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# Using Gradients to Construct Response Surface Models for High-Dimensional Design Optimization Problems

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# Using Gradients to Construct Response Surface Models for High-Dimensional Design Optimization Problems

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**The response surface method (RSM) is one of the most common techniques for building approximation models using values of sampled data alone. In this work, a method for using both function values and their gradients with respect to the design variables in the problem and construct response surface (RS) models has been developed. This approach improves on the efficiency of using the RSM for high-dimensional design optimization problems. Provided that gradient information is available through inexpensive algorithms such as the adjoint method, this approach significantly reduces the large computational cost needed for full RS model construction. The minimum number of function evaluations (CFD analyses, in our case) required for a full quadratic RS model increases with the square of the number of design variables, $N$, effectively preventing their use in high-dimensional design optimization. In contrast, the proposed modification to the RS model, which incorporates gradient information, can approximate the original function with order $N$ function evaluations, without significantly sacrificing the accuracy of the approximation. After validating the feasibility of the proposed method using simple one- and two-dimensional analytic functions, the approach is applied to the aerodynamic design of a supersonic business jet. The results of this 7-variable design problem indicates that the method can be effectively used to construct response surfaces with greatly reduced computational cost. The advantages of the method become much more significant as the number of design variables increases.**

## Nomenclature

| | |
|---|---|
| $\alpha$ | weighting factor controlling the contribution of gradient information for RS construction |
| $\boldsymbol{\beta}$ | vector of the unknown coefficients in a response surface model |
| $\mathbf{b}$ | vector of the least squares estimator of $\beta$ |
| $C_D$ | drag coefficient |
| $\epsilon$ | random error |
| $L$ | sum of the squares of the errors |
| $N$ | number of design variables |
| $n_s$ | number of sample points (also called sites) |
| $n_t$ | number of test sample points to evaluate modeling error |
| $RMS_{ub}$ | unbiased root mean square error |
| $RS$ | response surface |
| $x$ | scalar component of $\mathbf{x}$ |
| $\mathbf{x}$ | vector denoting locations (sites) in design space |
| $\mathbf{X}$ | matrix of sample sites for RS model |
| $y(.)$ | unknown function |
| $\hat{y}(.)$ | estimated model function for y(.) |

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## 1. Introduction

COMPUTATIONAL Fluid Dynamics (CFD) methods are recently gaining ground as a design tool for aerospace systems. The optimization of aerospace systems is an iterative process that requires computational models embodied in complex and expensive analysis software. This paradigm is well exemplified by the field of Multidisciplinary Design Optimization (MDO) which attempts to exploit the synergism of mutually interacting disciplines in order to improve the performance of a given design, while increasing the level of confidence that the designer places on the outcome of the design itself. However, MDO methods greatly increase the computational burden and complexity of the design process.[1,2] For this reason, high-fidelity analysis software typically used in single discipline designs may not be suitable for direct use in MDO.[3] Faced with these problems, the alternative of using approximation models of the actual analysis software has received increased attention in recent years. A second advantage of using approximation models during optimization process is that they can be used with optimization algorithms which do not rely on the computation of sensitivity derivatives.

One of the most common methods for building an approximate model is the response surface method

(RSM) in which a polynomial function of varying order (usually a quadratic function) is fitted to a number of sample data points using least squares regression. This method has achieved popularity since it provides an explicit functional representation of the sampled data, and is both computationally cheap to run and easy to use. However, response surface models have several key limitations: their accuracy is only guaranteed within a small trust region, and, by design, they are unable to predict multiple extrema. In addition, the use of these methods is limited to design optimization problems having only a small number of design variables, since the number of required function evaluations increases quadratically with the number of design variables. A modified RSM that requires fewer functional evaluations must be developed if the approximation method is to be used in a realistic MDO environment.

In this research, a modified RSM which uses gradient information is developed to reduce the computational cost of constructing traditional RS models. The finite difference method has often been used to calculate gradient information in a computational environment. This method results in a very high computational burden in high-dimensional problems since additional function evaluations are needed for each new variable. Therefore, the use of gradient information based on finite differencing to replace function evaluations does not result in improvements in computational performance. However, recently developed adjoint-based methods[7] can be used to compute gradient information of systems governed by PDEs with low computational cost. For a 7-dimensional problem, the complete gradient information at a given design point can be obtained with the equivalent of two function evaluations (one for the flow solution and the other for the adjoint calculation), whereas the finite difference approach requires 8 or N+1 (N being the number of design variables) function evaluations. At a given design point, a flow solver together with an adjoint method provides one function value and seven gradients in the direction of each design variable with the cost of *only* two function evaluations. Six flow calculations can be saved with the use of these seven gradients when constructing a RS model. The main idea of the modified RSM is to alleviate the high computational burden of constructing RS models for high-dimensional problems by using the gradient information calculated through a relatively inexpensive method instead of using function values. For the same example problem, the traditional RS method requires at least 36 flow solutions to construct the model. In contrast, the modified RS method with gradient information only requires as few as 5 function evaluations and 5 adjoint calculations. One adjoint calculation takes about same amount of computational effort as one function evaluation; therefore, the minimum possible computational cost to construct a RS model can be reduced to the equivalent of 10 flow solutions. This means that the required number of flow calculations for the proposed method is only linearly proportional to the number of design variables rather than quadratically proportional as needed for the original RSM. The benefit of the modified method will become more significant for problems involving large numbers of design variables.

In our work, the proposed concept was first tested using simple 1-D and 2-D analytic functions for validation and visualization purposes. The tests show excellent agreement between the original and modified RS models. The investigation of the applicability of this method to realistic problems was pursued by looking at the aerodynamic tailoring of the supersonic wing-body business jet mentioned above. Seven design variables were used to describe the aerodynamic shape in this test case.

# 2. Overview

## 2.1 Original RS Method

The response surface method (RSM) develops polynomial approximation models by fitting the sample data using a least squares regression technique. The true response can be written in the following form:

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

where $f(x)$ is an unknown response function and $\epsilon$ is the random error. The response surface model of equation (1) can be written in terms of a series of observations

$$y_i = \beta_0 + \sum_{j=1}^{k} \beta_j x_{ij} + \epsilon_i, \qquad i = 1, 2 \ldots n_s, \tag{2}$$

where $x_{ij}$ denotes the ith observation of variable $x_j$ and $n_s$ is the number of samples.

Equation (2) may be written in matrix form as

$$\boldsymbol{y} = \boldsymbol{X\beta} + \boldsymbol{\epsilon}, \tag{3}$$

where

$$\boldsymbol{y} = \left\{ \begin{array}{cccc} y_1 & y_2 & \ldots & y_n \end{array} \right\}^T, \qquad \text{and}$$

$$\boldsymbol{X} = \begin{bmatrix} 1 & x_{11} & x_{12} & \ldots & x_{1k} \\ 1 & x_{21} & x_{22} & \ldots & x_{2k} \\ . & . & . & & . \\ . & . & . & & . \\ . & . & . & & . \\ 1 & x_{n1} & x_{n2} & \ldots & x_{nk} \end{bmatrix}.$$

$\beta$ is a (k $\times$ 1) vector of the regression coefficients, and $\epsilon$ is an (n $\times$ 1) vector of random errors.

The vector of least squares estimators, **b**, is determined in a way that it minimizes

$$L = \sum_{i=1}^{n} \epsilon_i^2 = (\boldsymbol{y} - \boldsymbol{X\beta})^{\boldsymbol{T}}(\boldsymbol{y} - \boldsymbol{X\beta}). \tag{4}$$

This condition simplifies to

$$\boldsymbol{X^T X b = X^T y}. \tag{5}$$

Thus, the least squares estimator of $\beta$ is

$$\boldsymbol{b = (X^T X)^{-1} X^T y}. \tag{6}$$

The reader if referred to Ref.[5] for more details on the development of the RSM technique.

### 2.2 Modified RS Method

The modified RS method uses a reduced number of observations together with gradient information when constructing the vector, $\boldsymbol{y}$, and the matrix, $\boldsymbol{X}$, instead of using the full number of observations required for the original RS model. Equation (3) can be replaced by

$$\boldsymbol{y_m = X_m \beta + \epsilon}, \tag{7}$$

and $\mathbf{b}$, the vector of least squares estimators of $\beta$ can be obtained as

$$\boldsymbol{b = (X_m{}^T W X_m)^{-1} X_m{}^T W y_m}, \tag{8}$$

where, for a 2-D problem, $\boldsymbol{y_m}$, $\boldsymbol{X_m}$ and the weighting matrix, $W$, can be defined as

$$\boldsymbol{y}_m = \left\{ \begin{array}{cccccc} y_1 & y_2 & g_{11} & g_{21} & g_{12} & g_{22} \end{array} \right\}^T,$$

$$\boldsymbol{X}_m = \begin{bmatrix} 1 & x_{11} & x_{12} & x_{11}^2 & x_{12}^2 & x_{11}x_{12} \\ 1 & x_{21} & x_{22} & x_{21}^2 & x_{22}^2 & x_{21}x_{22} \\ 0 & 1 & 0 & 2x_{11} & 0 & x_{12} \\ 0 & 1 & 0 & 2x_{21} & 0 & x_{22} \\ 0 & 0 & 1 & 0 & 2x_{12} & x_{11} \\ 0 & 0 & 1 & 0 & 2x_{22} & x_{21} \end{bmatrix},$$

$$\boldsymbol{W} = \begin{bmatrix} \alpha & 0 & 0 & 0 & 0 & 0 \\ 0 & \alpha & 0 & 0 & 0 & 0 \\ 0 & 0 & (1-\alpha) & 0 & 0 & 0 \\ 0 & 0 & 0 & (1-\alpha) & 0 & 0 \\ 0 & 0 & 0 & 0 & (1-\alpha) & 0 \\ 0 & 0 & 0 & 0 & 0 & (1-\alpha) \end{bmatrix},$$

where $g_{ij}$ denotes the gradient of $y_i$ in the direction of variable $x_j$ ($\frac{\partial y_i}{\partial x_j}$), and $\alpha$ is a weighting factor controlling the contribution of gradient information to the least squares regression process.

The minimum number of observations needed to construct the original RS model is given by $(N+1)(N+2)/2$, where $N$ is the number of variables. This number increases quadratically with $N$, which prevents the RS method from being used for high-dimensional design applications. However, the proposed RS method needs only small fraction of the total observations needed for the original RS method since it also uses gradient information at the locations of the observations. This advantage of the modified RS method allows it to be effectively incorporated into high-dimensional design problems. For 2 variable cases, the original RS model needs at least 6 observations at different design points since there are six unknown coefficients in the quadratic function that is being fitted to the data. When utilizing gradient information, we can construct the $\boldsymbol{y_m}$ vector and $\boldsymbol{X_m}$ matrix with only two observations and four gradients, two with respect to each design variable. We can eliminate the required CFD analyses to compute the coefficients of cross product terms in the model equation by using gradient information obtained from an adjoint-based method. Assuming the gradient information can be obtained cheaply using an adjoint-based method, this newly proposed procedure greatly reduces the computational cost of generating accurate RS models.

### 2.3 Modeling Error Estimation

Each approximation model was constructed based on the CFD results obtained at $n_s$ sample points. To evaluate the modeling accuracy, another set of CFD calculations were performed at $n_t$ randomly selected validation points and the computed results of $C_D$ values were compared with the predictions from the approximation models at the same test locations. The accuracy of RS models were compared using the unbiased root mean squared (RMS) error, $RMS_{ub}$, and the average % error.

The modeling error at each test site is defined as the difference between the actual result from the CFD analysis ($\hat{y_i}$) and the predicted value from the RS model ($y_i$).

$$\delta_i = |\hat{y_i} - y_i|, \qquad i = 1, ..., n_t. \tag{9}$$

The average % error is defined as

$$\text{average \% error} = \frac{1}{n_t}\sum_{i=1}^{n_t}\left(\frac{\delta_i \times 100.0}{y_i}\right), \tag{10}$$

and RMS error is:

$$RMS_{ub} = \sqrt{\frac{\sum_{i=1}^{n_t}\delta_i^2}{n_t}}. \tag{11}$$

## 3. Test Problem : Supersonic Business Jet(SBJ) Design

The design problem in question involves the drag minimization of a supersonic business jet wing-body configuration at a specified lift coefficient. The aircraft geometry and flow conditions were parameterized with a total of 22 potential design variables.

For the initial test case, total of 7 geometric design variables were used. The chosen design variables represent the radii at three different stations along the axisymmetric fuselage, ($x_1 \sim x_3$), and the thickness to chord ratios at four span-wise stations ($x_4 \sim x_7$).

The airfoil shape for all wing stations was selected as a simple biconvex airfoil of varying thickness. Once the design variables were selected, an automatic mesh generation procedure that was able to handle the geometry variations imposed by the changes in the design variables was utilized to automatically generate different sets of meshes needed for the CFD calculations.

The three-dimensional Euler solver, FLO87, developed by Jameson [8,9] was used to calculate aerodynamic coefficients at sample design points chosen by incrementing each variable from the baseline design value using a design of experiments approach. The free-stream flow conditions were fixed at $M_\infty = 1.5$ and the coefficient of lift, based on the wing planform area was fixed at $C_L = 0.1$. Response surface models were built using drag output data from the Euler solver, and were incorporated into the nonlinear optimization code SNOPT which has been developed by Gill, et al.[10] to perform realistic design optimization calculations.

## 4. Design Tools

### 4.1 Grid Generator

A grid generator called CH-GRID developed by Reuther et al. was used for mesh generation for supersonic business jet wing-body configurations. CH-GRID is a stand-alone form of the C-H type grid generator for the adjoint-based, single-block wing-body design code, SYN87-SB. Figure 2 shows a typical wing-body mesh. A geometry generation engine was constructed for this work so that the input geometry for CH-GRID can be easily created using an input file that contains the values of the design variables described above.

### 4.2 Flow Solver and Gradient Module

The CFD flow solver must meet fundamental requirements of accuracy, efficiency, robustness, and fast convergence to be used in an high-dimensional design optimization problem. The accuracy is important because the approximation model accuracy and the improvement predicted by the optimization process using these models can only be as good as the accuracy of the flow analysis itself. Efficiency is also required when the number of design variables increases and the required number of the sample evaluations for constructing the approximation models increases accordingly. The robustness of the solver, i.e., its ability to obtain a flow solution for a variety of configuration shapes and flow conditions, is particularly critical for the construction of sample databases for the approximation models, in which large variations of the design variables is allowed. In addition, the benefit of aerodynamic optimization lies in obtaining the last few percentage points in aerodynamic efficiency. In such cases, the solution must be highly converged such that the noise in the figure of merit is well below the level of realizable improvement. [11]

Jameson's FLO87 code used in this study easily met all of the previously mentioned criteria. FLO87 solves the steady three-dimensional Euler equations using a modified explicit multistage Runge-Kutta time stepping scheme. FLO87 achieves fast convergence with the aid of multigridding and implicit residual smoothing. Also, a driver program called RS87 was developed to utilize multiprocessor computers for analyzing a number of different configurations simultaneously.

The necessary gradient information for the construction of the response surface models was obtained in the manner described earlier with the use of an adjoint-based method. Details of the adjoint methodology have been previously published in the literature and are mathematically involved. These details are omitted in this paper, but the reader is referred to[11–13] for more details. The particular implementation used in this work is that embodied in the SYN87-SB solver developed by Reuther and Jameson. The flow solver in this design code is effectively the FLO87 solver described above.

### 4.3 Optimization Procedure

Drag minimization of wing-body configurations was performed using the SNOPT program. SNOPT uses a sequential quadratic programming (SQP) algorithm that obtains search directions from a sequence of quadratic programming subproblems.[10] Nonlinear constraints were imposed on the minimization process by setting bounds for the values of the design variables and constraining the admissible ranges of wing (wv) and fuselage volume (fv). The optimization problem can be written as

$$\min_{x \in R^m} \; C_D(x), \tag{12}$$

subject to

$$\begin{aligned} 0.8\times wv_i \le wv \le 1.2\times wv_i, \\ 0.8\times fv_i \le fv \le 1.2\times fv_i, \\ x_{min} \le x \le x_{max}, \end{aligned}$$

where $wv_i$ and $fv_i$ are the initial wing and fuselage volumes.

## 5. Results and Discussion

### 5.1 Graphical Validation of Modified RS Method using Simple Analytic Test Functions

The modified RS technique was applied to approximate simple one- and two-dimensional analytic functions. The results were compared with those of the original RS method for validation purposes only. Figure 3 shows the results of the one-dimensional validation case. The original RS model was fitted to three sample data points while the modified RS model was constructed with only two sample sites and their corresponding gradients. Although the modified RS is far off from the actual function when the sample sites are separated by large distances, $\Delta x$, the two RS models become nearly identical as $\Delta x$ decreases. With proper selection of the optimization algorithm, the modified RS can effectively predict local extrema.

For two-dimensional graphical validation of original and modified RS models, an analytic test function called the *peaks* function was chosen from MATLAB User's Guide[14] as shown in Figure 4 (a). Results from this test case can also be seen in Figure 4. The original RS model was fitted to 6 sample points around the global minimum of the test function, while the modified RS model used 3 sample sites and their gradients in each direction, which make up a total of 9 pieces of information (3 function values and 6 gradients) available for surface fitting. Both approximation models accurately predicted the global minimum and the general shape of the test function. These graphical examples clearly demonstrate the applicability of the modified RS model for simple 1- and 2-dimensional function approximation. Although in these simple test cases, the computational savings are minimal, when the number of design variables grows, the use of the modified RS technique becomes compelling.

### 5.2 Graphical Validation of RS Models for SBJ Test Problem

To further investigate their ability to model the results of the original CFD code, 7-dimensional RS models were created for $C_D$ of the supersonic business jet test problem, using sample data obtained from CFD analysis. For the original RS model a total of 36 CFD analyses are necessary to obtain the coefficients of the functional fit. For the modified RS model, 15 sample points together with gradient information at these points were used. One-dimensional slices of the 7-dimensional RS models generated through both the original and modified methods are plotted in Figure 5 for the first and fifth design variables corresponding to the radius of a fuselage station ahead of the leading edge of the wing, and to the $t/c$ ratio of the wing station located right at the side-of-body. Additional runs of the flow solver are included to get a feeling for the accuracy of the presented techniques. The original and modified RS models appear to resolve the function of interest (coefficient of drag) quite well over a wide range of values of the design variables.

Figure 6 shows two-dimensional slices of original and modified RS models for the same test case. As in the one-dimensional surface cut case, the ability to locate a local minimum and the general shapes of two models are quite similar. Through these graphical comparisons, the authors have gained confidence on the fact that the modified RS model can approximate the response function as accurately as the original RS models could.

### 5.3 Design of Experiments and Modeling Accuracy Comparison

In general, the second-order RS model has the form

$$\hat{y} = \beta_0 + \sum_{j=1}^{N} \beta_j x_j + \sum_{i \leq j} \beta_{ij} x_i x_j, \tag{13}$$

in which there are $(N+1)(N+2)/2$ coefficients to be estimated, where $N$ is the number of variables. When constructing a quadratic model, the design variables need to be evaluated at least at 3 locations to estimate the coefficients in the model. This leads to a $3^N$ factorial design of experiments that requires $3^N$ data samples. However, the Central Composite Design (CCD) introduced by Box, et al.[15] has become a popular alternative for second-order RS models. CCDs are first-order ($2^N$) designs augmented by additional points to allow for the estimation of the second-order coefficients.[16] Unal, et al.[3] found out that CCD enabled the efficient construction of second-order RS models with significantly less effort than for a full factorial design. Moreover, the fitted model could be successfully used within an MDO process with reasonable accuracy for cases with four to six design variables. However, for design problems dealing with a large number of design variables, even CCD becomes unrealistic in the optimization process.

In this work, two design of experiments (DOE) methods for the original RS model were investigated and the results of their modeling accuracy were compared with those of the modified RS model constructed based on a star design in which only the central point and the axial points along the each variable direction were sampled. The first DOE tested for the original RS was CCD and the second one was the minimum point design (MPD). The number of functional evaluations needed for MPD is exactly equal to the number of coefficients in the RS model. Thus, the minimum number of CFD calculations needed to construct a RS model for the 7-dimensional design problem was 36 and that for CCD was 143 with only one center point. In contrast, only 8 or 15 sample data points were needed for the two variations of the star design with the modified RS model. The modified RS model was constructed with the CFD results from 15 design points selected from the original 36, and their gradients in each variable direction. The total number of pieces of the information used for the modified RS model is 120 (15 function values and 15*7 gradients) which are typically available inexpensively from an adjoint-based sensitivity calculation method such as the one described above. Figure 7 illustrates each DOE method mentioned above for a two-dimensional case.

The results of a comparison study of these different design of experiments methods are summarized in Table 1. RS models were constructed based on the sample data collected from CCD, MPD and a star design and their modelling accuracy was checked with CFD computations over a different set of 228 test points. The results show that the RS model using CCD generally has the lowest error when compared with models using MPD or the star design approaches. However, the difference between them is very small as seen by the results in the Table. Thus, we can conclude that the modified RS model based on the star design using only axial sample points can approximate the response function with similar accuracy to the original RS models using MPD or CCD, proving that the CFD calculations needed to fit cross product terms in the response surface approximation function can be reduced and/or eliminated and replaced by gradient information at a series of sites, where only one design variable is changed at a time.

Note that the accuracy of the modified RS model is even slightly better than that of the original RS model using MPD. The result is mainly due to the fact that the total number of data used in the modified RS method is much larger since the gradients along all the design variable directions at each sample point are used in addition to the function values at the same sample points. The result might also be attributed to the existence of the weighting factor, $\alpha$ in the modified RS method. $\alpha$ was chosen in such a way to minimize the average % error over the set of 228 test points. Therefore, the modified RS model has one more degree of freedom to adjust itself to the test data, which, in turn, reduces the error. However, the existence of the weighting brings about the problem of selecting the best value for $\alpha$. This is not a trivial problem, especially when information about the design space is not available. However, in typical design problems, similar designs are repeated several times. The results from earlier designs can serve to adjust the value of the $\alpha$ parameter.

For demonstration purposes, one optimization cycle for each case mentioned above was carried out and the results are also compared in Table 1. As can be seen, all three models have almost same trends in predicted optimum value ($C_D$) and the design variables. This result also contributes to the validation of the modified RS model for use in realistic design problems. One interesting point is that the results from the 1st optimization cycle using the CCD based RS model are really close to those from the 3rd optimization cycle using the minimum point design as shown in Table 2. Therefore, the conclusion is reached that the CCD based RS model generally has better chances of locating the minimum point in fewer optimization cycles; however, the sequential optimization process using the RS model with MPD has almost the same ability with less computational cost since the number of required CFD evaluations for three optimization cycles with MPD is 108 whereas CCD requires 143 computations for a single design cycle.

### 5.4 Optimization Results Comparison

The base design point for the SBJ design problem was chosen to be given by the following values of the design variables in the problem: $x_1$=0.45, $x_2$=0.45, $x_3$=0.3, $x_4 \sim x_7$=2.0(%). The design variables are defined in section 3. Design optimization was performed using three different RS models with the following limits on design variables and constraints. The results from three successive optimization cycles are presented in Table 2.

$$\begin{aligned}
0.8\times wv_i \le wv \le 1.2\times wv_i,\\
0.8\times fv_i \le fv \le 1.2\times fv_i,\\
0.35 \le x_1 \le 0.55,\\
0.35 \le x_2 \le 0.55,\\
0.20 \le x_3 \le 0.40,\\
1.60 \le x_4 \le 2.40,\\
1.60 \le x_5 \le 2.40,\\
1.60 \le x_6 \le 2.40,\\
1.60 \le x_7 \le 2.40,
\end{aligned}$$

where $wv_i$ and $fv_i$ are the initial wing and fuselage volumes.

Three test cases are chosen: the first consists of optimization based on the original RS model, the second is based on the modified RS model with 15 sample design points and their gradients, and the last is based on the modified RS model with 8 sample design points and their gradients. Three optimization cycles were performed for each test case.

As shown in Table 2, the predicted optimum design point and optimum value of $C_D$ for these cases become nearly identical after the 3rd cycle. The predicted $C_D$ for the original RS model case is 0.0072704 whereas that for the modified RS model with 15 sample points is 0.0072723 with almost same optimum design points. Note that the fuselage radii defined at just forward of wing ($x_1$) and aft of wing ($x_3$) tends to increase. This trend follows the well known supersonic area rule for the configuration in question. Also, the thickness-to-chord ratios except the one defined at inside of fuselage ($x_4$) all tend to decrease to the variable limit of 1.6% as expected. The reduced cross sectional volume will result in a reduction in the volume dependent supersonic wave drag. The total of 5.5 % $C_D$ reduction was achieved for the first case while the reduction for the second case was slightly lower at 5.4 %.

### 5.5 Further Error Estimates of Modified RS Model and Projected Gains for High-Dimensional Problems

The investigation of the effect of the number of sample sites on the accuracy of the modified RS method is presented in Figure 8. The average percentage error and RMS error over 108 randomly selected sample points are plotted against the the number of sample points used in the construction of the approximations. The number of sample points used in the construction of the approximation ranges from the minimum amount of 36 to only 5 points. The error is nearly constant up to the 15 point case and it increases sharply for fewer data points. The case with 15 sample data points requires taking the baseline design point $\pm$ a $\Delta x$ deviation from the base along all coordinate directions and the gradients at all of these locations. This figure clearly shows that the additional CFD calculations needed to account for the cross product terms in the RS model can be eliminated with the use of gradient information. The result illustrates the fact that the required number of sample data or CFD calculations for fitting a RS model increases only linearly with the number of design variables, as compared to the quadratic increase in the original RS method.

Projected computational savings for the modified RS method are plotted in Figure 9. For the more realistic case of 40 design variables, the required number of sampling points for the original RS model with MPD is 861, whereas for the modified RS model using gradient information obtained from an adjoint method it is only 162. Therefore a computational cost equivalent to about 700 CFD analyses can be realized. The graph shows the apparent advantage of the method in high-dimensional cases.

## Conclusions

In this study, a way to improve the efficiency of traditional RS method by using gradient information at the sampling sites was proposed and its applicability in a realistic design problem was evaluated for 7-dimensional Supersonic Business Jet Design problem. It was demonstrated that the modified RS method could generate approximation models as accurately and effectively as the original RS method with the greatly improved efficiency of the method in terms of reducing the computational cost for obtaining sample data. Confidence on the fact that the proposed method can be used efficiently in realistic high-dimensional design problems such as in complex multidisciplinary system design was gained. In particular, we are interested in using this type of procedure to extend the use of adjoint methods to more dramatic geometry changes such as those to be found in planform and geometry optimization. For design problems where larger areas of the design space are investigated, a procedure such as the one described in this work is likely to be more effective than traditional adjoint approaches where small steps for changes in the configuration are required.

## Future Work

The presented study identified the areas of further investigation. They include (1) the research on a robust method to determine the weighting factor, $\alpha$, (2) the testing of the modified RS method in more realistic design applications, (3) the investigation on various techniques of design of experiments (DOE) most suitable for the proposed method, and (4) the applicability test of using gradients in other approximation model techniques such as Kriging.

## References


[1]Thomas A. Zang and Lawrence L. Green. "Multidisciplinary Design Optimization Technique: Implications and Opportunities for Fluid Dynamics *30th AIAA Fluid Dynamics Conference*, Norfolk, Virginia, AIAA 99-3798, June 1999

[2]Jaroslaw Sobieszczanski-Sobieski and Raphael T. Haftka "Multidisciplinary Aerospace Design Optimization: Survey of Recent Developments," *34th AIAA Aerospace Sciences Meeting and Exhibit* , Reno, Nevada, AIAA 96-0711, January 1996.

[3]Resit Unal, Roger A. Lepsch, Jr. and Mark L. McMillin "Response Surface Model Building and Multidisciplinary Optimization Using Overdetermined D-Optimal Designs," *7th AIAA/USAF/NASA/ISSMO Symposium on Multidisciplinary Analysis and Optimization*, St. Louis, Missouri, AIAA 98-4759, September 1998

[4]Virginia Torczon and Michael W. Trosset "Using Approximation to Accelerate Engineering Design Optimization," *ICASE Report 98-33*, Hampton, Virginia, 1998

[5]Raymond H. Myers and Douglas C. Montgomery *Response Surface Methodology:Process and Product Optimization Using Designed Experiments*, John Wiley, New York, 1995.

[6]J. R. Koehler and A. B. Owen "Computer Experiments," *Handbook of Statistics Vol. 13*, pp. 261-308, Elsevier Science, New York, eds. S. Ghosh and C. R. Rao

[7]A. Jameson "Optimum Aerodynamic Design Using CFD and Control Theory" *AIAA 12th Computational Fluid Dynamics Conference* , AIAA paper 95-1729, San Diego, CA, June 1995.

[8]A. Jameson, W. Schmidt, and E. Turkel "Numerical Solutions of the Euler Equations by Finite Volume Methods with Runge-Kutta Time Stepping Schemes," *AIAA Paper 81-1259*, Jan. 1981.

[9]A. Jameson "Multigrid Algorithms for Compressible Flow Calculations," *Lecture Note in Mathematics* edited by W. Hackbusch and V. Trottenberg, Vol. 1228, Springer-Verlag, 1986.

[10]Philip E. Gill, Walter Murray and Michael A. Saunders "User's Guide for SNOPT 5.3: A Fortran Package for Large-scale Nonlinear Programming," *Technical Report* SOL 98-1 Dept. of Engineering Economic Systems and Operations Research, Stanford Univ., Stanford, CA, 1998

[11]James J. Reuther, Antony Jameson, and Juan J. Alonso "Constrained Multipoint Aerodynamic Shape Optimization Using an Adjoint Formulation and Parallel Computers, Parts I and II," *Journal of Aircraft* Vol 36, No 1, January-February, 1999

[12]A. Jameson, L. Martinelli and N. A. Pierce "Optimum Aerodynamic Design Using the Navier-Stokes Equations," *Theoretical and Computational Fluid Dynamics* Vol 10, pp. 231–237, 1998.

[13]A. Jameson, N. Pierce and L. Martinelli "Optimum Aerodynamic Design Using the Navier-Stokes Equations," *AIAA Paper 97-0101*, Jan. 1997.

[14]*MATLAB User's Guide for Unix Workstations*, The MathWorks, Inc. Mass., August 1992, January-February, 1999

[15]G. E. Box, and K. B. Wilson, "On the experimental Attainment of Optimum Conditions," *Journal of the Royal Statistical Society* Series B, 13, 1-45.

[16]G. E. Box, and N. R. Draper, *Empirical Model Building and Response Surfaces*, John Wiley, New York, NY, 1987.

| Design of Experiment | Model Accuracy Comparison | | | Optimization Comparison | | | |
|---|---|---|---|---|---|---|---|
| | RMS | Ave. % Error | Mean Error | 1st Design Cycle Results | Predicted Optimum ($C_D$) | Verified Optimum by CFD | % Error |
| **Central Composite Design** (143 Samples) | 1.1425E-4 | 0.4119 % | 3.7324E-5 | $x_1$ = 0.481<br>$x_2$ = 0.441<br>$x_3$ = 0.325<br>$x_4$ = 2.400<br>$x_5$~$x_7$ = 1.600 | 0.007276 | 0.007271 | 0.069 % |
| **Minimum Point Design** (36 Samples) | 8.8712E-5 | 0.7155 % | 5.9924E-5 | $x_1$ = 0.482<br>$x_2$ = 0.418<br>$x_3$ = 0.286<br>$x_4$ = 1.653<br>$x_5$~$x_7$ = 1.600 | 0.007287 | 0.007305 | 0.244 % |
| **Modified RS Method With Star Design** (15 Samples & Gradients) | 9.3684E-5 | 0.6259 % | 5.3025E-5 | $x_1$ = 0.474<br>$x_2$ = 0.431<br>$x_3$ = 0.303<br>$x_4$ = 2.400<br>$x_5$~$x_7$ = 1.600 | 0.007271 | 0.007288 | 0.225 % |

**Table 1. Comparison of Design of Experiments for RS**
**(Errors estimated over 228 test points)**

| | | 1st Design Cycle | 2nd Design Cycle | 3rd Design Cycle |
|---|---|---|---|---|
| **Original RS Method** (36 Sample Sites) | Optimum Design | $X_1$ = 0.4816<br>$X_2$ = 0.4177<br>$X_3$ = 0.2862<br>$X_4$ = 1.653<br>$X_5$ = 1.600<br>$X_6$ = 1.600<br>$X_7$ = 1.600 | $X_1$ = 0.4770<br>$X_2$ = 0.4460<br>$X_3$ = 0.3313<br>$X_4$ = 2.400<br>$X_5$ = 1.600<br>$X_6$ = 1.600<br>$X_7$ = 1.600 | $X_1$ = 0.4811<br>$X_2$ = 0.4425<br>$X_3$ = 0.3247<br>$X_4$ = 2.400<br>$X_5$ = 1.600<br>$X_6$ = 1.600<br>$X_7$ = 1.600 |
| | Predicted Optimum | 0.00728711 | 0.00727620 | 0.00726608 |
| | Verified Optimum* | 0.00730491 | 0.00727142 | 0.00727036 |
| | % Error (%) | 0.244 | 0.066 | 0.059 |
| **Modified RS Method** (15 Sample Sites and their Gradients) | Optimum Design | $X_1$ = 0.4740<br>$X_2$ = 0.4312<br>$X_3$ = 0.3029<br>$X_4$ = 2.400<br>$X_5$ = 1.600<br>$X_6$ = 1.600<br>$X_7$ = 1.600 | $X_1$ = 0.4803<br>$X_2$ = 0.4357<br>$X_3$ = 0.3237<br>$X_4$ = 1.600<br>$X_5$ = 1.600<br>$X_6$ = 1.600<br>$X_7$ = 1.600 | $X_1$ = 0.4828<br>$X_2$ = 0.4402<br>$X_3$ = 0.3243<br>$X_4$ = 2.193<br>$X_5$ = 1.600<br>$X_6$ = 1.600<br>$X_7$ = 1.600 |
| | Predicted Optimum | 0.00727141 | 0.00723918 | 0.00726102 |
| | Verified Optimum* | 0.00728779 | 0.00728161 | 0.00727234 |
| | % Error (%) | 0.225 | 0.583 | 0.156 |
| **Modified RS Method** (8 Sample Sites and their Gradients) | Optimum Design | $X_1$ = 0.4983<br>$X_2$ = 0.4419<br>$X_3$ = 0.3607<br>$X_4$ = 2.400<br>$X_5$ = 1.807<br>$X_6$ = 1.600<br>$X_7$ = 1.600 | $X_1$ = 0.4799<br>$X_2$ = 0.4391<br>$X_3$ = 0.3270<br>$X_4$ = 1.600<br>$X_5$ = 1.600<br>$X_6$ = 1.600<br>$X_7$ = 1.600 | $X_1$ = 0.4815<br>$X_2$ = 0.4484<br>$X_3$ = 0.3428<br>$X_4$ = 1.955<br>$X_5$ = 1.600<br>$X_6$ = 1.600<br>$X_7$ = 1.600 |
| | Predicted Optimum | 0.00722336 | 0.00721061 | 0.00727253 |
| | Verified Optimum* | 0.00732571 | 0.00728047 | 0.00727810 |
| | % Error (%) | 1.420 | 0.969 | 0.077 |

**Table 2. Optimization Results Comparison**
**(* Calculated using CFD analysis code with predicted optimum design)**

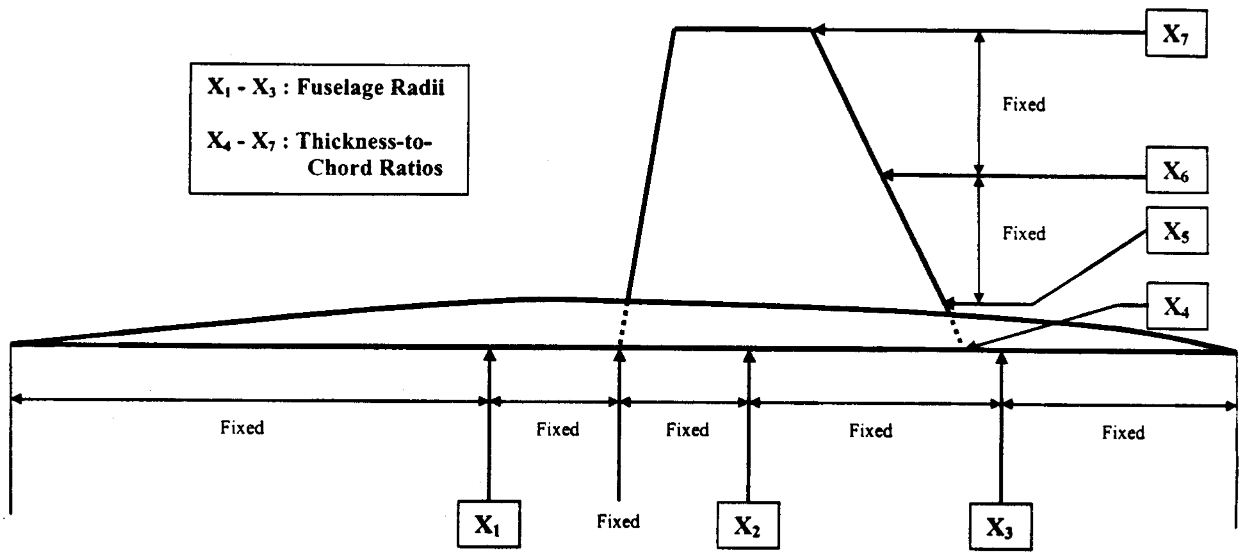



**Fig. 1 Definition of Design Variables for SBJ Wing-Body Configuration**

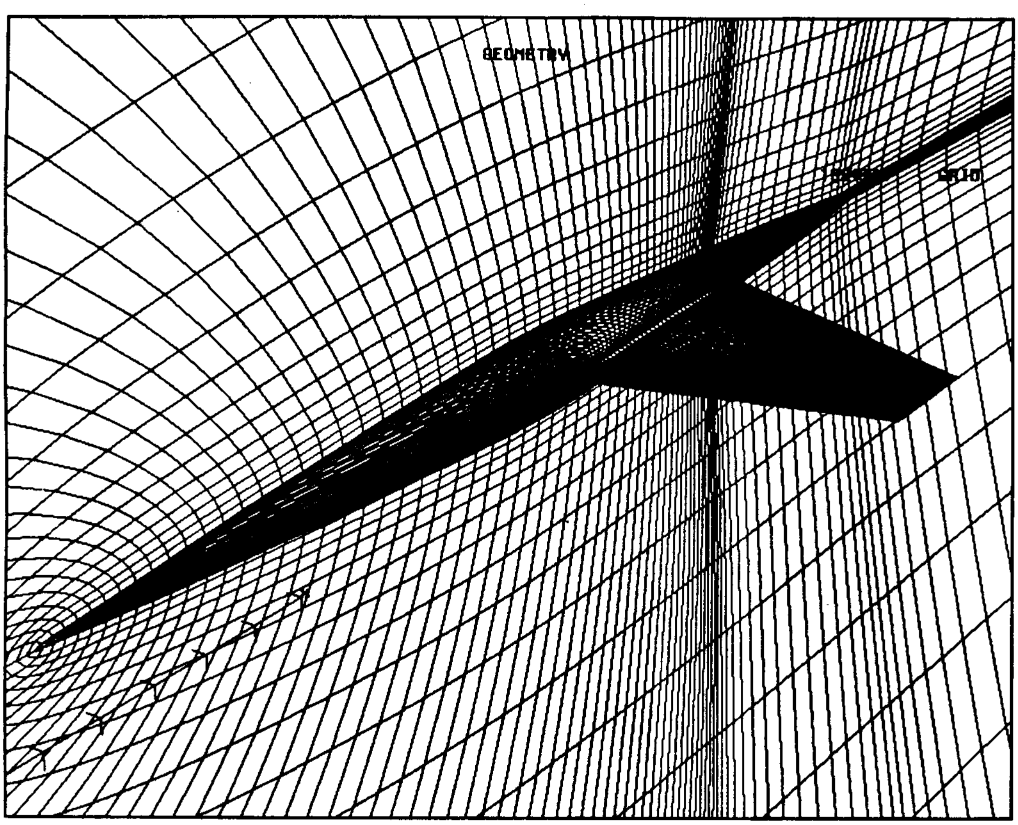
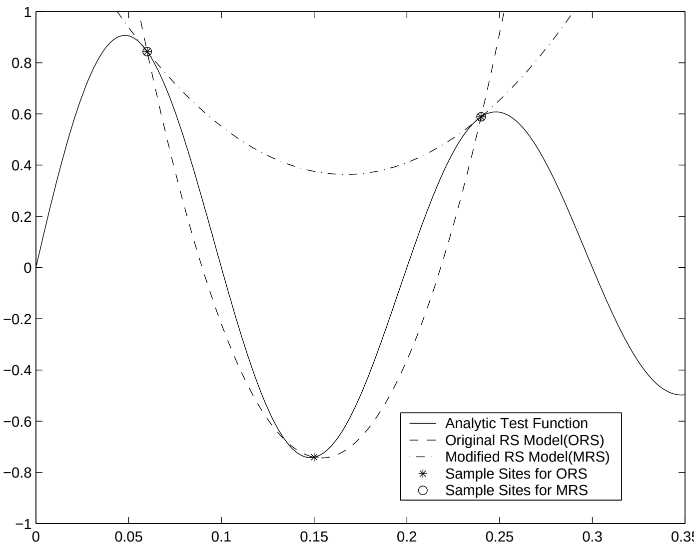
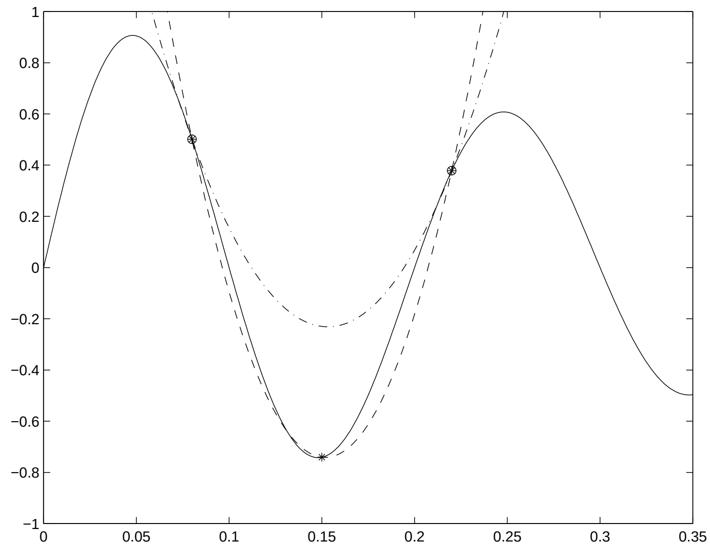


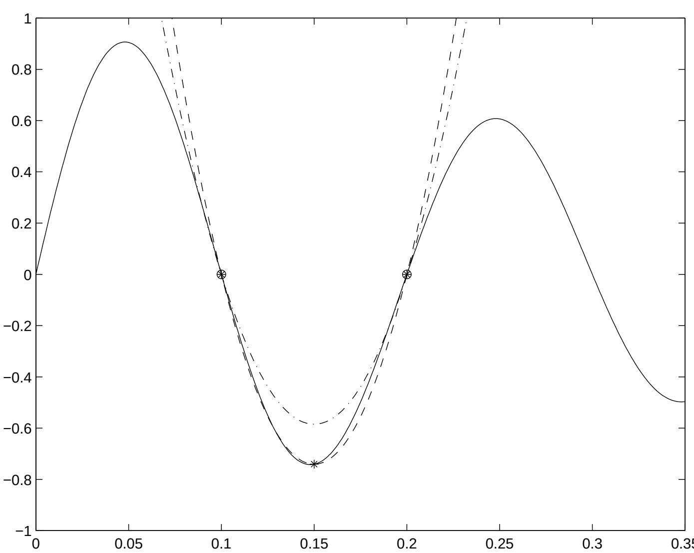
**Fig. 2 A Typical Supersonic Business Jet Mesh for CFD Calculation**



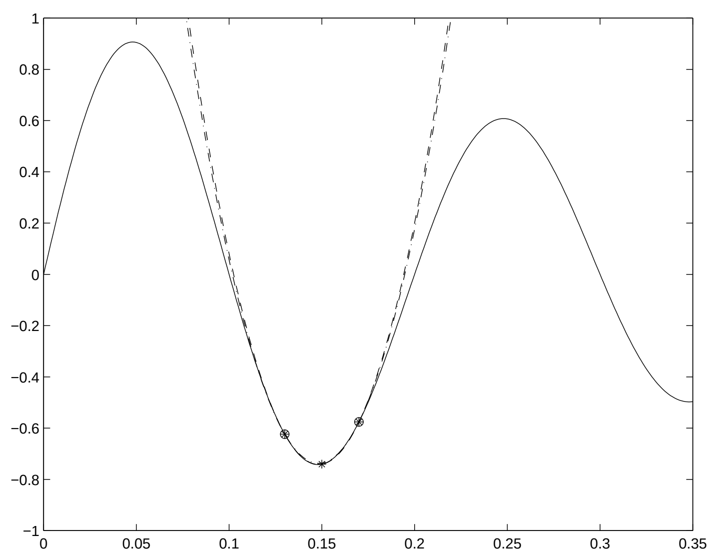

(a) Sample Sites x=[0.06, 0.15, 0.24]



(b) Sample Sites x=[0.08, 0.15, 0.22]

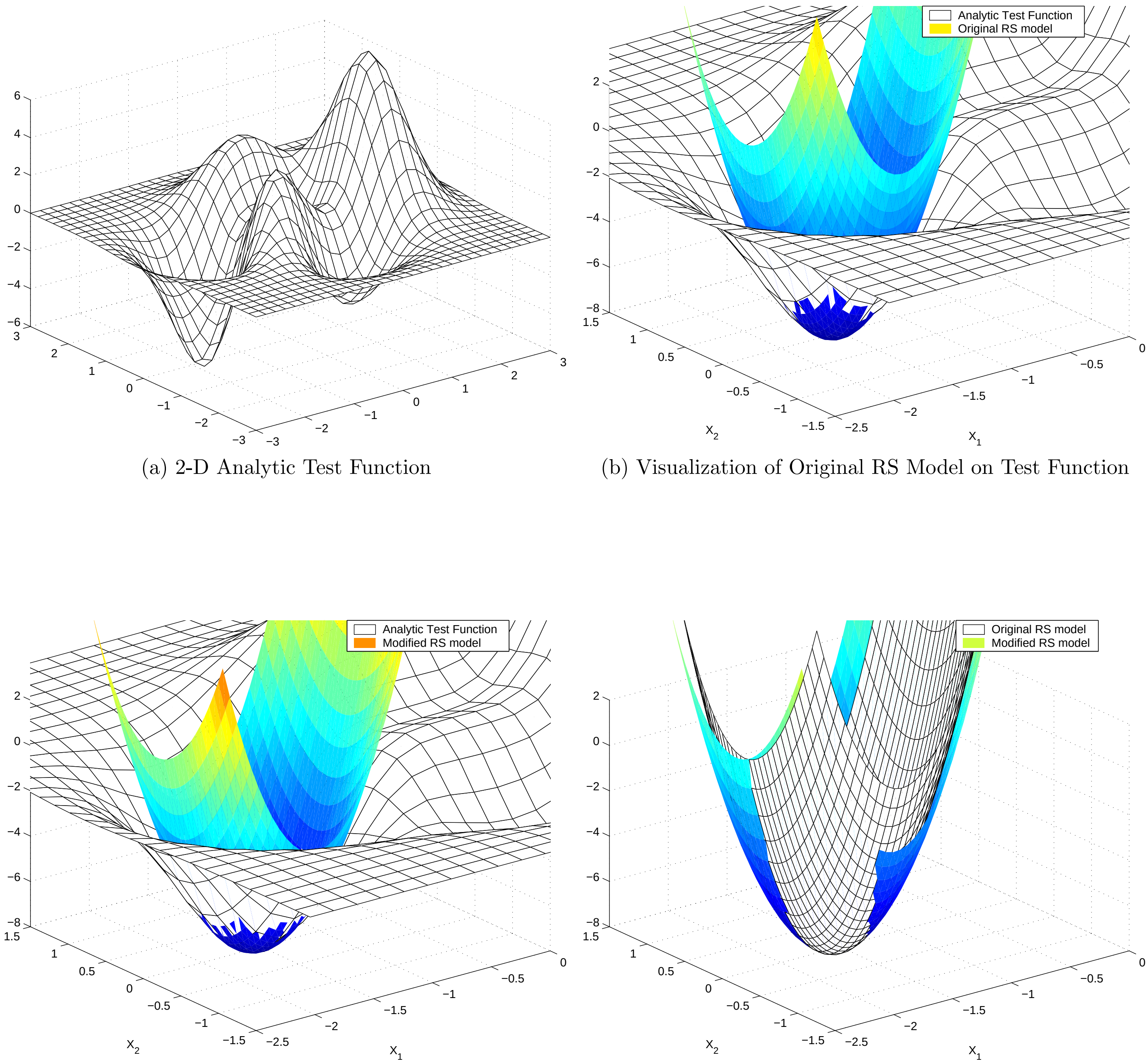


(c) Sample Sites x=[0.10, 0.15, 0.20]



(d) Sample Sites x=[0.13, 0.15, 0.17]

**Fig. 3 Modified RS Model Validation on One-Dimensional Analytic Test Function**



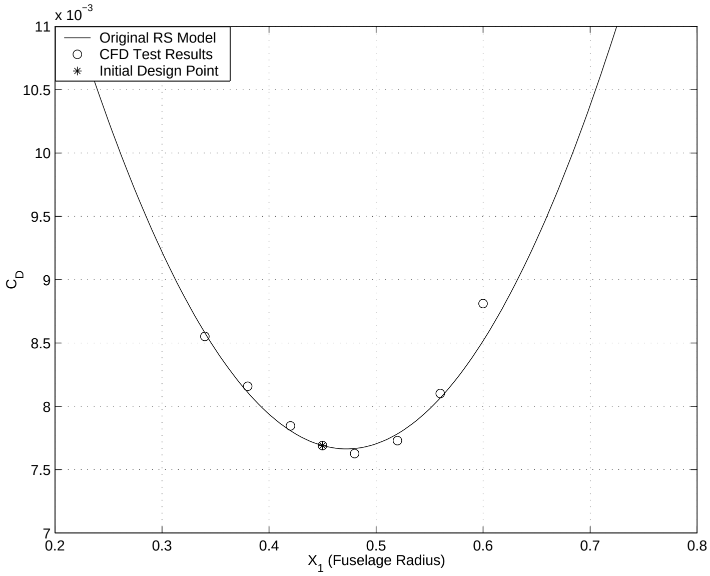

(a) 2-D Analytic Test Function

(b) Visualization of Original RS Model on Test Function

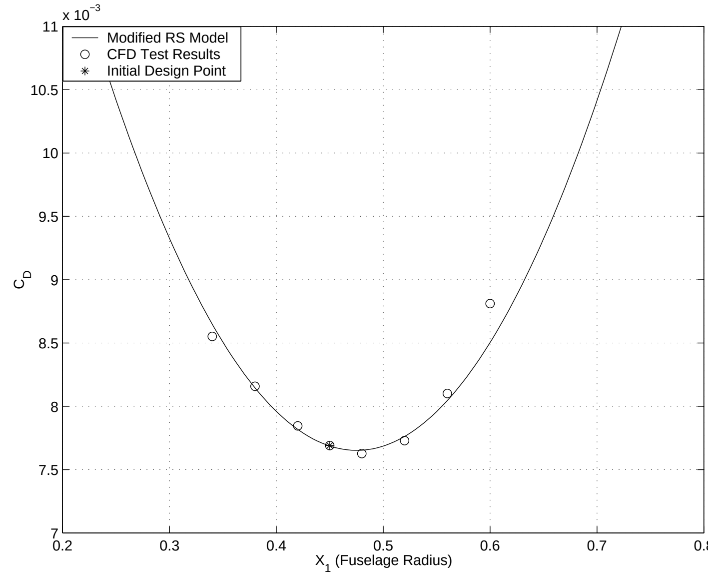
(c) Visualization of Modified RS Model on Test Function

(d) Comparison of Original and Modified RS Models

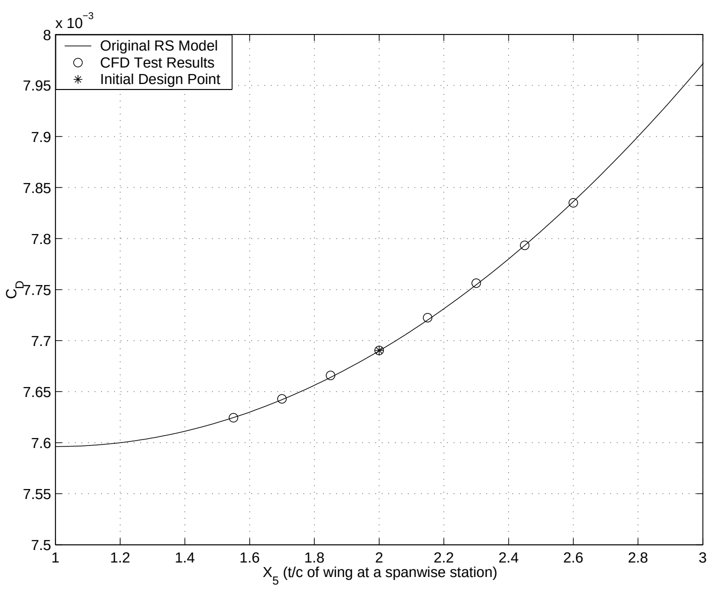
**Fig. 4 Modified RS Model Validation on Two-Dimensional Analytic Test Function**



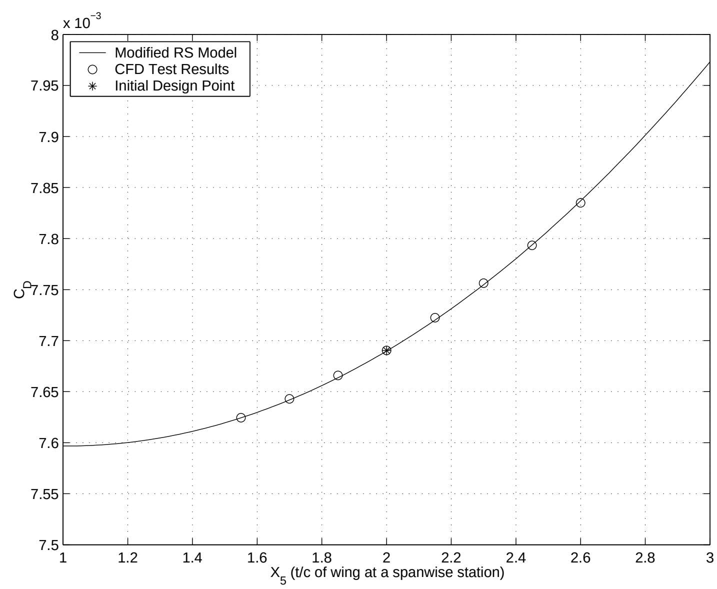

(a) Original RS Model 1-D Slice for $X_1$ (all other design variables fixed)




(b) Modified RS Model 1-D Slice for $X_1$ (all other design variables fixed)

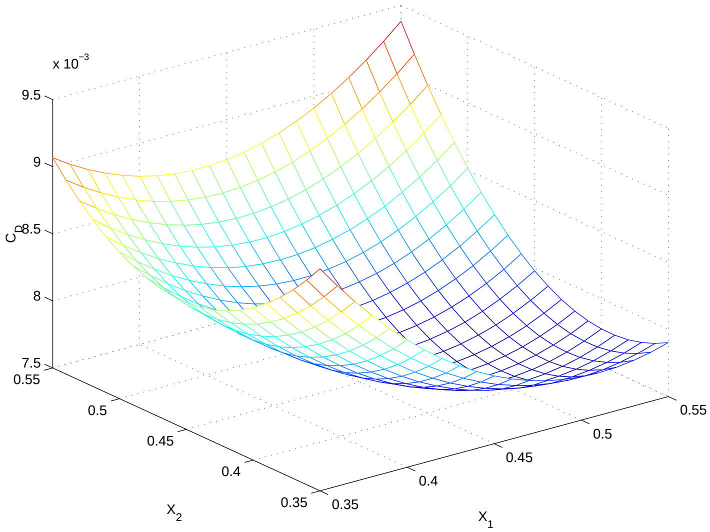



(c) Original RS Model 1-D Slice for $X_5$ (all other design variables fixed)

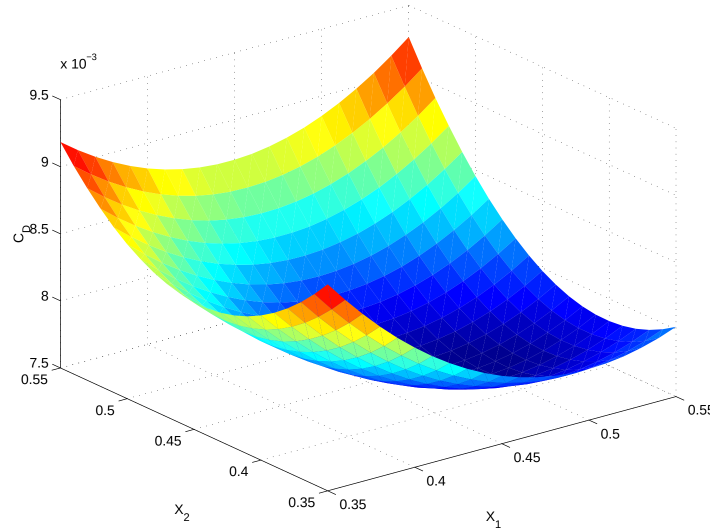



(d) Modified RS Model 1-D Slice for $X_5$ (all other design variables fixed)

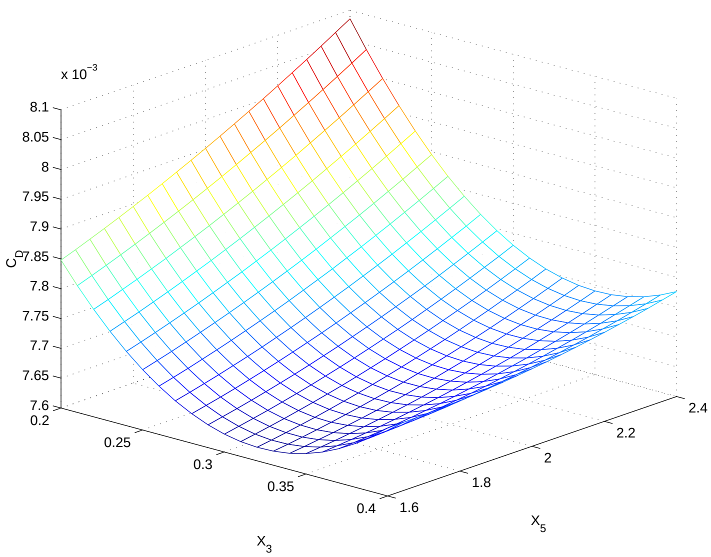
**Fig. 5 RS Model 1-D Slice Validation for SBJ Design Test Problem**



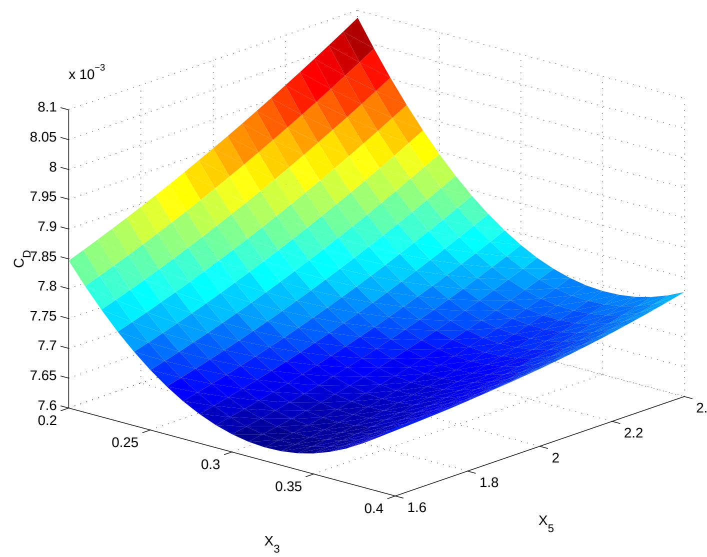

(a) $X_1$-$X_2$ Surface Slice of Original RS Model (all other design variables fixed)




(b) $X_1$-$X_2$ Surface Slice of Modified RS Model (all other design variables fixed)

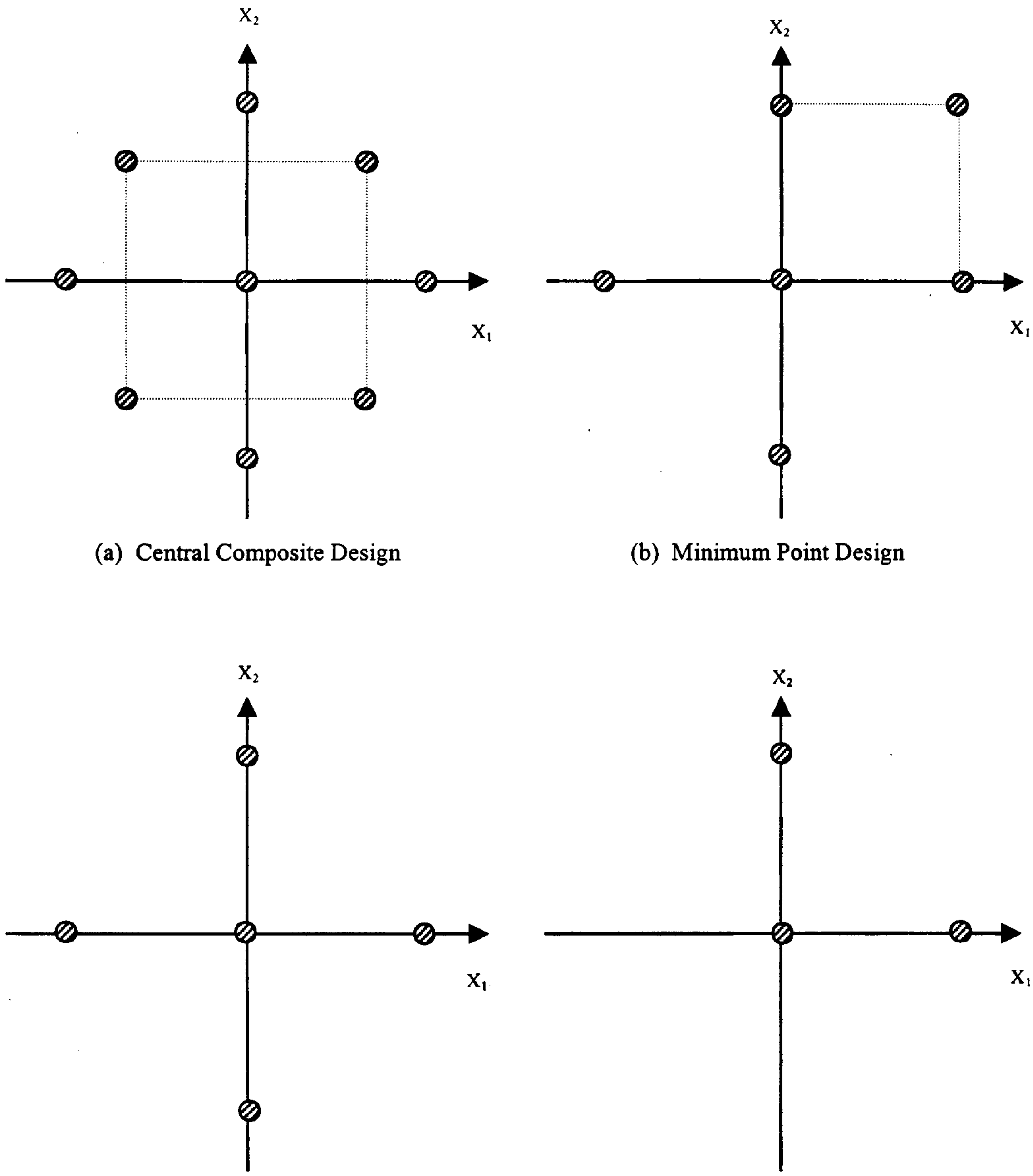



(c) $X_3$-$X_5$ Surface Slice of Original RS Model (all other design variables fixed)




(d) $X_3$-$X_5$ Surface Slice of Modified RS Model (all other design variables fixed)

**Fig. 6 RS Model 2-D Slice Validation for SBJ Design Test Problem**



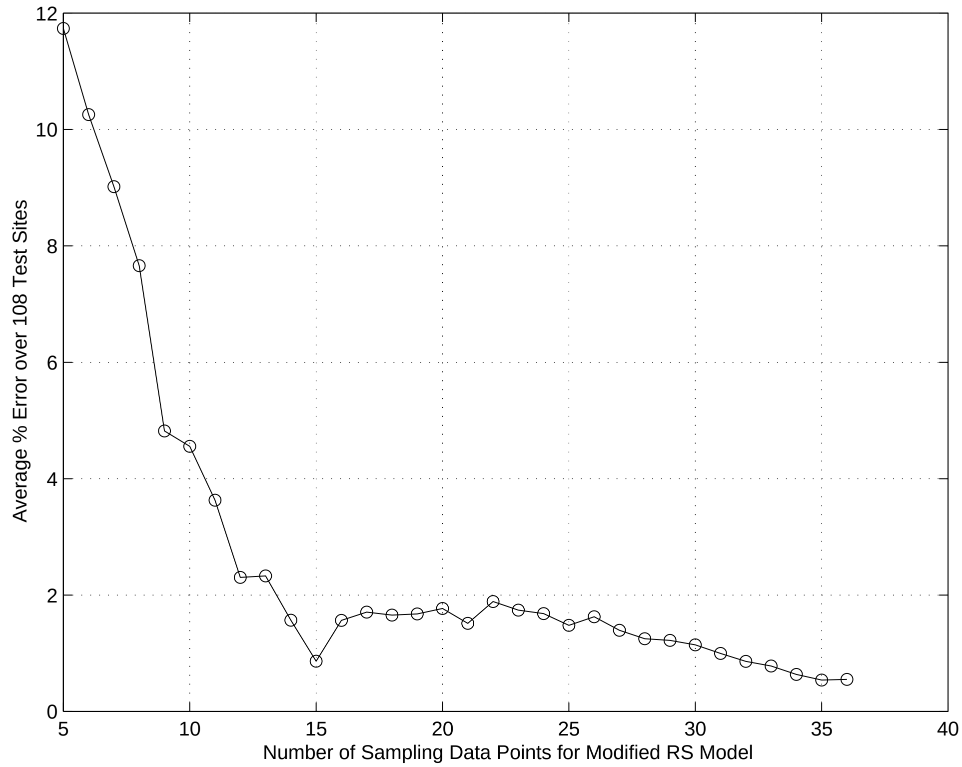

(a) Central Composite Design

(b) Minimum Point Design

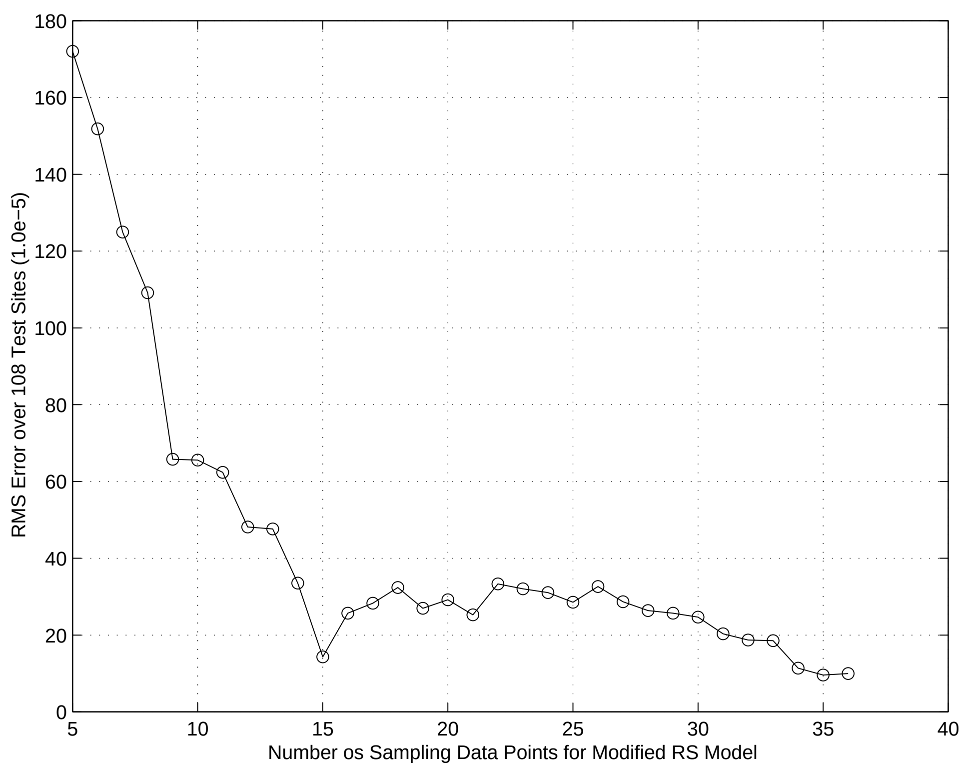
(c) Star Design (100% Axial Points Sampling)

(d) Star Design (50% Axial Points Sampling)

**Fig. 7 Various Designs of Experiment for a 2-dimensional problem**

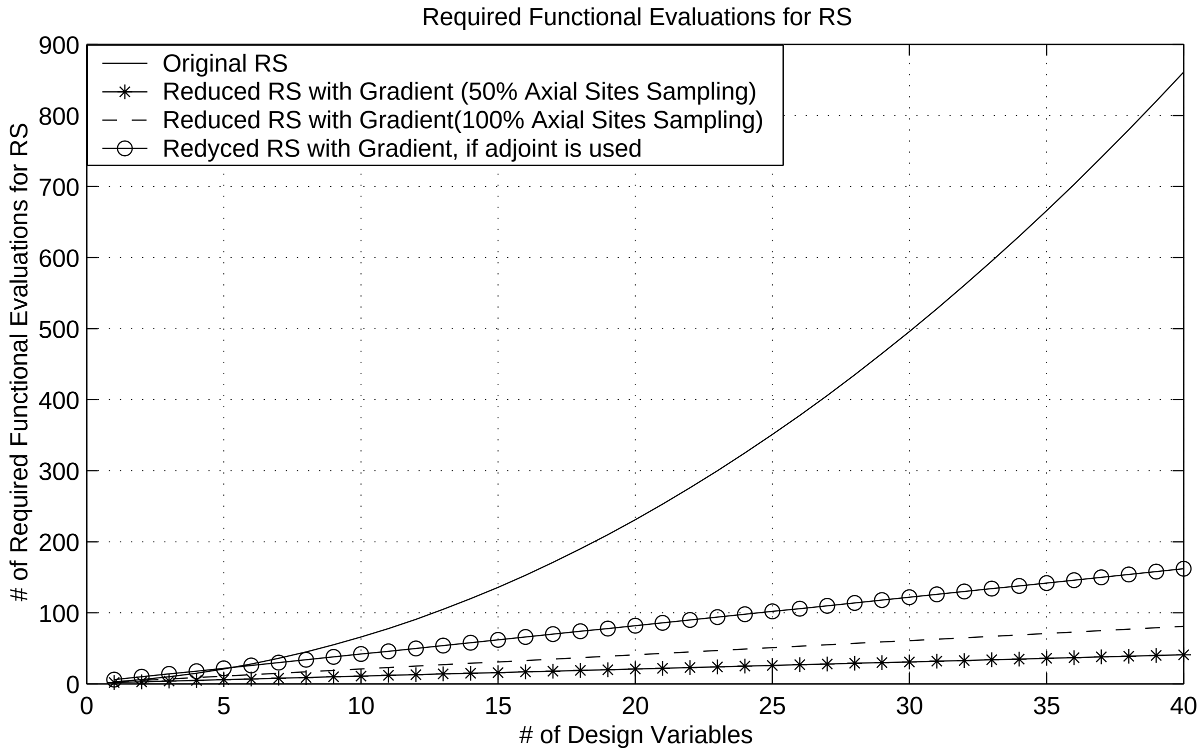



(a) Ave. % Error over 108 Random Test Sites vs. Number of Samples




(b) RMS Error over 108 Random Test Sites vs. Number of Samples

**Fig. 8 Modeling Accuracy of Modified RS Model vs. Number of Samples**



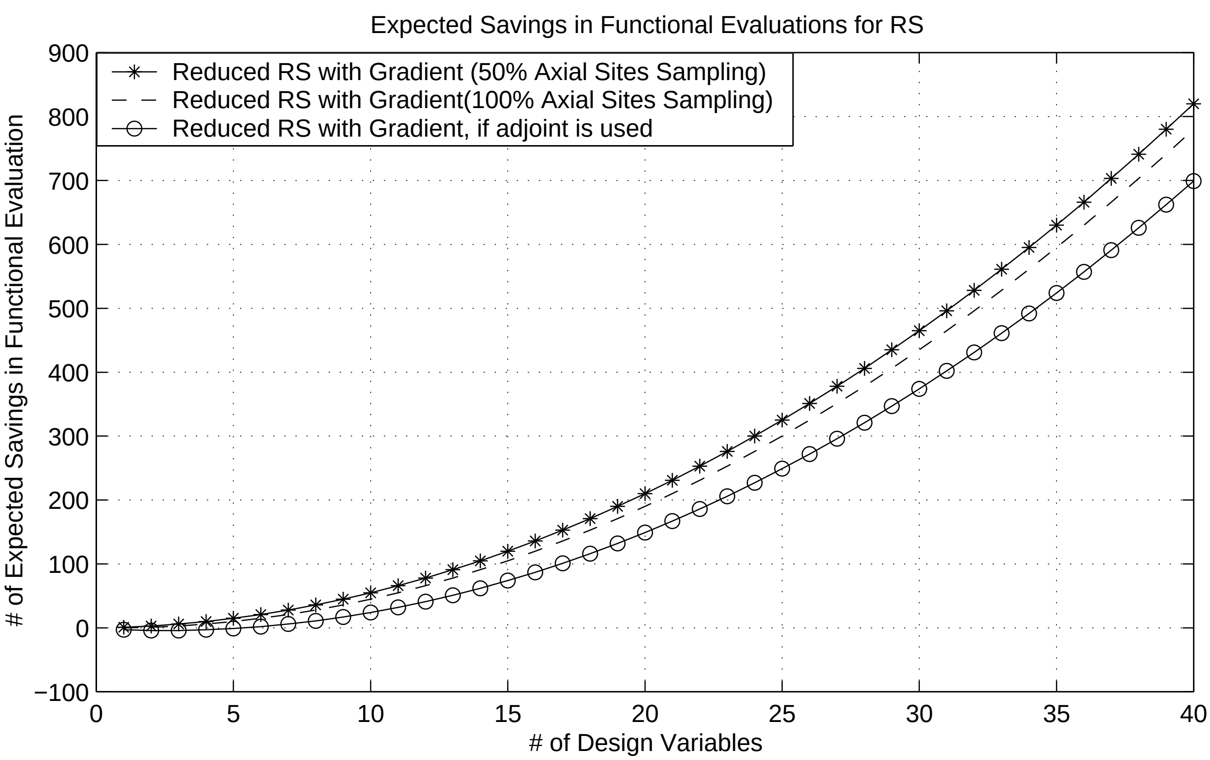




**Fig. 9 Projected Gain for Modified RS Method vs. Number of Design Variable**