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Using Genetic Algorithms to Generate D_w and G_w-Optimal Response Surface Designs in the Hypercube

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Abstract

This article proposes and develops a genetic algorithm (GA) for generating response surface designs using weighted D and G optimality criteria (D_w and G_w). The numbers of input variables are $k = 2,3$ and 4 with the number of design points $N = p, p+1,..., p+4$ with $p = 6,10$ and 16, respectively. In this research, weak heredity (WH) is assumed with 16 cases of prior probabilities assigned to the reduced models. For all cases, the designs are generated in a k-dimensional hypercube design region. The weighted optimality criterion are used to compare the performance of GA designs with computer-generated designs (SAS OPTEX procedure).

Keywords: Computer-generated design, experimental design, robustness, optimality criteria, weak heredity.

1. Introduction

Response surface methodology (RSM) is helpful in solving many types of experimental problems. For example, RSM can address the problem of fitting a model over a particular region of interest, the problem of determining the optimization of the response, and the problem is selection of operating conditions to achieve certain specifications. The major goal is to maintain an optimal or near-optimal value for the response function.

The second-order model is applied in RSM because it is very flexible and easy to estimate the parameters by the least squares method. When fitting the model, the use of coded variables instead of the actual experimental process variables facilitates the construction of response surface designs. The advantages of using coded variables include computational ease and enhanced ability to interpret the coefficient estimates in the model introduced by Khuri and Cornell (1996). The actual process variables $\varphi_1, \varphi_2, \ldots, \varphi_k$ are transformed into coded variables $x_1, x_2, \ldots, x_k$, and the coded variables can be written as

$$x_i = \frac{2\varphi_i - (L_i + H_i)}{H_i - L_i}, \quad i = 1, 2, ..., k, \tag{1}$$

where H_i and L_i are the experimental high and low levels of φ_i, respectively. For this coding, note $-1 \le x_i \le 1$ for all i. The second-order model in the coded variables is defined as

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

After considering practical design size limitations due to resources such as time and money, design optimality criteria are often used to evaluate a proposed experimental design. In this research use D and G optimality criteria are used to evaluate designs. Borkowski and Valeroso (2001) and Anderson-Cook et al. (2009) used optimality criteria to evaluate and compare response surface designs. The selection of a design via optimality criteria is dependent on the model, number of design points, ranges for the process variable levels, and possibly other constraints. Therefore, different models lead to different design optimality criteria values. After the model is fitted, many parameters may be deemed in significant, and a reduced model retaining only significant terms is adopted for practical applications. Therefore, a design should be robust over the set of potential reduced models as well as the full model, That is, the design's optimality criteria should remain high over a wide classification of potential models particularly for those models held a priori to be most likely.

Chipman (1996) presented two classes of reduced models based on the weak heredity (WH) and strong heredity (SH) principles. Borkowski et al. (2001) used weak and strong heredity to generate weighted design optimality criteria for response surface designs. This research will lead to the development and application of only weak heredity to calculate a weighted average of the efficiency values across all models given the assignment of prior probabilities to model effects. This research addresses model misspecification when the second-order model is over-parameterized. Based on weighted D and G optimality criteria, the robustness properties of several families of response surface designs over a collection of reduced models are evaluated.

Although the weighted optimality criteria can be used to evaluate and compare designs, the designs that optimize these weighted optimality criteria are the most desirable. Currently, the optimal designs based on weighted optimality criteria are not known. A genetic algorithm (GA) is a potentially useful method to generate these optimal designs.

The foundation of GAs were developed by Holland (1975) and provided solutions for complex problem in optimization machine learning, programming, and job scheduling. The GAs were adopted in many disciplines and include generation of optimal response surface designs. For example, Borkowski (2003) used a GA to generate small exact response surface designs.

This research proposes and develops a genetic algorithm (GA) for generating response surface designs using weighted D and G optimality criteria (D_w and G_w) and compares the performance of GA designs with computer-generated designs produced by the OPTEX procedure in SAS statistical software.

2. Materials and Methods

This research will be presented in two parts. The first part is the evaluation of the D_w and G_w criteria for computer-generated designs using the OPTEX procedure in SAS. The second part is the development of a GA for generating designs that optimize these weighted optimality criteria.

2.1. Methodology for finding the weighted optimality criteria

The following methodology was used to calculate the weighted D_w optimality criterion values for all possible WH reduced models of the designs.

1. For a given number of design variable k and design size N, generate an N point design using the OPTEX procedure with k and N.

2. Reduce the full model using the principles of weak heredity (WH). WH requires that

- If a model contains an x_i^2 term, then it must also contain the corresponding x_i term, and
- If a model contains an $x_i x_j$ term, then it must also contain either or both of the corresponding x_i and x_j terms.

3. Calculate the D-efficiency from each WH reduced model. For $k = 2,3$ and 4 design variables, there are, respectively, 17, 185, and 3905 WH reduced models.

4. Use the a priori researcher-assigned probabilities (i.e. weights) to each of the model effects to determine the a priori probability for each WH reduced model. For a given model, the set of effects present in the model can be represented by a δ vector

$$\delta = \left(\delta_1, \delta_2, \ldots, \delta_k, \delta_{12}, \delta_{13}, \ldots, \delta_{(k-1)k}, \delta_{11}, \delta_{22}, \ldots, \delta_{kk}\right), \tag{3}$$

such that an effect is in the model or active if its associated δ indicator value equals 1. Otherwise, the effect is not in the model or inactive, and δ equals 0. In this research, independence among certain model effects is assumed (Chipman 1996). Specifically, it is assumed:

1. The linear effects (or δ_i indicators) are independent.

2. The interaction effects (or δ_{ij} indicators) are independent of each other and only depend on the parents (or δ_i and δ_j indicators).

3. The second-order effects (or δ_{ii} indicators) are independent of each other and only depend on the parent (or δ_i indicator).

4. Assuming these three independence assumptions, the joint probability density function of indicator vector δ can be written as:

$$\Pr\left(\delta\right) = \left(\prod_{i=1}^{k} \Pr\left(\delta_i\right)\right) \times \left(\prod_{i<j}^{k} \Pr(\delta_{ij} \mid \delta_i, \delta_j)\right) \times \left(\prod_{i=1}^{k} \Pr(\delta_{ii} \mid \delta_i)\right), \tag{4}$$

where $\Pr\left(\delta_i\right)$, $\Pr\left(\delta_{ij} | \delta_i, \delta_j\right)$, and $\Pr(\delta_{ii} \mid \delta_i)$ are researcher-assigned prior probabilities that the x_i, x_{ij} and x_i^2 terms, respectively, are in the model. Although not required, it is also assumed that the input variables equally important so that prior probabilities do not depend on particular variables, but only on the type of model term. Therefore, the prior probabilities are equal for linear effects, interaction effects, and second-order effects. That is,

$$\Pr\left(\delta_i = 1\right) = p_l \quad \text{for all } i, \tag{5}$$

$$\begin{aligned} \Pr\left(\delta_{ij} = 1 \mid \delta_i, \delta_j\right) &= p_0 \quad \text{if } \left(\delta_i, \delta_j\right) = \left(0,0\right), \\ &= p_1 \quad \text{if } \left(\delta_i, \delta_j\right) = \left(0,1\right) \text{ or } \left(1,0\right), \\ &= p_2 \quad \text{if } \left(\delta_i, \delta_j\right) = \left(1,1\right), \end{aligned} \tag{6}$$

$$\Pr(\delta_{ii} = 1 \mid \delta_i) \quad = \quad p_q \quad \text{if } \delta_i = 1,$$
$$= \quad 0 \quad \text{if } \delta_i = 0. \tag{7}$$

For WH, $p_0 = 0$. Thus, the researcher will only need to assign the values of p_l, p_1, p_2 and p_q when designing the experiment. In this research, the sixteen combinations of $p_l = 0.5$ or 0.9, $p_1 = 0.1$ or 0.7, $p_2 = 0.35$ or 0.95, and $p_q = 0.35$ or 0.95 were used to study a variety of a priori probability assignments.

5. Calculate the weighted optimality criterion $D_w = \sum_{i=1}^{K^*} D(i)\Pr(\Delta_i^*)$, $D(i) = 100|X'X|^{1/p}/N$ is the D-efficiency of the i^{th} reduced model having model matrix X and p is the number of parameters associated with the model. K^* = 17, 185, and 3905 for $k = 2,3$ and 4 design variables, respectively.

If the researcher wants to use the weighted G-optimality criterion G_w, replace *D*-efficiency $D(i)$ with $G(i)$ in the equation of D_w, where $G(i) = 100\max\left[p/Nx'(X'X)^{-1}x\right]$ is the G-efficiency of the i^{th} reduced model having model matrix X, and the maximum is taken over all points in the design space.

2.2. Methodology for developing the genetic algorithm (GA) for generating designs

The methodology for generating an k-variable N-point design that optimize the D_w or G_w weighted optimality criterion by a GA is outlined as follows.

1. Specify the number of design variables ($k = 2,3$ or 4), and the design size $N = p$, $p+1$, $p+2$, $p+3$ or $p+4$ design points with $p = 6, 10$ and 16, respectively, for he initial GA population of $M = 9$ parent designs (which are referred to as chromosomes in the GA).

2. For each of the M chromosomes, calculate the objective function of the GA for the weighted optimality criterion of interest (D_w or G_w).

3. Find the elite chromosome that produces the largest the objective function value. The remaining $M - 1 = 8$ chromosomes randomly partitioned into $(M-1)/2 = 4$ pairs of parent chromosomes.

4. Apply the reproduction process to each of these parental pairs. The reproduction process will operate on the genes to produce offspring chromosomes (or designs). An operator will be applied if a probability test is passed (PTIP). A probability test is a Bernoulli trial with success probability α. Thus, a PTIP if $U \le \alpha$ where U ~ Uniform[0,1]. Six operators will be applied in the following order: blending, zero gene, extreme gene, sign change, crossover, and creep. The success probabilities of applying these operators are α = 0.10, 0.15, 0.15, 0.05, 0.10, and 0.05, respectively.

i. Blending operator: If a PTIP, combine row A_a of A with a random row of B, say B_b to form two new rows: $\boldsymbol{A_a^*}$ and $\boldsymbol{B_b^*}$ via the linear combinations:

$$A_a^* = \beta A_a + (1-\beta)B_b \quad \text{and} \quad B_b^* = \beta B_b + (1-\beta)A_a,$$

where A and B are two parent chromosomes paired in the reproduction process, and blending proportion β is a random [0, 1] uniform variate.

ii. Zero gene operator: If a PTIP for gene x_{ij}, then the gene is set to 0.

iii. Extreme gene operator: If a PTIP for gene x_{ij}, then the gene is randomly set to ± 1.

iv. Sign change operator: If a PTIP for gene x_{ij}, then the sign of gene is changed. That is, replace x_{ij} with $-x_{ij}$.

v. Crossover operator: If a PTIP, the crossover operator will change a gene of A with a random gene of B by exchanging trailing decimal place digits from the genes after a random cut-point. After applying the crossover, the new genes from A and B are $A(r,c) = cutA + B - cutB$ and $B(r,c) = cutB + A - cutA$ respectively, where *cutA* and *cutB* are the genes of *A* and *B* truncated to a random number of decimal places.

vi. Creep operator: If a PTIP for gene x_{ij}, then a random normal $N(0,\sigma^2)$ variate is added to x_{ij} to form a new gene $x_{ij}^* = x_{ij} + \varepsilon$. If the creep operator takes $x_{ij}^* > 1$ or $x_{ij}^* < -1$ it will be reset to the boundary value $x_{ij}^* = \pm 1$. The variance σ^2 is set by the researcher.

The elite chromosome from the present generation of parent and offspring chromosomes is retained to the next generation which guarantees that the most fit chromosome (design) that has evolved will survive to the next generation. The elite chromosome, however, is not allowed to participate in the reproduction process until some future chromosome with a better fitness (larger D_w or G_w) evolves to take its place. After the reproduction process, there are the 1 elite, ($M-1$) parents, and ($M-1$) offspring chromosomes for a total of $2M-1$ chromosomes (or designs).

5. Calculate the objective function for each of these $2M-1$ elite, parent, and offspring chromosomes.

6. For each of the M parent/offspring pairs of chromosomes, calculate the objective function values. For each pair, the chromosome with the larger objective function value survives to be a future parent and the other is removed from the population. Hence, at the end of each generation, there are M chromosomes (one elite and ($M-1$) future parents) that exist to form the next generation.

7. Sort the M objective function values for this next generation of chromosomes, and select the one with the largest objective function values to become the elite for this generation.

8. Iterate steps 4 to step 7 for a large number of generations. In this research, 2,500 generation are used to generate designs for 2, 3, and 4 input variables. If needed, the number of generations can be increased if convergence does not occur.

3. Results and Discussion

The objectives of this study are to find the weighted D_w or G_w efficiencies for computer-generated designs and to develop a genetic algorithm for generating designs that optimize the D_w or G_w optimality criterion for variety of response surface design situations in a k-dimensional hypercube design region.

The results are contained in the following three sections: the weighted D and G-optimality criteria values (I) for $k=2$ design variables, (II) for $k=3$ design variables, and (III) for $k=4$ design variables. Each boxplot summarizes the D_w or G_w optimality criterion values for the sixteen combinations of a priori assignments of probabilities ($p_l = 0.5$ or 0.9, $p_1 = 0.1$ or 0.7, $p_2 = 0.35$ or 0.95, and $p_q = 0.35$ or 0.95) for the model terms.

(I) The weighted D_w and G_w optimality criteria values for $k=2$ design variables

The boxplots of the weighted D_w-optimality criterion values for SAS OPTEX designs (light shade) are almost equal, but for the GA designs (dark shade) there is slight increase when N increases. The D_w values of the GA designs are larger than the D_w values of the OPTEX designs. This is shown in Figure 1.

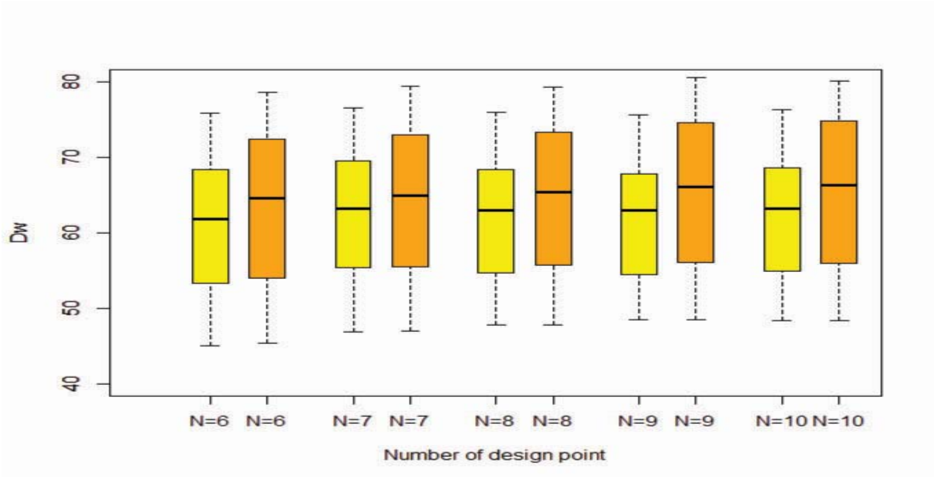

Figure 1 Boxplots for weighted D_w-optimality criterion values in a cuboidal region for OPTEX designs (light shade) and GA designs (dark shade) for $k=2$ design variables

The boxplots of the weighted G_w-optimality criterion values for SAS OPTEX designs (light shade) are and GA designs (dark shade) indicate there is slight increase when N increases. It is highest at $N=9$ and then decreased at $N=10$. The G_w values of GA designs are uniformly higher than the G_w values of OPTEX designs for all reduced models. This is shown in Figure 2.

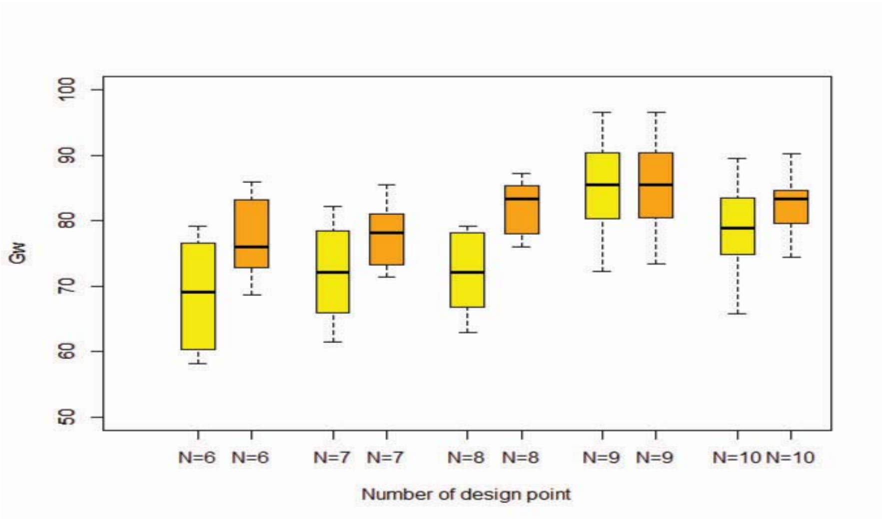

Figure 2 Boxplots for weighted G_w-optimality criterion values in a cuboidal region for OPTE designs (light shade) and GA designs (dark shade) for $k=2$ design variables

(II) The weighted D_w and G_w optimality criteria values for $k = 3$ factors

The boxplots of the weighted D_w optimality values for SAS OPTEX designs (light shade) indicate a slight increase from $N = 10$ to $N = 11$, and then decrease slightly for $N \geq 11$. The boxplots for the GA designs (dark shade) are almost equal for all N. The D_w values of GA designs are uniformly larger than the D_w values of the OPTEX designs. This is shown in Figure 3.

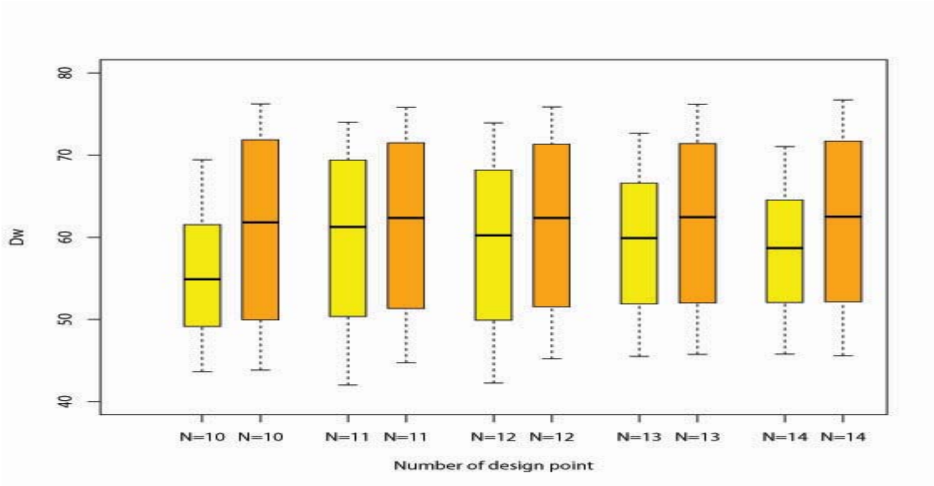

Figure 3 Boxplots for weighted D_w-optimality criterion values in a cuboidal region for OPTEX designs (light shade) and GA designs (dark shade) for $k = 3$ design variables

The boxplots of the weighted G_w optimality values for both SAS OPTEX designs (light shade) and GA designs (dark shade) increase when N increases. The G_w values of the GA designs are uniformly larger than the G_w values of the OPTEX designs, but are almost equal at $N = 14$. This is shown in Figure 4.

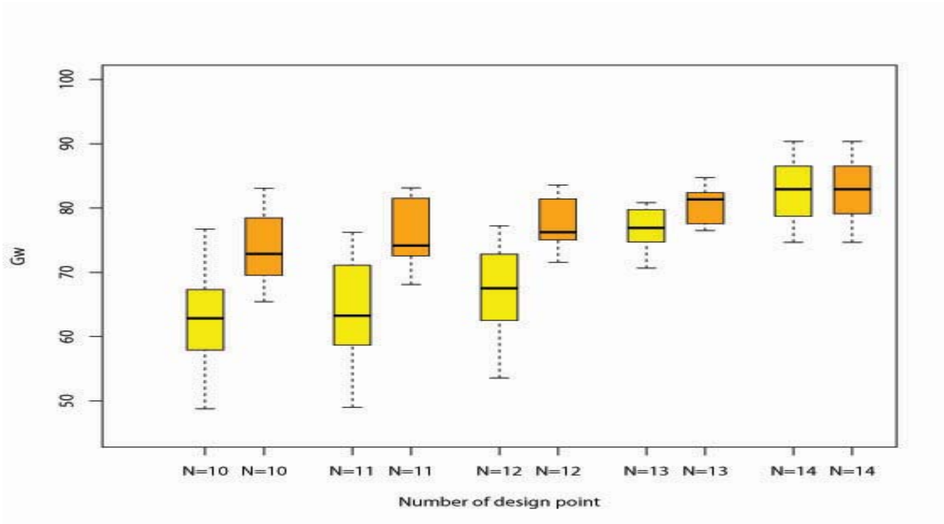

Figure 4 Boxplots for weighted G_w -optimality criterion values in a cuboidal region for OPTEX designs (light shade) and GA designs (dark shade) for $k = 3$ design variables

(III) The weighted D_w and G_w optimality criteria values for $k = 4$ factors

The boxplots of the weighted D_w optimality values for SAS OPTEX designs (light shade) form a small wave shape, but for the GA designs (dark shade) the D_w values are nearly constant and only very slightly increase when N increases. The D_w values of GA designs are larger than the D_w values of OPTEX designs. This is shown in Figure 5.

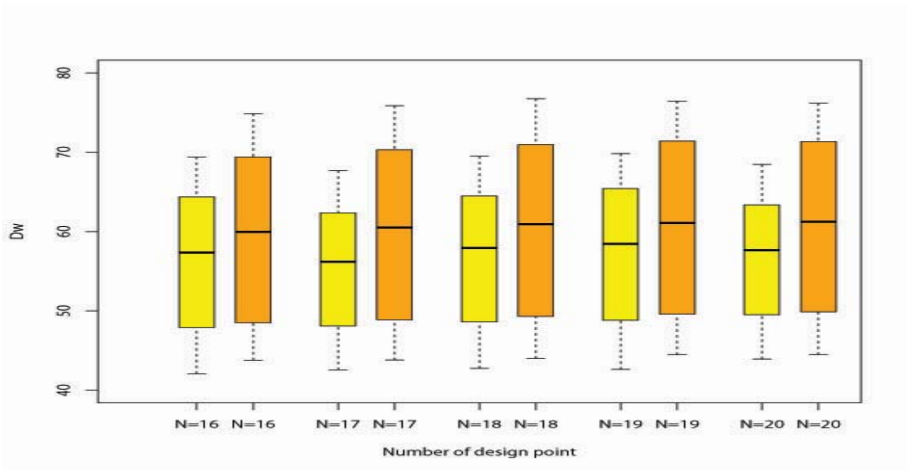

Figure 5 Boxplots for weighted D_w-optimality criterion values in a cuboidal region for OPTEX designs (light shade) and GA designs (dark shade) for $k = 4$ design variables

The boxplots of the weighted G_w optimality values for OPTEX designs (light shade) form a wave shape. The G_w values are smallest at $N = 16$ and $N = 18$. The G_w values for GA designs (dark shade) increase very slightly as N increases, and are larger than the G_w values of OPTEX designs. This is shown in Figure 6.

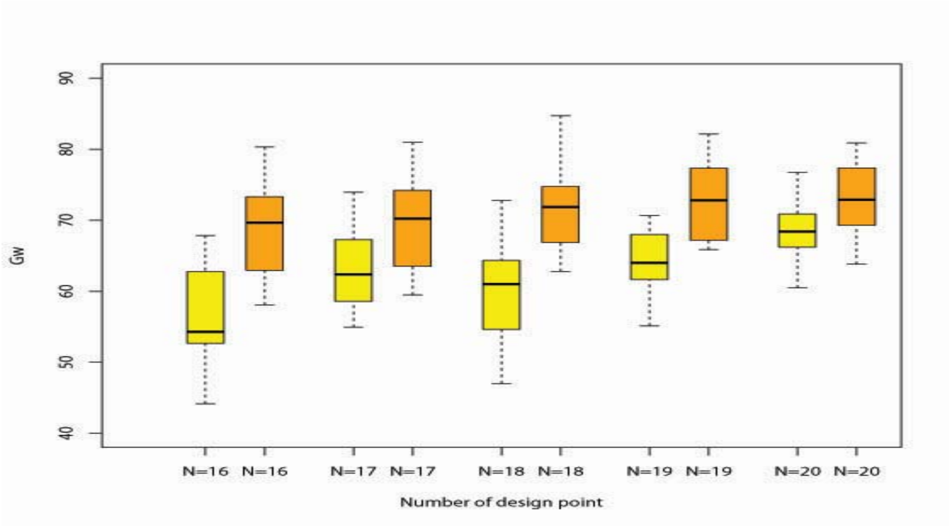

Figure 6 Boxplots for weighted G_w -optimality criterion values in a cuboidal region for OPTEX designs (light shade) and GA designs (dark shade) for $k = 4$ design variables

4. Conclusions

In this study, the weighted D_w and G_w optimality criteria for computer-generated designs and GA designs were found. The designs are in the k-dimensional hypercube, and the number of design variables k = 2, 3, or 4. Conclusions regarding design robustness and efficiency are shown in the Table 1.

Table 1 Conclusions regarding the robustness and efficiency of designs for each combination of weighted optimality criterion, design variables, and weighted optimality criterion

Criterion	Number of design variables					
	2		3		4	
	Robustness	Efficient	Robustness	Efficient	Robustness	Efficient
D_w	OPTEX GA	GA	GA	GA	OPTEX GA	GA
G_w	GA	GA	GA	GA	GA	GA

A design is considered robust if the weighted D_w and G_w values are not sensitive to changes across the sixteen a priori probabilities assigned to the model terms (See Equations (5), (6), and (7)). A design is considered efficient if the weighted D_w and G_w values remain relatively large compared other designs across the set of reduced WH models and assignment of a priori probabilities. It is clear that the GA designs are the more robust and efficient than the OPTEX designs for the G_w criterion for all k. The GA designs are more efficient and are equally or more robust than the OPTEX designs for the D_w criterion for all k. Hence, we recommend using GA designs over those generated by the OPTEX procedure.

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