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DUAL KRIGING: AN EXPLORATORY USE IN ECONOMIC METAMODELING

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Sensitivity analysis of capital investments can be effectively carried out by employing a metamodel approach and experimental designs. Although polynomial regression metamodels are popular and straightforward, they do not consider spatial relationships among the data. Dual kriging is an estimation technique that allows the incorporation of spatial correlation into the interpolation or estimation process and has been used primarily in geophysical statistical analysis. This article investigates the dual kriging approach as an alternative technique to polynomial regression and artificial neural networks for metamodel analysis of capital investments. It is observed that dual kriging shows potential in performing sensitivity analysis as its accuracy is as good as, or better than, other techniques, and, while model building and interpretation is more complicated than that of polynomial regression, it is significantly more straightforward than that of neural networks. Furthermore, this is the first known work of using kriging in the field of engineering economics; there may be other useful applications such as in cost estimation.

INTRODUCTION

Sensitivity analysis is crucial in deterministic capital investment evaluation since the estimates of input factors such as the interest rate and amount and

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timing of cash flows used in cash flow analysis are not known with certainty. Not only does sensitivity analysis allow the decision maker to determine the relative effect of changes in the input estimates on the indicated decision, but it can also be used to identify the input factors that are most influential to the investment decision. The aptness of the final decision depends on correctness of the estimates of these significant input factors. In addition, monitoring these factors during implementation of the investment will assist the decision maker in taking the right action in a timely manner. The drawback of traditional sensitivity analysis, such as one factor at a time and scenario generation, is that interactions among factors are not considered and it is difficult to derive useful information when three or more factors are considered.

In order to overcome the problem in traditional sensitivity analysis, Sartori and Smith [18] proposed a polynomial regression metamodel approach. A metamodel is an approximated model of a descriptive model and is constructed from input-output data generally gathered by design of experiments. The concept of a metamodel as defined by Kleijenen [11] can be explicitly described in terms of the capital investment problem as the following. Let X_j denote the value of a factor j influencing the economic measure, Y, of the investment under study where $\{X_j \mid j = 1, 2, \ldots, n\}$. The relationship between the input factors X_j and the output or economic measure Y can be represented as

$$Y = f_1(X_1, X_2, \ldots, X_n)$$

This relationship can be generalized to multiple outputs by representing Y as a response vector. A metamodel is usually developed separately for each output Y and only a single output metamodel is considered in this article. A metamodel is an approximation of the investment under study and may include a subset of the input factors $\{X_j \mid j = 1, 2, \ldots, m\}$, where $m \leq n$:

$$Y' = f_2(X_1, X_2, \ldots, X_m) + \varepsilon_m$$

The error term, ε_m, is composed of the effects of any excluded or unidentified input factors and the error of fitting the metamodel to the real input-output relationship of the investment.

The regression metamodel is the most popular metamodeling technique used in practice. A polynomial regression metamodel for m input factors, $(x_1, x_2, \ldots, x_m) = \mathbf{x}$, can be expressed as:

$$Y = \sum_{k=1}^{p} \beta_k Z_k(\mathbf{x}) + \varepsilon_p$$

where there are p power functions $Z_k(\mathbf{x})$; e.g., linear, quadratic, cross terms, etc. β_k are the regression coefficients, which are calculated from the observed pairs of data points via least-squares estimation. ε_p is a random error term composed of the error of any excluded or unidentified input factors and the error of fitting the polynomial. This latter component is assumed to distributed according to $N(0, \sigma)$.

Sartori and Smith [18] constructed a second-order polynomial regression metamodel from the input factor combinations and the corresponding measure of economic value (NPV) that were called for by an experimental design. The validated metamodel was used to carry out sensitivity analysis. It has been shown that this approach was more insightful than traditional sensitivity analysis. The combination of regression metamodeling and experimental design theory was also used in performing sensitivity analysis of capital investment evaluation by Van Groenendaal [24, 25]. The developed regression metamodels could be used to gain useful information contained in the experimental data while the use of experimental design theory allowed the estimation of interactions between factors, which was not possible in traditional sensitivity analysis. Chaveesuk and Smith [3] applied artificial neural networks (ANN) to economic metamodeling, which showed potential in certain situations.

Although a polynomial regression metamodel is straightforward to implement, it has restricting assumptions of uncorrelated error components and absence of multicollinearity. However, correlation might exist among the sample data observed from physical or social phenomena. Data close together, in time or in space, are likely to be correlated and should be modeled as such [4]. Kriging is an estimation technique that allows the incorporation of spatial correlation into the interpolation or estimation process. Accordingly, it might be an appropriate alternative metamodeling technique to represent the input-output relationship from cash flow analysis. Barton [1], in his review of metamodeling, includes spatial correlation models or kriging models among the most promising metamodeling techniques. Since its introduction into the simulation community by Sacks et al. [17], the use of classical kriging models for deterministic simulation metamodels has been limited [2, 19] due to the complexity of the method and intense computational effort. However, the dual formulation of kriging (dual kriging) was developed to alleviate the computational problems. Dual kriging has been adopted in diverse applications including stress analysis [15], a contouring program [21], shrinkage analysis [13], modeling of failure behavior for composite materials [6–8, 23], modeling and construction of material laws [20, 22], a surrogate for fitness landscape in evolutionary optimization [16], and modeling human radiographic images [5].

This article aims to examine the potential use of dual kriging in performing sensitivity analysis of a capital investment evaluation. The theory of classical kriging and its dual formulation (dual kriging) is reviewed. A methodology for incorporating a metamodel approach into the sensitivity analysis of capital investment evaluation is then described. The performance of dual kriging is investigated and compared to that of polynomial regression and artificial neural network metamodels through two case studies.

The following notation is used throughout the article:

$U(X)$	A random function at a specified point X
$U(X_i)$	A set of measurements or computed samples taken at point X_i
$u^*(X)$	The estimator of $U(X)$
λ_i	A set of weights
$E[U(X)]$	The expected value of $U(X)$
$Var[U(X)]$	The variance of $U(X)$
$a(X)$	The drift function
$b(X)$	A stationary fluctuation
$p_l(X)$	The basis function of the drift function
σ_R^2	The variance of the estimation error
$Cov[U(X), u^*(X)]$	The covariance between $U(X)$ and $u^*(X)$
u_l	The Lagrange multipliers
C_{ij}	The covariance between sample points X_i and X_j
C_i	The covariance between sample points X_i and X
$C(h)$	The covariance function
a_l and b_j	The coefficients of the dual kriging model

CLASSICAL KRIGING AND DUAL KRIGING

Kriging is an estimation technique proposed in 1951 by D.G. Krige, a mining engineer, for gold deposit evaluations. Similar to polynomial regression, the kriging technique is a BLUE, “Best Linear Unbiased Estimator” of a random function and is “best” in terms of aiming at minimizing the variance of estimation error among all linear estimators [15]. Geologists and environmental engineers have long used kriging to estimate the measurements or characteristics of hydraulic properties or contaminant concentrations in air, water, or soil in inaccessible or unobserved regions. More recently, its use was extended to the simulation community. Classical kriging (see Journel & Huijbregts [10] for a thorough treatment) is usually implemented as a local estimation method. That is, its procedure requires the solution of a new system of equations for each interpolated value. This is obviously untenable for metamodeling.

A global estimation kriging technique called “dual kriging” was developed in 1985 [21] where the kriging system is evaluated only once for the whole domain by simultaneously using the information provided by all data points. The development of classical kriging equations and derivation of dual kriging is presented in the following sections (based on Journel and Huijbregts [10], Porier and Tinawi [15], and Trochu [21]).

Theory of Classical Kriging

The purpose of kriging is to estimate the value of a random function $U(X)$ at a specified point or location X, given a set of measurements or computed samples $U(X_i)$ taken at location X_i for $i = 1, 2, \ldots, N$. The original theory of kriging was formulated for dealing with one-, two-, or three-dimensional problems, i.e., when X represents the position vector $X = x$ or $X = (x, y)$ or $X = (x, y, z)$. However, it can be generalized to an L dimension problem; i.e., $X = (x^1, x^2, \ldots, x^L)$ as will be done later in this article.

The estimation of $U(X)$ can be obtained as a linear combination of the observed data point X_i where $i = 1, 2, \ldots, N$:

$$u^*(X) = \sum_{i=1}^{N} \lambda_i U(X_i) \tag{1}$$

As a BLUE, a set of weights λ_i must be determined in such as way that (1) the expected values of $U(X)$ and $u*(X)$ are identical; i.e., $E[U(X)] = E[u^*(X)]$, and (2) the variance of the estimation error $Var[U(X) - u^*(X)]$ is minimized.

In kriging, the random function $U(X)$ is comprised of the sum of two terms:

$$U(X) = a(X) + b(X) \tag{2}$$

where $a(X)$ is a drift function representing the average behavior of $U(X)$ or $a(X) = E[U(X)]$, and $b(X)$ is a stationary fluctuation with $E[b(X)] = 0$.

The kriging system can be derived to minimize the variance of the estimation error under the constraints of unbiased conditions as follows: From the unbiased condition, $E[U(X)] = E[u^*(X)]$, Equation (1) can be expressed as

$$E[U(X)] = \sum_{i=1}^{N} \lambda_i E[U(X_i)] \tag{3}$$

Since the drift function represents the expected value of $U(X)$, Equation (3) can be represented by

$$a(X) = \sum_{i=1}^{N} \lambda_i a(X_i) \tag{4}$$

Usually, the drift function is built up from M basis functions, $p_l(X), l = 1, 2, \ldots, M$ and the conditions of unbiased become

$$p_l(X) = \sum_{i=1}^{N} \lambda_i p_l(X_i), \quad l = 1, 2, \ldots, M \tag{5}$$

The variance of the estimation error is calculated as follows

$$\begin{aligned} Var[U(X) - u^*(X)] = \sigma_R^2 &= Var[U(X)] - 2Cov[U(X), u^*(X)] \\ &\quad + Var[u^*(X)] \end{aligned}$$

with $Var[U(X)] = \sigma_{U(X)}^2$

$$\begin{aligned} Cov[U(X), u^*(X)] &= Cov\left\{\left[\sum_{i=1}^{N} \lambda_i U(X_i)\right], U(X)\right\} \\ &= \sum_{i=1}^{N} \lambda_i Cov[U(X), U(X_i)] \\ Var[u^*(X)] &= Var\left[\sum_{i=1}^{N} \lambda_i U(X_i)\right] \\ &= \sum_{i=1}^{N}\sum_{j=1}^{N} \lambda_i \lambda_j Cov[U(X_i), U(X_j)] \end{aligned}$$

Combining these three terms, the variance of estimation error can be expressed as

$$\begin{aligned} \sigma_R^2 = \sigma_{U(X)}^2 &- 2\sum_{i=1}^{N} \lambda_i Cov[U(X), U(X_i)] \\ &+ \sum_{i=1}^{N}\sum_{j=1}^{N} \lambda_i \lambda_j Cov[U(X_i), U(X_j)] \end{aligned} \tag{6}$$

This error variance is minimized subject to M unbiased conditions in (5). The constrained minimization problem is converted to an unconstrained one by introducing M Lagrange multipliers, $\mu_l, l = 1, 2, \ldots, M$, associated with the constraints. The solution is then characterized by a linear system of $N + M$ equations in $N + M$ unknowns $\lambda_1, \ldots, \lambda_N$ and $\mu_1, \ldots, \mu_M$:

$$\sum_{j=1}^{N} \lambda_j Cov[U(X_i), U(X_j)] + \sum_{l=1}^{M} \mu_l p_l(X_i) = Cov[U(X), U(X_j)], \quad i=1,2,\ldots,N$$

$$\sum_{j=1}^{N} \lambda_j p_l(X_j) = p_l(X), \quad l = 1, 2, \ldots, M. \tag{7}$$

This system is called the "kriging system" and can be written in matrix form

$$\begin{bmatrix} C_{11} & \cdots & C_{1N} & p_1(X_1) & \cdots & p_M(X_1) \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ C_{N1} & \cdots & C_{NN} & p_1(X_N) & \cdots & p_M(X_N) \\ p_1(X_1) & \cdots & p_1(X_N) & 0 & \cdots & 0 \\ \vdots & \ddots & \vdots & \vdots & \ddots & \vdots \\ p_M(X_1) & \cdots & p_M(X_N) & 0 & \cdots & 0 \end{bmatrix} \cdot \begin{bmatrix} \lambda_1 \\ \vdots \\ \lambda_N \\ \mu_1 \\ \vdots \\ \mu_M \end{bmatrix} = \begin{bmatrix} C_1 \\ \vdots \\ C_N \\ p_1(X) \\ \vdots \\ p_M(X) \end{bmatrix} \tag{8}$$

where C_{ij} denotes the covariance between sample points X_i and X_j, or $Cov[U(X_i), U(X_j)]$, and C_i is the covariance between sample points X_i and a point X, or $Cov[U(X), U(X_i)]$, in which the value of $U(X)$ is to be estimated. Solving this system yields the optimal values of the λ_i, $i = 1, 2, \ldots, N$, at the point X.

Dual Formulation of Kriging

The kriging system of Equation (8) depends on the covariance between the sample point X_i and the point X. That is, the solution of system λ_i depends on point X. Therefore, a new kriging system would be needed for each estimated value. The dual formulation of kriging was developed to provide independent λ_i thereby eliminating this limitation. Dual kriging can be formulated from Equation (8) as follows. When the matrix in system

(8) is inverted, the following expression is obtained:

$$\begin{bmatrix} \lambda_1 \\ \vdots \\ \lambda_N \\ - \\ \mu_1 \\ \vdots \\ \mu_M \end{bmatrix} = \left[\begin{array}{c|c} Q & R \\ \hline R^T & S \end{array}\right] \cdot \begin{bmatrix} C_1 \\ \vdots \\ C_N \\ - \\ p_1(X) \\ \vdots \\ p_M(X) \end{bmatrix} \tag{9}$$

By substituting this solution into Equation (1), the estimated value $u^*(X)$ can be expressed as:

$$\begin{aligned} u^*(X) &= [U(X_1) \cdots U(X_N)] \cdot Q \cdot \begin{bmatrix} C_1 \\ \vdots \\ C_N \end{bmatrix} \\ &\quad + [U(X_1) \cdots U(X_N)] \cdot R \cdot \begin{bmatrix} p_1(X) \\ \vdots \\ p_M(X) \end{bmatrix} \end{aligned} \tag{10}$$

Using the symmetry of the kriging matrix, a new set of coefficients is defined as:

$$\begin{bmatrix} b_1 \\ \vdots \\ b_N \end{bmatrix} = Q \cdot \begin{bmatrix} U(X_1) \\ \vdots \\ U(X_N) \end{bmatrix}, \quad \begin{bmatrix} a_1 \\ \vdots \\ a_M \end{bmatrix} = R^T \cdot \begin{bmatrix} U(X_1) \\ \vdots \\ U(X_N) \end{bmatrix} \tag{11}$$

and Equation (10) becomes

$$u^*(X) = \sum_{j=1}^{N} b_j C_j + \sum_{l=1}^{M} a_l p_l(X) \tag{12}$$

Equation (12) is called dual kriging. The coefficients a_l, $l = 1, \ldots, M$ and b_j, $j = 1, \ldots, N$ can be written in matrix form as:

$$\begin{bmatrix} b_1 \\ \vdots \\ b_N \\ - \\ a_1 \\ \vdots \\ a_M \end{bmatrix} = \left[\begin{array}{c|c} Q & A \\ \hline R_T & B \end{array}\right] \cdot \begin{bmatrix} U(X_1) \\ \vdots \\ U(X_N) \\ - \\ 0 \\ \vdots \\ 0 \end{bmatrix} \tag{13}$$

where the matrices A and B are arbitrary. By choosing $A = R$ and $B = S$, the matrix of Equation (9), which is the inverse kriging matrix, appears again in Equation (13). Therefore, the coefficients a_ls and b_js are solutions of

$$\left[\begin{array}{c|c} C_{ij} & p_l(X_i) \\ \hline p_l(X_j) & 0 \end{array}\right] \cdot \begin{bmatrix} b_1 \\ \vdots \\ b_N \\ - \\ a_1 \\ \vdots \\ a_M \end{bmatrix} = \begin{bmatrix} U(X_1) \\ \vdots \\ U(X_N) \\ - \\ 0 \\ \vdots \\ 0 \end{bmatrix} \tag{14}$$

This system of linear equations along with the dual kriging model in Equation (12) comprise the dual formulation of kriging.

The Drift Function and the Covariance Functions

According to Journel and Huijbregts [10], a polynomial drift function is normally used in geostatistics applications. This can be a complete polynomial of order k (k dimensions) composed of all possible subsets of variables of size 1 to k. For example, an order three basis is expressed as:

$$a(x) = a_0 + \sum_{i=1}^{L} a_i x_i + \sum_{i=1}^{L} \sum_{j=i}^{L} a_{ij} x_i x_j + \sum_{i=1}^{L} \sum_{j=i}^{L} \sum_{k=j}^{L} a_{ijk} x_i x_j x_k \tag{15}$$

Dual kriging also requires the knowledge of the covariance between two points or locations. The covariance between two points or locations is assumed to depend only on the Euclidean distance h between X_i and X_j, (and not on the particular positions X_i or X_j) and is represented by $C(h)$. Usually, the covariance function decreases from a maximum at $C(0)$ since the degree of correlation between two locations decreases as the distance h between them increases [10]. Ratle [16] summarizes two approaches for obtaining the covariance. The first approach is to use an arbitrary theoretical covariance function. These functions are called shape functions rather than covariance functions since they have no relationship to the actual covariance. Kriging under these conditions is considered to be an exact interpolator. The other approach is to use the estimation of an experimental covariance function from the observed data. Under this condition, kriging is employed as an estimator. However, it is difficult to estimate a covariance function from the experimental data because it requires the knowledge of the unknown mean. Consequently, only theoretical covariance will be considered in this article.

Ratle [16] has described three common theoretical covariance functions. The first is the pure nugget effect which is the limiting case where the fluctuations around the samples are assumed to be insignificant. This model is appropriate for noisy data as well as for problems where only a rough estimate of the solution is required. The pure nugget effect covariance is written as:

$$C(h) = \begin{cases} 1 & \textit{if} \qquad h = 0; \\ 0 & \textit{otherwise}. \end{cases} \tag{16}$$

Under the pure nugget effect, there is no correlation between two points regardless of distance h. The kriging model does not pass through all of the data points and it reduces to a simple polynomial regression on the drift function basis.

The other two functions use the notion of distance of influence as introduced by Trochu [21]. The models assume that the correlation or actual covariance between two very distance points is negligible or zero; that is, $C(h) = 0$ if $h > d$, where d is a predefined threshold. The first function is linear. It assumes that the covariance decreases linearly from a maximal value at $h = 0$ to zero at $h = d$. The linear covariance is expressed as:

$$C(h) = \begin{cases} 1 - h/d & \textit{if } h < d; \\ 0 & \textit{otherwise}. \end{cases} \tag{17}$$

The other function is cubic. This ensures continuity by imposing the nullity of the first derivative of $C(h)$ at the points $h = 0$ and $h = d$. Two other conditions are $C(0) = 1$ and $C(d) = 0$. The covariance function is defined as:

$$C(h) = \begin{cases} 1 - 3(h/d)^2 + 2(h/d)^3 & \textit{if } h < d; \\ 0 & \textit{otherwise}. \end{cases} \tag{18}$$

METHODOLOGY

The methodology for incorporating a metamodel approach into the sensitivity analysis of capital investment evaluations comprises two parts: developing appropriate metamodels and conducting sensitivity analysis using the validated metamodels.

Development of Metamodels

For the purpose of sensitivity analysis of investment evaluation, Sartori and Smith [18] summarize the general steps for metamodel construction as the following:

1. **Identify factors of the cash flow analysis that may be uncertain and influence the economic measure of an investment alternative.**
2. **Determine the reasonable range of values over which these factors may occur; this becomes the domain of applicability of the metamodel.**
3. **Generate a fitting (training) data set based on an appropriate design of experiments (DOE) that covers the factor ranges identified previously and compute the economic measure at each of the factor combinations called for by the experimental design.**
4. **Construct a metamodel to approximate the relationship between the economic measure and the corresponding factor combinations.**
5. **Validate the developed metamodel.**

In order to obtain reasonable ranges for influential factors of the investment under study, Eschenbach and McKeague [9] recommend selecting the most likely value of each factor then choosing reasonable upper and lower bounds relative to this value. It must be emphasized that choice of these reasonable ranges is very important. Should metamodel prediction be needed beyond any of these values (that is, need to be extrapolated), the results are apt to be incorrect and possibly misleading. Ranges should be chosen broadly enough to permit all useful predictions. However, ranges that are unnecessarily broad will result in the generation of additional data points or a decrease in prediction accuracy, or both.

Since a metamodel is constructed from the data, its performance also depends on the selection of an appropriate experimental design. A small design may impair model accuracy while a large design will require more effort in gathering the data. In this article, data is easily calculated as the NPV from values of the input factors. However, in modeling other economic scenarios, it may be necessary to simulate the economic relationship or produce physical prototypes, thus restricting the ability to generate data.

Dual kriging metamodels are built using the code developed by Ratle [16]. All variables are normalized between ± 1. The order of the drift basis function, the covariance function, and the Euclidean distance of influence are the key parameters. A second-order drift function is found to work best for all studies in this article. Linear or cubic covariance models and two values of distance of influence (d) are chosen, depending on the case study and data set.

For comparison, second-order polynomial regression and backpropagation artificial neural networks are selected to capture the nonlinearity that exists in most economic models. In order to minimize multicollinearity, each input factor is expressed as a deviation around its mean (i.e., a z value). The output or response of the metamodel is chosen as the NPV of each alternative. Forward and backward stepwise regression is used with the probability to enter and remove of 0.05. The aptness of the polynomial regression metamodel is investigated using residual normal probability plots and the variance inflation factor is calculated to examine multicollinearity. For the neural network metamodels, training is done with an ordinary backpropagation algorithm, which minimizes the squared error, as detailed in Chaveesuk and Smith [3]. One hidden layer is used in each ANN (number of hidden neurons are specified in each case study) and training occurs until the best set of weights (using the validation set) are found (the number of training iterations—passes through the training data set—is specified in each case study). Ten sets of initial random weights were trained for each ANN architecture and the best of these are chosen for the final metamodel. ANN can be sensitive to initial starting weights since the error minimization is by gradient descent, which terminates at a local minimum. Therefore, for the ANN models, number of hidden neurons, number of training iterations, and random initial weight set were experimental factors.

After metamodels are built from the fitting data sets, their accuracy must be assessed. This is accomplished by using a *validation data set* obtained by uniformly randomly selecting points from the sample space covered by the ranges identified prior to the experimental design. The predicted NPVs, together with the actual NPVs, are used to compute the average absolute error (AAE) and the relative average absolute error (RAAE). These error measures are defined as follows:

$$AAE = \frac{\sum_{i=1}^{n} |Y_i - \hat{Y}_i|}{n}$$

$$RAAE(\%) = \frac{\sum_{i=1}^{n} \frac{|Y_i - \hat{Y}_i|}{|Y_i|}}{n} \times 100$$

where

Y_i **denotes the actual response value of data point** i;
$\hat{Y}_i$ **denotes the predicted response value of data point** i;
n **denotes the number of data points over which the error is calculated.**

Once metamodel selection has been completed, a larger validation data set, termed the *generalization data set*, is used to compare the metamodels. The extent of model deterioration and overfit are examined by comparing the error measurements from this generalization data set with the ones computed from the fitting data set. In addition, the error measurements from the two validation data sets are used to compare the effect of various metamodel techniques and experimental designs on accuracy. Selecting the best metamodel can depend on its intended use: A high accuracy metamodel is critical for prediction while a crude metamodel may suffice for understanding the problem [12].

Sensitivity Analysis of a Capital Investment Using Metamodels

Sensitivity analysis of a capital investment includes what-if analysis, break even boundaries and identification of critical factors. A metamodel can be used to reveal the presence of interactions among factors as well as their degree of influence, which is not possible in traditional sensitivity analysis. For a stepwise polynomial regression metamodel, inference can be made from the magnitude of the standardized regression coefficients. A large coefficient indicates a significant effect of that variable. For dual kriging metamodels, the magnitude of the standardized coefficients of the drift function, which represents the average behavior of the economic data, can be used for this purpose. Similar to polynomial regression, a large coefficient is associated with a significant effect of the factor or interaction. For neural network metamodels, selection of important variables and effects is not straightforward since there is no ready interpretation of the trained weights. Instead, a laborious one variable at a time process must be undertaken to establish the relationship of the change in output variable for each change in input variable. For compound effects, this is further complicated by the need to alter multiple variables together, and observe the output.

CASE STUDIES AND DISCUSSION

Two case studies are selected from the engineering economy literature to illustrate and assess the potential use of kriging metamodels in sensitivity analysis of capital investment decisions. Both cases differ in problem size, which is characterized by the number of uncertain factors and have been studied using polynomial regression and ANN metamodels.

A Municipal Construction Case Study

This case study was originally taken from Sartori and Smith [18]. It involves the proposed construction of a new municipal building in a north Pittsburgh suburb. The first cost of this investment is estimated to be \$7,010 K. This investment is financed by a loan with an interest rate of 6%. The investment is expected to generate annual savings of \$350 K. The inflation rate is estimated to be 3%. Table 1 shows the cash flow analysis of this investment under the most likely condition.

Sartori and Smith identified four uncertain factors in this cash flow analysis: first cost (C), interest rate (I), initial operating saving (S), and inflation rate (R). The reasonable ranges of these variables are shown in Table 2. Two experimental designs are studied: a three-level fractional factorial 3^{4-1} with a mid range value design and a three-level full factorial 3^4 design. These designs generate 28 and 81 design points, respectively. A validation set of 40 observations and a generalization set of 200 observations are also generated. The kriging model for the 3^{4-1} data set uses a linear covariance function and distance of influence $= 1$. The ANN is best at 2 hidden neurons (after considering 1, 2, or 3) trained for 479 K iterations. The kriging model for the 3^4 data set uses a linear covariance function and distance of influence $=0.5$. The ANN is best at 5 hidden neurons (after considering 1 through 6) trained for 4,913 K iterations.

Table 3 shows the error in prediction of NPV of the metamodels. Since dual kriging is an exact interpolation technique, the metamodel exactly fits all data points in the fitting data set, thus leading to the absence of fitting errors. Dual kriging considerably outperforms the polynomial regression and the ANN metamodel in terms of prediction accuracy across all designs and data sets. Figure 1 shows the dual kriging predictions versus actuals for the 200 point validation set and it is seen that the predictions are uniformly good with no bias exhibited.

Table 1. Cash flow analysis for the municipal construction case from Sartori and Smith [18] (in $1000)

Year	Principal balance	Debt service	Principal payment	Operating savings	Other revenue	Net cash flow
0	7,010	0	0	0	280	280.000
1	7,010	(421)	0	350	140	69.400
2	7,010	(421)	0	361	35	(25.100)
3	7,010	(421)	0	371		(49.285)
4	7,010	(421)	0	382		(38.146)
5	7,010	(421)	0	394		(26.672)
6	7,010	(421)	0	406		(14.854)
7	7,010	(421)	0	418		(2.682)
8	7,010	(421)	0	430		9.856
9	7,010	(421)	0	443		22.770
10	7,010	(421)	0	457		36.071
11	7,010	(421)	0	470		49.771
12	7,010	(421)	0	484		63.882
13	7,010	(421)	0	499		78.416
14	7,010	(421)	0	514		93.387
15	7,010	(421)	0	529		108.806
16	7,010	(421)	0	545		124.689
17	7,010	(421)	0	562		141.047
18	7,010	(421)	0	578		157.897
19	7,010	(421)	0	596		175.252
20	7010	(421)	0	614		193.127
21	3,505	(421)	(3505)	632		(3293.461)
22	0	(210)	(3505)	651		(3064.197)
					NPV (6%)	(1103.607)

Identification of influential factors, nonlinear effects and their magnitudes are further insights gained from metamodels. Because of their prediction accuracy, the metamodels constructed from the 3^4 design are used for this purpose and shown in Table 4. In spite of the

Table 2. Estimated range of variation for each input factor of the municipal construction project from Sartori and Smith [18]

Factor	Lower bound	Mid-range	Upper bound
First costs (C)	5860	7010	8160
Interest rate (I)	4%	6%	8%
Initial operating savings (S)	100	350	600
Inflation rate (R)	1%	3%	5%

All money amounts are in thousands of dollars.

Table 3. NPV results of the metamodels (error in $1000)

DOE	Type of metamodel	Specification	Fitting set		Validation set		Generalization set	
			AAE	AARE (%)	AAE	AARE (%)	AAE	AARE (%)
3^{4-1}	Regression	2nd-order stepwise	107.18	8.70	169.94	30.94	86.63	25.12
	ANN	2 hidden neurons, 479 K iterations	88.29	43.94	123.03	17.06	114.31	20.64
	Dual kriging	2nd-order drift function, linear covariance function, $d = 1.0$	0.00	0.00	47.10	7.39	46.49	12.27
3^4	Regression	2nd-order stepwise	88.45	12.66	157.73	29.50	50.49	9.68
	ANN	5 hidden neurons, 4,913 K iterations	21.45	4.04	67.20	9.95	53.09	10.20
	Dual kriging	2nd-order drift function, linear covariance function, $d = 0.5$	0.00	0.00	6.01	0.95	18.14	3.85

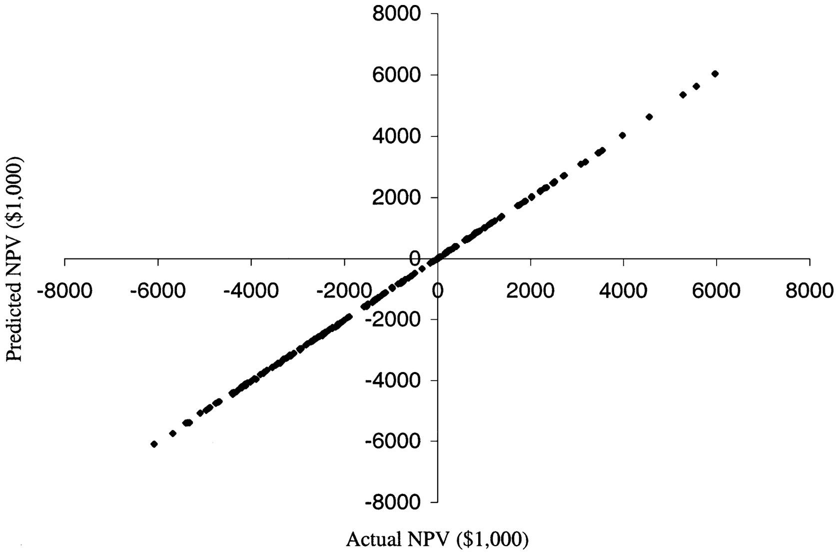

Figure 1. A scatter plot between the actual and predicted NPV of the dual kriging metamodel constructed from the 3^4 design for the first case study over the 200-point validation set.

difference in accuracy and method of identifying the critical factors, the dual kriging, ANN and regression metamodels all identify the savings (S) as the most influential factor. In terms of interactions, all metamodels signal that the interactions between I and S and between

Table 4. Significant factors, interactions, and nonlinear terms for the 3^4 construction case

	Regression		ANN		Dual kriging	
Rank	Factor	Magnitude[1]	Factor	Magnitude[2]	Factor	Magnitude[3]
1	S	0.89	S	55.47	S	0.89
2	C	0.25	C	19.91	C	0.25
3	I	0.24	I	11.95	I	0.24
4	R	0.23	R	7.90	R	0.23
1	II	0.02	II	9.66	II	0.26
2	RR	0.01	SS	6.07	RR	0.20
1	IS	0.14	IS	37.47	IS	1.28
2	SR	0.13	SR	15.17	SR	1.19
3	IR	0.05	CS	12.34	IR	0.46

[1]Magnitude of the standardized regression coefficient.
[2]Magnitude of the percentage change in the output.
[3]Magnitude of the standardized drift function coefficient.

Table 5. Comparison of the estimated cost structure of the CMT and the FMS systems from Park [14]

	CMT	FMS
Number of pieces produce/year	544,000	544,000
Variable labor cost/part	\$2.15	\$1.30
Variable material cost/part	\$1.53	\$1.10
Annual overhead	\$3.15M	\$1.95M
Annual tooling costs	\$470,000	\$300,000
Annual inventory costs	\$141,000	\$31,500
Investments	\$3.5M	\$10M
Salvage value	\$0.5M	\$1M
Service life	10 years	10 years
Depreciation method (MACRS)	7-year	7-year

S and R are the most important. The quadratic effect of I is also important.

An FMS Case Study

An FMS case was selected and modified from Park [14]. A U.S. company will determine whether to replace a conventional manufacturing technology (CMT) with a flexible manufacturing system (FMS). Table 5 shows the comparison of the estimated cost structure of both systems. The firm's marginal tax rate and MARR are projected to be 40% and 15%, respectively. The incremental cash flow analysis for CMT and FMS is shown in Table 6.

Park stated that the management of this company was very confident about all estimates for CMT. However, the firm did not have any previous experience in operating an FMS. Ten uncertain factors for the FMS are identified: variable labor cost per part (L), variable material cost per part (M), annual overhead (O), annual tooling costs (T), annual inventory costs (V), first investment (I), salvage value (S), tax rate (X), discount rate (D), and service life (L). Table 7 depicts a reasonable range for each factor. An experimental design of a three-level fractional factorial 3^{10-5} with a mid range value design is used and generates 257 design points. The validation data set has 120 data points and the generalization data set consists of 200 data points. Because ANN are sensitive to number of input variables, an ANN metamodel with all input variables is used to identify the critical factors, their quadratic effects, and their interactions. Then,

Table 6. An incremental cash flow analysis for CMT and FMS from Park [14] (in $1000)

Year	0	1	2	3	4	5	6	7	8	9	10
Income statement											
Revenue											
Labor		462.40	462.40	462.40	462.40	462.40	462.40	462.40	462.40	462.40	462.40
Material		233.92	233.92	233.92	233.92	233.92	233.92	233.92	233.92	233.92	233.92
Overhead		1200.00	1200.00	1200.00	1200.00	1200.00	1200.00	1200.00	1200.00	1200.00	1200.00
Tooling		170.00	170.00	170.00	170.00	170.00	170.00	170.00	170.00	170.00	170.00
Inventory		109.50	109.50	109.50	109.50	109.50	109.50	109.50	109.50	109.50	109.50
Depreciation		928.85	1591.85	1136.85	811.85	580.45	579.80	580.45	289.90		
Taxable income		1246.97	583.97	1038.97	1363.97	1595.37	1596.02	1595.37	1885.92	2175.82	2175.82
Income tax (40%)		498.79	233.59	415.59	545.59	638.15	638.41	638.15	754.37	870.33	870.33
Net income		748.18	350.38	623.38	818.38	957.22	957.61	957.22	1131.55	1305.49	1305.49
Cash flow statement											
Cash from operation											
Net income		748.18	350.38	623.38	818.38	957.22	957.61	957.22	1131.55	1305.49	1305.49
Depreciation		928.85	1591.85	1136.85	811.85	580.45	579.80	580.45	289.90		
Investment & salvage	(6500)										500.00
Gain tax (40%)											(200.00)
Net cash flow	(6500)	1677.03	1942.23	1760.23	1630.23	1537.67	1537.41	1537.67	1421.45	1305.49	1605.49
NPV (15%)	1756.225										

Table 7. Uncertain factors and their ranges for the FMS case from Park [14]

Factors	Lower bound	Mid-range	Upper bound
Variable labor cost/part (L)	\$1.04	\$1.3	\$1.56
Variable material cost/part (M)	\$0.88	\$1.1	\$1.32
Annual overhead (O)	\$1.56M	\$1.95M	\$2.34M
Annual tooling costs (T)	\$240,000	\$300,000	\$360,000
Annual inventory costs (V)	\$3.15M	\$3.15M	\$3.15M
Investments (I)	\$8M	\$10M	\$12M
Salvage value (S)	\$0.8M	\$1M	\$1.2M
Tax rate (X)	36%	40%	44%
Discount rate (D)	13.5%	15%	16.5%
Service life (Y)	8 years	10 years	12 years

the quadratic effects and two-factor interactions that do not appear to be significant are discarded from the input neuron representation. For this case study, 25 inputs were removed and therefore the number of input neurons was reduced from 65 (original ANN) to 40 (reduced ANN). Then the metamodel development process was carried out. The kriging model for the 3^{10-5} data set uses a cubic covariance function and distance of influence $= 0.7$. The original ANN is best at 2 hidden neurons (after considering 1 through 6) trained for 69,670 K iterations. The reduced ANN is best at 5 hidden neurons (after considering 1 through 6) trained for 159,486 K iterations.

Table 8 shows the error in prediction of NPV of the metamodels. The dual kriging metamodel predicts slightly better than the reduced ANN metamodel and somewhat better than the original ANN metamodel and the polynomial regression metamodel. Influential variables are identified in Table 9. Polynomial regression and dual kriging metamodels identify the same ordering of the top five influential factors as the investment (I), annual overhead (O), service life (Y), discount rate (D), and service life (L). The quadratic effects of Y and D are important. Both metamodels also pointed out that the top-five significant interactions are between O and Y, O and D, O and X, D and Y, and I and X. Although the tax rate (X) is not among the top-five critical factors, it must also be considered a key factor since it interacts with both I and O which are among top-two critical factors. The ANN metamodels identify some of the same factors but in different rank order than the regression or kriging metamodels. Since the ANN procedure for ranking significant factors is fairly ad hoc, one would place more confidence in those (and their order) selected by the regression and kriging metamodels.

Table 8. NPV results of the metamodels (error in \$1000)

		Fitting set		Validation set		Generalization set	
Type of metamodel	Specification	AAE	AARE (%)	AAE	AARE (%)	AAE	AARE (%)
Regression	2nd-order stepwise	10.29	1.85	5.67	2.26	5.83	1.77
ANN	2 hidden neurons, 69,670 K iterations	16.93	3.35	16.70	3.88	17.69	2.23
Reduced ANN	5 hidden neurons, 40 inputs, 159,486 K iterations	4.98	1.40	6.33	1.85	6.28	1.61
Dual kriging	2nd-order drift function, cubic covariance function, $d = 0.7$	0.00	0.00	5.67	1.83	5.48	1.63

Table 9. Significant factors, interactions, and nonlinear terms for the FMS case

	Regression		ANN		ANN reduced		Dual kriging	
Rank	Factor	Magnitude[1]	Factor	Magnitude[2]	Factor	Magnitude[2]	Factor	Magnitude[3]
1	I	0.70	Y	66.46	Y	49.29	I	0.70
2	O	0.54	O	37.48	O	39.35	O	0.54
3	Y	0.28	X	27.75	I	30.18	Y	0.28
4	D	0.21	I	25.34	L	9.81	D	0.21
5	L	0.20	D	21.63	X	7.89	L	0.20
1	YY	0.02	YY	14.59	YY	9.93	YY	0.49
2	DD	0.01	DD	7.22	XX	3.70	DD	0.12
1	OY	0.04	OX	24.58	ID	21.07	OY	0.65
2	OD	0.03	DY	22.46	OY	17.83	DY	0.48
3	OX	0.03	OD	18.88	DY	12.45	OX	0.46
4	DY	0.03	OY	18.68	LY	6.13	OD	0.40
5	IX	0.02	IX	15.60	MY	5.27	IX	0.28
6	LY	0.02	XY	11.96	LX	4.85	LY	0.24
7	XY	0.02	LX	10.20	XY	3.79	XY	0.23

[1] Magnitude of the standardized regression coefficient.
[2] Magnitude of the percentage change in the output.
[3] Magnitude of the standardized drift function coefficient.

CONCLUSIONS

The dual kriging metamodel decidedly outperforms polynomial regression and ANN metamodels in prediction accuracy when the number of uncertain factors is small (Case 1). In the larger case study, while the kriging metamodel was still the most accurate, its accuracy was closer to that of the polynomial regression and reduced ANN metamodels. Despite the difference in prediction accuracy, both polynomial regression and dual kriging metamodels identify the same sets of critical factors, non linear and interaction effects. It is easy to identify the importance of factors, terms and interaction from both dual kriging and polynomial metamodels from the coefficients. This is much more difficult in ANN metamodels, where importance usually needs to be ascertained in a laborious, empirical fashion.

In terms of ease of model building, many commercial software packages are available for polynomial regression. Most kriging software packages are aimed at its traditional use—geostatistics—but might be used for other applications including economic metamodeling. Widely available kriging software includes freeware (a version for Matlab can be found at http://globec.whoi.edu/software/kriging) and commercial software (an example is GS+ from RockWare, Inc.). There are not too many parameter choices for dual kriging and the method is computationally similar to a least squares regression method in terms of procedure and computational effort. ANN has widely available commercial software but the model building and validation are much more artful and laborious than in regression or kriging and require greater experiential knowledge in the field.

Since kriging leverages the spatial relationship among data, it may find particularly good application in engineering economics problems where observations are limited but there is definite (or assumed) correlation among the input data. Besides the metamodeling application herein, one could foresee the use of kriging for cost estimation.

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