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Using a genetic algorithm to generate D_s-optimal designs with bounded D-efficiencies for mixture experiments

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Abstract

We propose and develop a genetic algorithm (GA) to generate D_s-optimal designs for constrained mixture regions when quadratic terms are of primary interest. Our method does not limit the selection of design points from a finite candidate, but allows points to be select points throughout a continuous region in selection and reproduction process of GA. Summaries of GA designs are reported for 3 and 4 components. Moreover, efficiencies are used to compare the performance of GA designs with designs generated from an exchange algorithm (EA) and to computed-generated designs (CGDs).

Keywords: exchange algorithm, genetic algorithm, optimal design, mixture experiment, subset optimality.

1. Introduction

A mixture experiment is a special type of response surface (RS) experiment in which the controllable factors are ingredients or components of a mixture. In mixture experiments, the experimental region is defined by the following constraints:

$$x_i \geq 0, i = 1,2,.,q \quad \sum_{i=1}^{q} x_i = x_1 + \cdots + x_q = 1 \qquad (1)$$

where x_i represents the proportion of the *i*th component in a *q* component mixture.

The most commonly-used forms of the mixture model are the Scheffe' models. In many industrial or agricultural applications, the quadratic Scheffe' model has been used, and it has the form:

$$y = \sum_{i=1}^{q} \beta_i x_i + \sum \sum_{i<j}^{q} \beta_{ij} x_i x_j + \varepsilon \qquad (2)$$

where the β's are the parameter coefficients to be estimated, y is the response of interest and ε is a random error term.

Selection of experimental design is important for modelling a RS process. It involves selection of design points for the experimental trials, number of replications, and so forth. At present, there are statistical software packages and algorithms which are used to construct experimental designs based on methodologies for selecting experimental runs that optimize some design optimality criterion. The resulting design is called an optimal design. There are several popular optimality criteria, and the best-known and most often used criterion is *D*-optimality. Another optimality criterion of interest is D_s-optimality. This is an extension of *D*-optimality which focuses on a subset of model parameters.

Designs generated by software packages are called computer-generated designs. Currently, there is controversy about whether these designs are truly optimal exact designs or just near-optimal. Exchange algorithms (EAs) have been the most important algorithms for constructing exact *D*-optimal designs. EAs have evolved over the years. However, the disadvantages of EAs are long operating times when the number of factors increase and there is no guarantee that optimality will be achieved.

Genetic algorithms (GAs) have recently generated interest as an alternative way of constructing exact optimal designs because they have proven to be very effective in solving complex problems in other areas of science and engineering. For example, Borkowski [1] used a GA to generate near-optimal *D*, *A*, *G* and *IV* small exact response surface designs in the hypercube for the second-order model of 1, 2, 3 factors. Heredia-langner et al. [2] also used the GA for construction of exact *D*-optimal designs. They compared the performance of the GA with a family of EAs, and the results showed that

the performance of the GA was at least as good as those EAs. Alvarez et al. [3] reviewed previous studies using genetic algorithms in RSM. Limmun et al. [4] employed a GA to generate *D*-optimal designs for mixture experiments. The objective of this study is to develop a GA to generate D_s-optimal designs while simultaneously guaranteeing an acceptable lower bound for the *D*-efficiency for a mixture experiment. Moreover, the powerful advantages of a GA to generate a design are following:

- Unlike EAs, a GA does not need to select points from a finite user-defined candidate set.
- A GA allows movement through a continuous region.

A GA is suitable to produce a design which has numerous factors and highly constrained regions.

2. Genetic Algorithm (GA) Methodology

Genetic algorithms (GAs) were introduced by Holland [5] in 1975. Since then researchers across many disciplines have used GAs to solve difficult optimization problems. For a review of GAs and their applications, see Davis [6], Michalewicz [7], Haupt and Haupt [8], and Sivanandam and Deepa [9].

When using a GA, a chromosome represents a potential solution to an optimization problem and the objective function assesses the fitness of a chromosome as a solution. The goal is to find a chromosome that optimizes the fitness. The general steps of a GA include:

1. Starting population: Create an initial population of *N* parent chromosomes.
2. Selection process: Chromosomes with superior fitness in the population are retained so that their good characteristics can be passed to chromosomes in the next generation.
3. Reproduction process: Operators are applied to chromosomes to produce offspring chromosomes whose fitness is assessed relative to the parent population of chromosomes. The parent or offspring chromosome having the superior objective function value is retained for the next generation.
4. Convergence checking: After each generation, determine if the GA produced a chromosome that optimizes the objective function or stop if no further improvement is observed after some specified number of generations. Otherwise, repeat steps 2 and 3 with the chromosomes in the population at the end of the generation.

In developing the GA to construct D_s-optimal mixture designs, a chromosome is a mixture design, and the objective function will be a design optimality criterion which quantifies the fitness of a mixture design as a solution to the design problem. Thus, a chromosome is an $N \times q$ matrix representing the N design points in q components. A chromosome can then be expanded to the $N \times p$ model matrix X which include columns for all the p terms in the proposed Scheffe mixture model. Let x_{ij} be the real-value coded setting of the ith component in the jth experimental run. Each x_{ij} will be referred to as a gene of the chromosome. The main objective of this paper is to evolve a design (chromosome) that maximizes the D_s criterion (objective function) while simultaneously guaranteeing an acceptable D-efficiency for the mixture experiment.

Consider the X^TX matrix. A mixture design with model matrix X is said to be D-optimal if the design maximizes $D(X) = |X^TX|$, the determinant of the information matrix. The D-optimality criterion $D(X)$ is applicable when all p model parameters are to be estimated and the volume of the confidence ellipsoid is to be minimized. In certain cases, however, the experimenter may be interested in only a subset of s parameters with $s<p$. That is, the experimenter wants to minimizes the volume of the confidence ellipsoid for β_s where β_s is the vector of the subset of s model parameters of interest and β_r is the vector of the remaining $r = p-s$ model parameters. Rewrite β in partitioned form $\beta = [\beta_s| \beta_r]$. X^TX and $(X^TX)^{-1}$ are then rewritten in matrix portioned forms:

$$M(X) = \begin{bmatrix} M_{11}(X) & M_{12}(X) \\ M_{21}(X) & M_{22}(X) \end{bmatrix}$$

$$M^{-1}(X) = \begin{bmatrix} M^{11}(X) & M^{12}(X) \\ M^{21}(X) & M^{22}(X) \end{bmatrix}$$

The D_s-optimality criterion $D_s(X)$ is the minimization of the Determinant of $M^{11}(X)$, or, equivalently to maximize

$$|M_{11}(X) - M_{12}(X)M_{22}^{-1}(X)M_{12}^{T}(X)| = \frac{|M(X)|}{|M_{22}(X)|}$$

Therefore, the two optimality criteria will be considered in this constrained optimization problem: D_s-optimality criterion, $f_{Ds} = D_s(X)$, and the D-efficiency $f_D = D(X)$.

Let the lower bound constraint for the *D*-efficiency be denoted by *D*min. In this research, the values of *D*min considered are 0%, 25%, 50%, 75% and 100% of the *D*-efficiency values for *D*-optimal designs generated by the OPTEX procedure in *SAS* statistical software.

For these generated designs, note that a change in *D*-efficiency affects a D_S value for generating D_S-optimal designs for constrained mixture regions as follows: D_S increases when *D*-efficiency decreases, and vice versa.

The steps of the genetic algorithm are illustrated in Figure 1. Details of the steps are given in items *A*, *B*, *C* and *D*.

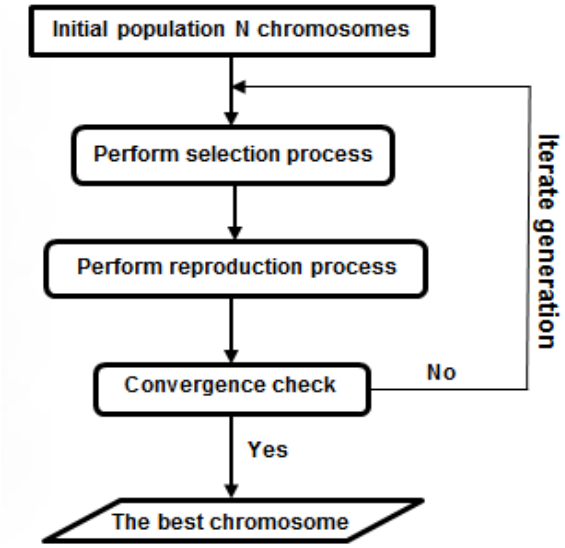


Figure 1. The steps of the genetic algorithm.

A. Creating an initial population of N chromosomes

To create an initial population of N chromosomes in this research, the1-point EA (EA1) is used. To start the EA1, n mixtures are randomly selected from a finite set of candidate mixtures to form an initial n-point design. Points are exchanged between the design and the candidate set, and the D-efficiency is re-calculated. Improved designs are retained, and the exchange process continues until no further improvement in D-efficiency occurs. If the final design has a D-efficiency value that is at least the specified Dmin value, it is retained. Otherwise, the design is discarded. The EA1 process is iterated until N designs satisfy the Dmin constraint. These N chromosomes form the initial population.

B. Selection process

The population at the start of every generation consists of an odd number of *N* chromosome (designs). Each chromosome is calculated for f_{Ds} and f_D values. The best or elite chromosome that has the highest f_{Ds} value is retained and left unchanged. The remaining *N-1* chromosomes are randomly divided into *(N-1)/2* pairs of a chromosome that are called the parent chromosomes. The *(N-1)/2* pairs of a parent chromosome are used to generate their offspring chromosomes by a reproduction process. At the end of the reproduction process in each generation, there are a total of *2N-1* chromosomes that are computed for f_{Ds} and f_D values for selection of the chromosomes to be the parent chromosomes in the next generation. For each parent-offspring pair, the chromosome with the better f_{Ds} value is kept to be a future parent whereas the other is discarded. Therefore, there exist *N-1* future parent chromosomes and the elite chromosome that will survive to the next generation. The *N* chromosomes are sorted and the chromosome that has the best f_{Ds} value becomes the elite for the next generation.

C. Reproduction process

This process was performed on the genes to produce offspring chromosomes. Generally, the process involves changing of the genes in the hope that the genes so evolved achieve the optimum of an objective function value. This change depends on the parameter values. The parameter value for this paper is a probability of success of a Bernoulli trial. The reproduction operator is applied when the parameter value is passed that it is within the range, $0 \leq \gamma \leq \alpha$,which γ is a random number form a [0,1] uniform distribution. On the other hand, if the parameter value is not passed, the reproduction operator is not utilized. This implies that the chromosome is left unchanged.

The blending, crossover, creep, and extreme operators as well as two new operators called mid-point and centroid will be used for this research.

D. The Reproduction Operators

The operators and their order used for the GA in this research are the blending, crossover, centroid gene, mid-point gene, extreme gene and creep gene. Let *u* be a random number from U(0,1). A probability test is passed (PTIP) if $u < \alpha$ where α is chosen by the researcher and will vary across operators. Let P1 and P2 represent two parent chromosomes.

- The blending operator combines row genes from P1 and P2 into new row genes in the offspring. Let A_m be the *m*th row of P1 and B_n be a random row of P2. If a PTIP, two new rows ,say A'_m and B'_n are formed as linear combinations

$$A'_m = \beta B_n + (1-\beta)A_m$$
$$B'_n = \beta A_m + (1-\beta)AB_n$$

where β is a random [0,1] uniform distribution.

- There are two crossover operators: between parents and within a parent.
    1. For the crossover operator between two parent chromosomes, if a PTIP, a row of P1 is exchanged with a random row of P2.
    2. For the crossover operator within a row of P1 or P2, if a PTIP, the genes within the row are permuted.
- For the centroid gene operator, if a PTIP, a gene x_{ij} is set to $1/q$ for a simplex region and it is set to an average of extreme vertices for a constrained mixture region.
- For the mid-point gene operator, if a PTIP, a gene x_{ij} is set to 1/2 for a simplex region and $(LB_i + UB_i)/2$ for a constrained mixture region where LB_i and UB_i are the lower and upper bounds of the i^{th} mixture component.
- For the creep gene operator, if a PTIP, a random ε such that $\varepsilon \sim N(0,\sigma^2)$ is added to a gene x_{ij} to form a new gene $x^*_{ij} = x_{ij} + \varepsilon$ If a new gene $x^*_{ij} < LB_i$ or $x^*_{ij} > UB_i$, it is reset to LB_i or UB_i, respectively. σ^2 is set by the researcher.

For each of these operators, the remaining $q-1$ genes in the i^{th} row operated are adjusted proportionally so that the mixture constraint $\sum_{i=1}^{q} x_{ij}^* = 1$ is satisfied. Specifically:

$$x_{kj}^* = x_{kj} + \frac{\left(1 - x_{ij}^*\right)}{\left(1 - x_{ij}\right)} \qquad (3)$$

where x_{kj} is the k^{th} gene in row j ($k \neq i$) before the operator is applied and x^*_{kj} is the new gene in row j after the operator is applied.

3. Results

Results for generating of the exact near D_s-optimal mixture designs for subsets of parameters from the Scheffe' quadratic mixture model

$$f(x) = \sum_{i=1}^{q} \beta_i x_i + \sum \sum_{i<j}^{q} \beta_{ij} x_i x_j$$

in a constrained mixture region will be presented. Designs generated by a GA and an EA will be compared in terms of D_s values and D-efficiencies. The primary $s=q(q-1)/2$ parameters to be estimated are the β_{ij}s while the remaining β_is are the $r=q$ nuisance parameters.

Consider two design cases: (C3) n = 6, 8 and 10 points for mixtures with q=3 components bounded by $0.2 \le x_1 \le 0.6$, $0.1 \le x_2 \le 0.6$, and $0.1 \le x_3 \le 0.5$ and (C4) n = 10 and 11 for the q=4 chemical constituents of a safety flare [10].

An empirical study is not feasible because of the time required for just one run of the GA, and that finding optimal parameter values with respect to program execution time is not required to find the D_s optimal designs.

The GA populations for design cases C3 and C4 have, respectively, 7 and 9 chromosomes. Let α_b, α_{cb}, α_{cwr}, α_{cp}, α_m, and α_{ct} represent probability test values for the blending, between-parent crossover, within-parent crossover, creep, midpoint, and centroid operators, respectively. For C3, each of these six α values were varied to be 0.05, 0.025 and 0.0125 across generations. For C4, α_b, α_{cb}, α_{cwr}, α_{cp} were varied to be 0.05, 0.025, 0.0125, and 0.003 across generations while α_m, and α_{ct} were varied between 0.003 and 0.007. For C3, σ=0.002 and for C4, $0.001 \le \sigma \le 0.003$. The GA was executed for 18000 and 23000 generations for C3 and C4, respectively.

The following notation is adopted: vertices (V), edge centroids (EC), near-edge centroids (NEC), overall centroid (OC), and near-overall centroid (NOC) for summaries of the GA, EA, and the SAS Proc OPTEX-generated design points.

- For C3 (q=3), the GA design points are V, NEC, and NOC points, the EA design points are V, EC, and OC points, and the SAS design points are V and EC points.
- For C4 (q=4), the GA and EA design points are V and NEC points, and the SAS design points are V and EC points.

Tables 1 and 3 contain list, respectively, the 3-component (Case C3) and 4-component (Case C4) mixtures that appeared as points in the designs generated by the GA or EA. All mixtures generated by SAS contain only vertices and edge centroids Tables 2 and 4 identify the specific design points using the coding given in Tables 1 and 3, respectively, for cases C3 and C4.

Table 1. List of points appearing in the q=3 components example (C3).

Label	x1	x2	x3	Label	x1	x2	x3
Vertices				**Other points**			
V1	0.3	0.6	0.1	O4	0.4	0.325	0.276
V2	0.4	0.1	0.5	O5	0.2	0.343	0.458
V3	0.6	0.1	0.3	O6	0.4	0.321	0.279
V4	0.6	0.3	0.1	O7	0.2	0.351	0.449
V5	0.2	0.6	0.2	O8	0.382	0.336	0.282
V6	0.2	0.3	0.5	O9	0.441	0.459	0.1
2-dimension centroids				O10	0.379	0.335	0.286
D1	0.25	0.6	0.15	O11	0.2	0.459	0.341
D2	0.2	0.45	0.35	O12	0.387	0.335	0.278
D3	0.45	0.45	0.1	O13	0.387	0.335	0.279
Other points				O14	0.383	0.334	0.283
O1	0.35	0.35	0.3	O15	0.383	0.334	0.283
O2	0.4	0.35	0.25				
O3	0.4	0.3	0.3				

Table 2. Summary of points appearing in the q=3 components example (C3).

Design	V1	V2	V3	V4	V5	V6	2-DC	Other points
GA6(0-75)	1	1	1	1				O4,O5
GA6(100)	1	1	1	1				O6,O7
EA6(0-100)		1	1	1		1	D1	O3
CGD6	1	1	1	1		1		O3
GA8(0-100)	1	1	1	1	1	1		O8
EA8(0-100)	1	1	1	1	1	1		O1,O2
CGD8	1	1	1	1	1	1		O1,O2
GA10(0,25,75)	1	1	1	1	1	1		O9,O10
GA10(50)	1	1	1	1	1	1		O11 to O13
GA10(100)	1	1	1	2	1	2		O14,O15
EA10(0-75)	1	1	1	1	1	1	D2,D3	O3
EA10(100)	1	1	1	2	1	2		O1,O2
CGD10	1	1	1	2	1	2		O1,O2

Table 3. List of points appearing in the chemical constituents of the flare example data (C4).

Label	x1	x2	x3	x4
Vertices				
V1	0.4	0.1	0.47	0.03
V2	0.4	0.1	0.42	0.08
V3	0.4	0.47	0.1	0.03
V4	0.4	0.42	0.1	0.08
V5	0.6	0.1	0.22	0.08
V6	0.6	0.1	0.27	0.03
V7	0.6	0.27	0.1	0.03
V8	0.6	0.22	0.1	0.08
(q-1)-dimension centroids				
D1	0.5	0.345	0.1	0.055
D2	0.5	0.1	0.345	0.055
Other points				
O1	0.6	0.1	0.25	0.05
O2	0.4	0.28	0.27	0.05
O3	0.5	0.35	0.1	0.05
O4	0.5	0.2	0.27	0.03
O5	0.6	0.25	0.1	0.05
O6	0.4	0.27	0.28	0.05
O7	0.5	0.1	0.35	0.05
O8	0.5	0.27	0.2	0.03
O9	0.4959	0.2743	0.1998	0.03
O10	0.4	0.2742	0.2751	0.0507
O11	0.5008	0.1	0.3444	0.0548
O12	0.6	0.2504	0.1	0.0496
O13	0.4958	0.2001	0.2741	0.03

Label	x1	x2	x3	x4
Other points				
O14	0.4055	0.2756	0.2691	0.0598
O15	0.5015	0.3437	0.1	0.0548
O16	0.4816	0.2297	0.2587	0.03
O17	0.5168	0.1	0.3032	0.08
O18	0.5021	0.3432	0.1	0.0547
O19	0.4	0.2717	0.2759	0.0524
O20	0.6	0.1	0.2521	0.0479
O21	0.4	0.275	0.275	0.05
O22	0.6	0.1	0.25	0.05
O23	0.485	0.225	0.26	0.03
O24	0.515	0.1	0.305	0.08
O25	0.6	0.25	0.1	0.05
O26	0.515	0.305	0.1	0.08
O27	0.485	0.26	0.225	0.03
O28	0.4	0.29	0.28	0.03
O29	0.43	0.11	0.38	0.08
O30	0.5	0.34	0.1	0.06
O31	0.52	0.1	0.35	0.03
O32	0.6	0.19	0.13	0.08
O33	0.4	0.1	0.43	0.07
O34	0.47	0.1	0.35	0.08
O35	0.53	0.1	0.34	0.03
O36	0.6	0.1	0.25	0.05

Table 4. Summary of points appearing in the chemical constituents of the flare example data (C4).

Design	V1	V2	V3	V4	V5	V6	V7	V8	DC	Other points
GA10 (0-50)	1	1	1	1	1	1				O9-O12
GA10 (75-100)	1	1	1	1		1	1	1		013-015
EA10 (0,100)	1	1	1	1			1	1		O1-O4
EA10 (25,50,75)	1	1	1	1	1	1				O5-O8
CGD10	1		1	1			1			028-O32, O36
GA11 (0-100)	1	1	1	1			1	1		O16-O20
EA11 (0,50,100)	1	1	1	1			1	1	D1	O21-O24
EA11 (25,75)	1	1	1	1	1	1			D2	O21, O25-O26
CGD11	1		1	1			1			O28, O30, O32-O36

Figures 2 and 3 show that the D_s-values of the GA designs are greater than those of the EA designs and the computed-generated designs (CDGs) from SAS. Figures 4 and 5 show that the *D*-efficiencies for C3 and C4, respectively.

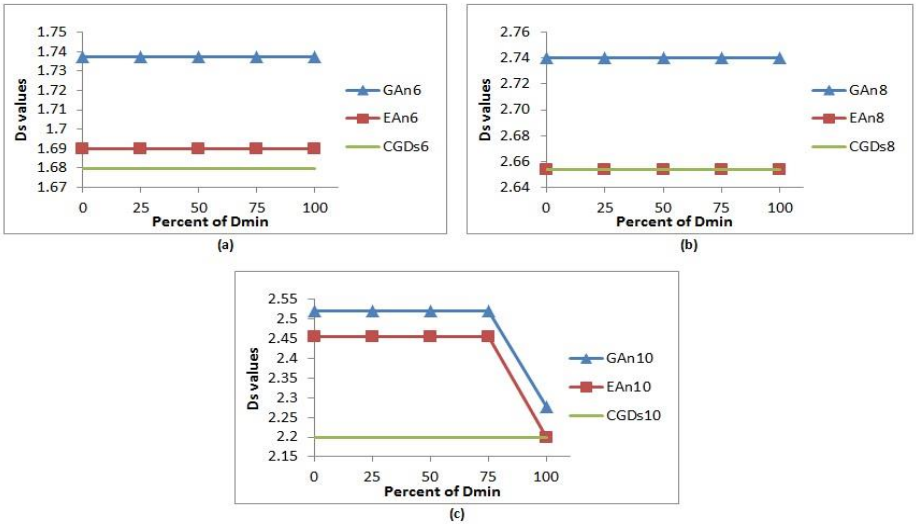


Figure 2. D_s values for case C3 (q=3).

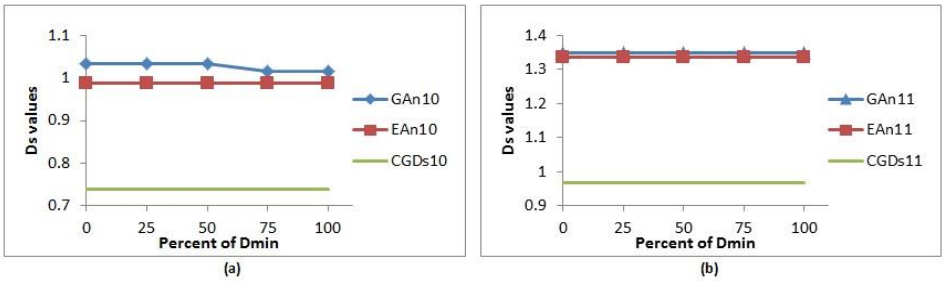


Figure 3. D_s values for case C4 (q=4).

For C3, the D-efficiencies at all percentages of $D_{\min}$ for the GA designs are less than those of the EA designs for n=6. For n=8, however, the D-efficiencies for the GA designs are greater than those of the EA designs. For n=10, all D- efficiencies at $D_{\min}$= 0, 25, 50 and 75 % for the GA designs are less than $D_{\min}$. However, the D-efficiencies at $D_{\min}$ = 100 % are mostly larger than $D_{\min}$.

For C4, the D-efficiencies at all percentages of D_{min} for the GA designs are equal to or greater than D_{min} except for n=15. Moreover, the D-efficiencies of both GA and EA designs are greater than D_{min}.

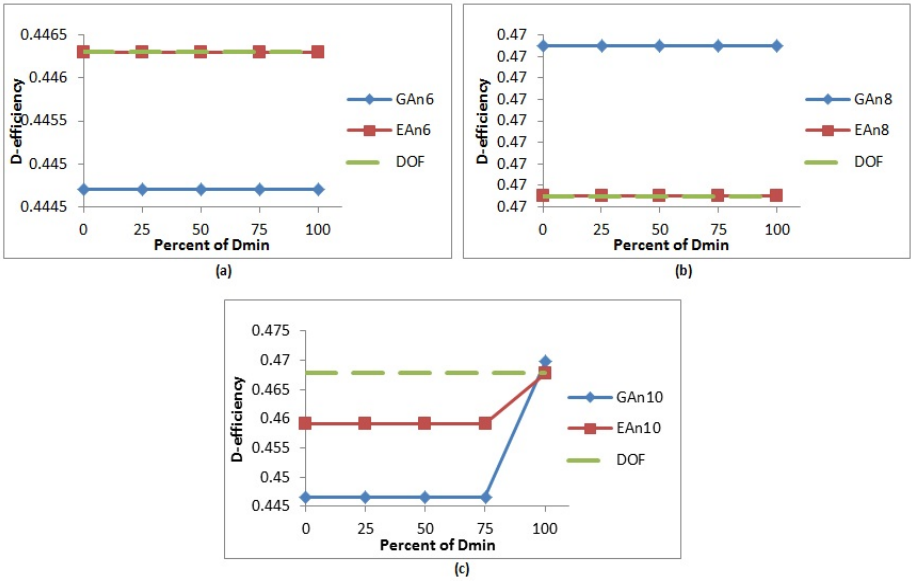


Figure 4. D-efficiencies for case C3 (q =3).

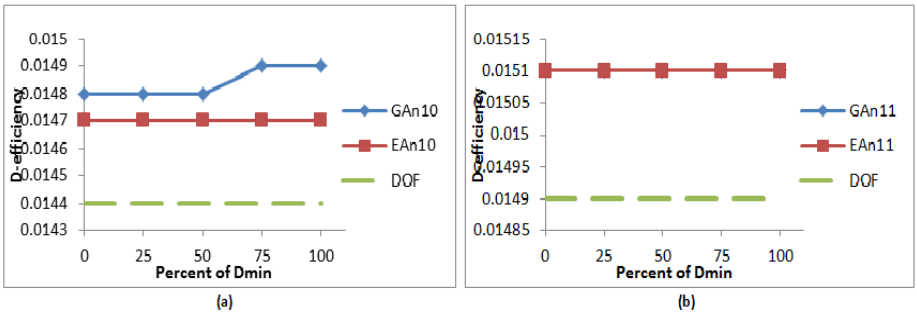


Figure 5. D-efficiencies for case C4 (q =4).

4. Conclusions and Recommendation

The primary goal of this research was to employ a GA to generate D_s-optimal or near-optimal mixture designs that are constrained by a lower bound on the D-efficiency. The D_s values of the GA designs are as good as, if not better than, those of the EA designs and the computed-generated SAS designs. However, the D-efficiencies of the GA are closer to the lower bound D_{min} than both the EA and the computed-generated SAS designs. Figures 6(a) and 6(b) show two patterns for the GA designs. The first pattern demonstrates that the GA designs obtain the same D_s values and the D- efficiencies at all percentages of D_{min}. Moreover, the D-efficiencies are equal to or slightly greater than the D-efficiencies of the full quadratic model from SAS. This implies that the designs are robust. The designs can give both the best D_s values and the best D-efficiencies. The designs from the second pattern yield similar D_s values and D-efficiencies at all percentages of D_{min} except 100 percent of D_{min}. The designs at 100 percent of D_{min} have the best D-efficiencies but the D_s values are slightly less than the best D_s values. Therefore, the suggestion in this case is to use the designs at 100 percent of D_{min}.

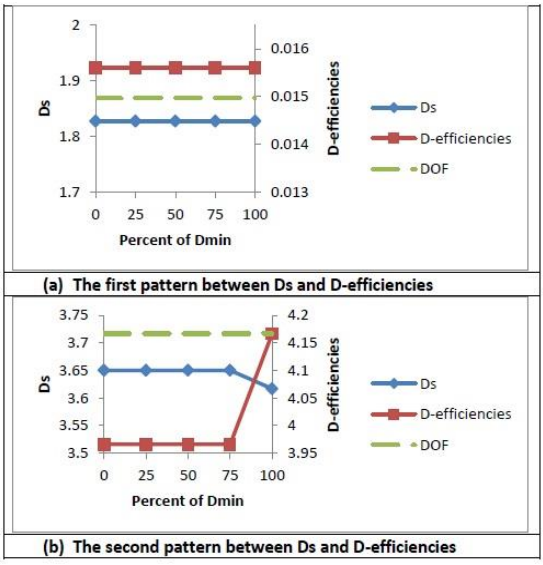


Figure 6. The pattern between D_s and D.

Acknowledgment

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