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# Multi-Optimal Designs for Second-Order Response Surface Models

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**Abstract**

A conventional single design optimality criterion has been used to select an efficient experimental design. But, since an experimental design is constructed with respect to an optimality criterion prespecified by investigators, an experimental design obtained from one optimality criterion which is superior to other designs may perform poorly when the design is evaluated by another optimality criterion. In other words, none of these is entirely satisfactory and even there is no guarantee that a design which is constructed from using a certain design optimality criterion is also optimal to the other design optimality criteria. Thus, it is necessary to develop certain special types of experimental designs that satisfy multiple design optimality criteria simultaneously because these multi-optimal designs (MODs) reflect the needs of the experimenters more adequately. In this article, we present a heuristic approach to construct second-order response surface designs which are more flexible and potentially very useful than the designs generated from a single design optimality criterion in many real experimental situations when several competing design optimality criteria are of interest. In this paper, over cuboidal design region for $3 \le k \le 5$ variables, we construct multi-optimal designs (MODs) that might moderately satisfy two famous alphabetic design optimality criteria, $G$- and $IV$-optimality criteria using a GA which considers a certain amount of randomness. The minimum, average and maximum scaled prediction variances for the generated response surface designs are provided. Based on the average and maximum scaled prediction variances for $k = 3$, 4 and 5 design variables, the MODs from a genetic algorithm (GA) have better statistical property than does the theoretically optimal designs and the MODs are more flexible and useful than single-criterion optimal designs.

Keywords: Multi-optimal designs, $G$-efficient design, $IV$-efficient design, genetic algorithms, cuboidal regions.

## 1. Introduction

Since the efficiency of the experiment is greatly affected by the values of the design factors selected from the design region of interest, the selection of proper experimental design points is very important. A certain design optimality criterion is often considered when deciding which response surface design to implement. There have been considerable studies in the problem of selecting efficient experimental designs and developing evaluation criteria for experimental designs. One of the most popular and commonly used classes of experimental design for fitting a second-order response surface model is the central composite designs (CCDs) which consist of factorial points, center points and axial points (Box and Wilson, 1951). A family of efficient three-level designs based on balanced incomplete block designs for fitting second-order response surfaces has been developed by Box and Behnken (1960), so called as Box-Behnken Designs (BBDs). Usually, in order to evaluate the developed experimental designs, certain optimality properties are used before running an experiment. In the next section, the details of several design optimality criteria and optimal design generation methods are presented.

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## 2. Optimal Design Theory and Optimal Design Generation Algorithms

### 2.1. Optimal design theory

There are several researches on the optimality properties and comparison of constructed experimental designs for second-order response surface models. Borkowski (1995a, 1995b, 1995c) theoretically developed analytical forms of the prediction variance properties for CCDs and BBDs. Borkowski and Valeroso (2001) addressed an overparameterization problem that usually happens when approximating the true response surface model and investigated robustness against many classes of misspecified response surface models (See, Lucas, 1974, 1976; Myers *et al.*, 1992 and Box and Draper, 1987). Hartley (1959) considered the smallest composite designs (SCDs) for $k = 3, 4$, and 5 and Hoke (1974) and Notz (1982) considered smaller designs consisting of a subset of the $3^k$ fractional design. See Myers and Montgomery (2002) for a more details on SCDs. Many researchers have studied various design evaluation criteria for the purpose of comparing designs and for constructing efficient experimental designs. The commonly used design optimality criteria for these purposes are alphabetic optimality criteria such as $D$-, $A$-, $G$- and $IV$-optimality criteria. Most of the design optimality criteria are based on the properties of the information matrix, $\mathbf{X}'\mathbf{X}$, where $\mathbf{X}$ is the expanded design matrix of an experimental design with associated response surface model on $k$ design variables. Among these, the most popular design optimality criterion for estimating coefficient parameters is $D$-optimality criterion when errors in the response surface model are assumed to be *iid.* normally distributed. $D$-optimal designs minimize the volume of the confidence ellipsoid of the parameters by minimizing the generalized variance. Because the inverse of the moment matrix, $\mathbf{M}^{-1} = n(\mathbf{X}'\mathbf{X})^{-1}$, (scaled dispersion matrix), contains variances and covariances of the regression coefficients, scaled by $n/\sigma^2$, control of the moment matrix by design implies control of the variances and covariances of regression coefficients (Kiefer, 1959, 1961; Wald, 1943). Thus, an upper bound for the prediction variance for a proposed experimental design which called as the maximum prediction variance over the design region is often used for evaluating experimental designs. So, two design optimality criteria that are particularly useful when interest lies in good prediction for the second-order response surface model are $G$-optimality and $IV$-optimality. The criterion which focuses on the maximum prediction variance over the design region is called $G$-optimality and the $G$-efficiency is defined as

$$G_{eff} = \frac{p}{\max_{\mathbf{x}\subset R}[v(\mathbf{x})]}, \tag{2.1}$$

where $v(\mathbf{x})$ is the scaled prediction variance (SPV) at the location of $\mathrm{x}^{(m)}$ and $p$ is the number of estimated coefficient parameters. A design is said to be $G$-optimal if the maximum value of the scaled prediction variance ($v(\mathbf{x})$) in Equation (2.1) is minimized. It can be shown that the maximum SPV for a $G$-optimal design is $p$. As an alternative to the single-value criterion approach, the variance dispersion graphs (VDGs) have been developed by Giovannitti-Jensen and Myers. VDGs show the prediction-variance properties throughout the experimental design region of interest. As another alphabetic optimality criterion related to prediction variance, $IV$-optimality has been developed. A design is said to be $IV$-optimal (also called $I$- and $Q$-optimal in the literature) if it minimizes the integrated SPV over the design region $R$. Specifically, the $IV$ criterion is

$$IV = n\int_R \mathrm{x}'^{(m)}(\mathrm{X}'\mathrm{X})^{-1}\mathrm{x}'^{(m)}d\mathrm{x}. \tag{2.2}$$

Here the design region is a cube or hypercube and $n$ is the number of runs in the design. Because the $G$ and $IV$-optimality criteria focus on optimizing functions of the prediction variance, they are a good choice of criterion for selecting a second-order response surface design. As another available tool to create optimal designs is to use computer using a specific design optimality criterion, so the created designs are called as computer-generated designs. $IV$-efficient designs can be constructed using JMP (2004) software or SAS. The designs created in JMP are not truly $IV$-optimal but represent the best design for this criterion found from among a number of candidate designs obtained with an exchange algorithm using the default parameters. By using a larger number of candidate designs with a richer set of candidate points, some improvement in performance is possible, which leads to designs that do have the best average scaled prediction variance values. However, this richer set of search options is considerably more computationally intensive. The size of the design was selected based on the prediction variance results obtained for the standard designs. In addition to these, there are huge amount of researches on optimal design theory (See, Atwood, 1969; Karlin and Studden, 1966; Myers and Montgomery, 2002; Stigler, 1971).

## 2.2. Optimal design generation algorithms

Several useful design generation algorithms have been developed and applied to obtain efficient designs reflecting good statistical properties. The most popular algorithms for constructing $D$-optimal designs are the exchange-type algorithms that find efficient designs by sequentially adding and removing experimental points to maximize the size of the variance-covariance matrix. Since the exchange-type algorithms are direct search methods, they usually only provide locally optimal solutions (Meyer and Nachtsheim, 1995). For more details on these algorithms, see Fedorov (1972), Mitchell (1974) and Wynn (1970). Cook and Nachtsheim (1980) compared algorithms for the computer generation of exact $D$-optimal experimental designs and evaluated a procedure for rounding off approximate designs as suggested by Kiefer (1959). Welch (1982) described a branch-and-bound algorithm for finding global $D$-optimum designs and Haines (1987) applied simulated annealing algorithm to the construction of exact $D$-, $IV$- and $G$-optimal designs for linear models. Montepiedra *et al.* (1998), Hamada *et al.*(2001), Borkowski (2003) and Heredia-Langner *et al.*(2003) applied genetic algorithms (GAs) to the problem of finding the efficient designs for many different kinds of models. Currently, computer-intensive optimization algorithms are utilized to construct efficient experimental designs and evaluate the important properties of the designs and also several computer packages are available that can generate optimal or near optimal designs for use in many industrial applications. However, the general approach which uses a single design optimality criterion for constructing an experimental design has been criticized because it does not simultaneously satisfy the various statistical design characteristics required by industrial practitioners. The design robust over the design optimality criteria will be potentially very useful in many practical experimental situations. When an experimental design is selected with respect to a single design optimality criterion, the design based on a prespecified optimality criterion could have inferior to other designs with respect to the other design optimality criterion. Thus, it is important to construct a certain superior response surface design which has moderately high efficiencies for different design optimality criteria of interest over a proposed response surface model. However, it may not be easy to characterize and optimize several competing objectives relevant in the design of an experiment simultaneously.

There have been many researches on taking more than one criterion into consideration and combining more than one criterion in optimal design problems and various design optimality measures have been developed and used to select optimal designs for this situation. One approach to the design problem is to create a new objective function based on a weighted average of a several design criteria; this has been termed either a compound or a weighted design problem (Cook and Nachtsheim, 1982). This approach is to weight each criterion and find the design that optimizes the weighted average of the criteria. An alternative approach is to optimize one primary design criterion, subject to constraints for a specified minimum efficiency of other criteria. This is known as the constrained design problem. This approach sets up a minimal quality of designs and then determines a design that is optimal with respect to a criterion among the designs that achieve the minimal quality. Stigler (1971) formulated a multipurpose optimality criterion for the standard univariate linear regression models, which is called $C$-restricted $D$- and $G$-optimality. Läuter (1974, 1976) suggested an approach that the true model is in a class of models specified in advance and then assigned a weight to each model and an adjustment to the different orders of magnitude of the determinant of information matrix under various response surface models. In this approach, $D$-optimality criterion is considered, and the design called multipurpose design which maximizes a combined weighted design optimality criterion is sought through a proposed design generating algorithm. Most of these researches have been used in discriminating between two or three competing models and finding efficient estimates of the coefficient parameters for a given model. The minimal qualities required in most optimal design problems are about the model discrimination that allows a check of whether or not the fitted model provides an adequate fit to the true model or that allows simultaneously good fit of a class of models. Lee (1988) considered a problem of combining optimality criteria using constrained optimization technique. Constraints can be due to some optimality criteria so that the designs satisfying the constraints will have at least the minimal quality that an investigator wishes to maintain. In this work, he provided multiple-objective designs for the quadratic and cubic models using Lagrange's multiplier techniques. Cook and Wong (1994) considered the problem of finding a two-objective optimal design and showed that two standard approach for constructing optimal designs to satisfy two objectives, that is, constrained and compound optimal design, are essentially equivalent. They provided an example that the design optimality criteria of interest are $A$- and $D$-optimality at the same time and plotted the efficiencies for the value of $\lambda$, where $\lambda$ is the weight assigned to each criterion. Clyde and Chaloner (1996) also showed that the equivalence between compound optimal designs and constrained optimal designs and then applied these approaches to Bayesian and nonlinear design problems with three or more design optimality criteria. They formulated the constrained design problem as a weighted design problem that allows the use of unconstrained optimization routines to find optimal design for the constrained optimal design problem. Huang and Wong (1998) proposed a sequential approach for constructing multiple-objective locally optimal designs for nonlinear models that satisfy multiple criteria simultaneously under the assumption that the initial estimates of parameters are known. However, in most cases, it is known that to generate even a compound optimal design requires quite a large amount of time if the conventional optimal design generation algorithms. Consequently, we can conclude that it is much harder to find multiple-objective optimal designs when there are more than two objectives. And, when compound optimal design approach is used, because of scaling in the utility functions, choosing the appropriate weights can be difficult work. Thus, we present a genetic algorithm (GA) approach which is known as a simple and quick approach to attack this type of optimal design problems. Using a GA for solving difficult combinatorial optimization problems, we generate second-order response surface designs that satisfy multi-optimal criteria simultaneously over a cuboidal region for $3 \leq k \leq 5$ variables. In next section, we provide a brief description of GAs and the operating characteristics as well as multi-objective optimization methods. Before finding multi-optimal response surface designs, we first need to specify a response surface model. In this research we focus on the second-order response surface model on $k$ variables given by:

$$y = \beta_0 + \sum_{i=1}^{k} \beta_i x_i + \sum_{i=1}^{k} \sum_{j=i+1}^{k} \beta_{ij} x_i x_j + \sum_{i=1}^{k} \beta_{ii} x_i^2 + \varepsilon, \tag{2.3}$$

where $y$ is the measured response, $\beta_0$ is the intercept term, $\beta_i$ are the coefficients of the first-order terms, $\beta_{ii}$ and $\beta_{ij}$ are the coefficients of the pure quadratic terms and the interaction terms and $\varepsilon$ is error term with NID(0, $\sigma^2$). This model is simple and very useful in many experimentation studies.

## 3. Multi-Objective Optimization Methods and Genetic Algorithms

Multi-objective optimization methods deal with searching optimal or nearly optimal solutions to problems having multiple objectives (see Evans, 1984). So the user is not satisfied by finding one optimal solution with respect to a single optimality criterion. In a single criterion optimization problem the main goal is to find the global optimal solution to a objective function, while, in a multi-criterion optimization problem, there is more than one objective function, each of which may have a different individual optimal solution. If there is a sufficient difference in the optimal solutions corresponding to different objective functions, then we can say that the objective functions are conflicting to each other. Multi-objective (or multi-criterion) optimization problems with such conflicting objective functions may provide a set of optimal solutions, instead of one optimal or nearly optimal solution. We call these optimal solutions as 'Pareto-optimal solutions' following the name of an economist Vilfredo Pareto who is known for 'Pareto optimality'. The concept of 'Pareto optimality' is that, generally, the solutions to a multi-objective optimization problem are not a single value but instead a set of values also called the 'Pareto set'. If we illustrate the 'Pareto optimal solutions' with cost and time (which are should be minimized in general) from an algorithm shown in Figure 1.

For example, in this problem we have to minimize both cost and time simultaneously. The point $p$ represents a solution to this problem, which has a minimal cost, but time is high. On the other hand, the point $r$ represents a solution with high cost but minimum time. Considering both objectives, no solution is optimal. So in this case we cannot say that solution $p$ is better than $r$ and also there exist many such solutions like $q$ also belong to the 'Pareto optimal set'. All of the solutions, on the curve, are known as 'Pareto-optimal solutions'. From the Figure 1 it is clear that there exist solutions, which does not belong to the 'Pareto optimal set', such as a solution like $t$. If we compare $t$ with solution $q$, $t$ is not better than $q$ with respect to any of the objectives. So we can say that $t$ is a 'dominated solution' or 'inferior solution'. In the next part, a brief description of GAs and the operating characteristics of GAs will be provided.

Generally, applying exhaustive search algorithm may be inefficient computationally in order to find the optimum or near optimum for the large-scale combinatorial optimization problems within acceptable computation time. So, we should consider a certain efficient search algorithm rather than exhaustive search algorithm for these cases. When dealing with large-scale combinatorial optimization problems, specialized procedures should be applied simply. The specialized procedures are usually called heuristic procedures that do not require a mathematical formulation since heuristic methods as a practical and quick method based on strategies are likely to (but not guaranteed to) lead to a solution that is approximately optimal or near optimal. Several different kinds of heuristic approaches have been developed for dealing with difficult combinatorial optimization problems. Many useful heuristic algorithms based on the general principle of local improvement have been developed. One of the famous heuristic algorithms is genetic algorithms (GAs). GAs that occur on a computer were motivated by an analogy of biological evolution and heredity: a population (a pool of individuals) undergoes some transformation and during this process, the individuals strive for survival. Usually through the artificial evolution operations, GAs iteratively seek to breed solutions that are optimal or nearly optimal. When applying GAs, we have to define a fitness measure or an evaluation criterion in order to determine whether a solution optimize the numerically predetermined fitness measure or not.

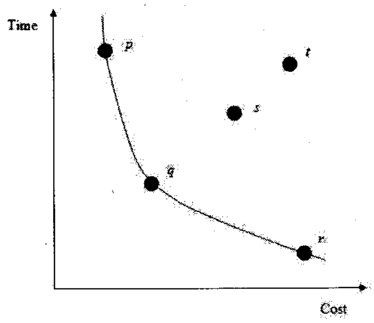


Figure 1: *Pareto optimal solutions*

Once all individual solutions in the population have been evaluated, their evaluated values, called as fitnesses, are used as the basis for selection of the next generation. Some of these selected individual solutions are carried forward into the next generation population intact. Others are used as the basis for generating new offspring individuals by applying artificial evolution operations (Forrest, 1993 and Montepiedra *et al.*, 1998). In this study, in order to select the required number of individual solutions of the next generation, we use three main genetic operations: cloning, crossover (mating) and mutation and we use real-value encoding scheme. For more details, see Park *et al.* (2005). However, it should be noted that GAs also have a possibility of getting trapped at a local optimum, since the considered problem in this study includes numerous locally optimal solutions. However, although GAs may not guarantee the optimal solution, GAs can be used for solving this problem since it strikes a balance between a direct search, leading to a systematic improvement of the criterion value and a stochastic search of the space of possible solutions.

## 4. Construction of Multi-Optimal Designs over Cuboidal Region Using GA

In this section, we present a detailed description of how a GA can be applied to the problem of finding the best experimental designs that have moderately high $G$- and $IV$-efficiency simultaneously when the number of factors is 3 to 5. Based on these two optimality criteria, maximum and average scaled prediction variances at the maximum shrinkage levels can be calculated and then be used to compare several designs. The robustness of a design against the design optimality can be quantified by calculating scaled prediction variances. For selecting the multi-optimal designs, we find non-dominated solutions that draw an efficient frontier. As generating initial populations, we consider two cases: (i) Random generation of initial populations; (ii) Random generation plus already developed best designs such as Hoke designs or Mitchell and Bayne's DETMAX designs or SCD or FCC. We analyze the maximum and average scaled prediction variances for second-order designs generated from the GA according to the number of design factors considered. For cuboidal regions, it is known that the design from Mitchell-Bayne's DETMAX (1978) algorithm is the most efficient in maximum scaled prediction variance point of view for $k$ = 4 and 24-run case and the Hoke designs (1974) are the most efficient in maximum scaled prediction variance point of view for $k$ = 3 with 14-run case and $k$ = 5 with 26-run cases, respectively. Table 1 summarizes the minimum, average and maximum of the scaled prediction variances for several designs and GA designs with different experimental runs for $k$ = 3 design variable case, where $n$ and $n_c$ represent the total number of experimental runs and the number of center points, respectively. In each table, we represent the newly generated experimental designs from GA by a sign. For example, the experimental design 'GA3F13R_01' for $k$ = 3 and

Table 1: Scaled prediction variances of current designs and GA-Designs for $k = 3$

| $k$ | $n$ | $n_c$ | Design Type | Scaled Prediction Variance at Shrinkage Level = 1 | | |
|---|---|---|---|---|---|---|
| | | | | Minimum | Average | Maximum |
| 3 | 13 | 3 | SCD | 8.175 | 22.955 | 90.737 |
| | | 0 | GA3F13R_01 | 4.690 | 7.452 | 15.364 |
| | | 1 | GA3F13R_02 | 3.572 | 7.255 | 16.545 |
| 3 | 14 | 0 | Hoke | 5.250 | 8.773 | 12.042 |
| | | 0 | $IV$-Efficient | 5.531 | 9.875 | 24.531 |
| | | 0 | GA3F14R_01 | 4.346 | 6.179 | 11.200 |
| 3 | 15 | 5 | AP | 5.518 | 97.092 | 1049.440 |
| | | 1 | GA3F15R_01 | 3.789 | 6.417 | 11.958 |
| 3 | 17 | 3 | FCC | 7.798 | 9.348 | 13.510 |
| | | 1 | GA3F17R_01 | 4.562 | 7.022 | 13.074 |
| | | 0 | GA3F17R_02 | 3.610 | 6.168 | 13.519 |
| 3 | 18 | 1 | MB-B | 6.221 | 8.747 | 15.646 |
| | | 0 | GA3F18R_01 | 4.445 | 6.791 | 12.514 |

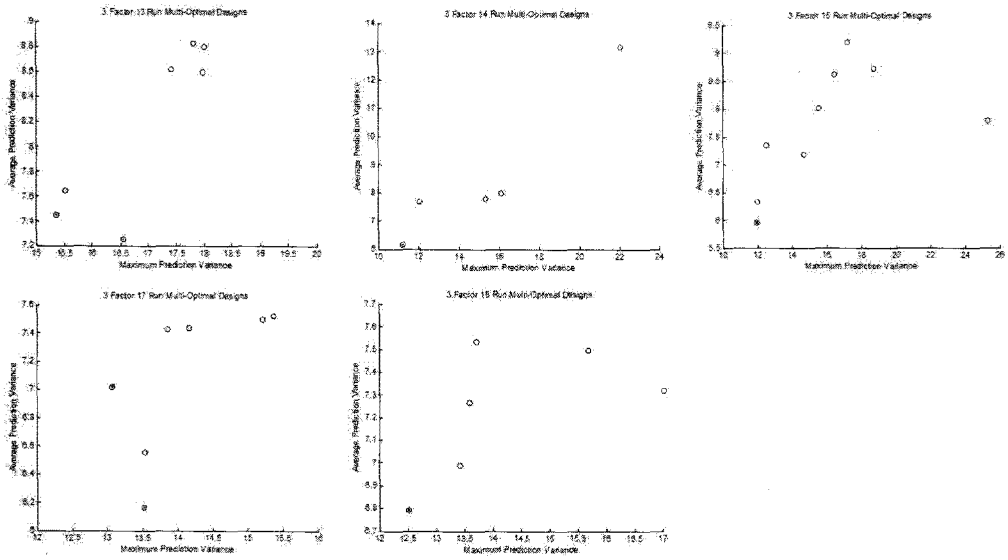


Figure 2: *Pareto optimal solutions for* $k = 3$

$n = 13$ stands for the first 'Pareto-optimal solution' (or Non-dominated solution) with 13 runs for 3 design variable case.

For $k = 3$ design variables, we consider five different cases, that is, $n = 13, 14, 15, 17$ and 18. The Pareto optimal solutions marked by '⊙' are plotted in Figure 2 and the minimum, average and maximum scaled prediction variance of the designs from a GA and theoretically optimal designs are shown in Table 1. As shown in Table 1, the newly generated experimental designs ('GA3F13R_01' and 'GA3F13R_02') are very efficient with respect to the $G$- and $IV$-optimality criteria for $n = 13$. For $n = 14$, the experimental design from GA, 'GA3F14R_01' without center points is superior to Hoke design that is known as both $G$- and $IV$-efficient for a second-order response surface model. For $n = 15$, the experimental design from GA, 'GA3F15R_01' is superior to AP design that is known as both G-efficient for a second-order response surface model. For $n = 17$, the experimental design from GA, 'GA3F17R_01' is superior to Face-centered cube (FCC) design that is known as both $G$-efficient for a second-order response surface model. The newly generated experimental design for $n = 17$, that is, 'GA3F17R_02' is superior to the FCC design with respect to the $IV$-optimality criterion. For $n = 18$, the experimental design from GA, 'GA3F18R_01' is superior to MB-B design that is known as both $G$-efficient for a second-order response surface model. The 'GA3F18R_01' design also has better efficiency than the MB-B with respect to the $IV$-optimality criterion. So, there are small improvements in both average and maximum scaled prediction variances of the response for all cases. For example, the average and maximum scaled prediction variances of Hoke design are 8.773 and 12.042, whereas those of GA design, 'GA3F14R_01', are 6.179 and 11.200. We could also see that the minimum scaled prediction variances of the designs from a GA for $n = 24$ and $n = 41$ are not much different from those of famous optimal designs such as MB-D and AP. Because the minimum scaled prediction variances of the constructed designs are not a matter of concern in the optimal design problem, only the average and maximum prediction variances of experimental designs should be considered. Among the multi-optimal designs, we present only some experimental designs in the Appendix.

For $k = 4$ design variables, we consider five different cases, that is, $n = 19, 21, 24, 29$ and 41. The Pareto optimal solutions marked by '⊙' are plotted in Figure 3 and the minimum, average and maximum scaled prediction variance of the designs from a GA and theoretically optimal designs are shown in Table 2. As shown in Table 2, the newly generated experimental designs ('GA4F19R_01' and 'GA4F19R_02') are very efficient compared to Hoke design with respect to the $G$- and $IV$-optimality criteria for $n = 19$. For $n = 21$, the experimental designs from GA, 'GA4F21R_01' and 'GA4F21R_02' are superior to small composite design (SCD) with respect to $G$- and $IV$-optimality criteria. For $n = 24$, none of the newly generated designs from GA is superior to MB-D and $IV$-efficient designs with respect to $G$- and $IV$-optimality criteria at the same time. But, all of newly generated designs from GA are superior to MB-D, $IV$-efficient and GA $G$-efficient designs with respect to $IV$-optimality criterion. For $n = 29$ and $n = 41$, all of the experimental design generated from GA are superior to Face-centered cube (FCC) design and AP design with respect to the $IV$-optimality criterion. So, there are small improvements in both average and maximum scaled prediction variances of the response for all cases. For example, the average and maximum scaled prediction variances of face-centered cube (FCC) are 15.061 and 22.237, whereas those of one GA design, 'GA4F29R_03', are 10.331 and 20.341.

For $k = 5$ design variables, we consider four different cases, that is, $n = 26, 30, 31$ and 41. The Pareto optimal solutions marked by '⊙' are plotted in Figure 4 and the minimum, average and maximum scaled prediction variance of the designs from a GA and theoretically optimal designs are shown in Table 3. As shown in Table 3, the newly generated experimental design, that is, 'GA5F26R_01' is very efficient compared to the other four designs with respect to the $G$- and $IV$-optimality criteria for $n = 26$. For $n = 30$ and $n = 31$, the four experimental designs from GA are superior to MB-D and FCC with respect to $G$- and $IV$-optimality criteria, respectively. For $n = 41$, all of the experimental design generated from GA are superior to AP design with respect to the $G$- and $IV$-optimality criterion. So, there are small improvements in both average and maximum scaled prediction variances of the response for all cases. For example, the average and maximum scaled prediction variances of Hoke design are 18.623 and 29.302, whereas those of the GA design, 'GA5F26R_01', are 13.476 and 27.776. Consequently, as we can see the results, since the efficiencies are not always monotonic when we consider two design optimality criteria simultaneously; the trade-off between the competing optimality criteria can not be easily assessed.

Table 2: Scaled prediction variances of current designs and GA-Designs for $k = 4$

| $k$ | $n$ | $n_c$ | Design Type | Scaled Prediction Variance at Shrinkage Level = 1 | | |
|---|---|---|---|---|---|---|
| | | | | Minimum | Average | Maximum |
| 4 | 19 | 0 | Hoke | 7.006 | 15.901 | 47.032 |
| | | 0 | GA4F19R_01 | 4.903 | 11.006 | 24.640 |
| | | 0 | GA4F19R_02 | 7.023 | 14.423 | 24.410 |
| 4 | 21 | 5 | SCD | 11.262 | 35.378 | 146.391 |
| | | 0 | GA4F21R_01 | 5.902 | 11.569 | 28.627 |
| | | 0 | GA4F21R_02 | 5.156 | 12.272 | 26.745 |
| 4 | 24 | 0 | MB-D | 7.258 | 12.665 | 20.813 |
| | | 0 | GA_$G$-efficient Design | 7.998 | 12.996 | 19.598 |
| | | 3 | $IV$-Efficient | 7.530 | 11.928 | 29.439 |
| | | 1 | GA4F24R_01 | 6.108 | 12.352 | 21.118 |
| | | 1 | GA4F24R_02 | 5.847 | 11.471 | 21.289 |
| | | 1 | GA4F24R_03 | 5.939 | 11.468 | 21.541 |
| | | 1 | GA4F24R_04 | 5.848 | 11.192 | 21.570 |
| | | 0 | GA4F24R_05 | 6.040 | 10.831 | 22.146 |
| | | 1 | GA4F24R_06 | 5.642 | 10.498 | 23.276 |
| | | 1 | GA4F24R_07 | 5.960 | 10.348 | 23.291 |
| | | 1 | GA4F24R_08 | 5.487 | 10.227 | 23.371 |
| 4 | 29 | 5 | FCC | 11.819 | 15.061 | 22.237 |
| | | 0 | GA4F29R_01 | 5.338 | 10.713 | 19.914 |
| | | 0 | GA4F29R_02 | 5.244 | 10.474 | 20.117 |
| | | 0 | GA4F29R_03 | 4.564 | 10.331 | 20.341 |
| 4 | 41 | 5 | AP | 7.440 | 13.510 | 37.799 |
| | | 0 | GA4F41R_01 | 7.166 | 11.807 | 18.325 |
| | | 0 | GA4F41R_02 | 6.643 | 10.003 | 18.907 |
| | | 0 | GA4F41R_03 | 5.593 | 9.529 | 20.101 |

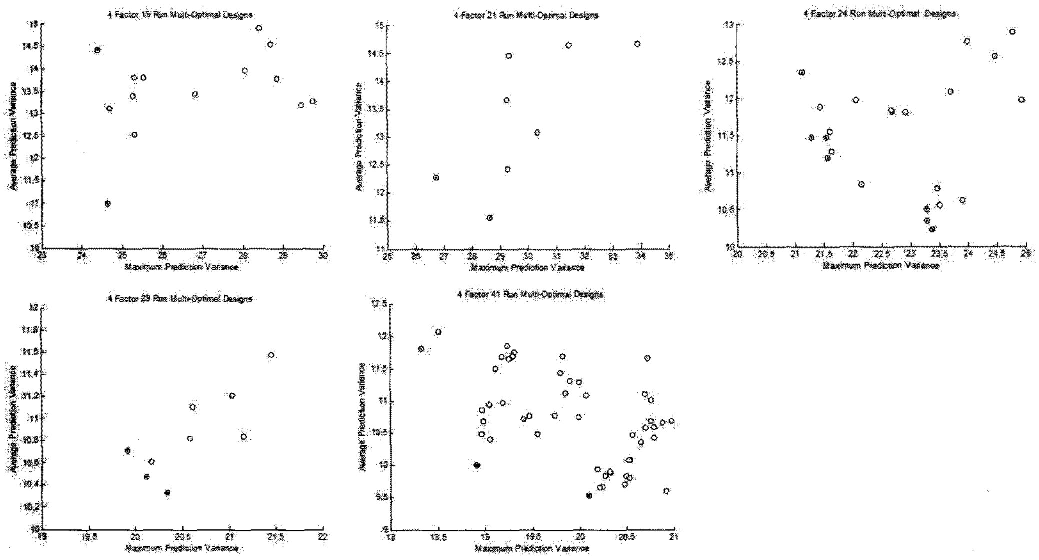

Figure 3: *Pareto optimal solutions for* $k = 4$

Table 3: Scaled prediction variances of current designs and GA-Designs for $k = 5$

| $k$ | $n$ | $n_c$ | Design Type | Scaled Prediction Variance at Shrinkage Level = 1 | | |
|---|---|---|---|---|---|---|
| | | | | Minimum | Average | Maximum |
| 5 | 26 | 0 | Hoke | 6.399 | 18.623 | 29.302 |
| | | 5 | SCD | 13.314 | 84.530 | 742.389 |
| | | 0 | GA_G-efficient Design | 9.403 | 16.594 | 28.795 |
| | | 0 | $IV$-efficient | 8.141 | 18.117 | 87.099 |
| | | 0 | GA5F26R_01 | 4.355 | 13.476 | 27.776 |
| 5 | 30 | 0 | MB-D | 9.371 | 22.757 | 46.595 |
| | | 0 | GA5F30R_01 | 8.517 | 18.635 | 37.272 |
| | | 0 | GA5F30R_02 | 8.659 | 18.445 | 37.528 |
| | | 0 | GA5F30R_03 | 7.910 | 18.042 | 38.242 |
| | | 0 | GA5F30R_04 | 7.531 | 16.768 | 43.685 |
| 5 | 31 | 5 | FCC | 14.254 | 19.953 | 32.165 |
| | | 0 | GA5F31R_01 | 8.357 | 16.761 | 30.721 |
| | | 0 | GA5F31R_02 | 8.542 | 16.581 | 30.924 |
| | | 0 | GA5F31R_03 | 7.703 | 16.125 | 31.546 |
| | | 0 | GA5F31R_04 | 7.156 | 15.941 | 32.127 |
| 5 | 41 | 5 | AP | 8.180 | 21.228 | 90.955 |
| | | 0 | GA5F41R_01 | 9.084 | 17.700 | 30.884 |
| | | 0 | GA5F41R_02 | 8.753 | 16.904 | 31.027 |
| | | 0 | GA5F41R_03 | 8.031 | 15.463 | 38.425 |

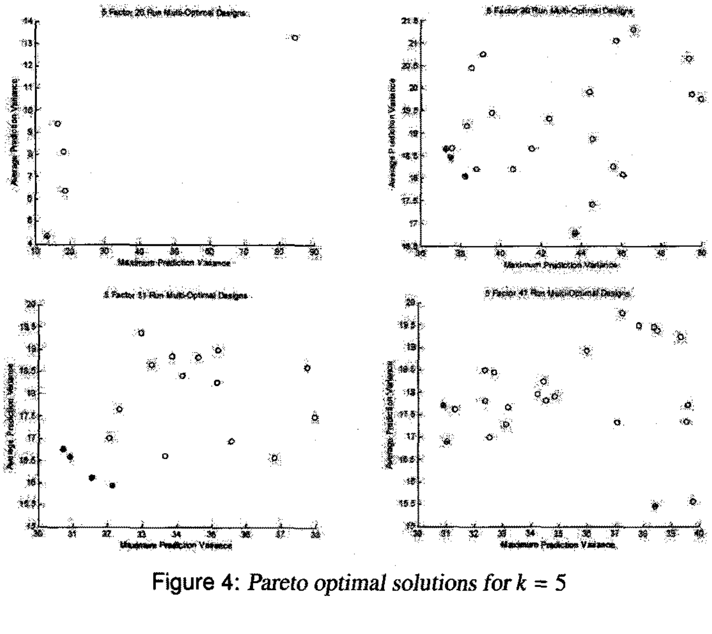

Figure 4: *Pareto optimal solutions for* $k = 5$

## 5. Conclusion

A major criticism is that optimal response surface designs developed under the assumption that the prespecified optimality criterion can have low efficiencies compared to another experimental design when another optimality criterion is employed. So, it is necessary to develop the multi-optimal (or multiple-objective) response surface designs which guarantee high design efficiencies (or low average or maximum scaled prediction variances) under many design criteria considered. In this paper, we discuss the construction of multi-optimal response surface designs and show that the use of the genetic algorithms to find $G$- and $IV$-efficient designs for three different number of design variable cases. Through the GA, we have shown that particular designs have outperformed over other designs with respect to $G$- and $IV$-optimality criteria. To assess the quality of the constructed designs over cuboidal region from genetic algorithms, by investigating the minimum, maximum and averages of the scaled prediction variances of the designs, we could reach the following conclusions:

Based on the average and maximum scaled prediction variances for $k$ = 3, 4 and 5 design variables, the computer generated designs from a genetic algorithm (GA) have better statistical property than does the theoretically optimal designs such as Hoke and Mitchell-Bayne's DETMAX algorithms (1978), FCC, SCD and AP designs and these multi-optimal designs (MODs) are more flexible and useful than single-criterion optimal designs, which have been increasingly criticized as being overly myopic. From the GA search procedure, we could conclude that the symmetrically distributed GA-designs without center point provides minimum of average and maximum scaled prediction variances at the same time. In conclusion, multi-optimal response surface designs can overcome some of the criticism when we find optimal experimental designs under single-objective optimal design criterion. They also can satisfy the practical needs of many researchers and are robust to various optimality criteria because the multiple-objective response surface designs provide more extensive availability in practice. We, however, should note that since the performance of designs can be changed by selecting number of experimental points and adding or removing center points in the considered designs, further investigation on the variance properties should be needed. Furthermore, since the selection of a design via an optimality criterion is dependent on an approximated response surface model proposed by experimenters prior to data collection, it should also be noted that different models lead to different design optimality values and thus different design should be selected.

## Appendix:

Table A.1: 3-Factor multi-optimal designs for $k$ = 14: GA3F14R_01

| $X_1$ | $X_2$ | $X_3$ |
|---|---|---|
| −1 | −1 | −1 |
| 1 | −1 | −1 |
| 0 | 0 | −1 |
| −1 | 1 | −1 |
| 1 | 1 | −1 |
| 0 | −1 | 0 |
| −1 | 0 | 0 |
| 1 | 0 | 0 |
| 0 | 1 | 0 |
| −1 | −1 | 1 |
| 1 | −1 | 1 |
| 0 | 0 | 1 |
| −1 | 1 | 1 |
| 1 | 1 | 1 |

Table A.2: 4-Factor multi-optimal designs for $k = 21$: GA4F21R_02

| $X_1$ | $X_2$ | $X_3$ | $X_4$ |
|---|---|---|---|
| −1 | −1 | −1 | −1 |
| 1 | 0 | −1 | −1 |
| −1 | 1 | −1 | −1 |
| −1 | 0 | 0 | −1 |
| −1 | −1 | 1 | −1 |
| 1 | −1 | 1 | −1 |
| −1 | 0 | 1 | −1 |
| 0 | 0 | 1 | −1 |
| 1 | 1 | 1 | −1 |
| −1 | 0 | −1 | 0 |
| 1 | 1 | −1 | 0 |
| 0 | −1 | 0 | 0 |
| 0 | 0 | 1 | 0 |
| 1 | 1 | 1 | 0 |
| 1 | −1 | −1 | 1 |
| −1 | 0 | −1 | 1 |
| 0 | 1 | −1 | 1 |
| 1 | 0 | 0 | 1 |
| −1 | −1 | 1 | 1 |
| 1 | 0 | 1 | 1 |
| −1 | 1 | 1 | 1 |

Table A.3: 5-Factor multi-optimal designs for $k = 26$: GA5F26R_01

| $X_1$ | $X_2$ | $X_3$ | $X_4$ | $X_5$ |
|---|---|---|---|---|
| −1 | −1 | −1 | −1 | −1 |
| 1 | 1 | −1 | −1 | −1 |
| 1 | −1 | 1 | −1 | −1 |
| −1 | 1 | 1 | −1 | −1 |
| 0 | 0 | 0 | 0 | −1 |
| 1 | −1 | −1 | 1 | −1 |
| −1 | 1 | −1 | 1 | −1 |
| −1 | −1 | 1 | 1 | −1 |
| 1 | 1 | 1 | 1 | −1 |
| 0 | 0 | 0 | −1 | 0 |
| 0 | 0 | −1 | 0 | 0 |
| 0 | −1 | 0 | 0 | 0 |
| −1 | 0 | 0 | 0 | 0 |
| 1 | 0 | 0 | 0 | 0 |
| 0 | 1 | 0 | 0 | 0 |
| 0 | 0 | 1 | 1 | 0 |
| 1 | −1 | −1 | −1 | 1 |
| −1 | 1 | −1 | −1 | 1 |
| −1 | −1 | 1 | −1 | 1 |
| 1 | 1 | 1 | −1 | 1 |
| 0 | 0 | 1 | 0 | 1 |
| −1 | −1 | −1 | 1 | 1 |
| 1 | 1 | −1 | 1 | 1 |
| 0 | 0 | 0 | 1 | 1 |
| 1 | −1 | 1 | 1 | 1 |
| −1 | 1 | 1 | 1 | 1 |

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