

Research Article

Robust D-optimal Designs for the First-degree and the Second-degree Kronecker Model for Mixture Experiments

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Abstract

Many practical problems are associated with the investigation of mixture of m ingredients, which are assumed to influence the response through the proportions in which they are blended together. Such problems lend their applicability to mixture experiments. Mixture experiments can be modeled using Scheffé' or Kronecker models. For the first-, second-, and third-degree Kronecker models, D-optimal designs for the mixture experiments have been derived by various authors. This creates uncertainties to an experimenter, hence the need for robust designs. The objective of this study is to derive robust D-optimal designs for mixture experiments in the first- and the second-degree Kronecker model for mixture experiments. In order to achieve this, the D-optimal weights for the designs in the first-degree and those of the second degree Kronecker models are obtained. The model robust D-Optimality criterion is then used. The D-Optimal designs are obtained by maximizing this criterion which involves differentiating, equating to zero and solving for α , r_1 and r_2 in order to obtain the optimal values. In conclusion the results of this study demonstrate the existence of model robust D-optimal Kronecker model mixture experiments for the first- and the second-degree Kronecker models.

Keywords

Mixture Experiment, Kronecker Product, Moment Matrix, D-optimal, Robust Designs

1. Introduction

This section gives brief background information on mixture experiments and their properties. The Kronecker model representation is also be discussed. Finally, problem statement of the study, objectives, significance of the study and the scope of the study will be stated.

2. Background Information

2.1. Mixture Experiments

A mixture experiment is an experiment which involves mixing of proportions of two or more ingredients to make different compositions of an end product. Consequently, many practical problems are associated with the investigation of mixture ingredients of m factors, assumed to influence the response through the proportions in which they are blended together. The m ingredient proportions, t_1, \dots, t_m form the column vector of experimental conditions, $t = (t_1, \dots, t_m)$ with $t_i \geq 0$ and further subject to the simplex restriction,

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that they sum up to unity. Let $1_m = (1, \dots, 1)' \in \mathfrak{R}^m$ be the unity vector, whence, $1_m' t$ is the sum of the ingredients of t . Therefore, the experimental conditions are points in the probability simplex, which constitute the independent and controlled variables with the experimental domain being the simplex, $T = \{t \in [0, 1]^m; 1_m' t = 1\}$. Under experimental conditions $t \in T$, the experimental response Y_t is taken to be a scalar random variable. Replications under identical experimental conditions or response from distinct experimental conditions are assumed to be of equal (unknown) variance, σ^2 , and uncorrelated. An experimental design τ is a probability measure on the experimental domain τ with finite support points of. If τ assigns weights w_1, w_2, \dots to its points of support in τ , then the experimenter is directed to draw proportions w_1, w_2, \dots of all observations under the respective experimental conditions.

2.2. Kronecker Products

The Kronecker product approach bases second-degree polynomial regression in m variables $t = (t_1, t_2, \dots, t_m)'$ on the matrix of all cross products:

$$tt' = \begin{matrix} & t_1 & t_2 & \cdots & t_m \\ \begin{matrix} t_1 \\ t_2 \\ \vdots \\ t_m \end{matrix} & \begin{pmatrix} t_1^2 & t_1 t_2 & \cdots & t_1 t_m \\ t_2 t_1 & t_2^2 & \cdots & t_2 t_m \\ \vdots & \vdots & \ddots & \vdots \\ t_m t_1 & t_m t_2 & \cdots & t_m^2 \end{pmatrix} \end{matrix}$$

rather than reducing them to the Box-hunter minimal set of polynomials $(t_1^2, \dots, t_m^2, t_1 t_2, \dots, t_{m-1} t_m)$. The benefits enjoyed are; that distinct terms are repeated appropriately according to the number of times they can arise, that transformational rules with a conformable matrix R become simple, $(Rt)(Rt)' = R(tt')R'$ and that the approach extends to third degree polynomial regression.

For a $k \times m$ matrix A and a $l \times n$ matrix B , their Kronecker product $A \otimes B$ is defined to be the $kl \times mn$ block matrix.

$$A \otimes B = \begin{pmatrix} a_{11}B & \cdots & a_{1m}B \\ \vdots & \ddots & \vdots \\ a_{k1}B & \cdots & a_{km}B \end{pmatrix}.$$

The Kronecker product of a vector $s \in \mathfrak{R}^m$ and another vector $t \in \mathfrak{R}^n$ then is simply a special case.

$$s \otimes t = \begin{pmatrix} s_1 t \\ \vdots \\ s_m t \end{pmatrix} = \left(s_i t_j \right)_{\substack{i=1, \dots, m, j=1, \dots, n \\ \text{in lexicographic order}}} \in \mathfrak{R}^{mn}.$$

A key property is their product rule $(A \otimes B)(s \otimes t) = (As) \otimes (Bt)$.

This has nice implications for transposition, $(A \otimes B)' = (A') \otimes (B')$ for Moore-Penrose inversion, $(A \otimes B)^+ = (A^+) \otimes (B^+)$ and if possible for regular inversion $(A \otimes B)^{-1} = (A^{-1}) \otimes (B^{-1})$.

It is of specific importance that the Kronecker product preserves orthogonality. That is, if A , and B are individual orthogonal matrices, then their Kronecker product $(A \otimes B)$ is also an orthogonal matrix.

Thus while the matrix tt' assembles the cross products $t_i t_j$ in an $m \times m$ array, the Kronecker square $t \otimes t$ arranges the same numbers as a long $m^2 \times 1$ vector. The transformation with a conformable matrix R simply amounts to $(Rt) \otimes (Rt) = (R \otimes R)(t \otimes t)$. This greatly facilitates the calculations we apply to response surface models.

2.3. Optimal Designs

In the design of experiments, optimal designs are a class of experimental designs that are optimal with respect to some statistical criterion. Optimal designs allow parameters to be estimated without bias and with minimum variance. The optimality of a design depends on the statistical model and is assessed with respect to a statistical criterion, which is related to the variance matrix of the estimator.

A family of scalar measurements for the amount of information inherent to $C_K(M(\tau))$ is provided by Kiefer's ϕ_p -criteria, with $p \in [-\infty, 1]$. These are defined by;

$$\phi_p(C) = \begin{cases} \lambda_{\min}(C) & \text{if } p = -\infty \\ (\det C)^{\frac{1}{p}} & \text{if } p = 0 \\ \left(\frac{1}{s} \text{tr} C^p \right)^{\frac{1}{p}} & \text{if } p \in (-\infty, 1] \setminus \{0\} \end{cases}$$

for all C in $\text{PD}(s)$, the set of positive definite $s \times s$ matrices. Here $\lambda_{\min}(C)$ stands for the smallest eigenvalue of C . By definition, $\phi_p(C)$ is a function of the eigenvalues of C for all $p \in [-\infty, 1]$ Pukelsheim [17]. The family of ϕ_p -criteria includes the often used T-, D-, A-, and E-criteria, corresponding to parameter values 1, 0, -1, and $-\infty$ respectively Klein (2001) [11].

2.4. Robust D-optimal Designs

Robust is a characteristic describing a model's, test's, or system's ability to effectively perform while its variables or assumptions are altered, so a robust concept can operate

without failure under a variety of conditions. It is the stability theory of statistical procedure, Hampel, Frank, [6]. A robust mathematical model is a model which takes into account uncertainties in the existing assumptions.

In most cases, the investigators assume that the fitted model is focused on a single regression function. However, in practice the experimenters are often uncertain about which model is suitable especially when there are several possible regression models in consideration. The experimenters do not know which model is proper before accomplishing the experiment. Box and Draper observes that if one uses a simple linear function to estimate the expected value of the response when the true model is quadratic, it would result in a large bias term for estimation [2]. Since then while designing an experiment for regression models, robustness has always been an important issue.

Mixture experiments were first discussed in Quenouille [18]. Later on, Scheffé made a systematic study and laid a strong foundation by proposing the model commonly known as Scheffé models or simply S-models [19, 20]. Draper and Pukelsheim proposed a set of mixture models referred to as Kronecker Models or simply K-models [3]. They are alternative representation of mixture models based on the Kronecker algebra of vectors and matrices. They offer alternative symmetries, compact notations and homogeneous in ingredients.

The first-degree model is;

$$E[Y_t] = \sum_{i=1}^m t_i \theta_i = t' \theta \quad (1)$$

For the second-degree model, Draper and Pukelsheim proposed a representation involving the Kronecker square $t \otimes t$, the $m^2 \times 1$ vector consisting of the squares and cross products of the components of t in the lexicographic order of the subscripts [2]. This is referred to as Kronecker-model with a Kronecker-polynomial as the regression function.

$$E[Y_t] = \sum_{i=1}^m \sum_{j=1}^m t_i t_j \theta_{ij} = (t \otimes t)' \theta \quad (2)$$

Optimal designs for mixture experiments have been investigated extensively in the literature; Chan's gave a comprehensive overview [1]. Kiefer derived D-optimal designs in Scheffé's second-degree model [8]. Galil and Kiefer presented numerical results on ϕ_p -optimal designs in that model [5]. Draper, Heiligers and Pukelsheim established the completeness results that reduce the optimal design problem to a mere allocation problem [4]. They obtained unique optimal designs in Scheffé's first-degree and the second-degree models.

For the Kronecker models proposed by Draper and Pukelsheim, Kinyanjui and Klein showed how invariance

results can be applied to analytical derivation of optimal designs [3, 9, 10]. Kinyanjui investigated ϕ_p -optimal weighted centroid designs for $K'\theta$ [9] by adopting the general equivalence theorem as given in Pukelsheim [16] and derive the general forms for the unique A-optimal, D-optimal, T-optimal, and E-optimal designs for $K'\theta$.

Later on, Ngigi give the optimality criteria for ϕ_p -optimal weighted centroid designs for $K'\theta$ and found that for second-degree model with $m \geq 2$ ingredients, a unique A-optimal, D-optimal, and T-optimal weighted centroid designs for $K'\theta$ exist [16]. E-optimal designs could only be derived for experiments with two ingredients. Koske, Kinyanjui, Mutiso and Cherutich derived designs with optimal values in the second-degree Kronecker model mixture experiments and obtain designs with maximum information on the parameter subsystem $K'\theta$ subject to the side condition [13]. Similarly, Kerich, Koske, Cherutich and Kungu investigate D-optimal designs for third-degree Kronecker model mixture experiments with an application to artificial sweetener experiment. Results on D-optimal designs for the third-degree Kronecker model are presented [7]. Koech E., Koech M., Koske, Kerich and Otieno investigate E-optimal designs for maximal parameter subsystem second degree Kronecker model mixture experiments and finds that E-optimal weighted centroid designs based on maximal parameter subsystem exists for the corresponding two, three and four ingredients [12]. Here, numerical optimal weights and optimal values for the weighted centroid designs are obtained.

The above literature is a clear indication that quite a considerable amount of research has been done on the theory of Kronecker model mixture experiments. This presents a wide range of Kronecker models presenting a situation where an experimenter finds a dilemma is selecting a particular model for application. This situation forms the basis for this study; to investigating the optimal designs for mixture experiments where there is uncertainty in the first-degree Kronecker model and the second-degree Kronecker model as well as investigating the optimal designs for mixture experiments where there is uncertainty in particular Kronecker models in the second-degree. In each case robust-optimal designs are derived.

Robust is a characteristic describing a model's, test's, or system's ability to effectively perform while its variables or assumptions are altered, so a robust concept can operate without failure under a variety of conditions. It is the stability of a statistical procedure, Hampel, Frank [6]. A robust mathematical model is a model which takes into account uncertainties in the existing assumptions. In most cases, the investigators assume that the fitted model is focused on a single regression function. However, in practice the experimenters are often uncertain about which model is suitable especially when there are several possible regression models in consideration. The experimenters do not know which model is proper before accomplishing the experiment. Box

and Draper observes that if one uses a simple linear function to estimate the expected value of the response when the true model is quadratic, it would result in a large bias term for estimation [2]. Since then while designing an experiment for regression models, robustness has always been an important issue.

For the Scheffé models, Hsiang-Ling Hsu and Mong-Na Lo Huang investigates Robust D-optimal designs for mixture experiments with consideration on uncertainties in the Scheffé linear, quadratic and cubic models without three-way effects [15]. They use D-optimal designs for each of the Scheffé to find robust D-optimal designs and showed that the optimal convex combination of the two model's D-optimal designs is a robust D-optimal design. Numerical results about the robust D-optimal designs for Scheffé linear and cubic model without three-way effects as well as that for Scheffé linear, quadratic and cubic model without three-way effects are presented. Furthermore, Hsiang-Ling Hsu, Mong-Na Lo Huang, Chao-Jin Chou and Thomas Klein investigates and establishes a complete class result for mixed design criteria. In their current paper, model-robust D- and A-optimal designs that are convex combinations of the D- and A-optimal designs in the first- and second-degree Scheffé models are derived [15].

Mahesh K. P. in his work discussed the aspect of model robust A-Optimal designs Criterion for the K-Models [14]. The results show that the support points for the simplex centroid designs are A-Optimal designs for K- and S-Models in the first- and second-degree models. It is further observed that an appropriately defined convex combination of the D-Optimal designs is model-robust D-Optimal designs for both K- and S-Models while in the case of the model-robust A-Optimality criterion, it holds only for the S-Models. This study therefore proposes to investigate model-robust optimal designs for mixture experiments for the Kronecker models with a view to obtaining model robust D-optimal designs.

3. Methodology

This section discusses the model-robust D-optimal designs for mixture experiments for the Kronecker model are investigated where the methodology employed in deriving these designs is discussed in detail. Secondly, this chapter also investigates mixture experiments with process variables for the Kronecker model. The Kronecker model mixture experiment in the presence of process variables is developed.

Model-robust D-optimal Designs

In deriving these designs, this study considers the unique D-optimal designs for the first-degree and the second-degree Kronecker models. Using the D-efficiencies for the first-degree and the second-degree Kronecker models, a weighted geometric average are obtained for the D-optimality criteria. These designs are then investigated for the case of two, three, four and a general case of m ingredients as shown in the following subsections.

Klein and Kinyanjui showed how invariance results can be applied to analytical derivations of optimal designs. The spectral analysis of invariant symmetric matrices yielded both eigenvalues and eigenvectors [9, 10].

For the first-degree Kronecker model for mixture, the D-optimal design η_1^D assigns a weight.

$$\eta_1^D(x) = \left\{ \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \\ \frac{1}{m} \end{pmatrix} \cdots \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ \frac{1}{m} \end{pmatrix} \right\}. \quad (3)$$

While for the second-degree Kronecker model for mixture experiments, the D-optimal design η_2^D assigns a weight.

$$\eta_2^D(x) = \left\{ \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \\ \frac{2}{m+1} \end{pmatrix} \cdots \begin{pmatrix} 0 \\ 0 \\ \vdots \\ 1 \\ \frac{2}{m+1} \end{pmatrix} \begin{pmatrix} \frac{1}{2} \\ \frac{1}{2} \\ \vdots \\ 0 \\ \frac{m-1}{m+1} \end{pmatrix} \cdots \begin{pmatrix} 0 \\ 0 \\ \vdots \\ \frac{1}{2} \\ \frac{m-1}{m+1} \end{pmatrix} \right\} \quad (4)$$

Klein (2004).

Model Robust D-criterion

For the first-degree Kronecker model, suppose that the D-optimal design η_1^D assigns equal weight w to each of the points in X . Therefore, the information matrix is given by

$$M_1(\eta_1^D) = \sum_{t_i \in \eta_1^D} w f_1(t_i) f_1'(t_i), \quad (5)$$

While the dispersion matrix is given by

$$d_1(t, \eta_1^D) = f_1'(t_i) M_1^{-1}(\eta_1^D) f_1(t_i) \quad (6)$$

On the other hand, for the second-degree Kronecker model, suppose that the D-optimal design η_2^D assigns equal weight w_1 to each of the points $T \leftrightarrow (1, 0, \dots, 0)$ and equal weight w_2 to each of the points $T \leftrightarrow \left(\frac{1}{2}, \frac{1}{2}, \dots, 0\right)$.

Then, the D-optimal information matrix as defined in Klein is given by [10].

$$M_2(\eta_2^D) = \sum_{t_i \in \eta_1^D} w f_1(t_i) f_1'(t_i), \quad (7)$$

$$d_2(t, \eta_2^D) = f_2'(t_i) M_2^{-1}(\eta_2^D) f_2(t_i) \quad (8)$$

While the dispersion matrix is given by

In order to obtain model robust D-optimal designs for the first- and the second-degree Kronecker models define,

$$\Psi_r(\eta_\alpha^D) = \left| M_1(\eta_\alpha^D) \right|^{\frac{r_1}{m_1}} \left| M_2(\eta_\alpha^D) \right|^{\frac{r_2}{m_2}} \text{ where } r_1 + r_2 = 1 \quad (9)$$

where, $M_1(\eta_\alpha^D) = \alpha M_1(\eta_1^D) + (1-\alpha)M_1(\eta_2^D)$, $M_2(\eta_\alpha^D) = \alpha M_2(\eta_1^D) + (1-\alpha)M_2(\eta_2^D)$ and $0 \leq \alpha \leq 1$.

This relation is called the model robust D-criterion. The model robust D-optimal designs are obtained by maximizing this criterion as follows.

Taking logarithm on both sides yields

$$\log \Psi_r(\eta_\alpha^D) = \frac{r_1}{m_1} \log \left(\left| M_1(\eta_\alpha^D) \right| \right) + \frac{r_2}{m_2} \log \left(\left| M_2(\eta_\alpha^D) \right| \right) \quad (10)$$

In order to find the optimal α_r^D which minimizes $\Psi_r(\eta)$, take derivative with respect to α and equate to zero. This yield

$$\frac{d}{d\alpha} \Psi_r(\eta_\alpha^D) = \frac{r_1}{m_1} \text{Tr} M_1^{-1}(\eta_\alpha^D) \left((M_1(\eta_1^D)) - (M_2(\eta_2^D)) \right) + \frac{r_2}{m_2} \text{Tr} M_2^{-1}(\eta_\alpha^D) \left((M_1(\eta_1^D)) - (M_2(\eta_2^D)) \right) \quad (11)$$

This form is provided by Mong-Na, L. H., Hsiang-Ling, H., Chao-Jin, C. and Klein, T. [15].

Robust D-optimal Designs for the First-degree and the Second-degree Kronecker Model for Mixture Experiments

For the second-degree Kronecker model, this study considers models with different parameter subspaces (subsystems) say, s_1 and s_2 with corresponding D-Optimal designs

η_1^D and η_2^D respectively.

Theorem 1

The robust D-optimal weight $\alpha_{r_1}^D$ for m ingredients for a given r_1 is given by

$$r_1 = \frac{\alpha_{r_1}^D \left[(21m^2 - 39m + 18) \alpha_{r_1}^{D2} + (10m^2 + 82m - 84) \alpha_{r_1}^D + (m^2 + 21m + 98) \right]}{(24m^2 - 38m + 16) \alpha_{r_1}^{D2} + (8m^2 + 88m - 76) \alpha_{r_1}^D + (14m + 92)}$$

Proof

By utilizing the weights given in equations (3) and (4) together with equations (5) and (7) and using m ingredients, the moment matrices for the designs η_1^D and η_2^D for the first- and second-degree Kronecker models are

$$M_1(\eta_1^D) = \frac{1}{m} I_m, \quad M_1(\eta_2^D) = \frac{1}{m+1} \left[\frac{15+m}{8m} I_m + \frac{1}{8m} U_2 \right]$$

$$M_2(\eta_1^D) = \begin{bmatrix} \frac{1}{m} I_m & 0 \\ 0 & 0 \end{bmatrix}, \quad M_2(\eta_2^D) = \frac{1}{m+1} \begin{bmatrix} \frac{15+m}{8m} I_m + \frac{1}{8m} U_2 & \frac{1}{4m} V_1' \\ \frac{1}{4m} V & \frac{1}{2m} I_{\binom{m}{2}} \end{bmatrix}$$

Now using equation (11) we have

$$M_1(\eta_\alpha^D) = \left[\frac{7m\alpha - 7\alpha + m + 15}{8m(m+1)} I_m + \frac{(1-\alpha)}{8m(m+1)} U_2 \right],$$

and

$$M_2(\eta_\alpha^D) = \begin{bmatrix} \frac{7m\alpha - 7\alpha + m + 15}{8m(m+1)} I_m + \frac{(1-\alpha)}{8m(m+1)} U_2 & \frac{(1-\alpha)}{4m(m+1)} V_1' \\ \frac{(1-\alpha)}{4m(m+1)} V & \frac{(1-\alpha)}{2m(m+1)} I_{\binom{m}{2}} \end{bmatrix}$$

Taking their inverses yields and utilizing equation (11) we find that

$$M_1^{-1}(\eta_\alpha^D) M_1(\eta_1^D) = \frac{1}{m} [aI_m + bU_2], \quad M_1^{-1}(\eta_\alpha^D) M_1(\eta_2^D) = \frac{1}{8m(m+1)} [((m+15)a + (m-1)b)I_m + (a + (2m+13)b)U_2],$$

$$M_2^{-1}(\eta_\alpha^D) M_2(\eta_1^D) = \begin{bmatrix} \frac{m+1}{(m-1)\alpha + 2} I_m & 0V_1' \\ \frac{-(m+1)}{2[(m-1)\alpha + 2]} V_1 & 0I_{\binom{m}{2}} \end{bmatrix}, \quad \text{and} \quad M_2^{-1}(\eta_\alpha^D) M_2(\eta_2^D) = \begin{bmatrix} \frac{2}{(m-1)\alpha + 2} I_m & 0V_1' \\ 0V_1 & \frac{1}{(1-\alpha)} I_{\binom{m}{2}} \end{bmatrix}$$

Hence,

$$TrM_1^{-1}(\eta(\alpha)) (M_1(\eta_1^D)) = \frac{8m(m+1)[(6m-5)\alpha + (2m+13)]}{(42m^2 - 78m + 36)\alpha_r^{D2} + (20m^2 + 164m - 168)\alpha_r^D + (2m^2 + 42m + 196)},$$

$$TrM_1^{-1}(\eta(\alpha)) (M_1(\eta_2^D)) = \frac{a(m+15) + b(m-1)}{8(m+1)}, \quad TrM_2^{-1}(\eta(\alpha)) (M_2(\eta_1^D)) = \frac{m(m+1)}{(m-1)\alpha + 2}, \quad \text{and}$$

$$TrM_2^{-1}(\eta(\alpha)) (M_2(\eta_2^D)) = \frac{m[(m^2 - 2m - 3)\alpha + (2m + 2)]}{2[(m-1)\alpha + 2](1-\alpha)}$$

Substituting these equations to equation (11), setting to zero and solving yields the following relationship between r_1 and $\alpha_{r_1}^D$

$$r_1 = \frac{\alpha_{r_1}^D [(21m^2 - 39m + 18)\alpha_{r_1}^{D2} + (10m^2 + 82m - 84)\alpha_{r_1}^D + (m^2 + 21m + 98)]}{(24m^2 - 38m + 16)\alpha_{r_1}^{D2} + (8m^2 + 88m - 76)\alpha_{r_1}^D + (14m + 92)}$$

Illustration 1

The robust D-optimal weight $\alpha_{r_1}^D$ for $m=3$ ingredients for a given r_1 is given by

$$r_1 = \frac{\alpha_{r_1}^D (180\alpha_{r_1}^{D2} + 504\alpha_{r_1}^D + 340)}{236\alpha_{r_1}^{D2} + 520\alpha_{r_1}^D + 268}$$

Proof

By utilizing the weights given in equations (3) and (4) together with equations (5) and (7) and setting $m=3$, the moment matrices for the designs η_1^D and η_2^D for the first- and second-degree Kronecker models are

$$M_1(\eta_1^D) = \frac{1}{3} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{bmatrix}, M_1(\eta_2^D) = \begin{bmatrix} \frac{18}{96} & \frac{1}{96} & \frac{1}{96} \\ \frac{1}{96} & \frac{18}{96} & \frac{1}{96} \\ \frac{1}{96} & \frac{1}{96} & \frac{18}{96} \end{bmatrix}$$

$$, M_2(\eta_1^D) = \frac{1}{3} \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 0 & 0 \end{bmatrix} \text{ and } M_2(\eta_2^D) = \begin{bmatrix} \frac{18}{96} & \frac{1}{96} & \frac{1}{96} & \frac{1}{48} & \frac{1}{48} & 0 \\ \frac{1}{96} & \frac{18}{96} & \frac{1}{96} & \frac{1}{48} & 0 & \frac{1}{48} \\ \frac{1}{96} & \frac{1}{96} & \frac{18}{96} & 0 & \frac{1}{48} & \frac{1}{48} \\ \frac{1}{48} & \frac{1}{48} & 0 & \frac{1}{24} & 0 & 0 \\ \frac{1}{48} & 0 & \frac{1}{48} & 0 & \frac{1}{24} & 0 \\ 0 & \frac{1}{48} & \frac{1}{48} & 0 & 0 & \frac{1}{24} \end{bmatrix}$$

Using equation (11) we have

$$M_1(\eta_\alpha^D) = \begin{bmatrix} \frac{14\alpha+18}{96} & \frac{1-\alpha}{96} & \frac{1-\alpha}{96} \\ \frac{1-\alpha}{96} & \frac{14\alpha+18}{96} & \frac{1-\alpha}{96} \\ \frac{1-\alpha}{96} & \frac{1-\alpha}{96} & \frac{14\alpha+18}{96} \end{bmatrix},$$

and

$$M_2(\eta_\alpha^D) = \begin{bmatrix} \frac{14\alpha+18}{96} & \frac{1-\alpha}{96} & \frac{1-\alpha}{96} & \frac{1-\alpha}{48} & \frac{1-\alpha}{48} & 0 \\ \frac{1-\alpha}{96} & \frac{14\alpha+18}{96} & \frac{1-\alpha}{96} & \frac{1-\alpha}{48} & 0 & \frac{1-\alpha}{48} \\ \frac{1-\alpha}{96} & \frac{1-\alpha}{96} & \frac{14\alpha+18}{96} & 0 & \frac{1-\alpha}{48} & \frac{1-\alpha}{48} \\ \frac{1-\alpha}{48} & \frac{1-\alpha}{48} & 0 & \frac{1-\alpha}{24} & 0 & 0 \\ \frac{1-\alpha}{48} & 0 & \frac{1-\alpha}{48} & 0 & \frac{1-\alpha}{24} & 0 \\ 0 & \frac{1-\alpha}{48} & \frac{1-\alpha}{48} & 0 & 0 & \frac{1-\alpha}{24} \end{bmatrix}$$

Taking their inverses yields

$$M_1^{-1}(\eta_\alpha^D) = \begin{bmatrix} \frac{96(13\alpha+19)}{180\alpha^2+504\alpha+340} & \frac{96(\alpha-1)}{180\alpha^2+504\alpha+340} & \frac{96(\alpha-1)}{180\alpha^2+504\alpha+340} \\ \frac{96(\alpha-1)}{180\alpha^2+504\alpha+340} & \frac{96(13\alpha+19)}{180\alpha^2+504\alpha+340} & \frac{96(\alpha-1)}{180\alpha^2+504\alpha+340} \\ \frac{96(\alpha-1)}{180\alpha^2+504\alpha+340} & \frac{96(\alpha-1)}{180\alpha^2+504\alpha+340} & \frac{96(13\alpha+19)}{180\alpha^2+504\alpha+340} \end{bmatrix}$$

$$M_2^{-1}(\eta_\alpha^D) = \begin{bmatrix} \frac{6}{\alpha+1} & 0 & 0 & \frac{-3}{\alpha+1} & \frac{-3}{\alpha+1} & 0 \\ 0 & \frac{6}{\alpha+1} & 0 & \frac{-3}{\alpha+1} & 0 & \frac{-3}{\alpha+1} \\ 0 & 0 & \frac{6}{\alpha+1} & 0 & \frac{-3}{\alpha+1} & \frac{-3}{\alpha+1} \\ \frac{-3}{\alpha+1} & \frac{-3}{\alpha+1} & 0 & \frac{21\alpha+27}{(1-\alpha)(\alpha+1)} & \frac{3}{2(\alpha+1)} & \frac{3}{2(\alpha+1)} \\ \frac{-3}{\alpha+1} & 0 & \frac{-3}{\alpha+1} & \frac{3}{2(\alpha+1)} & \frac{21\alpha+27}{(1-\alpha)(\alpha+1)} & \frac{3}{2(\alpha+1)} \\ 0 & \frac{-3}{\alpha+1} & \frac{-3}{\alpha+1} & \frac{3}{2(\alpha+1)} & \frac{3}{2(\alpha+1)} & \frac{21\alpha+27}{(1-\alpha)(\alpha+1)} \end{bmatrix}$$

Now, utilizing equation (11) we find that

$$TrM_1^{-1}(\eta(\alpha))(M_1(\eta_1^D)) = \frac{96(13\alpha+19)}{180\alpha^2+504\alpha+340}, \quad TrM_1^{-1}(\eta(\alpha))(M_1(\eta_2^D)) = \frac{3(236\alpha+340)}{180\alpha^2+504\alpha+340},$$

$$TrM_2^{-1}(\eta(\alpha))(M_2(\eta_1^D)) = \frac{6}{\alpha+1}, \quad \text{and} \quad TrM_2^{-1}(\eta(\alpha))(M_2(\eta_2^D)) = \frac{6}{(1-\alpha)(\alpha+1)}.$$

Substituting these equations to equation (11), setting to zero and solving yields the following relationship between $\alpha_{r_1}^D$ for $m=3$ and r_1 is given by

$$r_1 = \frac{\alpha_{r_1}^D (180\alpha_{r_1}^{D2} + 504\alpha_{r_1}^D + 340)}{236\alpha_{r_1}^{D2} + 520\alpha_{r_1}^D + 268}$$

This result can easily be verified using the results of theorem 1.

4. Results and Discussions

This section gives a detailed interpretation and explanation of findings of this study with regard to the objectives of this study.

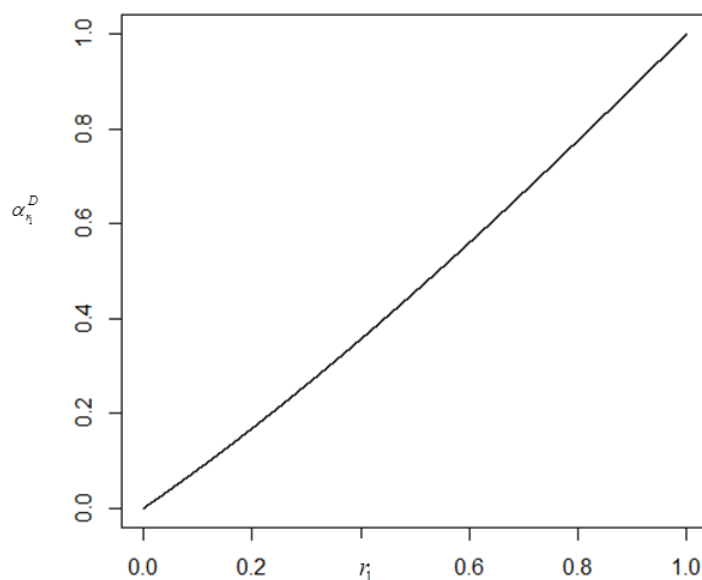
Robust D-optimal Designs for the First-degree and the Se-

cond-degree Kronecker Model for Mixture Experiments

This study in attempting to derive the D-optimal designs for the first-degree and the second-degree Kronecker model mixture experiments considered the D-optimal designs for these models. The corresponding D-optimal information matrices and the moment matrices were obtained for two, three, four and m ingredients were obtained in Theorem 1 and the illustration 1.

Table 1. Robust D-optimal weights for two, three, four and m ingredients.

No of ingredients (m)	Robust D-optimal weight (α_i^D)
2	$r_1 = \frac{2\alpha_i^D(\alpha_i^{D2} + 5\alpha_i^D + 6)}{3\alpha_i^{D2} + 11\alpha_i^D + 10}$
3	$r_1 = \frac{\alpha_i^D(180\alpha_i^{D2} + 504\alpha_i^D + 340)}{236\alpha_i^{D2} + 520\alpha_i^D + 268}$
4	$r_1 = \frac{\alpha_i^D(198\alpha_i^{D2} + 404\alpha_i^D + 198)}{248\alpha_i^{D2} + 404\alpha_i^D + 148}$
m	$r_1 = \frac{\alpha_i^D[(21m^2 - 39m + 18)\alpha_i^{D2} + (10m^2 + 82m - 84)\alpha_i^D + (m^2 + 21m + 98)]}{(24m^2 - 38m + 16)\alpha_i^{D2} + (8m^2 + 88m - 76)\alpha_i^D + (14m + 92)}$

**Figure 1.** The graph of the weight (α_i^D) as a function of $r_1 \in [0,1]$ for two ingredients.

The optimal values for the model-robust D-criterion for different values of r_1 , and α_i^D are as shown in the following table.

Table 2. The optimal values for the model-robust D-criterion for different values of r_1 , and α_i^D .

r_1	0	$\frac{1}{4}$	$\frac{1}{2}$	$\frac{3}{4}$	1
α_i^D	0	0.2197063	0.4610722	0.7219898	1
$\Psi_r(\eta_\alpha^D)$	0.209987	0.242075097	0.287512057	0.3574266	0.5

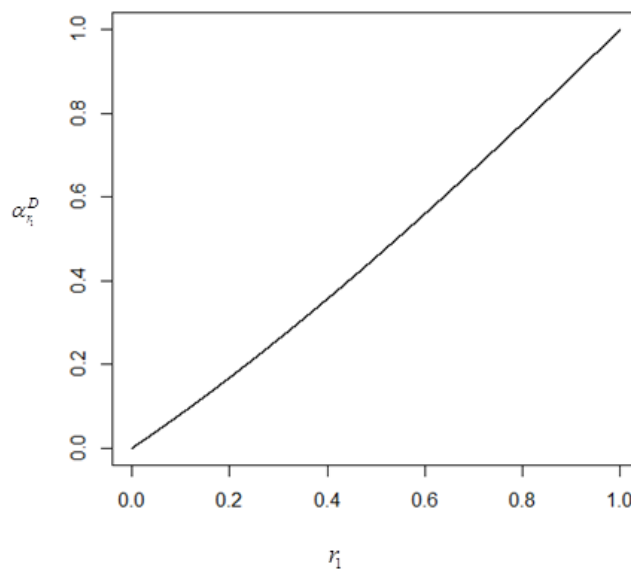


Figure 2. The graph of the weight (α_n^D) as a function of $r_1 \in [0,1]$ for three ingredients.

The optimal values for the model-robust D-criterion for different values of r , and α_r^D are as shown in the following table.

Table 3. The optimal values for the model-robust D-criterion for different values of r , and α_n^D .

r_1	0	$\frac{1}{4}$	$\frac{1}{2}$	$\frac{3}{4}$	1
α_n^D	0	0.2197063	0.4610722	0.7219898	1
$\Psi_r(\eta_\alpha^D)$	0.0833333	0.1041831	0.1371406	0.1950306	0.3333333

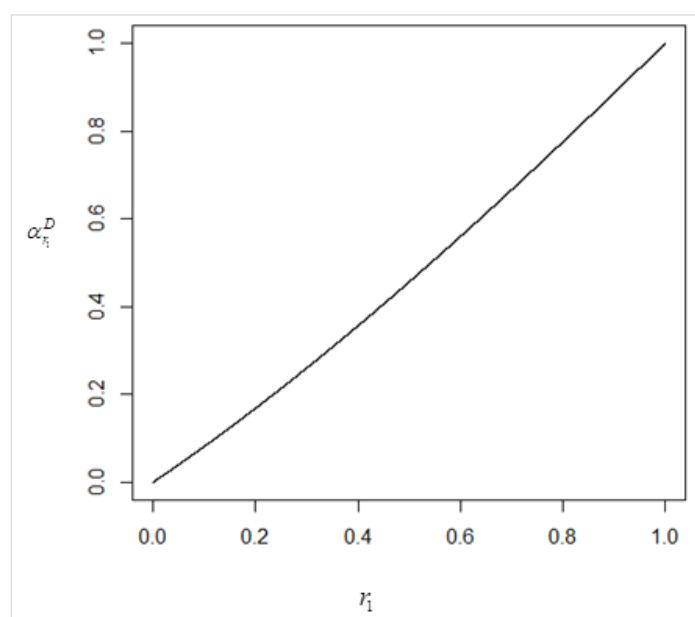


Figure 3. The graph of the weight (α_n^D) as a function of $r_1 \in [0,1]$ for four ingredients.

The optimal values for the model-robust D-criterion for different values of r_1 , and $\alpha_{r_1}^D$ are as shown in the following table.

Table 4. The optimal values for the model-robust D-criterion for different values of r_1 , and $\alpha_{r_1}^D$.

r_1	0	$\frac{1}{4}$	$\frac{1}{2}$	$\frac{3}{4}$	1
$\alpha_{r_1}^D$	0	0.2089266	0.4536888	0.7193914	1
$\Psi_r(\eta_a^D)$	0.04352753	0.05752092	0.08150017	0.1274106	0.25

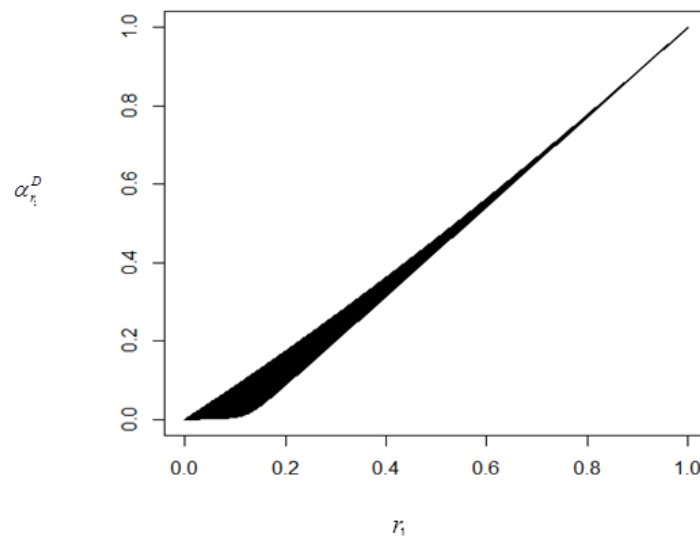


Figure 4. The graph of the weight ($\alpha_{r_1}^D$) as a function of $r_1 \in [0,1]$ for m ingredients.

Table 5. The optimal values for the model-robust D-criterion for different values of r_1 , and $\alpha_{r_1}^D$.

r_1	0	$\frac{1}{4}$	$\frac{1}{2}$	$\frac{3}{4}$	1
$\alpha_{r_1}^D$ m	0	0.2089266	0.4536888	0.7193914	1
2	0.209987	0.2420751	0.28751206	0.3574266	0.50
$\Psi_r(\eta_a^D)$ 3	0.0833333	0.10401831	0.1371406	0.1950306	0.333333
4	0.04352753	0.05752092	0.08150017	0.1274106	0.25

5. Conclusions and Recommendations

5.1. Conclusions

This paper demonstrates that robust D-optimal designs ex-

ist for the Kronecker model mixture experiments. The optimal designs were constructed for $m=2,3,4$ and the general number of ingredients at various values of the prior parameter r_1 . It is observed that the designs constructed perform better for higher values of r_1 .

5.2. Recommendations

From the results of this study, the following recommendations are made:

- 1) For the first- and second-degree K-models, robust models can be used as a guide in cases where the experimenter is uncertain of the model to use since the robust designs exist.
- 2) This study opens an avenue for a practical/experimental/ simulation study to be conducted in any field and make use of these results.
- 3) There is need to consider the model-robust A-optimal designs in future research since not much has been done.
- 4) There is need to consider the model-robust A-optimal and D-optimal designs for the second- and third- degree Kronecker models for mixture experiments in future research.

Abbreviations

- D Determinant
A Average

Author Contributions

Mike Cherutich: Conceptualization, Data curation, Formal Analysis, Funding acquisition, Investigation, Methodology, Resources, Software, Validation, Writing – review & editing

Conflicts of Interest

The authors declare no conflicts of interest.

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