations, and storing the matrix requires $\mathcal{O}(n^2)$ space. Hence, the matrix $(I + \frac{1}{2}\Delta t \hat{A})^{-1}$ should never be explicitly formed.
5. More pragmatically, to solve (8.7) using MATLAB, we first store I and A as sparse matrices using the `sparse` command. We then call

$$\tilde{u}^j \leftarrow (I + \frac{1}{2}\Delta t \hat{A}) \setminus ((I - \frac{1}{2}\Delta t \hat{A})\tilde{u}^{j-1} + \frac{1}{2}\Delta t(\hat{f}^j + \hat{h}^j + \hat{f}^{j-1} + \hat{h}^{j-1})),$$

where “ \setminus ” is the backslash operator, which automatically solves the system using the Thomas algorithm for tridiagonal systems. We should *never* use the `inv` function, which is very inefficient.

8.9 Example

We now consider the approximation of the heat equation on $(0, 1) \times (0, 1)$:

$$\begin{aligned} \frac{\partial u}{\partial t}(x, t) - \frac{\partial^2 u}{\partial x^2}(x, t) &= \cos(t/2) \exp(x^2), \quad \forall x \in (0, 1), t \in (0, 1], \\ u(x = 0, t) &= 0, \quad \forall t \in (0, 1], \\ \frac{\partial u}{\partial x}(x = 1, t) &= 0, \quad \forall t \in (0, 1], \\ u(x, t = 0) &= \frac{1}{2} \sin(3\pi x/2), \quad \forall x \in [0, 1]. \end{aligned} \tag{8.8}$$

Figure 8.2 shows the finite difference solution for two different grid spacings Δx and time steps Δt . We note that the arbitrary initial condition and the time-dependent source function can be handled without any difficulty using the numerical method. We also qualitatively observe that the approximation gets finer as Δx decreases.

Table 8.1 shows the maximum error

$$\|u - \tilde{u}\|_\infty \equiv \max_{\substack{i=1, \dots, n \\ j=1, \dots, J}} |u(x_i, t^j) - \tilde{u}_i^j|$$

as a function of Δx and Δt . We make some observations:

1. The solution accuracy can be limited by either the lack of the spatial resolution or the lack of the temporal resolution. We must decrease both Δx and Δt to control the error.
2. If Δt is sufficiently small such that the accuracy is limited by the spatial resolution — i.e., $\Delta t = 1/256$ which is the last column of the table — the error scales as $\mathcal{O}(\Delta x^2)$, which is consistent with the theory for the second-order accurate finite difference method.
3. If Δx is sufficiently small such that the accuracy is limited by the time resolution — i.e., $\Delta x = 1/64$ which is the last row of the table — the error scales as $\mathcal{O}(\Delta t^2)$, which is consistent with the theory for the second-order accurate Crank-Nicolson method.
4. To minimize the computational cost (i.e., the number of grid points or time steps) required to achieve a given accuracy, we wish to choose a combination of Δx and Δt such that the spatial and temporal errors are balanced and neither one is dominating the other.

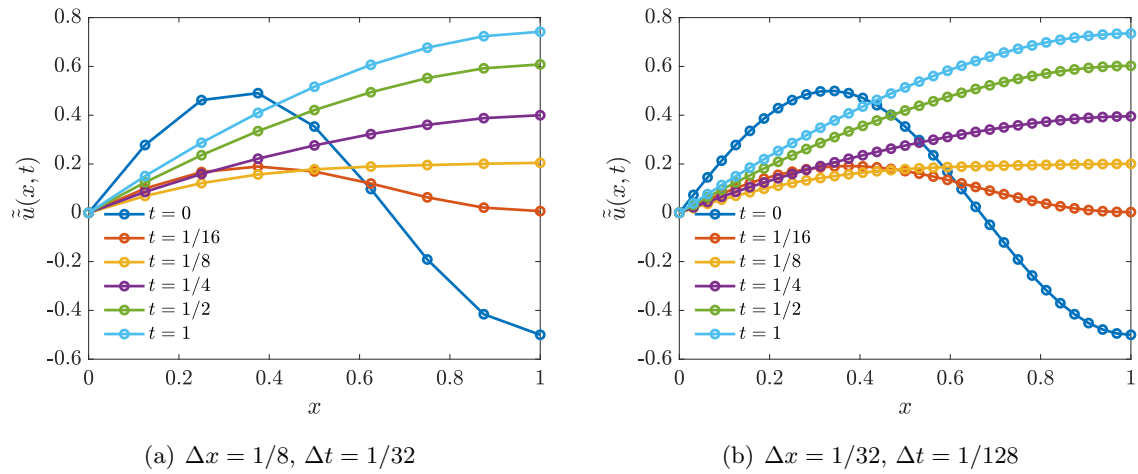


Figure 8.2: Approximation of the heat equation problem (8.8).

	$\Delta t = 1/32$	$\Delta t = 1/64$	$\Delta t = 1/128$	$\Delta t = 1/256$
$\Delta x = 1/8$	7.61×10^{-3}	7.54×10^{-3}	7.53×10^{-3}	7.52×10^{-3}
$\Delta x = 1/16$	7.75×10^{-3}	1.91×10^{-3}	1.89×10^{-3}	1.89×10^{-3}
$\Delta x = 1/32$	8.33×10^{-3}	1.84×10^{-3}	4.77×10^{-4}	4.73×10^{-4}
$\Delta x = 1/64$	8.47×10^{-3}	1.97×10^{-3}	4.48×10^{-4}	2.09×10^{-4}

Table 8.1: Maximum error for the heat equation problem (8.8) as a function of the grid spacing Δx and time stepping Δt .

8.10 Summary

We summarize key points of this lecture:

1. The finite difference method provides an approximation of the solution to the heat equation on a set of grid points in space and instances in time.
2. Given a function f , its derivative evaluated at a grid point x_i can be approximated as a linear combination of f evaluated at a set of grid points. The order of accuracy of the finite difference formula can be analyzed using Taylor series. The number of required grid points depends on the order of the derivative and the order of accuracy.
3. Semi-discrete form of a time-dependent PDE is a system ODEs (initial value problems) that has been discretized in space but remains continuous in time.
4. The semi-discrete equation can be discretized in time using a time marching method (e.g., the Crank-Nicolson method), which yields a fully discrete equation.
5. The fully discrete equation can be solved by starting with $t = 0$ and then marching forward in time. If the backward Euler method is used for the time discretization, we must solve a linear system at each time instance; the linear system can be solved efficiently because it is a sparse matrix.

Part III

Laplace's equation

Lecture 9

Laplace's equation: introduction

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9.1 Introduction

In this lecture we introduce and study Laplace's equation

$$-\Delta u = 0 \quad \text{in } \Omega \subset \mathbb{R}^n$$

and the closely related Poisson's equation

$$-\Delta u = f \quad \text{in } \Omega \subset \mathbb{R}^n$$

for some $f : \Omega \rightarrow \mathbb{R}$. Both equations are ubiquitous in science and engineering, and they are an archetype of elliptic PDEs. Following the approach used for the heat equation, we will first derive a number of properties associated with Laplace's and Poisson's equations without explicitly seeking the solution.

Classification. We recall the classification system introduced in Lecture 1. We immediately observe that Laplace's and Poisson's equations are second-order linear equations. Laplace's equation is homogeneous, while Poisson's equation is nonhomogeneous (for $f \neq 0$). Both equations are also elliptic. To see this, for simplicity we consider $n = 2$ and observe that the matrix associated with the second-order operator $-\Delta = -\frac{\partial^2}{\partial x_1^2} - \frac{\partial^2}{\partial x_2^2}$ is

$$A = \begin{pmatrix} -1 & 0 \\ 0 & -1 \end{pmatrix};$$

the associated eigenvalues are $\lambda_{1,2} = -1$. Because the eigenvalues have the same sign, the equation is elliptic. This argument would hold for an arbitrary n because the A matrix is $A = -I_{n \times n}$.

9.2 Laplace's and Poisson's equations in science and engineering

We provide a few applications of Laplace's and Poisson's equations in science and engineering.

- *Steady heat transfer.* The PDE that describes the steady temperature distribution u is obtained by setting the time derivative term $\frac{\partial u}{\partial t}$ of the heat equation to 0. The resulting equation is Laplace's equation $-\Delta u = 0$ if there is no (volume) heat source and Poisson's equation $-\Delta u = f$ if there is a source term f . We may obtain a boundary value problem by augmenting the PDE with some combination of the boundary conditions discussed in Section 5.3.
- *Steady diffusion.* The steady-state concentration of chemical species dispersed in a medium is described by Laplace's equation. The species concentration $u : \Omega \rightarrow \mathbb{R}$ satisfies the Laplace's equation $-\Delta u = 0$ if there is no volume chemical source and Poisson's equation $-\Delta u = f$ if there is a source term.
- *Potential flow.* Steady, inviscid, incompressible, and irrotational flows can be modeled using the potential flow theory. The velocity potential $\phi : \Omega \rightarrow \mathbb{R}$ satisfies Laplace's equation $-\Delta \phi = 0$. The velocity field is then given by $v = \nabla \phi$.
- *Electrostatics.* The electric field in a linear, isotropic, and homogeneous material is described by Poisson's equation. The electric potential $\phi : \Omega \rightarrow \mathbb{R}$ satisfies Poisson's equation $-\Delta \phi = \rho/\epsilon$, where ρ is the volumetric charge density and ϵ is the permittivity of the medium. The electric field is then given by $E = -\nabla \phi$.

Laplace's equation is also ubiquitous in mathematics, and its solution bears a special name.

Definition 9.1 (harmonic function). Let $\Omega \subset \mathbb{R}^n$. A function $u : \Omega \rightarrow \mathbb{R}$ that satisfies Laplace's equation $-\Delta u = 0$ in Ω is called a harmonic function.

Before we proceed with the solution of Laplace's and Poisson's equations, we make one remark about our choice of the sign. Laplace's and Poisson's equation are sometimes written without the negative sign in front of the differential operator; i.e., $\Delta u = 0$ instead of $-\Delta u = 0$. Throughout this course we will use the convention with the negative sign in front.

9.3 Mean-value formulas

Harmonic functions have a number of special properties. The first property is expressed in *mean value formulas*. (All proofs in this section and following sections should be considered optional.)

Definition 9.2 (ball in \mathbb{R}^n). A ball of radius r and centered at x_0 is an open subset of \mathbb{R}^n given by $B(x_0, r) \equiv \{x \in \mathbb{R}^n \mid \|x - x_0\|_2 < r\}$, where $\|\cdot\|_2$ is the Euclidean norm in \mathbb{R}^n . Its boundary is $\partial B(x_0, r) = \{x \in \mathbb{R}^n \mid \|x - x_0\|_2 = r\}$. The volume of the ball is denoted by $|B(x_0, r)|$, and the surface area of the ball is denoted by $|\partial B(x_0, r)|$.

Example 9.3. In two dimensions, $B(x_0, r)$ is a disk, and $\partial B(x_0, r)$ is a circle. Its "volume" (i.e., area in \mathbb{R}^2) is $|B(x_0, r)| = \pi r^2$, and its "surface area" (i.e., arc length in \mathbb{R}^2) is $|\partial B(x_0, r)| = 2\pi r$.

Theorem 9.4 (mean-value formula for harmonic functions). If u is harmonic in Ω , then for any ball $B(x_0, r) \subset \Omega$ and the associated boundary $\partial B(x_0, r)$ we have

$$u(x_0) = \underbrace{\frac{1}{|B(x_0, r)|} \int_{B(x_0, r)} u dx}_{\text{average over the volume}} = \underbrace{\frac{1}{|\partial B(x_0, r)|} \int_{\partial B(x_0, r)} u ds}_{\text{average over the surface}}.$$

Proof. We prove the formula in \mathbb{R}^2 ; the proof readily extends to higher dimensions. We first prove the relationship for the average over the circumference. Without loss of generality, we choose the coordinate system centered about the ball and introduce a function

$$\phi(r) = \frac{1}{2\pi r} \int_{\partial B(0,r)} u(y) ds(y) = \frac{1}{2\pi r} \int_{\theta=0}^{2\pi} u(r, \theta) r d\theta = \frac{1}{2\pi} \int_{\theta=0}^{2\pi} u(r, \theta) d\theta.$$

We then differentiate the function to obtain

$$\phi'(r) = \frac{1}{2\pi} \int_{\theta=0}^{2\pi} \frac{\partial u}{\partial r}(r, \theta) d\theta = \frac{1}{2\pi r} \int_{\theta=0}^{2\pi} \frac{\partial u}{\partial r}(r, \theta) r d\theta.$$

We now (i) recognize that the integration is over the circle $B(0, r)$, (ii) recognize $\frac{\partial u}{\partial r} = \nu \cdot \nabla u$ for ν the outward pointing unit normal on the circle, and (iii) invoke the divergence theorem to obtain

$$\phi'(r) = \frac{1}{2\pi r} \int_{\partial B(0,r)} \nu \cdot \nabla u ds = \frac{1}{2\pi r} \int_{B(0,r)} \Delta u dx = 0,$$

where the last equality follows from $\Delta u = 0$. Hence ϕ is a constant function and we can equate its value for any r to the limit of r going to 0, $\lim_{r \rightarrow 0} \phi(r)$:

$$\phi(r) = \lim_{a \rightarrow 0} \phi(a) = \lim_{a \rightarrow 0} \frac{1}{2\pi a} \int_{\partial B(0,a)} u(y) ds(y) = u(x=0),$$

which is the first relationship. (Note that we use a dummy variable a for the limit $\lim_{a \rightarrow 0} \phi(a)$ to avoid conflation with r about which ϕ is evaluated.)

To prove the second relationship we again use the polar coordinate to obtain

$$\int_{B(0,r)} u(x) dx = \int_{z=0}^r \left(\int_{\partial B(0,z)} u ds \right) dz = \int_{z=0}^r u(0) 2\pi z dz = u(0) \pi r^2,$$

which is the second relationship. □

Theorem 9.5 (Converse to mean-value theorem). If $u \in C^2(\Omega)$ satisfies

$$u(x_0) = \frac{1}{2\pi r} \int_{\partial B(x_0,r)} u(s) ds$$

for all balls $B(x_0, r) \subset \Omega$, then u is harmonic.

Proof. Proof is beyond the scope of this course. See, for example, *Partial Differential Equations* by Evans. □

Example 9.6 (mean-value formulas in \mathbb{R}^1). Let $u : \mathbb{R} \rightarrow \mathbb{R}$ be a harmonic function (i.e., u satisfies $-u'' = 0$ in \mathbb{R}). We introduce a ball $B(x_0 = 1, r = 2) = (-1, 3)$. (The ball is just an open line segment in \mathbb{R}^1 .) Suppose $u(x = -1) = 1$ and $u(x = 3) = 2$. Then by the mean value formula, the value at the center of the ball is given by

$$u(1) = \underbrace{\frac{1}{|\partial B(1,2)|} \int_{\partial B(1,2)} u ds}_{\text{ball surface average}} = \frac{1}{2}(u(-1) + u(3)) = \frac{3}{2}.$$

In addition, the average of u over the line segment $(-1, 3)$ is

$$\frac{1}{|B(x_0, r)|} \int_{B(x, r)} u dx = \frac{1}{4} \int_{-1}^3 u dx = \frac{3}{2}.$$

Note that we arrive at these conclusions *without knowing the precise form of the solution*.

(Note that explicit form of the solution is given by $u(x) = \frac{1}{4}x + \frac{5}{4}$, which yields the results that are consistent with the above. Harmonic functions are linear in \mathbb{R}^1 because $u'' = 0$.)

Example 9.7 (mean-value formulas in \mathbb{R}^2). Let $u : \mathbb{R}^2 \rightarrow \mathbb{R}$ be a harmonic function. We introduce a ball $B(0, 2) \subset \mathbb{R}^2$. Suppose along the surface of the ball (i.e., the circle) the function is given by

$$u(r = 2, \theta) = 1 + \cos(3\theta)$$

in the polar coordinates. Then, by the mean-value formula for the surface, the value at the center of the ball is

$$u(0) = \underbrace{\frac{1}{|\partial B(0, 2)|} \int_{\partial B(0, 2)} u ds}_{\text{average over circle}} = \frac{1}{2\pi \cdot 2} \int_{\theta=0}^{2\pi} (1 + \cos(3\theta)) 2 \cdot d\theta = 1.$$

Similarly, by the mean value formula for the volume,

$$\underbrace{\frac{1}{|B(0, 2)|} \int_{B(0, 2)} u dx}_{\text{average over disk}} = u(0) = 1.$$

We arrive at these results without knowing the explicit form of the solution.

(We will find an explicit form of the solution using separation of variables in Example 10.2. The solution as expected satisfies the above mean-value properties.)

9.4 Maximum principles

Similarly to the heat equation, Laplace's equation also satisfies certain maximum and minimum principles:

Theorem 9.8 ((weak) maximum principle). Let u be a harmonic function in a connected open domain $\Omega \subset \mathbb{R}^2$. Then

$$\max_{\bar{\Omega}} u = \max_{\partial\Omega} u;$$

the function attains the maximum value on the boundary of the domain.

Proof. Suppose $x^* \in \bar{\Omega}$ is the maximizer so that $u(x^*) = \max_{\bar{\Omega}} u \equiv M$. We have two cases: (i) x^* is an interior point, $x^* \in \Omega$; (ii) x^* is on the boundary, $x^* \in \partial\Omega$. If $x^* \in \Omega$, then by the strong maximum principle u is a constant function and hence the maximum is attained on everywhere including the boundary $\partial\Omega$. If $x^* \in \partial\Omega$, the statement is trivially satisfied because it is the statement itself. \square

Theorem 9.9 (strong maximum principle). Let u be a harmonic function in a connected open domain $\Omega \subset \mathbb{R}^n$. If there exists a point $x^* \in \Omega$ such that

$$u(x^*) = \max_{\bar{\Omega}} u,$$

then u is constant in Ω . (Note that x^* must lie in the open set Ω , which is strictly interior to $\bar{\Omega}$.)

Proof. Suppose $x^* \in \Omega$ is the maximizer so that $u(x^*) = \max_{\bar{\Omega}} u \equiv M$. Then, by the mean-value formula for the ball

$$M = u(x^*) = \frac{1}{|B(x^*, a)|} \int_{B(x^*, a)} u(x) dx \leq \max_{x \in B(x^*, a)} u(x) \leq M.$$

The last inequality holds as equality only if $u(x) = M$ for all $x \in B(x^*, a)$, and hence we conclude that u must be constant (and equal to M) in $B(x^*, a)$. We then repeat the same argument for a new ball with the center $x^{*'}$ and radius a' that lies in $B(x^*, a)$, from which we conclude $u(x) = M$ for all $x \in B(x^*, a) \cup B(x^{*'}, a')$. We repeat the same argument until we cover the whole domain and conclude that $u(x) = M$ for all $x \in \bar{\Omega}$. \square

Theorem 9.10 (weak and strong minimum principles). Let u be a harmonic function in a connected open domain $\Omega \subset \mathbb{R}^2$. Then

$$\min_{\bar{\Omega}} u = \min_{\partial\Omega} u.$$

In addition, if there exists a point $x^* \in \Omega$ such that

$$u(x^*) = \min_{\bar{\Omega}} u,$$

then u is constant in Ω .

Proof. We apply the weak and strong maximum principle, respectively, to $-u$. (See the same argument for the maximum/minimum principle for the heat equation for a complete proof.) \square

We make a few observations:

1. The weak maximum (resp. minimum) principle states that, if $u : \bar{\Omega} \rightarrow \mathbb{R}$ is a harmonic function, then it attains a maximum (resp. minimum) on the boundary $\partial\Omega$. In other words, for any $x \in \bar{\Omega}$ (including the boundary),

$$\min_{\partial\Omega} u \leq u(x) \leq \max_{\partial\Omega} u.$$

2. The strong maximum (resp. minimum) principle states that, if $u : \bar{\Omega} \rightarrow \mathbb{R}$ is a harmonic function, then the only way for it to attain a maximum (resp. minimum) in Ω — i.e., strictly inside of the domain and not on the boundary — is if u is a constant function. Conversely, if u is a non-constant function, then the function values in Ω are strictly less than (resp. greater than) the maximum (resp. minimum) value on the boundary. In other words, for a non-constant harmonic function u and for any $x \in \Omega$ (strictly inside),

$$\min_{\partial\Omega} u < u(x) < \max_{\partial\Omega} u.$$

We now provide an example:

Example 9.11 (maximum principle in \mathbb{R}^2). Suppose $u : \mathbb{R}^2 \rightarrow \mathbb{R}$ is a harmonic function. We introduce a ball $\Omega = B(0, 2) \subset \mathbb{R}^2$. Suppose along the surface of the ball (i.e., the circle) the function is given by

$$u(r = 2, \theta) = 2 + \cos(3\theta)^2$$

in the polar coordinates. Then by the weak maximum and minimum principles, for any $x \in \bar{\Omega}$ (including the boundary),

$$2 = \min_{\partial\Omega} u \leq u(x) \leq \max_{\partial\Omega} u = 3.$$

In addition, because u is a non-constant function, by the strong maximum and minimum principles, for any $x \in \Omega$ (strictly inside),

$$2 < u(x) < 3.$$

We conclude the section with a positivity result:

Corollary 9.12 (positivity). Let u is the solution to

$$\begin{aligned} -\Delta u &= 0 & \text{in } \Omega, \\ u &= g & \text{on } \partial\Omega. \end{aligned}$$

If $g \geq 0$, then $u \geq 0$ everywhere in $\bar{\Omega}$. In addition, if Ω is connected and $g(x) > 0$ for some $x \in \partial\Omega$, then $u > 0$ everywhere in Ω .

Proof. Non-negativity is a consequence of the (weak) minimum principle. If $u \geq 0$ on $\partial\Omega$ then $u(x) \geq \min_{x \in \Omega} u(x) \geq 0$.

Positivity is a consequence of the strong minimum principle. Suppose $g \geq 0$ and $g(x) > 0$ for some $x \in \partial\Omega$, and there exists $x^* \in \Omega$ such that $u(x^*) = 0 = \min_{\bar{\Omega}} u$. Then, by the strong maximum principle u must be a constant function, $u = 0$. However, this contradicts the fact $g(x) > 0$ for some $x \in \partial\Omega$. Hence u must be positive everywhere in Ω . \square

9.5 Uniqueness and uniform stability by maximum principle

We now assess two of the three conditions of well-posedness: uniqueness and stability. We appeal to the maximum principle to show Dirichlet boundary value problems associated with Laplace's equation satisfy both conditions. The approach is analogous to our proof of uniqueness and stability for the heat equation by its maximum principle.

Theorem 9.13 (uniqueness of the solution to Laplace's equation). Let $g \in C(\partial\Omega)$. There exists at most one solution $u \in C^2(\Omega) \cap C(\bar{\Omega})$ to the boundary value problem

$$\begin{aligned} -\Delta u &= 0 & \text{in } \Omega, \\ u &= g & \text{on } \partial\Omega. \end{aligned}$$

Proof. If both $u_1 \in C^2(\Omega) \cap C(\bar{\Omega})$ and $u_2 \in C^2(\Omega) \cap C(\bar{\Omega})$ are solutions to the boundary value problem, then $u_1 - u_2 \in C^2(\Omega) \cap C(\bar{\Omega})$ and by linearity

$$\begin{aligned} -\Delta(u_1 - u_2) &= 0 & \text{in } \Omega, \\ (u_1 - u_2) &= 0 & \text{on } \partial\Omega. \end{aligned}$$

By the maximum and minimum principle, $u_1 - u_2 = 0$ everywhere in $\bar{\Omega}$ and hence $u_1 = u_2$. \square

Theorem 9.14 (stability of the solution to Laplace's equation). Let u_1 and u_2 be the solutions to the boundary value problems associated with boundary data g_1 and g_2 , respectively:

$$\begin{aligned} -\Delta u_i &= 0 & \text{in } \Omega, \\ u_i &= g_i & \text{on } \partial\Omega \end{aligned}$$

for $i = 1, 2$. Then the solution depends continuously on data in the sense that

$$\max_{x \in \bar{\Omega}} |u_1(x) - u_2(x)| \leq \max_{x \in \partial\Omega} |g_1(x) - g_2(x)| \quad (9.1)$$

Proof. We appeal to the linearity of the Laplacian operator and take the difference of the two set of equations to obtain

$$\begin{aligned} -\Delta(u_1 - u_2) &= 0 & \text{in } \Omega, \\ (u_1 - u_2) &= (g_1 - g_2) & \text{on } \partial\Omega. \end{aligned}$$

The (weak) maximum (resp. minimum) principle require the maximum (resp. minimum) to occur at the boundary; i.e., for any $x \in \bar{\Omega}$,

$$\begin{aligned} u_1(x) - u_2(x) &\leq \max_{x \in \partial\Omega} (g_1(x) - g_2(x)), \\ u_1(x) - u_2(x) &\geq \min_{x \in \partial\Omega} (g_1(x) - g_2(x)). \end{aligned}$$

It follows that

$$\max_{x \in \bar{\Omega}} |u_1(x) - u_2(x)| \leq \max_{x \in \partial\Omega} |g_1(x) - g_2(x)|,$$

which is the desired inequality. \square

The left hand side of (9.1) measures the closeness of the two solutions, and the right hand side of (9.1) measures the closeness of the boundary data. The uniform stability result shows that the difference in the two solutions u_1 and u_2 over any point $x \in \bar{\Omega}$ is bounded by the maximum difference in the boundary data $g_1 - g_2$. Hence a small change in the data results in a small change in the solution; the problem is hence stable. We have seen in Lecture 5 that that the heat equation also enjoys a similar stability property; however, not all PDEs possesses the property, as we will see for the wave and transport equations.

9.6 Energy method: uniqueness

Similarly to the case of the heat equation, we can also prove the uniqueness of the solution to Laplace's equation using an energy method. Suppose u_1 and u_2 are two solutions to the same boundary value problem associated with Laplace's equation. Then their difference $w \equiv u_1 - u_2$ satisfies

$$\begin{aligned} -\Delta w &= 0 & \text{in } \Omega, \\ w &= 0 & \text{on } \partial\Omega. \end{aligned}$$

We then observe that

$$0 = - \int_{\Omega} w \Delta w dx = \int_{\Omega} \nabla w \cdot \nabla w dx,$$

where the second equality follows from integration by parts and the fact $w = 0$ on $\partial\Omega$. Hence $\nabla w = 0$ in Ω . Because $w = 0$ on $\partial\Omega$, we conclude $w = u_1 - u_2 = 0$ in Ω .

9.7 Summary

We summarize key points of this lecture:

1. Laplace's equation is ubiquitous in both engineering and mathematics. A function that satisfies Laplace's equation is called a harmonic function.
2. Harmonic functions satisfy mean-value properties. Given a harmonic function over a ball, the value of the function at the center is equal to both the mean of the function over the ball and the mean of the function over the surface of the ball.
3. Harmonic functions satisfy maximum principles. A harmonic function attains the maximum value somewhere on the boundary (i.e., the weak maximum principle); if the maximum is attained in an interior, then it must be a constant function (i.e., the strong maximum principle).
4. Harmonic functions also satisfy the weak and strong minimum principles.
5. Dirichlet boundary value problems associated with Laplace's equation have unique solutions. The proof follows from either the maximum principle or the energy method.
6. Dirichlet boundary value problems associated with Laplace's equation are stable in the sense that the solution depends continuously on the boundary data. The proof follows from the maximum principle.

Lecture 10

Laplace's equation: separation of variables

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10.1 Introduction

In this lecture, we seek the solution of Laplace's and Poisson's equations on bounded domains using *separation of variables*. While the technique is fundamentally the same as that considered for the heat equation, we pay particular attention on the extension of the technique to higher spatial dimensions ($n > 1$).

10.2 Laplace's equation on a rectangle

We now consider the solution of Laplace's equation on a rectangle $\Omega \equiv (0, L) \times (0, H)$ using separation of variables:

$$\begin{aligned} -\Delta u &= 0 && \text{in } \Omega \equiv (0, L) \times (0, H), \\ u &= g^1 && \text{on } \Gamma^1 \equiv \{x = 0\} \times (0, H), \\ u &= g^2 && \text{on } \Gamma^2 \equiv \{x = L\} \times (0, H), \\ u &= g^3 && \text{on } \Gamma^3 \equiv (0, L) \times \{y = 0\}, \\ u &= g^4 && \text{on } \Gamma^4 \equiv (0, L) \times \{y = H\}, \end{aligned} \tag{10.1}$$

where x and y denote the first and second spatial coordinates, respectively, and g^i , $i = 1, \dots, 4$, are some boundary functions. Note that the boundaries Γ^1 , Γ^2 , Γ^3 , and Γ^4 correspond to the left, right, bottom, and top boundaries, respectively.

To solve the boundary value problem (10.1), we again appeal to the principle of superposition. Namely, we decompose the solution u into two parts $u = u^{1,2} + u^{3,4}$, where $u^{1,2}$ is the solution to the boundary value problem with only g^1 and g^2 as the nonhomogeneous boundaries, and $u^{3,4}$ is the solution to the boundary value problem with only g^3 and g^4 as the nonhomogeneous boundaries.

More explicitly, $u^{1,2}$ is the solution to

$$\begin{aligned} -\Delta u^{1,2} &= 0 && \text{in } \Omega, \\ u^{1,2} &= g^1 && \text{on } \Gamma^1, \\ u^{1,2} &= g^2 && \text{on } \Gamma^2, \\ u^{1,2} &= 0 && \text{on } \Gamma^3 \cup \Gamma^4; \end{aligned} \tag{10.2}$$

similarly, $u^{3,4}$ is the solution to

$$\begin{aligned} -\Delta u^{3,4} &= 0 && \text{in } \Omega, \\ u^{3,4} &= g^3 && \text{on } \Gamma^3, \\ u^{3,4} &= g^4 && \text{on } \Gamma^4, \\ u^{3,4} &= 0 && \text{on } \Gamma^1 \cup \Gamma^2. \end{aligned}$$

We readily see $u = u^{1,2} + u^{3,4}$ by superposition.

We now consider the solution of (10.2) by separation of variables and linear superposition. We recall the two step procedure:

- *Step 1.* We find a family of separable solutions of the form

$$u_n(x, y) = X_n(x; C_n, D_n)Y_n(y), \quad n = 1, 2, \dots,$$

each of which satisfies the homogeneous boundary conditions on Γ^3 and Γ^4 for any choice of coefficients C_n and D_n , but not (in general) the nonhomogeneous boundary conditions on Γ^1 and Γ^2 . (As we have seen for the heat equation, Y_n will be a family of functions in y that satisfy homogeneous boundary conditions at $y = 0$ and $y = H$; hence, we associate the indeterminate coefficients C_n and D_n with functions X_n in x .)

- *Step 2.* We consider a particular choice of coefficients C_n and D_n such that

$$u^{1,2}(x, y) = \sum_{n=1}^{\infty} X_n(x; C_n, D_n)Y_n(y)$$

satisfies the nonhomogeneous boundary conditions on Γ^1 and Γ^2 . Note that the solution $u^{1,2}$ automatically satisfies the homogeneous boundary conditions on Γ^3 and Γ^4 since each u_n satisfies the homogeneous boundary condition.

To find the separable solution of the form $u_n(x, y) = X_n(x)Y_n(y)$, we substitute the expression into (10.2) and obtain

$$-X_n''Y_n - X_nY_n'' = 0 \quad \Rightarrow \quad \frac{X_n''}{X_n} = -\frac{Y_n''}{Y_n} = \alpha_n$$

for some constant $\alpha_n \in \mathbb{R}$. We have used the fact X_n''/X_n and Y_n''/Y_n depend on only x and y , respectively, and hence each of them must be a constant.

We now consider the boundary value eigenproblem associated with Y_n ; we solve for Y_n (instead of X_n) first because we wish to impose homogeneous boundary conditions at the endpoints $y = 0$ and $y = H$. We first observe that the boundary condition implies that

$$\begin{aligned} u_n(x, y = 0) &= X_n(x)Y_n(0) = 0, & \forall x \in (0, L) \\ u_n(x, y = H) &= X_n(x)Y_n(H) = 0, & \forall x \in (0, L). \end{aligned}$$

Since we seek a nontrivial solution, we require $X_n \neq 0$ and deduce $Y_n(0) = Y_n(H) = 0$. Our boundary value eigenproblem for Y_n is as follows:

$$\begin{aligned} -Y_n'' &= \alpha_n Y_n & \text{in } (0, H), \\ Y_n(0) &= Y_n(H) = 0. \end{aligned}$$

This is a Sturm-Liouville problem. In fact this is a scaled-version of the problem considered in Example 4.6, and the eigenpairs are given by

$$Y_n(y) = \sin(\lambda_n y) \quad \text{and} \quad \alpha_n = \lambda_n^2$$

for $\lambda_n = n\pi/H$, $n = 1, 2, \dots$

We next consider the ODE associated with X_n :

$$X_n'' = \alpha_n X_n \quad \Rightarrow \quad X_n'' = \lambda_n^2 X_n$$

for $\lambda_n = n\pi/H$. The general solution is given by

$$X_n(x) = C_n \sinh(\lambda_n x) + D_n \cosh(\lambda_n x).$$

We hence conclude that any solution of the form

$$u^{1,2}(x, y) = \sum_{n=1}^{\infty} (C_n \sinh(\lambda_n x) + D_n \cosh(\lambda_n x)) \sin(\lambda_n y)$$

satisfies Laplace's equation and the associated homogeneous boundary conditions on $y = 0$ and $y = H$.

We now enforce the nonhomogeneous boundary conditions on $x = 0$ and $x = L$. We first enforce $u(x = 0, y) = g_1(y)$ to obtain

$$u^{1,2}(x = 0, y) = \sum_{n=1}^{\infty} D_n \sin(\lambda_n y) = g^1(y)$$

for $\lambda_n = n\pi/H$. We recognize that this is a Fourier sine series and the coefficients are given by

$$D_n = \hat{g}_n^1 \equiv \frac{2}{H} \int_0^H \sin(n\pi y/H) g^1(y) dy, \quad n = 1, 2, \dots \quad (10.3)$$

We next enforce the boundary condition $u^{1,2}(x = L, y) = g^2(y)$ to obtain

$$u^{1,2}(x = L, y) = \sum_{n=1}^{\infty} (C_n \sinh(\lambda_n L) + \hat{g}_n^1 \cosh(\lambda_n L)) \sin(\lambda_n y) = g^2(y),$$

where we have set $D_n = \hat{g}_n^1$. We note that the ‘‘coefficient’’ ($C_n \sinh(\lambda_n L) + \hat{g}_n^1 \cosh(\lambda_n L)$) must be the n -th Fourier sine coefficient of g^2 . Hence

$$C_n \sinh(\lambda_n L) + \hat{g}_n^1 \cosh(\lambda_n L) = \hat{g}_n^2 \equiv \frac{2}{H} \int_0^H \sin(n\pi y/H) g^2(y) dy.$$

We rearrange the expression to obtain

$$C_n = \frac{\hat{g}_n^2 - \hat{g}_n^1 \cosh(\lambda_n L)}{\sinh(\lambda_n L)}. \quad (10.4)$$

We hence conclude that the solution $u^{1,2}$ is given by

$$u^{1,2}(x, y) = \sum_{n=1}^{\infty} \left(\frac{\hat{g}_n^2 - \hat{g}_n^1 \cosh(\lambda_n L)}{\sinh(\lambda_n L)} \sinh(\lambda_n x) + \hat{g}_n^1 \cosh(\lambda_n x) \right) \sin(\lambda_n y).$$

We may group the terms containing \hat{g}_n^1 and \hat{g}_n^2 to obtain

$$u^{1,2}(x, y) = \sum_{n=1}^{\infty} \left(\hat{g}_n^1 (\cosh(\lambda_n x) - \coth(\lambda_n L) \sinh(\lambda_n x)) + \hat{g}_n^2 \frac{\sinh(\lambda_n x)}{\sinh(\lambda_n L)} \right) \sin(\lambda_n y),$$

which may be further simplified using trigonometric identity to yields

$$u^{1,2}(x, y) = \sum_{n=1}^{\infty} \left(\hat{g}_n^1 \frac{\sinh(\lambda_n(L-x))}{\sinh(\lambda_n L)} + \hat{g}_n^2 \frac{\sinh(\lambda_n x)}{\sinh(\lambda_n L)} \right) \sin(\lambda_n y),$$

where $\lambda_n = n\pi/H$.

By the symmetry of the problem, we also find the solution to

$$\begin{aligned} -\Delta u^{3,4} &= 0 & \text{in } \Omega, \\ u^{3,4} &= g^3 & \text{on } \Gamma^3, \\ u^{3,4} &= g^4 & \text{on } \Gamma^4, \\ u^{3,4} &= 0 & \text{on } \Gamma^1 \cup \Gamma^2 \end{aligned} \quad (10.5)$$

is

$$u^{3,4}(x, y) = \sum_{n=1}^{\infty} \left(\hat{g}_n^3 \frac{\sinh(\mu_n(H-y))}{\sinh(\mu_n H)} + \hat{g}_n^4 \frac{\sinh(\mu_n y)}{\sinh(\mu_n H)} \right) \sin(\mu_n x),$$

where $\mu_n = n\pi/L$, and \hat{g}_n^3 and \hat{g}_n^4 are the Fourier sine series coefficients

$$\hat{g}_n^3 \equiv \frac{2}{L} \int_0^L \sin(n\pi x/L) g^3(x) dx \quad \text{and} \quad \hat{g}_n^4 \equiv \frac{2}{L} \int_0^L \sin(n\pi x/L) g^4(x) dx.$$

It follows that, by linear superposition, the solution to the original problem (10.1) is given by

$$\begin{aligned} u(x, y) &= u^{1,2}(x, y) + u^{3,4}(x, y) \\ &= \sum_{n=1}^{\infty} \left(\hat{g}_n^1 \frac{\sinh(\lambda_n(L-x))}{\sinh(\lambda_n L)} + \hat{g}_n^2 \frac{\sinh(\lambda_n x)}{\sinh(\lambda_n L)} \right) \sin(\lambda_n y) \\ &\quad + \sum_{n=1}^{\infty} \left(\hat{g}_n^3 \frac{\sinh(\mu_n(H-y))}{\sinh(\mu_n H)} + \hat{g}_n^4 \frac{\sinh(\mu_n y)}{\sinh(\mu_n H)} \right) \sin(\mu_n x) \end{aligned}$$

for $\lambda_n = n\pi/H$ and $\mu_n = n\pi/L$.

We make a few observations:

1. The solution is a linear combination of four harmonic functions associated with the four boundary functions g^1, \dots, g^4 ; i.e., $u = u^1 + u^2 + u^3 + u^4$ where

$$\begin{aligned} u^1(x, y) &= \sum_{n=1}^{\infty} \hat{g}_n^1 \frac{\sinh(\lambda_n(L-x))}{\sinh(\lambda_n L)} \sin(\lambda_n y), & u^2(x, y) &= \sum_{n=1}^{\infty} \hat{g}_n^2 \frac{\sinh(\lambda_n x)}{\sinh(\lambda_n L)} \sin(\lambda_n y), \\ u^3(x, y) &= \sum_{n=1}^{\infty} \hat{g}_n^3 \frac{\sinh(\mu_n(H-y))}{\sinh(\mu_n H)} \sin(\mu_n x), & u^4(x, y) &= \sum_{n=1}^{\infty} \hat{g}_n^4 \frac{\sinh(\mu_n y)}{\sinh(\mu_n H)} \sin(\mu_n x). \end{aligned}$$

2. We readily verify that the solution satisfy the boundary conditions:

$$\begin{aligned} u(x=0, y) &= \sum_{n=1}^{\infty} \hat{g}_n^1 \sin(\lambda_n y) = g^1(y), & u(x=L, y) &= \sum_{n=1}^{\infty} \hat{g}_n^2 \sin(\lambda_n y) = g^2(y), \\ u(x, y=0) &= \sum_{n=1}^{\infty} \hat{g}_n^3 \sin(\mu_n x) = g^3(x), & u(x, y=H) &= \sum_{n=1}^{\infty} \hat{g}_n^4 \sin(\mu_n x) = g^4(x). \end{aligned}$$

3. Figure 10.1 shows functions $\frac{\sinh(\lambda_n(L-x))}{\sinh(\lambda_n L)}$ and $\frac{\sinh(\lambda_n x)}{\sinh(\lambda_n L)}$ for $H = 1$, which dictate the decay of the n -th mode away from the $x = 0$ and $x = L$ boundaries, respectively. We observe that the functions decay exponentially away from the boundaries because $\sinh(\lambda_n x) \approx \exp(\lambda_n x)/2$ for $\lambda_n x \gg 1$. Moreover, higher modes (i.e., modes associated with a larger n) decay more rapidly away from the boundaries because the exponential factor is $\lambda_n x = n\pi/H$.
4. Figure 10.2 shows the solution associated with a nonhomogeneous boundary condition on $x = L$ and with the homogeneous boundary condition elsewhere: $u_n(x, y) = \hat{g}_n^2 \frac{\sinh(\lambda_n x)}{\sinh(\lambda_n L)} \sin(\lambda_n y)$ for $n = 1$ and 3. We observe that each mode is smooth and they decay exponentially away from the boundary.

Example 10.1 (Laplace's equation on a square). We consider Laplace's equation on the unit square $\Omega \equiv (0, 1)^2$. The boundary value problem is given by (10.1) for triangular boundary functions

$$\begin{aligned} g^2(y) &= 1 - 2|y - 0.5|, & y &\in (0, 1), \\ g^4(x) &= 1/2 - |x - 0.5|, & x &\in (0, 1), \end{aligned}$$

and $g^1 = g^3 = 0$. To find the solution, we first note that $\lambda_n = \mu_n = n\pi$ since $L = H = 1$. We then find the Fourier sine coefficients of g^2 and g^4 :

$$\begin{aligned} \hat{g}_n^2 &= \begin{cases} \frac{8(-1)^{(n-1)/2}}{n^2\pi^2}, & n \text{ odd}, \\ 0, & n \text{ even}, \end{cases} \\ \hat{g}_n^4 &= \begin{cases} \frac{4(-1)^{(n-1)/2}}{n^2\pi^2}, & n \text{ odd}, \\ 0, & n \text{ even}. \end{cases} \end{aligned}$$

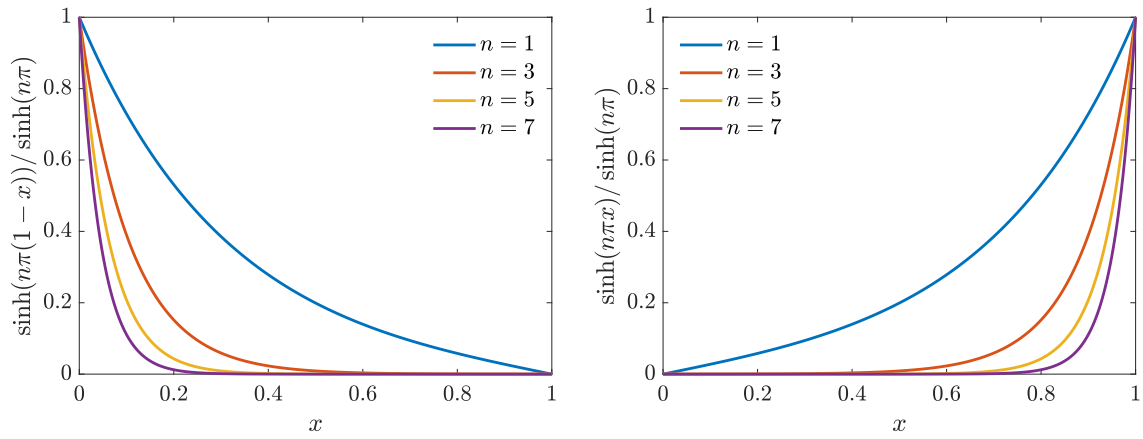


Figure 10.1: Functions $\sinh(n\pi(1-x))/\sinh(n\pi)$ and $\sinh(n\pi x)/\sinh(n\pi)$.

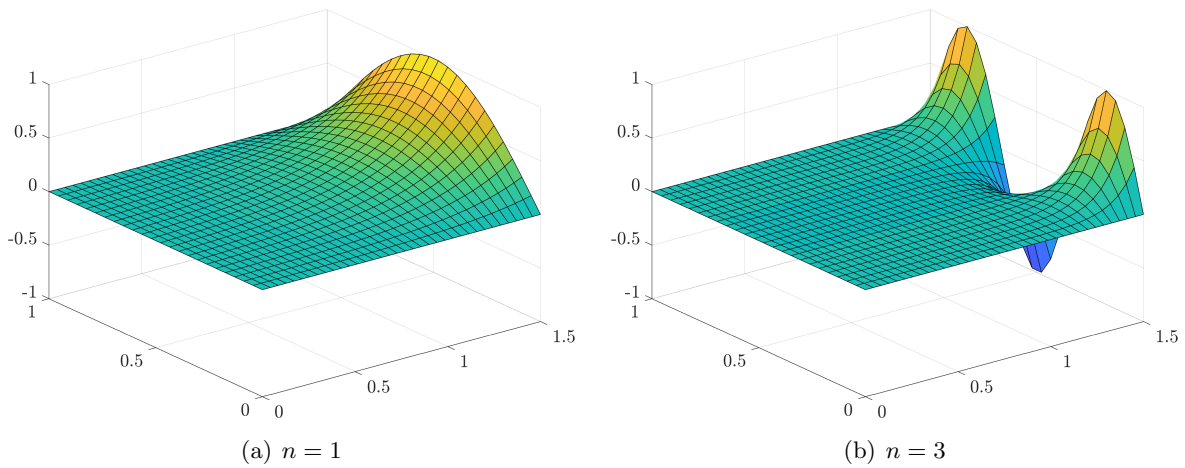


Figure 10.2: Solutions to Laplace's equation on $(0, 1.5) \times (0, 1)$ for $g^2(y) = \sin(n\pi y)$ and $g^i = 0$ for $i = 1, 3, 4$.

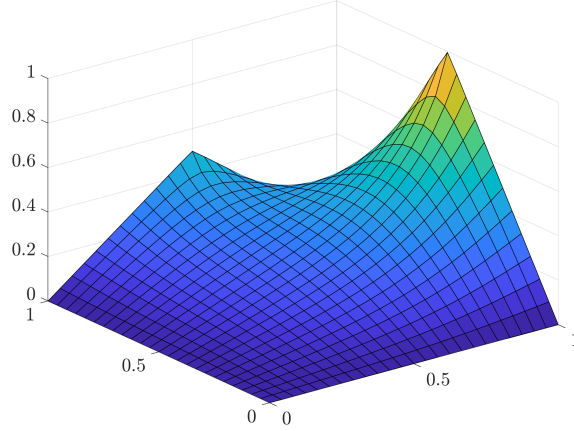


Figure 10.3: Solution to Laplace's equation on a square with triangular boundary functions.

We then substitute the coefficients to our general expression to find

$$u(x, y) = \sum_{n=1,3,5,\dots}^{\infty} \left(\frac{8(-1)^{(n-1)/2} \sinh(n\pi x)}{n^2\pi^2 \sinh(n\pi)} \sin(n\pi y) + \frac{4(-1)^{(n-1)/2} \sinh(n\pi y)}{n^2\pi^2 \sinh(n\pi)} \sin(n\pi x) \right).$$

Figure 10.3 shows the solution to the problem. We observe that even though the boundary functions are not smooth, the solution is smooth on Ω . In fact it can be shown that harmonic functions are infinitely continuously differentiable in Ω (but not necessarily on $\partial\Omega$). We also observe that the maximum (resp. minimum) principle is clearly satisfied and the maximum (resp. minimum) value is attained on the boundary.

10.3 Laplace's equation on a disk

We now consider the solution of Laplace's equation on a disk $\Omega \equiv \{x \in \mathbb{R}^2 \mid \|x\|_2 < a\}$:

$$\begin{aligned} -\Delta u &= 0 & \text{in } \Omega, \\ u &= g & \text{on } \partial\Omega. \end{aligned} \tag{10.6}$$

We again use separation of variables but now in polar coordinates. The Laplacian in polar coordinates is

$$\Delta u = \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial u}{\partial r} \right) + \frac{1}{r^2} \frac{\partial^2 u}{\partial \theta^2} = \frac{\partial^2 u}{\partial r^2} + \frac{1}{r} \frac{\partial u}{\partial r} + \frac{1}{r^2} \frac{\partial^2 u}{\partial \theta^2} = 0.$$

We substitute the separable form of the solution $u_n(r, \theta) = R_n(r)\Theta_n(\theta)$ and obtain

$$R_n''\Theta_n + \frac{1}{r}R_n'\Theta_n + \frac{1}{r^2}R_n\Theta_n'' = 0.$$

We multiply through by $r^2/(R_n\Theta_n)$ to obtain

$$r^2 \frac{R_n''}{R_n} + r \frac{R_n'}{R_n} + \frac{\Theta_n''}{\Theta_n} = 0 \quad \Rightarrow \quad r^2 \frac{R_n''}{R_n} + r \frac{R_n'}{R_n} = -\frac{\Theta_n''}{\Theta_n} = \alpha_n.$$

Since the left and right hand sides are functions of only r and θ , respectively, we deduce as before that they must be equal to some constant α_n .

We now consider the eigenproblem associated with Θ_n . Because the location of the “cut” that we make in the θ -coordinate is arbitrary, we impose periodic boundary conditions. In addition, we solve for Θ_n (instead of R_n) first because the periodic boundary condition can be readily incorporated into the separable form of the solution, just like the homogeneous boundary condition in the rectangular case. The resulting eigenproblem is given by

$$\begin{aligned} -\Theta_n'' &= \alpha_n \Theta_n \quad \text{in } (0, 2\pi), \\ \Theta_n(0) &= \Theta_n(2\pi), \\ \Theta_n'(0) &= \Theta_n'(2\pi), \end{aligned}$$

This is a periodic Sturm-Liouville problem. The general solution to the ODE is given by

$$\Theta_n(\theta) = A_n \cos(\lambda_n \theta) + B_n \sin(\lambda_n \theta)$$

for $\lambda_n = \sqrt{\alpha_n}$. We then impose the periodic boundary condition to find that $\lambda_n = n$, $n = 0, 1, 2, \dots$, and hence

$$\Theta_n(\theta) = A_n \cos(n\theta) + B_n \sin(n\theta),$$

and $\alpha_n = \lambda_n^2 = n^2$. (Note that $\Theta_{n=0} = A_n$ is a constant function, which of course is periodic.)

Having found $\alpha_n = n^2$, we next observe that the ODE for R_n must satisfy

$$r^2 R_n'' + r R_n' - n^2 R_n = 0.$$

This is a Cauchy-Euler equation of order two, whose solution is of the form $R_n(r) = r^m$ for some m . We substitute the form of the solution to obtain

$$m(m-1)r^m + mr^m - n^2 r^m = 0 \quad \Rightarrow \quad m^2 - n^2 = 0. \quad \Rightarrow \quad m = \pm n.$$

It follows that $R_n(r) = C_n r^n + D_n r^{-n}$ if $n \neq 0$. For $n = 0$, the solution is given by $R_{n=0}(r) = C_{n=0} + D_{n=0} \log(r)$. We now impose the condition that R_n should be bounded on $[0, a)$ and in particular at the origin; we hence reject the solution r^{-n} and $\log(r)$ which are unbounded at the origin. It follows that our solution is

$$R_n(r) = C_n r^n, \quad n = 0, 1, 2, \dots$$

Hence our family of separable solutions is

$$u_n(r, \theta) = R_n(r)\Theta_n(\theta) = r^n (A_n \cos(n\theta) + B_n \sin(n\theta)), \quad n = 0, 1, 2, \dots$$

We appeal to the principle of superposition and rescale the constant term by $1/2$ and all other terms by $1/a^n$ for convenience to obtain

$$u(r, \theta) = \frac{1}{2} A_0 + \sum_{n=1}^{\infty} \left(\frac{r}{a}\right)^n (A_n \cos(n\theta) + B_n \sin(n\theta)). \quad (10.7)$$

To find the coefficients $(A_n)_{n=0}^{\infty}$ and $(B_n)_{n=1}^{\infty}$, we apply the boundary condition at $r = a$:

$$u(r = a, \theta) = \frac{1}{2} A_0 + \sum_{n=1}^{\infty} (A_n \cos(n\theta) + B_n \sin(n\theta)) = g(\theta);$$

this is the Fourier series for g with the period of 2π and hence the coefficients are given by

$$\begin{aligned} A_n &= \frac{1}{\pi} \int_{-\pi}^{\pi} g(\theta) \cos(n\theta) d\theta, \quad n = 0, 1, \dots, \\ B_n &= \frac{1}{\pi} \int_{-\pi}^{\pi} g(\theta) \sin(n\theta) d\theta, \quad n = 1, 2, \dots \end{aligned} \quad (10.8)$$

Hence the Fourier series representation of the solution to (10.6) is given by (10.7) with coefficients (10.8). We make a few observations:

1. As the amplitude of the mode depends on $(r/a)^n$ with $r/a \leq 1$, high modes — modes with a large n that exhibit rapid oscillation on the boundary — decay rapidly away from the boundary. This behavior is shown in Figure 10.4 and is similar to the decay away from the boundary observed for rectangular domains.
2. The solution (as expected) satisfies the mean-value formulas over Ω and $\partial\Omega$. The value at the center of the disk is

$$u(r = 0, \theta) = \frac{1}{2}A_0.$$

The average of the solution over the disk is

$$\begin{aligned} \frac{1}{\pi a^2} \int_{\Omega} u dx &= \frac{1}{\pi a^2} \int_{\theta=-\pi}^{\pi} \int_{r=0}^a \left(\frac{1}{2}A_0 + \sum_{n=1}^{\infty} \left(\frac{r}{a}\right)^n (A_n \cos(n\theta) + B_n \sin(n\theta)) \right) r dr d\theta \\ &= \frac{1}{\pi a^2} \int_{\theta=-\pi}^{\pi} \int_{r=0}^a \frac{1}{2}A_0 r dr d\theta = \frac{1}{2}A_0, \end{aligned}$$

where the second equality follows because all of the sine and cosine integrals vanish when integrated over $(-\pi, \pi)$. The average over the circumference is

$$\begin{aligned} \frac{1}{2\pi a} \int_{\partial\Omega} u ds &= \frac{1}{2\pi a} \int_{\theta=-\pi}^{\pi} u(r = a, \theta) a d\theta \\ &= \frac{1}{2\pi a} \int_{\theta=-\pi}^{\pi} \left(\frac{1}{2}A_0 + \sum_{n=1}^{\infty} (A_n \cos(n\theta) + B_n \sin(n\theta)) \right) a d\theta \\ &= \frac{1}{2\pi a} \int_{\theta=-\pi}^{\pi} \frac{1}{2}A_0 a d\theta = \frac{1}{2}A_0, \end{aligned}$$

where the third equality again follows because all of the sine and cosine integrals vanish. Hence, we observe that, for any boundary condition g , the value of the solution at the center of the disk is equal to (i) its average over the disk and (ii) its average over the circumference, as expected from the mean-value formulas.

Example 10.2 (Laplace's equation on a disk). Let $\Omega \equiv \{x \in \mathbb{R}^2 \mid \|x\|_2 < 2\}$ and consider

$$\begin{aligned} -\Delta u &= 0 \quad \text{in } \Omega, \\ u(r = 2, \theta) &= 1 + \cos(3\theta), \quad \theta \in [-\pi, \pi]. \end{aligned}$$

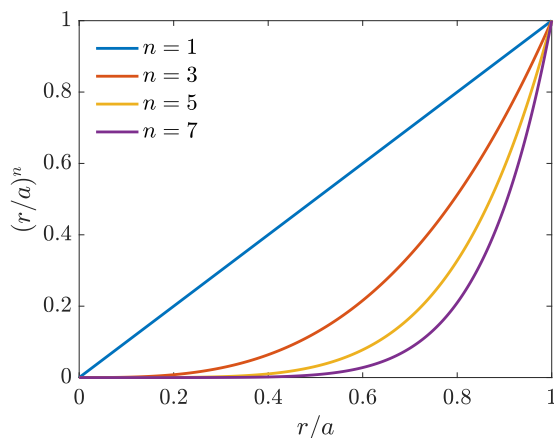


Figure 10.4: Function $(r/a)^n$.

We wish to find the solution to the boundary value problem. We could find the Fourier coefficients using the formula (10.8), but for this simple boundary condition we can find the coefficients by inspection. Namely, we wish to find $(A_n)_{n=0}^{\infty}$ and $(B_n)_{n=1}^{\infty}$ such that

$$u(r = 2, \theta) = \frac{1}{2}A_0 + \sum_{n=1}^{\infty} (A_n \cos(n\theta) + B_n \sin(n\theta)) = 1 + \cos(3\theta).$$

We match the coefficients on the left and right hand side to observe that $A_0/2 = 1$ (i.e., $A_0 = 2$), $A_3 = 1$, and all other coefficients should be zero. Hence the solution is

$$u(r, \theta) = 1 + \left(\frac{r}{2}\right)^3 \cos(3\theta).$$

Figure 10.5 shows the solution. We observe, as expected, the solution is smooth. In addition, we readily verify the (weak) maximum and minimum principles: the maximum and minimum of 2 and 0, respectively, occur on the boundary. The strong maximum and minimum principles are also satisfied: the solution strictly inside of the domain Ω (i.e., not on the boundary) are all strictly greater than 0 and strictly less than 2, since $(r/2)^3 < 1$ for all $r < 2$. Finally, we observe that the mean-value formulas are satisfied; the value at the center, the average over the disk, and the average over the circumference are all equal to 1.

10.4 Summary

We summarize key points of this lecture:

1. Separation of variables can be applied to solve Laplace's equation in two (or higher) dimensions.
2. The solution to Laplace's equation on a rectangle or disk can be expressed in terms of the Fourier coefficients of the boundary data.

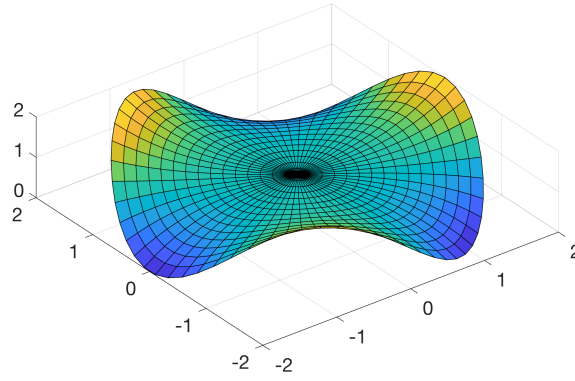


Figure 10.5: Solution to Laplace's equation on a disk.

3. The harmonic function on a rectangle or disk decays away from the boundary. The solution decays more rapidly for more oscillatory boundary functions; i.e., the effect of highly oscillatory boundary modes are confined to the thin region near the boundary.

Lecture 11

Laplace's equation: fundamental solutions and Green's functions

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11.1 Introduction

In this lecture we seek the *fundamental solution* of Laplace's equation and appeal to the principle of linear superposition to solve Laplace's and Poisson's equations. The technique allows us to naturally analyze the solution to Laplace's equation in unbounded domains. We will also apply the method of reflection to find *Green's functions* and solve boundary value problems.

11.2 Fundamental solution

We first introduce the Dirac delta distribution, which is important to characterize the fundamental solution.

Definition 11.1 (Dirac delta distribution). The Dirac delta distribution δ over \mathbb{R}^n is a distribution (or “function”) such that

$$\begin{aligned}\delta(x) &= 0, \quad x \neq 0, \\ \int_{\mathbb{R}^n} \delta(x) dx &= 1, \\ \int_{\mathbb{R}^n} f(x) \delta(x - a) dx &= f(a), \quad \forall a \in \mathbb{R}^n,\end{aligned}$$

where $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is continuous at a .

We wish to develop a better insight about the Dirac delta distribution. To this end, we restrict ourselves to \mathbb{R}^1 and recall the definition of a Gaussian $g : \mathbb{R} \rightarrow \mathbb{R}$ centered about the origin with a standard deviation σ :

$$g(x; \sigma) = \frac{1}{\sqrt{2\pi\sigma^2}} \exp\left(-\frac{1}{2} \frac{x^2}{\sigma^2}\right).$$

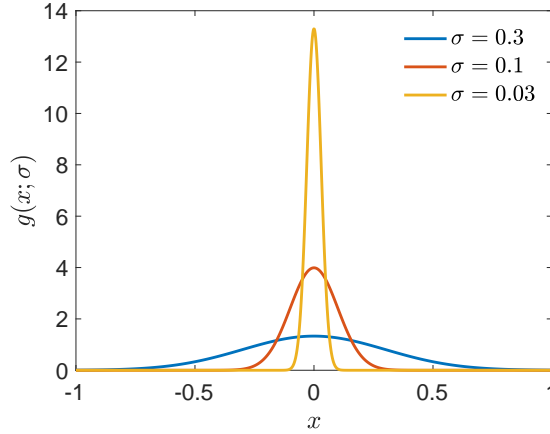


Figure 11.1: Gaussian functions for a few different values of σ .

Figure 11.1 shows Gaussian functions for a few different values of σ . The Dirac delta distribution can be thought of as a Gaussian in the limit of $\sigma \rightarrow 0$. To see this, we make three observations:

1. A Gaussian $g(x; \sigma)$ is nearly zero for any x such that $|x| \gg \sigma$. This becomes the first property of Dirac delta in the limit of $\sigma \rightarrow 0$; i.e., for $x \neq 0$, $\delta(x) \rightarrow 0$ as $\sigma \rightarrow 0$.
2. For any $\sigma > 0$, a Gaussian satisfies

$$\int_{\mathbb{R}} g(x, \sigma) dx = 1,$$

which is the second property of Dirac delta: $\int_{\mathbb{R}} \delta(x) dx = 1$.

3. The convolution of a Gaussian with a function,

$$\int_{\mathbb{R}} g(x - a, \sigma) f(x) dx,$$

provides an weighted average of f near a , where the nearness is defined by σ . In the limit of $\sigma \rightarrow 0$, this becomes the third property of Dirac delta: $\int_{\mathbb{R}} \delta(x - a) f(x) dx = f(a)$.

Having defined the Dirac delta distribution, we now introduce the fundamental solution of Laplace's equation.

Definition 11.2 (fundamental solution of Laplace's equation). The fundamental solution to Laplace's equation is the function $\Phi : \mathbb{R}^n \rightarrow \mathbb{R}$ such that

$$-\Delta \Phi = \delta \quad \text{in } \mathbb{R}^n,$$

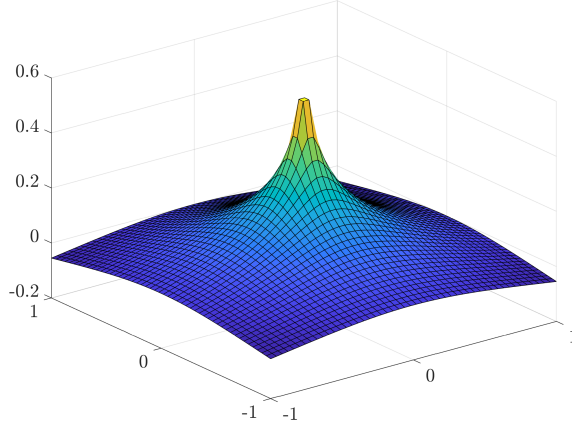


Figure 11.2: The fundamental solution of Laplace's equation in \mathbb{R}^2 . Note that the function is unbounded at the origin.

where δ is the Dirac delta function. The fundamental solutions are given by

$$\Phi(x) = \begin{cases} -\frac{1}{2}\|x\|, & n = 1, \\ -\frac{1}{2\pi} \log \|x\|, & n = 2, \\ \frac{1}{4\pi\|x\|}, & n = 3, \\ \frac{1}{\sigma_n(n-2)\|x\|^{n-2}}, & n \geq 4, \end{cases}$$

where σ_n is the surface area of the n -dimensional unit ball, and $\|x\| \equiv \sqrt{x_1^2 + \cdots + x_n^2}$.

First part of proof (for \mathbb{R}^2). We first prove the result for \mathbb{R}^2 for which $\Phi(x) = -\frac{1}{2\pi} \log \|x\| = -\frac{1}{2\pi} \log(r)$, where $r \equiv \|x\|$. We first verify that the Green's function satisfies Laplace's equation for any $r > 0$:

$$-\Delta\Phi = -\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial\Phi}{\partial r} \right) - \frac{1}{r^2} \frac{\partial^2\Phi}{\partial\theta^2} = -\frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{\partial}{\partial r} \left(-\frac{1}{2\pi} \log(r) \right) \right) = \frac{1}{2\pi} \frac{1}{r} \frac{\partial}{\partial r} \left(r \frac{1}{r} \right) = 0,$$

for $r > 0$, and hence $-\Delta\Phi(x) = 0$ for $x \neq 0$.

Showing $-\Delta\Phi = \delta$ requires the knowledge of distribution; this is beyond the scope of this course. \square

Figure 11.2 shows the fundamental solution of Laplace's equation in \mathbb{R}^2 . The function is unbounded at the origin and decays rapidly away from the origin. By definition, the function is harmonic everywhere except at the origin. In electrostatics, the fundamental solution represents the electric potential associated with a single point charge at the origin.

11.3 Poisson's equation in \mathbb{R}^n

We now use the fundamental solution to solve Poisson's problem in \mathbb{R}^n :

Theorem 11.3. Suppose $f : \mathbb{R}^n \rightarrow \mathbb{R}$ is twice continuously differentiable and has a compact support. Then a solution to Poisson's problem

$$-\Delta u = f \quad \text{in } \mathbb{R}^n$$

can be expressed as

$$u(x) = \int_{\mathbb{R}^n} \Phi(x - \xi) f(\xi) d\xi,$$

where $\Phi : \mathbb{R}^n \rightarrow \mathbb{R}$ is the fundamental solution to Laplace's equation.

Proof. The proof is beyond the scope of this course.

However, using the definition of the fundamental solution and the Dirac delta distribution, we may at least formally show

$$-\Delta u(x) = - \int_{\mathbb{R}^n} \Delta \Phi(x - \xi) f(\xi) d\xi = \int_{\mathbb{R}^n} \delta(x - \xi) f(\xi) d\xi = f(x),$$

and hence $-\Delta u(x) = f(x) \forall x \in \mathbb{R}^n$. □

11.4 Green's function

We now consider the solution of Laplace's (and Poisson's) equation in a domain Ω with a boundary using *Green's functions*, which are similar to the fundamental solution but incorporates the boundary condition.

Definition 11.4 (Green's function). A Green's function in Ω is a function $G : \Omega \times \Omega \rightarrow \mathbb{R}$ that satisfies, for each fixed $\xi \in \Omega$,

$$\begin{aligned} -\Delta G(x, \xi) &= \delta(x - \xi) \quad \forall x \in \Omega, \\ G(x, \xi) &= 0 \quad \forall x \in \partial\Omega. \end{aligned}$$

We can equivalently interpret $G(\cdot, \xi) : \Omega \rightarrow \mathbb{R}$ as a function that satisfies, for each fixed $\xi \in \Omega$,

$$\begin{aligned} -\Delta G(\cdot, \xi) &= \delta_\xi \quad \text{in } \Omega, \\ G(\cdot, \xi) &= 0 \quad \text{on } \partial\Omega, \end{aligned}$$

where δ_ξ is the Dirac delta distribution centered about ξ (i.e., $\delta_\xi(x) = \delta(x - \xi)$). Like the fundamental solution, a Green's function $G(\cdot, \xi)$ is harmonic everywhere except at ξ ; however, unlike the fundamental solution, the Green's function is associated with a particular domain with a boundary $\partial\Omega$. In electrostatics, the Green's function $G(\cdot, \xi)$ represents the electric potential associated with a single point charge at ξ inside a conducting boundary $\partial\Omega$ (where the potential vanishes).

We first note that Green's functions are symmetric.

Theorem 11.5 (symmetry of Green's function). For any $x, \xi \in \Omega$, $x \neq \xi$,

$$G(x, \xi) = G(\xi, x).$$

Proof. Proof is provided in Appendix 11.A. □

The symmetry of Green's functions is known as the *principle of reciprocity*. In electrostatics, the symmetry implies that (i) the potential at point a due to a point charge at b and (ii) the potential at point b due to a point charge at a are the same.

The Green's function provides the following solution representation for nonhomogeneous Dirichlet boundary value problem:

Theorem 11.6 (Green's representation formula). Let $G : \Omega \rightarrow \mathbb{R}$ be the Green's function associated with a domain Ω . Then the solution to the Poisson equation

$$\begin{aligned} -\Delta u &= f & \text{in } \Omega, \\ u &= g & \text{on } \partial\Omega \end{aligned}$$

can be expressed as

$$u(x) = \int_{\Omega} G(x, \xi) f(\xi) d\xi - \int_{\partial\Omega} \nu \cdot \nabla_{\xi} G(x, \xi) g(\xi) d\xi. \quad (11.1)$$

Proof. Proof is provided in Appendix 11.A.

We may also at least formally obtain the expression from the definition of the delta distribution and two successive applications of integration by parts:

$$\begin{aligned} u(\xi) &= \int_{\Omega} \delta(\xi - x) u(x) dx = - \int_{\Omega} \Delta G(x, \xi) u(x) dx \\ &= \int_{\Omega} \nabla G(x, \xi) \cdot \nabla u(x) dx - \int_{\partial\Omega} \nu \cdot \nabla G(x, \xi) u(x) dx \\ &= - \int_{\Omega} G(x, \xi) \Delta u(x) dx + \int_{\partial\Omega} G(x, \xi) \nu \cdot \nabla u(x) dx - \int_{\partial\Omega} \nu \cdot \nabla G(x, \xi) u(x) dx \\ &= \int_{\Omega} G(x, \xi) f(x) dx - \int_{\partial\Omega} \nu \cdot \nabla G(x, \xi) g(x) dx, \end{aligned}$$

where the last equality follows from $G(\cdot, \xi) = 0$ on $\partial\Omega$. We finally appeal to the symmetry of the Green's function to obtain the desired result. \square

The representation formula allows us to express the solution to the Poisson's problem as the convolution of the Green's function and the source/boundary data f and g . The Green's function for problems with boundaries (in Theorem 11.6) plays an analogous role as the fundamental solution for problems without boundaries (in Theorem 11.3).

11.5 Finding Green's functions: general formulation

In general, a Green's function, which satisfies Definition 11.4, can be expressed in terms of the fundamental solution Φ and a "correction function" Ψ . Namely, we consider the decomposition of the form

$$G(x, \xi) = \Phi(x - \xi) + \Psi(x, \xi).$$

We apply the Laplacian to the decomposition to obtain

$$-\Delta G(x, \xi) = -\Delta \Phi(x - \xi) - \Delta \Psi(x, \xi) = \delta(x - \xi) - \Delta \Psi(x, \xi) \quad \forall x, \xi \in \Omega.$$

Since we wish $-\Delta G(x, \xi) = \delta(x - \xi)$, we conclude that

$$-\Delta \Psi(x, \xi) = 0 \quad \forall x, \xi \in \Omega.$$

We next apply the boundary condition for the Green's function to the decomposition to obtain

$$G(x, \xi) = \Phi(x - \xi) + \Psi(x, \xi) = 0 \quad \forall x \in \partial\Omega, \forall \xi \in \Omega,$$

which implies that

$$\Psi(x, \xi) = -\Phi(x - \xi), \quad \forall x \in \partial\Omega, \forall \xi \in \Omega.$$

Thus, the correction function $\Psi : \Omega \times \Omega \rightarrow \mathbb{R}$ must satisfy, for each fixed $\xi \in \Omega$,

$$\begin{aligned} -\Delta_x \Psi(x, \xi) &= 0 \quad \forall x \in \Omega \\ \Psi(x, \xi) &= -\Phi(x - \xi) \quad \forall x \in \partial\Omega. \end{aligned}$$

The correction function, unlike the fundamental solution, does not contain a singularity and is harmonic everywhere in Ω .

11.6 Green's function for the upper half plane

We consider Laplace's problem on the upper half plane. To this end, we introduce the boundary $\Gamma \equiv \{(x_1, x_2) \mid x_2 = 0\}$ and the domain $\Omega \equiv \{(x_1, x_2) \mid x_2 > 0\}$. Poisson's problem is

$$\begin{aligned} -\Delta u &= 0 \quad \text{in } \Omega, \\ u &= g \quad \text{on } \Gamma. \end{aligned} \tag{11.2}$$

We solve the problem in two steps: we first find the Green's function; we then apply Green's representation formula.

To find the Green's function, we use *the method of images* (or *the method of reflection*) and express the Green's function as a sum of fundamental solutions. The idea is to choose an *image point* $\tilde{\xi} \in \mathbb{R}^2 \setminus \Omega$ associated with the reflection of ξ about the axis $x_2 = 0$; i.e.,

$$\tilde{\xi} = (\tilde{\xi}_1, \tilde{\xi}_2) \equiv (\xi_1, -\xi_2).$$

The image point $\tilde{\xi}$ associated with the point ξ has an important property that any point on the boundary Γ is equidistant from ξ and $\tilde{\xi}$; as we will see shortly, this property is important to enforce the boundary condition. We then choose the correction function

$$\Psi(x, \xi) = -\Phi(x - \tilde{\xi}),$$

so that the Green's function is

$$G(x, \xi) = \Phi(x - \xi) - \Phi(x - \tilde{\xi}) = -\frac{1}{2\pi} \log \|x - \xi\| + \frac{1}{2\pi} \log \|x - \tilde{\xi}\|.$$

We observe the following:

1. The Green's function $G(x, \xi)$ is harmonic everywhere in Ω except at ξ since (i) $\Phi(x - \xi)$ is harmonic everywhere except at ξ and (ii) $\Phi(x - \tilde{\xi})$ is harmonic everywhere (since $\tilde{\xi} \notin \Omega$).

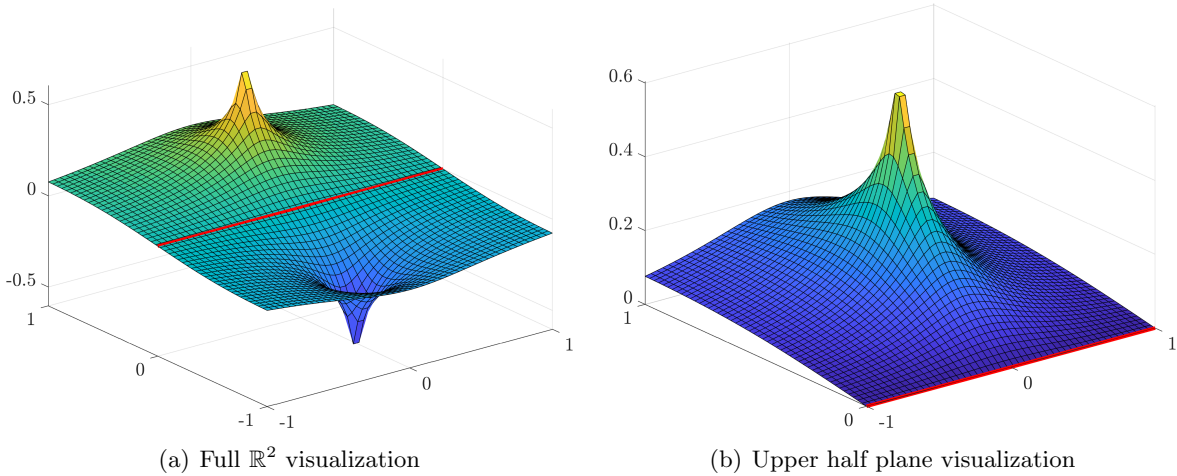


Figure 11.3: Green's function for the upper half plane $G(x, \xi \equiv (0, 0.5))$. The function is unbounded at $\xi = (0, 0.5)$ (and at the image point $\tilde{\xi} = (0, -0.5)$). The red line indicates the boundary.

2. The value of the fundamental solution depends only on the distance between two points, and the distance from x to ξ and from x to $\tilde{\xi}$ are the same for all $x \in \Gamma$. Hence, for any $x \in \Gamma$, $\Phi(x - \xi) = \Phi(x - \tilde{\xi})$, which implies $G(x, \xi) = \Phi(x - \xi) - \Phi(x - \tilde{\xi}) = 0$. Thus the boundary condition for the Green's function is satisfied.

Figure 11.3 shows the Green's function $G(x, \xi \equiv (0, 0.5))$ for the upper half plane.

We now wish to represent the solution to Laplace's problem (11.2) using the representation formula (11.1). To this end, we first evaluate the directional derivative $\nu \cdot \nabla_{\xi} G(x, \xi)$ to find

$$\nu \cdot \nabla_{\xi} G(x, \xi) = -\frac{\partial G(x, \xi)}{\partial \xi_2} = \frac{1}{2\pi} \frac{\partial}{\partial \xi_2} \left(\log \|x - \xi\| - \log \|x - \tilde{\xi}\| \right) = \frac{1}{2\pi} \left(\frac{\xi_2 - x_2}{\|x - \xi\|^2} - \frac{\xi_2 + x_2}{\|x - \tilde{\xi}\|^2} \right),$$

where the first equality follows from $\nu = (0, -1)$ on Γ for the upper half plane, and the last equality follows from $\tilde{\xi}_2 = -\xi_2$. For $\xi \in \Gamma$, $\xi = \tilde{\xi}$ and hence

$$\nu \cdot \nabla_{\xi} G(x, \xi) = -\frac{x_2}{\pi} \frac{1}{\|x - \xi\|^2}.$$

We appeal to (11.1) and find that the solution to (11.2) is

$$u(x) = \int_{\Omega} G(x, \xi) f(\xi) d\xi - \int_{\Gamma} \nu \cdot \nabla_{\xi} G(x, \xi) g(\xi) d\xi = \frac{1}{\pi} \int_{\Gamma} \frac{x_2}{\|x - \xi\|^2} g(\xi) d\xi,$$

where the integral over Ω vanished because $f = 0$. This solution representation is called *Poisson's formula for the upper half plane (in \mathbb{R}^2)*. The function

$$K(x, \xi) \equiv \frac{1}{\pi} \frac{x_2}{\|x - \xi\|^2},$$

which multiplies the boundary function g , is called *Poisson's kernel for the upper half plane (in \mathbb{R}^2)*.

We make a few observations

1. If $g \geq 0$ everywhere on Γ and $g > 0$ somewhere on Γ , then the solution is strictly positive ($u > 0$) everywhere in the upper half plane. This is consistent with the strong maximum principle.
2. Any disturbance in the boundary condition affects the solution everywhere in the upper half plane because Poisson's kernel is nonzero everywhere.
3. In \mathbb{R}^2 , the effect of the disturbance decays as $\sim 1/x_2$ as we move away from the plane. In other words, while the disturbance in the boundary condition affects solution everywhere in the domain, its effect decays away from the boundary.

Remark 11.7 (Poisson's formula for upper half plane in \mathbb{R}^n). Following the same derivation as the above, we can show that Poisson's formula for the upper half plane in \mathbb{R}^n is

$$u(x) = \frac{2}{n\alpha_n} \int_{\Gamma} \frac{x_n}{\|x - \xi\|^n} g(\xi) d\xi,$$

where α_n is the volume of the unit ball in \mathbb{R}^n (e.g., $\alpha_{n=2} = \pi$, $\alpha_{n=3} = 4/3\pi$).

Example 11.8 (Laplace's equation in the upper half plane). We consider a boundary-value problem

$$\begin{aligned} -\Delta u &= 0 & \text{in } \Omega \equiv \{(x_1, x_2) \mid x_2 > 0\}, \\ u &= g & \text{on } \Gamma \equiv \{(x_1, x_2) \mid x_2 = 0\}, \end{aligned}$$

where

$$g((x_1, 0)) \equiv \begin{cases} 1, & x_1 \in (-1/2, 1/2), \\ 0, & \text{otherwise.} \end{cases}$$

Using Poisson's formula for the upper half plane, we can express the solution as

$$u(x) = \frac{1}{\pi} \int_{\Gamma} \frac{x_2}{\|x - \xi\|^2} g(\xi) d\xi = \frac{1}{\pi} \int_{\xi_1=-1/2}^{1/2} \frac{x_2}{(x_1 - \xi_1)^2 + x_2^2} d\xi_1,$$

where the last equality follows from $\xi = (\xi_1, 0)$ on the boundary Γ . Figure 11.4 shows the solution. We observe that even though the boundary condition is discontinuous, the solution is smooth everywhere in the upper half plane (excluding the boundary). We also observe that the strong maximum principle is satisfied and the solution is strictly positive everywhere (excluding the boundary).

11.7 Green's function for a disk

We now consider the solution of Laplace's problem on a disk $\Omega \equiv B(0, a) = \{x \in \mathbb{R}^2 \mid \|x\| < a\}$ of radius a :

$$\begin{aligned} -\Delta u &= 0 & \text{in } \Omega, \\ u &= g & \text{on } \partial\Omega. \end{aligned} \tag{11.3}$$

We again solve the problem in two steps: we first find the Green's function; we then apply the Green's representation formula.

As before, to find the Green's function, we wish to find the correction function Ψ which takes on the same value as the fundamental solution Φ on the boundary. To this end, we first introduce the *dual point* with respect to the disk.

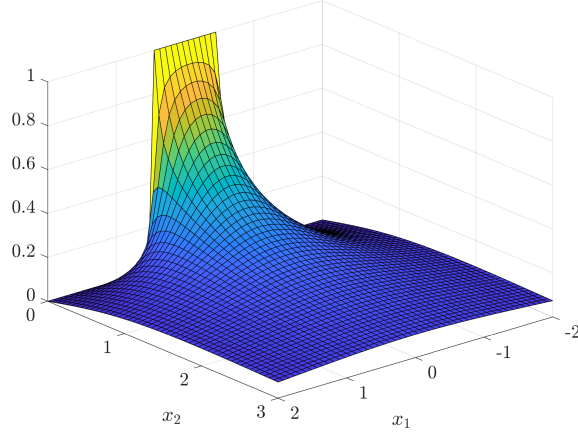


Figure 11.4: Solution to a Poisson's problem in the upper half plane.

Definition 11.9 (dual point with respect to a circle). The point

$$\tilde{\xi} \equiv \frac{a^2}{\|\xi\|^2} \xi.$$

is said to be dual to ξ with respect to the circle $\partial B(0, a)$. For any fixed $\xi \in B(0, a)$, the dual point satisfies for $x \in \partial B(0, a)$,

$$\|x - \xi\| = \frac{\|\xi\|}{a} \|x - \tilde{\xi}\|.$$

Proof. We first observe that

$$\frac{\|\xi\|}{a} \|x - \tilde{\xi}\| = \frac{\|\xi\|}{a} \left\| x - \frac{a^2}{\|\xi\|^2} \xi \right\| = \left\| \frac{\|\xi\|}{a} x - \frac{a}{\|\xi\|} \xi \right\| = \left(\frac{\|\xi\|^2}{a^2} x \cdot x - 2x \cdot \xi + \frac{a^2}{\|\xi\|^2} \xi \cdot \xi \right)^{1/2}.$$

Since $x \cdot x = a^2$ for $x \in \partial B(0, a)$,

$$\frac{\|\xi\|}{a} \|x - \tilde{\xi}\| = (\|\xi\|^2 - 2x \cdot \xi + \|x\|^2)^{1/2} = \|x - \xi\|,$$

which is the desired relationship. □

Given $\|x - \xi\| = \frac{\|\xi\|}{a} \|x - \tilde{\xi}\|$ for $x \in \partial B(0, a)$, we choose the correction function

$$\Psi(x, \xi) = -\Phi\left(\frac{\|\xi\|}{a}(x - \tilde{\xi})\right)$$

so that the Green's function is

$$G(x, \xi) = \Phi(x - \xi) - \Phi\left(\frac{\|\xi\|}{a}(x - \tilde{\xi})\right) = -\frac{1}{2\pi} \log(\|x - \xi\|) + \frac{1}{2\pi} \log\left(\frac{\|\xi\|}{a} \|x - \tilde{\xi}\|\right).$$

The Green's function then satisfies the boundary condition. Figure 11.5 shows the Green's function $G(x, \xi \equiv (0.4, 0))$ for the unit disk.

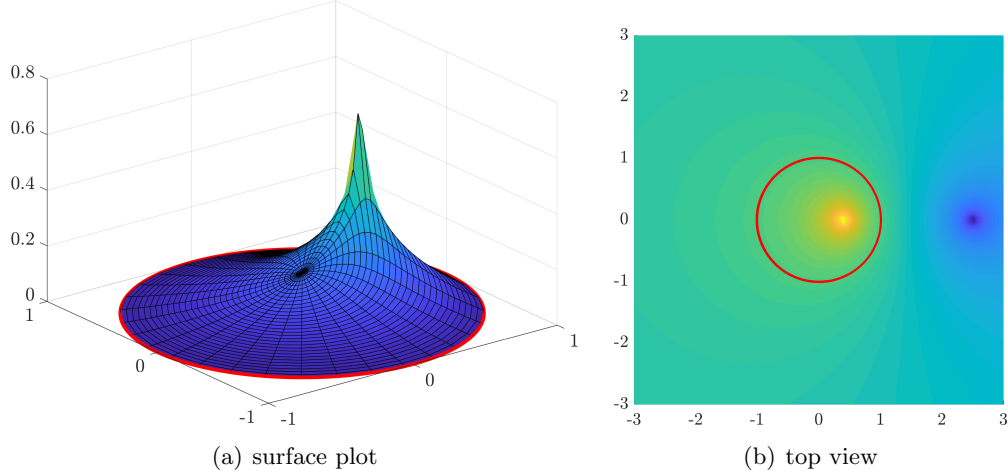


Figure 11.5: Green's function for the unit disk $G(x, \xi \equiv (0.4, 0))$. The function is unbounded at $\xi = (0.4, 0.0)$ (and at the dual point $\tilde{\xi} = (2.5, 0.0)$). The red line indicates the boundary.

We now wish to represent the solution to Laplace's problem (11.3) using the representation formula (11.1). After the tedious but straightforward evaluation of $\nu \cdot \nabla_{\xi} G(x, \xi)$ for $\xi \in \partial B(0, a)$, we find a solution representation:

$$u(x) = - \int_{\partial\Omega} \nu \cdot \nabla_{\xi} G(x, \xi) g(\xi) d\xi = \frac{a^2 - \|x\|^2}{2\pi a} \int_{\partial B(0, a)} \frac{g(\xi)}{\|x - \xi\|^2} d\xi.$$

This formula is called the *Poisson's formula for a disk (in \mathbb{R}^2)*. The function

$$K(x, \xi) \equiv \frac{a^2 - \|x\|^2}{2\pi a} \frac{1}{\|x - \xi\|^2},$$

which multiplies the boundary function g is called *Poisson's kernel for a disk (in \mathbb{R}^2)*.

Remark 11.10 (Poisson's formula for a ball in \mathbb{R}^n). Following the same derivation as the above, we can show that Poisson's formula for a ball $B(0, a) \subset \mathbb{R}^n$ is

$$u(x) = \frac{1}{n\alpha_n a} \int_{\partial B(0, a)} \frac{a^2 - \|x\|^2}{\|x - \xi\|^n} g(\xi) d\xi,$$

where α_n is the volume of the unit ball in \mathbb{R}^n .

Example 11.11 (Laplace's equation in a disk). We consider a boundary-value problem

$$\begin{aligned} -\Delta u &= 0 & \text{in } \Omega \equiv \{x \in \mathbb{R}^2 \mid \|x\| < 1\}, \\ u &= g & \text{on } \partial\Omega, \end{aligned}$$

where

$$g((r = 1, \theta)) \equiv \begin{cases} 1, & \theta \in (-\pi/10, \pi/10), \\ 0, & \text{otherwise.} \end{cases}$$

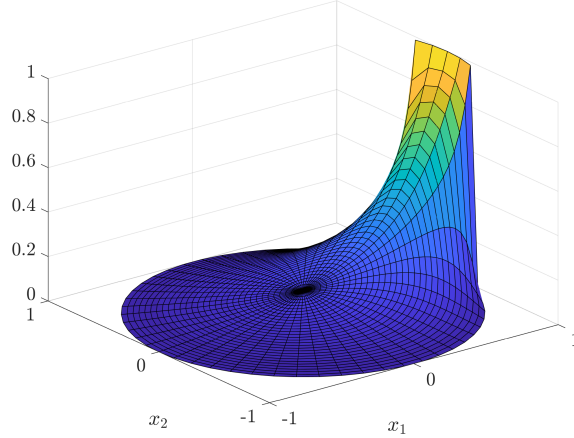


Figure 11.6: Solution to a Poisson's problem in a disk.

Using Poisson's formula for a unit disk, we can express the solution as

$$u(x) = \frac{a^2 - \|x\|^2}{2\pi a} \int_{\partial B(0,a)} \frac{g(\xi)}{\|x - \xi\|^2} d\xi = \frac{1^2 - \|x\|^2}{2\pi} \int_{-\pi/10}^{\pi/10} \frac{1}{(x_1 - \cos(\theta))^2 + (x_2 - \sin(\theta))^2} d\theta,$$

where the last equality follows from $\xi = (\cos(\theta), \sin(\theta))$ on $\partial B(0, a = 1)$. Figure 11.6 shows the solution. We observe that even though the boundary condition is discontinuous, the solution is smooth everywhere in the disk (excluding the boundary). We also observe that the strong maximum principle is satisfied and the solution is strictly positive everywhere (excluding the boundary).

Example 11.12 (proof of mean value formula by Poisson's formula). We evaluate Poisson's formula (for the disk) at the origin $x = 0$ to find that

$$u(0) = \frac{a^2}{2\pi a} \int_{\partial B(0,a)} \frac{g(\xi)}{a^2} d\xi = \frac{1}{2\pi a} \int_{\partial B(0,a)} g(\xi) d\xi,$$

which is the mean value formula.

11.8 Summary

We summarize key points of this lecture:

1. The Dirac delta distribution vanishes everywhere except at the origin and yet integrates to 1; it can be thought of as the Gaussian function in the limit of the standard deviation approaching 0.
2. The fundamental solution of Laplace's equation satisfies the Poisson's equation with the delta distribution as the source in \mathbb{R}^n . The fundamental solution decays rapidly away from the origin.
3. The solution to Poisson's equation in \mathbb{R}^n can be expressed as the convolution of the fundamental solution with the source function.

4. Green's function of Laplace's equation on $\Omega \subset \mathbb{R}^n$ satisfies the Poisson's equation with the Dirac delta distribution as the source and vanishes on $\partial\Omega$.
5. Green's function is symmetric. This is known as the principle of reciprocity.
6. The solution to Poisson's problem on $\Omega \subset \mathbb{R}^n$ with Dirichlet boundary conditions can be expressed using the Green's representation formula.
7. Green's function for a half plane can be found using the method of reflection (a.k.a. method of images).
8. Green's function for a disk can be found using the method of reflection using the concept of dual points.

11.A Proofs of properties of Green's functions

Before we prove properties of Green's function, we introduce Green's second identity, which helps us prove the properties.

Proposition 11.13 (Green's second identity). For all $w, u \in C^2(\Omega)$,

$$\int_{\Omega} (w\Delta u - u\Delta w) dx = \int_{\partial\Omega} (w(\nu \cdot \nabla u) - u(\nu \cdot \nabla w)) ds.$$

Proof. We invoke integration by parts twice to yield

$$\int_{\Omega} w\Delta u dx = \int_{\partial\Omega} w(\nu \cdot \nabla u) ds - \int_{\Omega} \nabla w \cdot \nabla u dx = \int_{\partial\Omega} (w(\nu \cdot \nabla u) - (\nu \cdot \nabla w)u) ds + \int_{\Omega} (\Delta w)u dx.$$

The subtraction of $\int_{\Omega} (\Delta w)u dx$ from both sides yields the desired result. \square

Proposition 11.14. Let $\Phi : \mathbb{R}^n \rightarrow \mathbb{R}$ be the fundamental solution of Laplace's equation. Then, for any continuously differentiable u ,

$$\lim_{\epsilon \rightarrow 0} \int_{\partial B(a, \epsilon)} (\Phi(x-a) \frac{\partial u}{\partial \nu}(x) - u(x) \frac{\partial \Phi}{\partial \nu}(x-a)) dx = u(a),$$

where $B(a, \epsilon)$ is the ball of radius ϵ centered about a , and $\frac{\partial u}{\partial \nu}(x) \equiv \nu \cdot \nabla u(x)$ for ν the outward-pointing normal on the surface of the ball.

Proof. We prove the result in two dimensions ($n = 2$), for which $\Phi(x) = -\frac{1}{2\pi} \log \|x\|$. The proof for other dimensions follows similarly. We first note that, for any fixed $\epsilon > 0$,

$$\begin{aligned} (\star) &\equiv \int_{\partial B(a, \epsilon)} (\Phi(x-a) \frac{\partial u}{\partial \nu}(x) - u(x) \frac{\partial \Phi}{\partial \nu}(x-a)) dx \\ &= -\frac{1}{2\pi} \log(\epsilon) \int_{\partial B(a, \epsilon)} \frac{\partial u}{\partial \nu}(x) dx + \frac{1}{2\pi\epsilon} \int_{\partial B(a, \epsilon)} u(x) dx, \end{aligned}$$

where the equality follows because (i) the fundamental solution depends only on the distance from a , and hence (ii) $\Phi(x-a) = -\frac{1}{2\pi} \log(\epsilon)$ and $\frac{\partial \Phi}{\partial \nu}(x-a) = \frac{\partial}{\partial r}(-\frac{1}{2\pi} \log(r))|_{r=\epsilon} = \frac{1}{2\pi\epsilon}$ for any $x \in \partial B(a, \epsilon)$. We now rewrite the integrals in terms of the mean over the surface of the ball to obtain

$$(\star) = -\frac{1}{2\pi} \log(\epsilon) 2\pi\epsilon \operatorname{mean}_{\partial B(a, \epsilon)} \left(\frac{\partial u}{\partial \nu} \right) + \frac{1}{2\pi\epsilon} 2\pi\epsilon \operatorname{mean}_{\partial B(a, \epsilon)} (u) = -\log(\epsilon) \operatorname{mean}_{\partial B(a, \epsilon)} \left(\frac{\partial u}{\partial \nu} \right) + \operatorname{mean}_{\partial B(a, \epsilon)} (u),$$

where $\operatorname{mean}_{\partial B(a, \epsilon)} \left(\frac{\partial u}{\partial \nu} \right) \equiv \frac{1}{2\pi\epsilon} \int_{\partial B(a, \epsilon)} \frac{\partial u}{\partial \nu}(x) dx$ and $\operatorname{mean}_{\partial B(a, \epsilon)} (u) \equiv \frac{1}{2\pi\epsilon} \int_{\partial B(a, \epsilon)} u(x) dx$. Since u continuously differentiable, $\frac{\partial u}{\partial \nu}$ and u are bounded and so are their means. Moreover, since $\lim_{\epsilon \rightarrow 0} \epsilon \log(\epsilon) = 0$, the first term is 0 in the limit of $\epsilon \rightarrow 0$. It follows that

$$\lim_{\epsilon \rightarrow 0} (\star) = \lim_{\epsilon \rightarrow 0} \operatorname{mean}_{\partial B(a, \epsilon)} (u) = u(a),$$

which is the desired result. \square

Proof of symmetry of Green's function. We first introduce $u(x) = G(x, a) = \Phi(x - a) + \Psi(x, a)$ and $w(x) = G(x, b) = \Phi(x - b) + \Psi(x, b)$, where $G(x, a)$ and $G(x, b)$ are Green's functions on Ω , and $\Psi(x, a)$ and $\Psi(x, b)$ are the associated correction functions. We next introduce a domain $\Omega_\epsilon \equiv \Omega \setminus (\overline{B(a, \epsilon)} \cup \overline{B(b, \epsilon)})$ for $\epsilon > 0$ but sufficiently small; i.e., Ω with two holes centered about a and b . Both u and w are harmonic in Ω_ϵ since the holes remove the singularity in the Green's functions. We now invoke the Green's second identity with u and w . The left hand side of the Green's second identity over Ω_ϵ is

$$(\text{LHS}) = \int_{\Omega_\epsilon} (G(x, b)\Delta G(x, a) - G(x, a)\Delta G(x, b))dx = 0;$$

the term vanishes because $G(x, a)$ and $G(x, b)$ are harmonic everywhere in Ω_ϵ and hence $\Delta G(x, a) = \Delta G(x, b) = 0$ for all $x \in \Omega_\epsilon$. We next note that the right hand side of the Green's second identity over Ω_ϵ is

$$\begin{aligned} (\text{RHS}) &= \int_{\partial\Omega_\epsilon} (w \frac{\partial u}{\partial \nu} - u \frac{\partial w}{\partial \nu})dx \\ &= \int_{\partial\Omega} (w \frac{\partial u}{\partial \nu} - u \frac{\partial w}{\partial \nu})dx - \int_{\partial B(a, \epsilon)} (w \frac{\partial u}{\partial \nu} - u \frac{\partial w}{\partial \nu})dx - \int_{\partial B(b, \epsilon)} (w \frac{\partial u}{\partial \nu} - u \frac{\partial w}{\partial \nu})dx \\ &\equiv C_\Omega - A_\epsilon - B_\epsilon, \end{aligned}$$

where ν is the outward-pointing normal with respect to Ω on $\partial\Omega$ and with respect to $B(a, \epsilon)$ on $\partial B(a, \epsilon)$. (In other words, ν is the inward-pointing normal with respect to Ω_ϵ on $\partial B(a, \epsilon)$.) The first term C_Ω vanishes because $u(x) = G(x, a) = 0$ and $w(x) = G(x, b) = 0$ for all $x \in \partial\Omega$. The second term simplifies to

$$\begin{aligned} \lim_{\epsilon \rightarrow 0} A_\epsilon &= \lim_{\epsilon \rightarrow 0} \int_{\partial B(a, \epsilon)} (w(x) \frac{\partial G}{\partial \nu}(x, a) - G(x, a) \frac{\partial w}{\partial \nu}(x))dx \\ &= \lim_{\epsilon \rightarrow 0} \int_{\partial B(a, \epsilon)} (w(x) \frac{\partial \Phi}{\partial \nu}(x - a) - \Phi(x - a) \frac{\partial w}{\partial \nu}(x))dx \\ &\quad + \lim_{\epsilon \rightarrow 0} \int_{\partial B(a, \epsilon)} (w(x) \frac{\partial \Psi}{\partial \nu}(x, a) - \Psi(x, a) \frac{\partial w}{\partial \nu}(x))dx \\ &= -w(a) = -G(a, b), \end{aligned}$$

where the second equality follows from the decomposition $G(x, a) = \Phi(x - a) + \Psi(x, a)$; the last equality follows from (i) the application of Proposition 11.14 to the first term and (ii) the fact that the second term vanishes as $\epsilon \rightarrow 0$ because $w(x) \frac{\partial \Psi}{\partial \nu}(x, a) - \Psi(x, a) \frac{\partial w}{\partial \nu}(x)$ is continuous. Similarly,

$$\lim_{\epsilon \rightarrow 0} B_\epsilon = u(b) = G(b, a).$$

It follows $0 = (\text{LHS}) = (\text{RHS}) = -A_\epsilon - B_\epsilon = G(a, b) - G(b, a)$, and hence $G(a, b) = G(b, a)$. \square

Proof of Green's representation formula. We first introduce $w(x) = G(x, \xi) = \Phi(x - \xi) + \Psi(x, \xi)$, where $G(x, \xi)$ is the Green's function on Ω and $\Psi(x, \xi)$ is the associated correction function. We next introduce a domain $\Omega_\epsilon \equiv \Omega \setminus \overline{B(\xi, \epsilon)}$ for $\epsilon > 0$ but sufficiently small. Note that w is harmonic

in Ω_ϵ since the hole removes the singularity in the Green's function. We now invoke the Green's second identity with $w(x) = G(x, \xi)$ and $u(x)$. The left hand side is given by

$$(\text{LHS}) = \int_{\Omega_\epsilon} (G(x, \xi)\Delta u(x) - u(x)\Delta G(x, \xi))dx = - \int_{\Omega_\epsilon} G(x, \xi)f(x)dx;$$

the second term vanishes because $G(x, \xi)$ is harmonic in Ω_ϵ . The right hand side is given by

$$\begin{aligned} (\text{RHS}) &= \int_{\Omega_\epsilon} (G(x, \xi)\frac{\partial u(x)}{\partial \nu} - u(x)\frac{\partial G}{\partial \nu}(x, \xi))dx \\ &= \int_{\partial\Omega} (G(x, \xi)\frac{\partial u(x)}{\partial \nu} - u(x)\frac{\partial G}{\partial \nu}(x, \xi))dx - \int_{\partial B(\xi, \epsilon)} (G(x, \xi)\frac{\partial u(x)}{\partial \nu} - u(x)\frac{\partial G}{\partial \nu}(x, \xi))dx \\ &\equiv C_\Omega - D_\epsilon, \end{aligned}$$

where ν is the outward-pointing normal with respect to Ω on $\partial\Omega$ and with respect to $B(a, \epsilon)$ on $\partial B(a, \epsilon)$. (In other words, ν is the inward-pointing normal with respect to Ω_ϵ on $\partial B(a, \epsilon)$.) The first term simplifies to

$$C_\Omega = - \int_{\partial\Omega} g(x)\frac{\partial G}{\partial \nu}(x, \xi)dx,$$

because $G(x, \xi) = 0$ and $u(x) = g(x)$ for all $x \in \partial\Omega$. The second term simplifies to

$$\lim_{\epsilon \rightarrow 0} D_\epsilon = u(\xi),$$

following the same argument used to simplify A_ϵ in the proof of symmetry of Green's functions. Equating the left and right hand sides, we obtain

$$u(\xi) = \int_{\Omega} G(x, \xi)f(x)dx - \int_{\partial\Omega} g(x)\frac{\partial G}{\partial \nu}(x, \xi)dx.$$

We switch the roles of x and ξ to obtain

$$u(x) = \int_{\Omega} G(\xi, x)f(\xi)d\xi - \int_{\partial\Omega} g(\xi)\frac{\partial G}{\partial \nu}(\xi, x)d\xi = \int_{\Omega} G(\xi, x)f(\xi)d\xi - \int_{\partial\Omega} g(\xi)\nu \cdot \nabla_\xi G(\xi, x)d\xi.$$

We appeal to the symmetry of the Green's function to obtain

$$u(x) = \int_{\Omega} G(x, \xi)f(\xi)d\xi - \int_{\partial\Omega} g(\xi)\nu \cdot \nabla_\xi G(x, \xi)d\xi,$$

which is the desired result. □

Lecture 12

Laplace's equation: finite difference method

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12.1 Introduction

In this lecture we consider finite difference approximations of Poisson's (and Laplace's) equation in two dimensions. Numerical methods are arguably a necessity for PDEs in two and higher dimensions, as there is no analytical means to find the solution for complex domain geometries. Building on our discussion on finite difference method for the one-dimensional heat equation in Lecture 8, in this lecture we focus on finite difference approximations in higher dimensions.

12.2 Problem statement

We introduce Poisson's equation in two dimensions:

$$\begin{aligned} -\frac{\partial^2 u}{\partial x^2} - \frac{\partial^2 u}{\partial y^2} &= f \quad \text{in } \Omega \equiv (0, 1) \times (0, 1), \\ u &= 0 \quad \text{on } \partial\Omega, \end{aligned}$$

where $f : \Omega \rightarrow \mathbb{R}$ is some forcing function. For simplicity, we consider a unit square domain and homogeneous Dirichlet boundary condition. We defer to Section 12.6 for the treatment of other boundary conditions.

12.3 Finite difference formulation

We approximate the two-dimensional Poisson's equation by a finite difference method. As we have done for the heat equation, we first introduce a computational grid over the domain Ω . The grid points are given by

$$(x_i, y_j) = (i\Delta x, j\Delta y), \quad i, j = 0, \dots, n+1,$$

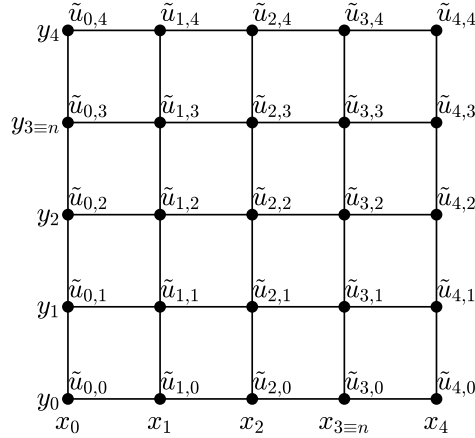


Figure 12.1: Computational grid for two-dimensional Poisson equation.

where $\Delta x = \Delta y = h = 1/(n + 1)$ is the spacing between any two grid points. We then denote our approximation of the solution by

$$\tilde{u}_{i,j} \equiv \tilde{u}(x_i, y_j), \quad i, j = 0, \dots, n + 1.$$

An example of computational grid for $n = 3$ is shown in Figure 12.1. (Note that our indices range from $i, j = 0$ to $n + 1$, so that the unknowns are at $i, j = 1, \dots, n$ after we impose the Dirichlet boundary conditions at $i, j = 0$ and $n + 1$. The indices are different from the mixed boundary condition case considered in Lecture 8, where the right most node was an unknown node because of the Neumann boundary condition. This also affects the relationship between the grid spacing Δx and n .)

We apply the second-order central difference formula to approximate the second derivatives

$$\begin{aligned} \left. \frac{\partial^2 u}{\partial x^2} \right|_{i,j} &\approx \frac{\tilde{u}_{i+1,j} - 2\tilde{u}_{i,j} + \tilde{u}_{i-1,j}}{\Delta x^2}, \\ \left. \frac{\partial^2 u}{\partial y^2} \right|_{i,j} &\approx \frac{\tilde{u}_{i,j+1} - 2\tilde{u}_{i,j} + \tilde{u}_{i,j-1}}{\Delta y^2}. \end{aligned}$$

We note that, because we are approximating *partial* derivatives, the finite difference step for $\frac{\partial^2 u}{\partial x^2}$ and $\frac{\partial^2 u}{\partial y^2}$ are taken (only) in the respective coordinate directions. We also recall that these approximations for the second-derivative are second-order accurate (Proposition 8.4); i.e., using the Taylor series, we can show that

$$\left| \left. \frac{\partial^2 u}{\partial x^2} \right|_{i,j} - \frac{\tilde{u}_{i+1,j} - 2\tilde{u}_{i,j} + \tilde{u}_{i-1,j}}{\Delta x^2} \right| = \mathcal{O}(\Delta x^2)$$

for sufficiently regular u .

Combining the two approximations of partial derivatives, we obtain an approximation of the Laplacian:

$$-\Delta u|_{i,j} = - \left. \frac{\partial^2 u}{\partial x^2} \right|_{i,j} - \left. \frac{\partial^2 u}{\partial y^2} \right|_{i,j} \approx - \frac{\tilde{u}_{i+1,j} - 2\tilde{u}_{i,j} + \tilde{u}_{i-1,j}}{\Delta x^2} - \frac{\tilde{u}_{i,j+1} - 2\tilde{u}_{i,j} + \tilde{u}_{i,j-1}}{\Delta y^2}.$$

Because the approximation of the Laplacian at (i, j) involves the solution values at five points (i.e. four neighbors and itself), the finite difference approximation is said to have a *five-point stencil*. The substitution of the finite difference formula to the Poisson equation yields

$$-\frac{\tilde{u}_{i+1,j} - 2\tilde{u}_{i,j} + \tilde{u}_{i-1,j}}{\Delta x^2} - \frac{\tilde{u}_{i,j+1} - 2\tilde{u}_{i,j} + \tilde{u}_{i,j-1}}{\Delta y^2} = \hat{f}_{i,j}, \quad i, j = 1, \dots, n, \quad (12.1)$$

where $\hat{f}_{i,j} = f(x_i, y_j)$. The homogeneous Dirichlet boundary conditions become

$$\begin{aligned} \tilde{u}_{0,j} = \tilde{u}_{n+1,j} = 0, \quad j = 0, \dots, n+1, \\ \tilde{u}_{i,0} = \tilde{u}_{i,n+1} = 0, \quad i = 1, \dots, n, \end{aligned}$$

Note that we have n^2 equations associated with the interior grid points. The difference equation can again be expressed in a matrix form:

$$\hat{A}\tilde{u} = \hat{f};$$

for instance, if $n = 3$ and $h \equiv \Delta x = \Delta y$, the matrix $\hat{A} \in \mathbb{R}^{9 \times 9}$ and the vectors $\tilde{u} \in \mathbb{R}^9$ and $\hat{f} \in \mathbb{R}^9$ are given by

$$\hat{A} = \frac{1}{h^2} \left(\begin{array}{ccc|cc} 4 & -1 & & -1 & & \\ -1 & 4 & -1 & & -1 & \\ & -1 & 4 & & & -1 \\ \hline -1 & & & 4 & -1 & -1 \\ & -1 & & -1 & 4 & -1 \\ & & -1 & & -1 & 4 \\ \hline & & & -1 & & \\ & & & & -1 & \\ & & & & & -1 \end{array} \right), \quad \tilde{u} = \begin{pmatrix} \tilde{u}_{11} \\ \tilde{u}_{21} \\ \tilde{u}_{31} \\ \tilde{u}_{12} \\ \tilde{u}_{22} \\ \tilde{u}_{32} \\ \tilde{u}_{13} \\ \tilde{u}_{23} \\ \tilde{u}_{33} \end{pmatrix}, \quad \hat{f} = \begin{pmatrix} \hat{f}_{11} \\ \hat{f}_{21} \\ \hat{f}_{31} \\ \hat{f}_{12} \\ \hat{f}_{22} \\ \hat{f}_{32} \\ \hat{f}_{13} \\ \hat{f}_{23} \\ \hat{f}_{33} \end{pmatrix}.$$

Note that we have ordered the grid points such that x -index is the faster changing index and y -index is the slower changing index; this choice is arbitrary.

Because we have employed a second-order accurate finite difference formula to approximate the Laplacian, it can be shown that this finite difference approximation is second-order accurate. If the exact solution is sufficiently regular, then the error is bounded by

$$\|u - \tilde{u}\|_\infty = \max_{i,j=1,\dots,n} |u(x_i, y_j) - \tilde{u}_{i,j}| \leq C\Delta x^2 + D\Delta y^2,$$

for some $C < \infty$ and $D < \infty$. We make two observations:

1. *Convergence:* the error $\|u - \tilde{u}\|_\infty \rightarrow 0$ as $\Delta x \rightarrow 0$ and $\Delta y \rightarrow 0$.
2. *Order of accuracy:* $\|u - \tilde{u}\|_\infty \leq C\Delta x^2 + D\Delta y^2$, and the scheme is second-order accurate. Decreasing both Δx and Δy by a factor of two results in the error to decrease by a factor of four.

We make one final remark on computational consideration. Similar to the case of one-dimensional heat equation, the matrix \hat{A} associated with two- (or higher-) dimensional Laplace's equation is *sparse* (i.e., mostly zero). It is important to take advantage of this sparsity in computation. Pragmatically, in MATLAB, we should (i) ensure that the matrix is stored as a sparse matrix using the `sparse` command and (ii) use the “\” backslash operator to solve the linear system $\hat{A}\tilde{u} = \hat{f}$. We should *never* use the `inv` function, which is very inefficient because the inverse of \hat{A} is a dense matrix.

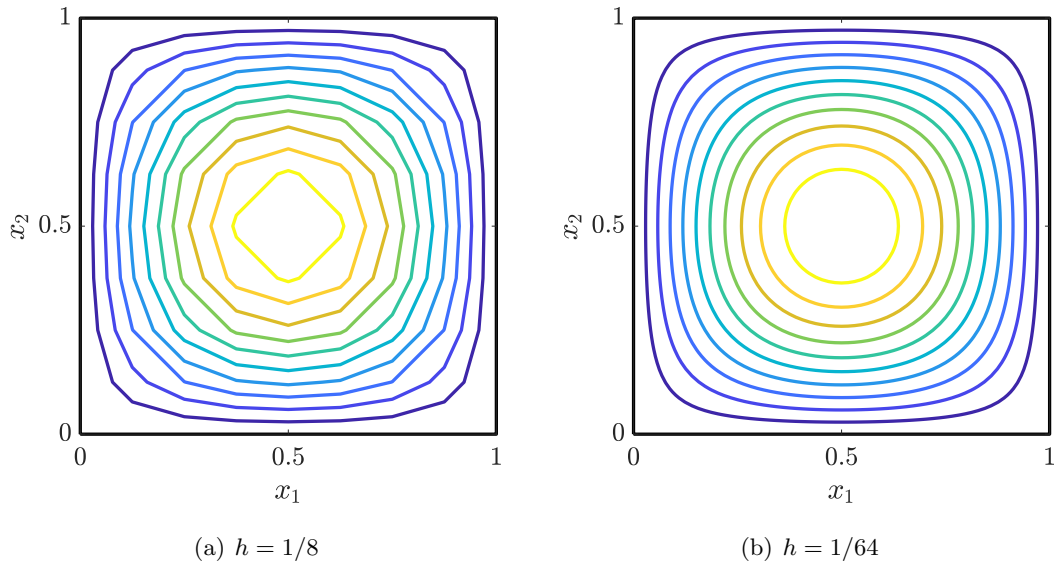


Figure 12.2: Finite difference approximations of Poisson's equation on the unit square domain.

h	$\ u - \tilde{u}\ _\infty$
1/4	2.69×10^{-3}
1/8	6.56×10^{-4}
1/16	1.63×10^{-4}
1/32	4.07×10^{-5}
1/64	1.02×10^{-5}

Table 12.1: Maximum error for finite difference approximations of Poisson's equation on the unit square domain as a function of the grid spacing.

12.4 Example: square domain

We consider a two-dimensional Poisson problem

$$\begin{aligned}
 -\Delta u &= \sin(\pi x) \sin(\pi y) \quad \text{in } \Omega \equiv (0, 1)^2, \\
 u &= 0 \quad \text{on } \partial\Omega.
 \end{aligned}$$

Finite difference approximations of the solution for two different values of the grid spacing $h = \Delta x = \Delta y$ are shown in Figure 12.2. The $h = 1/64$ approximation is noticeably smooth than the $h = 1/8$ approximation.

Table 12.1 shows the maximum error over all grid points as a function of the grid spacing. We observe that the maximum error decreases by approximately a factor of four whenever the grid spacing is decreased by a factor of two. This is consistent with the fact that the error scales as $\mathcal{O}(\Delta x^2, \Delta y^2)$ for the second-order accurate finite difference method for smooth problems.

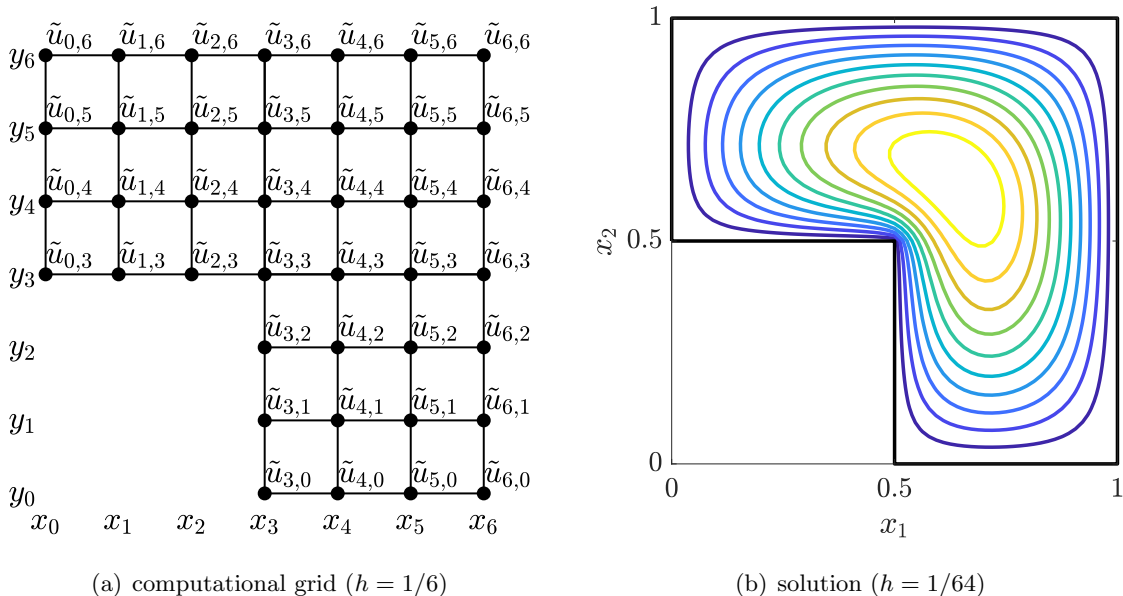


Figure 12.3: Computational grid and solution for the L -shaped domain problem.

12.5 Example: L -shaped domain

The finite difference approximation readily extends to non-square domains. We here consider Poisson's equation on a L -shaped domain $\Omega \equiv (0, 1)^2 \setminus [0, 1/2]^2$:

$$\begin{aligned} -\Delta u &= 1 && \text{in } \Omega, \\ u &= 0 && \text{on } \partial\Omega. \end{aligned}$$

An example of the computational grid for the L -shaped domain is shown in Figure 12.3(a). Note that there is no computational grid over $(0, 1/2)^2$, which is not part of the domain. The solution obtained on a finer grid is shown in Figure 12.3(b). The solution is in fact singular at the 270° corner; i.e., higher-order derivatives are not continuous at the corner. Table 12.2 shows that, due to the presence of the singularity, the finite difference error converges as $\mathcal{O}(h^{2/3})$ for $h = \Delta x = \Delta y$, which is (significantly) slower than the convergence of $\mathcal{O}(h^2)$ for smooth problems. The fact that the method does not achieve the design order of accuracy for problems with singularities is consistent with the fact that the finite difference formulas are derived using the Taylor series for smooth functions.

12.6 Treatment of various boundary conditions

The treatment of various boundary conditions in two dimensions is similar to their treatment the boundary condition in one dimension in Lecture 8.

1. *Dirichlet boundary.* Suppose we wish to impose a nonhomogeneous Dirichlet boundary condition on the $x = 0$ boundary:

$$u(x_{i=0}, y_j) = h(y_j).$$

h	$\ u - \tilde{u}\ _\infty$
1/4	1.79×10^{-3}
1/8	1.92×10^{-3}
1/16	1.40×10^{-3}
1/32	9.19×10^{-4}
1/64	5.80×10^{-4}

Table 12.2: Maximum error for the two-dimensional Poisson problem on the L -shaped domain as a function of grid spacing.

This boundary condition is incorporated in the finite difference equation associated with $(x_{i=1}, y_j)$. We substitute $u_{i=0,j} = h(y_j)$ to (12.1) evaluated at $(x_{i=1}, y_j)$,

$$-\frac{\tilde{u}_{2,j} - 2\tilde{u}_{1,j} + \tilde{u}_{0,j}}{\Delta x^2} - \frac{\tilde{u}_{1,j+1} - 2\tilde{u}_{1,j} + \tilde{u}_{1,j-1}}{\Delta y^2} = \hat{f}_{1,j},$$

to obtain

$$-\frac{\tilde{u}_{2,j} - 2\tilde{u}_{1,j} + h(y_j)}{\Delta x^2} - \frac{\tilde{u}_{1,j+1} - 2\tilde{u}_{1,j} + \tilde{u}_{1,j-1}}{\Delta y^2} = \hat{f}_{1,j}.$$

We move all known terms to the right hand side to obtain

$$-\frac{\tilde{u}_{2,j} - 2\tilde{u}_{1,j}}{\Delta x^2} - \frac{\tilde{u}_{1,j+1} - 2\tilde{u}_{1,j} + \tilde{u}_{1,j-1}}{\Delta y^2} = \hat{f}_{1,j} + \frac{h(y_j)}{\Delta x^2}.$$

We note that the expression is similar to the expression obtained for nonhomogeneous Dirichlet boundary condition for the one-dimensional heat equation.

2. *Neumann boundary.* Suppose we wish to impose a nonhomogeneous Neumann boundary condition on the $x = 0$ boundary:

$$-\frac{\partial u}{\partial x}(x_{i=0}, y_j) = h(y_j).$$

This boundary condition is incorporated in the finite difference equation associated with $(x_{i=0}, y_j)$. (Recall that, unlike the case of a Dirichlet boundary condition, the solution on the boundary $u(x_{i=0}, y_j)$ is unknown for a Neumann boundary.) The finite difference approximation of the boundary condition is

$$-\frac{\tilde{u}_{1,j} - \tilde{u}_{-1,j}}{2\Delta x} = h(y_j),$$

which implies $\tilde{u}_{-1,j} = \tilde{u}_{1,j} + 2\Delta x h(y_j)$. We substitute the (approximation of the) boundary condition to (12.1) evaluated at $(x_{i=1}, y_j)$,

$$-\frac{\tilde{u}_{1,j} - 2\tilde{u}_{0,j} + \tilde{u}_{-1,j}}{\Delta x^2} - \frac{\tilde{u}_{0,j+1} - 2\tilde{u}_{0,j} + \tilde{u}_{0,j-1}}{\Delta y^2} = \hat{f}_{0,j},$$

to obtain

$$-\frac{\tilde{u}_{1,j} - 2\tilde{u}_{0,j} + \tilde{u}_{1,j} + 2\Delta x h(y_j)}{\Delta x^2} - \frac{\tilde{u}_{0,j+1} - 2\tilde{u}_{0,j} + \tilde{u}_{0,j-1}}{\Delta y^2} = \hat{f}_{0,j}.$$

We again move known quantities to the right hand side to obtain

$$-\frac{2\tilde{u}_{1,j} - 2\tilde{u}_{0,j}}{\Delta x^2} - \frac{\tilde{u}_{0,j+1} - 2\tilde{u}_{0,j} + \tilde{u}_{0,j-1}}{\Delta y^2} = \hat{f}_{0,j} + \frac{2h(y_j)}{\Delta x}.$$

We note that the expression is similar to the expression obtained for nonhomogeneous Neumann boundary condition for the one-dimensional heat equation.

12.7 Time dependent problems: heat equation

We can readily apply the finite difference approximation of two-dimensional Laplace's equation to construct a semi-discrete equation for the two-dimensional heat equation. The resulting semi-discrete equation is

$$\frac{d\tilde{u}_{i,j}}{dt} - \frac{\tilde{u}_{i+1,j} - 2\tilde{u}_{i,j} + \tilde{u}_{i-1,j}}{\Delta x^2} - \frac{\tilde{u}_{i,j+1} - 2\tilde{u}_{i,j} + \tilde{u}_{i,j-1}}{\Delta y^2} = \hat{f}_{i,j}, \quad i, j = 1, \dots, n.$$

The associated matrix form of the equation is

$$\frac{d\tilde{u}}{dt} + \hat{A}\tilde{u} = \hat{f}.$$

We can then apply a time marching method discussed in Lecture 8 to the time derivative to obtain a fully discrete equation. We then solve the fully discrete equation, starting at time $t = 0$.

12.8 Other numerical methods for PDEs

While we have focused our discussion on the finite difference method in this course, there are many other numerical methods for PDEs. We here highlight several well-known approaches:

- *Finite element methods.* Finite element methods are derived from so-called weak form of the PDEs. Finite element methods permit the use of *unstructured meshes*, which facilitates the treatment of complex geometries; an example of unstructured meshes is shown in Figure 12.4(a). The method is also amenable to rigorous analysis using functional analysis techniques. The finite element method can be used to approximate PDEs of all types (i.e., parabolic, elliptic, and hyperbolic) and are used in many engineering applications including structures, fluids, acoustics, and electromagnetics. An example of finite element approximation of fluid flow is shown in Figure 12.4(b).
- *Finite volume methods.* Finite volume methods are derived from the integral (as opposed to differential) form of the PDEs and are particularly well-suited for hyperbolic conservation laws in fluid dynamics. Like finite element methods, finite volume methods also permit the use of unstructured meshes, which facilitates the treatment of complex geometries.
- *Boundary element methods.* Boundary element methods are designed for linear homogeneous PDEs. The method appeals to the fundamental solution of the PDE and the Green's representation formula to recast the PDE as a problem on boundaries. While applicable only to linear homogeneous PDEs, it provides efficient solution of these PDEs and are widely used in electromagnetics; the vortex-lattice method for potential flows in fluid dynamics is also an example of boundary element methods.

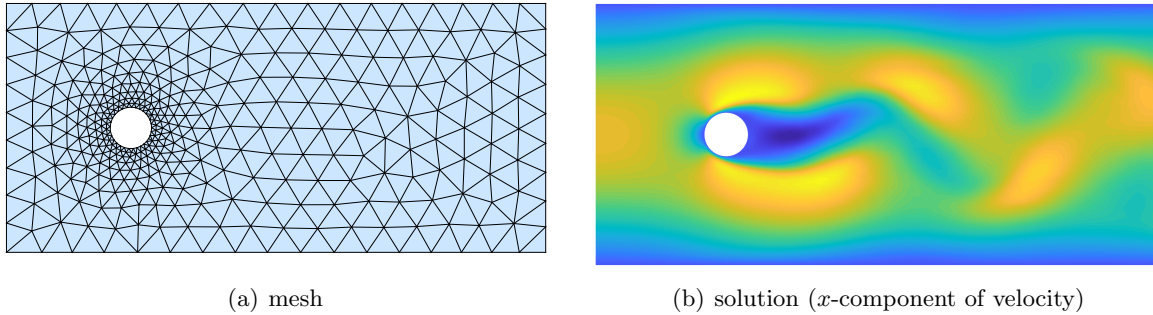


Figure 12.4: Example of a mesh and solution for flow past a cylinder.

12.9 Summary

We summarize key points of this lecture:

1. Finite difference methods readily extend to higher dimensions. To approximate a partial derivative in a given direction, a finite difference formula is applied in that direction.
2. If the Laplacian operator is approximated using the second-order accurate finite difference formula, the resulting finite difference approximation of Laplace's (or Poisson's) equation is second-order accurate.
3. Various boundary conditions can be treated. On a Dirichlet boundary, we simply replace the value of the solution on the boundary with the known value. On a Neumann (or Robin) boundary, we approximate the boundary condition using a finite difference formula and make an appropriate substitution.
4. Finite difference methods for higher spatial dimensions can also be used to identify a semi-discrete form of higher-dimensional time-dependent problems.
5. There are many numerical methods for PDEs, including finite element, finite volume, and boundary element methods.

Part IV

Hyperbolic equations

Lecture 13

Wave equation: introduction

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13.1 Introduction

We have so far considered parabolic equations in the heat equation and elliptic equations in Poisson’s (and Laplace’s) equation. We now consider a new class of equations: *hyperbolic equations*. Hyperbolic equations describe physical phenomena in which quantities are “transported” rather than “diffused.” The two model hyperbolic equations we consider in this course are the *wave equation* and the *transport equation*. In this lecture we focus on the wave equation; we introduce the equation and study the behavior of the equation without finding an explicit expression of the solution.

13.2 Derivation: vibrating string in $\mathbb{R} \times \mathbb{R}_{>0}$

We now derive the one-dimensional wave equation which models a vibrating string. We assume that the flexible string has a (per-length) density of ρ and is in tension T . We apply Newton’s law to a small segment (x_L, x_R) of the string shown in Figure 13.1 to obtain the equations of motion for the longitudinal (x) and transverse (y) motions:

$$\underbrace{0}_{\text{no movement in } x} = \underbrace{Tn_x|_{x_R} - Tn_x|_{x_L}}_{\text{longitudinal force}}, \quad (13.1)$$

$$\underbrace{\int_{x_L}^{x_R} \rho \frac{\partial^2 u}{\partial t^2} dx}_{\text{mass} \times \text{acceleration}} = \underbrace{Tn_y|_{x_R} - Tn_y|_{x_L}}_{\text{transverse force}}, \quad (13.2)$$

where n_x and n_y are the longitudinal and transverse components of the unit vector n pointing along the string. From the geometry of the problem, the unit vector $n = (n_x, n_y)$ must be proportional to (dx, du) or equivalently $(1, \frac{\partial u}{\partial x})$; hence, the components of the unit vector can be expressed as

$$n_x = \frac{1}{\sqrt{1 + \left(\frac{\partial u}{\partial x}\right)^2}} \quad \text{and} \quad n_y = \frac{\frac{\partial u}{\partial x}}{\sqrt{1 + \left(\frac{\partial u}{\partial x}\right)^2}}. \quad (13.3)$$

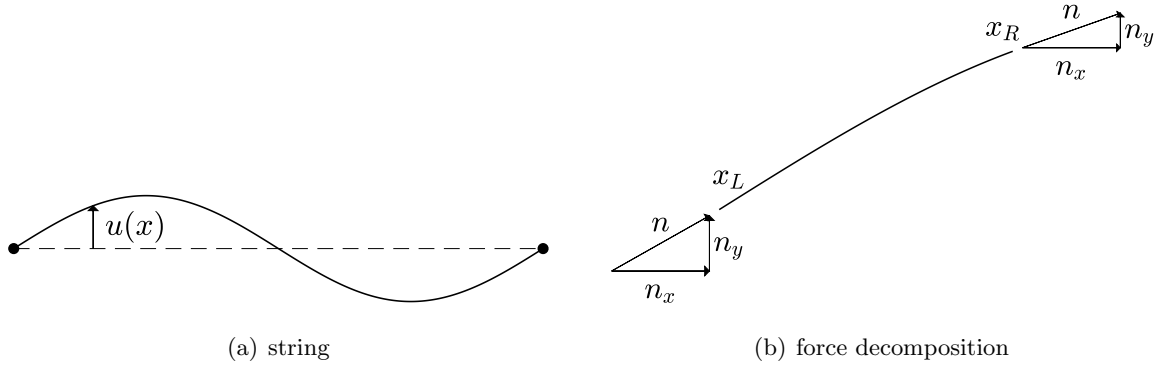


Figure 13.1: A vibrating string and the associated force decomposition of a segment.

We now assume that the displacement u and $\frac{\partial u}{\partial x}$ are small so that $\sqrt{1 + \left(\frac{\partial u}{\partial x}\right)^2} \approx 1$. This assumption simplifies the components of the unit vector to $n_x = 1$ and $n_y = \frac{\partial u}{\partial x}$. Consequently, the longitudinal equation of motion (13.1) simplifies to

$$T|_{x_R} - T|_{x_L} = 0;$$

since the choice of the segment (x_L, x_R) , we deduce that the tension is constant along the string. This further simplifies the transverse equation of motion (13.2) to

$$\rho \int_{x_L}^{x_R} \frac{\partial^2 u}{\partial t^2} dx = T \left(\frac{\partial u}{\partial x} \Big|_{x_R} - \frac{\partial u}{\partial x} \Big|_{x_L} \right)$$

We apply the divergence theorem to the right hand side to obtain

$$\rho \int_{x_L}^{x_R} \frac{\partial^2 u}{\partial t^2} dx = T \int_{x_L}^{x_R} \frac{\partial^2 u}{\partial x^2} dx.$$

Again, since the choice of the segment (x_L, x_R) is arbitrary, the integrands must be equal to each other and we obtain

$$\frac{\partial^2 u}{\partial t^2} = \frac{T}{\rho} \frac{\partial^2 u}{\partial x^2}.$$

We finally set $c \equiv \sqrt{T/\rho}$ and obtain

$$\frac{\partial^2 u}{\partial t^2} = c^2 \frac{\partial^2 u}{\partial x^2}.$$

This is the wave equation, where c is the wave speed.

13.3 Derivation: acoustic wave equation in $\mathbb{R}^3 \times \mathbb{R}_{>0}$

We now derive a multi-dimensional wave equation which models acoustic waves. The starting point for the acoustic wave equation is the Euler's equations for compressible flows:

$$\begin{aligned} \frac{\partial \rho}{\partial t} + \nabla \cdot \rho v &= 0, \\ \frac{\partial \rho v}{\partial t} + v \cdot \nabla \rho v + \nabla p &= 0; \end{aligned}$$

the first and second equations are the conservation of mass and momentum, respectively. We now express the density, velocity, and pressure as the perturbation ($\tilde{\rho}$, \tilde{v} , and \tilde{p}) about the background state (ρ_0 , v_0 , and p_0) that are invariant in space and time:

$$\begin{aligned}\rho &= \rho_0 + \tilde{\rho}, \\ v &= v_0 + \tilde{v} = \tilde{v}, \\ p &= p_0 + \tilde{p},\end{aligned}$$

where we have assumed that the background velocity is 0. We substitute the expressions to the Euler equations, appeal to the fact ρ_0 , v_0 , and p_0 are invariant in space and time, and neglect the product of two or more perturbation terms to obtain

$$\begin{aligned}\frac{\partial(\rho_0 + \tilde{\rho})}{\partial t} + \nabla \cdot ((\rho_0 + \tilde{\rho})\tilde{v}) &\approx \frac{\partial\tilde{\rho}}{\partial t} + \rho_0\nabla\tilde{v} = 0, \\ \frac{\partial((\rho_0 + \tilde{\rho})\tilde{v})}{\partial t} + \tilde{v} \cdot \nabla((\rho_0 + \tilde{\rho})\tilde{v}) + \nabla(p_0 + \tilde{p}) &\approx \rho_0\frac{\partial\tilde{v}}{\partial t} + \nabla\tilde{p} = 0.\end{aligned}$$

We next note that for isentropic flows $c^2 \approx \tilde{p}/\tilde{\rho}$. It follows that

$$\begin{aligned}\frac{1}{c^2}\frac{\partial\tilde{p}}{\partial t} + \rho_0\nabla \cdot \tilde{v} &= 0, \\ \rho_0\frac{\partial\tilde{v}}{\partial t} + \nabla\tilde{p} &= 0.\end{aligned}\tag{13.4}$$

We now wish to eliminate the velocity from the equations. To this end, we assume that both \tilde{p} and \tilde{v} are sufficiently smooth, differentiate the first equation in time, differentiate the second equation in space, and take the difference of the two equations:

$$\begin{aligned}0 &= \frac{\partial}{\partial t} \left(\frac{1}{c^2} \frac{\partial\tilde{p}}{\partial t} + \rho_0\nabla \cdot \tilde{v} \right) - \nabla \cdot \left(\rho_0\frac{\partial\tilde{v}}{\partial t} + \nabla\tilde{p} \right) \\ &= \frac{1}{c^2} \frac{\partial^2\tilde{p}}{\partial t^2} + \rho_0\frac{\partial}{\partial t}\nabla \cdot \tilde{v} - \rho_0\nabla\frac{\partial\tilde{v}}{\partial t} - \Delta\tilde{p} \\ &= \frac{1}{c^2} \frac{\partial^2\tilde{p}}{\partial t^2} - \Delta\tilde{p}.\end{aligned}$$

This is the acoustic wave equation for the (perturbation in the) pressure.

Following the convention that is used for all other PDEs in this course, we denote the solution — perturbation in the pressure — by the variable u and multiply through by c^2 to obtain

$$\frac{\partial^2 u}{\partial t^2} - c^2 \Delta u = 0.\tag{13.5}$$

This is the (dimensional form of the) wave equation.

13.4 Boundary conditions

To define a complete initial boundary value problem, we now complement the wave equation (13.5) with boundary and initial conditions. We consider two different types of boundary conditions for the wave equation.

1. *Dirichlet boundary condition* (e.g., prescribe pressure for the acoustic wave equation). We first recall that the solution to the (acoustic) wave equation represent the pressure perturbation. Hence, if the pressure perturbation at the boundary is prescribed, we obtain a boundary condition of the form

$$u = \tilde{p}^b \quad \text{on } \Gamma_D \times \mathbb{R}_{>0},$$

where Γ_D is the Dirichlet boundary, and \tilde{p}^b is the prescribed pressure perturbation. This is a Dirichlet boundary condition, as the equation depends only on the value of the solution (and not its derivative). If the pressure is fixed (i.e., there is no perturbation), then the equation simplifies to $u = 0$.

2. *Neumann boundary condition* (e.g., prescribed normal acceleration for the acoustic wave equation). The prescribed acceleration condition arises when we have, for instance, a speaker that vibrates at a known frequency and displacement. To prescribe the acceleration condition, we evaluate the linearized momentum equation (13.4) in the normal direction $\tilde{\nu}$ to obtain

$$\nu \cdot \nabla \tilde{p} = -\rho_0 \frac{\partial \nu \cdot \tilde{v}}{\partial t}.$$

Recalling $u = \tilde{p}$ we obtain

$$\nu \cdot \nabla u = -\rho_0 \frac{\partial \nu \cdot \tilde{v}}{\partial t} = -\rho_0 \nu \cdot \tilde{a}^b \quad \text{on } \Gamma_N \times \mathbb{R}_{>0},$$

where Γ_N is the Neumann boundary, and \tilde{a}^b is the prescribed acceleration of the wall. This is a Neumann boundary condition, as the equation depends only on the derivative (and not the value). If the wall is fixed (i.e., there is no acceleration), then the equation simplifies to $\nu \cdot \nabla u = 0$.

The wave equation, like the heat equation, is second order in space. Hence, we must enforce one and only one boundary condition at any point on $\partial\Omega$.

The wave equation, unlike the heat equation, is second order in time. Hence we must specify both the value and time derivative at the initial time to obtain a well posed problem; we impose

$$\begin{aligned} u &= g \quad \text{on } \Omega \times \{t = 0\}, \\ \frac{\partial u}{\partial t} &= h \quad \text{on } \Omega \times \{t = 0\}, \end{aligned}$$

for some prescribed initial state $g : \Omega \rightarrow \mathbb{R}$ and the time derivative of the state $h : \Omega \rightarrow \mathbb{R}$.

13.5 Nondimensionalization

As in the case for the heat equation, we may choose the nondimensionalization for the spatial and temporal variables so that the nondimensionalized equation has a unity wave speed. To demonstrate the idea, consider a wave equation

$$\frac{\partial^2 u}{\partial t^2} - c^2 \frac{\partial^2 u}{\partial x^2} = 0 \quad \text{in } (0, L) \times \mathbb{R}_{>0}.$$

We introduce the length scale L and the time scale $T \equiv L/c$, so that the nondimensionalized coordinate is $\tilde{x} = x/L$ and $\tilde{t} = t/T = ct/L$. The nondimensionalized wave equation is then

$$\frac{\partial^2 \tilde{u}}{\partial \tilde{t}^2} - \frac{\partial^2 \tilde{u}}{\partial \tilde{x}^2} = 0 \quad \text{in } (0, 1) \times \mathbb{R}_{>0}.$$

The choice of the time scale in particular reduces the wave speed to unity.

Example 13.1 (nondimensionalization). Suppose the solution to nondimensionalized wave equation is given by

$$\tilde{u}(\tilde{x}, \tilde{t}) = f(\tilde{x} - \tilde{t}) + \tilde{f}(\tilde{x} + \tilde{t}),$$

for some function $f : \mathbb{R} \rightarrow \mathbb{R}$. The solution to the original equation is then

$$u(x, t) = \tilde{u}(x/L, ct/L) = f((x - ct)/L) + \tilde{f}((x + ct)/L).$$

13.6 Energy conservation

In the derivation of the wave equation, we have seen that the equation is associated with phenomena such as the vibration of a string and acoustics, where the energy is propagated as waves. Our physical intuition suggests that, in the absence of friction, the energy should be conserved and simply propagate without any dissipation. Indeed the wave equation respects this physical intuition, as stated in the following theorem.

Theorem 13.2 (conservation of energy for the wave equation). Suppose u is the solution to the wave equation on Ω with homogeneous boundary conditions:

$$\begin{aligned} \frac{\partial^2 u}{\partial t^2} - \Delta u &= 0 & \text{in } \Omega \times \mathbb{R}_{>0}, \\ u &= 0 & \text{on } \Gamma_D \times \mathbb{R}_{>0}, \\ \frac{\partial u}{\partial n} &= 0 & \text{on } \Gamma_N \times \mathbb{R}_{>0}, \end{aligned}$$

where Γ_D and Γ_N are Dirichlet and Neumann boundaries, respectively, so that $\overline{\Gamma_D \cup \Gamma_N} = \partial\Omega$. Let $E(t)$ be the total energy at time t given by

$$E(t) \equiv \frac{1}{2} \int_{\Omega} \left(\left(\frac{\partial u}{\partial t} \right)^2 + \nabla u \cdot \nabla u \right) dx.$$

Then the total energy is conserved:

$$E(t) = E(t = 0) \quad \forall t \in \mathbb{R}_{>0}.$$

Proof. Let us introduce the kinetic and potential energy

$$\begin{aligned} K &\equiv \frac{1}{2} \int_{\Omega} \left(\frac{\partial u}{\partial t} \right)^2 dx, \\ P &\equiv \frac{1}{2} \int_{\Omega} \nabla u \cdot \nabla u dx, \end{aligned}$$

so that $E = K + P$. The change in the kinetic energy with time is

$$\begin{aligned}
\frac{dK}{dt} &= \frac{1}{2} \frac{d}{dt} \int_{\Omega} \left(\frac{\partial u}{\partial t} \right)^2 dx = \int_{\Omega} \frac{\partial u}{\partial t} \frac{\partial^2 u}{\partial t^2} dx = \int_{\Omega} \frac{\partial u}{\partial t} \Delta u dx \\
&= - \int_{\Omega} \left(\frac{\partial}{\partial t} \nabla u \right) \cdot \nabla u dx + \underbrace{\int_{\Gamma_D} \frac{\partial u}{\partial t} \frac{\partial u}{\partial n} ds}_{=0 \text{ as } u=0 \Rightarrow \frac{\partial u}{\partial t}=0} + \underbrace{\int_{\Gamma_N} \frac{\partial u}{\partial t} \frac{\partial u}{\partial n} ds}_{=0 \text{ as } \frac{\partial u}{\partial n}=0} \\
&= - \int_{\Omega} \frac{1}{2} \frac{\partial}{\partial t} (\nabla u \cdot \nabla u) dx = - \frac{1}{2} \frac{d}{dt} \int_{\Omega} (\nabla u \cdot \nabla u) dx = - \frac{dP}{dt};
\end{aligned}$$

here the third equality follows from the definition of the wave equation, the fourth equality follows from the integration by parts, and the last equality follows from the definition of the potential energy. The change in the kinetic energy is exactly the negative of the change in the potential energy. It follows that $\frac{dE}{dt} = \frac{dK}{dt} + \frac{dP}{dt} = 0$, which implies $E(t) = E(t=0)$. \square

We note that this energy conservation (or equality) for the wave equation is different from the energy stability (or inequality) for the heat equation. This again agrees with our physical intuition that in phenomena modeled by the wave equation the energy is conserved and propagated, whereas in phenomena modeled by the heat equation the energy is dissipated through diffusion.

13.7 Energy method: uniqueness

We now appeal to the energy conservation to show that the solution to an initial-boundary value problem for the wave equation, if it exists, is unique.

Theorem 13.3 (uniqueness of the solution to the wave equation). Let $\Omega \subset \mathbb{R}^n$ be a spatial domain and $\mathbb{R}_{>0}$ be the time interval. There is at most one solution $u : \Omega \times \mathbb{R}_{>0} \rightarrow \mathbb{R}$ that satisfies

$$\begin{aligned}
\frac{\partial^2 u}{\partial t^2} - \Delta u &= f \quad \text{in } \Omega \times \mathbb{R}_{>0}, \\
u &= h_D \quad \text{on } \Gamma_D \times \mathbb{R}_{>0}, \\
\frac{\partial u}{\partial n} &= h_N \quad \text{on } \Gamma_N \times \mathbb{R}_{>0}, \\
u &= g_0 \quad \text{on } \Omega \times \{t = 0\}, \\
\frac{\partial u}{\partial t} &= g_1 \quad \text{on } \Omega \times \{t = 0\},
\end{aligned}$$

where $f : \Omega \times \mathbb{R}_{>0} \rightarrow \mathbb{R}$ is a source function, $h_D : \Gamma_D \times \mathbb{R}_{>0} \rightarrow \mathbb{R}$ is the Dirichlet boundary function, $h_N : \Gamma_N \times \mathbb{R}_{>0} \rightarrow \mathbb{R}$ is the Neumann boundary function, and $g_0 : \Omega \rightarrow \mathbb{R}$ and $g_1 : \Omega \rightarrow \mathbb{R}$ specify the initial conditions.

Proof. Suppose u_1 and u_2 are two solutions to the heat equation initial-boundary value problem.

Then their difference $w \equiv u_1 - u_2$ satisfies

$$\begin{aligned} \frac{\partial^2 w}{\partial t^2} - \Delta w &= 0 && \text{in } \Omega \times \mathbb{R}_{>0}, \\ w &= 0 && \text{on } \Gamma_D \times \mathbb{R}_{>0}, \\ \frac{\partial w}{\partial n} &= 0 && \text{on } \Gamma_N \times \mathbb{R}_{>0}, \\ w &= 0 && \text{on } \Omega \times \{t = 0\}, \\ \frac{\partial w}{\partial t} &= 0 && \text{on } \Omega \times \{t = 0\}. \end{aligned}$$

The total energy of the difference w , for any $t \geq 0$, is

$$E(t) = \frac{1}{2} \int_{\Omega} \left(\left(\frac{\partial w}{\partial t} \right)^2 + \nabla w \cdot \nabla w \right) dx = \frac{1}{2} \int_{\Omega} \left(\left(\frac{\partial w}{\partial t} \right)^2 + \nabla w \cdot \nabla w \right) dx \Big|_{t=0} = 0,$$

where the second equality follows from energy conservation, and the third equality follows from (i) $\frac{\partial w}{\partial t}(t = 0) = 0$ by the initial condition and (ii) $\nabla w(t = 0) = 0$ since $w(t = 0) = 0$ by the initial condition. Since $E(t) = 0$ and the energy is sum of two non-negative terms, it follows that $\frac{\partial w}{\partial t} = 0$ for all $t \geq 0$. Since $w(t = 0) = 0$, we conclude that $w(t) = u_1(t) - u_2(t) = 0$ for all $t \geq 0$. \square

We recall that for the heat equation we could establish the uniqueness of the solution using either the energy method or the maximum principle. Unfortunately there is no property that is analogous to the maximum principle for the wave equation. The lack of maximum principle is one of the key differentiators between the heat and wave equations.

13.8 Summary

We summarize key points of this lecture:

1. The wave equation describes phenomena including the vibration of a taut string and the propagation of acoustic pressure wave.
2. Initial-boundary value problems associated with the wave equation is obtained by incorporating Dirichlet and/or Neumann boundary conditions and initial conditions on both the value and time derivative of the state.
3. The wave equation can be nondimensionalized such that the nondimensionalized equation has a unit wave speed.
4. The wave equation with homogeneous Dirichlet or Neumann boundary conditions conserves the total energy, which is the sum of the kinetic and potential energy.
5. The wave equation with an appropriate set of initial and boundary conditions has a unique solution. The uniqueness can be proven using the energy method.
6. There is no property that is analogous to the maximum principle for the wave equation.

Lecture 14

Wave equation: separation of variables and d'Alembert's formula

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14.1 Introduction

In this lecture we solve the wave equation in a bounded one-dimensional spatial domain using separation of variables. The procedure is identical to that used for the heat equation; however, we will find that the solution to the wave equation can be interpreted as a superposition of standing waves unlike the solution to the heat equation which decays in time. Moreover, we will find an alternative representation for the solution in terms of traveling waves. We will exploit this latter interpretation in the subsequent lectures.

14.2 Separation of variables

We consider a wave equation in $(0, 1) \times \mathbb{R}_{>0}$ with homogeneous Dirichlet boundary conditions:

$$\begin{aligned} \frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} &= 0 && \text{in } (0, 1) \times \mathbb{R}_{>0}, \\ u &= 0 && \text{on } \{0, 1\} \times \mathbb{R}_{>0}, \\ u &= g && \text{on } (0, 1) \times \{t = 0\}, \\ \frac{\partial u}{\partial t} &= h && \text{on } (0, 1) \times \{t = 0\}. \end{aligned} \tag{14.1}$$

We wish to find a series representation of the solution using separation of variables. We recall the two steps of the procedure:

1. We seek a family of solutions of separable form $u_n(x, t) = \phi_n(x)T_n(x)$, $n = 1, 2, \dots$, that satisfy the PDE and the boundary condition (but not necessarily the initial conditions).
2. We identify a linear combination of u_1, u_2, \dots that satisfies the initial conditions.

To begin, we substitute $u_n(x, t) = \phi_n(x)T_n(t)$ to the wave equation and obtain

$$\phi_n T_n'' - \phi_n'' T_n = 0.$$

We rearrange the expression to obtain

$$\frac{\phi_n''}{\phi_n} = \frac{T_n''}{T_n} = -\alpha_n;$$

here, we have appealed to the fact that ϕ_n''/ϕ_n depends on x only and T_n''/T_n depends on t only, and hence the expressions must be equal to a constant, which we denote by $-\alpha_n$. We then impose the boundary conditions to find

$$\begin{aligned} u_n(x=0, t) = \phi_n(0)T_n(t) = 0 &\Rightarrow \phi_n(0) = 0, \\ u_n(x=1, t) = \phi_n(1)T_n(t) = 0 &\Rightarrow \phi_n(1) = 0; \end{aligned}$$

note that we choose $\phi_n(0) = \phi_n(1) = 0$ because the other option, $T_n(t) = 0$, would result in the trivial solution $u_n = 0$. It follows that the spatial functions must satisfy the boundary value eigenproblem

$$\begin{aligned} -\phi_n'' &= \alpha_n \phi_n \quad \text{in } (0, 1), \\ \phi_n &= 0 \quad \text{on } \{0, 1\}. \end{aligned}$$

This is a Sturm-Liouville problem, and hence we expect ϕ_n to form a complete orthonormal functions. In fact, this very Sturm-Liouville problem was considered in Example 4.6: the eigenfunctions are given by

$$\phi_n(x) = \sin(n\pi x),$$

and eigenvalues are $\alpha_n = n^2\pi^2$, for $n = 1, 2, \dots$.

Given $\alpha_n = n^2\pi^2$, the temporal function must satisfy, for each n , the ODE

$$-T_n'' = \alpha_n T_n \quad \Rightarrow \quad -T_n'' = n^2\pi^2 T_n.$$

The solution to the ODE is of the form

$$T_n(t) = A_n \cos(n\pi t) + B_n \sin(n\pi t).$$

Hence our separable solutions that satisfy the wave equation and the boundary condition are of the form

$$u_n(x, t) = A_n \cos(n\pi t) \sin(n\pi x) + B_n \sin(n\pi t) \sin(n\pi x).$$

Note that because the wave equation is second-order in time, we obtain a family of functions with two unknown coefficients; this is unlike the heat equation which yields a family of functions with one unknown coefficient.

Our general solution is a linear combination of the separable solutions, hence

$$u(x, t) = \sum_{n=1}^{\infty} A_n \cos(n\pi t) \sin(n\pi x) + B_n \sin(n\pi t) \sin(n\pi x). \quad (14.2)$$

We now impose the initial conditions to obtain

$$u(x, t = 0) = \sum_{n=1}^{\infty} A_n \sin(n\pi x) = g(x),$$

$$\frac{\partial u}{\partial t}(x, t = 0) = \sum_{n=1}^{\infty} B_n n\pi \sin(n\pi t) = h(x);$$

here, we have assumed that the solution is sufficiently regular so that the series may be differentiated term by term. We note that the first and second equations are the Fourier sine series for g and h , respectively. We hence obtain

$$A_n = \hat{g}_n = 2 \int_0^1 \sin(n\pi x) g(x) dx,$$

$$B_n n\pi = \hat{h}_n = 2 \int_0^1 \sin(n\pi x) h(x) dx \quad \Rightarrow \quad B_n = \frac{\hat{h}_n}{n\pi} = \frac{2}{n\pi} \int_0^1 \sin(n\pi x) h(x) dx.$$

Hence the solution to (14.1) is given by

$$u(x, t) = \sum_{n=1}^{\infty} \left(\hat{g}_n \cos(n\pi t) + \frac{\hat{h}_n}{n\pi} \sin(n\pi t) \right) \sin(n\pi x), \quad (14.3)$$

where we have grouped the time-dependent terms. We make a few observations:

1. *Interpretation as standing waves.* Consider the special case where the initial condition is $g(x) = \sin(m\pi x)$ for some integer m and $h = 0$. The solution to the problem is then given by

$$u(x, t) = \cos(m\pi t) \sin(m\pi x).$$

For any fixed $t \in \mathbb{R}_{>0}$, the snapshot of the solution is $u(x, t) \propto \sin(m\pi x)$; i.e., the snapshot has the same shape (up to scaling) at any time. For any fixed $x \in (0, 1)$, the variation in the solution in time is $u(x, t) \propto \cos(m\pi t)$; i.e., the amplitude varies sinusoidally in time. Hence, as the name suggests, the wave equation admits standing waves as solutions.

2. *Oscillatory Fourier coefficients.* For any fixed t , the solution $u(\cdot, t)$ in (14.3) can be interpreted as the Fourier sine series $\sum_{n=1}^{\infty} a_n(t) \sin(n\pi x)$ with time-varying coefficients $a_n(t) = (\hat{g}_n \cos(n\pi t) + \frac{\hat{h}_n \sin(n\pi t)}{n\pi})$, which is oscillatory. This is in contrast to the coefficients for the heat equation, whose solution is given by

$$u(x, t) = \sum_{n=1}^{\infty} \hat{g}_n \exp(-n^2 \pi^2 t) \sin(n\pi x);$$

the Fourier coefficients for the heat equation, $a_n(t) = \hat{g}_n \exp(-n^2 \pi^2 t)$, decays exponentially in time.

3. *(Lack of) smoothness.* For any fixed t , the solution to the wave equation $u(\cdot, t)$ is not necessarily smooth if the initial conditions g and h are not smooth. This is in contrast to the solution to the heat equation which is infinitely differentiable for any $t > 0$ even if the initial condition is discontinuous. We recall that the solution of the heat equation is smooth

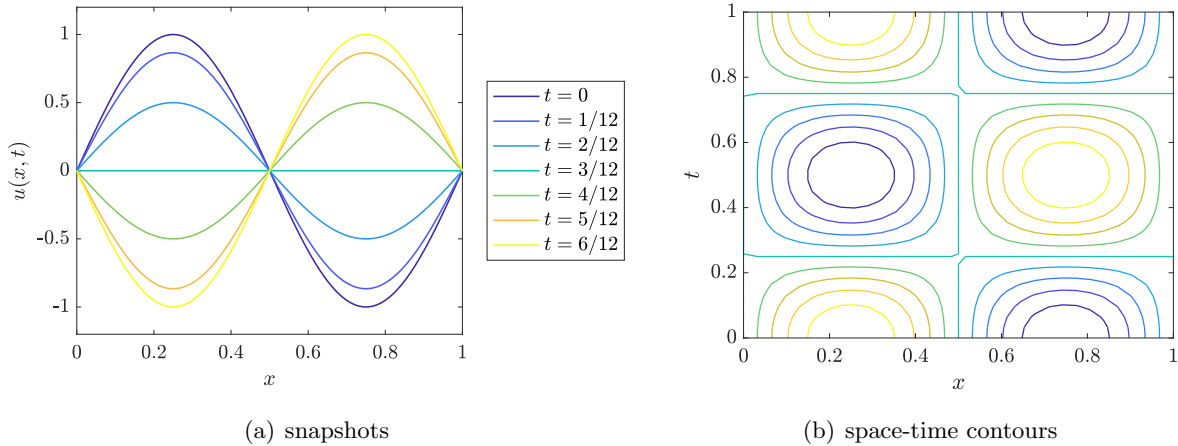


Figure 14.1: Solution to the one-dimensional wave equation with the initial condition $g = \sin(2\pi x)$ and $h = 0$.

because the Fourier coefficients decay exponentially with the mode number n for $t > 0$; as the wave equation does not have this property, the solution is not necessarily smooth. (This lack of smoothing effect will become more apparent for another solution representation that we introduce next.)

Example 14.1 (wave equation by separation of variables). We consider the solution of the initial-boundary value problem (14.1) for the initial condition $g(x) = \sin(2\pi x)$ and $h = 0$. By inspection, we find that the Fourier sine series coefficients are $\hat{g}_2 = 1$ and $\hat{g}_i = 0$, $i \neq 2$. The solution is hence given by

$$u(x, t) = \cos(2\pi t) \sin(2\pi x).$$

Figure 14.1 visualizes the solution as temporal snapshots and as a space-time contour. We observe a *standing wave* of with a unit wave length and a unit period.

14.3 d'Alembert's formula

We can further simplify the series solution (14.2) to derive *d'Alembert's formula*, which reveals more properties of the wave equation. To simplify the derivation we consider the solution for two cases — (i) $g \neq 0$ and $h = 0$ and (ii) $h \neq 0$ and $g = 0$ — and then take the superposition of the two solutions.

Case 1: $g \neq 0$ and $h = 0$. We set $\hat{h}_n = 0$ in (14.3) to obtain

$$u(x, t) = \sum_{n=1}^{\infty} \hat{g}_n \sin(n\pi x) \cos(n\pi t) = \frac{1}{2} \sum_{n=1}^{\infty} \hat{g}_n (\sin(n\pi(x-t)) + \sin(n\pi(x+t))),$$

where the second equality follows from $\sin(n\pi x) \cos(n\pi t) = \frac{1}{2}(\sin(n\pi(x-t)) + \sin(n\pi(x+t)))$. We recall that \hat{g}_n are the Fourier sine coefficients of g and hence, assuming $g^{0,p}$ is sufficiently regular,

$$\sum_{n=1}^{\infty} \hat{g}_n \sin(n\pi \xi) = g^{0,p}(\xi) \quad \forall \xi \in \mathbb{R},$$

where $g^{\text{o.p.}} : \mathbb{R} \rightarrow \mathbb{R}$ is the odd periodic extension of $g : (0, 1) \rightarrow \mathbb{R}$. Hence,

$$u(x, t) = \frac{1}{2} \sum_{n=1}^{\infty} \hat{g}_n (\sin(n\pi(x-t)) + \sin(n\pi(x+t))) = \frac{1}{2} [g^{\text{o.p.}}(x-t) + g^{\text{o.p.}}(x+t)].$$

Case 2: $h \neq 0$ and $g = 0$. We set $\hat{g}_n = 0$ in (14.3) to obtain

$$u(x, t) = \sum_{n=1}^{\infty} \frac{\hat{h}_n}{n\pi} \sin(n\pi x) \sin(n\pi t) = \frac{1}{2} \sum_{n=1}^{\infty} \frac{\hat{h}_n}{n\pi} (\cos(n\pi(x-t)) - \cos(n\pi(x+t))),$$

where the second equality follows from $\sin(n\pi x) \sin(n\pi t) = \frac{1}{2}(\cos(n\pi(x-t)) - \cos(n\pi(x+t)))$. We recall that \hat{h}_n are the Fourier sine coefficients of h and hence, assuming $h^{\text{o.p.}}$ is sufficiently regular,

$$h^{\text{o.p.}}(\xi) = \sum_{n=1}^{\infty} \hat{h}_n \sin(n\pi\xi) \quad \forall \xi \in \mathbb{R},$$

where $h^{\text{o.p.}} : \mathbb{R} \rightarrow \mathbb{R}$ is the odd periodic extension of $h : (0, 1) \rightarrow \mathbb{R}$. We integrate the expression over (a, b) to obtain

$$\int_a^b h^{\text{o.p.}}(\xi) d\xi = \sum_{n=1}^{\infty} \frac{\hat{h}_n}{n\pi} [-\cos(n\pi\xi)]_{\xi=a}^b = \sum_{n=1}^{\infty} \frac{\hat{h}_n}{n\pi} (\cos(n\pi a) - \cos(n\pi b)).$$

It hence follows that

$$u(x, t) = \frac{1}{2} \sum_{n=1}^{\infty} \frac{\hat{h}_n}{n\pi} (\cos(n\pi(x-t)) - \cos(n\pi(x+t))) = \frac{1}{2} \int_{x-t}^{x+t} h^{\text{o.p.}}(\xi) d\xi.$$

We take the superposition of the two solutions and find that the solution to the initial-boundary value problem (14.1) is

$$u(x, t) = \frac{1}{2} [g^{\text{o.p.}}(x-t) + g^{\text{o.p.}}(x+t)] + \frac{1}{2} \int_{x-t}^{x+t} h^{\text{o.p.}}(\xi) d\xi. \quad (14.4)$$

This is *d'Alembert's formula* for the wave equation.

We now use d'Alembert's formula to sketch the solution to the wave equation.

Example 14.2 (d'Alembert's formula: Dirichlet boundary condition). We consider the initial-boundary value problem (14.1) for the initial condition $g(x) = \exp(-(x-1/2)^2/0.05^2)$ and $h = 0$. We wish to sketch the solution at various times using d'Alembert's formula (14.4), as shown in Figure 14.2. We proceed as follows:

1. We first sketch two odd periodic extensions of $g(x, t=0)$, which has been scaled by the factor of $1/2$. In Figure 14.2, the right-traveling wave $\frac{1}{2}g^{\text{o.p.}}(x-t)$ and the left-traveling wave $\frac{1}{2}g^{\text{o.p.}}(x+t)$ are shown in blue and orange, respectively. The waves coincide at time $t = 0$.
2. To sketch the solution at time t , we now slide the right-traveling (blue) wave and left-traveling (orange) wave by t . Even though only the solution over $(0, 1)$ is physically relevant, we slide the entire periodic extension. The solution is given by the sum of the two waves: $u(x, t) = \frac{1}{2}(g^{\text{o.p.}}(x-t) + g^{\text{o.p.}}(x+t))$.

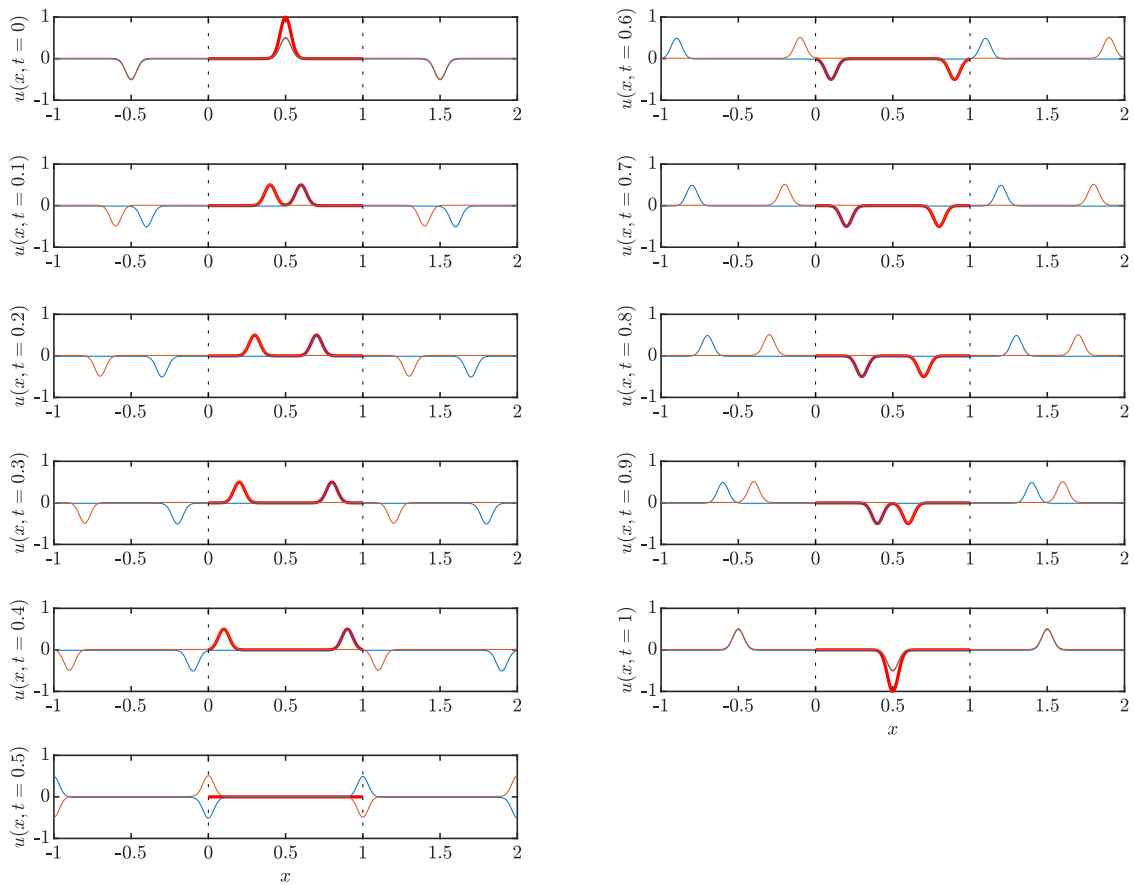


Figure 14.2: Solution to the one-dimensional wave equation with Dirichlet boundary conditions and the initial condition $g(x) = \exp(-(x - 1/2)^2/0.05^2)$ and $h = 0$. The blue and orange waves are the right- and left-traveling odd periodic extension $g^{o,p}$, respectively. The red wave is the sum of the two waves evaluated over the domain $(0, 1)$.

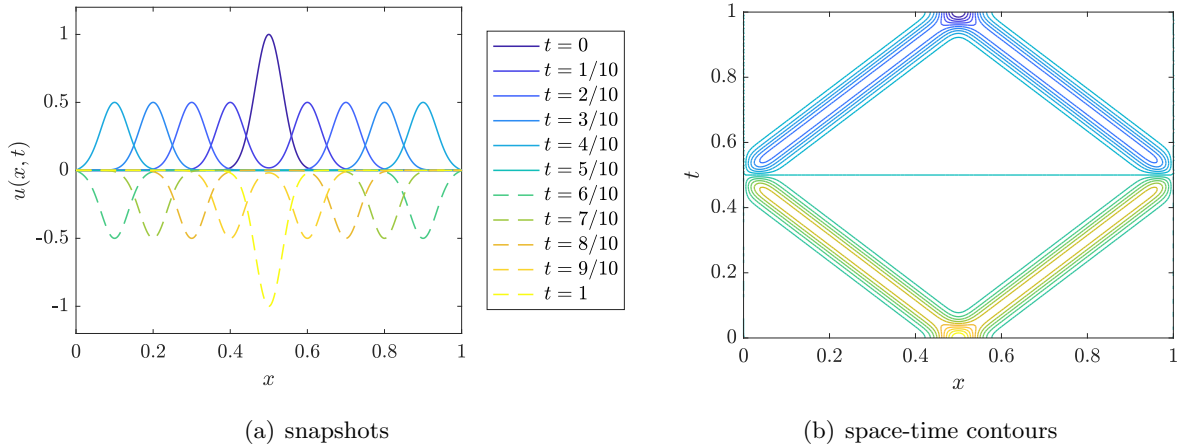


Figure 14.3: Solution to the one-dimensional wave equation with Dirichlet boundary conditions and the initial condition $g(x) = \exp(-(x - 1/2)^2/0.05^2)$ and $h = 0$. The snapshots are in $\Delta t = 1/10$ intervals.

This two-step procedure applies at any t . The effect of the wave reflecting off the boundary is captured by the odd periodic extension entering the physical domain $(0, 1)$. We observe that the solution “inverts” when it reflects at the boundary at $t \approx 1/2$; the wave is inverted because the odd-periodic extension is inverted in $(-1, 0)$ and $(1, 2)$, and these inverted waves enter the domain $(0, 1)$ for $t \in (1/2, 1)$.

Figure 14.3 shows the solution as snapshots and a space-time contour.

We conclude the section with a few observations about the d’Alembert’s formula:

1. *Interpretation as travel waves.* Consider the case $h = 0$. The solution is the superposition of two traveling waves: the left-traveling wave $\frac{1}{2}g^{o,p}(x + t)$ and the right-traveling wave $\frac{1}{2}g^{o,p}(x - t)$.
2. *Reflection at boundaries.* When the wave reflects off the boundary, the reflection induces a change of sign because we consider the odd periodic extension; i.e., the reflected wave is “inverted.”
3. *Lack of smoothness ($g \neq 0$ and $h = 0$).* Consider the case of $g \neq 0$ and $h = 0$. Because the solution is a superposition of two waves associated with the (odd periodic extension of the) initial condition, the solution $u(\cdot, t)$ at time t is in general no smoother than the initial condition g . For instance, if $g^{o,p}$ is (say) only twice differentiable, then $u(\cdot, t)$ is also only twice differentiable. This is unlike the heat equation, for which the solution $u(\cdot, t)$ is infinitely differentiable even if the initial condition is discontinuous.
4. *Lack of smoothness ($h \neq 0$ and $g = 0$).* Similar to the case above, the solution $u(\cdot, t)$ at time t is only once more differentiable than the initial function $h^{o,p}$. For instance, if $h^{o,p}$ is only once differentiable, then $u(\cdot, t)$ is only twice differentiable. (The additional regularity arises because we integrate h .)

We will later revisit d’Alembert’s formula and its interpretation using the method of characteristics.

14.4 Neumann boundary conditions

We now consider the solution of the wave equation with Neumann boundary conditions:

$$\begin{aligned} \frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} &= 0 \quad \text{in } (0, 1) \times \mathbb{R}_{>0}, \\ \frac{\partial u}{\partial x} &= 0 \quad \text{on } \{0, 1\} \times \mathbb{R}_{>0}, \\ u &= g \quad \text{on } (0, 1) \times \{t = 0\}, \\ \frac{\partial u}{\partial t} &= h \quad \text{on } (0, 1) \times \{t = 0\}. \end{aligned} \tag{14.5}$$

As many of the steps to solving the problem are identical to the Dirichlet boundary condition case, we provide an abbreviated exposition here. As before, we first find a family of separable solutions of the form $u_n(x, t) = \phi_n(x)T_n(t)$ that satisfies the homogeneous PDE and boundary conditions. The substitution of the separable form to the PDE and boundary conditions yield a spatial eigenproblem:

$$\begin{aligned} -\phi_n'' &= \alpha_n \phi_n \quad \text{in } (0, 1), \\ \phi_n' &= 0 \quad \text{on } \{0, 1\}. \end{aligned}$$

This is a Sturm-Liouville problem, whose solutions are given by

$$\phi_n(x) = \cos(n\pi x) \quad \text{and} \quad \alpha_n = n^2\pi^2 \quad \text{for } n = 0, 1, 2, \dots$$

The associated temporal ODE is

$$-T_n'' = \alpha_n T_n \quad \Rightarrow \quad -T_n'' = n^2\pi^2 T_n, \quad n = 0, 1, 2, \dots$$

The solutions are given by

$$T_n(t) = \begin{cases} \frac{1}{2}A_n + \frac{1}{2}B_n t, & n = 0, \\ A_n \cos(n\pi t) + B_n \sin(n\pi t), & n = 1, 2, \dots \end{cases}$$

(We here scale the $n = 0$ term by $1/2$ for convenience.) The general solution is hence given by

$$u(x, t) = \frac{1}{2}A_0 + \frac{1}{2}B_0 t + \sum_{n=1}^{\infty} (A_n \cos(n\pi t) + B_n \sin(n\pi t)) \cos(n\pi x).$$

We now impose the initial conditions:

$$\begin{aligned} u(x, t = 0) &= \frac{1}{2}A_0 + \sum_{n=1}^{\infty} A_n \cos(n\pi x) = g(x), \\ \frac{\partial u}{\partial t}(x, t = 0) &= \frac{1}{2}B_0 + \sum_{n=1}^{\infty} B_n n\pi \cos(n\pi x) = h(x). \end{aligned}$$

The first condition implies that A_n must be the Fourier cosine coefficients of g : i.e.,

$$A_n = \hat{g}_n \equiv 2 \int_0^1 \cos(n\pi x) g(x) dx, \quad n = 0, 1, 2, \dots$$

The second condition implies that B_0, B_1, B_2, \dots must be the Fourier cosine coefficients of h , and hence

$$B_n = \begin{cases} \hat{h}_n, & n = 0, \\ \frac{\hat{h}_n}{n\pi}, & n = 1, 2, \dots \end{cases} \quad \text{where} \quad \hat{h}_n \equiv 2 \int_0^1 \cos(n\pi x) h(x) dx.$$

The solution is hence given by

$$u(x, t) = \frac{1}{2}\hat{g}_0 + \frac{1}{2}\hat{h}_0 t + \sum_{n=1}^{\infty} (\hat{g}_n \cos(n\pi t) + \frac{\hat{h}_n}{n\pi} \sin(n\pi t)) \cos(n\pi x),$$

which is a series representation of the solution to (14.5).

We can also find d'Alembert's formula for the Neumann boundary condition case using a similar approach as the Dirichlet boundary condition case. First, for $g \neq 0$ and $h = 0$, we observe that

$$\begin{aligned} u(x, t) &= \frac{1}{2}\hat{g}_0 + \sum_{n=1}^{\infty} \hat{g}_n \cos(n\pi x) \cos(n\pi t) = \frac{1}{2}\hat{g}_0 + \frac{1}{2} \sum_{n=1}^{\infty} \hat{g}_n (\cos(n\pi(x+t)) + \cos(n\pi(x-t))) \\ &= \frac{1}{2}(g^{e,P}(x+t) + g^{e,P}(x-t)), \end{aligned}$$

where the second equality follows from a trigonometric identity, and the last equality follows from the fact that the Fourier cosine series of g converges to its even extension $g^{e,P}$ (assuming sufficient regularity). Second, for $g = 0$ and $h \neq 0$, we observe that

$$u(x, t) = \frac{1}{2}\hat{h}_0 t + \sum_{n=1}^{\infty} \frac{\hat{h}_n}{n\pi} \cos(n\pi x) \sin(n\pi t) = \frac{1}{2}\hat{h}_0 t + \frac{1}{2} \sum_{n=1}^{\infty} \frac{\hat{h}_n}{n\pi} (\sin(n\pi(x+t)) - \sin(n\pi(x-t))).$$

We also note that, assuming $h^{e,P}$ is sufficiently regular,

$$h^{e,P}(\xi) = \frac{1}{2}\hat{h}_0 + \sum_{n=1}^{\infty} \hat{h}_n \cos(n\pi\xi) \quad \forall \xi \in \mathbb{R},$$

and hence

$$\int_a^b h^{e,P}(\xi) d\xi = \frac{1}{2}\hat{h}_0(b-a) + \sum_{n=1}^{\infty} \frac{\hat{h}_n}{n\pi} (\sin(n\pi b) - \sin(n\pi a)).$$

We choose $a = x - t$ and $b = x + t$ to observe that

$$u(x, t) = \frac{1}{2}\hat{h}_0 t + \frac{1}{2} \sum_{n=1}^{\infty} \frac{\hat{h}_n}{n\pi} (\sin(n\pi(x+t)) - \sin(n\pi(x-t))) = \frac{1}{2} \int_{x-t}^{x+t} h^{e,P}(\xi) d\xi.$$

Combining the expression with the solution to the $g \neq 0$ and $h = 0$ case, we find that the solution to (14.5) can be expressed as

$$u(x, t) = \frac{1}{2}(g^{e,P}(x-t) + g^{e,P}(x+t)) + \frac{1}{2} \int_{x-t}^{x+t} h^{e,P}(\xi) d\xi, \quad (14.6)$$

which is d'Alembert's formula for the Neumann boundary condition problem (14.5). The formula is identical to the Dirichlet boundary case (14.4) with the exception of the use of the even periodic extension instead of the odd periodic extension.

We now use d'Alembert's formula to sketch the solution to the wave equation.

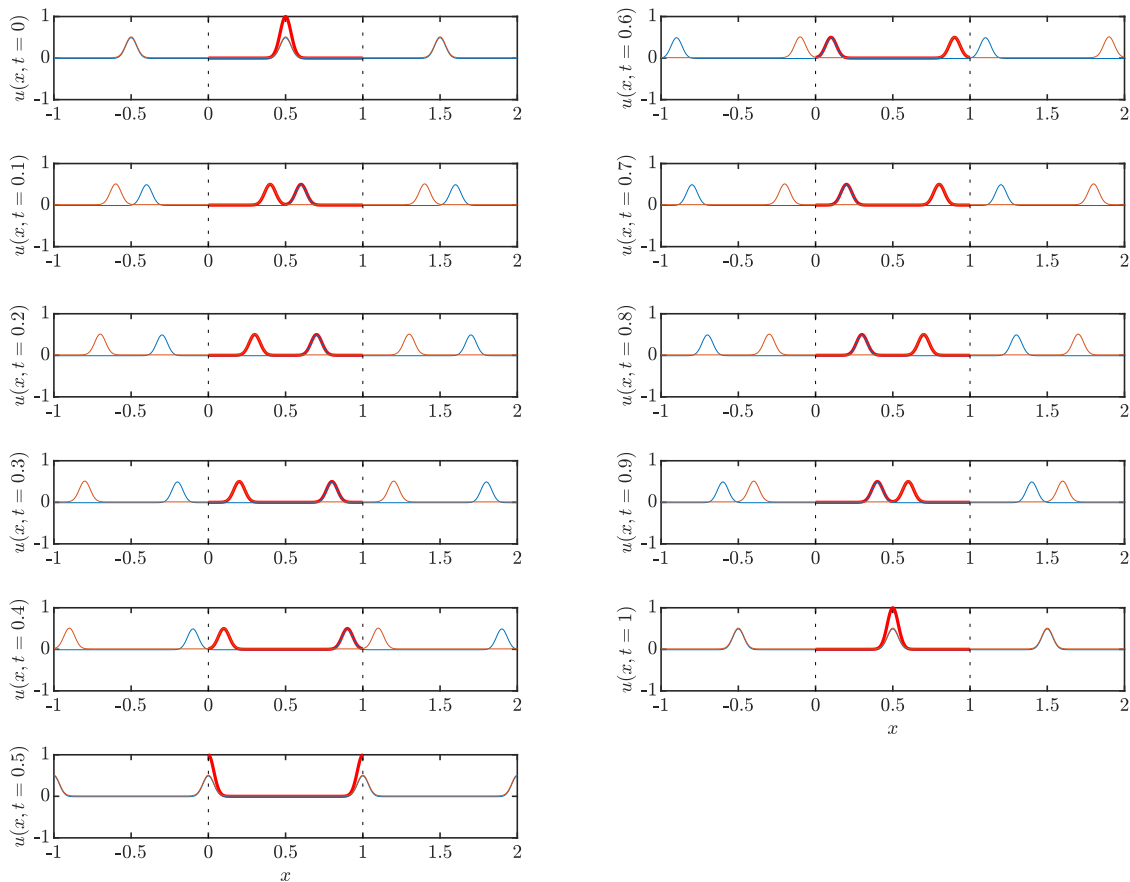


Figure 14.4: Solution to the one-dimensional wave equation with Neumann boundary conditions and the initial condition $g(x) = \exp(-(x - 1/2)^2/0.05^2)$ and $h = 0$. The blue and orange waves are the right- and left-traveling even periodic extension $g^{o,p}$, respectively. The red wave is the sum of the two waves evaluated over the domain $(0, 1)$.

Example 14.3 (d'Alembert's formula: Neumann boundary condition). We consider the solution of the initial-boundary value problem (14.5) for the initial condition $g(x) = \exp(-(x - 1/2)^2/0.05^2)$ and $h = 0$. We sketch the solution at various times using d'Alembert's formula (14.6). The resulting sketches are shown in Figure 14.4. The procedure to sketch the solutions is identical to Example 14.2, except that we consider the even periodic extension for the Neumann boundary condition. As a result, the solution does *not* invert when it reflects at the boundary at $t \approx 1/2$; the wave is not inverted because the even-periodic extension in $(-1, 0)$ and $(1, 2)$ are not inverted, and these waves enter the domain $(0, 1)$ for $t \in (1/2, 1)$.

Figure 14.5 shows the solution as snapshots and a space-time contour.

We make a few observations:

1. For the Neumann boundary problem, the series solution uses the Fourier cosine series and the associated d'Alembert's formula uses the even periodic extension of the initial conditions.

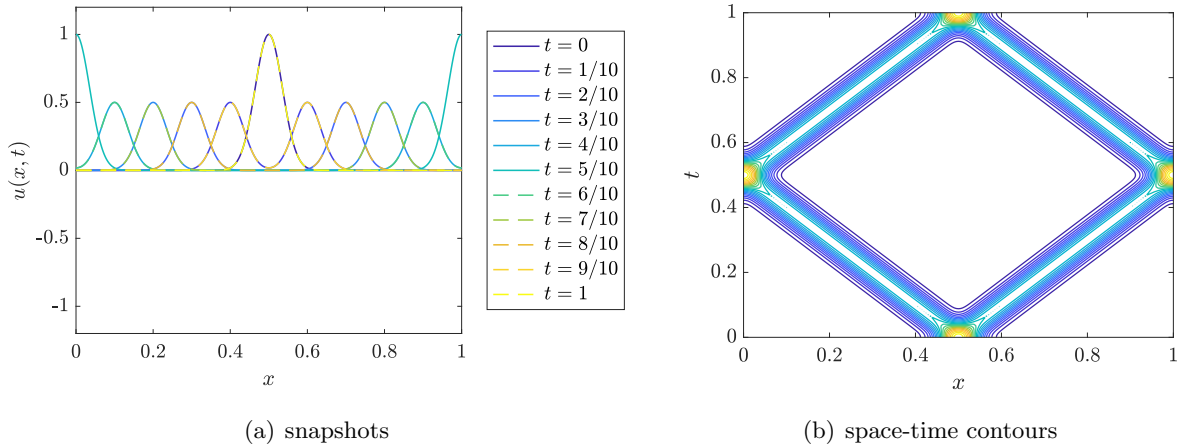


Figure 14.5: Solution to the one-dimensional wave equation with Neumann boundary conditions and the initial condition $g(x) = \exp(-(x-1/2)^2/0.05^2)$ and $h = 0$. The snapshots are in $\Delta t = 1/10$ intervals.

This is unlike the Dirichlet boundary problem which uses the Fourier sine series and the odd periodic extension of the initial conditions.

2. When the wave reflects off the boundary, the reflection does *not* induce a change of sign because we consider the even periodic extension. This is unlike the Dirichlet boundary problem in which the reflection induces a change of sign.
3. In general, the solution is not smooth; it is only as differentiable as $g^{e,P}$ and only once more differentiable than $h^{e,P}$.

14.5 Summary

We summarize key points of this lecture:

1. The one-dimensional wave equation can be readily solved using separation of variables. The solution is expressed in terms of the (generalized) Fourier coefficients of the initial conditions.
2. The Fourier coefficients for the wave equation are sinusoidal functions and oscillates in time, which may be interpreted as standing waves. This is unlike the Fourier coefficients for the heat equation which decays exponentially in time.
3. For any fixed t , the solution to the wave equation is not necessarily smooth if the initial condition is not smooth. This is again unlike the heat equation which smooths the solution.
4. d'Alembert's formula allows us to interpret the solution to the wave equation as a superposition of traveling waves associated with (appropriate periodic extensions of) the initial conditions.
5. The solutions to both Dirichlet boundary and Neumann boundary problems can be expressed as appropriate Fourier series or using d'Alembert's formula.

6. The reflection induces a change of sign at a Dirichlet boundary but not at a Neumann boundary.

Lecture 15

Transport equation: method of characteristics

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15.1 Introduction

In the previous lecture we considered the wave equation which is a second-order hyperbolic equation. In this lecture we consider (arguably) a simpler first-order hyperbolic equation: the transport equation. Transport equation, as the name suggests, describes the transport quantities in space. It also serves as a model equation for more complicated system of first-order hyperbolic equations, such as the Euler equations for compressible flows.

15.2 Derivation

We consider transport of some pollutant by fluid. To begin, we introduce a domain $\Omega \subset \mathbb{R}^n$ and the associated fixed subdomain $\omega \subset \Omega$. The density of the pollutant at any point in the domain is $u : \mathbb{R}^n \rightarrow \mathbb{R}$, and the (vector-valued) velocity field of the fluid is $b : \mathbb{R}^n \rightarrow \mathbb{R}^n$. We assume that the pollutant perfectly follows the motion of the fluid. (Physically this assumption is satisfied if the particles that constitute the pollutant are small enough.) We also assume that the velocity field is divergence free: $\nabla \cdot b = 0$. (Physically this corresponds to incompressible flows.)

We now appeal to the conservation of mass to derive the transport equation which describes the evolution of the pollutant density u . We first note that the total mass of the pollutant in Ω is $M = \int_{\Omega} u dx$. We next appeal to the conservation of mass to obtain

$$\underbrace{\frac{d}{dt} \int_{\omega} u dx}_{\text{change in pollutant mass}} = \underbrace{- \int_{\partial\omega} u(b \cdot \nu) ds}_{\text{net mass of pollutant entering } \omega},$$

where ν is the outward-pointing unit normal on $\partial\omega$. We then make two observations: (i) since ω is fixed in time the time derivative can be brought inside the integral; (ii) the integral over $\partial\omega$ can

be converted to an integral over ω using the divergence theorem. We hence obtain

$$\int_{\omega} \frac{\partial u}{\partial t} dx = - \int_{\omega} \nabla \cdot (bu) dx.$$

This relationship should hold for any $\omega \subset \Omega$, and hence the integrands must be equal to each other:

$$\frac{\partial u}{\partial t} = -\nabla \cdot (bu).$$

Because we assumed that the velocity field b is divergence free (i.e., $\nabla \cdot b = 0$), we obtain $\nabla \cdot (bu) = (\nabla \cdot b)u + b \cdot \nabla u = b \cdot \nabla u$ and hence

$$\frac{\partial u}{\partial t} + b \cdot \nabla u = 0.$$

This is the *transport equation*.

Remark 15.1 (transport equation and conservation principle). In the above, we have derived the transport equation using the conservation principle assuming the velocity field b is divergence-free. Following the convention, from hereon we *define* the transport equation as the PDE of the form $\frac{\partial u}{\partial t} + b \cdot \nabla u = 0$, regardless of whether b is divergence-free. Note that if b is not divergence-free, then the transport equation does *not* satisfy the conservation condition.

15.3 Generalized transport equation

Before we present a solution procedure for the transport equation, we first generalize the transport equation, as our procedure is quite flexible. Namely, we consider the case where the velocity b at the point (x, t) depends on both the position (x, t) and the state $u(x, t)$. Such a generalized transport equation is given by

$$\frac{\partial u}{\partial t}(x, t) + b(x, t, u(x, t)) \cdot \nabla u(x, t) = 0,$$

where $b : \mathbb{R}^n \times \mathbb{R}_{>0} \times \mathbb{R} \rightarrow \mathbb{R}^n$ is the velocity field. We consider three cases:

- *Case 1: b is constant.* This is a constant-coefficient transport equation.
- *Case 2: b depends on x and t but not on u .* This is a variable-coefficient transport equation.
- *Case 3: b depends on u .* This is a nonlinear transport equation. (More precisely, it is a *quasilinear* equation because it is linear in the derivatives $\frac{\partial u}{\partial t}$ and ∇u .)

15.4 Method of characteristics for homogeneous problems

We now present the method of characteristics for a homogeneous (generalized) transport equation. We first introduce an initial value problem

$$\begin{aligned} \frac{\partial u}{\partial t} + b \cdot \nabla u &= 0 && \text{in } \mathbb{R}^n \times \mathbb{R}_{>0}, \\ u &= g && \text{on } \mathbb{R}^n \times \{t = 0\}, \end{aligned} \tag{15.1}$$

where the transport field b in general depends on the point (x, t) and the state $u(x, t)$, and the initial condition $g : \mathbb{R}^n \rightarrow \mathbb{R}$ is given.

To solve the problem, let us first assume that the solution u is continuously differentiable: i.e., $u \in C^1(\mathbb{R}^n \times \mathbb{R}_{\geq 0})$. We then introduce a “trajectory” $x_c : \mathbb{R}_{\geq 0} \rightarrow \mathbb{R}^n$; note that this is a “curve” in space parametrized by time, or a point whose location depends on t . We next denote the associated solution along the trajectory by $u_c : \mathbb{R}_{\geq 0} \rightarrow \mathbb{R}^n$:

$$u_c(t) \equiv u(x_c(t), t).$$

We note that the solution u_c evolves along this trajectory as follows:

$$\frac{d}{dt}(u_c(t)) = \frac{d}{dt}u(x_c(t), t) = \frac{\partial u}{\partial t} + \frac{dx_c}{dt} \cdot \nabla u.$$

We compare the expression for $\frac{du_c}{dt}$ and the (generalized) transport equation (15.1) and note the following: if we choose a curve x_c such that $\frac{dx_c}{dt} = b(x_c(t), t, u(x_c(t), t))$, then

$$\frac{d}{dt}(u_c(t)) = \frac{d}{dt}u(x_c(t), t) = \frac{\partial u}{\partial t} + b(x_c(t), t, u(x_c(t), t)) \cdot \nabla u = 0. \quad (15.2)$$

Along the curve x_c such that $\frac{dx_c}{dt}(t) = b(x_c(t), t, u(x_c(t), t))$, the solution $u_c(t)$ is constant. The curve x_c is called the *characteristic*, and the pair of ODEs that govern the evolution of the solution along the characteristic is called the *characteristic equations*.

Definition 15.2 (characteristic equations for a homogeneous transport equation). The characteristic equations for a homogeneous transport equation $\frac{\partial u}{\partial t} + b \nabla u = 0$ is a pair of ODEs

$$\begin{aligned} \frac{dx_c}{dt}(t) &= b(x_c(t), t, u_c(t)), \quad t \in \mathbb{R}_{>0}, \\ \frac{du_c}{dt}(t) &= 0, \quad t \in \mathbb{R}_{>0}. \end{aligned}$$

The time-parametrized curve $x_c : \mathbb{R}^n \rightarrow \mathbb{R}_{\geq 0}$ is called the *characteristic*.

Note that this is a pair of ODEs — and not a PDE — that can be readily integrated in time. The solution at time t is given by

$$\begin{aligned} x_c(t) &= \int_{\tau=0}^t b(x_c(\tau), \tau, u_c(\tau)) d\tau + x_{c,0}, \\ u_c(t) &= u_c(0) = u(x_c(0), 0) = g(x_{c,0}), \end{aligned}$$

where $x_{c,0} \equiv x_c(t=0)$ is the initial point of the characteristic. The solution along the characteristic x_c is hence equal to the initial value $g(x_{c,0})$ at the point $x_{c,0}$.

Example 15.3 (constant-coefficient transport equation). We consider a transport equation

$$\begin{aligned} \frac{\partial u}{\partial t} + b \cdot \nabla u &= 0 \quad \text{in } \mathbb{R}^n \times \mathbb{R}_{>0}, \\ u &= g \quad \text{on } \mathbb{R}^n \times \{t=0\}, \end{aligned}$$

where $b \in \mathbb{R}^n$ is a (constant) velocity vector, and $g : \mathbb{R}^n \rightarrow \mathbb{R}$ is the initial condition. The characteristic takes a particularly simple form for this transport equation with a constant velocity. The characteristic equation is

$$\frac{dx_c}{dt}(t) = b \quad \forall t \in \mathbb{R}_{>0};$$

the direct integration of the ODE shows that the solution is given by

$$x_c(t) = \int_{\tau=0}^t b d\tau + x_{c,0} = bt + x_{c,0}.$$

Since the solution u is constant along the characteristic x_c (for a homogeneous equation), we obtain

$$u_c(t) = u(x_c(t), t) = u(bt + x_{c,0}, t) = g(x_{c,0}).$$

We propagate “backward” and choose $x_{c,0} = x - bt$ to obtain the solution

$$u(x, t) = g(x - bt).$$

This is a general solution to the homogeneous transport equation with a constant coefficient.

We now compare the behavior of the solutions to the transport equation and the heat equation. To this end, we note that the solutions to the two equations for a given initial condition g can be expressed as

$$\begin{aligned} \text{transport: } \quad u(x, t) &= g(x - bt), \\ \text{heat: } \quad u(x, t) &= \int_{\mathbb{R}^n} \Phi(x - \xi, t) g(\xi) d\xi, \end{aligned}$$

where Φ is the fundamental solution of the heat equation, which is smooth and nonzero everywhere. We make a few observations:

1. *Transport.* In the transport equation, the initial condition g is “transported” at the velocity b . This is consistent with our intuition for transport phenomena.
2. *Limited domain of influence/dependence.* The solution to the transport equation at (x, t) depends only on the initial condition at the point $x_{c,0} = x - bt$ from which the characteristic originates. Conversely, the initial condition at $\xi \in \mathbb{R}^n$ only affects the solution along its characteristic. This is unlike for the heat equation where the solution at (x, t) depends on the initial condition everywhere, and the initial condition at ξ affects the solution $u(\cdot, t)$ everywhere for any $t > 0$.
3. *Finite propagation speed.* For the transport equation, a change in the initial condition at point $x_{c,0}$ is felt only along the characteristic $x_c = bt + x_{c,0}$. As the point $x_c(t)$ moves at the velocity b (since $\frac{dx_c}{dt} = b$), the change in the initial condition also propagates at this finite velocity. This is unlike for the heat equation where the disturbance propagates at infinite speed.
4. *Lack of smoothness.* For the transport equation, the solution $u(\cdot, t)$ at time t has the same regularity as the initial condition g . If g is (only) once continuously differentiable, so is $u(\cdot, t)$. This is like the wave equation — another hyperbolic equation —, where the d’Alembert’s formula shows that the solution $u(\cdot, t)$ is only as regular as the initial condition. This is unlike the heat equation — a parabolic equation —, where the solution $u(\cdot, t)$ is smooth (i.e., infinitely differentiable) even if the initial condition is discontinuous.

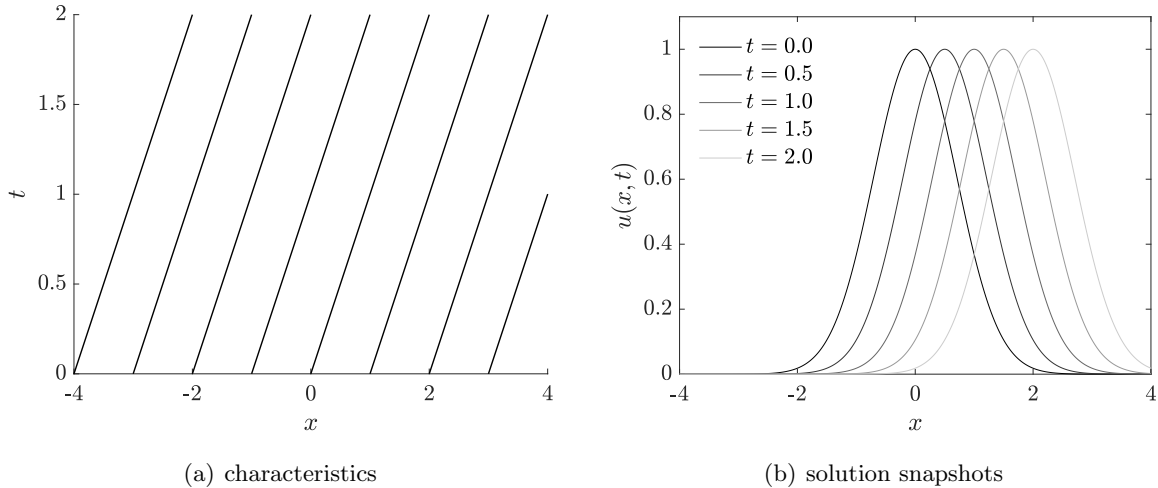


Figure 15.1: The characteristics and solution snapshots for the constant-coefficient transport equation in Example 15.3.

Example 15.4. Consider a one-dimensional transport equation

$$\begin{aligned} \frac{\partial u}{\partial t} + \frac{\partial x}{\partial t} &= 0 \quad \text{in } \mathbb{R} \times \mathbb{R}_{>0}, \\ u(x, t = 0) &= g(x) = \exp(-x^2), \quad \forall x \in \mathbb{R}. \end{aligned}$$

This is a homogeneous transport equation with constant coefficient of $b = 1$. Following the steps used in Example 15.3, we observe that the solution is given by

$$u(x, t) = g(x - t) = \exp(-(x - t)^2).$$

The characteristics and the snapshots of the solution are shown in Figure 15.1. The characteristics are parallel lines of slope 1 in the space-time domain, and the solution translates at a constant speed of 1.

Example 15.5. Consider an initial value problem associated with a homogeneous transport equation with variable coefficients:

$$\begin{aligned} \frac{\partial u}{\partial t} + x \frac{\partial u}{\partial x} &= 0 \quad \text{in } \mathbb{R} \times \mathbb{R}_{>0}, \\ u(x, t = 0) &= g(x) = \exp(-x^2), \quad x \in \mathbb{R}. \end{aligned}$$

The characteristics must satisfy

$$\frac{dx_c}{dt}(t) = x_c(t) \quad t \in \mathbb{R}_{>0}.$$

The solution to this ODE is of the form $x_c(t) = x_{c,0} \exp(t)$, where $x_{c,0}$ is the point from which the characteristic emanates. Since the PDE is homogeneous, the solution must be constant along each characteristic, and we find that

$$u(x_c(t), t) = u(x_{c,0} \exp(t), t) = u(x_{c,0}, t = 0) = g(x_{c,0}).$$

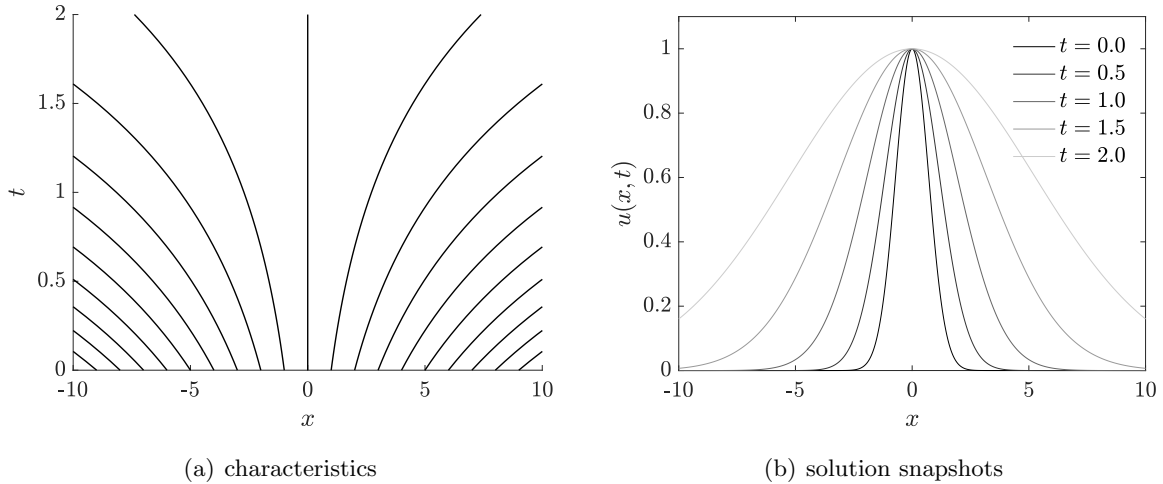


Figure 15.2: The characteristics and solution snapshots for Example 15.5.

We choose $x = x_{c,0} \exp(t)$ or $x_{c,0} = x \exp(-t)$ to obtain

$$u(x, t) = g(x \exp(-t)) = \exp(-x^2 \exp(-2t)).$$

The characteristics and the snapshots of the solution are shown in Figure 15.2. The characteristics spread at an increasingly faster rate over time. The accordingly the solution spread at an increasingly faster rate over time.

Remark 15.6. For the case with a constant coefficient, if $g \in C^1(\mathbb{R}^n)$, then $u \in C^1(\mathbb{R}^n \times \mathbb{R}_{>0})$, and our assumption on the smoothness of u is also satisfied. It turns out that the regularity condition can be relaxed if we consider *weak solutions*. We will consider this reformulation of the transport equation which admits not only nondifferentiable but also discontinuous solutions in a later lecture. The method of characteristics is in fact valid even if the initial condition (and hence the solution) is not differentiable.

15.5 Method of characteristics for nonhomogeneous problems

We now consider a initial value problem associated with a nonhomogeneous (generalized) transport equation

$$\begin{aligned} \frac{\partial u}{\partial t} + b \cdot \nabla u &= f \quad \text{in } \mathbb{R}^n \times \mathbb{R}_{>0}, \\ u &= g \quad \text{on } \mathbb{R}^n \times \{t = 0\}, \end{aligned} \tag{15.3}$$

where $b : \mathbb{R}^n \times \mathbb{R}_{>0} \times \mathbb{R} \rightarrow \mathbb{R}^n$ is the velocity field, $f : \mathbb{R}^n \times \mathbb{R}_{>0} \rightarrow \mathbb{R}$ is the source function, and $g : \mathbb{R}^n \rightarrow \mathbb{R}$ is the initial condition.

As before we define our characteristic as the time-parametrized curve which satisfies $\frac{dx_c}{dt} = b(x_c(t), t, u(x_c(t), t))$. We then observe that the solution along the characteristic evolves as follows

$$\frac{d}{dt}(u_c(t)) = \frac{d}{dt}u(x_c(t), t) = \frac{\partial u}{\partial t} + \frac{dx_c}{dt} \cdot \nabla u = f(x_c(t), t).$$

Hence we obtain the following characteristic equations:

Definition 15.7 (characteristic equations for a nonhomogeneous transport equation). The characteristic equations for a nonhomogeneous transport equation $\frac{\partial u}{\partial t} + b\nabla u = f$ is a pair of ODEs

$$\begin{aligned}\frac{dx_c}{dt}(t) &= b(x_c(t), t, u_c(t)), \quad t \in \mathbb{R}_{>0}, \\ \frac{du_c}{dt}(t) &= f(x_c(t), t), \quad t \in \mathbb{R}_{>0}.\end{aligned}$$

We note that the solution u_c along the characteristic is *not* a constant (since $\frac{du_c}{dt} \neq 0$ in general), but its value only depends on the initial condition and the value of f along the characteristic x_c . The pair of ODEs can be readily integrated in time to obtain

$$\begin{aligned}x_c(t) &= \int_{\tau=0}^t b(x_c(\tau), \tau, u_c(\tau))d\tau + x_{c,0} \\ u_c(t) &= \int_{\tau=0}^t f(x_c(\tau), \tau)d\tau + g(x_{c,0}),\end{aligned}$$

where $x_{c,0}$ is the starting point of the characteristic, and the second equation incorporates both the source function and the initial condition.

Example 15.8 (nonhomogeneous transport equation with a constant coefficient). We consider a transport equation

$$\begin{aligned}\frac{\partial u}{\partial t} + b \cdot \nabla u &= f \quad \text{in } \mathbb{R}^n \times \mathbb{R}_{>0}, \\ u &= g \quad \text{on } \mathbb{R}^n \times \{t = 0\}\end{aligned}$$

with a constant velocity field $b \in \mathbb{R}^n$, a source function $f : \mathbb{R}^n \times \mathbb{R}_{>0} \rightarrow \mathbb{R}$, and an initial condition $g : \mathbb{R}^n \rightarrow \mathbb{R}$. The characteristic must satisfy $\frac{dx_c}{dt} = b$, which for the constant velocity field yields $x_c(t) = bt + x_{c,0}$. It hence follows that

$$u_c(t) = u(bt + x_{c,0}, t) = g(x_{c,0}) + \int_{\tau=0}^t f(b\tau + x_{c,0}, \tau)d\tau.$$

We choose $x_{c,0} = x - bt$ to obtain

$$u(x, t) = g(x - bt) + \int_{\tau=0}^t f(x - b(t - \tau), \tau)d\tau. \quad (15.4)$$

As expected from linear superposition, the solution is the sum of the contributions from the initial condition g and the source term f .

Example 15.9. Consider a one-dimensional transport equation

$$\begin{aligned}\frac{\partial u}{\partial t}(x, t) + 2\frac{\partial u}{\partial x}(x, t) &= f(x, t) = \cos(x) \quad \forall x \in \mathbb{R}, t \in \mathbb{R}_{>0}, \\ u(x, t = 0) &= g(x) = \exp(-x^2) \quad \forall x \in \mathbb{R}.\end{aligned}$$

Following the procedure in the previous example for $b = 2$, we obtain

$$\begin{aligned}u(x, t) &= g(x - 2t) + \int_{\tau=0}^t f(x - 2(t - \tau), \tau)d\tau = \exp(-(x - 2t)^2) + \int_{\tau=0}^t \cos(x - 2(t - \tau))d\tau \\ &= \exp(-(x - 2t)^2) + \frac{1}{2} \sin(x - 2(t - \tau))|_{\tau=0}^t = \exp(-(x - 2t)^2) + \frac{1}{2}(\sin(x) - \sin(x - 2t)).\end{aligned}$$

15.6 Nonhomogeneous problems: Duhamel's principle revisited

We recall Duhamel's principle (Theorem 7.9), which allows us to express the solution to a non-homogeneous heat equation in terms of the solution to a family of homogeneous heat equations. Duhamel's principle in fact applies to any equations that is first-order in time. We here provide a general statement:

Theorem 15.10 (Duhamel's principle). Consider the initial value problem

$$\begin{aligned}\frac{\partial u}{\partial t} + \mathcal{L}u &= f \quad \text{in } \mathbb{R}^n \times \mathbb{R}_{>0}, \\ u &= g \quad \text{on } \mathbb{R}^n \times \{t = 0\},\end{aligned}\tag{15.5}$$

where \mathcal{L} is a linear differential operator (e.g., transport operator $b \cdot \nabla$ or Laplacian operator $-\Delta$), $f : \mathbb{R}^n \times \mathbb{R}_{>0} \rightarrow \mathbb{R}$ is the source function, and $g : \mathbb{R}^n \rightarrow \mathbb{R}$ is the initial condition. For any fixed $s \in \mathbb{R}_{>0}$, let $u_f^s : \mathbb{R}^n \times \mathbb{R}_{>s} \rightarrow \mathbb{R}$ be the solution to

$$\begin{aligned}\frac{\partial u_f^s}{\partial t} + \mathcal{L}u_f^s &= 0 \quad \text{in } \mathbb{R}^n \times \mathbb{R}_{>s}, \\ u_f^s &= f(\cdot, s) \quad \text{on } \mathbb{R}^n \times \{t = s\},\end{aligned}\tag{15.6}$$

and $u_g : \mathbb{R}^n \times \mathbb{R}_{>0} \rightarrow \mathbb{R}$ be the solution to

$$\begin{aligned}\frac{\partial u_g}{\partial t} + \mathcal{L}u_g &= 0 \quad \text{in } \mathbb{R}^n \times \mathbb{R}_{>0}, \\ u_g &= g \quad \text{on } \mathbb{R}^n \times \{t = 0\}.\end{aligned}\tag{15.7}$$

Then the solution to (15.5) is given by

$$u(x, t) = u_g(x, t) + \int_{s=0}^t u_f^s(x, t) ds, \quad x \in \mathbb{R}^n, t \in \mathbb{R}_{>0}.\tag{15.8}$$

Proof. We first consider the case of $f \neq 0$ and $g = 0$ (and hence $u_g = 0$). We differentiate (15.8) (for $u_g = 0$) in time to obtain

$$\begin{aligned}\frac{\partial u}{\partial t}(x, t) &= \frac{\partial}{\partial t} \left(\int_{s=0}^t u_f^s(x, t) ds \right) = u_f^t(x, t) + \int_{s=0}^t \frac{\partial u_f^s}{\partial t}(x, t) ds = f(x, t) - \int_{s=0}^t \mathcal{L}u_f^s(x, t) ds \\ &= f(x, t) - \mathcal{L} \left(\int_{s=0}^t u_f^s(x, t) ds \right) = f(x, t) - \mathcal{L}u(x, t).\end{aligned}$$

Here the first equality follows from the differentiation of (15.8) with respect to the integration bound and the integrand, the second equality follows from (15.6), the third equality follows from the fact that the integral does not depend on space, and the last equality follows from (15.8). Hence, the solution (15.8) satisfies the PDE. We also observe that

$$u(x, t = 0) = \int_{s=0}^{t=0} u^s(x, t = 0) ds = 0, \quad x \in \mathbb{R}^n,$$

as $u^s(\cdot, t = 0) = f(\cdot, s)$ is bounded; the solution hence satisfies the homogeneous initial condition $g = 0$ for this case.

We next consider the case of $f = 0$ and $g \neq 0$. This case is associated with (15.7), and hence the solution is given by u_g by definition.

We finally appeal to the linear superposition of the solutions to (i) $f \neq 0$ and $g = 0$ and (ii) $g \neq 0$ and $f = 0$ to obtain (15.8). \square

Example 15.11. We now apply Duhamel's principle to the transport equation with a constant velocity field:

$$\begin{aligned} \frac{\partial u}{\partial t} + b \cdot \nabla u &= f \quad \text{in } \mathbb{R}^n \times \mathbb{R}_{>0}, \\ u &= g \quad \text{on } \mathbb{R}^n \times \{t = 0\}, \end{aligned}$$

The family of homogeneous problems of interest is

$$\begin{aligned} \frac{\partial u^s}{\partial t} + b \cdot \nabla u^s &= 0 \quad \text{in } \mathbb{R}^n \times (s, \infty), \\ u^s &= f(\cdot, s) \quad \text{on } \mathbb{R}^n \times \{t = s\}. \end{aligned}$$

Using the method of characteristics, the solution, for any given s , is given by

$$u^s(x, t) = f(x - b(t - s), s).$$

We also recall that the solution to the homogeneous transport equation is given by

$$u_g(x, t) = g(x - bt).$$

The application of the Duhamel's principle thus yields the solution

$$u(x, t) = u_g(x, t) + \int_{s=0}^t u^s(x, t) ds = g(x - bt) + \int_{s=0}^t f(x - b(t - s), s) ds,$$

which, as we expect, is identical to (15.4) obtained using a more direct approach.

15.7 Initial-boundary value problems

We now consider an initial-boundary value problem in a bounded spatial domain $\Omega \subset \mathbb{R}^n$. Because the transport equation is first-order in space, a boundary condition is only imposed on an *inflow boundary*

$$\Gamma_{\text{in}} \equiv \{x \in \partial\Omega \mid b(x) \cdot \nu(x) < 0\},$$

where ν is the outward-pointing unit normal vector on the boundary. No boundary condition is imposed on an *outflow boundary*

$$\Gamma_{\text{out}} \equiv \partial\Omega \setminus \Gamma_{\text{in}}.$$

This agrees with our physical intuition that if u models the concentration of a pollutant, then we can only specify the concentration at the places where the pollutant enters, and not leaves, the domain. In addition, the only type of the boundary condition that can be imposed in the Dirichlet

type. Hence, given a spatial domain $\Omega \subset \mathbb{R}^n$, the initial-boundary value problem associated with the transport equation takes the following form:

$$\begin{aligned}\frac{\partial u}{\partial t} + b \cdot \nabla u &= f \quad \text{in } \Omega \times \mathbb{R}_{>0}, \\ u &= h \quad \text{on } \Gamma_{\text{in}} \times \mathbb{R}_{>0}, \\ u &= g \quad \text{on } \Omega \times \{t = 0\},\end{aligned}$$

where $f : \Omega \times \mathbb{R}_{>0} \rightarrow \mathbb{R}$ is the source function, $h : \Gamma_{\text{in}} \times \mathbb{R}_{>0} \rightarrow \mathbb{R}$ is the (in general time-dependent) boundary function, and $g : \Omega \rightarrow \mathbb{R}$ is the initial condition.

We can solve the initial-boundary value problem using the method of characteristics. We here provide a concrete one-dimensional example.

Example 15.12. We consider a one-dimensional initial-boundary value problem on a half line:

$$\begin{aligned}\frac{\partial u}{\partial t} - b \frac{\partial u}{\partial x} &= 0 \quad \text{in } \mathbb{R}_{>0} \times \mathbb{R}_{>0}, \\ u &= h \quad \text{on } \{x = 0\} \times \mathbb{R}_{>0}, \\ u &= g \quad \text{on } \mathbb{R}_{>0} \times \{t = 0\},\end{aligned}$$

where $b > 0$ is a fixed advection speed, $h : \mathbb{R}_{>0} \rightarrow \mathbb{R}$ is a boundary condition function, and $g : \mathbb{R}_{>0} \rightarrow \mathbb{R}$ is an initial condition function. Note that we require $b > 0$ so that $\{x = 0\}$ is an inflow boundary, where a boundary condition can be imposed.

To solve the problem, we again note that the ODE for characteristics is

$$\frac{dx_c}{dt}(t) = b.$$

We integrate the ODE from t_0 to t to obtain

$$x_c(t) = b(t - t_0) + x_c(t_0). \quad (15.9)$$

Because the solution to the homogeneous PDE is constant along each characteristic, we obtain

$$u(x_c(t), t) = u(x_c(t_0), t_0). \quad (15.10)$$

We now consider two cases distinguished by the point from which the characteristic emanates, as shown in Figure 15.3.

Case 1: $x > bt$. In this case, the characteristic that goes through (x, t) emanates from the initial-time boundary $\{t = 0\}$ of the space-time domain. (I.e., if we trace the characteristic backward from (x, t) , we intersect the initial-time boundary.) We hence set $x_c(t) = x$ and $t_0 = 0$ in (15.9) to obtain

$$x = bt + x_c(t_0) \quad \Rightarrow \quad x_c(t_0) = x - bt.$$

The substitution of the expressions to (15.10) yields

$$u(x, t) = u(x_c(t_0), t_0) = u(x - bt, 0) = g(x - bt).$$

Case 2: $x < bt$. In this case, the characteristic that goes through (x, t) emanates from the $\{x = 0\}$ boundary. (I.e., if we trace the characteristic backward from (x, t) , we intersect the $\{x = 0\}$ boundary.) We hence set $x_c(t) = x$ and $x_c(t_0) = 0$ in (15.9) to obtain

$$x = b(t - t_0) \quad \Rightarrow \quad t_0 = t - x/b.$$

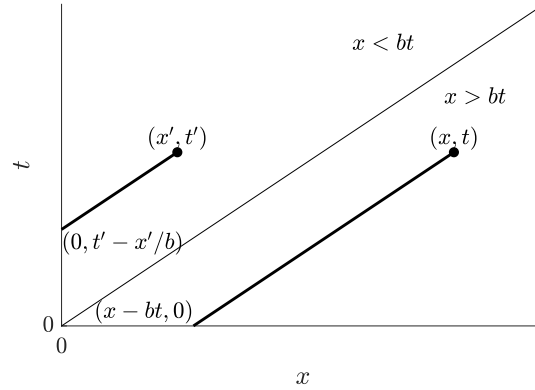


Figure 15.3: Characteristics for the transport equation on the half line $\mathbb{R}_{>0}$.

The substitution of the expressions to (15.10) yields

$$u(x, t) = u(x_c(t_0), t_0) = u(0, t - x/b) = h(t - x/b).$$

In summary, the solution is given by

$$u(x, t) = \begin{cases} g(x - bt), & x > bt, \\ h(t - x/b), & x < bt. \end{cases}$$

We note that the solution $u(x, t)$ for $x > bt$ depends only on the initial condition g ; it does not depend on the boundary condition h . Conversely, the solution $u(x, t)$ for $x < bt$ depends only on the boundary condition h ; it does not depend on the initial condition g . This is a direct consequence of the limited domain of influence and dependence that the transport equation exhibits. The result can be contrasted with the solution of the heat equation on the half line $\mathbb{R}_{>0}$, where the solution at any (x, t) depends on both the initial and boundary conditions.

15.8 Summary

We summarize key points of this lecture:

1. The transport equation models the transport of a conserved quantity by an advection field.
2. The generalized transport equation models transport equation with the advection field that may (i) be constant, (ii) depend on space and time, and (iii) depend on space, time, and the state.
3. The generalized transport equation can be solved using the method of characteristics. The method turns the PDE into a pair of ODEs along characteristics.
4. For homogeneous transport equations, the value of the solution along each characteristic is a constant. The characteristic can be found by integrating the advection field. If the advection field is constant, the solution is simply translated in time.

5. For nonhomogeneous transport equations, the value of the solution along each characteristic grows/decays depending the values of the source function along the characteristic.
6. The transport equation exhibits limited domain of influence and finite propagation speed. This is unlike the heat equation which exhibits unbounded domain of influence and infinite propagation speed.
7. The solution to the transport equation is not smooth if the initial condition is not smooth. This is unlike the heat (and Laplace's) equation for which the solution is always smooth even if the initial condition (or boundary condition) is discontinuous.
8. The solution to nonhomogeneous transport equations can also be obtained using Duhamel's principle.
9. If the spatial domain has a boundary, then Dirichlet boundary conditions are imposed on the inflow boundaries; no boundary conditions are imposed elsewhere.

Lecture 16

Wave equation: method of characteristics

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16.1 Introduction

In this lecture we analyze the wave equation in unbounded domain using the d'Alembert's formula derived using the method of characteristics. The method provides other physical insights that are not as obvious from the analysis based on separation of variables. Method of characteristics in fact provides a similar insight for the wave equation that the fundamental solution does for the heat equation. We will also study the behavior of the wave equation on a half line $\mathbb{R}_{>0}$ using the method of reflection, with a particular attention to the behavior of the function at the boundary.

16.2 d'Alembert's formula: revisited

We first consider the IVP for one-dimensional wave equation in $\mathbb{R} \times \mathbb{R}_{>0}$:

$$\begin{aligned}\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} &= 0 \quad \text{in } \mathbb{R} \times \mathbb{R}_{>0}, \\ u &= g \quad \text{on } \mathbb{R} \times \{t = 0\}, \\ \frac{\partial u}{\partial t} &= h \quad \text{on } \mathbb{R} \times \{t = 0\},\end{aligned}$$

for some functions $g : \mathbb{R} \rightarrow \mathbb{R}$ and $h : \mathbb{R} \rightarrow \mathbb{R}$. Our goal is to find a representation for u in terms of g and h using the method of characteristics. We will find that the resulting formula is the d'Alembert's formula, which we have derived for bounded domains using separation of variables in Lecture 14.

To this end, we first factor the second-order operator as a product of two first-order operators:

$$\frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} = \left(\frac{\partial}{\partial t} + \frac{\partial}{\partial x} \right) \underbrace{\left(\frac{\partial}{\partial t} - \frac{\partial}{\partial x} \right)}_{\equiv v} u = 0.$$

This “factorization” allows us to decompose the wave equation, which is a second-order PDE, into a pair of first-order PDEs:

$$\frac{\partial u}{\partial t} - \frac{\partial u}{\partial x} = v, \quad (16.1)$$

$$\frac{\partial v}{\partial t} + \frac{\partial v}{\partial x} = 0. \quad (16.2)$$

We recognize these are transport equations. We approach the problem in two steps: we first solve (16.2) for v ; we then solve (16.1) for u .

We first apply the method of characteristics to the one-dimensional homogeneous transport equation (16.2) (for which $b = 1$) to obtain

$$v(x, t) = v^0(x - t),$$

where $v^0(x) = v(x, t = 0) \forall x \in \mathbb{R}$ is the initial condition, which we later specify.

We next substitute the expression for v into (16.1) to obtain

$$\frac{\partial u}{\partial t}(x, t) - \frac{\partial u}{\partial x}(x, t) = v^0(x - t).$$

This is a nonhomogeneous transport equation with a constant coefficient $b = -1$ and the source function $v(x, t) = v^0(x - t)$. We again apply the method of characteristics to obtain

$$\begin{aligned} u(x, t) &= u(x - bt, 0) + \int_{\tau=0}^t v(x - b(t - \tau), \tau) d\tau \\ &= u(x - bt, 0) + \int_{\tau=0}^t v^0(x - b(t - \tau) - \tau) d\tau \\ &= u(x + t, 0) + \int_{\tau=0}^t v^0(x + t - 2\tau) d\tau. \end{aligned}$$

We now consider the change of variables $\xi = x + t - 2\tau$ to obtain

$$u(x, t) = u(x + t, 0) + \int_{x+t}^{x-t} v^0(\xi) \left(-\frac{1}{2} d\xi\right) = u(x + t, 0) + \frac{1}{2} \int_{x-t}^{x+t} v^0(\xi) d\xi. \quad (16.3)$$

We then appeal to the initial condition $u(x + t, 0) = g(x + t)$ and the definition of v^0 to obtain

$$v^0(\xi) = v(\xi, 0) = \frac{\partial u}{\partial t}(\xi, 0) - \frac{\partial u}{\partial x}(\xi, 0) = h(\xi) - g'(\xi).$$

The substitution of the relationship to (16.3) yields

$$u(x, t) = g(x + t) + \frac{1}{2} \int_{x-t}^{x+t} (h(\xi) - g'(\xi)) d\xi$$

which, by the fundamental theorem of calculus, simplifies to

$$\begin{aligned} u(x, t) &= g(x + t) - \frac{1}{2}g(x + t) + \frac{1}{2}g(x - t) + \frac{1}{2} \int_{x-t}^{x+t} h(\xi) d\xi \\ &= \frac{1}{2}(g(x + t) + g(x - t)) + \frac{1}{2} \int_{x-t}^{x+t} h(\xi) d\xi. \end{aligned} \quad (16.4)$$

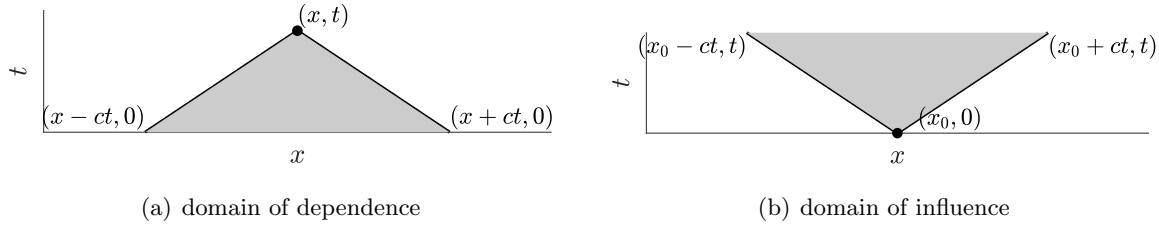


Figure 16.1: Domain of dependence and influence for the wave equation.

We have rederived the *d'Alembert's formula* using the method of characteristics. Note that the formula is now defined on the entire real line \mathbb{R} .

We now compare the behaviors of the wave equation (which is hyperbolic) and the heat equation (which is parabolic). To this end, we note that the solutions to the two equations for a given initial condition g (and h) can be expressed as

$$\begin{aligned} \text{wave: } u(x, t) &= \frac{1}{2}(g(x+t) + g(x-t)) + \frac{1}{2} \int_{x-t}^{x+t} h(\xi) d\xi, \\ \text{heat: } u(x, t) &= \int_{\mathbb{R}} \Phi(x-\xi, t) g(\xi) d\xi, \end{aligned}$$

where Φ is the fundamental solution of the heat equation, which is smooth and nonzero everywhere. We make a few observations:

1. *Limited domain of dependence.* The solution at (x, t) depends only on the initial position g at $x-t$ and $x+t$ and the initial velocity in $(x-t, x+t)$. (Note that in the dimensional form, the domain is $(x-ct, x+ct)$.) Figure 16.1(a) illustrates the *domain of dependence* for the wave equation in the space-time domain. The bounded domain of dependence is unlike the heat equation, in which the solution $u(x, t)$ depends on the initial condition everywhere.
2. *Limited domain of influence.* The *domain of influence* is the subset of the space-time domain that the initial values $g(x_0)$ and $h(x_0)$ affects the solution. Figure 16.1(b) illustrates the domain of influence for the wave equation. Again, because the wave propagates at the speed of at most $c = 1$, the initial condition at (x_0, t) only influences solutions in $[x_0 - t, x_0 + t]$ at time t . This is again unlike the heat equation, for which the initial condition $g(x_0)$ influences the entire solution for $t > 0$.
3. *Finite propagation speed.* The waves propagate at the speed of at most $c = 1$, and the initial condition outside of $[x-t, x+t]$ does not have time to influence the solution at (x, t) . This is again unlike the heat equation with the infinite propagation speed.
4. *Lack of smoothness.* The solution to the wave equation is only as regular as the initial condition g and only one order more regular than the initial condition h . If g is (only) twice continuously differentiable and h is (only) once continuously differentiable, then $u(\cdot, t)$ is (only) twice continuously differentiable. This is unlike the heat equation whose solution $u(\cdot, t)$ is smooth (i.e., infinitely differentiable) for any $t > 0$ even if the initial condition g is discontinuous.

16.3 Wave equation on $\mathbb{R}_{>0} \times \mathbb{R}_{>0}$: homogeneous Dirichlet BC

We now consider the wave equation on the half line $\mathbb{R}_{>0}$:

$$\begin{aligned} \frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} &= 0 && \text{in } \mathbb{R}_{>0} \times \mathbb{R}_{>0}, \\ u &= 0 && \text{on } \{x = 0\} \times \mathbb{R}_{>0}, \\ u &= g && \text{on } \mathbb{R}_{>0} \times \{t = 0\}, \\ \frac{\partial u}{\partial t} &= h && \text{on } \mathbb{R}_{>0} \times \{t = 0\}; \end{aligned} \tag{16.5}$$

note that homogeneous Dirichlet boundary condition is imposed at $x = 0$.

We wish to solve the problem using the method of reflection, which we have considered in the context of heat equation in Lecture 7. We recall the idea is to identify a problem on the entire real line \mathbb{R} whose solution restricted to the half line $\mathbb{R}_{>0}$ is the solution to (16.5). We also recall that we can impose the homogeneous Dirichlet boundary condition by considering the odd extension of the initial conditions, as the odd extension of a continuous function vanishes at the origin. We hence consider

$$\begin{aligned} \frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} &= 0 && \text{in } \mathbb{R} \times \mathbb{R}_{>0}, \\ u &= g^\circ && \text{on } \mathbb{R} \times \{t = 0\}, \\ \frac{\partial u}{\partial t} &= h^\circ && \text{on } \mathbb{R} \times \{t = 0\}, \end{aligned} \tag{16.6}$$

where $g^\circ : \mathbb{R} \rightarrow \mathbb{R}$ and $h^\circ : \mathbb{R} \rightarrow \mathbb{R}$ are the odd extensions of $g : \mathbb{R}_{>0} \rightarrow \mathbb{R}$ and $h : \mathbb{R}_{>0} \rightarrow \mathbb{R}$, respectively. We apply d'Alembert's formula to the extended problem to obtain

$$u(x, t) = \frac{1}{2}(g^\circ(x+t) + g^\circ(x-t)) + \frac{1}{2} \int_{x-t}^{x+t} h^\circ(\xi) d\xi.$$

We can simplify the formula with some manipulation specific to odd functions. To this end, we partition the space-time domain into two parts: the part not affected by the reflected wave ($x > t$) and the part affected by the reflected wave ($x < t$).

Case 1: $x > t$. In this case, all arguments of g° and h° are positive and hence we can simply substitute $g^\circ = g$ and $h^\circ = h$:

$$u(x, t) = \frac{1}{2}(g(x+t) + g(x-t)) + \frac{1}{2} \int_{x-t}^{x+t} h(\xi) d\xi, \quad x > t.$$

An illustration for the $x > t$ case is shown in Figure 16.2(a). Because the reflected wave does not reach $u(x, t)$, the solution is identical to what would have been obtained if the boundary did not exist.

Case 2: $x < t$. In this case, some of the arguments of g° and h° become negative. We appeal to the property of the odd extension to obtain, for $x - t < 0$,

$$g^\circ(x-t) = -g(t-x).$$

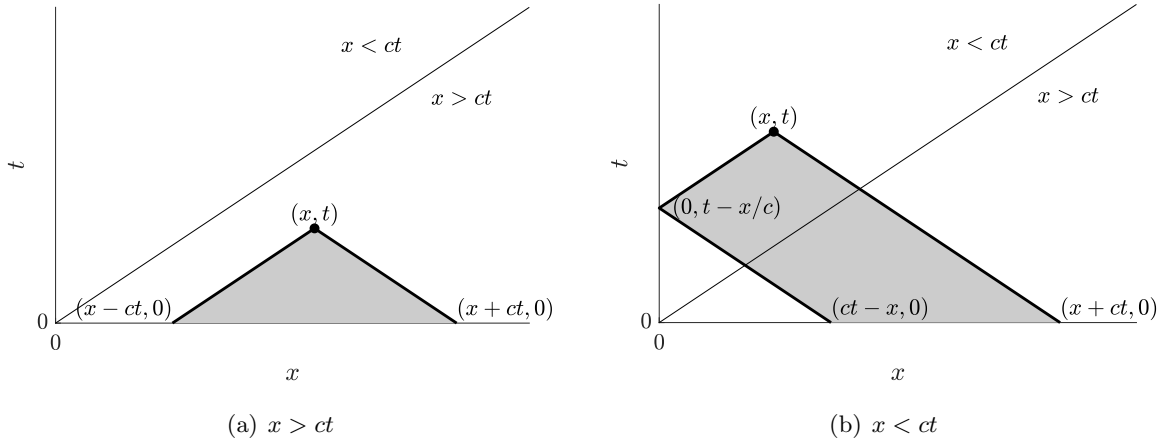


Figure 16.2: Visualization of the solution of the wave equation on the half line with homogeneous Dirichlet boundary condition at $x = 0$.

In addition, we split the integral on h° into three parts according to Figure 16.2(b) to obtain

$$\frac{1}{2} \int_{x-t}^{x+t} h^\circ(\xi) d\xi = \underbrace{\frac{1}{2} \int_{x-t}^0 h^\circ(\xi) d\xi + \frac{1}{2} \int_0^{t-x} h^\circ(\xi) d\xi}_{\text{equal and opposite}} + \frac{1}{2} \int_{t-x}^{x+t} h^\circ(\xi) d\xi = \frac{1}{2} \int_{t-x}^{x+t} h(\xi) d\xi;$$

here, the first two integrals cancel each other because h° is an odd function and the integration domains $(x-t, 0)$ and $(0, t-x)$ are symmetric about the origin. We hence obtain

$$u(x, t) = \frac{1}{2}(g(x+t) - g(t-x)) + \frac{1}{2} \int_{\xi=t-x}^{x+t} h(\xi) d\xi, \quad x < t.$$

An illustration for the $x < t$ case is shown in Figure 16.2(b).

We make a few observations:

1. For $x > t$, the solution $u(x, t)$ does not depend on the boundary condition, as the information does not reach (x, t) due to the finite propagation speed. This is unlike for the heat equation, where the boundary condition influences the solution everywhere due to the infinite propagation speed.
2. For $x < t$, the reflected wave that reaches (x, t) originates at $t-x$ and is inverted (i.e., the sign is changed).
3. For $x < t$, the integral of h over $(0, t-x)$ vanishes because it cancels with the odd extension over $(-(t-x), 0)$; hence the solution depends only on h over $(t-x, x+t)$.

16.4 Wave equation on $\mathbb{R}_{>0} \times \mathbb{R}_{>0}$: homogeneous Neumann BC

We now consider the wave equation on the half line $\mathbb{R}_{>0}$:

$$\begin{aligned} \frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} &= 0 \quad \text{in } \mathbb{R}_{>0} \times \mathbb{R}_{>0}, \\ \frac{\partial u}{\partial x} &= 0 \quad \text{on } \{x = 0\} \times \mathbb{R}_{>0}, \\ u &= g \quad \text{on } \mathbb{R}_{>0} \times \{t = 0\}, \\ \frac{\partial u}{\partial t} &= h \quad \text{on } \mathbb{R}_{>0} \times \{t = 0\}; \end{aligned}$$

note that homogeneous Neumann boundary condition is imposed at $x = 0$.

We again use the method of reflection. We recall that for homogeneous Neumann boundary condition, we consider the even extension of the initial conditions, as the even extension of a continuous function has a vanishing derivative at the origin. We hence consider

$$\begin{aligned} \frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} &= 0 \quad \text{in } \mathbb{R} \times \mathbb{R}_{>0}, \\ u &= g^e \quad \text{on } \mathbb{R} \times \{t = 0\}, \\ \frac{\partial u}{\partial t} &= h^e \quad \text{on } \mathbb{R} \times \{t = 0\}, \end{aligned} \tag{16.7}$$

where $g^e : \mathbb{R} \rightarrow \mathbb{R}$ and $h^e : \mathbb{R} \rightarrow \mathbb{R}$ are the even extensions of $g : \mathbb{R}_{>0} \rightarrow \mathbb{R}$ and $h : \mathbb{R}_{>0} \rightarrow \mathbb{R}$, respectively. We apply d'Alembert's formula to obtain

$$u(x, t) = \frac{1}{2}(g^e(x+t) + g^e(x-t)) + \frac{1}{2} \int_{x-t}^{x+t} h^e(\xi) d\xi.$$

We simplify the formula with some manipulation specific to even functions. We again partition the space-time domain into two parts: the part not affected by the reflected wave ($x > t$) and the part affected by the reflected wave ($x < t$).

Case 1: $x > t$. In this case, all arguments of g^e and h^e are positive and hence we can simply substitute $g^e = g$ and $h^e = h$:

$$u(x, t) = \frac{1}{2}(g(x+t) + g(x-t)) + \frac{1}{2} \int_{x-t}^{x+t} h(\xi) d\xi, \quad x > t.$$

As before, and as shown in Figure 16.3(a), the reflected wave does not reach $u(x, t)$ and hence the solution is identical to what would have been obtained if the boundary did not exist.

Case 2: $x < t$. In this case, some of the arguments of g^e and h^e become negative. We appeal to the property of the even extension to obtain, for $x - t < 0$,

$$g^e(x-t) = g(t-x).$$

In addition, we split the integral on h^e into three parts according to Figure 16.3(b) to obtain

$$\begin{aligned} \frac{1}{2} \int_{x-t}^{x+t} h^e(\xi) d\xi &= \frac{1}{2} \int_{x-t}^0 h^e(\xi) d\xi + \underbrace{\frac{1}{2} \int_0^{t-x} h^e(\xi) d\xi + \frac{1}{2} \int_{t-x}^{x+t} h^e(\xi) d\xi}_{\text{equal to each other}} \\ &= \int_0^{t-x} h^e(\xi) d\xi + \frac{1}{2} \int_{t-x}^{x+t} h(\xi) d\xi; \end{aligned}$$

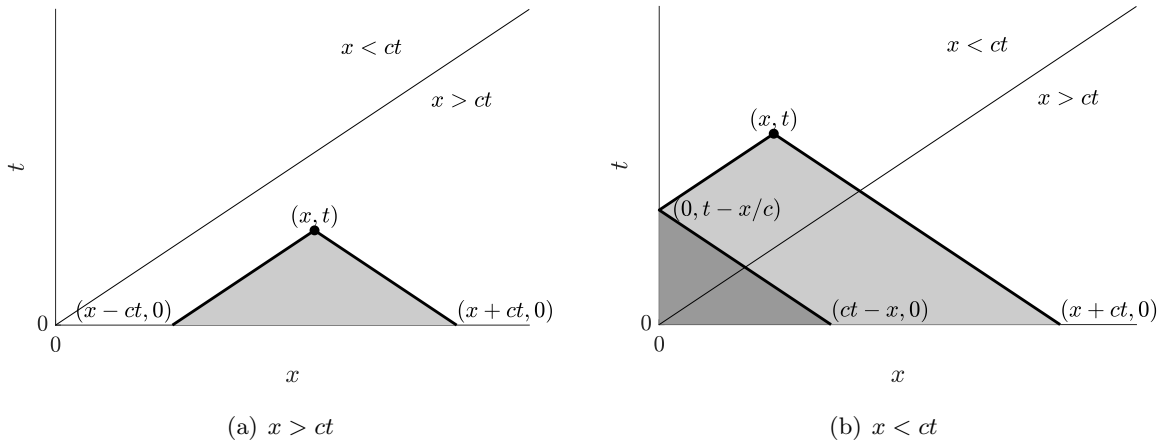


Figure 16.3: Visualization of the solution of the wave equation on the half line with homogeneous Neumann boundary condition at $x = 0$.

here the first two integrals are equal to each other because h^e is an even function and the integration domains $(x - t, 0)$ and $(0, t - x)$ are symmetric about the origin. We hence obtain

$$u(x, t) = \frac{1}{2}(g(x + t) + g(t - x)) + \int_0^{t-x} h(\xi) d\xi + \frac{1}{2} \int_{t-x}^{x+t} h(\xi) d\xi, \quad x < t.$$

An illustration for the $x < t$ case is shown in Figure 16.3(b).

We make a few observations:

1. For $x > t$, the solution $u(x, t)$ does not depend on the boundary condition (as before).
2. For $x < t$, the reflected wave that reaches (x, t) originates at $t - x$ and is *not* inverted (i.e., has the same sign). This is unlike at a homogeneous Dirichlet boundary where the reflected wave is inverted.
3. For $x < t$, the integral of h over $(0, t - x)$ is doubled because it must also account for the even extension over $(-(t - x), 0)$. The solution depends on h over $(0, x + t)$; this differs from the homogeneous Dirichlet boundary case, in which the solution depends on h over only $(t - x, x + t)$.

16.5 Wave equation on $(0, 1) \times \mathbb{R}_{>0}$

In a previous lecture we considered the solution of the wave equation on a bounded domain using separation of variables. We now revisit the problem, but now using the method of reflection. The

problem we consider is

$$\begin{aligned} \frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} &= 0 && \text{in } \mathbb{R}_{>0} \times (0, 1), \\ u &= 0 && \text{on } \{0, 1\} \times \mathbb{R}_{>0}, \\ u &= g && \text{on } (0, 1) \times \{t = 0\}, \\ \frac{\partial u}{\partial t} &= h && \text{on } (0, 1) \times \{t = 0\}; \end{aligned} \tag{16.8}$$

the homogeneous Dirichlet boundary condition is imposed at both $x = 0$ and 1 .

We again consider a problem on the entire real line \mathbb{R} whose solution restricted to $(0, 1)$ satisfies (16.8). To find the solution that vanishes at both $x = 0$ and 1 , we consider the initial condition that is odd with respect to both $x = 0$ and 1 . The odd extension $g : (0, 1) \rightarrow \mathbb{R}$ and $h : (0, 1) \rightarrow \mathbb{R}$ to $g^\circ : (0, 1) \rightarrow \mathbb{R}$ and $h^\circ : (0, 1) \rightarrow \mathbb{R}$ results in an odd function about $x = 0$. We then consider the periodic extension of g° and h° — which is the odd periodic extension of g and h — to obtain a function that is odd with respect to $x = 1$. Hence, the problem on the entire \mathbb{R} that we seek is

$$\begin{aligned} \frac{\partial^2 u}{\partial t^2} - \frac{\partial^2 u}{\partial x^2} &= 0 && \text{in } \mathbb{R} \times \mathbb{R}_{>0}, \\ u &= g^{\circ,p} && \text{on } \mathbb{R} \times \{t = 0\}, \\ \frac{\partial u}{\partial t} &= h^{\circ,p} && \text{on } \mathbb{R} \times \{t = 0\}, \end{aligned} \tag{16.9}$$

where $g^{\circ,p} : \mathbb{R} \rightarrow \mathbb{R}$ and $h^{\circ,p} : \mathbb{R} \rightarrow \mathbb{R}$ are the odd extensions of the $g : (0, 1) \rightarrow \mathbb{R}$ and $h : (0, 1) \rightarrow \mathbb{R}$, respectively. We had previously derived this result using separation of variables; we have now derived the result using the method of characteristics and the method of reflection. This approach based on the method of reflection readily extends to the case of homogeneous Neumann boundary conditions and mixed boundary conditions (i.e., Dirichlet on one end and Neumann on the other end).

16.6 Summary

We summarize key points of this lecture:

1. We can derive the d'Alembert's formula on the entire real line \mathbb{R} using the method of characteristics.
2. The wave equation exhibits a limited domain of influence, limited domain of dependence, and finite propagation speed. This is unlike the heat equation which exhibits unbounded domain of influence and dependence and infinite propagation speed.
3. The solution to the wave equation is in general not smooth if either of the initial conditions g or h is not smooth.
4. The solution to the wave equation on the half line $\mathbb{R}_{>0}$ can be obtained using the method of reflection. If homogeneous Dirichlet boundary condition is imposed at $x = 0$, then we consider the odd extension of the initial condition and find the reflected wave is inverted. If homogeneous Neumann boundary condition is imposed at $x = 0$, we consider the even extension of the initial condition and find the reflected wave is not inverted.

5. The solution to the wave equation on a bounded domain can be obtained using the method of reflection on both boundaries. The initial conditions are extended using appropriate odd/even periodic extensions.

Lecture 17

Weak solution of conservation laws

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17.1 Introduction

In this lecture we consider the solution of conservation laws, which play an important role in fluid mechanics. We first provide an abstract form of conservation laws and then provide a few concrete model problems. We then introduce the notion of weak solution; a weak solution may contain discontinuities and allows us to analyze phenomena such as shock and rarefaction waves. We conclude the lecture with a discussion of entropy-satisfying (i.e., physically relevant) solutions to conservation laws in the presence of discontinuities.

17.2 Conservation laws

To consider the idea of weak solution in a general but simple setting, we first introduce a general conservation law in one dimension:

$$\begin{aligned} \frac{\partial u}{\partial t} + \frac{\partial}{\partial x} F(u) &= 0 \quad \text{in } \mathbb{R} \times \mathbb{R}_{>0}, \\ u &= g \quad \text{on } \mathbb{R} \times \{t = 0\}, \end{aligned} \tag{17.1}$$

where u is the conserved state, and $F : \mathbb{R} \rightarrow \mathbb{R}$ is a flux function. We assume that the flux is continuous in u . This general form of the equation encompasses many relevant PDEs; we provide a few examples.

Example 17.1 (transport equation). The constant-coefficient transport equation $\frac{\partial u}{\partial t} + b \frac{\partial u}{\partial x} = 0$ for $b \in \mathbb{R}$ is a conservation law with the flux $F(u) = bu$. (More generally in higher dimensions, transport equation with any divergence free velocity field $\nabla \cdot b = 0$ is a conservation law with the flux $F(u) = bu$.)

Example 17.2 (Burgers' equation). The Burgers' equation $\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = 0$ is a model equation for compressible flows, which exhibits phenomena such as shock waves and rarefaction waves. We observe that $u \frac{\partial u}{\partial x} = \frac{\partial}{\partial x} (\frac{1}{2}u^2)$, and hence the Burgers' equation is a conservation law with the flux $F(u) = \frac{1}{2}u^2$.

Example 17.3 (traffic flow equation). The traffic flow equation models the density of cars on a one-way road. The conserved state u is the density of the cars and the flux is given by $F(u) = uv_{\max}(1 - u/u_{\max})$, where v_{\max} is the maximum velocity of the traffic and u_{\max} is the maximum density of the cars.

17.3 Weak solution

We have observed that the solution to the transport equation $\frac{\partial u}{\partial t} + b\frac{\partial u}{\partial x} = 0$ is in general not smooth. This is unlike the solution to the heat equation $\frac{\partial u}{\partial t} - \frac{\partial^2 u}{\partial x^2} = 0$ for which the solution is smooth (i.e., $u(\cdot, t) \in C^\infty(\mathbb{R})$) for any $t > 0$. This lack of smoothness is in fact a property of conservation laws, where the solution is “transported” instead of “diffused”. However, as it stands, the PDE $\frac{\partial u}{\partial t} + b\frac{\partial u}{\partial x} = 0$ does not even make sense unless the solution is at least once differentiable in both space and time. It turns out we can relax this differentiability requirement and pose a different form of the PDE, called the *weak form*, so that the problem admits less regular solutions (and initial and boundary conditions), which includes discontinuous solutions. In this section we introduce this weak form of conservation laws.

To begin, we introduce a space of *test functions*, which comprises smooth space-time functions $v \in C^\infty(\mathbb{R} \times \mathbb{R}_{\geq 0})$. We (for now) assume the solution is differentiable — and hence $\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}F(u) = 0$ makes sense —, multiply our strong form by the test function, and integrate by parts to obtain

$$\begin{aligned} 0 &= \int_0^\infty \int_{-\infty}^\infty v \left(\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}F(u) \right) dxdt \\ &= - \int_0^\infty \int_{-\infty}^\infty \frac{\partial v}{\partial t} u dxdt - \int_{-\infty}^\infty v u dx|_{t=0} - \int_0^\infty \int_{-\infty}^\infty \frac{\partial v}{\partial x} F(u) dxdt. \end{aligned}$$

We finally substitute the initial condition $u = g$ on $\mathbb{R} \times \{t = 0\}$ to obtain

$$\int_0^\infty \int_{-\infty}^\infty \left(\frac{\partial v}{\partial t} u + \frac{\partial v}{\partial x} F(u) \right) dxdt + \int_{-\infty}^\infty v g dx|_{t=0} = 0.$$

This is the weak form of the conservation law.

Definition 17.4 (weak solution). The bounded solution $u \in L^\infty(\mathbb{R} \times \mathbb{R}_{>0})$ such that

$$\int_0^\infty \int_{-\infty}^\infty \left(\frac{\partial v}{\partial t} u + \frac{\partial v}{\partial x} F(u) \right) dxdt + \int_{-\infty}^\infty v g dx|_{t=0} = 0 \quad \forall v \in C^\infty(\mathbb{R} \times \mathbb{R}_{\geq 0})$$

is called a weak solution of the conservation law $\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}F(u) = 0$ with the initial condition $u = g$ at $t = 0$.

We now analyze the behavior of the weak solution for three cases with increasingly less regular solutions: smooth solution, continuous but nondifferentiable solution, and discontinuous solution.

Smooth solution. Any solution u that satisfies the strong form of the conservation law (17.1) is a solution to the weak form; we integrate by parts in both space and time to obtain

$$\begin{aligned} &\int_0^\infty \int_{-\infty}^\infty \left(\frac{\partial v}{\partial t} u + \frac{\partial v}{\partial x} F(u) \right) dxdt + \int_{-\infty}^\infty v g dx|_{t=0} \\ &= - \int_0^\infty \int_{-\infty}^\infty v \left(\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}F(u) \right) dxdt + \int_{-\infty}^\infty v(g - u) dx|_{t=0} = 0, \end{aligned}$$

where the first and second terms vanish because u satisfies the strong form of PDE and the initial condition, respectively.

Continuous but nondifferentiable solution. We now consider the case where u is not differentiable across some space-time curve and hence the strong form (17.1) does not make sense. For instance, for the transport equation, such a nondifferentiable solution would arise if the initial condition is not differentiable. We will show that a weak solution exists even in this case. To begin, we introduce a space-time curve $x = \xi(t)$ and the associated space-time unit normal vector $n \equiv (n_x, n_t) = \frac{1}{\sqrt{1+(\xi')^2}}(1, -\xi')$ that points outward from the “left” domain $\{(x, t) \in \mathbb{R} \times \mathbb{R}_{>0} \mid x < \xi(t), \forall t \in \mathbb{R}_{>0}\}$ into the “right” domain. Note that $\xi' = \frac{d\xi}{dt}$ is the velocity at which the nondifferentiable point moves. We assume that the solution u satisfies $\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}F(u) = 0$ everywhere except on the curve $x = \xi(t)$ and observe that

$$\begin{aligned} 0 &= \int_0^\infty \int_{-\infty}^\infty \left(\frac{\partial v}{\partial t} u + \frac{\partial v}{\partial x} F(u) \right) dx dt \\ &= \int_0^\infty \int_{-\infty}^{\xi(t)} \left(\frac{\partial v}{\partial t} u + \frac{\partial v}{\partial x} F(u) \right) dx dt + \int_0^\infty \int_{\xi(t)}^\infty \left(\frac{\partial v}{\partial t} u + \frac{\partial v}{\partial x} F(u) \right) dx dt \\ &= - \int_0^\infty \int_{-\infty}^{\xi(t)} v \left(\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} F(u) \right) dx dt + \int_{x=\xi(t)} (vu^- n_t + vF(u^-) n_x) ds \\ &\quad - \int_0^\infty \int_{\xi(t)}^\infty v \left(\frac{\partial u}{\partial t} + \frac{\partial}{\partial x} F(u) \right) dx dt - \int_{x=\xi(t)} (vu^+ n_t + vF(u^+) n_x) ds \\ &= \int_{x=\xi(t)} (v((u^- - u^+) n_t + (F(u^-) - F(u^+)) n_x)) ds. \end{aligned}$$

Because v is arbitrary, we require the solution to satisfy

$$(u^- - u^+) n_t + (F(u^-) - F(u^+)) n_x = 0$$

along the nondifferentiable curve $x = \xi(t)$. We now substitute $n_t/n_x = -\xi'$ to obtain

$$F(u^-) - F(u^+) = \xi'(u^- - u^+). \quad (17.2)$$

If u is continuous but not differentiable across $x = \xi(t)$, we observe that the condition at the nondifferentiable interface (17.2) is automatically satisfied because (i) $u^- = u^+$ since u is continuous and (ii) $F(u^-) = F(u^+)$ since $F : \mathbb{R} \rightarrow \mathbb{R}$ is continuous on its argument and u is continuous. In addition, we note that the above argument can be generalized to any finite number of nondifferentiable curves. Hence we conclude that if the solution u is (i) continuous everywhere and (ii) satisfies the strong form $\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}F(u) = 0$ everywhere except on a finite number of space-time curves on which u is not differentiable, then u is a weak solution.

Discontinuous solution. We now consider the case where u is discontinuous across some space-time curve. We follow the same argument as the case above for nondifferentiable solution and find that the condition across the space-time curve $x = \xi(t)$ is

$$F(u^-) - F(u^+) = \xi'(u^- - u^+).$$

However, now that u is discontinuous, this condition is not automatically satisfied. This is in fact the *Rankine-Hugoniot condition*, which the weak solution must satisfy across a discontinuity or *shock*.

Theorem 17.5 (Rankine-Hugoniot condition). Given a conservation law $\frac{\partial u}{\partial t} + \frac{\partial}{\partial x}F(u) = 0$, the discontinuous solution across the shock curve $\{(x, t) \mid x = \xi(t), t \in \mathbb{R}_{>0}\}$ satisfies

$$F(u^-) - F(u^+) = s(u^- - u^+)$$

for the shock speed $s = \xi'$.

Hence, if the solution is discontinuous along a finite number of space-time curves, the weak solution must (i) satisfy the strong form of the equation everywhere it is continuous and differentiable and (ii) the Rankine-Hugoniot condition across the discontinuities.

17.4 Weak solutions of transport equation

We now seek the weak solution of the transport equation with nondifferentiable initial conditions.

Example 17.6 (transport equation with a nondifferentiable initial condition). Consider the transport equation $\frac{\partial u}{\partial t} + b\frac{\partial u}{\partial x} = 0$ on $\mathbb{R} \times \mathbb{R}_{>0}$ with the initial condition

$$g(x) = \begin{cases} 1 - |x|, & x \in (-1, 1), \\ 0, & x \in (-\infty, 0) \cup (1, \infty). \end{cases}$$

The initial condition is continuous but not differentiable at $x = -1, 0$, and 1 . We use the method of characteristics to find that the solution is

$$u(x, t) = g(x - bt),$$

which is a triangular wave that propagates at the speed b . Because u is continuous, this is a weak solution to the problem.

Example 17.7 (transport equation with a discontinuous initial condition). Consider the transport equation $\frac{\partial u}{\partial t} + b\frac{\partial u}{\partial x} = 0$ on $\mathbb{R} \times \mathbb{R}_{>0}$ with the initial condition

$$g(x) = \begin{cases} 1, & x \in (-1, 1), \\ 0, & x \in (-\infty, 0) \cup (1, \infty). \end{cases}$$

The initial condition is discontinuous at $x = -1$ and 1 . We use the method of characteristics to find that the solution is $u(x, t) = g(x - bt)$, which is a square wave that propagates at the speed b . Because u is discontinuous, we must check that the Rankine-Hugoniot condition is satisfied. We observe that the discontinuities must propagate at the speed of

$$s = \frac{F(u^-) - F(u^+)}{u^- - u^+} = \frac{bu^- - bu^+}{u^- - u^+} = \frac{b(u^- - u^+)}{u^- - u^+} = b.$$

The discontinuity in the solution $u(x, t) = g(x - bt)$ indeed propagates at the speed b , the Rankine-Hugoniot condition is satisfied, and u is a weak solution to the problem.

We recall that the characteristic equations were obtained assuming the solution is differentiable. However, the above two examples show that the solution to the characteristic equation, $u(x, t) = g(x - bt)$, is indeed a weak solution even if the initial condition is nondifferentiable and hence the solution is nondifferentiable.

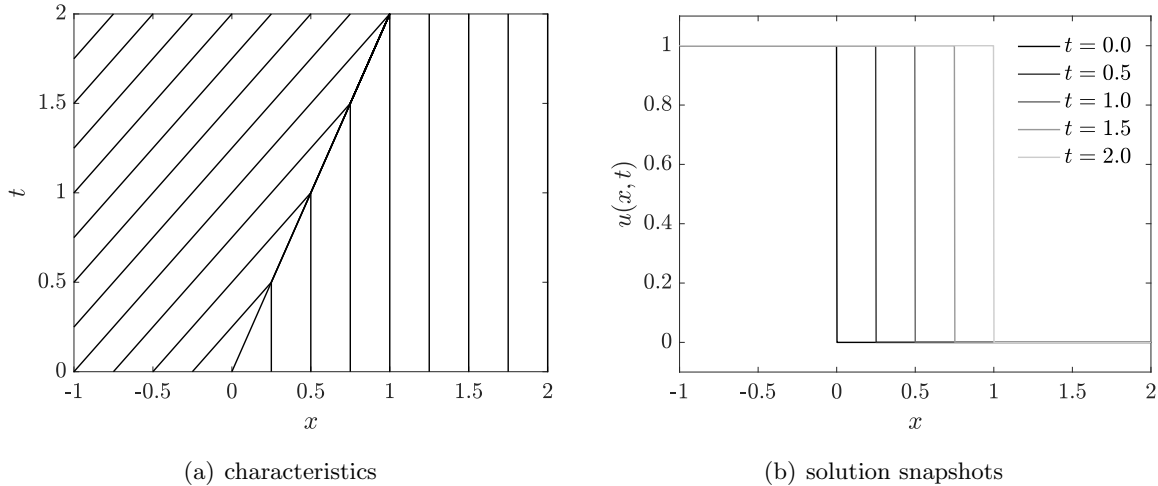


Figure 17.1: The characteristics and solution snapshots for the Burgers' problem with a shock in Example 17.8.

17.5 Weak solution of Burgers' equation: shocks

We now seek a weak solution of Burgers' equation.

Example 17.8 (shock in Burgers' equation). Consider the initial value problem: Burgers' equation

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = \frac{\partial u}{\partial t} + \frac{\partial}{\partial x} \left(\frac{1}{2} u^2 \right) = 0 \quad \text{in } \mathbb{R} \times \mathbb{R}_{>0}$$

with the initial condition

$$g(x) = \begin{cases} 1, & x < 0 \\ 0, & x > 0. \end{cases}$$

Because $1 = u(x = 0^-) > u(x = 0^+) = 0$, the characteristic curve intersect for any $t > 0$ and there is no continuous solution. However, there is a discontinuous solution given by

$$u(x, t) = \begin{cases} 1, & x < st \\ 0, & x > st, \end{cases}$$

where the shock speed s is given by the Rankine-Hugoniot condition

$$s = \frac{F(u^-) - F(u^+)}{u^- - u^+} = \frac{\frac{1}{2}1^2 - \frac{1}{2}0^2}{1 - 0} = \frac{1}{2}.$$

Figure 17.1 shows the characteristics and the solution snapshots. The characteristics collapse into the shock at $x = st = t/2$; the snapshots also show the traveling shock.

17.6 Entropy condition

We now consider another initial value problem: Burgers' equation on \mathbb{R} with the initial condition

$$g(x) = \begin{cases} 0, & x < 0, \\ 1, & x > 0. \end{cases}$$

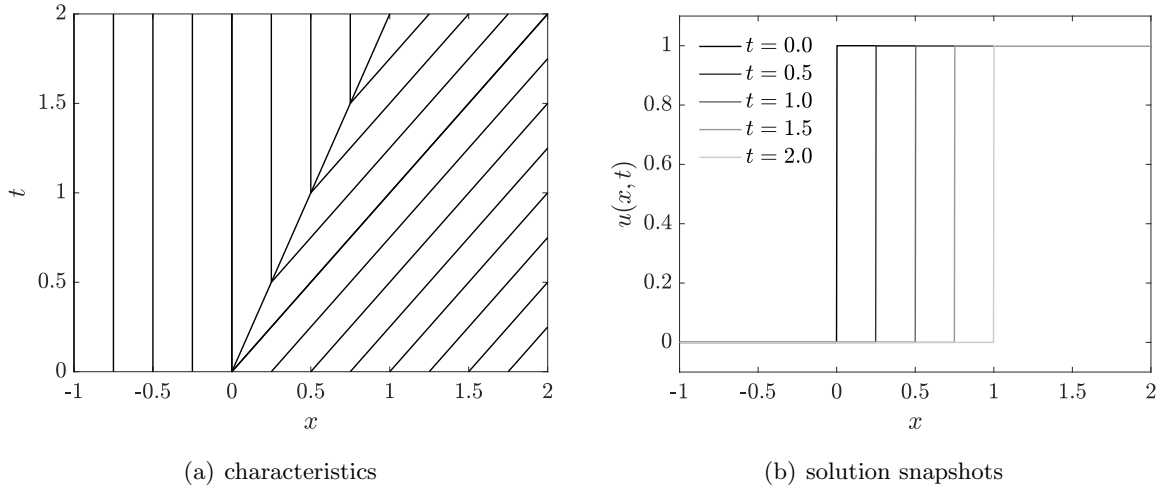


Figure 17.2: The characteristics and solution snapshots for a Burgers' problem with a nonphysical shock wave.

We apply the method of characteristics to find that

$$u(x, t) = \begin{cases} 0, & x < 0, \\ 1, & x > t. \end{cases}$$

However, the method of characteristics does not inform us how the solution in the wedge $\{(x, t) \mid 0 < x < t, t \in \mathbb{R}_{>0}\}$.

Solution 1. One potential solution is to fill the wedge with a discontinuous solution

$$u_1(x, t) = \begin{cases} 0, & x < t/2, \\ 1, & x > t/2. \end{cases}$$

We readily verify that the solution satisfies the Burgers' equation outside of the discontinuity. The solution also satisfies the Rankine-Hugoniot condition across the discontinuity:

$$s = \frac{F(u^-) - F(u^+)}{u^- - u^+} = \frac{\frac{1}{2}0^2 - \frac{1}{2}1^2}{0^2 - 1^2} = \frac{1}{2}.$$

Hence, this is a weak solution to the initial value problem. Figure 17.2 shows the characteristics and the solution snapshots.

Solution 2. Another potential solution is to fill the wedge with a continuous solution

$$u_2(x, t) = \begin{cases} 0, & x \in (-\infty, 0), \\ x/t, & x \in (0, t), \\ 1, & x \in (t, \infty). \end{cases}$$

We first note that the solution is continuous. We second observe that the Burgers' equation is satisfied for $x \in (-\infty, 0)$ and $x \in (t, \infty)$ where the solution is constant. We finally observe that for $x \in (0, t)$,

$$\frac{\partial u}{\partial t} + u \frac{\partial u}{\partial x} = -\frac{x}{t^2} + \frac{x}{t} \frac{1}{t} = 0.$$

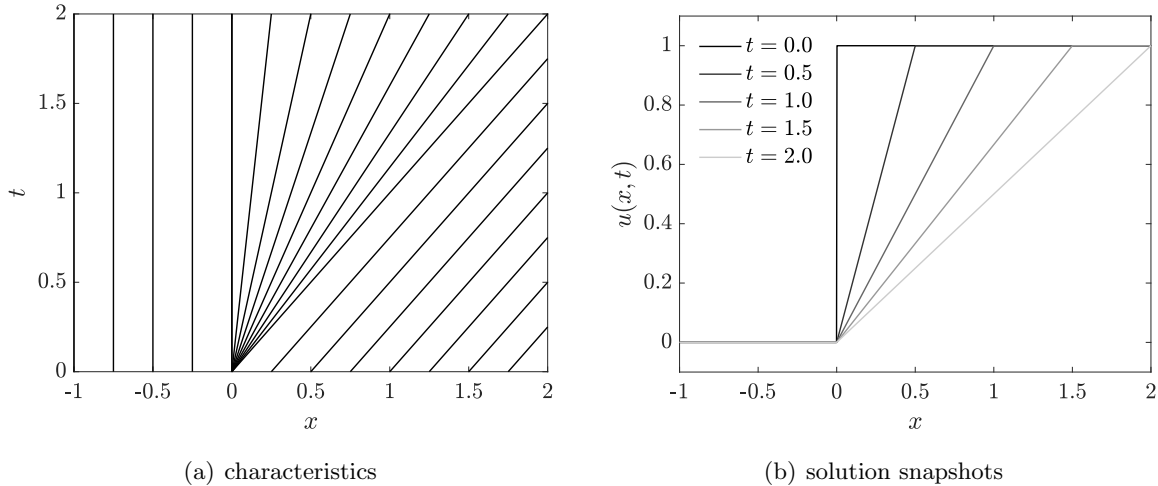


Figure 17.3: The characteristics and solution snapshots for a Burgers' problem with a rarefaction wave.

Hence the continuous solution satisfies the strong form of the Burgers' equation everywhere except along the two nondifferentiable curves; this is a weak solution of the Burgers' equation. Figure 17.3 shows the characteristics and the solution snapshots.

We have shown that there are at least two weak solutions to the Burgers' equation; in fact we can show that there are infinitely many weak solutions. However, only one of these solutions are physically relevant. It turns out there is an additional condition, called the *entropy condition*, that a physically relevant solution must satisfy. While there are a few different characterizations of the condition, one interpretation is that information cannot be created when we march forward in time. Mathematically, this translates to a condition that if we start at a point $(x, t) \in \mathbb{R} \times \mathbb{R}_{>0}$ and march *backward* in time along the characteristic, then we would not cross any other characteristics. In other words, if we start at a point $(x, t) \in \mathbb{R} \times \mathbb{R}_{>0}$ and march *backward* in time along the characteristic, we would not encounter any discontinuities. Note that, as we have seen, if we march *forward* in time along the characteristic, we may cross another characteristic at which point a discontinuity is formed. The characteristic terminating at a discontinuity when marching forward in time corresponds to the loss of information, which is permissible. However, characteristics terminating at a discontinuity when marching *backward* in time — or equivalently characteristics emanating from a discontinuity when marching *forward* in time — corresponds to the creation of information, which is not permissible. Because each characteristic has a moves at the speed of $F'(u)$, we arrive at the following mathematical condition:

Definition 17.9 (entropy condition). Along a discontinuity, a physically relevant weak solution to a conservation law must satisfy

$$F'(u^-) > s > F'(u^+),$$

where s is the shock speed given by the Rankine-Hugoniot condition.

Applying the entropy condition to Solutions 1 and 2 above, we find that Solution 1 is nonphysical since $0 = F'(u^-) < F'(u^+) = 1$. On the other hand, Solution 2 satisfies entropy condition at all discontinuities (because it has no discontinuity). Hence the solution shown in Figure 17.3 is the physically relevant solution to the weak form.