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Integrating Experimental Data and Mathematical Models in Simulation of Physical Systems

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Nomenclature

A	= matrix with components $G(x_k, x_m)$
$B[\cdot]$	= boundary operator of mathematical model
$b\langle\cdot, \cdot\rangle$	= symmetric form associated with boundary operator B
c_m	= basis expansion coefficients
\bar{c}	= vector with components c_m
$E[\cdot]$	= mathematical expectation operator
F	= response of physical system
f	= arbitrary function exactly satisfying boundary operator B
\tilde{f}	= hypersurface that gives global minimum of Eq. (5)
f_a	= network response; numerical approximation of \tilde{f}
f_{cor}	= correction of f_0 using experimental data
$f_e(x_i)$	= experimental measurements of $F(x_i)$
\tilde{f}_e	= vector with components $f_e(x_i)$
f_0	= response of mathematical model
\tilde{f}_0	= vector with components $f_0(x_j)$
$G(\cdot, \cdot)$	= Green's function of mathematical model
g	= algebraic function

I	= identity matrix
$L[\cdot]$	= linear self-adjointed differential operator
$l\langle\cdot, \cdot\rangle$	= quadratic symmetric energy form associated with L
p	= weighting function
q	= Lagrange multiplier function
R^d	= d -dimensional Euclidean space
$R(\alpha)$	= residual of Eq. (20)
s	= parameter related to operator L , where $s > 0$
$\text{Var}[\cdot]$	= variance of a random variable
$x = (x_1, \dots, x_d)$	= d -dimensional spatial coordinate
α	= regularization parameter where $\alpha \geq 0$
β	= set of general artificial neural network parameters; set of basis function parameters and basis expansion coefficients
Δ_k	= radial basis function parameter
$\delta(\cdot)$	= Dirac delta function
δ_{ji}	= $\delta(x - x_j, x - x_i)$
$\epsilon(\cdot)$	= objective function
η_k	= radial basis function parameter
κ	= positive constant
$\Lambda[\cdot]$	= smoothness-based Tikhonov regularization functional
μ	= noise of measurement
ξ	= arbitrary variable
ρ	= positive constant
σ	= basis function
$\Phi(\cdot)$	= energy functional of mathematical model
ϕ, ψ	= arbitrary functions
Ω	= spatial domain of mathematical model
$\partial\Omega$	= spatial boundary of mathematical model
$\ \cdot\ _{H^s(\Omega)}$	= norm in Sobolev space of order s
$\langle\cdot, \cdot\rangle$	= inner product

I. Introduction

THE goal of engineering analysis is to obtain a comprehensive description of a physical system of interest. Three approaches to this goal exist: theoretical analysis of mathematical models, physical experimentation, and computational mechanics.¹ None of these approaches is superior, and they should be used in combination. Though it is known in the engineering community that successful analyses rest upon the proper balance of all three approaches, few attempts have been made in uniting experimental, theoretical, and numerical methods in the literature. It is the objective of this Note to develop a method that effectively combines all available information, from both experimental data and mathematical models, in the emulation of physical systems.

The technical approach utilizes a common tool borrowed from artificial neural network (ANN) applications, the theory of Tikhonov regularization of ill-posed problems.² Specifically, the problem of mathematical analysis of experimental data is treated as an ill-posed problem. Its regularization involves the introduction of additional information regarding the physical system. It is proposed that a priori mathematical models of physical systems be utilized at appropriate degrees of fidelity for regularization. The example problem is used to illustrate two major benefits of the approach: 1) to show the benefit of employing a priori mathematical models of low degree of fidelity for extrapolation from sparse data, and 2) to show the usefulness of incorporating a priori mathematical models in the processing of experimental data corrupted by noise. The radial basis expansion is used as the numerical approximation tool in the developed method.

II. Method for Data Analysis: Regularization by A Priori Mathematical Models

The popular Tikhonov regularization method² was originally adopted for ANN systems by Poggio and Girosi³ and extensively used in ANN applications.^{4,5} In this case, a set of constraints on the network approximation $f_a(x, \beta)$ is introduced through the Tikhonov regularization functional $\Lambda[f_a(x, \beta)]$, which specifies the penalty

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given to the oscillatory behavior of $f_a(x, \bar{\beta})$; the network parameters can be determined by minimizing the objective function

$$\epsilon(f_a) = \sum_{i=1}^N |f_e(x_i) - f_a(x_i, \bar{\beta})|^2 + \alpha \Lambda[f_a(x, \bar{\beta})] \quad (1)$$

Unfortunately, conventional smoothness-based Tikhonov regularization of the Poggio–Girosi method may not be consistent with the smoothness required in emulating a physical system and so would be unable to properly approximate with noisy experimental data. Instead, the authors believe that the regularization should be based on an a priori mathematical model of some level of fidelity. This regularized model then can be approximated by more conventional computational methods.

A large class of mechanics problems can be described by the equations

$$L[f_0(x)] = g(x), \quad x \in \Omega \quad \text{and} \quad B[f_0(x)] = 0, \quad x \in \partial\Omega \quad (2)$$

The solution to Eq. (2) also can be determined by minimizing the following quadratic (energy) form:

$$\Phi(f) = \frac{1}{2} I\langle f, f \rangle - \langle g, f \rangle \quad (3)$$

Because for any f that satisfies the boundary conditions

$$I\langle f_0, f \rangle = \langle g, f \rangle \quad (4)$$

substituting Eq. (4) into Eq. (3) yields

$$\begin{aligned} \Phi(f) &= \frac{1}{2} I\langle f - f_0, f - f_0 \rangle - \frac{1}{2} I\langle f_0, f_0 \rangle \\ &= \frac{1}{2} I\langle f - f_0, f - f_0 \rangle + \text{constant} \end{aligned}$$

From a physical perspective, the functional $\Phi(f)$ penalizes the mechanical energy of the discrepancy between the function f and the response of a mathematical model f_0 .

With the use of f and the energy functional of Eq. (3), regularized modeling can be formulated as the minimization of the objective function

$$\epsilon(f) = \sum_{i=1}^N |f_e(x_i) - f(x_i)|^2 + \alpha \left(\frac{1}{2} I\langle f, f \rangle - \langle g, f \rangle \right) \quad (5)$$

which combines information from experimental data and the a priori mathematical model. Note that α represents the degree of reliance on the a priori mathematical model of the physical system relative to the reliability of the experimental data.

A. Analytical Approximation of Regularized Mechanical Systems

The formation of a regularized model of a mechanical system is identical to approximating the hypersurface $\tilde{f}(x)$ that gives the global minimum of Eq. (5). In this context, analytical study of $\tilde{f}(x)$ is essential for evaluating the properties of the regularized model.

Because $\tilde{f}(x)$ is the global minimum of Eq. (5),

$$L[\tilde{f}] = g + \frac{2}{\alpha} \sum_{i=1}^N (\tilde{f}(x_i) - f_e(x_i)) \delta(x - x_i), \quad x \in \Omega$$

and

$$B[\tilde{f}] = 0, \quad x \in \partial\Omega \quad (6)$$

From Eq. (6) it can be deduced that \tilde{f} contains two components:

$$\tilde{f}(x) = f_0(x) + f_{\text{cor}}(x) \quad (7)$$

These components can be determined by the equations

$$f_0(x) = \int_{\Omega} G(x, \xi) g(\xi) d\xi$$

and

$$f_{\text{cor}}(x) = \frac{2}{\alpha} \sum_{i=1}^N (f_e(x_i) - \tilde{f}(x_i)) G(x, x_i) \quad (8)$$

where the Green's function $G(x, \xi)$ satisfies the boundary value problem

$$L[G(x, \xi)] = \delta(x - \xi), \quad x \in \Omega$$

and

$$B[G(x, \xi)] = 0, \quad x \in \partial\Omega$$

Substituting Eq. (8) into Eq. (7) yields

$$\tilde{f}(x) = f_0(x) + \sum_{i=1}^N c_i G(x, x_i) \quad (9)$$

where the coefficients are defined as

$$c_j = (2/\alpha) (f_e(x_j) - \tilde{f}(x_j)) \quad (10)$$

The coefficients can be evaluated by substituting Eq. (9) into Eq. (10), resulting in

$$c_j = \frac{2}{\alpha} \left(f_e(x_j) - f_0(x_j) - \sum_{i=1}^N c_i G(x_j, x_i) \right) \quad j = 1, \dots, N \quad (11)$$

with which \bar{c} can be isolated. With the substitution of \bar{c} into Eq. (9), \tilde{f} can be written as

$$\tilde{f}(x) = f_0(x) + \sum_{i=1}^N G(x, x_i) \left[\left(A + \frac{\alpha}{2} I \right)^{-1} (\bar{f}_e - \bar{f}_0) \right]_i \quad (12)$$

Note that the matrix A of Eq. (12) is positive definite because, for an arbitrary function $\phi(x)$, we can write

$$\begin{aligned} \int_{\Omega} \int_{\Omega} G(x, \xi) \phi(\xi) \phi(x) d\xi dx &= \int_{\Omega} \psi(x) \phi(x) dx \\ &= \int_{\Omega} \psi(x) L[\psi(x)] dx = I\langle \psi, \psi \rangle \end{aligned}$$

where $\psi(x)$ is the solution to Eq. (2) for $g(x) = \phi(x)$ and satisfies the boundary condition. Therefore, because the quadratic form $I\langle \cdot, \cdot \rangle$ is strictly elliptic,

$$\int_{\Omega} \int_{\Omega} G(x, \xi) \phi(\xi) \phi(x) d\xi dx \geq \kappa \|\psi\|_{H^1(\Omega)}^2 > 0 \quad (13)$$

Substituting

$$\phi(x) = \sum_{i=1}^N c_i \delta(x - x_i)$$

into Eq. (13) yields

$$\int_{\Omega} \int_{\Omega} G(x, \xi) \phi(\xi) \phi(x) d\xi dx = \bar{c}^T A \bar{c} > 0$$

Because A is a positive-definite matrix, the matrix $(A + \alpha I/2)$ is also positive definite for any positive value of the parameter α . As a result, the vector \bar{c} can be evaluated in a computationally stable manner.

Because the range of the regularizing parameter α is the set of all positive numbers, it is prudent to obtain qualitative results for the limits of α . Equation (12) indicates that, as $\alpha \rightarrow \infty$, $\tilde{f}(x) \rightarrow f_0(x)$, as expected, because, with $\alpha \rightarrow \infty$, experimental data become less relevant and \tilde{f} emulates more of the a priori mathematical model.

For $\alpha \rightarrow 0$, the a priori model of the mechanical system is assumed to be increasingly unreliable compared to the experimental data. Equation (12) gives

$$\tilde{f}(x) \rightarrow f_0(x) + \sum_{i=1}^N G(x, x_i) [A^{-1} (\bar{f}_e - \bar{f}_0)]_i$$

so that the regularized solution interpolates the data $f_e(x_j)$ exactly because

$$\begin{aligned} f_0(x_j) + \sum_{i=1}^N G(x_j, x_i) [A^{-1}(\tilde{f}_e - \tilde{f}_0)]_i \\ = f_0(x_j) + \sum_{i=1}^N \delta_{ji} [\tilde{f}_e - \tilde{f}_0]_i = f_e(x_j) \end{aligned}$$

As a result, the a priori mathematical model of the mechanical system does not contribute to \tilde{f} in the region of adequate data. However, the mathematical model is not eliminated from the modeling procedure; it is used by \tilde{f} to extrapolate the data to the regions lacking data. In an alternative perspective, as $\alpha \rightarrow 0$, the function \tilde{f} can be thought of as a response of the a priori model attached to the data points.

B. Numerical Approximation of Regularized Mechanical Systems

The radial basis expansion used to approximate \tilde{f} can be described by the equations

$$f_a(x, \tilde{\beta}) = \sum_k c_k \sigma\left(\frac{|x - \eta_k|}{\Delta_k}\right) \quad \text{and} \quad \sigma(\xi) = e^{-\xi^2/2} \quad (14)$$

Because the basis expansion of Eq. (14) does not satisfy the boundary conditions of the mathematical model for arbitrary $\tilde{\beta}$, the objective function of Eq. (5) is augmented to incorporate the boundary conditions. Specifically,

$$\begin{aligned} \epsilon(f_a) = \sum_{i=1}^N |f_e(x_i) - f_a(x_i, \tilde{\beta})|^2 \\ + \alpha \left(\frac{1}{2} l \langle f_a, f_a \rangle - \langle g, f \rangle + b \langle f_a, q \rangle \right) \end{aligned} \quad (15)$$

where $b\langle \cdot, \cdot \rangle$ can be defined as

$$b\langle f, q \rangle = \int_{\partial\Omega} B[f(\xi)] q(\xi) d\xi$$

By preselecting the distribution and localization properties of the radial basis functions, Eq. (15) is minimized with respect to the remaining unknowns, c_k , resulting in

$$\begin{aligned} \sum_j^M \left(\alpha l \langle \sigma_j(x), \sigma_k(x) \rangle + 2 \sum_{i=1}^N \sigma_j(x_i) \sigma_k(x_i) \right) c_j \\ + \alpha b \langle \sigma_k(x), q \rangle = \alpha \langle g, \sigma_k(x) \rangle + 2 \sum_{i=1}^N f_e(x_i) \sigma_k(x_i) \end{aligned}$$

for $k = 1, \dots, M$ (16)

and

$$\sum_j^M c_j b \langle \sigma_j(x), p \rangle = 0 \quad (17)$$

where p and q belong to an appropriate finite dimensional subspace. Equations (16) and (17) are known as the Galerkin method.⁶ This observation provides a useful link between the proposed method of data analysis and methods in computational mechanics.

III. Example Problem

Consider a one-dimensional engineering system governed by the differential equation

$$-\frac{d}{dx} \left[a(x) \frac{d}{dx} F(x) \right] = x, \quad x \in (0, 1), \quad F(0) = F(1) = 0$$

For this example problem, the value of $a = 1$ is selected for the exact system. An a priori mathematical model with $a_0 = 1.3$ is used along with the regularizing functional

$$\begin{aligned} \Phi(f) &= \frac{1}{2} \int_0^1 a_0 \left(\frac{df}{dx} \right)^2 dx - \int_0^1 x f dx \\ &= \frac{1}{2} \int_0^1 a_0 \left(\frac{df}{dx} - \frac{df_0}{dx} \right)^2 dx + \text{constant} \end{aligned} \quad (18)$$

Regularization by the functional of Eq. (18) suppresses oscillations of the experimental data that are dissimilar to the oscillatory behavior of the a priori model. Consequently, the approximation of a regularized mechanical system should filter the data noise.

A. Results from Analytical Approximation

The experimental data for the extrapolation study are obtained from the physical system response at $x = 0.25$ and 0.75 , which are shown as triangles in Fig. 1. The optimal curve \tilde{f} , regularized by the a priori mathematical model, is evaluated from Eq. (12) and is shown in Fig. 1 for the regularization parameter $\alpha = 0.01$. By selecting values of α , Eq. (12) acts as a penalty method. The optimal curve passes through the data points; the curvature in the region between data matches the curvature of the a priori mathematical model. This can be shown by noting that the function $f_{\text{cor}}(x)$ is a piecewise linear function in the regions between data points.

As mentioned earlier, the use of Eq. (18) for regularization should filter data noise. Noisy experimental data were generated for this study by adding random noise μ to the response of the physical system; the random noise was statistically independent of location and uniformly distributed between $\pm d/2$, where $d = 0.025$, and with variance $\text{Var}[\mu] = d^2/12$. The generated data points are displayed as triangles in Fig. 2. Unlike the extrapolation example, the value of the regularization parameter α was determined such that Eq. (12) and the constraint

$$\sum_{i=1}^N |f_e(x_i) - f(x_i)|^2 = E \left[\sum_{i=1}^N \mu_i^2 \right] = N \cdot \text{Var}[\mu] = \rho \quad (19)$$

were satisfied for $f = \tilde{f}$. More specifically, α minimized the magnitude of the equation residual $R(\alpha)$, where

$$\begin{aligned} R(\alpha) &= \sum_{k=1}^N \left| f_e(x_k) - f_0(x_k) - \sum_{i=1}^N G(x_k, x_i) \right. \\ &\quad \times \left[\left(A + \frac{\alpha}{2} I \right)^{-1} (\tilde{f}_e - \tilde{f}_0) \right]_i \Big|^2 - \rho \end{aligned} \quad (20)$$

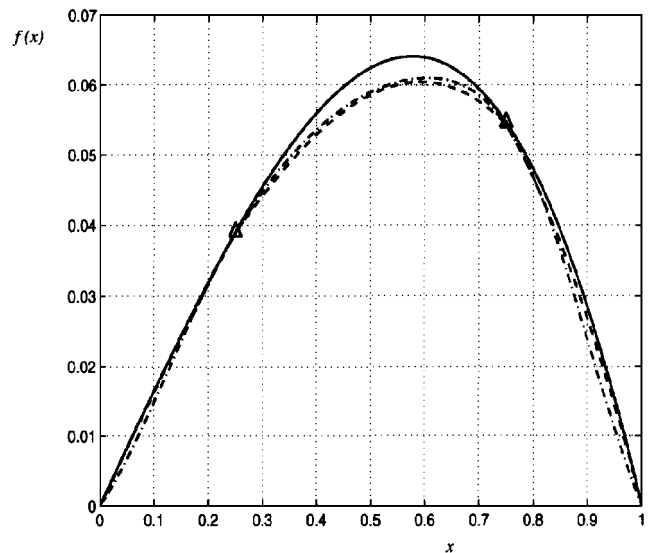


Fig. 1 Extrapolation from insufficient data for $\alpha = 0.01$: —, mechanical system $F(x)$; ---, regularized approximation $\tilde{f}(x)$; and - · -, numerical approximation $f_a(x)$.

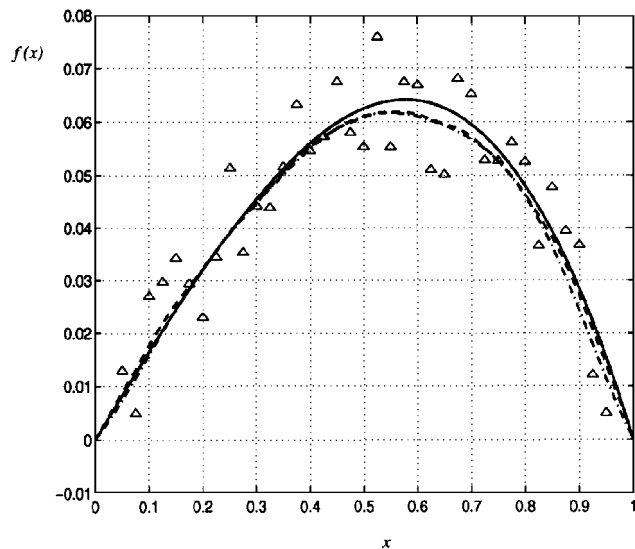


Fig. 2 Interpolation of data with noise for optimal α : —, $F(x)$; ---, $\hat{f}(x)$; and - · -, $f_a(x)$.

Use of Eq. (20) requires a priori knowledge regarding the intensity of the random noise in measurements. This is usually available in engineering applications. The optimal α , which acts as a Lagrange multiplier, was determined through the dichotomous search technique.⁷ The regularized curve of Fig. 2 (---) shows that the developed method of data analysis can successfully discriminate between noise and the physical system response.

B. Results from Numerical Approximation

The numerical approximation by basis expansion consisted of seven ($M = 7$) Gaussian radial basis functions in which the transfer function centers were uniformly distributed in the segment $[0, 1]$ with the center of the two boundary functions located at $x = 0$ and 1, respectively. The parameters Δ_k of Eq. (14), describing the localization properties of the Gaussian function, were all selected to be equal to $\frac{1}{6}$. Figure 1 illustrates the acceptable matching between the analytical solution of the regularization problem and the numerical approximation. Figure 2 shows that the performance of the basis expansion in modeling with the noisy data of Sec. III.A is satisfactory. In the interpolation study, α was determined such that Eqs. (16) and (17) were satisfied with Eq. (19) for $f = f_a$.

IV. Summary

A method of combining experimental data and physical models is presented. Specifically, physical models of engineering interest can be expressed in the form of empirical, differential, and/or integral equations of varying degrees of fidelity. These model equations can be incorporated in the form of a regularizing functional for a robust matching of experimental data. The method can be viewed as the adjustment of a low-fidelity, and computationally inexpensive, mathematical model response by experimental data. The developed method also can be viewed as an efficient procedure for interpolating experimental data by utilizing physically motivated criteria. Further, it has been shown how the developed method can be used to successfully extrapolate the physical system response at unmeasured coordinates and filter noisy experimental measurements. The radial basis expansion has been examined as the computational apparatus of the developed method. However, the developments of the paper retain a sufficient level of generality and can be implemented in conjunction with any of the commonly used methods, including finite difference and conventional finite elements.

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Application of Dual Sorption Theory to Pressure-Sensitive Paints

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Introduction

THIS Note describes the application of a nonlinear dual sorption theory^{1,2} for modeling the steady-state emission of pressure-sensitive paints (PSPs). Calibration comparisons with polynomial expansion models are presented over a 1-atm pressure range for two PSP formulations.

Theoretical Background

PSPs are composed of probe molecules—luminophors—doped into an oxygen permeable binder and dissolved in a thinning agent that forms a coating when sprayed onto a surface of interest. The luminescent intensity variation of most PSPs used in aerodynamic applications is described by the Stern–Volmer relation^{3–5}

$$I_0/I = 1 + K[\text{O}_2] \quad (1)$$

where I_0 is the unquenched intensity, I is the quenched intensity, K is the Stern–Volmer coefficient, and $[\text{O}_2]$ is the oxygen concentration within the coating. The concentration of sorbed oxygen in a liquid is related to the partial pressure of oxygen by Henry's law:

$$[\text{O}_2] = \sigma(T)P_{\text{O}_2} \quad (2a)$$

where

$$P_{\text{O}_2} = \chi_{\text{O}_2}P \quad (2b)$$

and where σ is the solubility coefficient (modeled as a function of temperature only), P is pressure, T is temperature, and χ is the mole fraction of the penetrant. When ratioing intensities at two pressure levels, one designated as a reference (ref), the common form^{3–6} of the intensity–pressure relationship for PSPs is derived from Eqs. (1) and (2a):

$$(I_{\text{ref}}/I) = A + B(P/P_{\text{ref}}) \quad (3)$$

where the coating sensitivities A and B are functions of temperature and reference conditions if all other conditions are held constant, e.g., illumination intensity.

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