RESPONSE SURFACE MODEL BUILDING USING ORTHOGONAL ARRAYS FOR COMPUTER EXPERIMENTS

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Abstract: This study investigates response surface methods for computer experiments and discusses some of the approaches available. Orthogonal arrays constructed for computer experiments are studied and an example application to a technology selection and optimization study for a reusable launch vehicle is presented.

I. Introduction

Multidisciplinary design optimization (MDO) is an important step in the conceptual design and evaluation of launch vehicles since it has a significant impact on performance and lifecycle cost. The objective in MDO is to search the design space efficiently to determine the values of design variables that optimize performance characteristics subject to system constraints. In launch vehicle conceptual design, system performance can generally be determined by the use of computerized analysis tools available in many disciplines. However, these complex sizing and performance evaluation computer programs utilize iterative algorithms. In many cases, they are expensive and difficult to integrate and use directly for MDO.

An alternative is to utilize response surface methodology to obtain mathematical models that approximate the functional relationships between performance characteristics and design variables. A common approach used in response surface model building is to utilize central composite designs (CCD) from the design of experiments literature (Box and Draper, 1987) to sample the design space efficiently. With this approach, design analyses (experiments) are performed at the statistically selected points specified by a CCD matrix. The resulting data is used to construct response surface approximation models using least squares regression analysis. These response surface equations are then used for MDO and for rapid sensitivity studies.

However, like most experimental designs, CCD are designed with the physical experiments in mind where the dominant issue is the variance of measurements

of the response (Sharifzadeh, Koehler, Owen and Shott, 1989). In an physical experiment, there is usually some variability in the output response with the experiment repeated with the same inputs. In contrast, the output of computer experiments is (in almost all cases) deterministic. Generally, there is no measurement error or no variability in analysis outputs. Therefore, experimental designs constructed to minimize variability of measurements may not be the best choice for computer experiments (Sacks, Welch, Mitchell and Wynn, 1989; Sacks, Schiller and Welch, 1989; Currin, Mitchell, Morris and Ylvisaker, 1991; Owen, 1991, 1994).

In this study response surface methods for computer experiments are investigated and some of the approaches available in the literature are disscussed. The focus is on response surface model building using orthogonal arrays designed for computer experiments. An example application to a parametric cost optimization study for a reusable launch vehicle is presented.

II. Response Surface Model Building Using Central Composite Designs

Response surface methods (RSM) can be utilized for MDO in cases where computerized design tool integration is difficult and design effort is costly. The first step in RSM, is to construct polynomial approximations to the functional relationships between design variables and performance characteristics (e.g. weight, cost) (Craig, 1978; Joyner and Sabatella, 1990; Stanley, et. al., 1993). In the next step, these parametric models are used for MDO and to determine variable sensitivities. A quadratic approximation model in the form given below (1) is commonly used since it can account for individual parameter effects, second-order curvature or non-linearity (square terms), and for two-parameter interactions (cross terms).

$$Y = b_o + \Sigma\, b_i\, x_i + \Sigma\, b_{ii} x_i^{\,2} + \Sigma\, \Sigma\, b_{ij}\, x_i\, x_j \qquad (1)$$

In this model, the x_i terms are the input variables that influence the response Y (the performance characteristic to be optimized); and b_o, b_i and b_{ij} are estimated least squares regression coefficients, based on the design and analysis data obtained by sampling the design space (or by conducting experiments).

This second-order model (1) can be constructed efficiently by utilizing central composite designs (CCD) from design-of-experiments (DOE) literature (Myers, 1971: Box and Draper, 1987: Khuri and Cornell, 1987; Cornell, 1990). CCD are first-order (2^n) designs augmented by additional points to allow estimation of the coefficients of a second-order model (Cornell, 1990; Box and Draper, 1987). CCD enables the efficient construction of a second-order response surface model with significantly less effort than would be required by a full factorial study (3^n). CCD have been successfully utilized in response surface model building and MDO in

many aerospace design applications using computerized design analysis tools (Schnackel and Dovenmuehle, 1990; Lepsch, Stanley and Unal, 1995: Unal and Stanley, 1993: Unal, Lepsch, Engelund and Stanley, 1996: Venter, Haftka and Starnes, 1996).

In some cases, however, RSM using CCD may not result in a good representation of the response surface as may be evidenced by poor predictions of the design analysis results. The reasons for this problem can be mainly due to;

1) The response surface is more complex than can be represented by a second order approximation model given by equation (1),
2) There are other influential design variables and interactions other than those currently under study,
3) The sample design points (experiments) specified by a CCD may not be suitable in terms of selection of these specific points for experimentation with computerized design analysis tools.

The third problem is directly related to the choice of specific experimental design points. In order to address this problem and to improve response surface model building using computer experiments, a study was conducted. A literature search on this subject is summarized in section III.

III. Response Surface Model Building Methods for Computer Experiments

For computer experiments, commonly used in aerospace design, there is generally no measurement error or no variability in analysis outputs, given a specific set of inputs. On the other hand, in a physical experiment, there is some variability in the output response with the experiment repeated with the same inputs. In other words, the distinguishing characteristic of a computer experiment is that the output is deterministic (Sacks, Welch, Mitchell and Wynn, 1989).

Even though the outputs from computer experiments are deterministic, the problem of selection of inputs at which to run a computer code is still an (statistical) experimental design problem. The quantification of uncertainty associated with predictions from fitted models is also a statistical problem (Sacks, Schiller and Welch, 1989).

For computer experiments, it seems necessary to introduce randomness in order to gauge how much an estimate using a model may differ from the true value obtained from an experiment (Owen, 1991). There appear to be two main statistical approaches to computer experiments, one based on Bayesian statistics and a frequentist approach based on sampling techniques (Owen, 1991).

The Bayesian approach models a computer code as if it were a realization of a stochastic process (Owen, 1991). Bayesian approach treats the bias, or the

systematic departure of the response surface from a linear model, as the realization of a stationary random function (Owen, 1991). This model has exact predictions at the observed responses and predicts with increasing error variance as the prediction point move away from all design points (Owen, 1991). The approaches for design and analysis of computer experiments using Bayesian statistics are given by Sacks et al (1989), Chaloner and Verdinelli (1995), Currin, Mitchell, Morris and Ylvisaker (1991), and Welch et al, (1992) in some detail. Bayesian approach to experimental design appear to be a growing area of research. However, the application of Bayesian experimantal design methods in real design analysis and optimization problems have been limited partly due to the lack of user friendly software (Chaloner and Verdinelli, 1995). Further development appears to be needed before they can be applied to practical design optimization problems.

The frequentist approach, surveyed by Owen (1991) on the other hand, introduces randomness by taking function values that are partially determined by pseudo-random number generators. Then this randomness is propagated through to randomness in the estimate (Owen, 1991). Owen, (1994) lists a set of randomized orthogonal arrays for computer experiments. The Statlib computer programs (http://lib.stat.cmu.edu/designs/) to generate these orthogonal arrays are also listed (Koehler and Owen, 1991).

The use of these orthogonal arrays in practice for response surface model building would be similar to utilizing central composite designs, with a potential of improving model accuracy for computer experiments. Further work is needed to study the advantages and limitations of these arrays for approximation model building and MDO in launch vehicle design. In the following section, an example application to a technology selection and optimization study for a reusable launch vehicle is presented.

IV. Example Application: Launch Vehicle Technology Selection Study

The complete design of a launch vehicle is a multidisciplinary process in which aerodynamics, propulsion, weights and sizing, structures, performance, heating, controls, operations and cost must be addressed (Stanley et al, 1993). While it is essential that each of these disciplines be addressed at the conceptual design level, it is equally vital to be able to perform this multidisciplinary analysis and optimization efficiently such that the numerous design options may be evaluated and understood rapidly.

Traditionally, the objective in a MDO study has been to search the design space to determine the values of design variables that optimize a performance characteristic (such as weight) subject to system constraints. However, research shows that up to 85 percent of the life cycle cost is committed during the early design phase (Fabrycky and Blanchard, 1991). Therefore, significant cost savings

could be realized if designers were better able to evaluate their designs on a cost basis.

This study focuses on rapid multidisciplinary analysis and evaluation-on-a-cost-basis for technology selection of a dual-fuel, rocket-powered, single-stage-to-orbit launch vehicle (SSV) (Unal, Braun, Moore and Lepsch, 1995). Different material and technology options, together with critical design variables, are studied to optimize design, development, test and evaluation (DDT&E) cost using orthogonal arrays for computer experiments. Calculus-based optimizers could not have been used in this case since material and technology options selection require the study of design variables that have discrete values. This study has the following steps:

1. Identify the design variables to be studied and alternative levels

In this study, design of a single-stage-to-orbit launch vehicle referred to determination of the appropriate component weights, sizes, and reference costs. To simplify the analysis such that the problem is tractable, several design disciplines were decoupled from the present analysis (Unal, Braun, Moore and Lepsch, 1995). An existing vehicle geometry, aerodynamics database, and internal packaging analysis were used (Engelund, Stanley, McMillin and Unal, 1993). Data from aerodynamics, structures, heating, and other subsystems were fixed or scaled appropriately. Furthermore, the ascent flight-path and propulsion system were fixed at a set of previously computed optimum values (Braun, Powell, Lepsch, Stanley and Kroo, 1995: Lepsch, Stanley and Unal, 1993).

Seven major vehicle sections accounting for most of the empty weight were selected for optimization. These were the liquid hydrogen tank (Lh2/Tank), liquid oxygen tank (Lox/Tank), hydrocarbon fuel tank (Lhc/Tank), wing section structure (Wing), wing tip-fin section structure (Tip-fin), basic structure (Basic) and secondary structure (Second). Each of these variables were studied at three technology levels represented by three different materials. The material options were aluminum (Al), aluminum-lithium (Al-li) and composite material (Comp). The objective of this investigation was then to determine the best combination of material options for the seven major vehicle sections optimized for DDT&E cost and empty weight.

2. Design the experiment and select an appropriate orthogonal array

Owen, (1994) lists a set of orthogonal arrays for computer experiments. For this study, an orthogonal array that enables the study of seven variables was selected (http://lib.stat.cmu.edu/designs/owen.small). Using this orthogonal array (Addelman and Kempthorne, 1961), the seven design variables can be studied at three levels (values) by conducting 18 design experiments. A full factorial design where all possible variable/material combinations are studied would have

required 2,187 (3^7) experiments. Variable interactions were assumed to be insignificant for this study.

Table 1: Seven Variable Orthogonal Array (Owen, 1994)

	A	B	C	D	E	F	G
1	1	1	3	2	3	1	1
2	3	2	2	1	1	3	1
3	2	3	1	3	2	2	1
4	1	2	1	1	2	1	2
5	3	3	3	3	3	3	2
6	2	1	2	2	1	2	2
7	1	3	2	1	3	2	3
8	3	1	1	3	1	1	3
9	2	2	3	2	2	3	3
10	1	3	1	2	1	3	1
11	3	1	3	1	2	2	1
12	2	2	2	3	3	1	1
13	1	1	2	3	2	3	2
14	3	2	1	2	3	2	2
15	2	3	3	1	1	1	2
16	1	2	3	3	1	2	3
17	3	3	2	2	2	1	3
18	2	1	1	1	3	3	3

3. Conduct the orthogonal array experiments

The eighteen matrix experiments were conducted using a weights and sizing routine and parametric cost estimating relationships (CER). The Configuration Sizing program (CONSIZ) developed at NASA Langley Research Center, is used to size the vehicle and determine the component weights. Within CONSIZ, the vehicle is modeled as a collection of components representing structure, subsystem, and propulsion elements.

For the cost analysis, a set of parametric CERs were developed (Moore, Braun and Powell, 1995). These equations model reference DDT&E costs specific to the reusable single-stage-to-orbit vehicle described earlier. The CERs include only those costs that are directly related to design variables contained in the study. Other cost elements, such as system level program management and programmatic costs, software costs, fees, etc., are not included. For the purpose of this study, these other cost elements are considered to be independent of the design trades over which the optimization occurs.

The CERs estimate reference DDT&E costs as a function of technology readiness level and weight. For major structural elements, the technology readiness level is a function of material choice: aluminum, aluminum-lithium or composite. The material cost differences reflect the differences in raw material cost, tooling costs and fabrication complexities between these three materials. The NASA technology readiness scale was used as the technology indicator.

The analysis results of the 18 experiments for DDT&E costs and vehicle dry weight (empty vehicle without propellants) are presented in Table 2.

Table 2: Analysis Results

	Lh2	Lhc	Lox	Wing	Tip-fin	Basic	Second	DDT&E Cost (%)	Dry Weight (lb)
1	1	1	3	2	3	1	1	90.51	281680
2	3	2	2	1	1	3	1	84.79	235518
3	2	3	1	3	2	2	1	87.66	248010
4	1	2	1	1	2	1	2	91.27	331372
5	3	3	3	3	3	3	2	80.34	182707
6	2	1	2	2	1	2	2	81.66	250502
7	1	3	2	1	3	2	3	94.44	260794
8	3	1	1	3	1	1	3	83.14	231724
9	2	2	3	2	2	3	3	82.99	195852
10	1	3	1	2	1	3	1	87.89	257717
11	3	1	3	1	2	2	1	85.05	248926
12	2	2	2	3	3	1	1	89.77	256285
13	1	1	2	3	2	3	2	83.91	219808
14	3	2	1	2	3	2	2	85.19	239077
15	2	3	3	1	1	1	2	81.72	273576
16	1	2	3	3	1	2	3	84.11	217207
17	3	3	2	2	2	1	3	82.58	231244
18	2	1	1	1	3	3	3	92.94	233486

In Table 2, level 1 corresponds to material choice one (Al), level 2 corresponds to material choice two (Al-Li) and level 3 corresponds to material choice three (Comp). The cost values are normalizedand displayed as a percentage of the highest DDT&E cost vehicle. For the 18 material combinations shown in Table 2, the lowest cost is 80.34 % (experiment number five).

4. Analyze the data to determine the optimum levels and verify results

The average cost (%) for each variable for each of the three levels are calculated and displayed in the response table given in Table 3. This response table shows the cost effects of the variables at each level. These are separate effects of each parameter and are commonly called main effects (Phadke, 1989). The average costs shown in the response table are calculated by taking the average for a variable at a given level, every time it was used. As an example, the variable Lh2 was at level 2 in experiments 3, 6, 9, 12, 15 and 18. The average of corresponding costs is 86.12 (%) which is shown in the response table (Table 3) under Lh2 at level 2. This procedure is repeated and the response table is completed for all variables at each level.

Table 3: Response table

Level	Lh2	Lhc	Lox	Wing	Tip-fin	Basic	Second
1	88.69	86.20	88.02	88.36	**83.91**	86.51	87.61
2	86.12	86.35	86.19	85.14	85.58	86.35	**84.02**
3	**83.52**	**85.77**	**84.12**	**84.82**	88.72	**85.50**	86.70

The optimum level for the design variables can now be selected by choosing the level with the lowest relative cost percentage. For example the lowest cost occured when variable Lh2 was at level 3 at 83.52 % as opposed to 88.69 % at level 1, and 86.12 % at level 2. Similarly, the levels that optimize total DDT&E cost were chosen. The optimum levels are indicated by bold in Table 3.

As the next step, least squares regression analysis is used to fit the second order approximation model (Equation 1) to the cost data (Y_i) given in Table 2 in terms of the seven design variables (X_i). This parametric model accounts for the response surface curvature (square terms) and two factor interactions (cross terms).

$$\begin{aligned}\text{DDT\&E Cost} = \; & 111.71 - 2.58\,(\text{lh2}) + 1.22\,(\text{lhc}) - 1.95\,(\text{Lox}) - 7.61\,(\text{Wing}) \\ & - 0.69\,(\text{Tip-fin}) + 0.94\,(\text{Basic}) - 13.04\,(\text{Second}) - 0.36\,(\text{lhc})^2 \\ & + 1.46\,(\text{Wing})^2 + 0.79\,(\text{Tip-fin})^2 - 0.36\,(\text{Basic})^2 \\ & + 3.15\,(\text{Second})^2\end{aligned}$$

Note that, in this response surface approximation model, the parameter values are restricted to 1 (Al), or 2 (Al-Li), or 3 (composite).

Table 4: Minimum cost value and corresponding material choices

Lh2/Tank	Lhc/Tank	Lox/Tank	Wing	Tip-fin	Basic	Second	Cost	Weight (lb)
Comp	Comp	Comp	Comp	Al	Comp	Al-li	76.29	185275

At these levels, the DDT&E cost was predicted to be 75.02 % using a second order prediction model. As a next step, a verification analysis was performed. The weight and cost of a vehicle constructed from these material choices were computed to be 185,275 lb. and 76.29 % recpectively (Table 4).

V. Conclusions

This study presents a brief overview of the response surface methods (RSM) for computer experiments available in the literature. The Bayesian approach and orthogonal arrays constructed for computer experiments (OACE) were briefly discussed. An example application of OACE to a cost optimization study for a launch vehicle was also given. In this case study, an orthogonal array for computer experiments was utilized to build a second order response surface model. Gradient-based optimization algorithms could not be utilized in this case study since the design variables were discrete valued.

Using OACE, optimum combination of material choices for seven launch vehicle technologies that minimize DDT&E cost were determined. Similar results were obtained in a previous study using a three level fractional factorial experimental design (Unal, Braun, Moore and Lepsch, 1996). Specifically, the fractional factorial design used in the prior study was a Taguchi (L18) orthogonal array (Taguchi and Konishi, 1987).

The use of OACE in this case for RSM did not show any advantage over the use of three level orthogonal arrays. The results obtained were the same in both methods. This perhaps could be expected in this case since the variables studied could only take three discrete values and variable interactions were assumed to be insignificant. However, the OACE listed by Owen (1991) seem to offer an efficient alternative to Taguchi's multilevel (three or more levels) orthogonal arrays (Taguchi and Konishi, 1987) for MDO cases that require the study of discrete-valued variables. Further work is needed in applying OACE to test cases with continuous variables to determine the advantages and limitations of OACE.

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