A Model–Data Weak Formulation for Simultaneous Estimation of State and Model Bias

Estimation de la variable d'état et du biais de modèle par une formulation faible incorporant les données.

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Abstract

We introduce a Petrov-Galerkin regularized saddle approximation which incorporates a "model" (partial differential equation) and "data" (M experimental observations) to yield estimates for both state and model bias. We provide an *a priori* theory which identifies two distinct contributions to the reduction in the error in state as a function of the number of observations, M: the stability constant increases with M; the model-bias best-fit error decreases with M. We present results for a synthetic Helmholtz problem and an actual acoustics system.

Résumé

Nous présentons une approximation de Petrov-Galerkin pour un problème de point selle incorporant un "modèle" (équation aux dérivées partielles) et des "données" (M observations expérimentales) afin d'obtenir une estimation conjointe de la variable d'état et du biais de modèle. Notre théorie *a priori* identifie deux contributions à la décroissance de l'erreur sur l'état en fonction du nombre d'observations expérimentales, M: la croissance de la constante stabilité avec M; la décroissance de l'estimation par moindre carré du biais de modèle avec M. Nous présentons des résultats pour un problème de Helmholtz synthétique ainsi que pour un système acoustique réel.

1. Problem Statement

We are given Hilbert spaces \mathcal{X} , \mathcal{Y} (with associated inner products $(\cdot, \cdot)_{\mathcal{X}}$, $(\cdot, \cdot)_{\mathcal{Y}}$ and induced norms $\|\cdot\|_{\mathcal{X}}$, $\|\cdot\|_{\mathcal{Y}}$) and respective dual spaces $\mathcal{X}', \mathcal{Y}'$ (with associated dual norms $\|\cdot\|_{\mathcal{X}'}$, $\|\cdot\|_{\mathcal{Y}'}$). We introduce an inverse Riesz representation operator $X : \mathcal{X} \to \mathcal{X}'$ that satisfies, for each $w \in \mathcal{X}$, $\langle Xw, v \rangle_{\mathcal{X}' \times \mathcal{X}} = (w, v)_{\mathcal{X}}, \forall v \in \mathcal{X}$, and an inverse Riesz representation operator $Y : \mathcal{Y} \to \mathcal{Y}'$ that satisfies, for each $w \in \mathcal{Y}, \langle Yw, v \rangle_{\mathcal{Y}' \times \mathcal{Y}} = (w, v)_{\mathcal{Y}}, \forall v \in \mathcal{Y}$.

We first postulate a linear operator $A: \mathcal{X} \to \mathcal{Y}'$ which is inf-sup stable and continuous such that $\beta_0 \equiv \inf_{w \in \mathcal{X}} \sup_{v \in \mathcal{Y}} \langle Aw, v \rangle_{\mathcal{Y}' \times \mathcal{Y}} / (\|w\|_{\mathcal{X}} \|v\|_{\mathcal{Y}}) > 0 \text{ and } \gamma_0 \equiv \sup_{w \in \mathcal{X}} \sup_{v \in \mathcal{Y}} \langle Aw, v \rangle_{\mathcal{Y}' \times \mathcal{Y}} / (\|w\|_{\mathcal{X}} \|v\|_{\mathcal{Y}}) < 0$

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 ∞ ; we also define a functional $f \in \mathcal{Y}'$. The pair $\{A, f\}$ defines a mathematical *model* which reflects our "best knowledge" of a physical system; we then introduce $u^{bk} \in \mathcal{X}$ solution of $Au^{bk} = f$ in the weak sense, $\langle Au^{bk}, v \rangle_{\mathcal{Y}' \times \mathcal{Y}} = \langle f, v \rangle_{\mathcal{Y}' \times \mathcal{Y}}, \forall v \in \mathcal{Y}$.

We now introduce a field $u^{\text{true}} \in \mathcal{X}$ which represents the true state of the physical system of interest and subsequently a model bias $g \equiv Au^{\text{true}} - f$; we also define a model-bias representation $p \equiv X^{-1}A^*Y^{-1}g$, where * denotes adjoint. We shall refer to both $g \in \mathcal{Y}'$ and $p \in \mathcal{X}$ as model bias with the context to determine the particular representation of interest. The model bias reflects the effects not included in the "best-knowledge" model $\{A, f\}$; note that u^{true} satisfies $Au^{\text{true}} =$ f + g, and hence $u^{\text{bk}} = u^{\text{true}}$ if and only if g = 0. Finally, we introduce observation functionals $\ell_m^{\text{o}} \in \mathcal{X}', 1 \leq m \leq M \leq \dim(\mathcal{X})$. In any given experiment we invoke observations $\ell_m^{\text{o}}(u^{\text{obs}})$, $m = 1, \ldots, M$, where $u^{\text{obs}} = u^{\text{true}} - q^{\text{obs}}$ is the experimentally observable state; we presume the "observation perturbation" q^{obs} is bounded in \mathcal{X} .

Our goal is to estimate u^{true} and g — both assumed deterministic and stationary — from the model $\{A, f\}$ and M experimental observations. Most state and bias estimation, and related parameter estimation, approaches ([5, 7, 6, 4]) are informed by minimization of a least-squares objective function which reflects regularization and model-observation misfit. One (Galerkin) version of our method, too, can be derived from such a least-squares formulation. However, we pose the problem in a (regularized) saddle form which thus admits interpretation and analysis from a variational approximation perspective ([10]); the latter, in turn, suggests and permits extensions and improvements — and, in particular, Petrov-Galerkin formulations which can not be derived from a least-squares minimization principle.

2. Model-Data Weak Formulation

We first consider a least-squares minimization: for given $\nu \in \mathbb{R}_{>0}$, find $u_M \in \mathcal{X}$ such that

$$u_M = \arg\min_{w \in \mathcal{X}} (\|f - Aw\|_{\mathcal{Y}'}^2 + \nu^{-1} \|\Pi_M (u^{\text{obs}} - w)\|_{\mathcal{X}}^2) ; \qquad (1)$$

here $\Pi_M : \mathcal{X} \to \mathcal{X}_M$ is the projection operator onto an *M*-dimensional subspace \mathcal{X}_M defined shortly, and, for any given $z \in \mathcal{X}$, $\Pi_M z \in \mathcal{X}_M$ satisfies $(\Pi_M z, v)_{\mathcal{X}} = (z, v)_{\mathcal{X}}$, $\forall v \in \mathcal{X}_M$. We then state the Euler-Lagrange equation, written in a mixed form, associated with the minimization problem: find $(u_M, \chi_M) \in \mathcal{X} \times \mathcal{X}_M$ such that

$$s(u_M, v) - (\chi_M, v)_{\mathcal{X}} = \langle A^* Y^{-1} f, v \rangle_{\mathcal{X}' \times \mathcal{X}}, \quad \forall v \in \mathcal{X}, -(u_M, \phi)_{\mathcal{X}} - \nu(\chi_M, \phi)_{\mathcal{X}} = -(u^{\text{obs}}, \phi)_{\mathcal{X}}, \quad \forall \phi \in \mathcal{X}_M,$$
(2)

where $s(w,v) \equiv \langle A^*Y^{-1}Aw, v \rangle_{\mathcal{X}' \times \mathcal{X}}, \forall w, v \in \mathcal{X}$. We choose $\mathcal{X}_M = \mathcal{E}_M^{\{\ell_m^o\}} \equiv \operatorname{span}\{\phi_m\}_{m=1}^M = \operatorname{span}\{X^{-1}\ell_m^o\}_{m=1}^M$ such that $(u^{\operatorname{obs}}, \phi_m)_{\mathcal{X}}$ can be evaluated as $(u^{\operatorname{obs}}, \phi_m)_{\mathcal{X}} = \langle X\phi_m, u^{\operatorname{obs}} \rangle_{\mathcal{X}' \times \mathcal{X}} = \ell_m^o(u^{\operatorname{obs}})$; in other words, the inner product that constitutes the right-hand side of the second equation is experimentally observable in the appropriate basis. Equation (2) constitutes a *Galerkin approximation* in the sense that the trial and test spaces are identical.

However, we may also consider different trial and test spaces, $\mathcal{X}_M^{\text{trial}} \neq \mathcal{X}_M^{\text{test}}$, to obtain a *Petrov-Galerkin approximation*: find $(u_M, \chi_M) \in \mathcal{X} \times \mathcal{X}_M^{\text{trial}}$ such that

$$s(u_M, v) - (\chi_M, v)_{\mathcal{X}} = \langle A^* Y^{-1} f, v \rangle_{\mathcal{X}' \times \mathcal{X}}, \quad \forall v \in \mathcal{X}, -(u_M, \phi)_{\mathcal{X}} - \nu(\chi_M, \phi)_{\mathcal{X}} = -(u^{\text{obs}}, \phi)_{\mathcal{X}}, \quad \forall \phi \in \mathcal{X}_M^{\text{test}};$$
(3)

here we choose $\mathcal{X}_M^{\text{test}} = \mathcal{E}_M^{\{\ell_m^o\}}$, the experimentally observable space, but $\mathcal{X}_M^{\text{trial}} \neq \mathcal{X}_M^{\text{test}}$ need no longer be an experimentally observable space. The Galerkin approximation (2) is a particular instance of the Petrov-Galerkin approximation (3) with $\mathcal{X}_M^{\text{trial}} = \mathcal{X}_M^{\text{test}} \equiv \mathcal{X}_M$. Note that u_M and χ_M depend on $\nu \in \mathbb{R}_{\geq 0}$, which we will specify in each instance as required. Alternative saddle formulations may also be pursued and several advantageous choices are described in [11].

To facilitate the error analysis of (3), we may now introduce an abstract variational problem: find $(u, \chi) \in \mathcal{X} \times \mathcal{X}$ such that

$$s(u,v) - (\chi,v)_{\mathcal{X}} = \langle A^* Y^{-1} f, v \rangle_{\mathcal{X}' \times \mathcal{X}} , \quad \forall v \in \mathcal{X} ,$$

$$-(u,\phi)_{\mathcal{X}} - \nu(\chi,\phi)_{\mathcal{X}} = -(u^{\text{obs}} + q^{\text{obs}},\phi)_{\mathcal{X}} - \nu(p,\phi)_{\mathcal{X}} \quad \forall \phi \in \mathcal{X} .$$
(4)

We readily verify that the solution to the abstract problem is given by $u = u^{\text{true}}$ (the true state) and $\chi = p$ (the true model bias). Note that the Petrov-Galerkin approximation (3) results from (*i*) neglecting the perturbation terms νp and q^{obs} in (4), and (*ii*) replacing the trial space for the model bias, and the test space for the second equation of (4), with respective *M*-dimensional subspaces $\mathcal{X}_M^{\text{trial}} \subset \mathcal{X}$ and $\mathcal{X}_M^{\text{test}} \subset \mathcal{X}$. Hence, (3) constitutes our "limited-observations" approximation to the unlimited-observations problem (4); note also that $u^{\text{bk}} = u_{M=0}$.

In the Galerkin case we can demonstrate stability; however we can not expect rapid convergence for the *de rigeur* experimentally observable trial spaces, as demonstrated in [11] for certain illustrative cases. In the Petrov-Galerkin case, we choose a suitable trial space for model-bias approximation and then choose the associated test space to provide maximum stability [2, 3]; although we cannot generally demonstrate stability for arbitrary spaces, the Petrov-Galerkin formulation offers the advantage of potentially rapidly convergent trial spaces.

3. Analysis: Galerkin Formulation

We now proceed to the *a priori* analysis of the error in the state estimate $u_M \in \mathcal{X}$ and the model-bias estimate $\chi_M \in \mathcal{X}_M^{\text{trial}}$ with respect to the true state $u^{\text{true}} \in \mathcal{X}$ and true model bias $p \in \mathcal{X}$, respectively. We shall restrict our analysis (but not numerical results) in this Note to the Galerkin case. By way of preliminaries, we first introduce an energy norm

$$|||w|||_{M,\nu} \equiv \left(s(w,w) + \nu^{-1} ||\Pi_M w||_{\mathcal{X}}^2\right)^{1/2}, \quad \forall w \in \mathcal{X} ,$$
(5)

parametrized by M and ν . We may then define our stability constant

$$\beta_{M,\nu} \equiv \inf_{w \in \mathcal{X}} \frac{\|w\|_{M,\nu}}{\|w\|_{\mathcal{X}}} .$$

$$(6)$$

We in addition introduce a continuity constant associated with the $s(\cdot, \cdot)$ bilinear form, γ , which in fact is the square of the continuity constant of A: $\gamma = \gamma_0^2$.

We then have the following proposition for the error in our state and model-bias estimates:

Proposition 1. In the Galerkin case, the state error $u^{\text{true}} - u_M \in \mathcal{X}$ and the model-bias error $p - \chi_M \in \mathcal{X}$ satisfy

$$\|u^{\text{true}} - u_M\|_{\mathcal{X}} \leq \frac{1}{\beta_{M,\nu^{\text{opt}}}} \left(\frac{1}{\beta_{M,2\nu^{\text{opt}}}^2} \|p - \Pi_M p\|_{\mathcal{X}}^2 + 8\|p\|_{\mathcal{X}} \|q^{\text{obs}}\|_{\mathcal{X}} \right)^{1/2}, \\\|p - \chi_M\|_{\mathcal{X}} \leq \frac{\gamma}{\beta_{M,\nu^{\text{opt}}}} \left(\frac{1}{\beta_{M,2\nu^{\text{opt}}}^2} \|p - \Pi_M p\|_{\mathcal{X}}^2 + 8\|p\|_{\mathcal{X}} \|q^{\text{obs}}\|_{\mathcal{X}} \right)^{1/2},$$
(7)

respectively, for $\nu^{\text{opt}} \equiv ||q^{\text{obs}}||_{\mathcal{X}}/||p||_{\mathcal{X}}$.

There are three contributions to the error in the state: the observation perturbation term $||q^{\text{obs}}||_{\mathcal{X}}$, which we do not control and which ultimately dictates the achievable error; the error in the best-fit approximation to p in $\mathcal{X}_M(=\mathcal{X}_M^{\text{trial}})$; and finally, the stability constant $\beta_{M,\nu^{\text{opt}}}$. As regards the latter, we can prove

Proposition 2. For given $\nu \in \mathbb{R}_{\geq 0}$,

$$\beta_{M',\nu} \ge \beta_{M'-1,\nu}, \quad M' = 1, \dots, M$$
 (8)

Furthermore, $\beta_{M=0,\nu} = \beta_0$ and $\beta_{M',\nu} \ge \beta_0$, $M' = 1, \ldots, M$, where β_0 is the inf-sup constant of the operator A (hence absent any observations).

It is possible based on SVD considerations [1] to prove that for certain idealized hierarchical test spaces $\mathcal{X}_{M'}^{\text{test}}$ that include the M' least stable trial singular functions of $A \in \mathcal{L}(\mathcal{X}, \mathcal{Y}')$, the stability constant $\beta_{M',\nu=0}$ is equal to the (M'+1)th generalized singular value of A: a form of E-stability from design of experiments [4]. We may devise an SVD-based anti-node heuristic for development of experimentally observable spaces which roughly replicates the ideal trial singular function choice; we may alternatively choose the observation locations based on other methods, for example the Empirical Interpolation Method [8, 9].

Finally, we may consider the special but important "perfect-observations" case in which $q^{\text{obs}} \equiv 0$ and we may hence choose $\nu = 0$. In this case our state and model-bias approximation (2) reduces to a true saddle problem which in the Galerkin case furthermore corresponds to constrained least squares (or constrained estimation). We may then demonstrate

Proposition 3. For the Galerkin case, and $q^{\text{obs}} \equiv 0$ and $\nu = 0$, the state error, $u^{\text{true}} - u_M \in \mathcal{X}$, and model-bias error, $p - \chi_M \in \mathcal{X}$, satisfy

$$|u^{\text{true}} - u_M|_{\mathcal{X}} \leq \frac{1}{\beta_{M,\nu=0}^2} ||p - \Pi_M p||_{\mathcal{X}}$$
$$||p - \chi_M||_{\mathcal{X}} \leq \frac{\gamma}{\beta_{M,\nu=0}^2} ||p - \Pi_M p||_{\mathcal{X}} .$$
(9)

Proof. Application of the Brezzi-Babuška theory (for example, Theorem 7.4.3 of [10]) to the saddle problem (2) (for $q^{\text{obs}} \equiv 0$, $\nu = 0$) yields the desired result.

The general result of Proposition 1 reduces to the perfect-observations case of Proposition 3 in the limit $q^{\text{obs}} \to 0$. In both Proposition 1 and Proposition 3, in fact we can sharpen the bound: we can transfer the A^* in $s(\cdot, \cdot)$ to the test function to reduce the dependence on the inf-sup constant from quadratic to linear [11].

4. Computational Results

We first consider a synthetic model Helmholtz problem over $\Omega \equiv]0, 1[^2$ in which we specify not only the best-knowledge model $\{A, f\}$ and observation functionals but also the quantities which in actual practice would be "provided" by the physical system (and unknown to us): the model bias g, which (with A and f) determines u^{true} from $Au^{\text{true}} = f + g$; and the actual experimental

	trial space I			trial space II	
M	$\beta_{M,\nu=0}$	$\ u^{\text{true}} - u_M\ _{\mathcal{X}}$	$\ p - \chi_M\ _{\mathcal{X}}$	$\ u^{\text{true}} - u_M\ _{\mathcal{X}}$	$\ p - \chi_M\ _{\mathcal{X}}$
0	0.0011	5.9134	0.0591	5.9134	0.0591
1	0.0011	5.2537	0.0591	6.5791	2.8844
2	0.0147	0.7396	0.0591	8.0641	1.8068
5	0.0589	0.3053	0.0557	0.2020	0.1499
10	0.0700	0.2636	0.0537	0.0889	0.0358
20	0.1946	0.0931	0.0391	0.0110	0.0032

Table 1: The stability constant $\beta_{M,\nu=0}$, state error $||u^{\text{true}} - u_M||_{\mathcal{X}}$, and model-bias error $||p - \chi_M||_{\mathcal{X}}$ as a function of the number of observations M for the synthetic two-dimensional Helmholtz problem.

observations, which we presume are perfect $(q^{\text{obs}} \equiv 0, \text{ and hence } \nu^{\text{opt}} = 0)$. In what follows $k \in \mathbb{R}$ denotes the reduced frequency or wavenumber; we shall choose $k = 3\pi + 0.01$ which lies slightly above a resonance. We further set $\mathcal{X} \equiv H^1(\Omega)$ and $\mathcal{Y} \equiv H^1(\Omega)$ and equip both spaces with inner product $\int_{\Omega} \nabla w \cdot \nabla v dx + k^2 \int_{\Omega} wv dx$ and induced norm $\|w\|_{\mathcal{X}} \equiv \|w\|_{\mathcal{Y}} \equiv \sqrt{(w, w)_{\mathcal{X}}}$. (In practice, and in general, we replace the continuous spaces \mathcal{X} and \mathcal{Y} with a discrete counterpart, for this problem a 512-element \mathbb{P}^5 continuous finite element space.)

We first specify the best-knowledge model $\{A, f\}$: the Helmholtz operator $A: \mathcal{X} \to \mathcal{Y}'$ is given by $\langle Aw, v \rangle_{\mathcal{Y}' \times \mathcal{Y}} = \int_{\Omega} \nabla w \cdot \nabla v dx - k^2 \int_{\Omega} wv dx$, $\forall w \in \mathcal{X}, \forall v \in \mathcal{Y}$; the functional f is given by $\langle f, v \rangle_{\mathcal{Y}' \times \mathcal{Y}} = \int_{\Omega} (2x^2 + y)v dx$, where (x, y) denotes a point in Ω ; we impose homogeneous Neumann boundary conditions everywhere on $\partial \Omega$. We next specify the observation functionals ℓ_m^{o} , m = $1, \ldots, M$: functional ℓ_m^{o} is a bivariate Gaussian with center \mathbf{x}_m^{o} and standard deviation 0.02; the centers \mathbf{x}_m^{o} are obtained by application of the Empirical Interpolation Method [8] to $\mathbb{P}^{p(M)}(\Omega)$, the space spanned by the first M hierarchically ordered members of the bivariate (complete, not tensorized) polynomials $(1, x, y, x^2, xy, y^2, x^3, x^2y, \ldots)$. Finally, we prescribe the synthetic model bias as $\langle g, v \rangle_{\mathcal{Y}' \times \mathcal{Y}} = \int_{\Omega} (\cos(1.3\pi x) + y^{7/2})v dx$.

It remains to choose the approximation spaces. The test space $\mathcal{X}_{M}^{\text{test}}$ is completely determined by the observation functionals: $\mathcal{X}_{M}^{\text{test}} = \text{span}\{\phi_m\}_{m=1}^{M} = \text{span}\{X^{-1}\ell_m^{\text{o}}\}_{m=1}^{M}$. For the trial space we consider two options: for trial space I, in the Galerkin framework, we choose $\mathcal{X}_{M}^{\text{trial}} \equiv \mathcal{X}_{M}^{\text{test}}$; for trial space II, now in the Petrov-Galerkin framework, we choose $\mathcal{X}_{M}^{\text{trial}} \equiv \mathbb{P}^{p(M)}(\Omega)$, the aforementioned hierarchical polynomial space.

The results are summarized in Table 1. For trial space I, Galerkin, we expect from Proposition 2 an improvement in the stability constant and indeed we observe a rapid decrease in error for small M. (Note that $k = 3\pi$ is a degenerate resonance wave number with multiplicity two, for which (special) reason the stability constant $\beta_{M,\nu=0}$ improves only with the second observation.) However, the asymptotic convergence rate is slow given the relatively poor approximation properties of experimentally observable spaces. In contrast, for trial space II, Petrov-Galerkin, we can not yet prove and hence presume a uniform improvement in the stability constant, and indeed we do not observe any significant decrease in error for small M. However, the asymptotic convergence rate is rapid given the high–order approximation spaces (accommodated by the Petrov-Galerkin recipe) and the quite regular model bias, p.

We now consider a second problem for which we invoke real data: a raised-box acoustic resonator [11]. In this three-dimensional acoustic problem with real data, we apply the complex-field extension of the framework developed in Sections 1 and 2. The physical system is a bottomless (5-sided) acrylic box of interior dimensions $12 \times 7 \times 5$ inches and wall thickness 0.06 inches which is



Figure 1: (a) Pressure response (normalized by $Z_0^{\dim} V_{\text{spk}}^{\dim}$, where Z_0^{\dim} is the acoustic impedance of air and V_{spk}^{\dim} is the speaker diaphragm velocity) as a function of frequency at a particular assessment point in the raised box as predicted by the "best-knowledge" model (M = 0) and our model-data weak formulation (M = 5) and as measured in practice (experiment). (b) The stability constant $\beta_{M,\nu}$ as a function of frequency for M = 0 and M = 5. Note $(\cdot)^{\dim}$ refers to dimensional quantities.

raised 0.22 inches above a larger acrylic floor panel; a speaker (Tang Band W2-1625SA) is placed symmetrically in one of the two 7 × 5 "end-walls" of the raised box to serve as a mono-chromatic sound source of prescribed frequency (in Hz). The pressure may be measured by a microphone as a function of time at any spatial point and then reduced to complex form (frequency description) by standard regression methods. The errors in the observations are quite small relative to the desired accuracy [11] such that (*i*) we may assume q^{obs} is effectively zero, $u^{\text{obs}} \approx u^{\text{true}}$, and choose $\nu = 0$ in our formulation, and furthermore (*ii*) experiment may serve as a surrogate for the truth for purposes of assessment.

We choose for our best-knowledge model A and f the Helmholtz operator with Neumann conditions on the speaker (inhomogeneous, uniform) and walls (homogeneous) and radiation conditions in the farfield. Note that the speaker is modeled as a calibrated electromechanical harmonic oscillator from which we derive a transfer function from speaker input voltage (measured) to normal diaphragm velocity — which is then incorporated in f [11]. In the best-knowledge model the walls are of finite thickness but rigid.

We consider M = 5 experimental observation Gaussians (at randomly selected centers, $\{\mathbf{x}_m^{\alpha}\}_{m=1}^5$) and apply the Galerkin framework (for $\nu = 0$, as motivated above). We plot in Figure 1(a) the amplitude of the state estimate, as a function of frequency, calculated as the application of an assessment Gaussian with center $\mathbf{x}^a = (8.60, 2.82)$ (a distance of 1.46 inches from the nearest observation Gaussian center); we also present the corresponding experimental observations at this same spatial point. The dramatic improvement in the prediction of the pressure by incorporation of just M = 5 experimental observations is due to the sizable increase of the stability constant, as demonstrated in the plot of $\beta_{M,\nu=0}$ in Figure 1(b).

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