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Domain Segmentation based on Uncertainty in the Surrogate (DSUS)

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This paper develops a novel approach to characterize the uncertainty in the accuracy of surrogate models. This technique segregates the design domain based on the level of cross-validation errors; the overall framework is called Domain Segmentation based on Uncertainty in the Surrogate (DSUS). The estimated errors are classified into physically meaningful classes based on the user's understanding of the system and/or the accuracy requirements for the concerned system analysis. In each class, the distribution of the cross-validation errors is estimated to represent the uncertainty in the surrogate. Support Vector Machine (SVM) is implemented to determine the boundaries between error classes, and to classify any new design (point) into a meaningful class. The DSUS framework is illustrated using two different surrogate modeling methods: (i) the Kriging method, and (ii) the Adaptive Hybrid Functions (AHF). We apply the DSUS framework to a series of standard problems and engineering problems. The results show that the DSUS framework can successfully classify the design domain and quantify the uncertainty (prediction errors) in surrogates. More than 90% of the test points could be accurately classified into its error class. In real life engineering design, where we use predictive models with different levels of fidelity, the knowledge of the level of error and uncertainty at any location inside the design space is uniquely helpful.

Keywords: Pattern classification, response surface, support vector machine, surrogate modeling, uncertainty, Kriging

I. Introduction

Uncertainties in a system may come from cognitive (qualitative) and noncognitive (quantitative) sources.[1] Noncognitive, or quantitative, sources of uncertainty can be classified into three types: (i) inherent randomness in all physical observation; (ii) statistical uncertainty; and (iii) modeling uncertainty.[1] Since a surrogate model is an approximation to an unknown function, prediction errors are generally present in the estimated function values. The three major sources of uncertainty in surrogate modeling are: (i) uncertainty in the observations (when they are noisy), (ii) uncertainty due to finite sample, and (iii) uncertainty as a result of **approximate** representation of the system behavior. One of the major challenges in surrogate modeling is to accurately quantify these uncertainties, and how these uncertainties vary in the design space.[2]

The fundamental purpose of a surrogate model is to provide a cheaper and/or a more convenient representation of the actual system. Substantial research has been done in past two decades to improve the

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fidelity and the robustness of surrogates. However, the most advanced surrogate modeling techniques currently available are still subject to the principles of "no free lunch" theorems.[3] In addition, the adoption of the more sophisticated methods often compromises the generality of application.[3] As a result, it would be uniquely helpful to be able to quantify what level of uncertainty is expected in the surrogate model. Additionally, the knowledge of **how the surrogate uncertainty and the levels of errors vary in the variable space** will introduce more confidence in the usage of the surrogate (irrespective of its overall level of fidelity). The latter remains a largely uncharted territory in Multidisciplinary Design Optimization.

A. An Overview of Surrogate Modeling

The need to quantify economic and engineering performance of complex products often demands highly complex and computationally expensive simulations and/or expensive experiments. Among the various approaches to deal with this problem, surrogate models (or metamodels) have gained wide acceptance from the design community. Surrogate modeling is concerned with the construction of approximation models to estimate the system performance, or to develop relationships between specific system inputs and outputs.

A wide variety of surrogate modeling techniques have been reported in the literature, such as: (*i*) Polynomial Response Surface Model (PRSM),[4] (*ii*) Kriging,[5–7] (*iii*) Radial Basis Functions (RBF),[8,9] (*iv*) Extended Radial Basis Functions (E-RBF),[10] (*v*) Artificial Neural Networks (ANN),[11,12] and (*vi*) Support Vector Regression (SVR).[13–15] In the literature, the accuracy and the effectiveness of various surrogate models for linear, nonlinear, smooth, and noisy responses have also been investigated.[16–19]

PRSM is a statistical tool, primarily developed for fitting analytical models (typically quadratic polynomials) to an available data set. Owing to its tractability, the classical PRSM is still one of the most widely used forms of surrogate models in engineering design.[16,17] PRSM can capture the global trend, and generally involves a smaller set of parameters (unknown coefficients) compared to other advanced models, such as Kriging and RBF. However, PRSM (quadratic polynomial) is often not adequate for capturing the local accuracy, particularly in the case of highly nonlinear functional relationships. The challenge of exact fitting has inspired researchers to explore the so-called kernel-based surrogate modeling techniques, which can provide an interpolating surface through the entire training data set. Kernel-based surrogate modeling techniques offer critical advantages over the traditional PRSM, such as the ease of extending the estimated function to higher dimensions and representation of highly nonlinear functional relationships. Kernel-based surrogate modeling methods typically make use of local information related to each training data point, and combine this information to define the overall surrogate model. Kriging, RBF and E-RBF are among the popular kernel-based surrogate modeling techniques.[10] More recently, researchers have combined different approximate models into a single hybrid model for developing weighted average surrogates.[20–23]

B. Uncertainty in Surrogate Modeling

Uncertainties can generally be classified into two categories: (i) aleatoric, or statistical, uncertainties; and (ii) epistemic, or systematic, uncertainties. Epistemic uncertainty represents a lack of knowledge about the appropriate value to use for a quantity, which can be reduced through increased or more relevant data. This paper will focus on the epistemic uncertainty to quantify prediction uncertainties in surrogate models.

In addition, uncertainty and error quantification is a classical theme in surrogate modeling. In surrogate modeling, the uncertainty arises from not knowing the output of the simulation code, except at a finite set of training points. Apley et al.[24] referred to this type of uncertainty as "interpolation uncertainty". In this paper, we use the term "prediction uncertainty", because we believe that surrogate modeling is one type of predictive models. Kennedy and O'Hagan[25] developed a Bayesian approach to calibrate a computer code by using observations from the real process, and subsequent prediction and uncertainty analysis of the process. Neufeld et al.[26] assessed the uncertainty introduced by a surrogate model in the conceptual design of the wing box of a generic light jet, by applying Reliability Based Design Optimization (RBDO) to obtain a feasible solution. Picheny[2] showed that uncertainty can be compensated by adding bias to the surrogate models in order to increase safety, using constant or pointwise margins.

Surrogate-based optimization under uncertainty has been conducted in the literature.[27–31] Uncertainty estimates are used in adaptive sampling and optimization methods to select the next sampling point(s). The Efficient Global Optimization (EGO) approach[28] and the Sequential Kriging Optimization (SKO) algorithm[32] use the Kriging uncertainty to seek the point of maximum expected improvement as the next infill point. Viana and Haftka[29] proposed the importation of uncertainty estimates from one surrogate to another.

A Support Vector Regression (SVR) with an uncertainty model was developed by combining the prediction from SVR and the standard error from Kriging. Xiong et al.[30] developed cheap surrogate models to integrate information from both low-fidelity and high-fidelity models based on the Bayesian-Gaussian process modeling. The interpolation uncertainty of the surrogate model due to the lack of sufficient high-fidelity simulations is quantified in the Bayesian-Gaussian process modeling.

C. Research Objectives

The existing surrogate-based uncertainty modeling methods are model-dependent. A generalized methodology that can be applied to a majority of surrogate models to characterize the surrogate-based uncertainty will be more helpful. To this end, this paper develops an innovative approach to segregate the design domain based on levels of fidelity, and quantify the uncertainty in the surrogate model. This technique, Domain Segmentation based on Uncertainty in the Surrogate (DSUS) framework, estimates the relative errors of a surrogate by investigating the cross-validation errors. The uncertainty in the surrogate is represented by the distribution of the errors. Assuming that the designer/researcher does not have a definitive insight into the functional relationships that we are seeking to model, the measured (or simulated) sample data is all the information that we have at our disposal. A broad objective of evaluating the uncertainty in a surrogate is to characterize the uncertainty that is introduced during the surrogate modeling process itself. An uncertainty modeling technique like the one presented in this paper is expected to streamline the overall system-design efforts, by providing the user more confidence in the surrogates being used.

The errors in the surrogate are stochastic. Therefore, the accuracy of the response is uncertain. Key features of the DSUS framework are:

1. This method segregates the design domain into regions based on the level of errors (or level of fidelity). Pattern classification methods are used for this purpose.

2. This method can classify any point/design, for which the actual functional response is not known, into an error class, and quantify the uncertainty in its predicted function response.

3. This method is readily applicable to a majority of interpolative surrogate models.

It is important to note that, in this paper, the term "prediction uncertainty" denotes the distribution of errors of the surrogate model prediction. The remainder of the paper is organized as follows: Section II presents the details of the DSUS framework; Section III describes different standard problems and engineering problems to which the DSUS framework is applied; the numerical settings and results of case studies are shown and discussed in Section IV; and Section V provides concluding remarks.

II. Domain Segmentation based on Uncertainty in the Surrogate (DSUS)

In this section, we develop a framework to segregate the design domain of a surrogate into classes based on the prediction errors. The uncertainty in each class is defined by the distribution of cross-validation errors. The development and the application of the DSUS model are followed by a description of the components of the DSUS framework: (i) surrogate modeling, (ii) cross-validation, and (iii) pattern classification.

A. Development of the DSUS Model

For an engineering design model, it is important to balance the accuracy of model predictions with the computational complexity of the model used. Model prediction errors that lie within a specified range may be acceptable. Based on the current level of knowledge regarding the design problem, the designer may know what levels of errors are acceptable for particular design purposes. For instance, for a wind farm power generation model,[33] 2 percent estimation error might be desirable; 2-10 percent error is acceptable; and higher than 10 percent error is unlikely acceptable. If the whole design domain can be divided into physically meaningful classes based on the level of prediction errors, new designs can be classified into a given class. Figure 1 illustrates the concept of determining the predictive modeling errors in a two design variable system. In Fig. 1, the errors of the model are classified into three classes, and each color represents one class of errors. The boundaries between classes can be determined using pattern classification methods. The designer can estimate the confidence of a new design based on the region into which the design point is classified; these regions can correspond to "good", "acceptable", and "unacceptable" levels of accuracy.

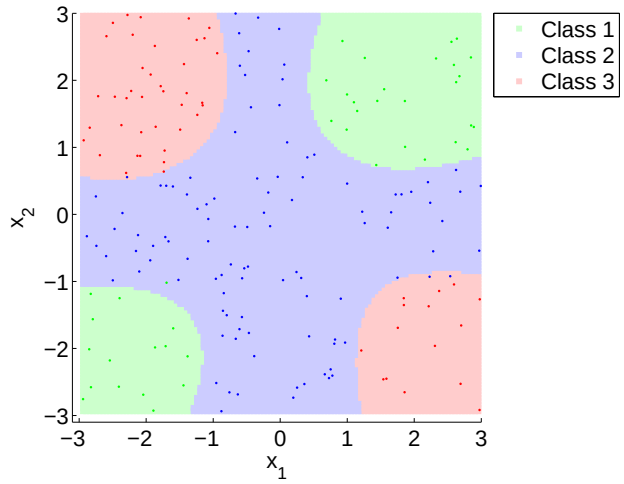


Figure 1. The illustration of the *prediction uncertainty* modeling (class 1: low error; class 2: medium error; class 3: high error)

The DSUS framework is implemented by observing the following sequence of four steps.

1. An interpolating surrogate modeling method is used to develop the predictive model: e.g. Kriging, RBF, or AHF.
2. Cross-validation errors are evaluated using the leave-one-out strategy; and we classify the training points into classes based on the cross-validation error at each training point. Within each class, the distribution of the cross-validation errors are represented using a Gaussian distribution.
3. A model is developed to determine the class boundaries in the input variable space using Support Vector Machines (SVM). The input variables of the surrogates are thus considered as input features in the classification process.
4. Stochastic models are developed (using Gaussian probability density functions) to represent the surrogate uncertainty in each error class.

It is important to note that in steps 1 and 2, approximating surrogates or regression models (e.g. PRSM) can also be used. However, in that case, a direct error estimation at each training point may be used instead of cross-validation errors. The development of the DSUS framework is illustrated in Fig. 2. In the following sections, we discuss the details of the DSUS framework.

B. Applications of the DSUS Model

The DSUS framework is useful for a variety of applications, such as optimization, system analysis (involving unknown functional relationships), and surrogate modeling improvement. In surrogate based optimization, optimal solutions in regions with smaller errors are more reliable than solutions in regions with larger errors. If optimal solutions are in a region with large errors, the user may add more training points in that region to improve the local surrogate accuracy. In addition, the DSUS framework can be used to quantify the uncertainty in the optimal solutions based on their locations in the design space. For instance, in surrogate based wind farm layout optimization,[34] power generation is represented as a function of turbine locations. The uncertainty in the power generation can be estimated based on the corresponding candidate farm layout design.

In surrogate-based system analysis, the knowledge of the errors and uncertainties in the surrogate (determined by DSUS) is helpful for the user/designer. For example, in the Response Surface-based Wind Farm Cost (RS-WFC) model, DSUS can quantify the the errors and uncertainties in the predicted wind farm cost. Using this information, the farm designer/analyst can estimate the uncertainty in the payback period and the associated risk of the wind farm project.

The design-domain-based uncertainty information provided by DSUS can be used to implement adaptive sampling strategies during surrogate development.

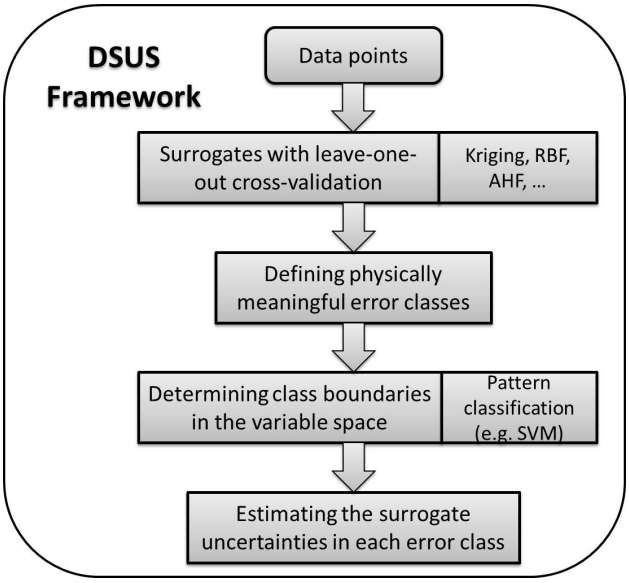


Figure 2. The framework of the DSUS methodology

C. Surrogate Modeling

The DSUS framework can be applied in conjunction with a majority of standard surrogate modeling methods. Table 1 provides a list of standard sampling techniques, surrogate modeling methods, and function-coefficient estimation methods. This list is an extended version of the one reported by Simpson et al.[35]

Table 1. Techniques for response surface

Sampling/Design of Experiments	Surrogate Modeling	Coefficient Estimation
(Fractional) factorial	Polynomial (linear, quadratic)	Least Squares Regression
Central composite	Splines (linear, cubic)	Best Weighted Least Squares Regression
Latin Hypercube	Kriging	Best Linear Predictor
Hammersley sequence	Radial Basis Functions (RBF)	Log-likelihood
Uniform designs	Extended RBF	Multipoint approximation
Sobol sequence	Support Vector Regression (SVR)	Adaptive response surface
Random selection	Neural Network (NN)	Back propagation
Box-Behnken	Hybrid models	Entropy
Plackett-Burman		Linear Unbiased Predictor
Orthogonal arrays		

D. Cross-Validation

Cross-validation errors are used in this paper as a measure of the accuracy of the surrogate. Cross-validation is a technique that is used to analyze and improve the accuracy of a surrogate model. Cross-validation error is the error estimated at a data point, when the response surface is fitted to all the data points except that point (also called the leave-one-out strategy). A vector of cross-validation errors, $\tilde{e}$, can be obtained, when the response surfaces are fitted to all the other points. This vector is known as the prediction sum of squares (the PRESS vector).

In the case of problems where the surrogate modeling process has a significant time expense, the leave-one-out strategy can be computationally expensive for a large number of training points. This issue can be overcome by using the q-fold strategy. Q-fold strategy involves (i) splitting the data randomly into q (approximately) equal subsets, (ii) removing each of these subsets in turn, and (iii) fitting the model to the remaining $q-1$ subsets. A loss function L can be computed to measure the error between the predictor and

the points in the subset that we set aside at each iteration; the contributions to L are then summed up over the q iterations.

In order to obtain the error at each training point, the leave-one-out strategy is adopted in the DSUS framework. The Relative Accuracy Error (RAE) is used to classify the training points into classes. The RAE is evaluated at each training point as

$$RAE(x^k) = \frac{|\tilde{f}_c(x^k) - f(x^k)|}{f(x^k)} \tag{1}$$

where $f(x^k)$ represents the actual function value at the training point x^k, the term $\tilde{f}_c(x^k)$ is the corresponding function value at x^k, estimated by the surrogate. That is developed using all training points except x^k, using the leave-one-out cross-validation strategy. According to the RAE values, we can manually classify the training points into error classes, and define the lower and upper limits of each class. The definition of the error levels (error ranges) depends on how the user intends to use the domain-based surrogate uncertainty information, e.g., use it for increasing the confidence of a particular system analysis.

E. Pattern Classification

The classes generated in the previous step are used to determine the classification boundaries. A wide variety of pattern classification methods are available in the literature,[11] such as (i) Linear discriminant analysis (LDA); (ii) Principal Components Analysis (PCA); (iii) Kernel estimation and K-nearest-neighbor algorithms; (iv) Perceptrons; (v) Neural Network; and (vi) Support Vector Machine (SVM). In this paper, the uncertainty classification in surrogate modeling is a multiclass classification problem. Support Vector Machine (SVM), which has been reported to be a competitive approach for multiclass classification problem,[36] is adopted in this paper.

1. Support Vector Machine (SVM)

Support Vector Machine (SVM) is a popular machine learning technique that has been used for classification, regression, and other learning tasks. Given a training set of instance-label pairs $(x_i, y_i),\ i = 1, \cdots, m$ where $x_i \in R^n$ and $y \in \{1, -1\}^m$, the determination of the support vectors requires the solution of the following optimization problem:

$$\begin{aligned} \min_{w,b,\xi} \quad & \frac{1}{2} w^T w + C \sum_{i=1}^{m} \xi_i \\ \text{subject to} \quad & y_i \left(w^T \phi(x_i) + b \right) \geq 1 - \xi_i \\ & \xi_i \geq 0 \end{aligned} \tag{2}$$

Here, training vectors x_i are mapped onto a higher (maybe infinite) dimensional space by the function ϕ. SVM finds a hyperplane with the maximum margin in this higher dimensional space. The vector w denotes the normal vector to the hyperplane; and the parameter $\frac{b}{\|w\|}$ determines the offset of the hyperplane from the origin along the normal vector w. The parameter $C > 0$ is the penalty parameter in the error term. The generic term ξ is a slack variable, which measures the degree of misclassification of the datum x_i. The function, $K(x_i, x_j) \equiv \phi(x_i)^T \phi(x_j)$ is called the kernel function. Four kernels that are popularly used are:

1. Linear: $K(x_i, x_j) = x_i^T x_j$
2. Polynomial: $K(x_i, x_j) = \left(\gamma x_i^T x_j + r \right)^d,\ \gamma > 0$
3. Radial basis function: $K(x_i, x_j) = \exp\left(-\gamma \|x_i - x_j\|^2 \right),\ \gamma > 0$
4. Sigmoid: $K(x_i, x_j) = tanh\left(\gamma x_i^T x_j + r \right)$

where γ, r, and d are the kernel parameters.

The support vector machine is a powerful tool for binary classification, which is capable of generating fast classifier functions following a training period. There exist several advanced SVM approaches to solve classification problems that involves three or more classes:[37]

1. One-against-all classification, in which one binary SVM is used to separate members of each class from the members of other classes.

2. One-against-one classification, which constructs $k(k-1)/2$ classifiers where each classifier is trained on data from two classes (k is the number of classes).

3. Directed acyclic graph SVM (DAGSVM), in which the training phase is the same as the one-against-one method.

Hsu and Lin[37] provided a detailed comparison of the above three approaches and concluded that "one-against-one" classification is a competitive approach; this approach is adopted in this paper. For training data from the i^{th} and the j^{th} classes, the following two-class classification problem is solved:[38]

$$\begin{aligned} \min_{w^{ij},b^{ij},\xi^{ij}} \quad & \frac{1}{2}\left(w^{ij}\right)^T w + C\sum_t \left(\xi^{ij}\right)_t \\ \text{subject to} \quad & \\ & \left(w^{ij}\right)^T \phi(x_t) + b^{ij} \geq 1 - \xi_t^{ij}, \quad \text{if } x_t \text{ in the } i^{th} \text{ class} \\ & \left(w^{ij}\right)^T \phi(x_t) + b^{ij} \leq -1 + \xi_t^{ij}, \quad \text{if } x_t \text{ in the } j^{th} \text{ class} \\ & \xi_t^{ij} \geq 0 \end{aligned} \tag{3}$$

A voting strategy is used in classification. Each binary classification is considered to be a voting process where votes can be cast for all data points x; and in the end a point is designated to be in the class with the maximum number of votes.[38] In this paper, we have used an efficient SVM package, LIBSVM (A Library for Support Vector Machines), developed by Chang and Lin.[38]

III. Case Studies

In this section, the DSUS framework is illustrated using two different surrogate modeling methods: (i) the Kriging method, and (ii) a newly developed hybrid surrogate, the Adaptive Hybrid Functions (AHF).[34,39] We apply the DSUS framework to a series of standard problems, including (i) 1-variable function,[40] and (ii) 2-variable Dixon & Price function. The prediction uncertainties in (i) the *Response Surface-Based Wind Farm Cost (RS-WFC) model*, and (ii) the *commonality representation in product family design* are characterized for engineering systems design.

A. Surrogate Modeling Methods

1. Kriging

Kriging[5,6] is an approach to approximate irregular data. The kriging approximation function consists of two components: (*i*) a global trend function, and (*ii*) a functional departure from the trend function. The trend function is generally a polynomial (e.g., constant, linear, or quadratic). The general form of the kriging surrogate model is given by:

$$\tilde{f}(x) = G(x) + Z(x) \tag{4}$$

where $\tilde{f}(x)$ is the unknown function of interest, $G(x)$ *is the user-defined approximation (usually polynomial) function*, and $Z(x)$ is the realization of a stochastic process with a zero mean and a nonzero covariance.

2. Adaptive Hybrid Functions (AHF)

The AHF methodology, recently developed by Zhang et al.,[39,41] formulates a reliable trust region, and adaptively combines characteristically different surrogate models. The weight of each contributing surrogate model is represented as a function of the input domain, based on a local *measure of accuracy* of that surrogate model. Such an approach exploits the advantages of each component surrogate, thereby capturing both the global and the local trend of complex functional relationships. In this paper, the AHF combines three component surrogate models by characterizing and evaluating the local *measure of accuracy* of each model. The three models are (i) RBF, (ii) E-RBF, and (iii) Kriging. The AHF methodology introduces a three-step approach:

1. Determination of a trust region: numerical bounds of the estimated parameter (output) as functions of the independent parameters (input vector).
2. Definition of a local *measure of accuracy* (using kernel functions) of the estimated function value, and representation of the corresponding distribution parameters as functions of the input vector.
3. Weighted summation of characteristically different surrogate models (component surrogates) based on the local *measure of accuracy* (defined in the previous step).

The development of the AHF surrogate model is illustrated in Fig. 3.

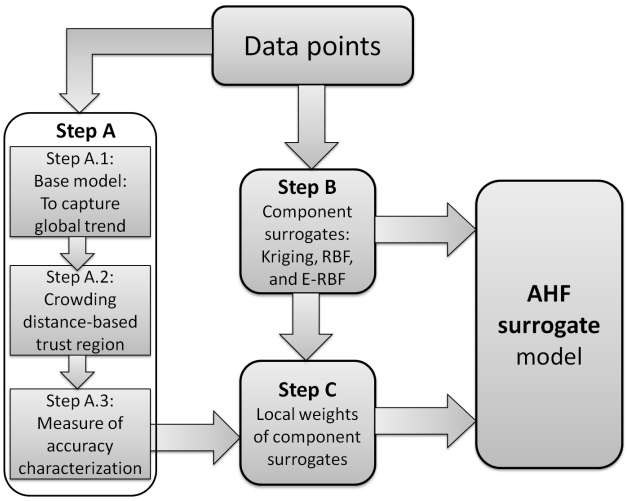


Figure 3. The framework of the AHF surrogate model

The AHF is a weighted summation of function values estimated by the component surrogates, as given by

$$\tilde{f}_{AHF} = \sum_{i=1}^{n_s} w_i(x)\tilde{f}_i(x) \tag{5}$$

where n_s is the number of component surrogates in the AHF, and $\tilde{f}_i(x)$ represents the value estimated by the i^{th} component surrogate. The weights, w_i, are expressed in terms of the estimated *measure of accuracy*, which is given by

$$w_i(x) = \frac{P_i(x)}{\sum_{i=1}^{n_s} P_i(x)} \tag{6}$$

where $P_i(x)$ is the *measure of accuracy* of the i^{th} surrogate for point x. The detailed formulation of the AHF method can be found in the paper by Zhang et al.[39]

B. Standard Test Problems

The performance of the new DSUS framework is illustrated using the following analytical test problems: (i) 1-variable function,[40] and (ii) 2-variable Dixon & Price function. Surrogate models (Kriging and AHF) are developed for each problem; and are evaluated using the DSUS framework. These problems are expressed as follows.

Test Function 1: 1-Variable Function

$$\begin{aligned} &f(x) = (6x_1 - 2)^2 \sin\left[2\,(6x_1 - 2)\right] \\ &where \quad x_1 \in [0 \;\; 1] \end{aligned} \tag{7}$$

Test Function 2: 2-Variable Dixon & Price Function

$$\begin{aligned} &f(x) = (x_1 - 1)^2 + 2\left(2x_2^2 - x_1\right)^2 \\ &where \quad x_i \in [-10 \;\; 10] \end{aligned} \tag{8}$$

C. Onshore Wind Farm Cost Model

A Response Surface-Based Wind Farm Cost (RS-WFC) model was developed by Zhang et al.[42] The RS-WFC model for onshore wind farms in the U.S. was implemented using the Extended Radial Basis Functions (E-RBF). The RS-WFC model estimates *the total annual cost of a wind farm per kilowatt installed*.

The input parameters to the RS-WFC total annual cost model are (*i*) the number, and (*ii*) the rated power of each wind turbine installed in the wind farm; and the output is the total annual cost of the wind farm. Data points collected for the state of North Dakota are used to develop the cost model.

D. Commonality Representation in Product Family Design

A product family is a group of related products that are derived from a common product platform to satisfy a variety of market niches. The sharing of a common platform by different products is expected to result in: (i) reduced overhead, (ii) lower per-product cost, and (iii) increased profit. The recently developed Comprehensive Product Platform Planning (CP^3) framework[43] formulated a generalized mathematical model to represent the complex platform planning process.

The CP^3 model formulates a generic equality constraint (the *commonality constraint*) to represent the variable-based platform formation. The presence of a combination of integer variables (specifically binary variables) and continuous variables can be attributed to the combinatorial process of platform identification. The authors[44] developed a methodology to reduce the high dimensional binary integer problem to a more tractable integer problem, where the commonality matrix is represented by a set of integer variables.

The detailed formulation of the *commonality matrix* can be found in the paper by Chowdhury et al.[43] Khajavirad and Michalek[45] illustrated that the commonality index introduced by Martin and Ishii[46] is an effective metric to meaure the tooling cost savings owing to commonality. This commonality index is essentially based on the ratio of "the number of unique parts" to "the total number of parts" in the product family. In this paper, we develop a surrogate model to represent the *commonality index* as a function of the integer variables.

E. Sampling Strategies

In the case of problems where the user has control over the design of experiments, the choice of an appropriate sampling technique is generally considered crucial. Two efficient sampling methods are adopted in this paper: (i) Latin Hypercube Sampling, and (ii) Sobol's Quasirandom Sequence Generator.

IV. Results and Discussion

The results from the application of the DSUS methodology are discussed in this section. The parameter selections and numerical settings of the DSUS framework are also summarized. In addition, we define the measure of *prediction uncertainty* in the surrogate. The SVM kernels and parameters are determined for the studied cases, followed by the discussion of the uncertainty prediction results.

A. Selection of Parameters

The AHF surrogate is an ensemble of RBF, E-RBF and Kriging methods. Detailed formulations of RBF and E-RBF can be found in the paper by Zhang et al.[39] The parameter values are the same as specified in that paper.

For the Kriging method used in this paper, we have used an efficient MATLAB implementation, DACE (design and analysis of computer experiments), developed by Lophaven et al.[47] The bounds on the correlation parameters in the nonlinear optimization, θ_l and θ_u, are selected as 0.1 and 20. Under the kriging approach, the order of the global polynomial trend function was specified to be zero. The parameters of the SVM depend on the kernel used. The selection of the parameters is provided in the following section.

B. Numerical Settings

The numerical settings for each problem are summarized in Table 2, which includes (i) the number of input variables, (ii) the number of training points, (iii) the number of test points, and (iv) the SVM kernel. The sampling points for the first two analytical problems (1-variable function, and 2-variable Dixon & Price

function) are generated using the Latin hypercube sampling method. The data used to develop and test the RS-WFC model is obtained from the Energy Efficiency and Renewable Energy Program at the U.S. Department of Energy.[48] For the *Commonality Representation in Product Family Design* problem, two different sampling methods are used to generate training and test points. The training points are generated using Sobol's quasirandom sequence generator; and test points are generated using the Latin hypercube sampling method. This sampling strategy differentiates the training points and the test points. We select the kernel function through numerical experiments. The linear kernel is selected for the 1-variable function; and the radial basis function kernel is adopted for the other problems.

Table 2. Numerical setup for test problems

Problem	No. of variables	No. of training points	No. of test points	SVM kernel
1-variable function	1	15	20	linear
Dixon & Price function	2	60	20	radial basis function
Wind farm cost	2	60	20	radial basis function
Commonality (2 products)	7	105	35	radial basis function
Commonality (3 products)	7	105	21	radial basis function

We classify the training points into different physically meaningful classes based on the RAE values. The user-defined lower and upper limits of each class are listed in Table 3. It can be seen from Table 3 that (i) two classes are selected for the 1-variable problem; and (ii) three classes are defined for the other problems. However in real life engineering design, the user is expected to specify the classes based on the physical implication of the errors (e.g., good, acceptable, unacceptable).

Table 3. The uncertainty scale in each class

Problem	Class 1	Class 2	Class 3
1-variable function	RAE<10%	RAE $\geq$ 10%	-
Dixon & Price function	RAE<25%	25% $\leq$ RAE<50%	RAE $\geq$ 50%
Wind farm cost	RAE<0.5%	0.5% $\leq$ RAE<1%	RAE $\geq$ 1%
Commonality (2 products)	RAE<0.5%	0.5% $\leq$ RAE<1%	RAE $\geq$ 1%
Commonality (3 products)	RAE<5%	5% $\leq$ RAE<10%	RAE $\geq$ 10%

C. Representation of Prediction Uncertainty

To represent the uncertainty in the prediction accuracy of the surrogate, Gaussian distribution is adopted. Tables 4 and 5 show the uncertainty in each class, in terms of the mean and standard deviation values of the prediction errors. Classes 1, 2 and 3 represent uncertainty levels of low errors, medium errors and high errors, respectively. For any new point (design) candidate, the DSUS framework can classify that point into one of these error classes. In addition, the *prediction uncertainty* of the new design is given by the mean (μ) and the standard deviation (σ) of errors in that class.

The prediction uncertainties in the surrogates for all the test problems are illustrated in Figs. 4-8. For the 1-variable problem, the Relative Accuracy Errors (RAEs) are classified into two classes that represent low and high errors, respectively. For the other problems, the RAEs are classified into three classes to respectively represent low, medium and high errors of the surrogate. In real life engineering design, the user might use "good", "acceptable", and "unacceptable" levels to characterize the system design.

It is observed that the prediction uncertainties vary significantly from problem to problem. For example, in the case of the Dixon & Price function (Fig. 5), the difference in mean values between classes 1 and 2 is significantly smaller than that between classes 2 and 3. With the AHF surrogate, the value of ($\mu_2^{Dixon} - \mu_1^{Dixon}$) is 0.1646, while the value of ($\mu_3^{Dixon} - \mu_2^{Dixon}$) is 2.7573. With the Kriging surrogate, the value of ($\mu_2^{Dixon} - \mu_1^{Dixon}$) is 0.1862, while the value of ($\mu_3^{Dixon} - \mu_2^{Dixon}$) is 2.1215. However, for the wind farm cost model (Fig. 6(a)), the three mean values are more uniformly distributed. The mean value of each

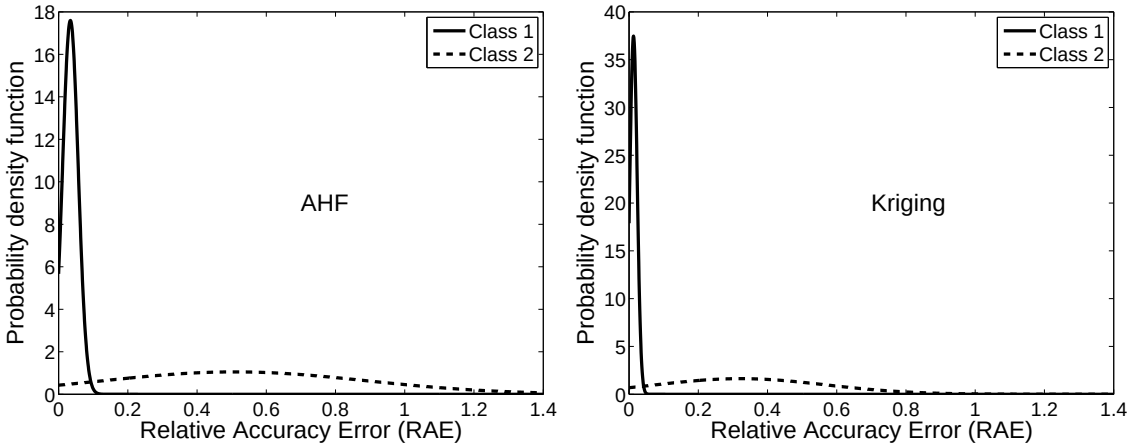
class is estimated to be 0.0018, 0.0066 and 0.0216, when the AHF method is used. It is also observed that, the standard deviation of class 3 for all test problems is generally larger than that of classes 1 and 2. Overall, it is interesting to note that (from Tables 4 and 5), the mean error in the class 3 level is an order of magnitude higher than those in classes 1 and 2. **This observation shows that there is significant scope to improve the surrogate accuracies in class 3 regions. This uniquely helpful design-space information provided by DSUS pushes the paradigm in advanced surrogate modeling and surrogate-based optimization.**

Table 4. Uncertainty scale (mean and standard deviation) of each class with AHF surrogate

Problem	Class 1		Class 2		Class 3	
	μ_1	σ_1	μ_2	σ_2	μ_3	σ_3
1-variable function	0.0341	0.0227	0.5092	0.3791	-	-
Dixon & Price function	0.0409	0.0293	0.2055	0.0838	2.9628	2.5012
Wind farm cost	0.0018	0.0011	0.0066	0.0013	0.0216	0.0102
Commonality (2 products)	0.0027	0.0012	0.0063	0.0011	0.0506	0.0536
Commonality (3 products)	0.0242	0.0124	0.0740	0.0149	0.1590	0.0906

Table 5. Uncertainty scale (mean and standard deviation) of each class with Kriging surrogate

Problem	Class 1		Class 2		Class 3	
	μ_1	σ_1	μ_2	σ_2	μ_3	σ_3
1-variable function	0.0129	0.0106	0.3224	0.2445	-	-
Dixon & Price function	0.0106	0.0200	0.1968	0.0863	2.3183	2.3530
Wind farm cost	0.0018	0.0015	0.0069	0.0015	0.0179	0.0080
Commonality (2 products)	0.0024	0.0011	0.0061	0.0009	0.0829	0.0204
Commonality (3 products)	0.0257	0.0145	0.0708	0.0162	0.1861	0.1126

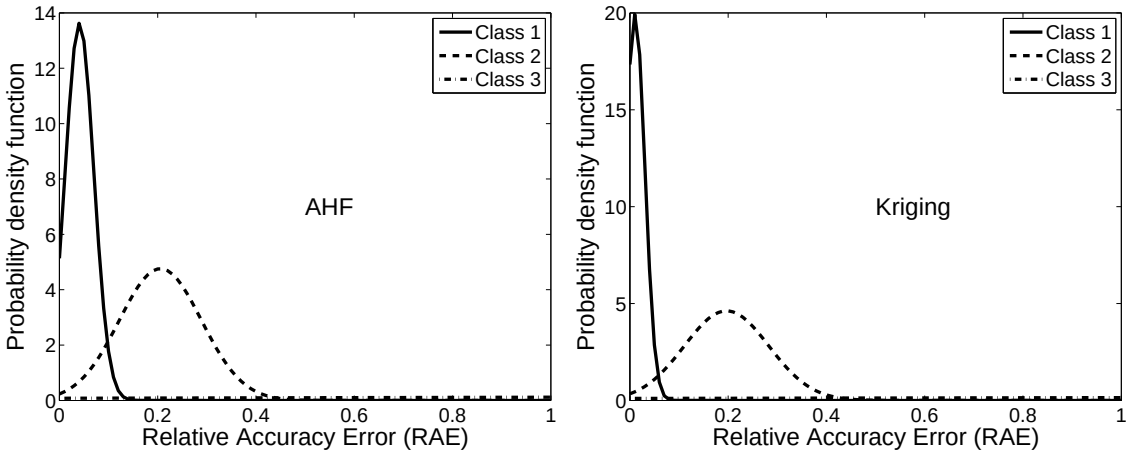


(a) AHF (b) Kriging

Figure 4. Distributions of errors (uncertainy) in each class for the 1-variable function

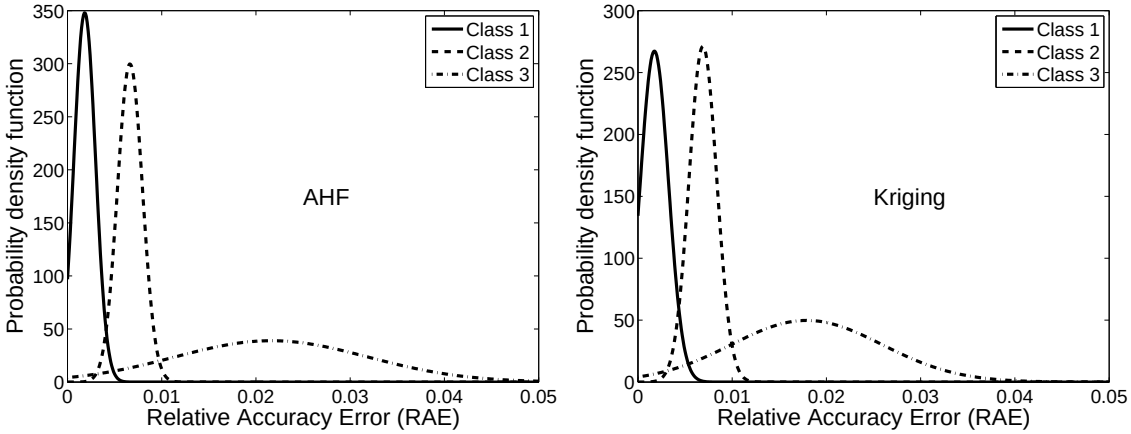
D. Determining the SVM Parameters

There are (i) one parameter for the SVM linear kernel, C; and (ii) two parameters for the SVM radial basis function kernel: C and γ. Cross-validation technique[38] is used to achieving high training accuracy. A grid-search technique[38] is performed on C and γ using cross-validation. Various pairs of (C, γ) values are



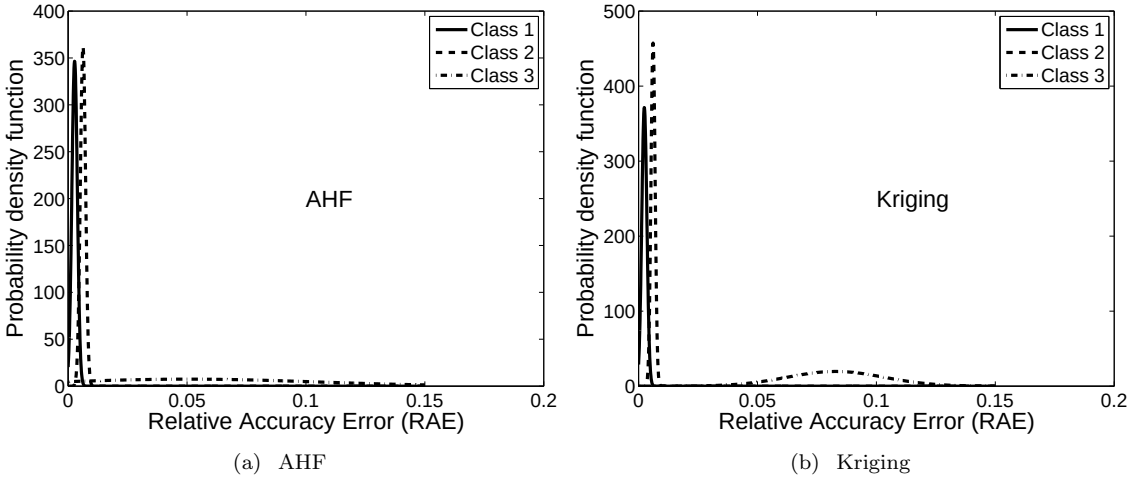
(a) AHF (b) Kriging

Figure 5. Distributions of errors (uncertainy) in each class for the Dixon & Price function



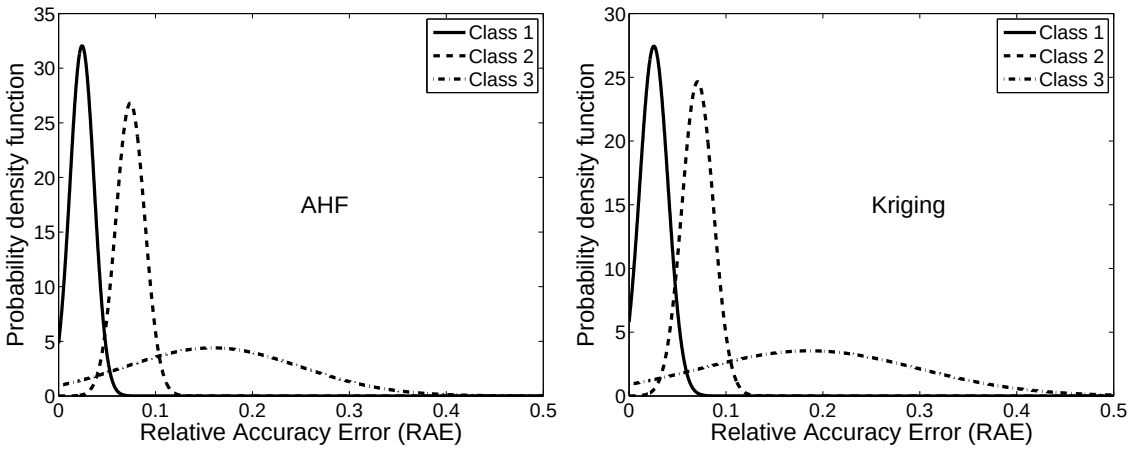
(a) AHF (b) Kriging

Figure 6. Distributions of errors (uncertainy) in each class for the wind farm cost model



(a) AHF (b) Kriging

Figure 7. Distributions of errors (uncertainy) in each class for the commonality matrix (2 products)



(a) AHF (b) Kriging

Figure 8. Distributions of errors (uncertainy) in each class for the commonality matrix (3 products)

tested and the one with the best cross-validation accuracy is selected. Figure 9 illustrates the cross-validation result with the grid-search on C and γ for the wind farm cost model. In Fig. 9, the horizontal and vertical axes denotes the $\log_2(C)$ and $\log_2(\gamma)$ values, respectively. It is observed that the cross-validation accuracy reaches 95% with the values $C = 0.83$ and $\gamma = 0.0078$. In addition, Table 6 gives the best C and γ values for all problems. It is important to note that the cross-validation used to determine the SVM parameter values does not have any connection with the cross-validation error of the surrogates.

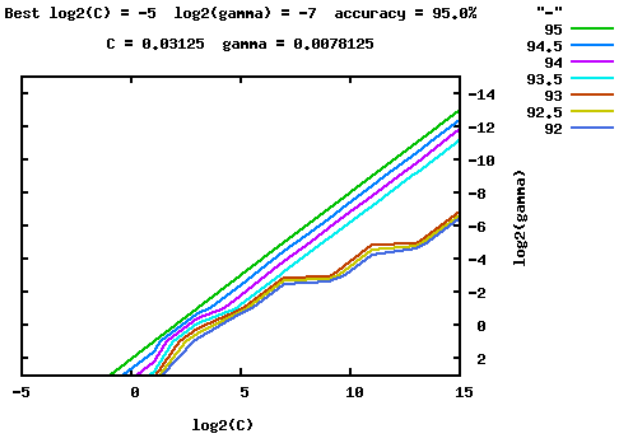


Figure 9. Cross-validation accuracy with the grid-search on $C = 2^{-5}, 2^{-3}, ..., 2^{15}$ and $\gamma = 2^{-15}, 2^{-13}, ..., 2^{3}$

E. Uncertainty Prediction Results

Table 6 shows the prediction accuracy of each problem. It can be seen that the DSUS framework performs fairly well for all the problems. The classification accuracy of the DSUS prediction is more than 90% for most test problems. The DSUS framework characterized the uncertainty levels with 100% accuracies in three cases: (i) Dixon & Price function with Kriging surrogate; (ii) wind farm cost with AHF surrogate; and (iii) commonality (2 products) index approximation with Kriging surrogate.

The number of training points required to obtain an acceptable surrogate accuracy may be significantly different from that required for developing classification. We should increase the number of training points if it is not enough for classification. Future research should investigate the training points balance between surrogate modeling and pattern classification, to promote acceptable accuracy both in the surrogate modeling stage and the classification stage, while maintaining acceptable system evaluation expense.

Table 6. Prediction accuracy of each problem

Problem	AHF		Kriging	
	Parameters	Accuracy	Parameters	Accuracy
1-variable function	C=1	90% (18/20)	C=1	95% (19/20)
Dixon & Price function	C=0.0313, γ=0.0078	75% (15/20)	C=0.0313, γ=0.0078	100% (20/20)
Wind farm cost	C=1, γ=0.8	100% (20/20)	C=1, γ=0.8	95% (19/20)
Commonality (2 products)	C=0.0313, γ=0.0078	94% (33/35)	C=0.0313, γ=0.0078	100% (35/35)
Commonality (3 products)	C=2, γ=0.12	95% (20/21)	C=2, γ=0.06	86% (18/21)

V. Conclusion

This paper develops a method to characterize the uncertainty attributable to surrogate models, which we call the Domain Segmentation based on Uncertainty in the Surrogate (DSUS) framework. In this framework, the whole design domain can be divided into physically meaningful classes. The uncertainty in each class is represented by Gaussian distribution (in terms of the mean and standard deviation values). Support Vector Machine (SVM) is implemented to model the boundaries between error classes in the design variable space, and classify any new point/design into the appropriate class. The system design can be evaluated by the designer based on the error and the uncertainty information.

The DSUS framework was applied to a series of standard problems and engineering problems, in conjunction with two surrogate modeling methods. The results show that the DSUS framework can successfully characterize and quantify the uncertainty (predictive errors) in surrogates.

Future research should investigate: (i) the training points balance between surrogate modeling and pattern classification; (ii) the physical implications of error class definitions; and (iii) the selection of surrogate modeling and pattern classification tools for the DSUS framework.

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