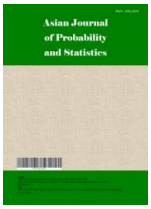

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Exploration of D-, A-, I- and G- Optimality Criteria in Mixture Modeling

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Authors' contributions

This work was carried out in collaboration among all authors. Author SWW designed the study, performed the statistical analysis, wrote the protocol, and wrote the first draft of the manuscript. Author AAO managed the analyses of the study. Author JKK managed the literature searches. All authors read and approved the final manuscript.

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Abstract

A design optimality criterion, such as D-, A-, I-, and G- optimality criteria, is often used to analyze, evaluate and compare different designs options in mixture modeling test. A mixture test is an experiment where the descriptive variable and response rely only on the mixture's relative ratio in the mix but not its composition. The study geared toward exploring D-, A-, I-, and G- optimality criteria and their efficiency in determining an optimal split-plot design in mixture modeling within the presences of process variables. We evaluated and discussed in detail D-, A-, I-, and G- optimality criteria based on literature review. We also explored and examine why I- and D-optimal criteria are often involved within the formulation of an optimal design in the context of mixture process variable settings. We recommend that optimality criterion must always be used when assessing the various styles of designs so as to search out a desirable design that matches a combination model.

Keywords: mixture designs; optimality criteria; optimal designs, split-plot designs, process variable.

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1 Introduction

A design optimality criterion, such as A-optimality, I-optimality, E-optimality, V-optimality, G-optimality, Q-optimality, and D-optimality, is typically used to analyze evaluate and compare designs. Myer et al. [1] include a more comprehensive discussion of the other design optimality. When the hypothesized model is of degree j and$1 \leq j \leq k \leq 8$, Wong [2] investigated the optimal criterion A, D, E, and G efficiencies for polynomial regression models of degree k. Most optimal designs are model-based and consider different model assumptions since, in practice, a true model is always uncertain. The robustness of properties of the optimal designs are normally evaluated under different optimality criteria. Wong, W. K [2] again in his paper posited that the optimality with respect to any criterion usually represents an estimate to some vague notion of 'goodness' of the model. This sometimes results in a design that meets many optimality requirements without being overly emphasized. The analysis of data resulting from many experimental designs normally depends on model assumption as described by Prescott, P. [3]. Therefore, this is always vital to examine different optimality criteria based on their model assumptions. The efficiencies of various types of optimal designs are typically compared numerically under the assumption that the true model $h_j(x)$ is j^{th} degree polynomial model given$1 \leq j \leq 8$. The collection of data in the designed experiment follows the assumption that the errors in the observations and the response are uncorrected with zero and constant variance [4]. In the absences of loss in generality, the symbol Ω is used in this paper to denote the design space that lies between -1 and 1. The use of optimal design for $h_k(x)$ is a good idea for the assumed model $h_j(x)$, $k > i$ as described by Kussmaul, K. [5], Kendall and Stuart [6], among others. This is because it always enables the researchers at least to perform a lack of fit test to various models being applied in order to determine the best model [7].

However, all designs are always considered continuous whenever the optimality criteria on different types of designs is being applied [4, 7]. This is normally aid in treating Ω as probability measure and ξ as a design with mass m_i at $x_i \epsilon\, \Omega, i = 1,2, \ldots, k$ subject to the constraints, $\sum_{i=1}^{k} nm_i = 1, n \epsilon N$ and $nm_i \in R$ where n is the planned observations that is taken at x_i under the assumption that $nm_i = N$ (total observations observed) [4]. Whenever this symbol $M(\xi)$ is applied usually represent the important amount of information contain in a continuous of the designξ. According to the standard optimal design theory by Fedorov $M(\xi)$ is also known as information matrix and is defined as

$$M_j(\xi) = \int_{\Omega} h_j(x) h_j'(x) \xi dx, \tag{1.1}$$

In addition, this information matrix also contains the main practical objective of an experiment [8]. Most optimality criteria for various designs have been discussed by various researchers [9, 10, 11, 12]. Therefore, the study explores and examine D-, A-, I-, and G- optimality criteria on how they contribute in selecting an optimal mixture process variable (MPV) designs according to the literature review.

1.1 Theory behind MPV within Split-plot Designs

Cornell [13] presents detailed information about mixture and MPV experiments. When the process variable is hard to change (Noise variable). Myers et al. [1], Goos and Donev [14], Cho [15], and Wanyonyi et al. [12] examined and evaluated robust MPV designs taking into account the usual process means and the Variance. The research begins at this MPV design entailing a hard-to-change process variable and adapts the MPV with split-plot designs structure. Hence, we present the articles as our selected papers for this study. Also, other more papers, which are nearly related to our purpose of the study.

However, the first Key articles focus on MPV design with hard change factor, commonly known as noise variable. In these papers, the researchers aimed to develop a model comprising mixture blends and controllable and uncontrollable process variables. The controllable process variables are easy to change factors, whereas uncontrollable factors are hard to change. They also took into account the models, which allow correlations between hard-to-change factors. They used a study technique involving a robust process in establishing variable levels, responsive to alterations in the uncontrollable process variable. In a situation involving rigorous analysis, the delta method was used to evaluate the Variance and mean of a targeted variable. The researchers often use this technique to find the best combinations that generate the desired mean value while reducing Variance.

The graphical technique paper presented by Njoroge et al. [16] is another essential paper relevant to this research. Fraction design space (FDS) plots for MPV designs are the focus of this approach in conjunction with design optimality criterion in finding an optimal design. Furthermore, Myers et al. [1] concentrate on prediction variances over design space using a variance dispersion graph (VDG), which allows the experimenter to see patterns of prediction variance in the design space. The FDS plots were initially introduced by Zahran *et al.* [17], not as a substitute for VDGs but complementary approach. The FDS plots provide sufficient information on the prediction variance distribution over the experimental area. This method was used by Goldfarb *et al.* [18] to create FDS plots for mixture designs. They showed that Piepel and Anderson's [19] random sampling technique and shrunken area approach yield equivalent results for fraction design space values and plots. They also provided the global FDS plot and sliced FDS plot over different process area shrinkage values for MPV designs. FDS plots for split-plot designs are discussed in Liang et al. [20]. When the design is entirely well randomized, the scaled prediction variance (SPV) is usually based on the experimental design and presumed model. Due to the covariance of the response affecting the entire plot error variance and subplot error variance, SPV becomes more complicated when SPD is taken into account. To study the relationship between fundamental plot errors and split-plot (subplot) errors, several researchers used the paradigm of variable variance ratio (d) as the basis for FDS plots.

$$d = \frac{\sigma_\delta^2}{\sigma_\varepsilon^2}, \tag{1.2}$$

where σ_δ^2 is the whole plot error variance and σ_ε^2 the subplot error variance. They also used sliced FDS plots at different whole plot levels to investigate prediction capability across the entire split-plot area in the design space. They also considered the influence of the variance ratio factor on design efficiency.

However, in this paper, the study majorly focus on design optimality criterion in determining an optimal design in the context of MPV settings within SPD instead of graphical techniques (VDG and FDS).

2 Statistical Modeling in the Context of Mixture Design

A mixture test is an experiment where the descriptive variable (factors) and response rely only on the mixture's relative ratio in the mix but not its composition. For example, the yield of crops may be the maximum number of Glycine per stem or the number of seeds per stem. In the most basic mixture design test, the q component in the compound meets the following barriers.

$$0 \le x_i \le 1 \sum_{i=1}^{q} x_i = 1 \tag{2.1}$$

The proportion of each blend must be between 0 and 1. Also, the proportions of the q blends in the mixture must total up to unity. The factor components space for an experiment with constraints (2.1) is a $q-1$ dimensional simplex that may include the design space's edge and interior. However, experiment with mixtures was officially formalized by Henry Scheffe in 1958 [21], where the simplex lattice design (SLD) and corresponding Scheffe canonical polynomial model was formally introduced [22]. Scheffe defines a (q, m) lattice to fit the design where q and m represent the number of components in the mixture and the polynomial model's degree, respectively. They are $\binom{m+q-1}{m}$ candidate points in a simplex lattice design [13]. The proportions applied for each component have $m+1$ equally spaced values from 0 to 1 of $x_i = 0, \frac{1}{m}, \frac{2}{m}, \ldots, 1$. One-to-one correspondence of candidates points to the polynomial model parameters, as pointed out by Cornell [13]. For instance, in a $(q, 1)$, SLD is the form:

$$\eta = \sum_{i=1}^{q} \gamma_i x_i \tag{2.2}$$

Subject to the substitution

$$x_q = 1 - \sum_{i=1}^{q} x_i \tag{2.3}$$

Into the standard polynomial model form:

$$\eta_1 = \beta_0 + \sum_{i=1}^{q} \beta_i x_i \tag{2.4}$$

According to Cornell [13] and Goos et al. [22], the Polynomial coefficient has a one-to-one correspondence with the points in the design. As mentioned above, there are q candidate points in a $(q, 1)$ SLD; hence for a three-mixture blend, there are three candidate points, and in the corresponding Polynomial, three parameters to be approximated. Enables for the coefficients to be compared employing least squares (MLS) regression, Maximum likelihood method (MLM), restricted maximum likelihood (REML), and ordinary least squares (OLS) as described in Wanyonyi *et al*. [12, 23]. Scheffe defines a second-order polynomial model for mixtures where the anticipated response to take on a nonlinear form as:

$$\eta = \sum_{i=1}^{q} \gamma_i x_i + \sum_{i=1}^{q-1} \sum_{j=i+1}^{q} \gamma_{ij} x_{ij} \tag{2.5}$$

In this polynomial model, the pure quadratic terms are combined with the two-factor quadratic terms owing to the substitution

$$x_i^2 = x_i \left(1 - \sum_{i=1, j \neq i}^{q} x_j \right) \tag{2.6}$$

As described by Goos et al. [22], in addition to the substitution used in the model (2.4). However, with this substitution, the Polynomial degree remains unchanged, and the number of terms $\binom{m+q-1}{m}$ maintaining the one-to-one correspondence of design points and parameters in the model.In mixture design experiments, the interaction terms in the model are commonly known as nonlinear blending terms. However, the nonlinear blending terms, response to binary and ternary or quinary mixtures, can be perceived and illustrated as being either a synergistic effect or an antagonistic effect. These interpretations of binary, ternary, and quinary mixture terms are broadly used in describing the impact of components on the characteristics of a mixture.

Response surface methodology traditionally applies a second-order Taylor series as the appropriate model basis for process optimization [14, 24]. This assumption relies typically on sufficient background knowledge besides knowing the experimental region that supports an accurate second-order model described by Kowalski et al. [25]. The mixture elements, process variable, and mixture by process variable interaction are always equal. In reality, according to Goos and Donev [14] and Cho [15], the mixture process variables interaction terms also provide considerable insight into optimal operating conditions.

In the polymer experiments proposed by Cornell [13] and Myers et al. [1], the experimenter may be interested in learning about a particular mixture component that makes the reaction particularly sensitive to the reaction temperature. This experimental situation led some authors (14, 15) to propose a new model for approaching the mixture process variable (MPV) experiments simplex centroid design with the split-plot structure experiments. However, the critical concern MPV design is the estimation variance at a particular location; design efficiency is often the best choice for comparing, analyzing, and assessing various design options. G-, I-, V-, and Q-optimality are architecture optimality parameters that rely on prediction variance. We therefore, discuss the role played by optimality criteria when comparing different mixture models.

3 Exploration D-, A-, I-, and G- Optimality Criteria

3.1 D-optimality Criterion

The D-optimality criterion is the determinant of the matrix $M_j(\xi_j)$for all the set χ for all continuous designs on Ω.

$$M_j(\xi) = Max_{\xi}\epsilon\chi\left|M_j(\xi)\right|, \tag{3.1}$$

where $\left|M_j(\xi)\right| = det\left(M_j(\xi)\right)$ denotes the the determinant of the information matrix [2, 26]. The moment matrix is another name for the information matrix denoted as $M = \frac{X'X}{N}$ wherethe concept matrix is represented by X, and its transpose is represented by X'. This optimality criterion normally focuses on good model parameter estimation. More so it makes both variance and covariance among the model parameter estimates small.

However, Chasiotis et al. [27, 28] proved that two saturated ± 1 designs of order 22, already existing in the current literature, are the D-optimal ones. They performed an exhaustive search for potential Gram matrices with determinant exceeding those of the provided designs, finding 25 such matrices. Each of these was excluded from being a Gram matrix, and so the maximum determinant of the provided designs was proved.

Furthermore, a design is D-optimal as described in Goos *et al*. (2016) if it reduces the overall variance of the model parameter estimates. The criterion function, on the other hand, defines this criterion as [26]:

$$\phi\left(M_j(\xi)\right) = Max_{\xi}\{M_j(\xi)\} = Min_{\xi}\{det\ det(M^{-1}(\xi))\}, \tag{3.2}$$

The D- efficiency of any design can also be obtained for the purpose of numerical comparison of various designs. This D- efficiency is given as

$$D\left(M_j(\xi)\right) = \left[Min_{\xi}\{det\ det(M^{-1}(\xi))\}\right]^{P^{-1}}, \tag{3.3}$$

Computation of relative D-efficiency is quite very important when it comes in comparing more than two designs at any given time and only one design needs to be selected [2]. In addition, relative D-efficiency (RD) plays a big role in determining best design among other designs with missing observations. Therefore, this leads to computation of loss in relative D-efficiency due to incomplete observations in any given design. The missing observations in a design experiment often drastically results in relative of D-efficiency as described by Iwundu, M. P. [26]. For the purpose of computing RD, we first start by letting a design with complete observations as $M(\xi_N)$ and the one with missing observations as $M(\xi_{N-m})$ where ξ_N indicates information matrix with full observations while ξ_{N-m} with missing observations. The D-efficiency is computed in both cases as

$$D(M(\xi_N)) = \left[Min_{\xi}\{det\ det(M^{-1}(\xi_N))\}\right]^{P^{-1}}, \tag{3.3}$$

$$D(M(\xi_{N-m})) = \left[Min_{\xi}\{det\ det(M^{-1}(\xi_{N-m}))\}\right]^{P^{-1}} \tag{3.4}$$

In (3.3) and (3.4) represent RD with complete and incomplete observations respectively. The RD is obtained by using (1.2.2.1) and (1.2.2.2 as follows

$$RD = \left\{\frac{\left[Min_{\xi}\{det\ det(M^{-1}(\xi_{N-m}))\}\right]^{P^{-1}}}{\left[Min_{\xi}\{det\ det(M^{-1}(\xi_N))\}\right]^{P^{-1}}}\right\} = \frac{D(M(\xi_{N-m}))}{D(M(\xi_N))}, \tag{3.5}$$

The RD in (3.5) is used to compare designs, and the better design has the highest D-efficiency value. The RD of a designs lies between 0 and 1 such that $0 \le RD \le 1$. If $RD < 0$ implies that the design ξ_{N-m} is better than the design ξ_N. Therefore, the relative loss in D-efficiency in the case of missing observations is given as

$$RD_{Loss} = 1 - \frac{D\big(M(\xi_{N-m})\big)}{D\big(M(\xi_N)\big)}. \tag{3.6}$$

3.2 G-optimality Criterion

The G-optimality criterion is a criterion that researchers can use to reduce the overall variance of the approximated response surface across all variables. The quantity of information matrix becomes G-optimal design when $Max\ \big(d_j(X,\xi)X\epsilon\ \Omega\big) = h_j'(x)M_j^{-1}(\xi)h_j$ over χ is minimized. Wong [2] argued that this design is more useful and important when the main goal is to estimate the entire response using the homoscedasticity assumption. As define.

d by the criterion function, the G-optimal design is

$$\phi\big(M(\xi)\big) = Min\{Max\ V(x)x\epsilon R\}, \tag{3.7}$$

where the scaled prediction variance is denoted by V(x) in this case. Prior to running the test and taking measurements, the scaled prediction variance (SPV) is used to analyze a planned experiment [25, 15]. This is because it describes and elucidates the error involved with making a prediction using a regression model. Moreover, this optimality criterion considers a design where maximum SPV in the region of interest is not too large and hence it maximizes the maximum SPV. When there are *P* parameters in the model and maximum SPV ($V(x)$), the G-efficiency can be calculated as

$$G_{eff} = P\big[V(x)_{Max(\xi)}\big]^{-1}, \tag{3.8}$$

Furthermore, the G-efficiency can also be computed in the case of missing observations. If we let the expected design beξ_N and observed design beξ_{N-m}, then relative G-efficiency (**RG**) can be obtained for *P* parameter model. This is done by first determining G-efficiency for a design with incomplete observations as

$$G_{eff(\xi_{N-m})} = P\big[V(x)_{Max(\xi_{N-m})}\big]^{-1}. \tag{3.9}$$

This $G_{eff(\xi_{N-m})}$ enables to compute the **RG** which is defined as

$$\mathbf{RG} = \frac{G_{eff(\xi_{N-m})}}{G_{eff(\xi_N)}} = \frac{V(x)_{Max(\xi_N)}}{V(x)_{Max(\xi_{N-m})}}. \tag{3.10}$$

Moreover, this **RG** aid in comparing design and the best design is known with the largest G-efficiency such that $0 \le RG \le 1$ but when $RG \le 0$ the design ξ_{N-m} with missing observations is better than the design ξ_N with complete observations. Besides calculating RG, the relative loss in G_{eff} due to missing observations is obtained as [26]

$$RG_{loss} = 1 - \frac{V(x)_{Max(\xi_N)}}{V(x)_{Max(\xi_{N-m})}} \tag{3.11}$$

3.3 A-Optimality Design Criterion

Researchers use the A-optimality criterion in planned experiments to reduce the variance of parameter estimates while ignoring model parameter covariance [2, 13, 15, 26]. Jones et al. [29] provided evidence that screening designs under the A-optimality criterion are more desirable than the ones under the D-optimality criterion, and so they advised experimenters to choose A-optimal designs rather than D-optimal ones for screening experiments. Also, they concluded that A-optimal designs generally perform better in terms of other optimality criteria than D-optimal designs.

Furthermore, the number of the variances of the model co-efficient is minimized whenever this optimality criterion is used as described in Iwundu [26]. This criterion for optimality is as follows:

$$\phi\big(M(\xi)\big) = Min\{tr[M^{-1}(\xi)]Over\ \chi\}, \tag{3.12}$$

where tr represent the trace and χ indicates all the set for all continuous designs on Ω. The A-efficiency in general is defined as

$$A_{eff}(\xi) = \frac{tr[M^{-1}(\xi^*)]}{tr[M^{-1}(\xi)]}, \tag{3.13}$$

where ξ^* in this case indicates A-optimal. However, the A-efficiency for a design with incomplete and complete observations is computed respectively as

$$A_{eff}(\xi_{N-m}) = \frac{tr[M^{-1}(\xi^*)]}{tr[M^{-1}(\xi_{N-m})]}, \tag{3.14}$$

And

$$A_{eff}(\xi_N) = \frac{tr[M^{-1}(\xi^*)]}{tr[M^{-1}(\xi_N)]}. \tag{3.15}$$

Therefore, the relative A-efficiency for P-parameter model is obtained as

$$RA_{eff}(\xi) = \left(\frac{\left\{\frac{trace[M^{-1}(\xi^*)]}{trace[M^{-1}(\xi_{N-m})]}\right\}}{\left\{\frac{trace[M^{-1}(\xi^*)]}{trace[M^{-1}(\xi_N)]}\right\}}\right) = \frac{tr[M^{-1}(\xi_N)]}{tr[M^{-1}(\xi_{N-m})]}. \tag{3.16}$$

This $RA_{eff}(\xi)$ aid in comparing the design. The best design is known with the largest $A_{eff}(\xi)$ value where $RA_{eff}(\xi)\ \epsilon\ [0, 1]$. If $RA_{eff}(\xi) < 0$ shows that the design ξ_{N-m} is better than ξ_N.

3.4 I -Optimal Criterion

I -optimal is an optimality criterion that minimizes the average predicted relative variance [2, 26]. Over centuries ago, G- optimality criterion has often been used since it minimizes the overall prediction variance over the experimental area as a prediction-based criterion for selecting experimental design. Recent research has shown that in more than 90% of experimental areas, reducing the overall prediction variance occurs as a result of increasing the prediction variance as described in Sitinjak and Syafitri [30]. As a result, as Goos et al. [22] point out, most writers prefer I-optimal designs to G-optimal designs. This is evident from the contour plots of the objective function for three criteria (D-, I- and G-optimal) using a very simple model function that was done by Crary et al. [31]. This simple model function was $Y = \beta_0 + \beta_1 X$and $n = 2$ experiments where the optimal design for three criteria placed one experiment at -1 and the other at +1 as it is supposed to be. Their findings indicate that the contours for G -optimality have discontinuous slope because of the minimax nature of the criterion.

The average variance prediction over the entire range of χ is minimized using the appropriate objective function as described by Crary et al. [31]. This appropriate objective function is defined as

$$Min_Q \int_{x\in\Xi} E\left\{\left[\hat{Y}(x) - Y(x)\right]^2\right\} d\mu(x) = Min \int_{x\in\Xi} [h'(x)(x'x)^{-1}h(x)]d\mu(x), \tag{3.17}$$

$Min\ trace\ A(x'x)^{-1}$,where

$$A = \int_{x\in\Xi} h(x)h'(x)d\mu(x).$$

A is the matrix that contains all of the model's dependencies. The minimization case of the integral over the set of points $s \in \Xi$ for the experimental design Q is denoted by Min Q. However, the estimated response within different experiment regions can be weighted through the differential $d\mu(x)$.

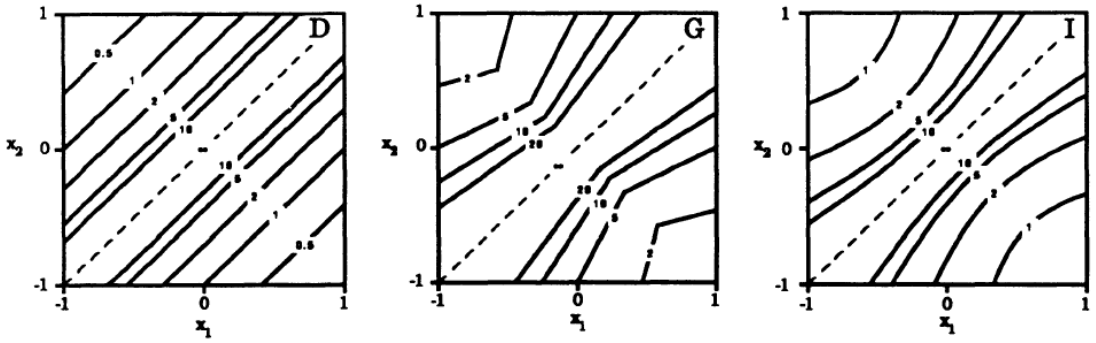

Fig. 1. The contours plots presented by Crary et al. [31] for objective function space for D-, G- and I-optimality for a straight- line regression with $n = 2$

Computing I -efficiency for designs is always important since it aids in selecting the appropriate design. I-efficiency for a design is obtained by the average of predicted relative variance (Goos et al. [22]**.** Therefore, a design with complete observations(ξ_N), I -efficiency can be computed as

$$I_{eff\,(\xi_N)} = \{2^k\}^{-1} trace\,[(X'X)^{-1} M\,(\xi_N)]. \tag{3.18}$$

However, for the case of a design with missing observations, I -efficiency can be obtained as

$$I_{eff\,(\xi_{N-m})} = \{2^k\}^{-1} trace\,[(X'X)^{-1} M\,(\xi_{N-m})]. \tag{3.19}$$

Furthermore, the relative I -efficiency and relative of I -efficiency loss after missing observations is obtained as follows

$$\begin{aligned} RI_{eff\,(\xi_{N-m}|\xi_N)} &= \frac{\{2^k\}^{-1} trace\,[(X'X)^{-1} M\,(\xi_{N-m})]}{\{2^k\}^{-1} trace\,[(X'X)^{-1} M\,(\xi_N)]}, \\ &= \frac{trace\,[(X'X)^{-1} M\,(\xi_{N-m})]}{trace\,[(X'X)^{-1} M\,(\xi_N)]}, \\ &= \frac{I_{eff\,(\xi_{N-m})}}{I_{eff\,(\xi_N)}}. \end{aligned} \tag{3.20}$$

Thus, the relative of I -efficiency loss is given as

$$RI_{loss\,(\xi_{N-m}|\xi_N)} = 1 - \frac{trace\,[(X'X)^{-1} M\,(\xi_{N-m})]}{trace\,[(X'X)^{-1} M\,(\xi_N)]}, \tag{3.21}$$

where $0 \leq RI_{eff\,(\xi_{N-m}|\xi_N)} \leq 1$. If $RI_{eff\,(\xi_{N-m}|\xi_N)} < 0$, then the design ξ_{N-m} is better than ξ_N. We also note that if they are two different designs for instance say Q_1 and Q_2 with each having relative I -efficiency RI_{Q_1} and RI_{Q_2} respectively, then relative I -efficiency of Q_1 versus Q_2 is given as $\frac{RI_{Q_2}}{RI_{Q_1}}$. Hence, if $\frac{RI_{Q_2}}{RI_{Q_1}} > 1$ implies that design $Q_1$is better than design Q_2.

3.5 Application D- optimal criteria in Construction of Mixture Designs

In this section, we look at the involvement of continuous or exact D- optimal criteria in construction of mixture designs based on pre-existing results on D- optimality. When the design space is the $q-1$ dimensional simplex, Goos *et al*. [10] point out that continuous D- optimal parameters for the models (2.2) to (2.5) are known. This criterion generally has two main characteristics. First, in D-optimal designs, the weight of each candidate point is equal to the inverse of the model parameters$\left(\frac{1}{P}\right)$. Second, they are minimum support designs, where d the number of distinct candidate points and P is the number of model parameters. The same $d = P$ design points are used in both continuous and exact D-optimal designs. When the budgeted number of runs in a mixture blend experiment, n, is an integer multiple of the D-optimal continuous configuration, $n/d = n/P$ runs are performed at each of the candidate points.

However, if n is not an integer multiple of $d = P$, the situation can be addressed by having as many equireplicated constant $d = P$ design points as possible, as Goos *et al*. advocate (2016). Some authors say that it doesn't matter the design points are repeated the most since the D-optimality criterion is their only concern [26]. The D- optimality of the $(q, 1)$ and $(q, 2)$SLDs for model (1) and (2), respectively, was defined by Kiefer [32]. After that, Uranis [33] demonstrated that the $(q, 3)$ are D- optimal for a special cubic model. D-optimal designs, according to Goos et al. [22], includes$q$ pure blends, $(q, 2)$ mixtures involving 0.2764 percent of one mixture blend and 0.7236 percent of another mixture blend, with exact proportions given by $\frac{\left(1\pm\frac{1}{\sqrt{5}}\right)}{2}$, and $(q, 3)$ ternary mixtures.

When it comes to constructing D- optimal designs for complete cubic models, the $\{q, 3\}$ simplex lattice design (SLDs) by 0.2764 and 0.7236 can be replaced by the proportions $\frac{1}{3}$ and$\frac{2}{3}$, respectively, based on Mikaeilli [34]. He proved the complete cubic models with all derivations in a general way. In contrast to other optimality designs, Goos et al. [22] found that D- optimal designs perform remarkably well in terms of the I–optimality criterion.

3.6 Application I-optimal Criteria in Construction of Mixture Designs

Only a small number of theoretical findings on the I-optimal design of mixture experiments have been reported. As Goos et al. [22] point out, all of the outcomes require continuous designs. Some researchers used the terms V- optimal, I- optimal, and all variance design interchangeably to refer to I- optimal designs, citing Sinha et al. [35]'s Theorem 12.1.1, which states that the continuous I- optimal design for a first order model in q mixture blends has a weight of $1/q$ at each stage of the $(q, 1)$ SLD. Furthermore, the q pure Mixture blends are the best candidate points, and each of them should be used equally. Goos et al. [22] published the analytical expression Laake [36], and Goos and Safifri [37] obtained for the I– optimal weights. The overview of numerical values as obtained for a second order degree model employing SLD techniques by Laake [36] and Goos et al. [22] for I-optimal weights for values q that ranges from three to six are given in Table 1. This value aids in constructing an ideal mixture design.

:

Table 1. I-optimal weights for second order mixture model [22]

	$q=3$			$q=4$			$q=5$			$q=6$		
i	k_i	Φ_i	$k_i\Phi_i$	k_i	Φ_i	$k_i\Phi_i$	k_i	Φ_i	$k_i\Phi_i$	k_i	Φ_i	$k_i\Phi_i$
1	3	0.1007	0.3022	4	0.0560	0.2240	5	0.0400	0.2000	6	0.0328	0.1968
2	3	0.2326	0.6978	6	0.1293	0.7760	10	0.0800	0.8000	15	0.0536	0.8032
$\boldsymbol{d}$	6			10			15			21		

The weight Φ_1 denotes the number of runs that must be completed with each other pure mixture blend, while the weight Φ_2 denotes the number of runs that must be completed with each binary mixture. The number of pure blends (k_1) and $(k_2)$for binary mixture blends are also mentioned in Table 1, as well as the concinnity of experimental runs involving pure mixture blends $(k_1\Phi_1)$ and $(k_2\Phi_2)$for binary mixture blends. The number of distinct candidate points is given by $d = (k_1 + k_2 + k_3)$on the last line of Table 1. Furthermore, as Goos

(2016) points out, each pure blend in Laake's design has a weight of less than $1/d$, while each binary mixture has a weight of more than $1/d$, in comparison to the continuous D- optimal designs for the second order model.

As Goos *et al*. (2016) points out, Laake's proposal for a second order model never considered the case of two ingredients ($q = 2$). Liu and Neudecker [38] analytically derived continuous I -optimal designs by considering the case of two ingredients ($q = 2$). The I- optimal weights for two pure mixture blends and a binary mixture were $\Phi_2 = 0.3$ and$\Phi_2 = 0.4$, respectively, as a result of their analytical expression.

Many scholars, however, believe that the designs advocated by Laake [36] and Goos *et al*. (2016) are much superior to Lambrakis' [39]. However, Chalikias [40, 41] later proposed mixture modelling criteria as a way of finding an optimal design in presences of process variables.

3.7 Comparison of D- and I- optimal designs

In this section, we illustrate how I-optimal design created is preferred to D-optimal designs when the scaled prediction variance (SPV) becomes the key in finding optimal design. The SPV is a prediction-based criterion that provides more information and details about designs. It examines a planned experiment before running the experimental test and collecting data. It also explains the error that comes with using a regression model to make a precise prediction. However, both D- and I-optimal design employ SPV. Therefore, using Fig. 2 described in Goos *et al*. [22] and findings from Laake [36] we found that both I-and D-optimal criteria are crucial for the construction of an optimal design as each criterion plays a unique role. Therefore, the choice between one of them is determined by researcher's needs. Therefore, choosing between one of them is determined with the researcher wants.

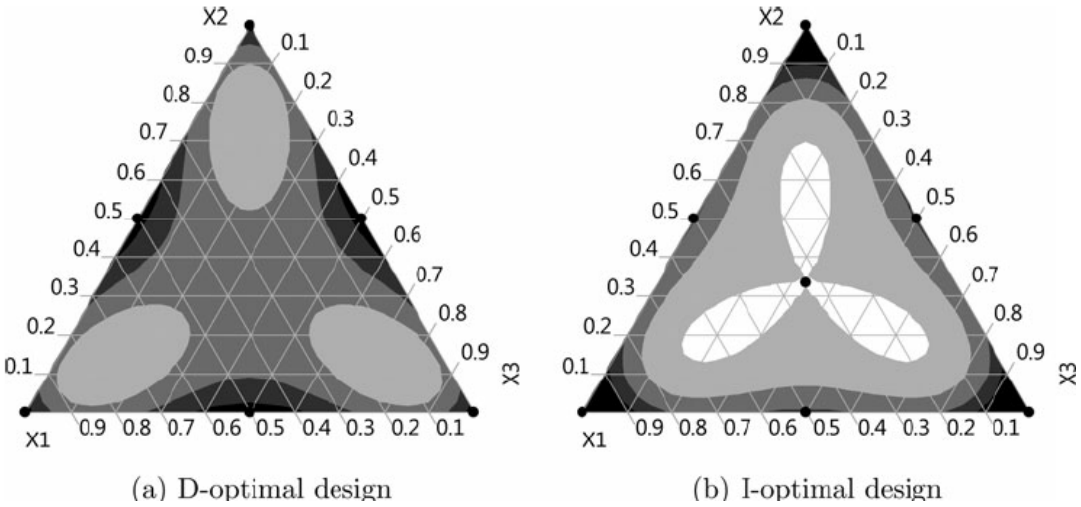

Fig. 2. The entire designs, Goos et al. [22] compared the SPV created by the two optimal designs

For instance, the prediction variances provided by two designs are compared in this Fig. 2 over the entire experimental area. Fig. 2's white, dark gray, and black areas correspond to an SPV of less than 2.5 to 3.5, 4.5 to 5.5, and above 5.5, respectively. However, as demonstrated by Laake [36] and Goos et al. [22] I-optimal designs result in lower prediction variance over the majority of the design space as compared to D-optimal designs.

Furthermore, as shown in Fig. 2, D- optimal designs collect information in the center of the experimental area, while I-optimal designs do not. However, according to the findings of Iwundu [26] D- efficiency of I- optimal designs relative to D- optimal designs is approximately 89.02 percent, while I- efficiency of optimal designs criteria relative to I- optimal designs is symmetric and unique. In addition, they discover that the average SPV for D- and I-optimal designs is 0.125 and 0.1086, respectively, as defined in Goos *et al*. [22]. We can therefore conclude both D- and I- optimal should considered when determining an optimal design since all plays a vital role in reducing variance prediction. However, Njoroge et al. [16] applied these two optimal criteria to construct two mixture process variable designs within a split plot design in which they later determined that model one

constructed using D-optimal design outperforms I-optimal designs. We conclude that both D- and I- optimal should considered when determining an optimal design since both of them play a vital role

4 Application of D-, A-, I-, and G-Relative Efficiency in Determining an Optimal MPV Design within SPD

This section outline the results described in Wanyonyi et al. [12] in finding an optimal design among six different designs option in the context split-plot structure arrangements they had. The results were as follows using JMP 15 software.

Table 2. Optimality criterion efficiency of design ξ_4Relative to design $\xi_1, \xi_2, \xi_3, \xi_5$ and ξ_6

Optimality Criterion Efficiency	Efficiency of ξ_4 Relative to 1	2	3	5	6
D-efficiency	1.450	1.328	1.067	1.159	1.239
G-efficiency	2.572	2.567	1.758	1.834	1.176
A-efficiency	2.007	1.807	1.507	1.307	1.395
I-efficiency	1.298	1.277	1.207	1.181	1.119

Table 3. The optimality criterion efficiency of design ξ_6Relative to design $\xi_1, \xi_2, \xi_3, \xi_4$ and ξ_5

Optimality Criterion Efficiency	Efficiency of ξ_6 Relative to 1	2	3	4	5
D-efficiency	1.171	1.072	0.861	0.935	0.807
G-efficiency	2.104	2.100	1.438	1.534	0.812
A-efficiency	1.439	1.296	1.080	0.937	0.717
I-efficiency	1.178	1.149	1.069	1.044	0.891

Table 4. Optimality criterion efficiency of design ξ_5Relative to design $\xi_1, \xi_2, \xi_3, \xi_4$ and ξ_6

Criterion Efficiency	Efficiency of ξ_5 Relative to 1	2	3	4	6
D-efficiency	1.252	1.146	0.921	0.863	1.069
G-efficiency	1.402	1.399	0.958	0.545	0.667
A-efficiency	1.536	1.383	1.153	0.765	1.067
I-efficiency	1.121	1.102	1.024	0.843	0.957

Table 5. The optimality criterion efficiency of design ξ_3Relative to design $\xi_1, \xi_2, \xi_4, \xi_5$ and ξ_6

Criterion Efficiency	Efficiency of ξ_3 Relative to 1	2	4	5	6
D-efficiency	1.359	1.245	0.937	1.086	1.161
G-efficiency	1.463	1.460	0.569	1.043	0.695
A-efficiency	1.332	1.199	0.664	0.867	0.926
I-efficiency	1.085	1.071	0.828	0.975	0.924

Table 6. The Optimality criterion efficiency of design ξ_2Relative to design $\xi_1, \xi_3, \xi_4, \xi_5$ *and* ξ_6

Criterion Efficiency	Efficiency of ξ_2 Relative 1	3	4	5	6
D-efficiency	1.092	0.803	0.753	0.872	0.933
G-efficiency	1.002	1.685	0.378	0.715	0.476
A-efficiency	1.111	0.834	0.553	0.723	0.772
I-efficiency	1.000	0.923	0.766	0.918	0.867

From Table 2, 3, 4, 5, 6 and 7, we can observe that the efficiency of design $\boldsymbol{\xi_4}$relative to $\xi_1, \xi_3, \xi_4, \xi_5$ and ξ_6 for all the D-, A-, I-, and G- efficiency is greater 1.0. This indicates that $\boldsymbol{\xi_4}$ is better than the other design. Therefore, we conclude that design $\boldsymbol{\xi_4}$ an optimal split-plot design that support and fit combined second order mixture process variable model.

Table 7. The optimality criterion efficiency of design ξ_1 Relative to design $\xi_2, \xi_3, \xi_4, \xi_5$ and ξ_6

Criterion Efficiency	Efficiency of ξ_1 Relative to 2	3	4	5	6
D-efficiency	0.916	0.736	0.690	0.799	0.854
G-efficiency	0.998	0.683	0.389	0.713	0.475
A-efficiency	0.900	0.751	0.498	0.651	0.695
I-efficiency	0.975	0.916	0.762	0.898	0.862

5 Conclusion

We explored and discussed in detail D-, A-, I-, and G- optimality criteria and their efficiency in determining a good mixture process variable (MPV) designs. We recommend that an optimality criterion should always be used when assessing different type designs in order to find a desirable design that fits a mixture model.

Competing Interests

Authors have declared that no competing interests exist.

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