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Identifying Feasible Design Concepts for Products with Competing Performance Requirements by Metamodeling of Loss-Scaled Principal Components

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Abstract

Engineering design often involves the determination of design variable settings to optimize competing performance requirements. In the early design stages we propose narrowing down the domain of design solutions using metamodels of principal components of the multiple performance levels that have been scaled by a multivariate quadratic loss function. The multivariate quadratic loss function is often used as the objective function in reaching optimal solutions because it utilizes the correlation structure of the design's performance metrics and penalizes off-target performance in a symmetrical manner. We also compare the computational performance of these loss-scaled principal components when used to solve for the design with minimal expected multivariate quadratic loss under three modeling approaches: response surface methodology, multivariate adaptive regression splines, and spatial point modeling. We demonstrate the technique on the design of the mechanical frame of an electric vehicle with six desired performance levels determined simultaneously by the dimensions of eight mechanical design elements. The method is the focus in this work.

Keywords

multiple response; multivariate quadratic loss function; optimal solutions; robust engineering design

INTRODUCTION

Often in the early stages of a sequential design process, the designer is first interested in restricting the broader design space to a smaller, localized region, which experimentation reveals as potentially containing the best response levels. It is common in these early stages to fit metamodels; that is, models obtained from the application of statistically oriented

modeling techniques to deterministic data, to approximate the very accurate, albeit computationally intensive, engineering design packages. The huge savings in computational time afforded by the metamodels more than compensates for their loss of accuracy during the early stages of the design timeline. In some cases with many interrelated responses, only highly complex models of system performance are available. This is particularly true for fluid systems and others modeled by finite elements as discussed in Rolander et al. (2006). In this article we propose a technique for the early stages of static multivariate robust design using metamodels of loss-scaled principal components of each potential design's performance levels. To simulate the uncontrollable variability introduced by manufacturing processes and use-related degradation, we inject internal noise around the nominal values of each design vector chosen by the optimization algorithm.

In the following section we introduce the technical elements that comprise the proposed method and the next section shows how they fit into a metamodel-based procedure for static multivariate robust design. Then we describe a product design problem with eight predictor variables and six responses that motivated the proposed method. We then present the results yielded from application of our procedure to the product design problem presented in the previous section. In the final section we make concluding remarks on the analytical and practical characteristics of the proposed approach.

DEFINING THE TECHNICAL ELEMENTS OF THE PROPOSED APPROACH

In this section we introduce the basic technical elements comprising the early stage design approach proposed in this article. We define the optimal solution as the vector of design variable settings that minimizes the expected value of the multivariate quadratic loss function MQL . We start by briefly defining the multivariate quadratic loss and its attractive mathematical properties.

Multivariate Quadratic Loss and Its Use in Robust Design

In the multiresponse situation it is assumed that a set of r performance responses ($Y_1, \dots, Y_r$) is affected by design and noise factors as follows:

$$Y_i = f_i(\mathbf{x}, \mathbf{N}, \theta_i) + \varepsilon_i, \quad i = 1, \dots, r,$$

where $\mathbf{x} = (x_1, \dots, x_p)^T$ is the vector of fixed design factor settings, $\mathbf{N} = (N_1, \dots, N_q)^T$ is the vector of noise factors, θ_i is the vector of unknown response model parameters, and f_i is the transfer function for Y_i . The noise factors $\mathbf{N}$ are assumed to be random and represent the uncontrolled sources of variability in production. The pure error ε_i represents the remaining variability of the manufacturing process that is not captured by the noise factors and is assumed to be normally distributed with zero mean and finite variance. A loss occurs if any of the responses (Y_i) deviate from their target t_i . Please note that we will use the terms *performance measures* and *responses* synonymously throughout.

For univariate responses, expected squared-error loss is a convenient way to evaluate the loss caused by deviation from target because of its decomposition into squared off-target and variance terms. A natural extension of this loss function to a set of r correlated responses is the multivariate quadratic function of the deviation vector $(\mathbf{Y} - \boldsymbol{\tau})$ where $\mathbf{Y} = (Y_1, \dots, Y_r)^T$ and $\boldsymbol{\tau} = (t_1, \dots, t_r)^T$; that is,

$$MQL(\mathbf{Y}, \boldsymbol{\tau}) = (\mathbf{Y} - \boldsymbol{\tau})^T \mathbf{A} (\mathbf{Y} - \boldsymbol{\tau}), \quad [1]$$

where $\mathbf{A}$ is a positive definite constant matrix. The values of the constants in $\mathbf{A}$ are related to the costs of a nonoptimal design, such as the costs related to repairing and/or scrapping noncompliant product. In general the diagonal elements of $\mathbf{A}$ represent the weights of the r characteristics and the off-diagonal elements represent the costs related to pairs of responses being simultaneously off-target.

In Murphy et al. (2005) it was shown that if $\mathbf{Y}$ follows a multivariate normal distribution with mean vector $E(\mathbf{Y})$ and covariance matrix $\Sigma_{\mathbf{Y}}$, the average (expected) loss can be written as:

$$\begin{aligned} E(MQL) &= E(\mathbf{Y} - \boldsymbol{\tau})^T \mathbf{A} (\mathbf{Y} - \boldsymbol{\tau}) \\ &= \text{trace}[\mathbf{A} \Sigma_{\mathbf{Y}}] + [E(\mathbf{Y}) - \boldsymbol{\tau}]^T \mathbf{A} [E(\mathbf{Y}) - \boldsymbol{\tau}]. \end{aligned} \quad [2]$$

Referring to the univariate squared-error loss function in [1], the $\text{trace}[\mathbf{A} \Sigma_{\mathbf{Y}}]$ is the multivariate counterpart to univariate variance, and the $[E(\mathbf{Y}) - \boldsymbol{\tau}]^T \mathbf{A} [E(\mathbf{Y}) - \boldsymbol{\tau}]$, which we call the *off-target vector product (OTVP)*, is the multivariate analog to the squared off-target component.

The simplest approach to solve the robust design problem is to apply algorithms to directly minimize the average loss function in Eq. [2]. Because the mean vector and covariance matrix are usually unknown, they can be estimated by the sample mean vector and sample covariance matrix or a fitted model based on a sample of observations of the multivariate responses. This strategy of optimizing the multivariate quadratic loss function directly employs the correlation structure of the responses in the trace component.

One sees from this decomposition that moving all response means to target simplifies the expected multivariate loss to the $\text{trace}[\mathbf{A} \Sigma_{\mathbf{Y}}]$ term. The trace-covariance term shows how the values of $\mathbf{A}$ and the covariance matrix $\Sigma_{\mathbf{Y}}$ directly affect the expected multivariate loss. Higher variances and covariances of the individual responses raise expected loss, and the $\mathbf{A}$ values can be seen as weights of the individual response variances and two-response interactions. Weighting or prioritization of the individual responses within the multivariate loss function is determined by the values in the $\mathbf{A}$ matrix.

Loss-Scaled Principal Components

In the previous subsection Eq. [2] showed the decomposition of the expected value of multivariate quadratic loss into terms representing covariance and the off-target vector product. Because we are seeking the vector of design variables settings that minimize expected multivariate quadratic loss, the design must find design variable settings that simultaneously reduce covariance as well as the bias of the design's performance levels. To minimize the two terms of the expected multivariate quadratic loss, one must simultaneously consider the contributions of the loss matrix $\mathbf{A}$ as well as the response covariance/correlation matrix.

Since their introduction in Pearson (1901), principal components are among the most widely used of the multivariate statistical techniques. Because the loss constant matrix $\mathbf{A}$ is assumed to be symmetric and positive definite it can be decomposed by either Cholesky decomposition or diagonalized in the following way:

$$\mathbf{G}^T \mathbf{A} \mathbf{G} = \Lambda_A,$$

where the columns of $\mathbf{G}$ are the eigenvectors of $\mathbf{A}$ and $\Lambda_{\mathbf{A}}$ is a diagonal matrix, whose diagonal elements are the eigenvalues of $\mathbf{A}$. This diagonalization allows $\mathbf{A}$ to be expressed as

$$\begin{aligned}\mathbf{A} &= \mathbf{G} \Lambda_{\mathbf{A}} \mathbf{G}^T \\ \mathbf{A} &= (\mathbf{G} \Lambda_{\mathbf{A}}^{\frac{1}{2}}) (\mathbf{G} \Lambda_{\mathbf{A}}^{\frac{1}{2}})^T.\end{aligned}$$

If we then define $\mathbf{q} = (\mathbf{G} \Lambda_{\mathbf{A}}^{\frac{1}{2}})^T$, we can express $\mathbf{A}$ in the following way:

$$\mathbf{A} = \mathbf{q} \mathbf{q}^T.$$

This allows Eq. [2] to be written as follows:

$$\begin{aligned}E(MQL) &= E(\mathbf{Y} - \boldsymbol{\tau})^T \mathbf{A} (\mathbf{Y} - \boldsymbol{\tau}) \\ &= E(\mathbf{q}^T \mathbf{Y} - \mathbf{q}^T \boldsymbol{\tau})^T (\mathbf{q}^T \mathbf{Y} - \mathbf{q}^T \boldsymbol{\tau}) \\ &= \text{trace}[\mathbf{q}^T \sum_y \mathbf{q}] + (E \mathbf{q}^T \mathbf{Y} - \mathbf{q}^T \boldsymbol{\tau})^T (E \mathbf{q}^T \mathbf{Y} - \mathbf{q}^T \boldsymbol{\tau}) \quad [3] \\ &= \text{trace}[\mathbf{q}^T \sum_y \mathbf{q}] + (\mathbf{q}^T (E \mathbf{Y} - \boldsymbol{\tau}))^T [\mathbf{q}^T (E \mathbf{Y} - \boldsymbol{\tau})].\end{aligned}$$

Therefore, multiplying the original response vectors by the matrix $\mathbf{q}^T$ incorporates the contents of matrix $\mathbf{A}$ and $\Sigma_{\mathbf{Y}}$ directly into the matrix $\mathbf{q}^T \Sigma_{\mathbf{Y}} \mathbf{q}$.

Loss-scaled responses are simply $\mathbf{q}^T \mathbf{Y}$ and their principal components are formed by multiplying the transpose of the eigenvectors of $\mathbf{q}^T \Sigma_{\mathbf{Y}} \mathbf{q}$ by $\mathbf{Y}$. If we use $\mathbf{Z}$ to denote the full set of loss-scaled principal components (*LSPC*) formed from the covariance matrix of the loss-scaled responses, that is, $\mathbf{q}^T \Sigma_{\mathbf{Y}} \mathbf{q}$, then Eq. [3] can be expressed as:

$$\begin{aligned}E(MQL) &= E[(\mathbf{Z} - \boldsymbol{\tau}_z)^T (\mathbf{Z} - \boldsymbol{\tau}_z)] \\ &= \text{trace}[\sum_z] + (E \mathbf{Z} - \boldsymbol{\tau}_z)^T (E \mathbf{Z} - \boldsymbol{\tau}_z).\end{aligned}$$

Metamodeling

As mentioned in the Introduction, in early design stages engineers commonly build metamodels using statistical model fitting techniques as a faster way to approximate accurate, deterministic design packages. Though there are many possible model fitting paradigms, we are limiting our discussion to three of the most common, namely, response surface methodology (RSM); spatial point modeling, also known as *kriging*; and multivariate adaptive regression splines (MARS). The metamodels created with these model-fitting approaches will be used to approximate “true” responses; that is, the output of a deterministic design package.

Each of these modeling techniques has been widely described and employed in the literature and are used here to provide some insight as to the computational efficiencies afforded by each in combination with the proposed metamodeling of loss-scaled principal components.

Because of the deterministic nature of the computational output, metamodels stray from a key underlying statistical assumption for linear models; that is, the response being a random variable with inherently constant variance. In this situation the variance in the responses is entirely a function of the variability in the supposedly fixed design variable values rather

than of the response itself. However, because these metamodels are being used to narrow down a large design space rather than for inferential purposes, this is a very useful application of the model-fitting techniques as described in Murphy (2004).

To fully utilize the robust design techniques, we inject random noise that follows a uniform distribution of values centered around the nominal design variable settings chosen by an optimization algorithm. We effectively analyze a distribution of several design settings centered around the nominal design setting of each dimension during each iteration of the optimization process. The process of minimizing the expected value of the multivariate quadratic loss will therefore provide insight as to the solution space that simultaneously considers off-target performance as well as insensitivity; that is, robustness to uncontrollable sources of variability. Our choice of taking values within a range of $\pm 5\%$ around the nominal design settings represents random noise introduced by manufacturing processes that is explicitly acknowledged in manufacturing tolerances.

Though metamodels built around these deterministic processes are not valid for statistical inference, they are often of sufficient accuracy to be useful in early design stages. Later design stages rely on sophisticated modeling programs to verify mature designs, thereby removing any risk incurred by use of metamodels early in the sequential design process.

A CONCEPTUAL DESIGN PARADIGM BASED ON METAMODELS OF LOSS-SCALED PRINCIPAL COMPONENTS

In lieu of the common practice of building discrete metamodels of predictably correlated responses, employing metamodels of principal components of the responses might permit a reduction of dimensionality of the problem, leading to faster solution of the optimization problem. In the previous section we have shown that loss-scaled principal components are a special case of principal components that incorporates the covariance information as well as the loss constant matrix associated with the multivariate quadratic loss. The models constructed for the loss-scaled principal components are assumed to provide a consistently good approximation throughout the design space. The same assumption applies to the metamodels representing the true response over the entire design space being considered.

The justification for direct modeling of principal components is from Pearson (1901), who proved the following with regard to an r -dimensional set of data. The hyperplane defined by the first $p < r$ eigenvectors is that p -dimensional surface that, out of all possible p -dimensional surfaces, minimizes the sum of squared orthogonal distances between itself and the data set. This concept is illustrated in Figure 1, which shows how a two-dimensional plane approximates a three-dimensional scatterplot by minimizing the sum of squared orthogonal distances between individual points and the plane formed by the first two eigenvectors of the covariance matrix of the data.

Pearson's (1901) proof of this property makes no parametric assumption regarding the data other than the existence of finite variances and covariances of the variables concerned. Therefore, assuming good model fit, models of the minimally orthogonal hyperplanes of the loss-scaled principal components will theoretically converge more quickly than a linear combination of models of the unscaled performance metrics.

In Murphy (2004) it was shown that the fraction of the trace covariance of expected multivariate quadratic loss accounted for by a subset of the loss-scaled principal components is easily calculated. Depending on the nature of the specific off-target vector being considered, the same subset of loss-scaled principal components also accounts for some fraction of the off-target vector product. Therefore, though the full set of loss-scaled

principal components completely replicates the value of multivariate quadratic loss, there is some loss of information associated with any formal subset of the loss-scaled principal components.

Defining $\mathbf{Z}_p$ as a subset of $p < r$ of the loss-scaled principal components, and $\hat{\mathbf{Z}}_p$ as the corresponding vector of metamodels, the expected multivariate quadratic loss can be expressed and approximated as

$$\begin{aligned} E(MQL) &= E(\mathbf{Y} - \tau)^T \mathbf{A} (\mathbf{Y} - \tau) \\ &= \text{trace}[\mathbf{A} \Sigma_Y] + [E(\mathbf{Y}) - \tau]^T \mathbf{A} [E(\mathbf{Y}) - \tau] \\ &\approx \text{trace}[\Sigma_{\hat{\mathbf{Z}}_p}] + [\hat{\mathbf{Z}}_p - \tau_{Z_p}]^T [\hat{\mathbf{Z}}_p - \tau_{Z_p}]. \end{aligned}$$

where $\text{trace}[\Sigma_{\hat{\mathbf{Z}}_p}]$ corresponds to the trace-covariance term of expected multivariate quadratic loss and $(\hat{\mathbf{Z}}_p - \tau_{Z_p})^T (\hat{\mathbf{Z}}_p - \tau_{Z_p})$ corresponds to the off-target vector product of expected multivariate quadratic loss.

We propose a robust design optimization procedure that approximates the expected multivariate quadratic loss with metamodels of a subset of the loss-scaled principal components as follows:

1. Select the first $p < r$ loss-scaled principal components according to a predetermined criterion. We define this group of p loss-scaled principal components as

$$\begin{aligned} \mathbf{Z}_p &= \mathbf{V}_p^T (\mathbf{q}^T \mathbf{Y}) \\ &= (Z_1, \dots, Z_p)^T. \end{aligned}$$

2. Build a metamodel for each loss-scaled principal component as a function of the design vector $\mathbf{x}$ as follows:

$$\begin{aligned} \hat{Z}_1 &= f_{Z_1}(\mathbf{x}) \\ &\vdots \\ \hat{Z}_p &= f_{Z_p}(\mathbf{x}). \end{aligned}$$

3. Approximate expected multivariate quadratic loss with the metamodels of the p loss-scaled principal components,

$$E(\mathbf{Y} - \tau)^T \mathbf{A} (\mathbf{Y} - \tau) \approx \text{trace}[\Sigma_{\hat{\mathbf{Z}}_p}] + [\hat{\mathbf{Z}}_p - \tau_{Z_p}]^T [\hat{\mathbf{Z}}_p - \tau_{Z_p}].$$

4. Solve for the design vector $\mathbf{x}$,

$$\min_{\mathbf{x} \in \Omega} \left\{ \text{trace}[\Sigma_{\hat{\mathbf{Z}}_p}] + [\hat{\mathbf{Z}}_p - \tau_{Z_p}]^T [\hat{\mathbf{Z}}_p - \tau_{Z_p}] \right\}.$$

Potential Advantages and Disadvantages of this Approach

There are two significant potential advantages to modeling the loss-scaled principal components over modeling of the standardized responses to emulate a direct search for the design vector minimizing expected multivariate quadratic loss:

- Assuming $p < r$ and reasonable models for the loss-scaled principal components per some criteria such as R^2 , there may be reduced computational time.
- By exploiting the correlation structure of the responses, the loss-scaled principal components metamodels may provide more accurate approximations of the true process than metamodels of the original responses.

The disadvantage of this approach is

- The accuracy of the approximation of off-target vector product by a formal subset of loss-scaled principal components varies with the specific off-target vector being evaluated and is therefore not estimable beforehand.

DESCRIPTION OF A DESIGN PROBLEM WITH COMPETING PERFORMANCE REQUIREMENTS

The problem that motivated the approach proposed in this article involves finite-element and geometric simulation models using the engineering simulation program *NX-Ideas* (refer to Siemens-AG 2007) for six characteristics of the chassis of an electric vehicle. The following diagrams and description are informed by Ortega (1998) and Lin (2000). Each of the eight design variables is a characteristic of a structural element of the vehicle chassis. The design variables and their ranges are described in Table 1. Each of the six desired performance metrics are functions of these eight design variables. Figure 2 shows the location of all the design factors within the context of the vehicle chassis. The numbered items correspond to the design variables described in Table 1.

The six desired performance characteristics are highly correlated and are related to safety, strength, and weight requirements of the final product. We will describe the responses below with some of their functional context in the following paragraphs.

1. BEND is the mid-span bending of the vehicle and refers to the amount of deformation in the middle of the chassis in the event of a collision. This is a safety concern because less deformation translates into higher safety for vehicle passengers.
2. CURB represents the magnitude of the force exerted on the vehicle's front wheels when the vehicle hits a bump or curb straight on with the brakes applied. This force has components directed vertically upward and horizontally in the rear direction. A designer wants to minimize both components of this force to provide the driver with as much vehicle control as possible during this sort of collision.
3. FRONT is the amount of deformation to the front of the chassis due to frontal impact during a head-on collision. This deformation is to be minimized to provide the passenger with the largest "crush-free" zone possible.
4. MASS is the mass of the chassis and for purposes of fuel efficiency and vehicle longevity is to be minimized. Though an important consideration to the consumer, it is typically of lower economic priority than responses directly related to passenger safety.
5. ROLL is related to the vehicle's deformation during vehicle rollover and is to be minimized to afford the passenger greater protection.

6. TOR is the vehicle's torsional stiffness, which is related to strength of the structural elements and is to be maximized.

The ranges and targets of the responses are characterized in Table 2. Per the Taguchi terminology (see Taguchi 1986), the first five responses are smaller-the-better (STB) and TOR is larger-the-better (LTB). Our original space-filling design was a Latin hypercube that had specific upper and lower bounds of the responses for which the metamodels were fit. One of the problems with using metamodels to solve robust design problems that have STB and LTB targets is that the metamodels are fit across only the reasonable range of possible design variable settings. This implies that even though the optimization algorithm is searching for the values of the design variable settings that achieve either the maximum possible (LTB) or the minimum possible (STB) response, the metamodels themselves are only credibly able to predict values of the outcomes across the range of explanatory variables for which they were fit. In short, we need to prevent the optimization algorithm from asking the metamodels to extrapolate response values. For this reason, we converted each response into a nominal-the-best (NTB) type response whose target is near the relevant extreme of the modeling space of the initial Latin hypercube design. This was intuitively more reasonable from both engineering and metamodeling perspectives.

In order to provide some prioritization on different responses, we defined the loss constant matrix **A** for this example as follows:

$$\mathbf{A} = \begin{pmatrix} 2 & 2 & 0 & 1 & 1 & 1 \\ 2 & 9 & 1 & 0 & 1 & 1 \\ 0 & 1 & 4 & 1 & 1 & 1 \\ 1 & 0 & 1 & 4 & 1 & 1 \\ 1 & 1 & 1 & 1 & 4 & 1 \\ 1 & 1 & 1 & 1 & 1 & 1 \end{pmatrix}.$$

Note that for purposes of safety we have placed the highest weight on the curb response, followed in magnitude by equal weightings of front and roll (safety) and mass (gas mileage). We have placed the lowest priority on torsional stiffness. In this case these weights are for demonstrational purposes only and can be chosen according to the desired profile of the product responses.

With *NX-Ideas*, (Siemens-AG 2007) calculating a vector of the six response values from a design vector with eight design variables takes approximately 4 min. Solving for the design vector that optimizes some objective function of the six responses when starting from the center of the design space usually takes several hundred cycles. This equates to more than a day of computational time. Adding an “external noise” matrix designed around the values of the design vector multiplies the time needed by *NX-Ideas* even more. Note that in the context of multiple response design problems, this is a very small project. A metamodel of each response is used to compute each value in a few seconds, allowing the same optimization problem to be solved in a few hours. In the early stages of design this rapid identification of a promising design region provides time and flexibility to other design stakeholders to react to the evolving design region. We limited our model-fitting techniques to response surface modeling, kriging, and MARS.

Response surface models use ordinary least squares that minimize the sum of squared error between the true responses and their predicted values. Kriging models assume a particular covariance structure of the multivariate data, typically normal, and form an interpolating model that correctly predicts each of the points in the training data set used to build them.

MARS is fundamentally an extension of ordinary least squares that builds the piecewise polynomial that minimizes squared error or some other criterion.

Figure 3 depicts the implementation of the proposed technique for solving the robust design (i.e., optimization) problem with metamodels of the loss-scaled principal components. The models referenced in the second step of Figure 3 are plugged directly into the second component of multivariate quadratic loss, which estimates the off-target vector product. The $trace[\Sigma \hat{\mathbf{z}}_p]$ component is calculated by injecting a uniform design built around each design vector chosen by the optimization algorithm. This uniform design chooses from among four levels evenly spaced between 0.95 and 1.05 times the nominal values of each design vector. These runs are analogous to the outer design array of Taguchi designs, and the covariance matrix of these “noise” replicates represents the sensitivity to unavoidable variation in the design settings. These are intended to represent variation in the manufacture of mechanical components, so we chose a range of exaggerated manufacturing variability such as $\pm 5\%$. The trace term was then added to the estimate of off-target vector product ($\widehat{OTVP}$) to yield a metamodel-based estimate of multivariate quadratic loss ($\widehat{MQL}$) for each particular design vector.

This procedure can be used iteratively for moving from global to localized design spaces.

Robust design concerns random variables possessing the $trace[\mathbf{A} \Sigma \hat{\mathbf{y}}_{(x)}]$ term of multivariate quadratic loss calculated from the “noise replicates” associated with each particular design vector selected by the optimization algorithm. So far we have described only a purely deterministic optimization problem. This is a type II robust design problem per the terminology of Chen et al. (1996) where the response variance induced by each fixed design vector is artificially created. Note that $\pm 5\%$ was used for demonstrational purposes here; other values can be selected by the designer. These values are centered on the nominal design values and are meant to represent exaggerated manufacturing tolerances for mechanical components.

We chose a four-level uniform design constructed with 32 runs representing internal noise within each of the eight design variables because it provided a range of noise values with fast computation. This uniform design was run for each design vector $\mathbf{x}$ chosen by the optimization software iSIGHT (see Dassault-Systemes 2009). The trace term was calculated from the covariance matrix of the 32 resulting internal noise response vectors generated from each design vector considered. The trace term was then added to the $\widehat{OTVP}$ to yield $\widehat{MQL}$ for each particular design vector.

RESULTS OF THE ELECTRIC VEHICLE CHASSIS DESIGN WITH METAMODELS OF ORIGINAL, STANDARDIZED RESPONSES AND LOSS-SCALED PRINCIPAL COMPONENTS

We solved the design problem by minimizing the multivariate quadratic loss estimated by the metamodels of the standardized responses fit with three different modeling approaches. Note that $\widehat{MQL}$ is the estimated value of multivariate quadratic loss calculated with the metamodels, whereas multivariate quadratic loss is taken as the true loss value because it is derived through *NX-Ideas* rather than a metamodel. Table 3 compares the optimal solution vectors and corresponding $\widehat{MQL}$ values chosen by the three sets of response metamodels with those of the true optimal response calculated by *NX-Ideas*. The design values chosen by *NX-Ideas* and the modeling approach with the lowest multivariate quadratic loss, that is,

the value of multivariate quadratic loss calculated by plugging the optimal solution vector into *NX-Ideas*, are in boldface print.

It is interesting to note that the more sophisticated modeling approaches, namely, kriging and MARS, selected the individual variable design settings closest to those chosen by *NX-Ideas* in all cases. Response surface models (RSMs) tied MARS in selecting the best approximation for x_8 . This is not surprising given that the RSM model was limited to a second-order form with no interactions, whereas kriging and MARS allow for higher levels of curvature in the models.

We then fit models of the full set of six loss-scaled principal components using the same three types of models and used these within the optimization algorithm to solve for the optimal solution vector. We are interested in the final design vectors and the number of optimization cycles needed to find them. We repeated the process respectively with subsets of five and four loss-scaled principal component models to compare the resulting savings in computation and loss of accuracy.

A key concern when considering the use of principal components is whether to derive them from the covariance or correlation matrix of the data. Jackson (1985) stated that when the data (i.e., responses) are measured in different units or of greatly different magnitudes of variance, principal components should be derived from the correlation matrix. Otherwise, the covariance matrix is preferred for retention of original units. The widely varying response ranges in Table 3 mandated the derivation of our principal components from the response correlation matrix.

Choosing the correlation matrix implies the use of standardized response values that require that the values of the loss constant matrix (i.e., $\mathbf{A}$) are defined accordingly. Whereas Pignatiello (1993) explained in detail how the values of the loss constant matrix reflect the cost of being one unit off-target for the nonstandardized responses, this data set requires that our loss constant matrix values be defined as the cost of poor quality from being one standard deviation off-target in either direction. The off-diagonal values reflect the additional cost penalty incurred from that pair of responses being simultaneously one standard deviation off-target.

In order to measure consistency between the three model-fitting approaches we generated a 64-test combination Latin hypercube across the design space for purposes of estimating the accuracy of prediction. This Latin hypercube design was run in *NX-Ideas* and the response values were compared to the values predicted by each model type. The maximum differences in residual errors between the different modeling approaches were in all cases less than or equal to 1.7 standard deviations and most times within fractions of a standard deviation. This indicated no substantive differences in their predictive ability across the 64-point verification design space. These differences are documented in Murphy (2004).

Design Vectors That Minimize Multivariate Quadratic Loss Estimated from Metamodels of Loss-Scaled Principal Components

A comparison of the resulting estimate of multivariate quadratic loss along with the corresponding design vectors and respective computation times yielded by metamodels of the loss-scaled principal components will allow us to judge the utility of our approach in this problem. Three tables are presented that compare the design vectors selected by combinations of model type and metamodel as follows. Table 4 compares optimal solution vector and computational time for the set of metamodels of all six loss-scaled principal components using the three modeling approaches and *NX-Ideas*. Tables 5 and 6 do the same

for formal subsets consisting of the first five and four loss-scaled principal components, respectively.

Each of these tables compares the design vector as well as the number of optimization cycles needed to solve. Each table compares the true solution chosen by *NX-Ideas* with the solutions chosen by their analogues among the different model approaches. Boldface print is used for the design solution values corresponding to the model-fitting approach producing the lowest value of multivariate quadratic loss as calculated by *NX-Ideas* as well as values chosen by *NX-Ideas*.

SUMMARIZING RESULTS AND CONCLUSIONS

The use of loss-scaled principal components is moderately successful in producing similar results in a shorter period of time. Due to time constraints, we only obtained the *NX-Ideas* solution corresponding to the off-target component of multivariate quadratic loss. This solution was obtained in 525 iterations over a period of 29 h. The robust solution includes the evaluation of a design vector's off-target component of loss followed by evaluation of 32 internal noise vectors centered around that same design vector. An individual cycle of evaluating the off-target component of loss takes approximately 4 min. Adding the noise replicates multiplies that computational time by a factor of 16, meaning that an individual cycle with noise replicates takes approximately 65 min. The estimated solution time for this robust design problem in *NX-Ideas*, assuming the same number of iterations as for the deterministic off-target component of loss, is approximately 22 days. All past experiments have shown that the trace-covariance component of loss in this problem makes up a small fraction of 1% of the multivariate quadratic loss associated with an optimal solution vector.

The metamodels each take less than half a minute to calculate the responses and noise replicates for each design vector selected by the optimization algorithm. This resulted in total solution time of a few hours for each of the metamodel-based techniques. Though the metamodels of the responses provide significant savings in computational time, those savings can be extended by using either the full set or a subset of the loss-scaled principal components of the data. For this example only, the following high-level observations are noted:

1. The full set of response metamodels yields design vector values very close to those of the *NX-Ideas* simulations.
2. The full set of response metamodels identifies the optimal solution vector much faster than *NX-Ideas* but not as accurately.
3. Using the full set of loss-scaled principal components models typically yields a design vector as close or closer to *NX-Ideas* than those chosen with the response models.
4. Using the full set of MARS models of loss-scaled principal components yielded a design vector close to optimal in less than half the number of optimization runs and hence computational time of the analogous response models.
5. For response surface models and kriging models, approximately the same number of optimization runs were required by the full sets of responses and loss-scaled principal components.
6. In all three modeling approaches, significant reductions in the number of optimization cycles was achieved by using either the full set or a subset of the models of the loss-scaled principal components. This gain in computation time is typically accompanied by some loss of accuracy in the design vector.

7. In this example, the use of loss-scaled principal components is feasible and useful in early design stages.

In the introduction of this article we defined our goal as restriction of the broader design space to a smaller region, which experimentation reveals as likely to contain the optimal solution to the design problem. The design solutions offered in Tables 3 and 4 are the full information solutions and define the most likely local region of ideal solutions. The first dimension is consistently the largest of all eight and the optimal solution space seems to be rather tightly restricted to 6mm+/-1 mm. Values in Tables 3 and 4 suggest that ideal solutions for dimensions 2, 4, 5, and 6 most likely reside in the range of 3.5–5.5 mm. In contrast, values in Tables 3 and 4 suggest that ideal solutions for dimension 3 range from 1.5 to 5.5 mm, perhaps indicating less sensitivity to noise variables, whereas the ideal solution for dimension 8 appears to reside in the smaller range of values between 3 and 4 mm. In summary, the solutions offered in Tables 3 and 4 provide a very useful restriction of the overall design space from which designers can more confidently start honing in on final solutions that are obtained with substantial reduction in computational time.

References

- Chen W, Allen J, Tsui K, Mistree F. A procedure for robust design: Minimizing variation caused by noise factors and control factors. *Transactions of the ASME*. 1996; 118:478–485.
- Dassault-Systemes. [accessed on April 30, 2009] iSIGHT. 2009. Available at: <http://www.simulia.com>
- Jackson JE. Multivariate quality control. *Communications in Statistics-Theory and Methods*. 1985; 14(11):2657–2688.
- Lin, Y. Master's thesis. Georgia Institute of Technology, School of Mechanical Engineering Theses and Dissertations; 2000. Robust design goal formulations and metamodeling techniques. URI:<http://hdl.handle.net/1853/15908>
- Murphy, T. PhD thesis. Georgia Institute of Technology, School of Industrial & Systems Engineering; 2004. Multivariate quality control using loss-scaled principal components. <http://smartech.gatech.edu/handle/1853/4916>
- Murphy T, Tsui K-L, Allen J. A review of robust design methods for multiple responses. *Research in Engineering Design*. 2005; 15:201–215.
- Ortega, RA. Master's thesis. Georgia Institute of Technology, School of Mechanical Engineering Theses and Dissertations; 1998. Robust design goal formulations and metamodeling techniques. URI:<http://hdl.handle.net/1853/18175>
- Pearson K. On lines and planes of closest fit to systems of points in space. *Philosophical Magazine*. 1901; 2:559–572.
- Pignatiello J. Strategies for robust multiresponse quality engineering. *IIE Transactions*. 1993; 25(3):5–15.
- Rolander N, Rambo J, Joshi Y, Allen J, Mistree F. An approach to robust design of turbulent convective systems. *Transactions of the ASME*. 2006; 128:844–855.
- Siemens, AG. [accessed on April 30, 2009] Nx-ideas. 2007. Available at: <http://usa.siemens.com>
- Taguchi, G. *Introduction to Quality Engineering: Designing Quality into Products and Processes*. White Plains, NY: Kraus International Publications; 1986.

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FIGURE 1.
Approximation of three-dimensional space with minimally orthogonal plane.

FIGURE 2.
Design factor locations on electric vehicle chassis.

FIGURE 3.

Using loss-scaled principal components (LSPC) Metamodels in estimated multivariate quadratic loss ($\widehat{MQL}$) to solve for design vector $\mathbf{x}$ for electric vehicle chassis (OTVP/off-target vector product).

TABLE 1**Design Variables and Ranges for Chassis Design**

Design variable	Part name	Geometry	Minimum (mm)	Maximum (mm)
x_1	Lower chassis structure	Rect. tube $w70 \times h100 \times x_1$	1.0	8.0
x_2	Rear end long. frame	Rect. tube $w70 \times h80 \times x_2$	1.0	8.0
x_3	Upper front end structure	Rect. tube $w50 \times h70 \times x_3$	1.0	8.0
x_4	Lower front end support structure	Rect. tube $w50 \times h50 \times x_4$	1.0	8.0
x_5	Floor structure and lower B-pillar	Hat $w120 \times h70 \times b40 \times x_5$	1.0	8.0
x_6	Upper front B-pillar	Hat $w120 \times h20 \times b40 \times x_6$	1.0	8.0
x_7	Upper rear B-pillar	Hat $w60 \times w20 \times h40 \times x_7$	1.0	8.0
x_8	Floor panels	Thin shell x_8	1.0	8.0

Data from Ortega (1998).

TABLE 2

Competing Performance Characteristics of the Electric Vehicle Chassis

Responses	Taguchi type	Product significance	Range	Target
BEND	NTB	Safety	0.00054–0.00125	0.00058
CURB	NTB	Safety	189 <i>M</i> –546 <i>M</i>	192 <i>M</i>
FRONT	NTB	Safety	125 <i>M</i> –406 <i>M</i>	130 <i>M</i>
MASS	NTB	Gas mileage	235–656	240
ROLL	NTB	Safety	18 <i>M</i> –61 <i>M</i>	20 <i>M</i>
TOR (stiffness)	NTB	Vehicle strength	0.00035–0.00129	0.00125

TABLE 3

Design Vectors and Computational Time from Metamodels of Original, Standardized Responses Bold Values Yielded by *NX-Ideas* and Kriging Produce Minimal Loss; Values for x_1 – x_8 in Millimeters

Design variable	<i>NX-Ideas</i> (off-target only)	RSM (robust)	Kriging (robust)	MARS (robust)
x_1 Lower chassis structure	0.0055264	0.0050753	0.0056379	0.0068702
x_2 Rear longframe	0.0030129	0.0046911	0.0038799	0.0030789
x_3 Upper front end	0.0015371	0.001	0.0027962	0.0011942
x_4 Lower front end	0.0039918	0.0046741	0.0041407	0.0038379
x_5 Floor and lower B-pillar	0.0042753	0.0049817	0.0036714	0.0031200
x_6 Upper front B-pillar	0.0045712	0.0051376	0.0047241	0.0051831
x_7 Upper rear B-pillar	0.0010877	0.0011156	0.001001	0.0011943
x_8 Floor panels	0.0044559	0.004	0.0057058	0.004
<i>MQL</i> Multivariate quadr. loss (NX-Ideas)	17.6368 (off-target only)	19.1172	18.066811	19.43
$\widehat{MQL}$ Est. of multivar. quadr. loss (metamodels)	Not used	18.2130	18.0982	17.5035
Runs to solve = (comp. time with iSIGHT software)	525 (29 h)	576 (81 min)	595 (342 min)	553 (314 min)

TABLE 4

Design Vectors and Computational Time from Full Set of Loss-Scaled Principal Components Metamodels
 Bold Values Yielded by *NX-Ideas* and Kriging Produce Minimal Loss; Values for x_1 – x_8 in Millimeters

Design variable	<i>NX-Ideas</i> (off-target only)	RSM (robust)	Kriging (robust)	MARS (robust)
x_1 Lower chassis structure	0.0055264	0.0049422	0.0052196	0.0063381
x_2 Rear long, frame	0.0030129	0.0044993	0.0042574	0.0035278
x_3 Upper front end	0.0015371	0.001	0.001	0.0013883
x_4 Lower front end	0.0039918	0.0048697	0.0053654	0.0041146
x_5 Floor and lower B-pillar	0.0042753	0.0048905	0.0044986	0.0039165
x_6 Upper front B-pillar	0.0045712	0.0051205	0.0052613	0.0041814
x_7 Upper rear B-pillar	0.0010877	0.001	0.001001	0.0013006
x_8 Floor panels	0.0044559	0.004	0.0020382	0.004
MQ_L Multivariate quadr. loss (NX-Ideas)	17.6368 (off-target only)	18.6257	18.4772	19.0712
$\widehat{MQ_L}$ Est. of multivar. quadr. loss (metamodels)	Not used	17.7158	17.8017	20.3608
Runs to solve = (comp. time with iSIGHT software)	525 (29 h)	566 (114 min)	714 (460 min)	235 (126 min)

TABLE 5

Design Vectors and Computational Time from Subset of Five Loss-Scaled Principal Components Models
 Bold Values Yielded by *NX-Ideas* and Kriging Produce Minimal Loss; Values for x_1 – x_8 in Millimeters

Design variable	<i>NX-Ideas</i>	RSM (robust)	Kriging (robust)	MARS (robust)
x_1 Lower chassis structure	0.0055264	0.0049496	0.0052916	0.0063913
x_2 Rear long, frame	0.0030129	0.0045719	0.0043554	0.0034834
x_3 Upper front end	0.0015371	0.001	0.001	0.0013882
x_4 Lower front end	0.0039918	0.0048394	0.0051764	0.0039860
x_5 Floor and lower B-pillar	0.0042753	0.0048741	0.0044571	0.0039031
x_6 Upper front B-pillar	0.0045712	0.0050785	0.0052396	0.0042977
x_7 Upper rear B-pillar	0.0010877	0.001	0.0010092	0.0013005
x_8 Floor panels	0.0044559	0.004	0.0021167	0.004
<i>ML</i> Multivariate quadr. loss (NX-Ideas)	17.6368	18.6531	18.5196	19.1005
$\widehat{ML}$ Est. of multvar. quadr. loss (metamodels)	Not used	15.6985	15.5207	18.1618
Runs to solve = (comp. time with iSIGHT software)	525 (29 h)	513 (98 min)	229 (141 min)	280 (149 min)

TABLE 6

Design Vectors and Computational Time from Subset of Four Loss-Scaled Principal Components Models
 Bold Values Yielded by *NX-Ideas* and RSM Produce Minimal Loss; Values for x_1 – x_8 in Millimeters

Design variable	<i>NX-Ideas</i> (off-target only)	RSM (robust)	Kriging (robust)	MARS (robust)
x_1 Lower chassis structure	0.0061328	0.0056615	0.0065985	0.0064214
x_2 Rear long, frame	0.0041071	0.0043851	0.0040401	0.0037083
x_3 Upper front end	0.0019598	0.0040582	0.0053019	0.0029500
x_4 Lower front end	0.0034235	0.0041176	0.0039482	0.0047322
x_5 Floor and lower B-pillar	0.0041462	0.0052525	0.0045717	0.0046497
x_6 Upper front B-pillar	0.0051624	0.0041565	0.0047048	0.0044643
x_7 Upper rear B-pillar	0.0014794	0.0015581	0.0018469	0.0018830
x_8 Floor panels	0.0030897	0.004	0.0040139	0.004
<i>MQL</i> Multivariate quadr. loss (NX-Ideas)	17.6368 (off-target only)	22.6823	25.5888	23.5363
$\widehat{MQL}$ Est. of multivar. quadr. loss (metamodels)	Not used	0.098	0.0094	0.1062
Runs to solve = (comp. time with iSIGHT software)	525 (29 h)	139 (17 min)	100 (59 min)	184 (96 min)