INTEGRATING EXPERIMENTAL DATA AND MATHEMATICAL MODELS IN THE SIMULATION OF PHYSICAL SYSTEMS

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NOMENCLATURE

Symbols	**Explanation**
$B(\cdot)$	boundary operator of the mathematical model
$b\langle\cdot,\cdot\rangle$	symmetric form associated with the boundary operator B
c_m	basis expansion coefficients
$\overline{c}$	vector with components c_m
$E[\cdot]$	mathematical expectation operator
F	response of the physical system
f	arbitrary function satisfying the boundary operator B exactly
$\tilde{f}$	hypersurface that gives the global minimum of Eq. (5)
f_0	response of the mathematical model
$\overline{f_0}$	vector with components $f_0(x_j)$
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 $F(x_i)$
$\overline{f_e}$	vector with components $f_e(x_i)$
$G(\cdot,\cdot)$	Green's function of the mathematical model
$\mathbf{G}$	matrix with components $G(x_k, x_m)$
g	algebraic function
$\mathbf{I}$	identity matrix
$L(\cdot)$	linear self-adjoined 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 Euclidian space
$R(\alpha)$	residual of Eq. (20)
s	parameter related to the operator L where $s > 0$
$Var[\cdot]$	variance of a random variable
$x = (x_1, ..., x_d)$	d-dimensional spatial coordinate

Symbols	**Explanation**
$\|\cdot\|_{H^s(\Omega)}$	norm in the Sobolev space of order s
$\langle\cdot,\cdot\rangle$	inner product
α	regularization parameter where $\alpha \geq 0$
$\overline{\beta}$	set of the general ANN parameters / set of basis function parameters and basis expansion coefficients
Δ_k	radial basis function parameter
$\delta(\cdot)$	Dirac delta function
δ_{ji}	$\delta\left(x - x_j\ ,\ x - x_i\right)$
$\epsilon(\cdot)$	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 the mathematical model
ϕ	arbitrary function
ψ	arbitrary function
Ω	spatial domain of the mathematical model
$\partial\Omega$	spatial boundary of the mathematical model

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1 INTRODUCTION

The goal of engineering analysis is to obtain a comprehensive description of a physical system of interest. Three approaches to this goal exist: 1) theoretical analysis of mathematical models, 2) physical experimentation and 3) 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, it is noted that few attempts have been made in uniting experimental, theoretical and numerical methods in the literature. It is the objective of this paper to develop a method which effectively combines all available information, from both experimental data and mathematical models, in the emulation of physical systems.

The technical approach developed in this paper 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 to utilize a-priori mathematical models of physical systems at appropriate degrees of fidelity for regularization. The example problem considered in this paper is used to illustrate two major benefits of the approach. First, to show the benefit of employing a-priori mathematical models of low degree of fidelity for extrapolation from sparse data. Second, 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.

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2 A METHOD FOR DATA ANALYSIS: REGULARIZATION BY A-PRIORI MATHEMATICAL MODELS

The popular Tikhonov regularization method [2] was originally adopted for ANN systems by Poggio and Girosi [3] and extensively used in ANN applications [4], [5]. In this case a set of constraints on the network approximation $f_a(x,\overline{\beta})$ is introduced through the Tikhonov regularization functional $\Lambda\left(f_a(x,\overline{\beta})\right)$ which specifies the penalty given to the oscillatory behavior of $f_a(x,\overline{\beta})$; the network parameters can be determined by minimizing the objective function

$$\epsilon(f_a) = \sum_{i=1}^{N} \left| f_e(x_i) - f_a(x_i,\overline{\beta}) \right|^2 + \alpha\Lambda\left(f_a(x,\overline{\beta})\right) \quad . \tag{1}$$

Unfortunately, conventional smoothness based Tikhonov regularization of Poggio and Girosi 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 can then be approximated by more conventional computational methods.

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

$$Lf_0(x) = g(x)\ ,\ x \in \Omega \quad \text{and} \quad Bf_0(x) = 0\ ,\ x \in \partial\Omega \quad , \tag{2}$$

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

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

Since for any f that satisfies the boundary conditions

$$l\langle f_0, f\rangle = \langle g, f\rangle \quad , \tag{4}$$

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

$$\Phi(f) = \frac{1}{2} l\langle f - f_0, f - f_0\rangle - \frac{1}{2} l\langle f_0, f_0\rangle = \frac{1}{2} l\langle f - f_0, f - f_0\rangle + \text{constant} \quad .$$

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 modelling can be formulated as the minimization of the objective function

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

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.

2.1 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.

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

$$L\tilde{f} = g + \frac{2}{\alpha} \sum_{i=1}^{N} \left(\tilde{f}(x_i) - f_e(x_i) \right) \delta(x - x_i) \ , \ x \in \Omega \quad \text{and} \quad B\tilde{f} = 0 \quad , x \in \partial\Omega \ . \tag{6}$$

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

$$\tilde{f}(x) = f_0(x) + f_{cor}(x) \ . \tag{7}$$

These components can be determined by the equations $f_0(x) = \int_\Omega G(x, \xi) g(\xi) \mathrm{d}\xi$ and

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

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

$$LG(x, \xi) = \delta(x - \xi) \ , \ x \in \Omega \quad \text{and} \quad BG(x, \xi) = 0 \ , \ x \in \partial\Omega \quad .$$

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

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

where the coefficients are defined as

$$c_j = \frac{2}{\alpha} \left(f_e(x_j) - \tilde{f}(x_j) \right) \quad . \tag{10}$$

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

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

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

$$\tilde{f}(x) = f_0(x) + \sum_{i=1}^{N} G(x, x_i)\left[\left(\mathbf{G} + \frac{\alpha}{2}\mathbf{I}\right)^{-1}\left(\overline{f_e} - \overline{f_0}\right)\right]_i \quad . \tag{12}$$

It is noted that the matrix $\mathbf{G}$ of Eq. (12) is positive definite since for an arbitrary function $\phi(x)$ we can write

$$\int_\Omega \int_\Omega G(x,\xi)\phi(\xi)\phi(x)\mathrm{d}\xi \;\mathrm{d}x = \int_\Omega \psi(x)\phi(x)\mathrm{d}x = \int_\Omega \psi(x)L\psi(x)\mathrm{d}x = l\langle\psi,\psi\rangle \quad ,$$

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

$$\int_\Omega \int_\Omega G(x,\xi)\phi(\xi)\phi(x)\mathrm{d}\xi \;\mathrm{d}x \geq \kappa\|\psi\|^2_{H^s(\Omega)} > 0 \quad . \tag{13}$$

Substituting $\phi(x) = \sum_{i=1}^{N} \; c_i\delta(x - x_i)$ into Eq. (13) yields

$$\int_\Omega \int_\Omega G(x,\xi)\phi(\xi)\phi(x)\mathrm{d}\xi \;\mathrm{d}x = \overline{c}^T\mathbf{G}\overline{c} > 0 \quad .$$

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

Since 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 $\alpha \to \infty$ then $\tilde{f}(x) \to f_0(x)$, as expected, since with $\alpha \to \infty$ experimental data becomes less relevant and $\tilde{f}$ emulates more of the a-priori mathematical model.

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

$$\tilde{f}(x) \to f_0(x) + \sum_{i=1}^{N} G(x, x_i)\left[\mathbf{G}^{-1}\left(\overline{f_e} - \overline{f_0}\right)\right]_i$$

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

$$f_0(x_j) + \sum_{i=1}^{N} G(x_j, x_i)\left[\mathbf{G}^{-1}\left(\overline{f_e} - \overline{f_0}\right)\right]_i = f_0(x_j) + \sum_{i=1}^{N} \delta_{ji}\left[\overline{f_e} - \overline{f_0}\right]_i = f_e(x_j) \quad .$$

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

2.2 Numerical Approximation of Regularized Mechanical Systems

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

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

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

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

where $b\langle \cdot, \cdot \rangle$ may be defined as $b\langle f, q \rangle = \int_{\partial\Omega} (Bf(\xi))\, q(\xi) \mathrm{d}\xi$.

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

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

$$\alpha \langle g, \sigma_k(x) \rangle + 2 \sum_{i=1}^{N} f_e(x_i) \sigma_k(x_i) \ \ , \text{ for } \ k = 1, ..., M \tag{16}$$

$$\text{and} \quad \sum_{j}^{M} c_j b \langle \sigma_j(x), p \rangle = 0 \tag{17}$$

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.

3 Example Problem

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

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

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

$$\Phi(f) = \frac{1}{2}\int_0^1 a_0 \left(\frac{\mathrm{d}f}{\mathrm{d}x}\right)^2 \mathrm{d}x - \int_0^1 xf\mathrm{d}x = \frac{1}{2}\int_0^1 a_0 \left(\frac{\mathrm{d}f}{\mathrm{d}x} - \frac{\mathrm{d}f_0}{\mathrm{d}x}\right)^2 \mathrm{d}x + \text{constant} \ . \tag{18}$$

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.

3.1 Results from the Analytical Approximation

The experimental data for the extrapolation study are obtained from the physical system response at $x = 0.25$ and $x = 0.75$, 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 while 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 $f_{cor}(x)$ is a piece-wise linear function in the regions between data points.

As previously mentioned, the use of Eq. (18) for regularization should filter data noise. Noisy experimental data was generated for this study by adding random noise μ, to the response of the physical system, that was statistically independent of location and uniformly distributed between $\pm d/2$, where $d = 0.025$, and with variance $Var[\mu] = d^2/12$. 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

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

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

$$R(\alpha) = \sum_{k=1}^{N} \left| f_e(x_k) - f_0(x_k) - \sum_{i=1}^{N} G(x_k, x_i) \left[\left(\mathbf{G} + \frac{\alpha}{2}\mathbf{I}\right)^{-1} \left(\overline{f_e} - \overline{f_0}\right)\right]_i \right|^2 - \rho \ . \tag{20}$$

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 (dash) shows that the developed method of data analysis can successfully discriminate between noise and the physical system response.

3.2 Results from the Numerical Approximation

The numerical approximation by basis expansion consisted of seven ($M = 7$) Gaussian radial basis functions where 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 $x = 1$, respectively. The parameters Δ_k of Eq. (14), describing the localization properties of the Gaussian function, were all selected to be equal to 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 modelling with the noisy data of Section 3.1 is satisfactory. In the interpolation study, α was determined such that Eqs. (16) and (17) were satisfied with Eq. (19) for $f = f_a$.

4 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 can also 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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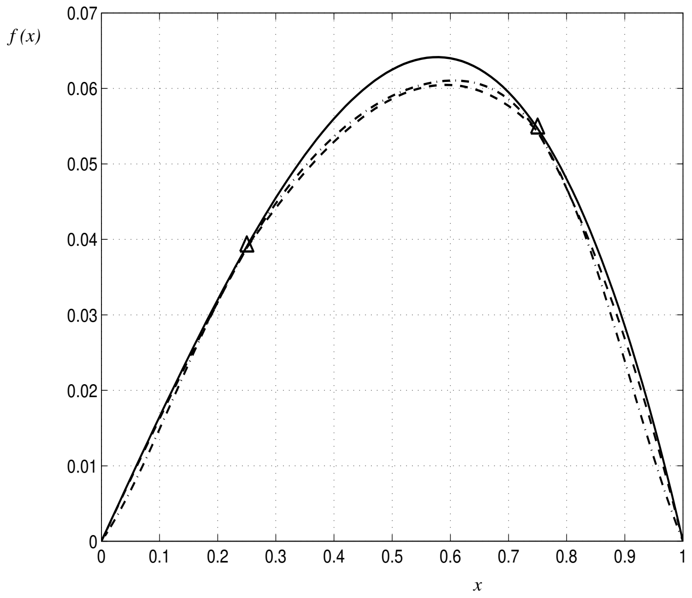

Figure 1: Extrapolation from insufficient data for $\alpha = 0.01$; (solid) the mechanical system $F(x)$, (dash) the regularized approximation $\tilde{f}(x)$, (dash-dot) the numerical approximation $f_a(x)$.

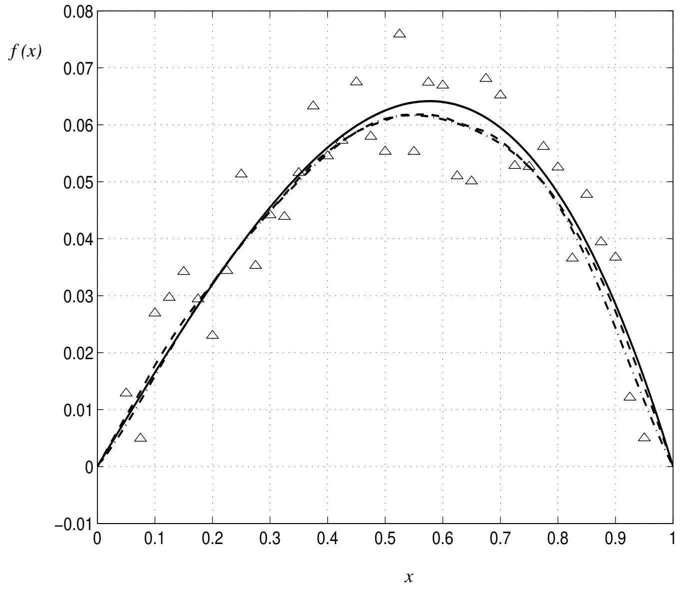

Figure 2: Interpolation of data with noise for optimal α; (solid) $F(x)$, (dash) $\tilde{f}(x)$, (dash-dot) $f_a(x)$.

FIGURE CAPTIONS

Figure 1: Extrapolation from insufficient data for $\alpha = 0.01$; (solid) the mechanical system $F(x)$, (dash) the regularized approximation $\tilde{f}(x)$, (dash-dot) the numerical approximation $f_a(x)$.

Figure 2: Interpolation of data with noise for optimal α; (solid) $F(x)$, (dash) $\tilde{f}(x)$, (dash-dot) $f_a(x)$.