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Choice of Optimality Criteria for the Simplex Centroid Design

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ABSTRACT

Mixture experiment involves mixing many or more ingredient proportions together to obtain the best product quality known as the response. In this study, we tried to obtain the best optimality choice for the simplex centroid design. The A, D and G optimality criteria for the simplex centroid design was obtain at n = 3 and 4. For each n, the design was replicated two times, three times and four times and for replicated, the linear, quadratic and cubic model was obtain. The result obtained indicates that under a, D and G optimality criteria, a better design will be obtained when the experiment is replicated 3 times without the quadratic and the cubic effects. The efficiency values and mean efficiency values were obtained and used to decide a suitable design for the simplex centroid design. Of the 3 optimality criteria used, the G optimality criteria proved to be the best.

KEYWORD: Mixture experiment, Simplex centroid design, optimality criteria

1. INTRODUCTION

Mixture experiment is an experimental design that involves the mixture of different proportion of components or ingredient. The response measured as a result of these mixtures is dependent on the percentage or proportion of the different ingredients. Where the amount of the mixture has an effect on the response, then the amount is kept fixed for all blends. The response changes as the proportion of the ingredients varies. The aim of mixture experiment is to obtain that proportion of ingredients that will produce the highest response in the experiment and also to understand better the effect of the individual ingredients. The proportion of the ingredients mixed must be nonnegative and they must sum to unity.

$$i.e\ x_i \geq 0\ and \sum_{i=1}^{q} x_i = x_1 + x_2 + \cdots + x_q = 1$$

Where q is the number of ingredients to be mixed in a mixture experiment, the levels chosen for any ingredient or factor are dependent on the levels chosen for the factors.

Many works have been done in relation to simplex lattice design and simplex centroid design.

In the works of Bondari(2005), Mixture experiments are appropriate to use when a researcher wishes to determine if synergism exists in mixing components which increases productivity or desirability of a product. An important property of the mixture experiment is that the change in the response depends on proportionality of the individual components present in the mixture and not on the amount of the mixture.

Coetzer(2010) used optimal designs in estimating the parameters in the generalized weighted -power-mean mixture model. In his conclusion, he derived locally optimal designs, that are those designs which depend on an initial guess for the parameter. He also concluded that the common mixture designs such as the simplex-lattice and simplex-centroid designs, have high efficiency for estimating most of the special forms of the weighted power-mean mixture models that are nonlinear in the parameters.

Sameera and Jaya Raju (2016) applied simplex lattice mixture design in the production of L-Gluta,imase using oil cake mixture. They concluded that there is a variation in glutaminase yield with different substrate under similar fermentation condition and this suggest the importance of substrate composition on fermentative. Peter Goss states that I-Optimal design minimizes the average variance of prediction and therefore seems appropriate for mixture experiments than the commonly used D-optimal design.

MandlikSatish etal (2012), also applied the simplex lattice design in formulation and development of buoyant matrices of Dipyridamole. The study indicates that buoyant matrices of Dipyridamole can successfully be employed as floating controlled release drug delivery with minimum experimentation using simplex-lattice design.

Dannis K. Murithi (2019) applied the simplex lattice design in watermelon production. He fitted a mathematical model to express response variables as functions of the proportions of the mixture components of organic manure and optimizes the multiple responses of watermelon to organic manure. In his conclusion, out of the three components (poultry manure, cow manure and goat manure), he concluded that goat manure played an important role in watermelon production.

Ronald (1971) presented some practical ideas on the design and analysis of mixture experiments. He concluded that efficient experimentation with mixtures require new statistical tools and different applications and interpretations of the results of existing techniques.

Schalkwyk (1971) examined the variance function of the expected mean response in the 3-components factor and under linear, quadratic and cubic mixture models and he also presented the generalization for designing D-optimum experiments for a simplex design space of more than three components under a linear model. In his conclusion, he said that when designing mixture experiments for simplex design space only the full simplex lattice design need to be considered since the design for a simplex subspace is a suitably scaled version of the design for the full simplex design space are D-optimum only for linear and quadratic models.

DRahayeetal (2019) examined the D-optimal design for ordinal response in mixture experiments. They developed a point exchange algorithm for the D-optimal design for ordinal response, the parameters estimates was obtained using simulation and these parameter were used to find the optimal design points with the D-optima criterion after which a twelve optimal design points were obtained.

Cheruiyot (2017) obtained the I-optimal designs for two, three and four mixture components for both weighted simplex centroid design and uniform weighted simplex centroid design for third degree kroncker model for mixture experiments. He stated that I-Optimality criterion is more appropriate for mixture experiments for precise predictions of responses. J.I Arimanwaetal assessed the suitability of run-off sand for concrete production and they used the simplex lattice design models for the determination of modulus of rupture of concrete beam made from fine aggregates sourced from two rivers and run-off sand from three locations. The formulated models predict the modulus of rupture of concrete made from fine aggregate of similar characteristics.

Wanida Limmun (2019). developed a weighted G-optimality criterion, which aims at minimizing the weighted average of the maximum scaled prediction variance (SPV) in design space on a set of reduced models they used fedorov's algorithm to find the D-optimal design. In their result, the weighted G-optimal designs appeared to have model robustness this was because their designs started with small values of the SPV and remained relatively flat throughout the design space across a set of possible reduced models.

Dennis K. Munithi (2019) used the simplex lattice design to conduct an experiment on the yield of watermelon with an objective of optimizing the multiple responses of watermelon to organic manure (poultry manure, cow manure and goat manure). He used multiple regression models to develop an equation of the model, the dependent variables are the watermelon fruit weight and the number of watermelon per plant. In his conclusion, he states that goat manure has a more important role on the watermelon production.

2. METHODOLOGY

In a {q, m} simplex lattice design, q is the number of components in the mixture and m is the degree of the model. For q = 3 components mixture, m can take values from 1 to any value, but in this study, the value of m will range from 1 to 3. The number of design points in any {q, m} simplex can be obtained using the following formula;

$$\binom{q+m-1}{m} = \frac{(q+m-1)!}{m!\,(q-m)!}$$

The form of the mathematical model used in a {q, m} simplex lattice to predict the response at a given mixture is called the canonical polynomial. We will take the values of $m = 1,2,3$ and derive the canonical equation for each.

2.1 SIMPLEX CENTROID DESIGN

A simplex-centroid design with q-components has a 2^q -1 distinct points, that corresponds to q permutations of (1, 0, … ,0) called the single component blend, the $\binom{q}{2}$ permutations of (½ , ½, 0, … ,0), the $\binom{q}{3}$ permutations of (1/3 , 1/3, 0, … ,0) and finally (1/3 , 1/3, 0, … ,0) called the q mixture (Cornel 2002). The mixtures in the simplex centroid design occur at equal proportion. This type of mixture cannot be used to estimate the full cubic model, but the special cubic can be estimated. The simplex centroid and the simplex lattice design are both boundary design except for the overall centroid (Cornel 2002). The polynomial equation is given below as,

$$y = \sum_{i=1}^{q} \beta_j + \sum_{i<}\sum_{j} \beta_{ij}\, x_i x_j + \sum_{i<}\sum_{j<}\sum_{k} \beta_{ijk}\, x_i x_j x_k + \cdots + \sum_{1} \dots \sum_{q} \beta_{1,2\dots q}\, x_1 \dots x_q \quad (1)$$

$where;$ β_i is the linear blend which represents the expected response to the pure component.

β_{ij} represents the coefficient of the nonadditive blending components of i and j.

β_{ijk} represents the ternary blending among the components i, j and k.

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$\beta_{1,2,\dots q}$ represents the coefficient of the blending components $1,2,\dots,q$.

The parameters in the polynomial are expressible as linear functions of the expected response (Cornel 2002). The parameters can be estimated as follows;

$$\beta_i = \hat{y} \quad (2)$$

$$\beta_{ij} = 2\left(2\hat{y}_{ij} - (\hat{y}_i + \hat{y}_j)\right) \quad (3)$$

$$\beta_{ijk} = 3\left(3^2\hat{y}_{ijk} - 2^2\left(\hat{y}_{ij} + \hat{y}_{ik} + \hat{y}_{jk}\right) + \left(\hat{y}_i + \hat{y}_j + \hat{y}_k\right)\right) \quad (4)$$

2.2 OPTIMALITY CRITERION

This is a value that tells us how good an experimental design is. Jasbir Singh Arora (2017) defines optimality criteria as a condition a function has to satisfy at its minimum point. Boonorm Chomtee (2003), in his words state that apart from considering money and other constraints, design optimality criteria should be used to evaluate a proposed experimental design. Design optimality criteria are used to evaluate which experimental design is best out of many proposed designed. This is done by studying the optimality properties of the proposed design.

In this research, we will study 3 types of design optimality criteria namely A, D and G optimality criteria.

2.2.1 A-OPTIMALITY CRITERIA: The A-optimality criteria minimizes the trace of the inverse of the X (information matrix), that is, it minimizes trace)

Where X is the design matrix

Trace is the sum of the scaled variances of the regression coefficients.

The A-Optimality is based on the sum of the variances of the estimated regression coefficients which is also the sum of the diagonal elements or trace of $(X'X)^{-1}$.

The efficiency measure is given as $\frac{100p}{trace[N(X'X)^{-1}]}$

Where p is the number of parameters and N the total runs

2.2.2 D-OPTIMALITY: The D-optimality is obtained using the determinant of the information matrix of the design, this is the same as the inverse of the determinant of the variance-covariance matrix for the estimate of the linear regression coefficients i.e. $|X'X| = \frac{1}{|(X'X)^{-1}|}$

It evaluates how well the coefficients were estimated; hence a smaller $|X'X|$ or a larger $|(X'X)^{-1}|$ implies poor estimation of the parameters. The aim of D-Optimality is to maximize $|X'X|$ or minimize $|(X'X)^{-1}|$.

The D efficiency is given as $\frac{100|X'X|^{\frac{1}{p}}}{N}$

Where p is the number of parameters and N the total runs

2.2.3 G-OPTIMALITY CRITERION: The G-efficiency is a known criterion for optimal design and it is based on the prediction variance property of the response. The G-Optimality criterion is used to obtain a set of points that will minimize the maximum scaled prediction variance (SPV) over the entire design space. Therefore the G-efficiency is based on the performance of SPV.

the scaled prediction variance (SPV) is given as

$$SPV = \frac{Nvar(\hat{y}(x))}{\sigma^2}$$

Where $\hat{y}(x)$ is the prediction equation

$var(\hat{y}(x))$ is the variance of the prediction response at a given point x

N is the number of design points

Then the G-efficiency is given as follows

$G - efficiency = \frac{100p}{\max(SPV)}$

Where p is the number of the parameters in the model

3.0 Illustrative example

Table 3.1 Optimality criteria values for a 3 components simplex centroid design

NO OF COMPTS	NO OF REP	ORDER OF THE MODEL	A-OPTIMAL	D-OPTIMAL	G-OPTIMAL
3	0	Linear	2.03	2.74286E-1	0.6762
	0	Quadratic	65.89	2.51345E3	0.9924
	0	Special cubic	1263.00	2.98598E6	1.00
	1	Linear	1.74	1.63636E-1	0.6670
	1	Quadratic	61.95	1.26151E3	0.9924
	1	Special cubic	1254	1.49299E6	1.00
	2	Linear	1.46	9.81595E-2	0.6564
	2	Quadratic	58.00	6.3316E2	0.9924

	2	Special cubic	1245	7.46496E5	1.00
	3	Linear	1.19	5.92593E-2	0.3963
	3	Quadratic	54	3.17793E2	0.8774
	3	Special cubic	1236	3.73248E5	1.00

Table 3.1 above displays the values of the A, D and G optimality criteria for a 3 components simplex centroid design when replicated and at different order of the design model. From the table above, when the 3 components were not replicated the optimal values of A-optimality criteria are as follows (2.03, 65.89, 1263.00). A-optimality criteria seeks to minimize the trace of the information matrix, from the values of the A-optimality criteria the min is 2.03 which means that the design is more optimal when there is no quadratic and the cubic effects in the model. When replicated once, the values for A-Optimal are (1.74, 61.95 and 1254). the minimum value is 1.74 which means that the design is better when there is no quadratic and cubic effect in the design. Also when replicated twice and three times, the value for A-optimal indicates we will have a better design when there is no quadratic and cubic effects. To compare the 4 designs under A-optimal, we will conclude that in a 3 components simplex centroid mixture experiment, the design should be replicated 3 times without the quadratic and special cubic effects, this is because it has the lowest value (1.19).

Under the D-optimal, with no replicate the optimal values are (2.74286E-1, 2.51345E3, 2.98598E6) this also indicates that we will have a better design under pure blending mixtures with no quadratic and cubic effects. This result also applies when the experiment is performed with one, two and three replications. The lowest value under D-optimal column is 5.92593E-2, which means that in a 3 components design, the optimum design will be achieved when it is replicated 3 times without quadratic and special cubic effects.

Under the G-optimal, with no replicate the optimal values are (0.6762, 0.9924, 1.00) this also indicates that we will have a better design under pure blending mixtures with no quadratic and special cubic effects. This result also applies when the experiment is performed with one, two and three replications. The lowest value under D-optimal column is 0.3963, which means that in a 3 components design, the optimum design will be achieved when it is replicated 3 times without quadratic and special cubic effects.

Table 3.2 Optimality criteria values for a 4 components simplex centroid design

NO OF COMPTS	NO OF REP	ORDER OF THE MODEL	A-OPTIMAL	D-OPTIMAL	G-OPTIMAL
4	0	Linear	2.13	6.37665E-2	0.5322
	0	Quadratic	112.77	2.19765E6	0.9771
	0	Special cubic	4329.93	2.62276E18	0.9999
	1	Linear	1.93	4.1618E-2	0.5271
	1	Quadratic	107.86	1.11153E6	0.9770
	1	Special cubic	4311.17	1.31147E17	0.9999
	2	Linear	1.73	2.72535E-2	0.5213
	2	Quadratic	102.93	5.62215E5	0.9769
	2	Special cubic	4292.41	6.5578E17	0.9999
	3	Linear	1.54	1.79142E-2	0.5148
	3	Quadratic	98	2.84386E5	0.9768
	3	Special cubic	4273.64	3.27911E17	0.9999

Table 4.4 above displays the values of the A, D and G optimality criteria for a 4 components simplex centroid design when replicated and at different order of the design model. From the table above, when the 4 components were not replicated the optimal values of A-optimality criteria are as follows (2.13, 112.77,4329.93). A-optimality criteria seeks to minimize the trace of the information matrix, from the values of the A-optimality criteria the min is 2.13 which means that the design is more optimal when there is no quadratic and the cubic effects in the model. When replicated once, the values for A-Optimal are (1.93, 107.86 and 4311.17). the minimum value is 1.93 which means that the design is better when there is no quadratic and cubic effect in the design. Also when replicated twice and three times, the value for A-optimal indicates we will have a better design when there is no quadratic and cubic effects. To compare the 4 designs under A-optimal, we will conclude that in a 4 components simplex centroid mixture experiment, the design should be replicated 3 times without the quadratic and special cubic effects, this is because it has the lowest value (1.54).

Under the D-optimal, with no replicate the optimal values are (6.37665E-2, 2.19765E6, 2.62276E18) this also indicates that we will have a better design under pure blending mixtures with no quadratic and cubic effects. This result also applies when the experiment is performed with one, two and three replications. The lowest value under D-optimal column is 1.79142E-2, which means that in a 4 components design, the optimum design will be achieved when it is replicated 3 times without quadratic and special cubic effects.

Under the G-optimal, with no replicate the optimal values are (0.5322, 0.9771, 0.9999) this also indicates that we will have a better design under pure blending mixtures with no quadratic and special cubic effects. This result also applies when the experiment is performed with one, two and three replications. The lowest value under G-optimal column is 0.5148, which means that in a 4 components design, the optimum design will be achieved when it is replicated 3 times without quadratic and special cubic effects.

Simplex centroid Design Optimal Criteria Comparison for n = 3 and 4.

To obtain the best optimality criteria that gives the best simplex centroid design, table 4.8 be used to compare the mean efficiency based on ranking.

Table 3.3 Simplex centroid Design Optimal Criteria Comparison for n = 3 and 4.

No of components	A-Efficiency	D-Efficiency	G-Efficiency
3	25.21	25.41	75.7
4	14.43	15.19	43.16
Mean	19.82	20.3	59.43
	3	2	1

From the above table, the G optimality criterion proved to be the best among the three optimality criteria studied for the simplex centroid design.

4.0 DISCUSION OF FINDING

The result show that replicating the simplex centroid design 3 times without the quadractic and cubic effect will produce the best design and in comparing the design for A, D and G optimality criterion, the G optimality criteria proved to be the best criteria.

5.0 CONCLUSION

In conclusion, our study shows that when designing the simplex centroid mixture design, the experiment irrespective of the number of components in the experiment should be replicated 3 times without the quadratic and cubic effects and that this design should be done using the G optimality criteria.

REFERENCES

Bondari (2005), *Mixture experiments and their applications in agricultural research.* SAS publishing

Cheruiyot (2017), Slope Optimal Designs for Third Degree Kronecker Model Mixture. *American journal of theoretical and applied statistics, pp: 170-175*

Coetzer (2010), Optimal Designs for estimating the parameters in weighted power-mean-mixture model. *Jounal of Chemometri. 24(1), p. 34 - 42*

Cornel (2011), Experiments with mixtures, *3rd edition. A wiley-interscience publication*

Dennis K. Murithi(2019). Application of simplex Lattice Design in Watermelon Production. *Journal of International knowledge sharing platform. 9(1)p. 2225 – 0522*

Jasbir Singh Arora (2017)

Mandlik Satish K, Adhikari Saugat, Deshpande Ameya, (2012). Application of Simplex Lattice Design in Formulation and Development of Bouyant Matrices of Dipyridamole. *Journal of applied Pharmaceutical Science.2(12): 107 – 111.*

Montegomery D.C (2005), Design and Analysis of Experiments, *6th edition. John Wiley & Son, New York*

Ngonadi, Lilian Oluebube (2019), A comparison of some varieties of central composite design using alphabetic optimality criteria.

Ronald D. Snee (1971). Design and Analysis of Mixture Experiments. *Journal of Quality Technnology, 3:4, 159 – 169,DOI: 10.1080/00224065.1971.11980489*

Schalkwyk (1971). On the Design of Mixture Experiments. *A thesis submitted for the Diploma of membership of Imperial College and the degree of doctor of philosophy in the university of London*

V. Sameera and K. Jaya Raju (2016). Simplex Lattice Mixture Design Approach for the production of L-Glutaminase using oil cake Mixture. *Imperial Journal of interdisplinary Research. 2(7), 2454 -1362*