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A Decision Theoretic Method For Surrogate Model Selection

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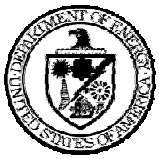

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A decision-theoretic method for surrogate model selection

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Abstract

The use of surrogate models to approximate computationally expensive simulation models, *e.g.*, large comprehensive finite element models, is widespread. Applications include surrogate models for design, sensitivity analysis, and/or uncertainty quantification. Typically, a surrogate model is defined by a postulated functional form; values for the surrogate model parameters are estimated using results from a limited number of solutions to the comprehensive model. In general, there may be multiple surrogate models, each defined by possibly a different functional form, consistent with the limited data from the comprehensive model. We refer to each as a candidate surrogate model. Methods are developed and applied to select the optimal surrogate model from the collection of candidate surrogate models. The classical approach is to select the surrogate model that best fits the data provided by the comprehensive model; this technique is independent of the model use and, therefore, may be inappropriate for some applications. The proposed approach applies techniques from decision theory, where postulated utility functions are used to quantify the model use. Two applications are presented to illustrate the methods. These include surrogate model selection for the purpose of: (1) estimating the minimum of a deterministic function, and (2) the design under uncertainty of a physical system.

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A decision-theoretic method for surrogate model selection

1 Introduction

Most systems in science and engineering can be described by an input/output relationship of the type shown in Fig. 1, where input **x** and operator **f** are, in general, vector valued. Typically, **f** is defined by a collection of differential, integral, and/or algebraic equations with (possibly) random coefficients. The objective is to calculate properties of an output vector, **y**. For example, **f** can be a finite element model of a spacecraft that maps an applied pressure field, **x**, to the displacement response, **y**, of an internal component. Properties of **y**, *e.g.*, the maximum in time, can then be calculated.

Mathematical models for the system shown in Fig. 1 are developed for one or more reasons, what we refer to as the **model use**. For example, we may use the models described above to select the appropriate stiffness and/or location of the internal component attachment point such that maximum in time of its response to the prescribed load is less than some critical value. In this case, we say the model use is design.

Real physical systems such as the example described above are often very complex. The models developed to study such systems can therefore involve a large number of equations that can only be solved numerically with a computer, requiring many hours to obtain an accurate solution. We refer to models of this type as **comprehensive models** for the system. Circumstances may require a simplified approximation for the comprehensive model; we refer to this approximation as a **surrogate model** for the system. To illustrate, consider the case where multiple solutions of the large finite element model for the spacecraft are necessary. This can occur, for example, if the applied pressure field is random in space and/or time, and Monte Carlo simulation is used as

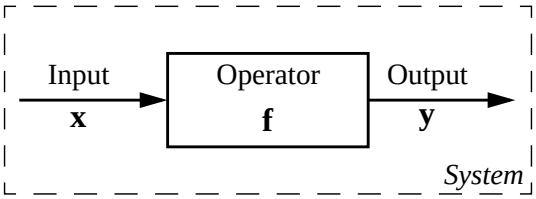

Figure 1. Model for a system as an input/output relationship.

the method for analysis. Optimization and sensitivity analyses also often require multiple model solutions to estimate, for example, the gradient of the output to changes in one or more design variables.

Surrogate models are typically based on a limited number of calculations from the comprehensive models they approximate. Because of this, there may be more than one surrogate model that is consistent with the available information. We refer to the collection of these models as the **collection of candidate surrogate models** for the system. Typical surrogate models include, but are not limited to, polynomials functions [7], radial basis functions [1, 16], Kriging interpolation [3, 11], and multivariate adaptive regression splines [6]. One type of surrogate model for non-Gaussian random variables and stochastic processes is the polynomial chaos approximation [8, 15].

Most often, one surrogate model from the collection of candidate surrogate models is selected and used for analysis. Classical methods to select a surrogate, such as the approaches discussed in [7], Chapter 2, and/or [14], typically do not consider the model use. It has been demonstrated (see [5], Section 3.1.3) that this limitation may render classical methods for surrogate model selection inappropriate for some applications. Herein, we apply a decision-theoretic method, introduced in [5, 13], to select a surrogate model for the system; the proposed approach uses elements from decision theory [2], where the model use is included via an appropriate utility function. We apply the methods for surrogate model selection to applications in design and prediction under uncertainty; the method has been developed and applied to more general classes of models [5].

2 The model selection problem

Consider the following input/output relationship motivated by Fig. 1

$$\mathbf{y} = \mathbf{f}(\mathbf{x}), \tag{1}$$

where $\mathbf{f}\colon \mathbb{R}^d \to \mathbb{R}^l$ is a deterministic, measurable mapping, and $\mathbf{x} = (x_1, \ldots, x_d)^T$ and $\mathbf{y} = (y_1, \ldots, y_l)^T$ are $\mathbb{R}^d-$ and $\mathbb{R}^l-$valued vectors, respectively. Vectors $\mathbf{x}$ and $\mathbf{y}$ may be deterministic or random; for the latter case, we replace $\mathbf{x}$ and $\mathbf{y}$ with $\mathbf{X}$ and $\mathbf{Y}$, respectively. We assume: (i) $\mathbf{f}$ is the comprehensive model for a physical system developed for a specific purpose, *i.e.*, the model use, (ii) the functional form for $\mathbf{f}$ is not explicitly known, but given a value for $\mathbf{x}$, we can calculate the corresponding value for $\mathbf{f}(\mathbf{x})$, and (iii) limited information on $\mathbf{f}$ is available.

The limited information on $\mathbf{f}$ is of two types: (a) calibration data, denoted by $(\mathbf{z}_i, \mathbf{w}_i)$, $i = 1, \ldots, n$, where $\mathbf{z}_i \in \mathbb{R}^d$ and $\mathbf{w}_i = \mathbf{f}(\mathbf{z}_i)$, and (b) prior knowledge, *i.e.*, any information, other than data, on the underlying physics of the system shown in Fig. 1. Prior knowledge is made up by the opinions and theories of experts, as well as any literature on the subject; the fact that $\mathbf{f}$ is nonnegative is one example of prior knowledge. We refer to items (a) and (b) collectively as the available information on $\mathbf{f}$. Note that by assumptions (ii) and (iii), the effects of any solution error are not included; the extension of the methods that follow to the case of nonzero error is straightforward.

2.1 Candidate models

There may be more than one surrogate model for $\mathbf{f}$ that is consistent with the available information. Define

$$\mathcal{G} = \{\mathbf{g}_1, \mathbf{g}_2, \ldots\} \tag{2}$$

where, for each j, $\mathbf{g}_j\colon \mathbb{R}^d \to \mathbb{R}^l$ denotes a surrogate model for $\mathbf{f}$. We refer to $\mathcal{G}$ as the collection of surrogate models for $\mathbf{f}$. Each $\mathbf{g}_j \in \mathcal{G}$ must be consistent with the available information on $\mathbf{f}$, meaning that: (i) any surrogate model that violates the prior knowledge on $\mathbf{f}$ is excluded from the collection, and (ii) given a functional form for $\mathbf{g}_j$, we estimate values for the coefficients of $\mathbf{g}_j$ using the calibration data. For example, consider the case where each $\mathbf{g}_j$ is a polynomial function of the coordinates of $\mathbf{x} \in \mathbb{R}^d$ up to and including order j; the coefficients of surrogate model $\mathbf{g}_j$ can be estimated using, for example, the method of least squares.

The objective is to select the optimal surrogate model for $\mathbf{f}$, denoted $\mathbf{g}^\star \in \mathcal{G}$; this requires a procedure to rank or order the members of $\mathcal{G}$. One way to order the collection of candidate surrogate models is to assess the accuracy of each $\mathbf{g}_j \in \mathcal{G}$ at various values for $\mathbf{x} \in \mathbb{R}^d$. A comparison of the

surrogate models at the calibration data alone may be inadequate since, in many cases, two candidate surrogate models may give the same results, *i.e.*, $\mathbf{g}_i(\mathbf{z}_k) = \mathbf{g}_j(\mathbf{z}_k)$, for $i \neq j$ and $k = 1, \ldots, n$. We therefore introduce validation data, denoted by $(\mathbf{z}'_k, \mathbf{w}'_k)$, $k = 1, \ldots, m$, where $\mathbf{z}'_k \in \mathbb{R}^d$ and $\mathbf{w}'_k \in \mathbb{R}^l$.

Validation data may originate from two sources: (i) solutions of $\mathbf{f}$ at values for $\mathbf{x}$ that do not coincide with the calibration data, *i.e.*, $\mathbf{w}'_k = \mathbf{f}(\mathbf{z}'_k)$, $\mathbf{z}'_k \neq \mathbf{z}_i$, $i = 1, \ldots, n$, $k = 1, \ldots, m$, and/or (ii) experimental observations of the system shown in Fig. 1. As the name implies, validation data may not be used for surrogate model calibration. The concept of using validation data to assess the accuracy of a surrogate model is common; see, for example, [14].

Define

$$p_j \propto \left(\lambda \sum_{k=1}^{m} \|\mathbf{w}'_k - \mathbf{g}_j(\mathbf{z}'_k)\|^2 + (1-\lambda) \sum_{i=1}^{n} \|\mathbf{w}_i - \mathbf{g}_j(\mathbf{z}_i)\|^2 \right)^{-1/2} \tag{3}$$

where $\propto$ is used to imply that p_j is proportional to the RHS of Eq. (3), $\lambda \in (0,1)$ is a deterministic constant, and $\|\boldsymbol{\zeta}\|^2 = \sum_{i=1}^{d} \zeta_i^2$ denotes the square of the $2-$norm of vector $\boldsymbol{\zeta} \in \mathbb{R}^d$. We scale Eq. (3) such that $\sum_j p_j = 1$ and interpret p_j to be the probability that surrogate model $\mathbf{g}_j \in \mathcal{G}$ is true. The values for $p_1, p_2, \ldots$ therefore define an ordering for the members of $\mathcal{G}$.

2.2 Optimal model by classical method

One technique to select $\mathbf{g}^\star \in \mathcal{G}$ is to consider only the model probabilities defined by Eq. (3). We refer to this approach as the classical method for surrogate model selection and note that, with this method, the optimal model is independent of the model use.

By the classical method, surrogate model $\mathbf{g}_i \in \mathcal{G}$ is optimal and denoted by $\mathbf{g}^\star$ if

$$p_i \geq p_j, \ j = 1, 2, \ldots \tag{4}$$

We note that by Eq. (3) if validation data is unavailable, p_j depends on the calibration data alone. If, in addition, we have $\mathbf{w}_i = \mathbf{g}_j(\mathbf{z}_i)$, $i = 1, \ldots, n$, $j = 1, \ldots$, meaning that each $\mathbf{g}_j \in \mathcal{G}$ interpolates the calibration data, we cannot rank any surrogate model higher than any other; in this case the models are assumed equally likely, *i.e.*, $p_1 = p_2 = \cdots$.

2.3 Optimal model by decision-theoretic method

Consistent with the approach developed in [5, 13] we propose to instead assess the utility of each candidate surrogate model for the intended model use, then select $\mathbf{g}^\star \in \mathcal{G}$ that has the least expected utility. We refer to this approach as the decision-theoretic method for surrogate model selection.

Let $U(\mathbf{g}_i, \mathbf{g}_j) \geq 0$ denote the utility of $\mathbf{g}_i \in \mathcal{G}$, if $\mathbf{g}_j \in \mathcal{G}$ is true. Surrogate model $\mathbf{g}_i \in \mathcal{G}$ is optimal and denoted by $\mathbf{g}^\star$ if, and only if

$$u_i \leq u_j, \ j = 1, 2, \ldots, \tag{5}$$

where

$$u_i = \mathrm{E}[U(\mathbf{g}_i, \mathcal{G})] = \sum_j U(\mathbf{g}_i, \mathbf{g}_j) \ p_j \tag{6}$$

denotes the expected utility of surrogate model $\mathbf{g}_i$. The utility, U, is sometimes referred to as the "opportunity loss" (see [17], p. 60) so that the solution to Eq. (5) agrees with intuition, *i.e.*, $\mathbf{g}^\star \in \mathcal{G}$ minimizes the expected loss. For the special case where $U(\mathbf{g}_i, \mathbf{g}_j) = 1 - \delta_{ij}$, where $\delta_{ij} = 1$ for $i = j$ and zero otherwise, the optimal surrogate model by the classical method (Eq. (4)) is recovered (see [12], p. 23).

The functional form for U depends on the model use, meaning that different models may be selected for a different model use. In Section 4 we apply the decision-theoretic method for surrogate model selection for two distinct types of model use: prediction and design.

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3 Surrogate models

Three classes of surrogate models are briefly reviewed. Detailed descriptions of these models can be found in, for example, [7], Chapter 2, and [14]. The purpose here is not to present an exhaustive list of the numerous types of surrogate models used in practice, but rather to present an overview of a few simple relevant models so as to illustrate the concept of surrogate model selection. We restrict our discussion to the case of scalar output $\mathbf{y}$; we therefore replace $\mathbf{f}$, $\mathbf{g}$, and $\mathbf{y}$ defined in Section 2 with f, g, and y, respectively.

We consider surrogate models for $y = f(\mathbf{x})$, $\mathbf{x} \in \mathbb{R}^d$, of the following type

$$g(\mathbf{x}; \mathbb{H}_d^r) = \sum_{j=1}^{r} c_j h_j(\mathbf{x}) = \mathbf{c}^T \mathbf{h}(\mathbf{x}), \tag{7}$$

where $\mathbf{c} = (c_1, \ldots, c_r)^T$ denotes a deterministic vector of coefficients that must be determined, and $\mathbf{h}(\mathbf{x}) = (h_1(\mathbf{x}), \ldots, h_r(\mathbf{x}))^T$ denotes an array of deterministic vector-valued basis functions. We explicitly write g as a function of the collection $\mathbb{H}_d^r = \{h_1(\mathbf{x}), \ldots, h_r(\mathbf{x}); \mathbf{x} \in \mathbb{R}^d\}$ to denote the dependence of the surrogate model on the choice of basis.

The method of least-squares can be used to solve for the coefficients of Eq. (7), *i.e.*,

$$\mathbf{c} = \left(\mathbf{a}^T \mathbf{a}\right)^{-1} \mathbf{a}^T \mathbf{w}, \tag{8}$$

where $\mathbf{a}$ is an $n \times r$ matrix with elements $a_{ij} = h_j(\mathbf{z}_i)$, $\mathbf{w} = (w_1, \ldots, w_n)^T$, and $(\mathbf{z}_i, w_i)$, $i = 1, \ldots, n$, denotes the calibration data defined in Section 2. For the special case when $r = n$ and $\mathbf{a}$ has full rank, Eq. (8) reduces to

$$\mathbf{c} = \mathbf{a}^{-1} \mathbf{w}. \tag{9}$$

Many of the surrogate models used in practice assume the calibration data, $(\mathbf{z}_i, w_i)$, $i = 1, \ldots, n$, satisfy the following criteria:

$$\begin{aligned} &\sum_{j=1}^{n} w_j = \sum_{j=1}^{n} z_{k,j} = 0, \; k = 1, \ldots, d, \text{ and} \\ &\sum_{j=1}^{n} w_j^2 = \sum_{j=1}^{n} z_{k,j}^2 = 1, \; k = 1, \ldots, d, \end{aligned} \tag{10}$$

where $z_{k,j}$ denotes the $k-$th coordinate of vector $\mathbf{z}_j$. When necessary, we will make the same assumption; the extension to the case where the calibration data do not satisfy Eq. (10) is straightforward.

As noted, the surrogate model for f defined by Eq. (7) depends on the choice of basis, $\mathbb{H}_d^r$. We next discuss some properties of g for three different choices for $\mathbb{H}_d^r$, where each choice is commonly used in practice. The bases studied include polynomial, exponential, and indicator functions of $\mathbf{x}$, and are discussed in Sections 3.1 – 3.3, respectively.

3.1 Polynomial basis

Let $\mathbb{P}_d^r = \{h_1(\mathbf{x}), \ldots h_r(\mathbf{x}),\ \mathbf{x} \in \mathbb{R}^d\}$ denote the collection of multidimensional polynomials of $\mathbf{x}$ up to, and including, order q, where

$$h_j(\mathbf{x}) = x_1^{q_1} x_2^{q_2} \cdots x_d^{q_d}, \tag{11}$$

each $q_i \in \{0, 1, \ldots, q\}$, and $\sum_{i=1}^d q_i \leq q$. It follows that r, the number of terms in Eq. (7), is given by $r = \prod_{j=1}^q (1 + d/j)$. For example, consider the case of $d = q = 2$ so that $r = (1+2)(1+2/2) = 6$. The corresponding collection of basis functions is given by $\mathbb{P}_2^6 = \{h_1(x_1, x_2), \ldots, h_6(x_1, x_2)\}$, where

$$\begin{aligned} h_1(x_1, x_2) &= 1 \\ h_2(x_1, x_2) &= x_1 \\ h_3(x_1, x_2) &= x_2 \\ h_4(x_1, x_2) &= x_1^2 \\ h_5(x_1, x_2) &= x_1 x_2 \\ h_6(x_1, x_2) &= x_2^2. \end{aligned} \tag{12}$$

The polynomial basis, perhaps the most frequently used approximation for dealing with functions on bounded domains, has some interesting properties. First, in general $g(\mathbf{z}_i; \mathbb{P}_d^r) \neq w_i$, meaning that a surrogate model defined on $\mathbb{P}_d^r$ does not necessarily interpolate f. Second, by Weierstrass's theorem, as $r \to \infty$, any continuous f can be approximated on a finite interval with arbitrary precision (see [19], p. 159).

3.2 Exponential basis

Assume $r = n$ and let $\mathbb{E}_d^n = \{h_1(\mathbf{x}), \ldots, h_n(\mathbf{x}),\ \mathbf{x} \in \mathbb{R}^d\}$ denote a collection of exponential functions of $\mathbf{x}$, where

$$h_j(\mathbf{x}) = \exp\left(-\theta_j \|\mathbf{x} - \mathbf{z}_j\|^2\right),\ j = 1, \ldots, n, \tag{13}$$

and $\theta_j > 0$ is a deterministic parameter. An alternative collection of basis functions, denoted by $\tilde{\mathbb{E}}_d^n = \{\tilde{h}_1(\mathbf{x}), \ldots, \tilde{h}_n(\mathbf{x})\}$, can be considered, where

$$\tilde{h}_j(\mathbf{x}) = h_j(\mathbf{x}) + \frac{1 - \mathbf{1}^T \mathbf{a}^{-1} \mathbf{h}(\mathbf{x})}{\mathbf{1}^T \mathbf{a}^{-1} \mathbf{1}} \tag{14}$$

$\mathbf{1} = (1, 1, \ldots, 1)^T$ denotes an $n \times 1$ vector of ones, and $\mathbf{h}(\mathbf{x})$ is defined by Eq. (7).

The bases defined by Eqs. (13) and (14) are similar. Because $r = n$, g interpolates f for either basis, meaning that $g(\mathbf{z}_i; \mathbb{E}_d^n) = g(\mathbf{z}_i; \tilde{\mathbb{E}}_d^n) = w_i$, $i = 1, \ldots, n$. The second term on the RHS of Eq. (14) is zero for $\mathbf{x} = \mathbf{z}_i$, $i = 1, \ldots, n$; it follows that $\tilde{h}_j(\mathbf{z}_i) = h_j(\mathbf{z}_i)$, $i, j = 1, \ldots, n$, and the coefficients of Eq. (7) are therefore identical under basis $\mathbb{E}_d^n$ and $\tilde{\mathbb{E}}_d^n$. The surrogate models defined above have special names in the literature. Equation (13) is a particular type of radial basis function (RBF), and under basis $\tilde{\mathbb{E}}_d^n$, Eq. (7) is a Kriging approximation for f [11, 16]. The RBF and Kriging approximations are commonly used in practice as surrogate models for large, complex finite element models (see, for example, [4]).

3.3 Indicator basis

Assume $r = n$ and let $\mathbb{I}_d^n = \{h_1(\mathbf{x}), \ldots, h_n(\mathbf{x}),\ \mathbf{x} \in \mathbb{R}^d\}$ denote a collection of basis functions, where

$$h_j(\mathbf{x}) = 1\left(\mathbf{x} \in \rho_j\right), \tag{15}$$

and $\rho_1, \ldots, \rho_r \subseteq \mathbb{R}^d$ denote non-overlapping subsets of $\mathbb{R}^d$. The function $1(A) = 1$ if event A is true, and $1(A) = 0$ otherwise, is referred to as an indicator function. We consider the special case where each ρ_j is a rectangle in $\mathbb{R}^d$ with center $\mathbf{x} = \mathbf{z}_j$ and size $\phi_1 \times \cdots \times \phi_d$, *i.e.*,

$$\rho_j = \bigtimes_{k=1}^{d} \left[z_{k,j} - \phi_k/2, z_{k,j} + \phi_k/2\right],\ j = 1, \ldots, n, \tag{16}$$

and

$$\phi_k = \min_{z_{k,i} \neq z_{k,j}} |z_{k,i} - z_{k,j}|. \tag{17}$$

By Eqs. (16) and (17), $\mathbf{a} = \mathbf{i}_n$, where $\mathbf{i}_n$ denotes the $n \times n$ identity matrix, so that, by Eq. (9), $\mathbf{c} = \mathbf{w}$. More sophisticated techniques are available to select both the number of basis functions, r, and the subsets, $\rho_1, \ldots, \rho_r$; one popular approach is the Multivariate Adaptive Regression Spline (MARS) [6].

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4 Applications

Two applications are provided to demonstrate the methods for surrogate model selection. They include: (i) deterministic prediction, and (ii) design under uncertainty. For (i), we consider a collection of surrogate models for f, a deterministic, 4-th order polynomial function of two variables. For (ii), we consider the design of a structural dynamics application, namely the response of a structural system to a time-varying forcing function, where one of the system parameters is modeled as a random variable. Applications (i) and (ii) are discussed in Sections 4.1 and 4.2, respectively.

4.1 Deterministic prediction

Let

$$f(x_1,x_2) = 100\left(x_2 - x_1^2\right)^2 + (1-x_1)^2,\ \mathbf{x} \in D, \tag{18}$$

where $D = [-2,2]\times[-2,2]$, be the comprehensive model of interest. This particular example has been extensively studied by the optimization community and is commonly known as the Rosenbrock test function [9, 10]. The function f is illustrated in Fig. 2; a contour plot is also shown. The objectives are: (i) select the optimal surrogate model for f, and (ii) predict

$$\min_{\mathbf{x}\in D} f(\mathbf{x}), \tag{19}$$

where, by (ii) the model use is prediction. The exact solution to Eq. (19) is $\min_{\mathbf{x}\in D} f = 0$ at $\mathbf{x} = (1,1)^T$, as denoted by the solid circle in Fig. 2.

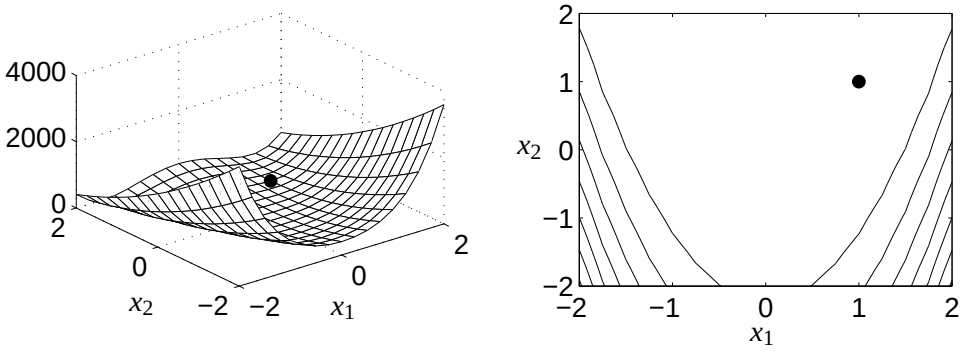

Figure 2. The Rosenbrock function, $f(x_1,x_2)$.

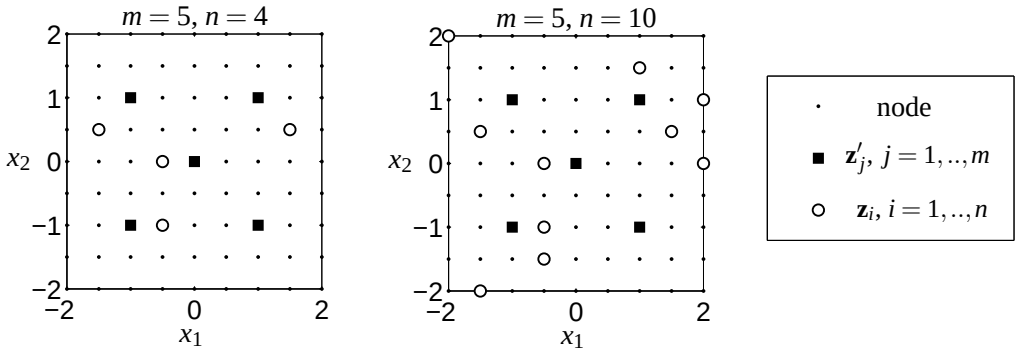

Figure 3. Locations of calibration data, $\mathbf{z}_i$, and validation data, $\mathbf{z}'_j$, for application #1.

4.1.1 Candidate models

The available information on f is limited to n calibration data, denoted by $(\mathbf{z}_i, w_i)$, $i = 1,\ldots,n$. We assume m validation data, denoted by $(\mathbf{z}'_j, w'_j)$, $j = 1,\ldots,m$, where $w'_j = f(\mathbf{z}'_j)$ and $\mathbf{z}'_j \neq \mathbf{z}_i$, $i = 1,\ldots,n$, $j = 1,\ldots,m$. The values for $\mathbf{z}_i$ and $\mathbf{z}'_j$ are illustrated by Fig. 3, where domain D is discretized into 64 non-overlapping $1/2 \times 1/2$ regions, defined by the 81 nodes in the figure. As denoted by the black squares in Fig. 3, $m = 5$ of the 81 nodes are reserved for surrogate model validation. The calibration points are selected at random from the remaining 76 nodes. The values for $\mathbf{z}_1,\ldots,\mathbf{z}_n$ for the case of $n = 4$ and $n = 10$ are shown on the left and right sides of Fig. 3, respectively, where the calibration data is denoted by a circle.

Six candidate surrogate models for f are considered, *i.e.*,

$$\begin{aligned}\mathcal{G} &= \{g_1,\ldots,g_6\} \\ &= \left\{g(\mathbf{x};\mathbb{P}_2^6), g(\mathbf{x};\mathbb{P}_2^{10}), g(\mathbf{x};\mathbb{P}_2^{15}), g(\mathbf{x};\mathbb{E}_2^n), g(\mathbf{x};\tilde{\mathbb{E}}_2^n), g(\mathbf{x};\mathbb{I}_2^n)\right\},\end{aligned} \tag{20}$$

where the functional form for each surrogate is defined by Eq. (7), and the parameters for each surrogate are estimated from the calibration data shown in Fig. 3. By Eq. (20), g_1, g_2, and g_3 are second-, third-, and fourth-order polynomial functions of $\mathbf{x} \in \mathbb{R}^2$, respectively. Surrogate models g_4 and g_5 are defined on the exponential basis defined by Eqs. (13) and (14), respectively, with $\theta_j = 1$, $j = 1,\ldots,n$; g_6 is defined on the indicator basis discussed in Section 3.3.

We refer to $g_3 \in \mathcal{G}$ as the "true surrogate model" for f because, by Eq. (18), f is a fourth-order polynomial in $\mathbf{x}$. Surrogates g_1, g_3, g_4, and g_6 are shown in Fig. 4 for the case of $n = 15$, illustrating that the candidate models can be very different, but each is consistent with the available information.

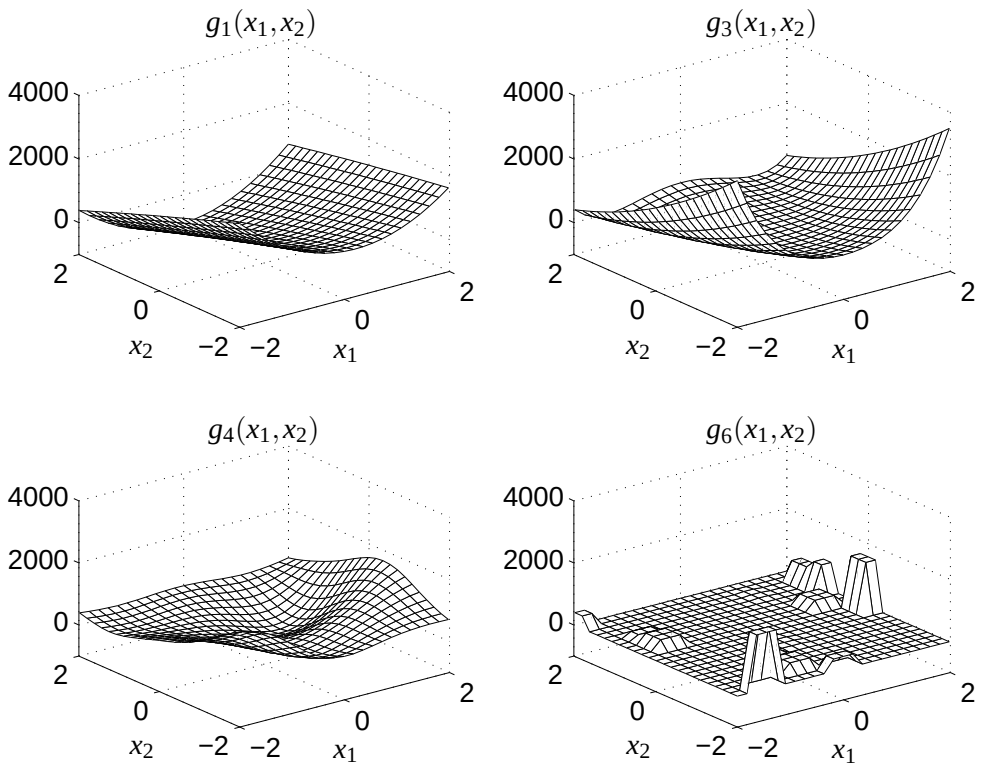

Figure 4. Candidate surrogate models for f assuming $n = 15$.

4.1.2 Optimal model

We apply the classical and decision-theoretic methods to select optimal surrogate models for f. Further, we study the evolution of the optimal model as the number of calibration data, n, increases.

As discussed in Section 2, the decision-theoretic method for model selection requires a utility function. Let

$$\xi_i = \min_{\mathbf{x}\in D} g_i(\mathbf{x}), \tag{21}$$

so that ξ_i denotes the estimate of Eq. (19) under surrogate $g_i \in \mathcal{G}$. Assuming surrogate $g_j \in \mathcal{G}$ is true, we say $g_i \in \mathcal{G}$ is conservative if it over-predicts the minimum, *i.e.*, if $\xi_i \geq \xi_j$. We assume conservative models are preferable to non-conservative models and use this assumption as the basis for our interpretation of surrogate model utility.

An appropriate value for the utility of surrogate model $g_i \in \mathcal{G}$, assuming surrogate $g_j \in \mathcal{G}$ is true, is given by

$$U(g_i, g_j) = \tilde{U}(\xi_i, \xi_j) = \begin{cases} \beta_1(\xi_i - \xi_j)^2 & \text{if } \xi_i \geq \xi_j \\ \beta_2(\xi_i - \xi_j)^2 & \text{if } \xi_i < \xi_j \end{cases} \tag{22}$$

where $\beta_2 \geq \beta_1 \geq 0$ are deterministic parameters, and we replace U with $\tilde{U}$ to denote that the utility function can be expressed as a function of ξ_i and ξ_j alone. By Eq. (22), non-conservative models are assigned a large utility; overly conservative models are also subject to penalty. We note that definitions of model utility are problem-dependent; alternative definitions can be used. The utility used here is consistent with the formulation for general problems in prediction discussed in [5], Section 2.3.2.3.

The surrogate model probabilities, $p_1, \ldots, p_6$, are shown on the left side of Fig. 5 for $4 \leq n \leq 20$; shown on the right are the expected utilities of each surrogate model, $u_1, \ldots, u_6$. Parameters $\lambda = 1/2$, $\beta_1 = 1$, and $\beta_2 = 10$ were used for calculations. The optimal surrogate model, $g^\star \in \mathcal{G}$, using the classical method (by Eq. (4)) and decision-theoretic method (by Eq. (5)) are shown in Fig. 6 for $4 \leq n \leq 20$. As the number of calibration data, n, increases, different surrogate models are selected. For $n < 15$, different surrogate models for f are optimal under the two methods for model selection. For $n \geq 15$, $p_3 = 1$ so that the true model, g_3, is selected by both methods; this is because g_3 is a fourth-order polynomial requiring $r = 15$ coefficients (see Section 3.1).

Recall that only the decision-theoretic method includes the model use and, therefore, assigns a large utility to those models that provide non-conservative predictions of Eq. (19). To illustrate this, let

$$\xi^\star = \min_{\mathbf{x}\in D} g^\star(\mathbf{x}) \tag{23}$$

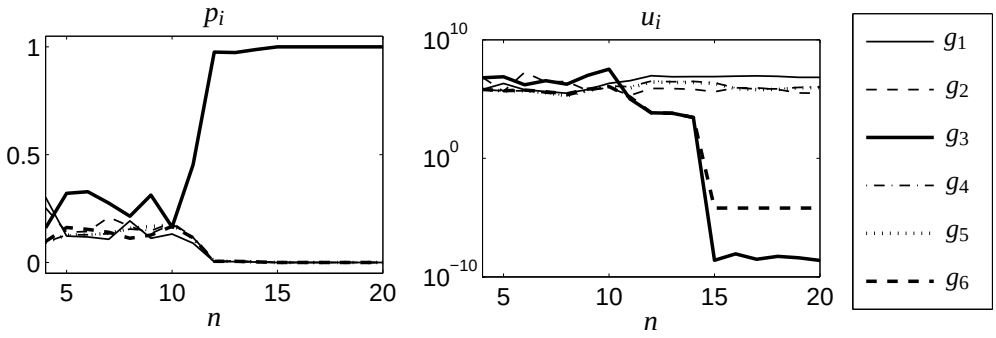

Figure 5. Model probabilities (left) and expected utilities (right) for each surrogate.

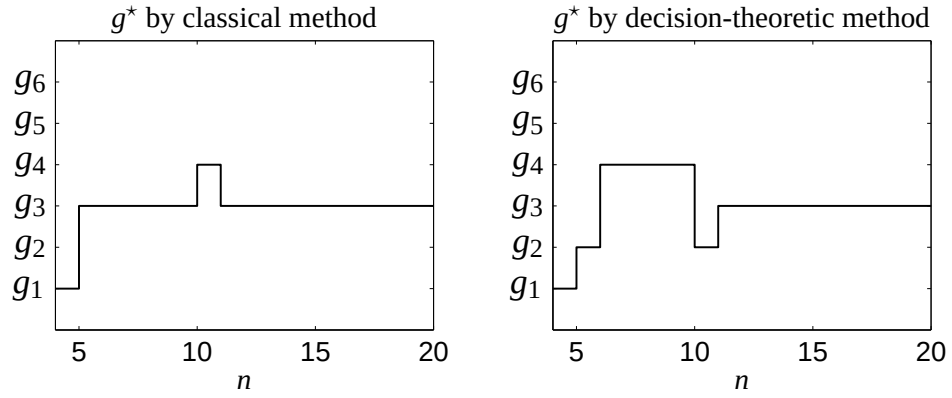

Figure 6. $g^\star \in \mathcal{G}$ using classical method (left) and decision-theoretic method (right).

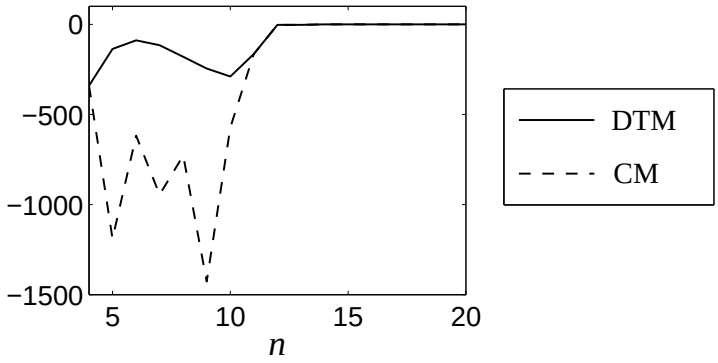

Figure 7. $\xi^\star$ vs. n under decision-theoretic (DTM) and classical (CM) method.

denote the prediction of Eq. (19) under the optimal model, $g^\star \in \mathcal{G}$. Values for $\xi^\star$ using the classical method and proposed decision-theoretic method are shown in Fig. 7. Note that with the classical method, a non-conservative model, *i.e.*, one that under-predicts the minimum, may be selected for $n < 15$. For $n \geq 15$, $\xi^\star = \min_{\mathbf{x}\in D} f(\mathbf{x}) = 0$ using both methods for surrogate model selection.

We remark that the results presented depend on the: (i) location and number of the validation data, (ii) order in which the calibration data is selected (see Fig. 3), and (iii) utility function. More sophisticated methods are available to select locations for calibration and validation data (see, for example, [18], Section 4.3); these methods can easily be included in the model selection framework presented here. A discussion on the sensitivity of the optimal model by the decision-theoretic method to changes in the utility function are discussed in [5], Sections 2.3.1.5, 2.4, 5.6.4, and 5.8.4.

4.2 Design under uncertainty

We next consider the 2 degree-of-freedom oscillator shown in Fig. 8, a model commonly used for applications in structural dynamics, where ζ denotes the forcing function, X denotes the value for a spring constant, m_1 and m_2 denote the values for the two masses, and v denotes the relative displacement of the two masses. We assume: (i) input $\zeta(t)$ is a perfectly known and deterministic function of time, t, (ii) the value for one of the spring constants is known and fixed, (iii) X is a uniform random variable on $[1500, 2500]$, and (iv) the values for the two masses are deterministic

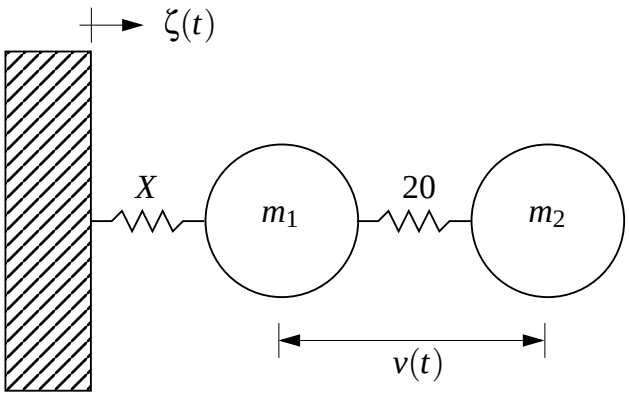

Figure 8. Two degree-of-freedom oscillator.

design parameters that must satisfy the following constraints:

$$m_1 + m_2 = 100 \tag{24a}$$

$$\frac{1}{99} \leq \frac{m_2}{m_1} \leq 1 \tag{24b}$$

The objectives are to: (a) select the optimal surrogate model for the comprehensive system model, and (b) design the structure, *i.e.*, select values for m_1 and m_2, such that certain properties of v satisfy a prescribed set of conditions. By (b), the model use is design.

Let **m**, **d**, and **k** denote the 2×2 mass, damping, and stiffness matrices, respectively, of the two degree-of-freedom oscillator shown in Fig. 8, *i.e.*,

$$\mathbf{m} = \begin{bmatrix} \dfrac{100}{1+\delta} & 0 \\ 0 & \dfrac{100\delta}{1+\delta} \end{bmatrix} \text{ and } \mathbf{k} = \begin{bmatrix} X+20 & -20 \\ -20 & 20 \end{bmatrix} \tag{25}$$

where $\delta = m_2/m_1$ is the ratio of the two masses, and **d** is such that the system is classically damped with a constant damping ratio of 4% for each mode. The relative displacement of the two masses, assuming zero initial conditions, is given by [20], p. 167,

$$v(t, X, \delta) = \mathbf{c} \int_0^t \exp\left[\mathbf{a}(t-\tau)\right] \mathbf{b} \zeta(\tau) \mathrm{d}\tau, \tag{26}$$

where

$$\mathbf{a} = \begin{bmatrix} \mathbf{0} & \mathbf{i} \\ -\mathbf{m}^{-1}\mathbf{k} & -\mathbf{m}^{-1}\mathbf{d} \end{bmatrix}, \; \mathbf{b} = \begin{bmatrix} 0 & 0 & -1 & -1 \end{bmatrix}^T,$$
$$\mathbf{c} = \begin{bmatrix} -1 & 1 & 0 & 0 \end{bmatrix}, \tag{27}$$

and **i** denotes the 2×2 identity matrix. We consider two metrics of system performance, given by

$$P(Y \leq \bar{y}), \text{ and} \tag{28a}$$
$$\mathrm{E}[Y], \tag{28b}$$

where $\bar{y} \geq 0$ is a prescribed deterministic parameter, and

$$Y = f(X, \delta) = \max_{t \geq 0} \mid v(t, X, \delta) \mid \tag{29}$$

is the output of interest. We write $Y = f(X, \delta)$ in Eq. (29) to be consistent with the general input/output relationship described by Fig. 1, and we replace $\mathbf{x}$ with (X, δ) and $\mathbf{y}$ with Y; capital letters for X and Y are used to denote that these two quantities are random variables.

To estimate the performance metrics defined by Eq. (28), it is convenient to approximate Eq. (29) with a surrogate model; approximation may become necessary when we consider nonlinear systems or linear systems with many degrees-of-freedom. Herein, we employ methods for surrogate model selection for the purpose of design under uncertainty. We consider two cases:

$$\text{Case \#1: select } \delta \in [1/99, 1] \text{ such that } P(Y \leq \bar{y}) = \bar{q} \tag{30a}$$
$$\text{Case \#2: select } \delta \in [1/99, 1] \text{ such that } \mathrm{E}[Y] = \bar{r} \tag{30b}$$

where $\bar{q}$ and $\bar{r}$ denote prescribed deterministic parameters that define the design constraints. By Eq. (30), the model use for Case #1 is different than for Case #2. Optimal surrogate models for Case #1 and Case #2 are discussed in Sections 4.2.2.1 and 4.2.2.2, respectively. A discussion on a related problem, where $\delta = 1/99$ is fixed and the model use is to predict the metrics defined by Eq. (28), is discussed in [5], Section 3.3.

4.2.1 Candidate models

The available information on f is limited to n calibration data, denoted by $(\mathbf{z}_i, w_i)$, $i = 1, \ldots, n$, and m validation data, denoted by $(\mathbf{z}'_k, w'_k)$, $k = 1, \ldots, m$. We assume the latter is given by simulated experimental observations of the system shown in Fig. 8. For calculations, we model each experimental observation as the solution of the comprehensive model at one of the calibration points, subject to additive noise, *i.e.*, for $k = 1, \ldots, m$, w'_k is one sample of random variable

$$f(\mathbf{z}'_k) + E_k, \tag{31}$$

where $\{E_k\}$ denotes a sequence of zero-mean iid Gaussian random variables with variance σ^2, each $\mathbf{z}'_k$ coincides with one of $\mathbf{z}_i$, $i = 1, \ldots, n$, and $m \leq n$. The data are illustrated by Fig. 9 for $m = 5$ and $n = 10$. The values for $\mathbf{z}'_1, \ldots, \mathbf{z}'_5$, the validation data, are shown in the left plot, while the values for $\mathbf{z}_1, \ldots, \mathbf{z}_{10}$, the calibration data, are shown in the right plot. For calculations, the forcing function, $\zeta(t)$, is given by one sample of Gaussian white noise with intensity $10000/\pi$ (see [20], p. 29).

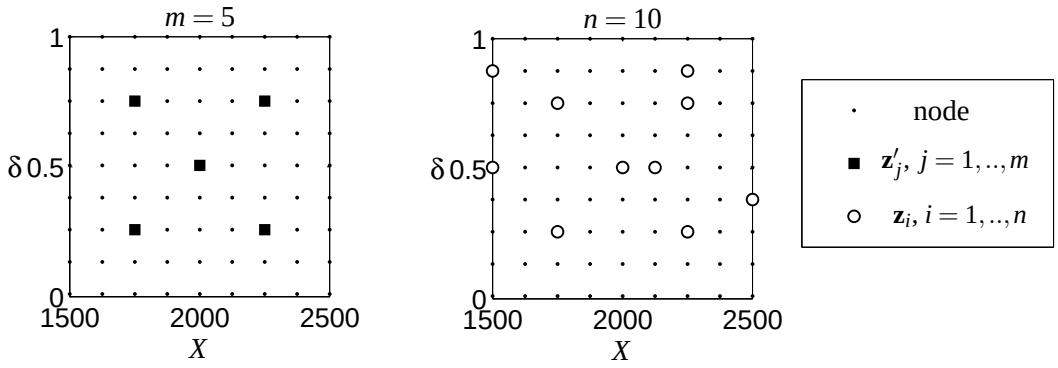

Figure 9. Locations of validation data (left) and calibration data (right) for application #2.

We consider 6 candidate surrogate models for f, *i.e.*,

$$\begin{aligned}\mathcal{G} &= \{g_1,\ldots,g_6\} \\ &= \left\{g(X,\delta;\mathbb{P}_2^6), g(X,\delta;\mathbb{P}_2^{10}), g(X,\delta;\mathbb{P}_2^{15}), g(X,\delta;\mathbb{E}_2^n), g(X,\delta;\tilde{\mathbb{E}}_2^n), g(X,\delta;\mathbb{I}_2^n)\right\} \end{aligned} \tag{32}$$

where the functional form for each surrogate is defined by Eq. (7), and the parameters for each surrogate are estimated from the calibration data shown on the right side of Fig. 9. Note the the functional form for each surrogate considered is identical to the functional form considered in Section 4.1.1. Unlike the example of Section 4.1, there is no true surrogate model for f. Surrogates g_1, g_2, g_4, and g_6 are shown in Fig. 10 for the case of $n = 15$, illustrating that the candidate surrogate models for f are very different, but each is consistent with the available calibration data.

4.2.2 Optimal model

We first apply the classical method for model selection; results using the decision-theoretic method, which depend on the model use, are discussed in Sections 4.2.2.1 and 4.2.2.2. The surrogate model probabilities, $p_1,\ldots,p_6$, are shown on the left side of Fig. 11 for $5 \le n \le 81$; the optimal surrogate model for f using the classical method, *i.e.*, by Eq. (4), is also shown. Parameters $\lambda = 1/2$ and $\sigma^2 = 10$ were used for calculations. For $n < 16$, any surrogate model can be selected. For $n \ge 16$, values for p_1, p_2, and p_3, which correspond to the polynomial models, approach zero, while values for p_4, p_5, and p_6 are nearly identical and nonzero. Hence, among models $\{g_4, g_5, g_6\}$ there is no strong preference of one over another for $n \ge 16$; this is further demonstrated by the oscillatory behavior of $g^\star$ on the left side of Fig. 11.

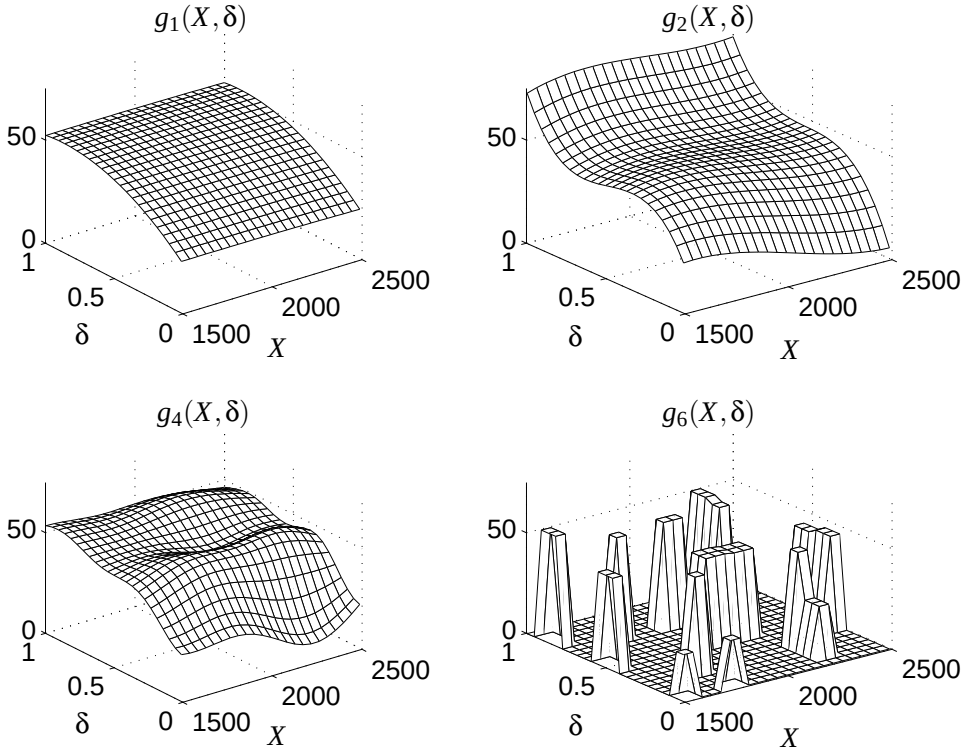

Figure 10. Candidate surrogate models for f assuming $n = 15$.

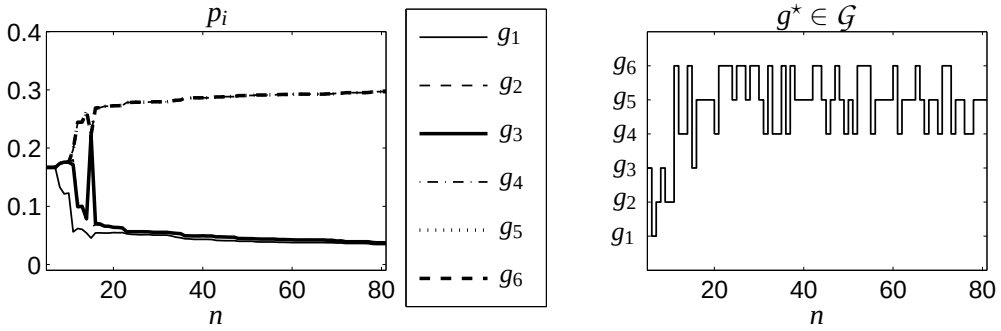

Figure 11. Model probabilities (left) and optimal model (right) using classical method.

4.2.2.1 Case #1 As discussed in Section 2, the decision-theoretic method for model selection requires a utility function; we next develop such a function to quantify the utility of each surrogate that is consistent with the model use (Eq. (30a)).

Assuming it exists, we define a_i such that

$$P\left(g_i(X,a_i) \leq \bar{y}\right) = \bar{q}, \tag{33}$$

so that a_i is the value for δ that satisfies design condition #1, defined by Eq. (30a), under surrogate model g_i. In the case of a non-unique solution, we choose the minimum a_i that satisfies Eq. (33). The performance of design a_i, assuming model $g_j \in \mathcal{G}$ is true, is given by

$$\xi_{ij} = P\left(g_j(X,a_i) \leq \bar{y}\right), \tag{34}$$

which may or may not equal the required reliability, $\bar{q}$. We say design a_i is conservative if the reliability exceeds $\bar{q}$, and non-conservative otherwise. We assume models that favor conservative designs are favorable to models that favor non-conservative designs and use this assumption as the basis for our interpretation of surrogate model utility.

An appropriate value for the utility of surrogate model $g_i \in \mathcal{G}$, if surrogate model $g_j \in \mathcal{G}$ is true, is given by

$$U(g_i,g_j) = \tilde{U}(a_i,a_j) = \begin{cases} \beta_1\left(a_i - a_j\right)^2 & \text{if } \xi_{ij} \geq \bar{q} \\ \beta_2\left(a_i - a_j\right)^2 & \text{if } \xi_{ij} < \bar{q} \end{cases} \tag{35}$$

where $\beta_2 \geq \beta_1 \geq 0$ are deterministic parameters, and we replace U with $\tilde{U}$ to denote that the utility function can be expressed as a function of a_i and a_j. By Eq. (35), models that favor non-conservative designs are assigned a large utility; models that favor overly conservative designs are also subject to penalty. The utility used here is consistent with the formulation for general design problems discussed in [5], Section 2.3.2.2.

The expected utility of each surrogate model, denoted by $u_1,\ldots,u_6$, is shown on the left side of Fig. 12 for $5 \leq n \leq 81$; shown on the right is the optimal surrogate model, $g^\star$, for each value for n. Parameters $\beta_1 = 1$, $\beta_2 = 100$, $\bar{q} = 0.9$, and $\bar{y} = 50$ were used for calculations. The results are different than those shown in Fig. 11 because the optimal model under the decision-theoretic method depends on the model use. For example, surrogate model g_1, a second-order polynomial, is often optimal because it results in a conservative design of the system.

4.2.2.2 Case #2 By Eq. (30), the model use for Case #2 is different than for Case #1; our definition for the utility function must therefore reflect this. Assuming it exists, we define a_i such that

$$\mathrm{E}\left[g_i(X,a_i)\right] = \bar{r}, \tag{36}$$

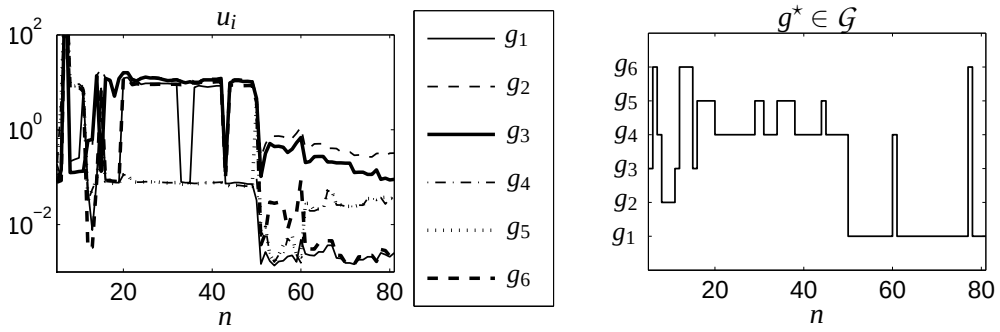

Figure 12. Expected utilities (left) and optimal model (right) for case #1.

so that a_i is the value for δ that satisfies design condition #2, defined by Eq. (30b), under surrogate model g_i. As before, in the case of a non-unique solution, we choose the minimum a_i that satisfies Eq. (36). The performance of design a_i, assuming model $g_j \in \mathcal{G}$ is true, is given by

$$\xi_{ij} = \mathrm{E}\left[g_j(X, a_i)\right], \tag{37}$$

which may or may not be equal to $\bar{r}$, the design requirement. We say design a_i is non-conservative if the mean value exceeds $\bar{r}$, and conservative otherwise; we assume models that favor conservative designs are favorable to models that favor non-conservative designs.

An appropriate value for the utility of surrogate model $g_i \in \mathcal{G}$, if surrogate model $g_j \in \mathcal{G}$ is true, is given by

$$U(g_i, g_j) = \tilde{U}(a_i, a_j) = \begin{cases} \beta_1 \left(a_i - a_j\right)^2 & \text{if } \xi_{ij} \leq \bar{r} \\ \beta_2 \left(a_i - a_j\right)^2 & \text{if } \xi_{ij} > \bar{r} \end{cases} \tag{38}$$

where $\beta_2 \geq \beta_1 \geq 0$ denote deterministic parameters. The expected utility of each surrogate model, denoted by $u_1, \ldots, u_6$, is shown on the left side of Fig. 13 for $5 \leq n \leq 81$; shown on the right is the optimal surrogate model, $g^\star$, for each value for n. Parameter $\bar{r} = 30$ was used for calculations. In general, we note that by Figs. 12 and 13, different surrogate models are optimal under different model use. The expected utilities are undefined for $n < 12$ since no value for δ exists to satisfy the design requirement given by Eq. (30b); $g^\star$ is therefore identical to results using the classical method (Fig. 11) for $n < 12$.

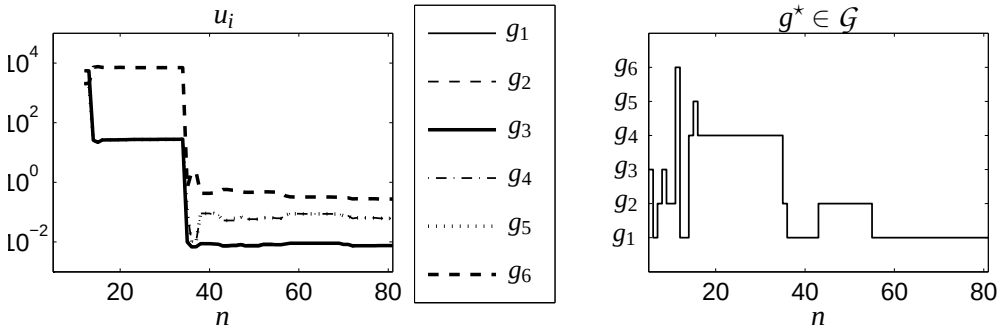

Figure 13. Expected utilities (left) and optimal model (right) for case #2.

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5 Conclusions

Methods were developed and applied to select the optimal member from a collection of candidate surrogate models, where each is an approximation for a single comprehensive model. Each model in the collection was consistent with limited information provided by the comprehensive model. Classical methods select the surrogate model that best fits the data provided by the comprehensive model; it was shown that this technique is independent of the model use and, therefore, was inappropriate for some applications. The proposed approach applied techniques from decision theory, where postulated utility functions were used to quantify the model use. Two applications were presented to illustrate the methods. These included surrogate model selection for the purpose of: (1) estimating the minimum of a deterministic function, and (2) the design under uncertainty of a physical system.

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