Augmented Designs for Mixture Experiments

मिश्रण परीक्षण के लिए संवर्धित अभिकल्पनाएं

By

DEBOPAM RAKSHIT

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Approved By:

Chairperson: **Dr. Baidya Nath Mandal**
Co-chairman: **Dr. Rajender Parsad**
Member: **Dr. Sukanta Dash**
Member: **Dr. Mukesh Kumar**

ICAR- INDIAN AGRICULTURAL STATISTICS RESEARCH INSTITUTE
LIBRARY AVENUE, PUSA, NEW DELHI- 110012

Dr. Baidya Nath Mandal
Scientist
Division of Design of Experiments
ICAR- I.A.S.R.I , Library Avenue
Pusa, New Delhi- 110012

CERTIFICATE

This is to certify that the work incorporated in the thesis entitled ***"Augmented Designs For Mixture Experiments"*** *submitted in partial fulfilment of the requirement for the degree of* ***Master of Science in Agricultural Statistics*** *of the* ***Post-Graduate School, ICAR-Indian Agricultural Research Institute, New Delhi****, is a record of bona fide research carried out by* ***Debopam Rakshit*** *under my guidance and supervision and no part of this dissertation has been submitted for any other degree or diploma.*

All assistance and help received during the course of this investigation has been duly acknowledged.

Date: 26/10/18
Place: New Delhi

(Dr. Baidya Nath Mandal)
Chairperson
Advisory Committee

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Debopam Rakshit

(Debopam Rakshit)

CONTENTS

CHAPTER I

INTRODUCTION

This chapter gives an introduction to mixture experiments, its properties, different designs of mixture experiments, and their applications. After that, the motivation of research work is introduced followed by thesis objectives and scope of the present investigation.

1.1 Introduction

There are many experiments where a fixed amount of inputs, such as a fixed dose of fertilizer, insecticide or pesticide, or a fixed quantity of irrigation water etc. are used. Here, the fixed amount of input may be a mixture of several ingredients. For example, a fixed quantity of nitrogen, P_2O_5 and K_2O can be taken from various sources of nitrogenous/ phosphoric/ potassic fertilizers. Similar things also happen in case of pesticide or insecticide trial by mixing several chemicals. For making a mixed fruit juice consisting of four fruits (say) pineapple, banana, guava and pomegranate, all the fruits are mixed in pre-defined proportions. In this situation the taste and flavour are totally dependent upon the proportions. All the above mentioned experiments are done using mixture experiments. Mixture experiments are performed for product development and its quality improvement. Two or more components or ingredients are blended in various proportions to get an end product. Mixture experiments are very useful in agriculture, horticulture, plant protection, food processing etc. Let us consider an example.

Example 1: Let two chemical pesticides P_1 and P_2 will be used to control any insect by spraying pesticides on plants. The objective of the experiment is to find out if a combination of P_1 and P_2 is more effective than either of pesticides used separately. Experimenter may take five different combinations of P_1 and P_2 where each of the blends has the fixed amount. The five mixes may be (1.0 : 0), (0.75 : 0.25), (0.50 : 0.50), (0.25 : 0.75), (0 : 1.0). The difference in effectiveness of controlling insects is due to relative proportions of P_1 and P_2 present in the blends and does not depend on the total amount of pesticides applied. Therefore, for such situations, experiments with mixtures methodology should be used. Out of these 5 blends above, two blends namely first and fifth one consist of a single component. These blends are known as "pure blends" or "single-component blends". The experimenter may take other proportions of P_1 and P_2 also based on the experimental situations.

1.2 Mixture Experiments

In mixture experiments, it is assumed that the observed response depends on the proportions of the ingredients present in the mixture and it does not depend on the amount of the mixture (Cornell, 1981).

Mixture experiments along with their analysis methods are aimed to develop a functional relationship between responses and the corresponding proportions of various inputs used to produce the responses. This functional relationship is helpful to obtain the responses at these proportions, which are not included in the experiments by interpolation.

In mixture experiments, the proportions of constituent components are expressed as fractions of a mixture and they are always non-negative and their total is always one, i.e.

$$0 \leq x_i \leq 1.0 \quad \text{and} \quad \sum_{i=1}^{q} x_i = 1; \qquad i = 1, 2, \ldots, q \tag{1.1}$$

where q is the number of components in the mixture. Here, x_i, $i = 1, 2, \ldots, q$ represents the proportion of component i forming the mixture.

1.3 Models for Experiments with Mixture

Let the functional relationship between observed response (η) and the proportions of ingredients $x_1, x_2, \ldots, x_q$ is

$$\eta = \varphi(x_1, x_2, \ldots, x_q) + \varepsilon, \quad \varepsilon \sim i.i.d\ \mathrm{N}(0, \sigma^2) \tag{1.2}$$

A very basic assumption is made that the response surface, denoted by the function φ, is a continuous function of the x_i, $i = 1, 2, \ldots, q$.

The problem of determining the shape of the response surface with the component compositions depends on finding the mathematical equation that satisfactorily describe the function φ in Eq. (1.2). Due to the constraint of mixture experiment i.e. $\sum_{i=1}^{q} x_i = 1$, these polynomial functions are different from the usual regression equations.

To deal with data obtained from mixture experiments, Scheffé (1958, 1963) derived the canonical polynomial by applying the constraint (1.1) in a standard polynomial. These polynomials are devoid of any intercepts.

Linear: $$\eta = \sum_{i=1}^{q} \beta_i x_i + \varepsilon \qquad (1.3)$$

Quadratic: $$\eta = \sum_{i=1}^{q} \beta_i x_i + \sum_{i}^{q} \sum_{j>i}^{q} \beta_{ij} x_i x_j + \varepsilon \qquad (1.4)$$

where $\varepsilon \sim$ *i.i.d* N $(0, \sigma^2)$

For a q = 3 components system, linear and quadratic polynomials are given by:

Linear: $$\eta = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \varepsilon$$

Quadratic: $$\eta = \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_3 + \beta_{12} x_1 x_2 + \beta_{13} x_1 x_3 + \beta_{23} x_2 x_3 + \varepsilon$$

where $\varepsilon \sim$ *i.i.d* N $(0, \sigma^2)$

The terms present in canonical polynomials (linear and quadratic) can be interpreted as usual regression coefficients. The coefficients of x_i, i = 1, 2,…, q denote the effects due to the i^{th} component, whereas the coefficients of x_{ij} denote the joint effect of the components i and j.

When the mixtures of components are strictly additive in nature, linear canonical polynomial (first degree) is best suitable to represent the surface, whereas canonical polynomials of higher degree are being used to represent the surface with curvature due to non-linear blending between the pairs of components. Positive sign of β_{ij} indicates synergistic relationship between components and vice versa.

1.4 Basic Designs for Experiments with Mixture

There are two very important classes of designs used in mixture experiments. These are

- Simplex-lattice designs (Scheffé, 1958, 1963) and
- Simplex-centroid designs (Scheffé, 1963)

If there is a constraint imposed on *n* variables, then it can be represented by ($n - 1$) dimensional factor space, which is known as simplex. For 2 components it is a straight line, for 3 components it is an equilateral triangle.

When a polynomial equation is used to characterize the response surface over the entire simplex region, the design should be so chosen that the points are spread uniformly over the whole simplex factor space. An ordered arrangement with uniformly distributed points on a simplex is known as a *lattice.* The name lattice always represents an array of points.

1.4.1 Simplex-Lattice Designs

To fit a polynomial model of degree *m* in *q* components mixture experiment over the simplex, the lattice, is referred to as a $\{q, m\}$ simplex-lattice. It consists of points where the proportions of each component take the $m + 1$ equally spaced values from 0 to 1, i.e.

$$X_i = 0, 1/m, 2/m, \ldots, 1 \tag{1.5}$$

and the $\{q, m\}$ simplex-lattice design consists of all possible combinations (mixtures) of each of the components with proportions presented in (1.5) . The total number of design points in the $\{q, m\}$ simplex-lattice is ${}^{q+m-1}C_m$.

For example, the $\{3, 3\}$ simplex-lattice consists of ${}^5C_3 = 10$ points (Figure 1).

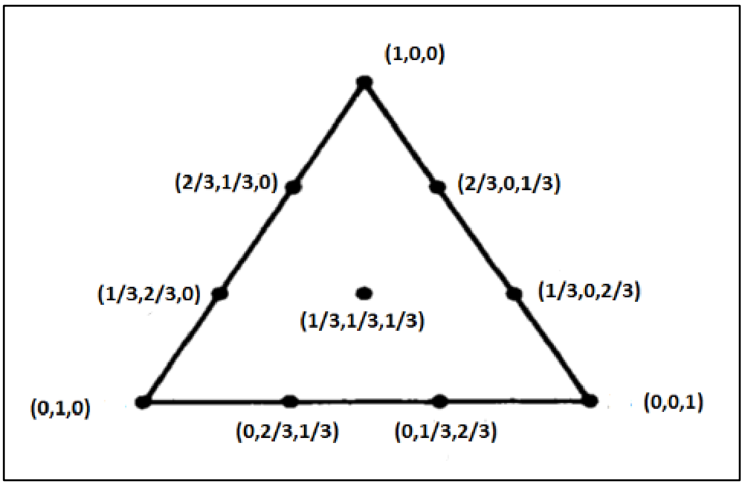

Figure 1: Three-component 10-point design, a $\{3, 3\}$ simplex-lattice design.

1.4.2 Simplex-Centroid Designs

Scheffé (1963) introduced simplex-centroid designs. A simplex-centroid design for q components mixture experiment consists of all possible subsets of these q components present in equal proportions. The design contains only one full mixture blend and that point is the overall centroid. It has a total number of (2^q – 1) design points which are given by ${}^qC_1$ permutations of (1, 0,…, 0), ${}^qC_2$ permutations of (1/2, 1/2, 0,…, 0), ${}^qC_3$ permutations of (1/3, 1/3, 1/3, 0,…, 0), so on, and finally the overall centroid of the triangle (1/q, 1/q,…, 1/q). For example, a three-component simplex-centroid design consists of $2^3 – 1 = 7$ points (Figure 2).

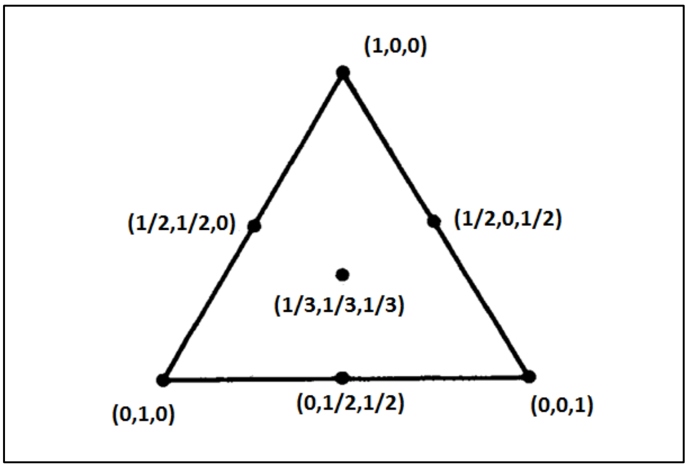

Figure 2: A simplex-centroid design with 3 components containing 7 points

1.5 Motivation and Objectives

Cornell (1986) suggested the augmentation of simplex-centroid designs. Augmentation is suggested in those situations where researcher is fitting a low degree (first or second) canonical polynomial but is uncertain about the shape of the surface above the simplex region. If the design consists of a smaller or equal number of points than the number of parameters in the fitted model, test for the significance of the parameters of the fitted model cannot be conducted. The design may be augmented by adding extra points so that the augmented design have more number of points than the number of parameters in the fitted model and then the test of significance of the parameters can be conducted. Further, designs with augmented points permit better exploration of the entire design space. Thus, efforts are needed to be made for obtaining suitable ways to augment a standard simplex-lattice design and a simplex-centroid design so that the testing of significance of the parameters can be performed and testing of hypothesis that there is no lack of fit of the model being used with replicated points can be done.

Keeping in mind the above research gap, following objectives have been proposed:

1. To develop a method for constructing augmented simplex-lattice designs for three-component mixture experiments.

2. To obtain a methodology for constructing augmented simplex-centroid designs.

1.6 Scope of the Present Investigation

The main purpose of this thesis is to develop suitable methods for augmentation of standard simplex-lattice designs and simplex-centroid designs for mixture experiments. Efforts have been made to obtain a method of construction of augmented simplex-lattice designs under objective 1. Proposed method of construction is utilized to construct augmented simplex-lattice designs. A catalogue of augmented simplex-lattice designs is prepared. D-efficiency and G-efficiency of the designs are also computed to see the quality of the constructed designs.

Method of obtaining augmented simplex-centroid designs is explored under objective 2. Proposed method is used to construct augmented simplex-centroid designs and the designs are catalogued. D-efficiency and G-efficiency of the augmented simplex-centroid designs as compared to the standard designs are investigated.

Chapter 1 gives introduction to mixture experiments along with an example of mixture experimental situation in agricultural research. A brief description of canonical polynomials used in mixture experiment is given. Detailed description of simplex-lattice designs, simplex-centroid designs, and motivation to undertake this topic as a research work are also provided. Chapter 2 gives a brief review of the work done on mixture experiments, simplex-lattice designs and simplex-centroid designs, Scheffé’s polynomial, restricted mixture designs, etc. Chapter 3 includes material and methods for obtaining augmented simplex-lattice and simplex-centroid designs. The concept of canonical polynomials and their derivations are discussed in this chapter. Design evaluation criteria D-efficiency per point and G-efficiency are also discussed in brief along with their calculation procedures. Chapter 4 comprises of the results and discussions of this study. The thesis ends with abstract written in both English and Hindi and finally bibliography.

CHAPTER II

REVIEW OF LITERATURE

This Chapter includes the review of available literatures regarding the topics related to this study. The review relates to general overview of mixture experiments, simplex-lattice designs, simplex-centroid designs, Scheffé's polynomial, restricted mixture designs and mixture experiments with process variables.

Scheffé (1958, 1963) introduced two important classes of mixture designs namely simplex-lattice designs and simplex-centroid designs. These two designs are used to know about the 'factor-response' relationship in the simplex region. Linear and quadratic canonical polynomials were used for this purpose for q-component mixture experiment. Scheffé (1963) also studied the problem of experimentation using simplex-centroid design with process variables for q-component mixture system where each of these n ($n > 0$) process variables are with two levels. Hence it was a simplex-centroid × 2^n factorial design.

McLean and Anderson (1966) proposed extreme vertices designs for restricted mixture designs. These type of designs are applied when at least for one component either an upper bound and/or a lower bound is present. The constraints are imposed to reduce the size of the factor space. They obtained a design method to determine a unique set of treatment combinations by selecting the vertices and different centroids from the resulting reduced simplex space.

Murty and Das (1968) obtained the generalized version of Scheffé's designs, known as systematic simplex design. In these designs the design points are scattered evenly throughout the simplex to explore the whole simplex space uniformly. A simple method of analysis and estimation was also provided by them with the help of symmetrically distributed design points.

Nigam (1969) proposed the estimation procedure of parameters in four types of mixture models and provided the blocks structure in presence of process variables. These four models were the all possible combination of linear and quadratic model of mixture and process variables.

Nigam (1970) has shown that without transforming the mixture experiments, orthogonal blocking is not possible to estimate the regression parameters, which are not dependent on the block effects. Nigam (1976) obtained the corrections for the blocking conditions of mixture experiments.

Snee and Marquardt (1974) developed XVERT algorithm for obtaining extreme vertices designs for restricted mixture designs. This proposed algorithm selects only a subgroup of extreme vertices from a large number of candidate vertices. These designs generally have small trace$(\mathbf{X'X})^{-1}$, which indicates that the average variance of the estimated parameters of the linear model is small.

Cornell (1973, 1979) wrote two reviews and bibliography of experiments with mixture experiments. His first review (1973) includes twenty research papers started with the work of Scheffé (1958) and the last one appeared in October, 1971. The second review (1979) is the sequel of the first one. It includes twenty two papers from 1971 to 1979. Research papers regarding analysis of mixture data, additional design configurations to cover the whole simplex and restricted simplex designs are discussed here in brief. Suggestions for future research aspects are also discussed.

Hare (1979) obtained some designs by using a special geometric approach, where some set of mixture blends are not repeated. Alternative procedures for minimizing the loss of simplex space were obtained in this study. All possible combinations of three and four mixture variables, each are of with and without a centre point, and with and without upper and/or lower bounds comprising a total number of eight cases were studied. The solution co-ordinate points of the simplex space were represented in the paper.

Nigam *et al*. (1983) proposed XVERT1 algorithm to obtain extreme vertices designs which are useful for restricted mixture designs. This new algorithm needs less computational effort. This proposed algorithm is as efficient as the XVERT algorithm of Snee and Marquardt (1974).

Cornell (1986) presented two designs with ten points for mixture experiments with three components. The first design was a {3, 3} simplex-lattice design where nine points are uniformly distributed on the perimeter of the triangular simplex region and the remaining one was the centroid of the triangle. In the second design, a simplex-centroid design with 3 components was augmented with three more points inside the triangle. These two designs were compared based on the variance and bias of fitted canonical models i.e. Scheffé first-degree model, second-degree model and special cubic model.

Draper *et al*. (1993) developed four components mixture designs with two or more orthogonal blocks by using quadratic models. They used the properties of Latin squares of side four to quickly obtain the designs with specific properties. Orthogonal blocks can also be obtained when higher order models are fitted.

Prescott *et al*. (1993) extended the four components mixture designs with orthogonal blocks developed by Draper *et al*. (1993) to a mixture of five components. The properties of five sided Latin squares was used to quickly obtain the designs with specific properties. While fitting higher order models it was seen that these designs also produced orthogonal blocks.

Lewis *et al*. (1994) generalized methods for constructing orthogonal block for q-component ($q \geq 3$) mixture system. These designs were the generalized version of four and five components mixture designs obtained by Draper *et al*. (1993) and Prescott *et al*. (1993) respectively.

Khuri and Cornell (1996) obtained techniques for designing experiments which yield adequate and reliable measurements of responses, and helps for fitting and testing of suitable models to make decisions concerning the system under investigation.

Batra *et al*. (1999a) and Batra *et al*. (1999b) have shown that for the fertilizer experiments with fertilizer application in split doses at different crop growth stages, restricted mixture designs are more appropriate. They suggested to apply XVERT1 algorithm for these purpose. Responses from those design points, that were not included as treatment in the experiments, were interpolated.

Deka *et al*. (2001) used mixture experiments to assess quality of ready to serve beverages of lime, aonla, grape, pineapple and mango juice/pulp with varying proportions (5 to 95%). Data were collected on the likeliness of these beverages on three different age groups (22-34 years, 35-44 years and 45-54 years). The collected data were analysed by using response surface model. It was observed that lime 95% + aonla 5% combination was supposed to be the best.

Dhekale (2001) fitted the canonical quadratic model including one process variable. An illustration was given using an intercropping experiment, where sorghum and green gram were cultivated and spacing between rows was considered as a process variable.

Cornell (2002, 2011) gave detailed explanation of origin of mixture experiment, mixture designs and canonical polynomials that are being used for searching the entire simplex factor space, restricted mixture experiments where some constraints are imposed on at least one of the component proportions, analysis of mixture experiment data, other mixture model forms, mixture experiments with process variables etc.

Aggarwal and Singh (2003) projected four different types of standard 3 level designs into the design space and provided various efficiency measures of the obtained mixture designs by fitting Scheffé's canonical quadratic model and Darroch's quadratic models. They also tabulated and compared the uniformity measures for these designs.

Parsad *et al*. (2004) developed response surface designs for both response optimization and slope estimation when factors are with equi-spaced levels, response optimization of mixture experiments with qualitative-cum-quantitative factors and studied the robustness aspects of response surface designs against single missing observation.

Alam (2010) developed construction methods of designs for multi-factor mixture experiments with fewer number of runs and second order mixture model was fitted. The designs were evaluated with various efficiency measures. Methods of construction of designs were also developed with restricted upper or lower bound of one component of each factor and for both restricted upper and lower bound of some of the components for each factor. Two different types of models, used for multifactor mixture experiment when process variable(s) are present, were discussed. In one model only the liner effect of process variable(s) and in the other model both the linear effect and the interaction effect of mixture components with the process variable(s) were considered.

Lal *et al*. (2010) obtained efficient mixture experiment in smaller number of runs. They developed two construction methods of mixture designs with process variables. In the first method, orthogonally blocked response surface designs and projection matrices was used while in second method blocking criteria of response surface designs suggested by Wu and Ding (1998) was used.

Khattree (2015) developed a class of mixture designs which is known as yantram designs. These designs always contain a complete mixture. These designs can be directly derived from the Hindu yantrams. These designs are also suitable for situations when there are some constraints imposed on components. Leverage values for these designs are more uniformly distributed in the interior part of the simplex space as compared to simplex-lattice designs or simplex-centroid designs.

Pradhan *et al*. (2016) obtained a construction method of efficient mixture with process variable with minimum number of runs by using the projection matrix, which are useful when resources are limited. They constructed efficient designs for three, four and five components mixture experiment system with one process variable.

Hasan *et al*. (2018) introduced shrinkage simplex-centroid designs. These designs contain complete blends of mixture. G-efficiency of these designs are stable but there are some loss of D-efficiency. They also generated component-amount designs by using the proposed designs by their projections.

CHAPTER III

MATERIALS AND METHODS

3.1 Introduction

The material and methods for obtaining augmented simplex-lattice and simplex-centroid designs, concept of canonical polynomials and various optimality measures are discussed in this chapter.

In mixture experiments, the response is not a function of the total amount of the mixture but the relative proportion of its ingredients. Experimentation is done with some design points and the responses are collected for these design points.

3.2 Models for Mixture Experiments

An important problem in mixture experiments is to develop a suitable model or mathematical equation that adequately describe the shape of response surface as a function of ingredient compositions. Scheffé (1958, 1963) has obtained the canonical polynomial for problems with mixture experiments after incorporating the constraints that sum of mixture components proportions adds to one in a standard polynomial. First degree (Linear) and Second degree (Quadratic) canonical polynomial models are described below.

3.2.1 First degree (Linear) Model

The first degree regression model for a mixture experiment with q components is

$$E(Y) = \beta_0 + \sum_{i=1}^{q} \beta_i x_i$$

where β_0 and β_i are the unknown coefficients of the model. The coefficients are estimated using regression analysis procedure.

Substituting β_0 by β_0 $(x_1 + x_2 + \ldots + x_q)$ due to the constraint $\sum_{i=1}^{q} x_i = 1$; condition (1.1), we can write,

$$E\,(Y) = \beta_0(x_1 + x_2 + \ldots + x_q) + \sum_{i=1}^{q} \beta_i x_i$$

= (β_0+β_1) x_1 + (β_0+β_2) x_2 +…+ (β_0+β_q) x_q

= $\beta'_1 x_1$ + $\beta'_1 x_1$ +…+ $\beta'_q x_q$ (where β'_i = β_0 +β_i)

This is known as canonical polynomial of first degree (Linear model) for mixture experiment.

3.2.2 Second degree (Quadratic) Model

The second degree regression model for a mixture experiment with q components is given by

$$E(Y) = \beta_0 + \sum_{i=1}^{q} \beta_i x_i + \sum_{i<j}^{q} \beta_{ij} x_i x_j + \sum_{i=1}^{q} \beta_{ii} {x_i}^2$$

Replacing β_0 by $\beta_0\left(x_1 + x_2 + \cdots + x_q\right)$ and ${x_i}^2$ by $x_i\left(1 - \sum_{j\neq i=1}^{q} x_j\right)$ we get,

$$E(Y) = \sum_{i=1}^{q} (\beta_\circ + \beta_i) x_i + \sum_{i<j}^{q} \beta_{ij} x_i x_j + \sum_{i=1}^{q} \beta_{ii} x_i \left(1 - \sum_{i\neq j}^{q} x_j\right)$$

$$= \sum_{i=1}^{q} (\beta_0 + \beta_i + \beta_{ii}) x_i + \sum_{i<j}^{q} \beta_{ij} x_i x_j + \sum_{i=j}^{q} \left(\beta_{ij} - \beta_{ii} - \beta_{jj}\right) x_i x_j$$

$$= \sum_{i=1}^{q} {\beta_i}' x_i + \sum_{i<j}^{q} {\beta_{ij}}' x_i x_j$$

(where ${\beta_i}' = \beta_0 + \beta_i + \beta_{ii}$, ${\beta_{ii}}' = \beta_{ij} - \beta_{ii} - \beta_{jj}$)

For a q-component mixture experiment, linear and quadratic canonical polynomials are given by:

Linear: $\eta = \sum_{i=1}^{q} \beta_i x_i + \varepsilon$ (3.1)

Quadratic: $\eta = \sum_{i=1}^{q} \beta_i x_i + \sum_{i}^{q} \sum_{j>i}^{q} \beta_{ij} x_i x_j + \varepsilon$ (3.2)

In similar way special cubic model is obtained as,

Special cubic: $\eta = \sum_{i=1}^{q} \beta_i x_i + \sum_{i}^{q} \sum_{j>i}^{q} \beta_{ij} x_i x_j + \sum_{i}^{q} \sum_{j}^{q} \sum_{k}^{q} \beta_{ijk}\, x_i x_j x_k + \varepsilon$ (3.3) where $\varepsilon \sim i.i.d\ N(0, \sigma^2)$

In these canonical polynomial the intercept term is not present. The coefficients of canonical polynomials can be viewed as regression coefficients where the coefficients of x_i, $i = 1, 2,\dots, q$ denote the effect due to the i^{th} component and the coefficients of x_{ij} denote the joint effect of components i and j. In case of strictly additive blending, the linear canonical polynomial is best suitable to represent the response surface. But curvature of response surface due to non-linear blending cannot be represented by this linear model. Second-degree or higher-degree canonical polynomials are used for representation of the curvature. For synergistic relation between i^{th} and j^{th} component, β_{ij} is positive and for antagonistic relation, it is negative.

3.3 Methodology

A simplex-lattice and simplex-centroid design for three components are represented by equilateral triangles. From the geometry of triangles, it is known that any equilateral triangle can be partitioned into t^2 equilateral triangles, where t is a positive integer. So the simplex design space of a simplex-lattice and simplex-centroid design for three components can be partitioned into t^2 equilateral triangles. Centroids of these t^2 equilateral triangles can be used as augmented points of the design. This principle may be used for augmentation of standard designs for three-component mixture experiments.

A standard simplex-lattice design for {3, 2} system is given in Figure 3.1.

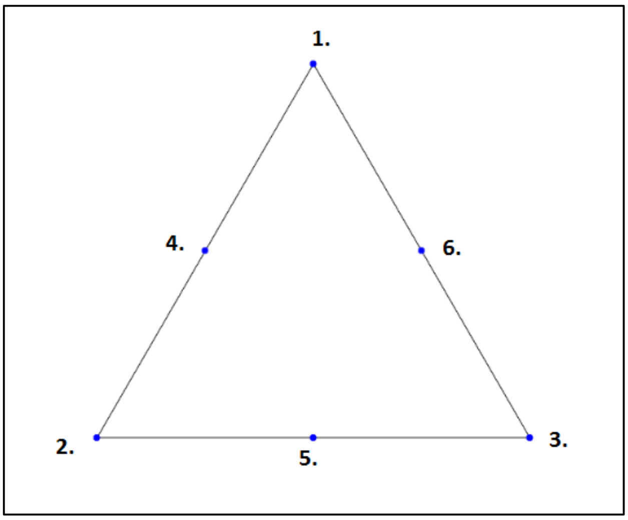

Figure 3.1: A standard simplex-lattice design with 6 points for 3-component mixture

A {3, 2} simplex-lattice design has $^{3+2-1}C_2$= 6 design points and the co-ordinates of the candidate points are as below.

Table 3.1: Co-ordinates of the candidate points of 6-point simplex-lattice design for three-component mixture experiment

Points	x_1	x_2	x_3
1	1	0	0
2	0	1	0
3	0	0	1
4	1/2	1/2	0
5	0	1/2	1/2
6	1/2	0	1/2

This standard simplex-lattice design for three components may be augmented as follows,

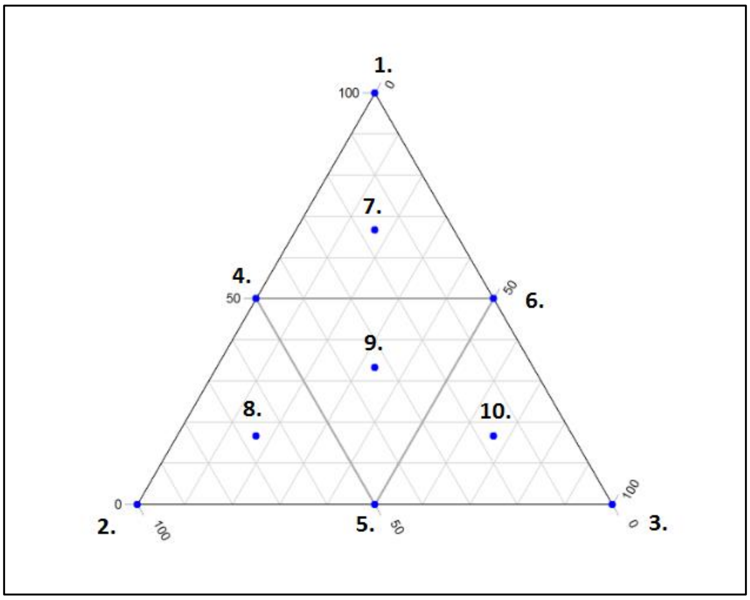

Figure 3.2: Three-component 10-point design, an augmented simplex-lattice design

Here we consider $t = 2$, hence the triangle has been partitioned into $t^2 = 4$ equilateral triangles. For each smaller interior triangle, their centroid points are included in the design points. Hence, we obtain four additional points inside the simplex design space and the total number of the design points is ten. The co-ordinates of these ten design points are given in Table 3.2.

Table 3.2: Co-ordinates of the candidate points of three-component 10-point augmented simplex-lattice design

Points	x_1	x_2	x_3
1	1	0	0
2	0	1	0
3	0	0	1
4	1/2	1/2	0
5	0	1/2	1/2
6	1/2	0	1/2
7	2/3	1/6	1/6
8	1/6	2/3	1/6
9	1/3	1/3	1/3
10	1/6	1/6	2/3

These candidate points are included in the design points and responses are measured.

For our current study, we consider only quadratic and special cubic model. Model matrix **X** is obtained for each augmented design for the study. Various efficiency measures such as D-efficiency per point and G-efficiency per point are computed for each design. Given below is the model matrix **X** of the above mentioned augmented simplex-lattice design while considering the quadratic model.

$$\mathbf{X} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 & 0 \\ 1/2 & 1/2 & 0 & 1/4 & 0 & 0 \\ 0 & 1/2 & 1/2 & 0 & 0 & 1/4 \\ 1/2 & 0 & 1/2 & 0 & 1/4 & 0 \\ 2/3 & 1/6 & 1/6 & 1/9 & 1/9 & 1/36 \\ 1/6 & 2/3 & 1/6 & 1/9 & 1/36 & 1/9 \\ 1/3 & 1/3 & 1/3 & 1/9 & 1/9 & 1/9 \\ 1/6 & 1/6 & 2/3 & 1/36 & 1/9 & 1/9 \end{bmatrix}$$

All these mathematical operations are done by R software using ‘matlib’ package. ‘Ternary’ package has been used for the visualization of the augmented designs. R code for D-efficiency per point and G-efficiency per point are attached at the end of the results and discussions chapter.

3.4 Design Evaluation Criteria

Proposed experimental designs will be evaluated using suitable design evaluation criteria. Two such important measures of design efficiency in mixture experiments are D-efficiency and G-efficiency. These two measures can be used to compare different designs for mixture experiments with same number of design points.

D-efficiency per point and G-efficiency per point of these augmented designs are studied and they are compared with the un-augmented designs. These measures are given by

D-efficiency per point = $\left(\frac{|\boldsymbol{X'X}|^{1/p}}{n}\right)$ x 100

G-efficiency per point = $\left(\frac{p}{nd}\right)$ x 100

where n denotes the number of points in the design, p denotes the number of parameters in the model and d denotes the maximum value of var[$\hat{y}(\mathbf{X})$]/σ^2 over all candidate points.

D-efficiency is related to the D-optimality criterion. D-optimal designs are defined as those that will minimize the generalized variance of the estimated parameters. G-efficiency is related to the G-optimality criterion. A G-optimal design is defined as one that minimizes the maximum value of the standard error of the predicted response.

As a thumb rule, Wheeler (1972) has advocated that a design with G-efficiency more than or equal to 50% may be considered as “good” for practical purposes and has shown that efforts to obtain designs with higher efficiencies may not be justified in practice.

CHAPTER IV

RESULTS AND DISCUSSIONS

In this chapter, we have described the results and discussions of augmented simplex-lattice designs and augmented simplex-centroid designs in Sections 4.1 and 4.2, respectively. Both these classes of designs have been obtained using the proposed methods described in Chapter III.

4.1 Augmented Simplex-Lattice Designs

Augmented simplex-lattice designs for both {3, 2} and {3, 3} systems are described in sequel.

4.1.1 Augmented Simplex-Lattice Designs for Scheffé Quadratic Model

At first we are considering a standard simplex-lattice design for {3, 2} system.

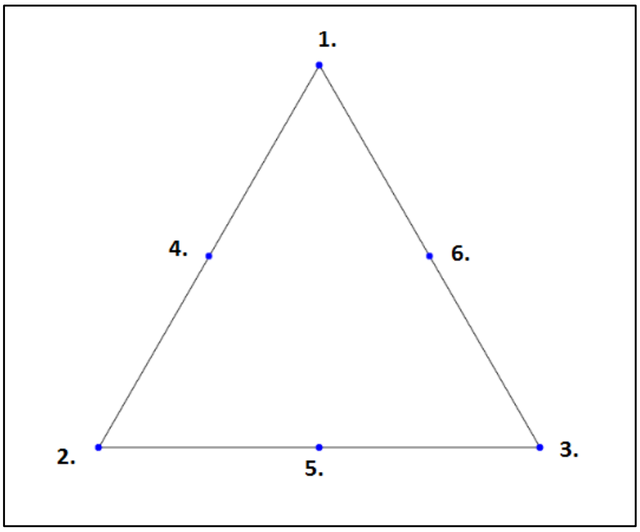

Figure 4.1: Three-component 6-point design, a standard simplex-lattice design

A standard simplex-lattice design with 3 components has six design points and the co-ordinates of the candidate points are given in Table 4.1.

Table 4.1: Co-ordinates of the candidate points of three-component 6-point simplex-lattice design

Points	x_1	x_2	x_3
1	1	0	0
2	0	1	0
3	0	0	1
4	1/2	1/2	0
5	0	1/2	1/2
6	1/2	0	1/2

Now we consider t = 1, then the triangle has been partitioned into t^2 = 1 equilateral triangle, i.e., the triangle itself. Here, the centroid point of the triangle is being included as a design point. Figure 4.2 gives the pictorial representation of the design.

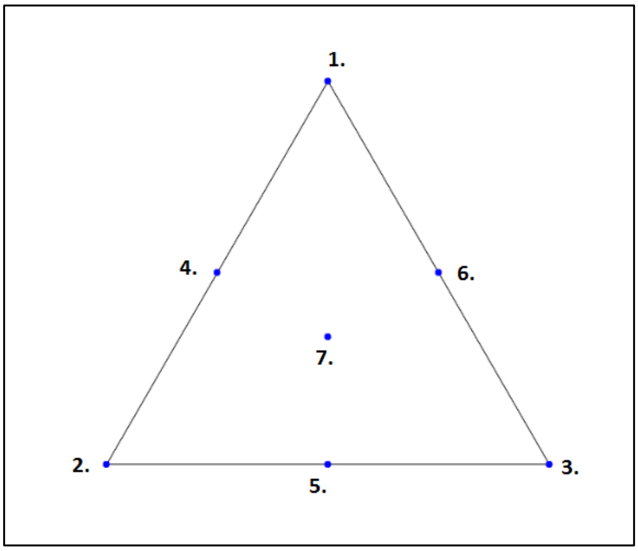

Figure 4.2: Three-component 7-point design, an augmented simplex-lattice design

Design points of the augmented design are shown in Table 4.2.

Table 4.2: Co-ordinates of the candidate points of three-component 7-point augmented simplex-lattice design

Points	x_1	x_2	x_3
1	1	0	0
2	0	1	0
3	0	0	1
4	1/2	1/2	0
5	0	1/2	1/2
6	1/2	0	1/2
7	1/3	1/3	1/3

For considering $t = 2$, the triangle has been partitioned into $t^2 = 4$ equilateral triangles. For each smaller interior triangle, their centroid points are included in the design points. Hence, we have obtained four additional points inside the simplex design space. The agumented design is shown in Figure 4.3.

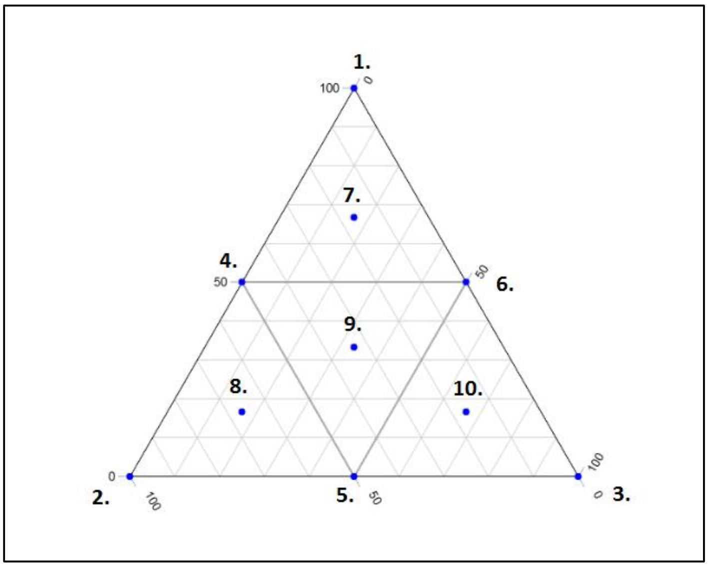

Figure 4.3: Three-component 10-point design, an augmented simplex-lattice design

Designs points in the augmented design are displayed in Table 4.3. The R code for visualization of augmented design points in the simplex region for {3, 2} simplex-lattice design for $t = 2$ is given in the end of this chapter.

Table 4.3: Co-ordinates of the candidate points of three-component 10-point augmented simplex-lattice design

Points	x_1	x_2	x_3
1	1	0	0
2	0	1	0
3	0	0	1
4	1/2	1/2	0
5	0	1/2	1/2
6	1/2	0	1/2
7	2/3	1/6	1/6
8	1/6	2/3	1/6
9	1/3	1/3	1/3
10	1/6	1/6	2/3

While considering t = 3, the triangle has been partitioned into t^2 = 9 equilateral triangles. For each nine smaller interior triangle, their centroid points are included in the design points. Hence, we have obtained nine additional points inside the simplex design space and the total number of the design points are fifteen. The design is shown in Figure 4.4.

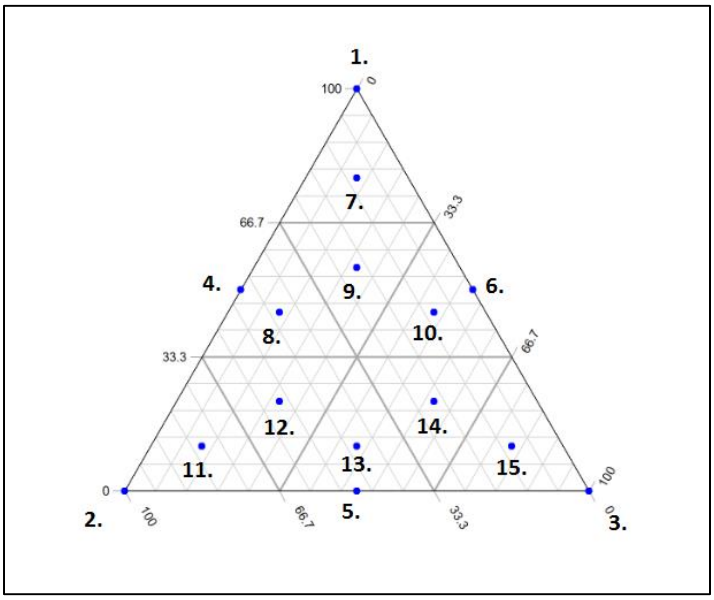

Figure 4.4: Three-component 15-point design, an augmented simplex-lattice design

Table 4.4 gives the design points of the augmented simplex-lattice design with t = 3.

Table 4.4: Co-ordinates of the candidate points of three-component 15-point augmented simplex-lattice design

Points	x_1	x_2	x_3
1	1	0	0
2	0	1	0
3	0	0	1
4	1/2	1/2	0
5	0	1/2	1/2
6	1/2	0	1/2
7	7/9	1/9	1/9
8	4/9	4/9	1/9
9	5/9	2/9	2/9
10	4/9	1/9	4/9
11	1/9	7/9	1/9
12	2/9	5/9	2/9
13	1/9	4/9	4/9
14	2/9	2/9	5/9
15	1/9	1/9	7/9

For $t = 4$, the triangle has been partitioned into $t^2 = 16$ equilateral triangles. For each sixteen smaller interior triangle, their centroid points are included in the design points. Hence, we have obtained sixteen additional points inside the simplex design space and the total number of the design points are twenty-two. The design is shown in Figure 4.5 and the design points are displayed in Table 4.5.

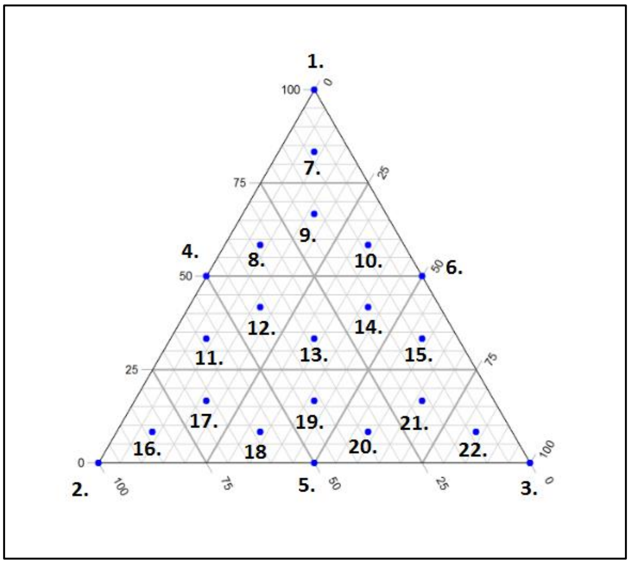

Figure 4.5: Three-component 22-point design, an augmented simplex-lattice design

Table 4.5: Co-ordinates of the candidate points of three-component 22-point augmented simplex-lattice design

Points	x_1	x_2	x_3
1	1	0	0
2	0	1	0
3	0	0	1
4	1/2	1/2	0
5	0	1/2	1/2
6	1/2	0	1/2
7	5/6	1/12	1/12
8	7/12	1/3	1/12
9	2/3	1/6	1/6
10	7/12	1/12	1/3
11	1/3	7/12	1/12
12	5/12	5/12	1/6
13	1/3	1/3	1/3
14	5/12	1/6	5/12
15	1/3	1/12	7/12
16	1/12	5/6	1/12
17	1/6	2/3	1/6
18	1/12	7/12	1/3
19	1/6	5/12	5/12
20	1/12	1/3	7/12
21	1/6	1/6	2/3
22	1/12	1/12	5/6

For $t = 5$, the triangle has been partitioned into $t^2 = 25$ equilateral triangles. For each twenty-five smaller interior triangle, their centroid points are included in the design points. Hence, we have obtained twenty-five additional points inside the simplex design space and the total number of the design points are thity-one. The design is shown in Figure 4.6 and the design points are displayed in Table 4.6.

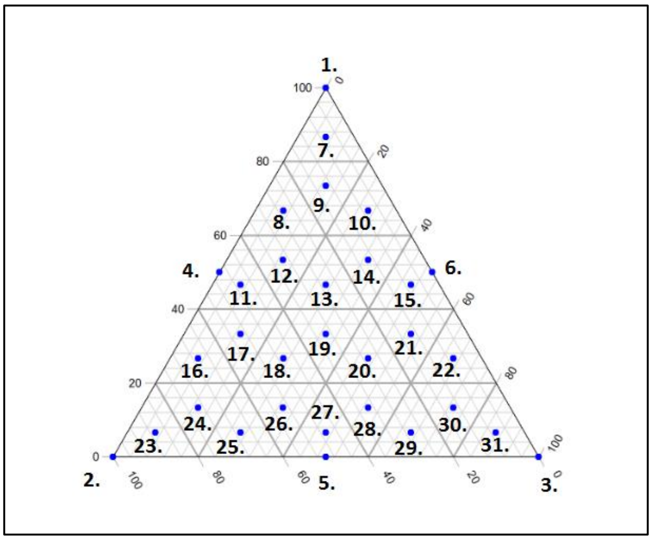

Figure 4.6: Three-component 31-point design, an augmented simplex-lattice design

Table 4.6: Co-ordinates of the candidate points of three-component 31-point augmented simplex-lattice design

Points	x_1	x_2	x_3
1	1	0	0
2	0	1	0
3	0	0	1
4	1/2	1/2	0
5	0	1/2	1/2
6	1/2	0	1/2
7	13/15	1/15	1/15
8	2/3	4/15	1/15
9	11/15	2/15	2/15
10	2/3	1/15	4/15
11	7/15	7/15	1/15
12	8/15	1/3	2/15
13	7/15	4/15	4/15
14	8/15	2/15	1/3
15	7/15	1/15	7/15
16	4/15	2/3	1/15
17	1/3	8/15	2/15
18	4/15	7/15	4/15
19	1/3	1/3	1/3
20	4/15	4/15	7/15
21	1/3	2/15	8/15
22	4/15	1/15	2/3
23	1/15	13/15	1/15
24	2/15	11/15	2/15

25	1/15	2/3	4/15
26	2/15	8/15	1/3
27	1/15	7/15	7/15
28	2/15	1/3	8/15
29	1/15	4/15	2/3
30	2/15	2/15	11/15
31	1/15	1/15	13/15

4.1.2 Augmented Simplex-Lattice Designs for Scheffé Cubic Model

Let us consider a standard simplex-lattice design for {3, 3} system given in Figure 4.7.

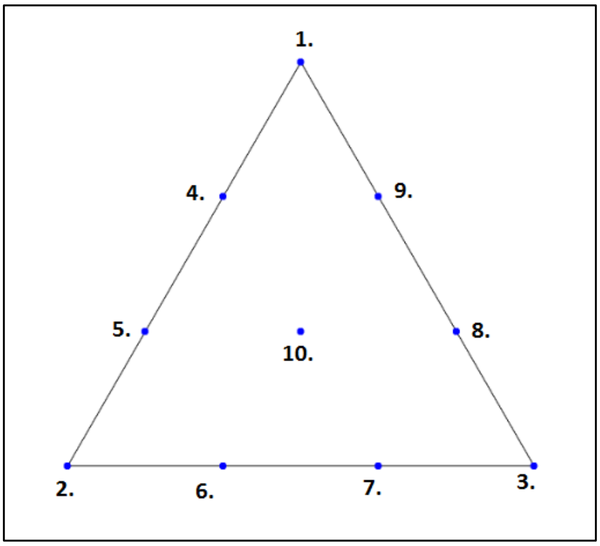

Figure 4.7: Three-component 10-point design, a simplex-lattice design with 3 components

Corresponding design points are shown in Table 4.7.

Table 4.7: Co-ordinates of the candidate points of three-component 10-point simplex-lattice design

Points	x_1	x_2	x_3
1	1	0	0
2	0	1	0
3	0	0	1
4	2/3	1/3	0
5	1/3	2/3	0
6	0	2/3	1/3
7	0	1/3	2/3
8	1/3	0	2/3
9	2/3	0	1/3
10	1/3	1/3	1/3

Now we consider $t = 1$, then the triangle has been partitioned into $t^2 = 1$ equilateral triangle, i.e., the triangle itself. Here, the centroid point of the triangle, which we supposed to be included as a candidate point to the design, is already been there. Hence, the design is same as of non-augmented one.

For considering $t = 2$, the triangle has been partitioned into $t^2 = 4$ equilateral triangles. From each of the four smaller interior triangle, four centroid points are considered for inclusion. Here, it is seen that centroid of one smaller triangle is same as the centroid of the triangle itself. Hence, we have obtained three more additional points inside the simplex design space. The design is showed in Figure 4.8.

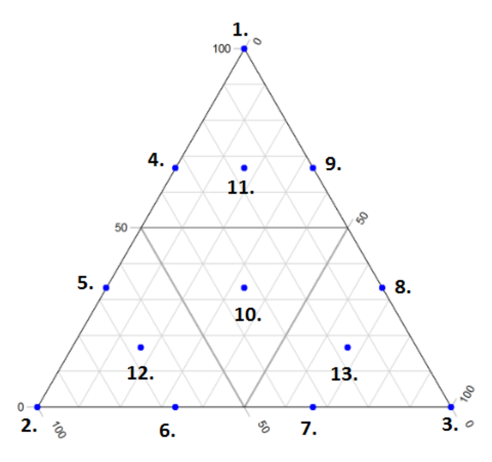

Figure 4.8: Three-component 13-point design, a simplex-lattice design with 3 components

The design points are displayed in Table 4.8.

Table 4.8: Co-ordinates of the candidate points of three-component 13-point simplex-lattice design

Points	x_1	x_2	x_3
1	1	0	0
2	0	1	0
3	0	0	1
4	2/3	1/3	0
5	1/3	2/3	0
6	0	2/3	1/3
7	0	1/3	2/3
8	1/3	0	2/3
9	2/3	0	1/3
10	1/3	1/3	1/3
11	2/3	1/6	1/6
12	1/6	2/3	1/6
13	1/6	1/6	2/3

While considering t = 3, the triangle has been partitioned into t^2 = 9 equilateral triangles. For each nine smaller interior triangle, their centroid points are included in the design points. Hence, we have obtained nine additional points inside the simplex design space and the total number of the design points are nineteen. The design points are shown in Figure 4.9 and in Table 4.9.

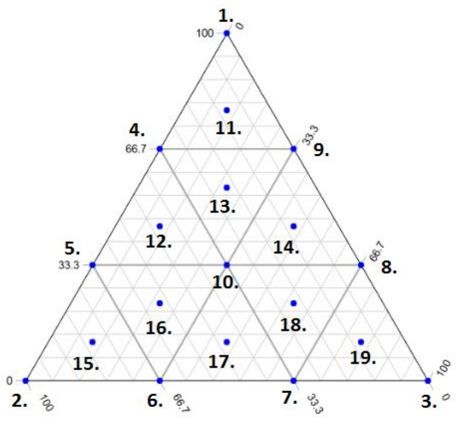

Figure 4.9: Three-component 19-point design, a simplex-lattice design with 3 components

The R code for visualization of augmented design points in the simplex region for {3, 3} simplex-lattice design for $t = 3$ is given in the end of this chapter.

Table 4.9: Co-ordinates of the candidate points of three-component 19-point simplex-lattice design

Points	x_1	x_2	x_3
1	1	0	0
2	0	1	0
3	0	0	1
4	2/3	1/3	0
5	1/3	2/3	0
6	0	2/3	1/3
7	0	1/3	2/3
8	1/3	0	2/3
9	2/3	0	1/3
10	1/3	1/3	1/3
11	7/9	1/9	1/9
12	4/9	4/9	1/9
13	5/9	2/9	2/9
14	4/9	1/9	4/9
15	1/9	7/9	1/9
16	2/9	5/9	2/9
17	1/9	4/9	4/9
18	2/9	2/9	5/9
19	1/9	1/9	7/9

For $t = 4$, the triangle has been partitioned into $t^2 = 16$ equilateral triangles. From each of the sixteen smaller interior triangle, sixteen centroid points are considered for inclusion. But, it is seen that centroid of one smaller triangle is same as the centroid of the triangle itself. Hence, we have obtained fifteen more additional points inside the simplex design space and the total number of design points are twenty-five. The design is shown in Figure 4.10 and the design points are displayed in Table 4.10.

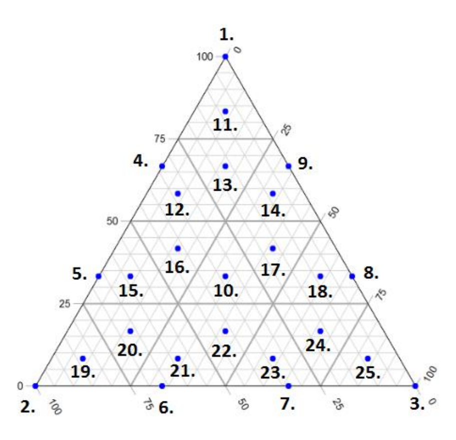

Figure 4.10: Three-component 25-point design, a simplex-lattice design with 3 components

Table 4.10: Co-ordinates of the candidate points of three-component 25-point simplex-lattice design

Points	x_1	x_2	x_3
1	1	0	0
2	0	1	0
3	0	0	1
4	2/3	1/3	0
5	1/3	2/3	0
6	0	2/3	1/3
7	0	1/3	2/3
8	1/3	0	2/3
9	2/3	0	1/3
10	1/3	1/3	1/3
11	5/6	1/12	1/12
12	7/12	1/3	1/12
13	2/3	1/6	1/6
14	7/12	1/12	1/3
15	1/3	7/12	1/12
16	5/12	5/12	1/6
17	5/12	1/6	5/12
18	1/3	1/12	7/12
19	1/12	5/6	1/12
20	1/6	2/3	1/6
21	1/12	7/12	1/3
22	1/6	5/12	5/12
23	1/12	1/3	7/12
24	1/6	1/6	2/3
25	1/12	1/12	5/6

For $t = 5$, the triangle has been partitioned into $t^2 = 25$ equilateral triangles. From each of the twenty-five smaller interior triangle, twenty-five centroid points are considered for inclusion. But again, it is seen that centroid of one smaller triangle is same as the centroid of the triangle itself. Hence, we have obtained twenty-four more additional points inside the simplex design space and the total number of design points are thirty-four. The design is shown in Figure 4.11 and the design points are displayed in Table 4.11.

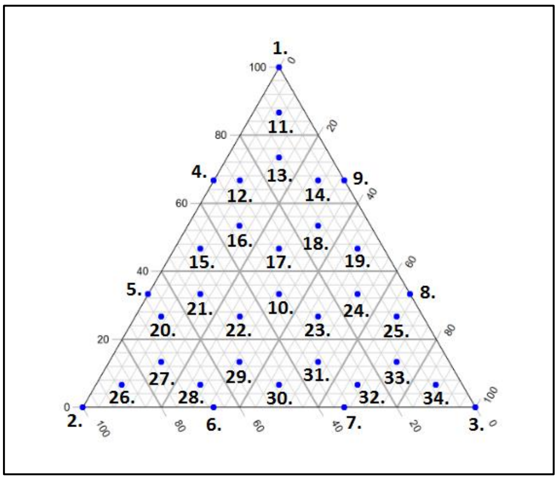

Figure 4.11: Three-component 34-point design, an augmented simplex-lattice design

Table 4.11: Co-ordinates of the candidate points of three-component 34-point augmented simplex-lattice design

Points	x_1	x_2	x_3
1	1	0	0
2	0	1	0
3	0	0	1
4	2/3	1/3	0
5	1/3	2/3	0
6	0	2/3	1/3
7	0	1/3	2/3
8	1/3	0	2/3
9	2/3	0	1/3
10	1/3	1/3	1/3
11	13/15	1/15	1/15
12	2/3	4/15	1/15
13	11/15	2/15	2/15
14	2/3	1/15	4/15
15	7/15	7/15	1/15
16	8/15	1/3	2/15

17	7/15	4/15	4/15
18	8/15	2/15	1/3
19	7/15	1/15	7/15
20	4/15	2/3	1/15
21	1/3	8/15	2/15
22	4/15	7/15	4/15
23	4/15	4/15	7/15
24	1/3	2/15	8/15
25	4/15	1/15	2/3
26	1/15	13/15	1/15
27	2/15	11/15	2/15
28	1/15	2/3	4/15
29	2/15	8/15	1/3
30	1/15	7/15	7/15
31	2/15	1/3	8/15
32	1/15	4/15	2/3
33	2/15	2/15	11/15
34	1/15	1/15	13/15

4.2 Augmented Simplex-Centroid Designs

A standard simplex-centroid design for three components system is shown in Figure 4.12.

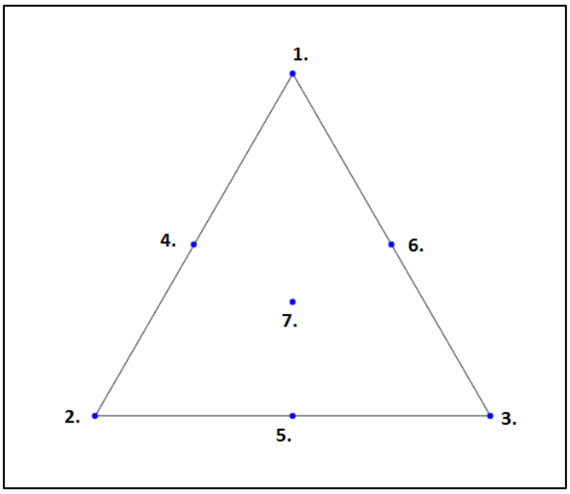

Figure 4.12: Three-component 7-point standard simplex-centroid design.

The design points of this design are given in Table 4.12.

Table 4.12: Co-ordinates of the candidate points of three-component 7-point standard simplex-centroid design

Points	x_1	x_2	x_3
1	1	0	0
2	0	1	0
3	0	0	1
4	1/2	1/2	0
5	0	1/2	1/2
6	1/2	0	1/2
7	1/3	1/3	1/3

For t = 1, the triangle has been partitioned into t^2 = 1 equilateral triangle, i.e., the triangle itself. As simplex-centroid design always include the overall centroid, the centroid point of the triangle, which we supposed to be included as a candidate point to the design, is already been there. Hence, augmentation does not produce any new design points and the design is same as of the non-augmented one.

For considering t = 2, the triangle has been partitioned into t^2 = 4 equilateral triangles. From each of the four smaller interior triangle, four centroid points are considered for inclusion. Here, it is seen that centroid of one smaller triangle is same as the centroid of the triangle itself, which is already there in simplex-centroid design. Hence, we have obtained three more additional points inside the simplex design space. Figure 4.13 gives the layout of the design.

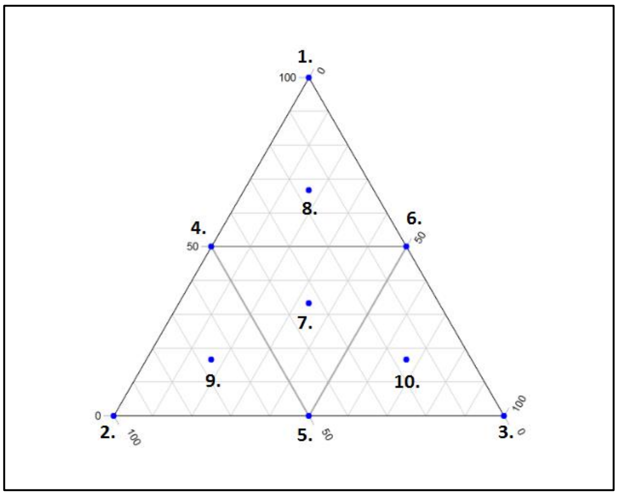

Figure 4.13: Three-component 10-point design, a simplex-centroid design with 3 components

Table 4.13: Co-ordinates of the candidate points of three-component 10-point simplex-centroid design

POINTS	x_1	x_2	x_3
1	1	0	0
2	0	1	0
3	0	0	1
4	1/2	1/2	0
5	0	1/2	1/2
6	1/2	0	1/2
7	1/3	1/3	1/3
8	2/3	1/6	1/6
9	1/6	2/3	1/6
10	1/6	1/6	2/3

It is seen that this design is same as a {3, 2} simplex-lattice design augmented with four points.

While considering $t = 3$, the triangle has been partitioned into $t^2 = 9$ equilateral triangles. For each nine smaller interior triangle, their centroid points are included in the design points. These centroid points are totally different from the overall centroid point. Hence, we have obtained nine additional points inside the simplex design space and the total number of the design points are sixteen. The design is shown in Figure 4.14 and the design points are displayed in Table 4.14.

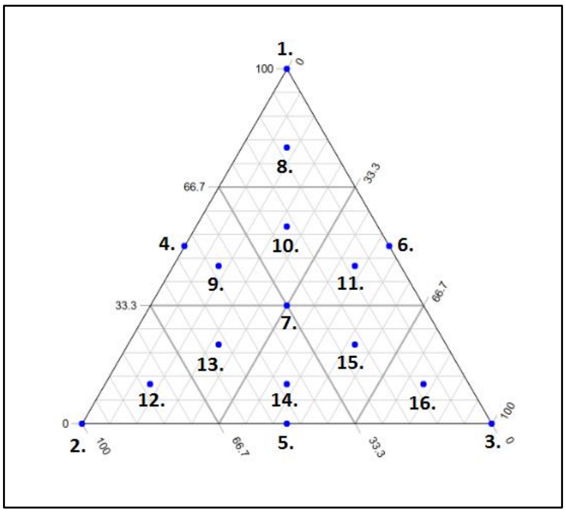

Figure 4.14: Three-component 16-point design, a simplex-centroid design with 3 components

Table 4.14: Co-ordinates of the candidate points of three-component 16-point simplex-centroid design

Points	x_1	x_2	x_3
1	1	0	0
2	0	1	0
3	0	0	1
4	1/2	1/2	0
5	0	1/2	1/2
6	1/2	0	1/2
7	1/3	1/3	1/3
8	7/9	1/9	1/9
9	4/9	4/9	1/9
10	5/9	2/9	2/9
11	4/9	1/9	4/9
12	1/9	7/9	1/9
13	2/9	5/9	2/9
14	1/9	4/9	4/9
15	2/9	2/9	5/9
16	1/9	1/9	7/9

For t = 4, the triangle has been partitioned into t^2 = 16 equilateral triangles. From each of the sixteen smaller interior triangle, sixteen centroid points are considered for inclusion. But, it is seen that centroid of one smaller triangle is same as the centroid of the triangle itself, which is already there in simplex-centroid design. Hence, we have obtained fifteen more additional points inside the simplex design space and the total number of design points are twenty-two. The design is shown in Figure 4.15.

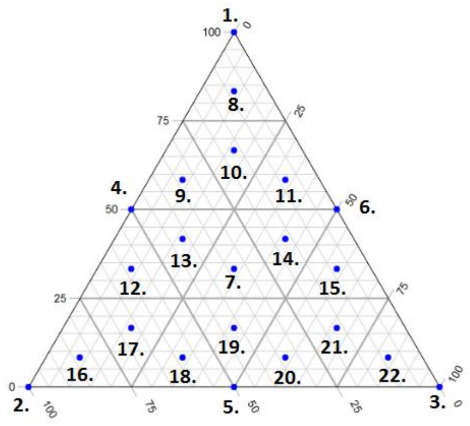

Figure 4.15: Three-component 22-point design, a simplex-centroid design with 3 components

The R code for visualization of augmented design points in the simplex region for simplex-centroid design for $t = 4$ is given in the end of this chapter. The design points are displayed in Table 4.15.

Table 4.15: Co-ordinates of the candidate points of three-component 22-point simplex-centroid design

Points	x_1	x_2	x_3
1	1	0	0
2	0	1	0
3	0	0	1
4	1/2	1/2	0
5	0	1/2	1/2
6	1/2	0	1/2
7	1/3	1/3	1/3
8	5/6	1/12	1/12
9	7/12	1/3	1/12
10	2/3	1/6	1/6
11	7/12	1/12	1/3
12	1/3	7/12	1/12
13	5/12	5/12	1/6
14	5/12	1/6	5/12
15	1/3	1/12	7/12
16	1/12	5/6	1/12
17	1/6	2/3	1/6
18	1/12	7/12	1/3
19	1/6	5/12	5/12
20	1/12	1/3	7/12
21	1/6	1/6	2/3
22	1/12	1/12	5/6

It is seen that this design is same as a {3, 2} simplex-lattice design augmented with sixteen points.

For $t = 5$, the triangle has been partitioned into $t^2 = 25$ equilateral triangles. From each of the twenty-five smaller interior triangle, twenty-five centroid points are considered for inclusion. But again, it is seen that centroid of one smaller triangle is same as the centroid of the triangle itself, which is already there in simplex-centroid design. Hence, we have obtained twenty-four more additional points inside the simplex design space and the total number of design points are thirty-one. The design is shown in Figure 4.16 and the design points are displayed in Table 4.16.

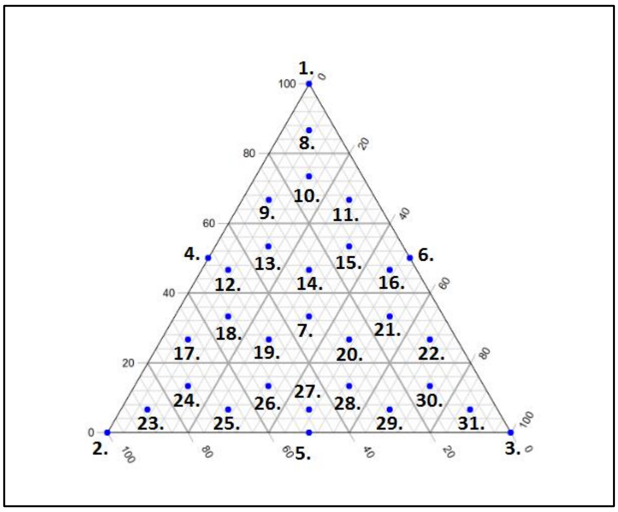

Figure 4.16: Three-component 31-point design, an augmented simplex-centroid design

The R code for visualization of augmented design points in the simplex region for simplex-centroid design for *t* = 5 is given in the end of this chapter.

Table 4.16: Co-ordinates of the candidate points of three-component 31-point augmented simplex-centroid design

Points	x_1	x_2	x_3
1	1	0	0
2	0	1	0
3	0	0	1
4	1/2	1/2	0
5	0	1/2	1/2
6	1/2	0	1/2
7	1/3	1/3	1/3
8	13/15	1/15	1/15
9	2/3	4/15	1/15
10	11/15	2/15	2/15
11	2/3	1/15	4/15
12	7/15	7/15	1/15
13	8/15	1/3	2/15
14	7/15	4/15	4/15
15	8/15	2/15	1/3
16	7/15	1/15	7/15
17	4/15	2/3	1/15

18	1/3	8/15	2/15
19	4/15	7/15	4/15
20	4/15	4/15	7/15
21	1/3	2/15	8/15
22	4/15	1/15	2/3
23	1/15	13/15	1/15
24	2/15	11/15	2/15
25	1/15	2/3	4/15
26	2/15	8/15	1/3
27	1/15	7/15	7/15
28	2/15	1/3	8/15
29	1/15	4/15	2/3
30	2/15	2/15	11/15
31	1/15	1/15	13/15

Again, it is seen that this design is same as a {3, 2} simplex-lattice design augmented with twenty-five points.

4.3 D-efficiency and G-efficiency of the Designs

D-efficiency per point and G-efficiency per point of the augmented mixture designs have been calculated for each of the augmented as well as non-augmented designs. They are represented in tabular form below. The R codes for computing D-efficiency and G-efficiency of augmented mixture designs are given in end of this chapter.

Table 4.17: D-efficiency per point and G-efficiency per point of augmented simplex-lattice designs for Scheffé quadratic model

	Total design points (n)	$|\boldsymbol{X}'\boldsymbol{X}|^{1/p}$	D-efficiency per point (%)	G-efficiency per point(%)
Non-augmented	6 + 0 = 6	0.250	4.167	100
$t = 1$	6 + 1 = 7	0.271	3.869	86.360
$t = 2$	6 + 4 = 10	0.315	3.148	64.509
$t = 3$	6 + 9 = 15	0.406	2.707	48.655
$t = 4$	6 + 16 = 22	0.529	2.404	38.606
$t = 5$	6 + 25 = 31	0.681	2.198	32.322

Table 4.18: D-efficiency per point and G-efficiency per point of augmented simplex-lattice designs for Scheffé cubic model

	Total design points (n)	$\lvert \boldsymbol{X}'\boldsymbol{X}\rvert^{1/p}$	D-efficiency per point(%)	G-efficiency per point(%)
Non-augmented	10 + 0 = 10	0.151	1.511	70
t = 1	10 + 0 = 10	0.151	1.511	70
t = 2	10 + 3 = 13	0.172	1.320	62.580
t = 3	10 + 9 = 19	0.216	1.139	47.503
t = 4	10 + 15 = 25	0.258	1.030	40.905
t = 5	10 + 24 = 34	0.322	0.947	34.488

Table 4.19: D-efficiency per point and G-efficiency per point of augmented simplex-centroid designs for Scheffé quadratic model

	Total design points (n)	$\lvert \boldsymbol{X}'\boldsymbol{X}\rvert^{1/p}$	D-efficiency per point(%)	G-efficiency per point(%)
Non-augmented	7 + 0 = 7	0.271	3.869	86.360
t = 1	7 + 0 = 7	0.271	3.869	86.360
t = 2	7 + 3 = 10	0.315	3.148	64.509
t = 3	7 + 9 = 16	0.416	2.600	45.897
t = 4	7 + 15 = 22	0.529	2.404	38.606
t = 5	7 + 24 = 31	0.681	2.198	32.322

Table 4.20: D-efficiency per point and G-efficiency per point of augmented simplex-centroid designs for Scheffé cubic model

	Total design points (n)	$\lvert \boldsymbol{X}'\boldsymbol{X} \rvert^{1/p}$	D-efficiency per point(%)	G-efficiency per point(%)
Non-augmented	7 + 0 = 7	0.119	1.697	100
$t = 1$	7 + 0 = 7	0.119	1.697	100
$t = 2$	7 + 3 = 10	0.138	1.378	74.910
$t = 3$	7 + 9 = 16	0.181	1.130	52.823
$t = 4$	7 + 15 = 22	0.223	1.013	44.181
$t = 5$	7 + 24 = 31	0.288	0.928	36.404

Batra *et al.* (1996b) provided 5 mixture designs out of which, one is standard simplex-lattice design with 6 points, one is standard simplex-centroid design with 7 points and rest of the three designs are custom made. Out of these three custom made designs, two are with 7 points and one is with 10 points. Design points of these designs are given below.

Ref. No. 69(38): Standard simplex-lattice design

Ref. No. 57(6), 57(69): Standard simplex-centroid design

Ref. No. 66(196), 67(182), 65(191):

Points	x_1	x_2	x_3
1	1	0	0
2	1/2	1/2	0
3	1/2	1/4	1/4
4	1/2	1/3	1/6
5	1/2	1/6	1/3
6	1/3	1/3	1/3
7	1/3	1/2	1/6

Ref. No. 71(28):

Points	x_1	x_2	x_3
1	1	0	0
2	3/4	1/4	0
3	3/4	0	1/4
4	1/2	1/2	0
5	1/2	0	1/2
6	1/2	1/4	1/4
7	1/4	1/2	1/4

Ref. No. 69(7):

Points	x_1	x_2	x_3
1	1	0	0
2	3/4	1/4	0
3	3/4	0	1/4
4	1/2	1/2	0
5	1/2	0	1/2
6	1/2	1/4	1/4
7	1/4	3/4	0
8	0	1	0
9	0	3/4	1/4
10	0	1/2	1/2

Table 4.21 gives the D-efficiency per point and G-efficiency per point of the designs of Batra *et al*. (1999b). A comparison of the proposed augmented designs in this study is made with the designs given by Batra *et al.* (1999b) in terms of D-efficiency per point and G-efficiency per point. It can be seen that for both the seven-point and ten-point designs, proposed designs are better than the designs of Batra *et al.* (1999b) in terms of D-efficiency per point. In terms of G-efficiency per point proposed seven-point design is superior to the designs of Batra *et al.* (1999b) but the proposed ten-point design is inferior.

Table 4.21: D-efficiency per point and G-efficiency per point of the designs used by Batra *et al*. (1999b) for Scheffé quadratic model

Ref. No.	Total design points (n)	$\lvert \boldsymbol{X}'\boldsymbol{X} \rvert^{1/p}$	D-efficiency per point(%)	G-efficiency per point(%)
69(38)	6	0.250	4.167	100
57(6),57(69)	7	0.271	3.869	86.360
66(196),67(182), 65(191)	7	0.028	0.393	85.744
71(28)	7	0.061	0.875	85.714
69(7)	10	0.203	2.033	72.736

In Table 4.22, we give the D-efficiency per point and G-efficiency per point of the various mixture designs based on different Yantrams proposed by Khattree (2015). It can be seen that proposed ten-point augmented design is always better than all the Yantram Designs in terms of D-efficiency per point, as well as G-efficiency per point.

Table 4.22: Comparison between Yantram Designs (Khattree, 2015) with three components and augmented 10-point simplex-lattice design

Ref. No.	Design points(n)	$\lvert \boldsymbol{X}'\boldsymbol{X} \rvert^{1/p}$	D-efficiency per point(%)	G-efficiency per point(%)
$t = 2$	10	0.315	3.148	64.509
Surya Yantram	10	0.044	0.439	61.388
Mangala Yantram	10	0.019	0.191	61.953
Budh Yantram (Y1)	10	0.015	0.153	61.705
Sukra Yantram (Y2)	10	0.007	0.070	61.113
Sani Yantram (Y3)	10	0.005	0.045	60.000
Sukra/2 (Y4)	10	0.007	0.069	61.922
2Surya + 1 (Y5)	10	0.036	0.360	60.703

Yantram designs for three-component mixture experiments are of basically eight-point designs. To do the comparison, two additional design points are obtained by taking the diagonal element of the Yantram in reverse order so that the designs become ten-point designs.

4.4 Discussions

In non-augmented standard designs, most of the design points for mixture experiments with three components are distributed on the edge of the triangular design space. More design points inside the simplex design space are helpful for better exploration of the response surface inside the simplex region. When the shape of the response surface inside the triangle is expected to be quite different from the shape of the surface near the boundaries of the triangle, augmented design can be used (Cornell, 1986). In this study, design space of a simplex-lattice and simplex-centroid design for three components are partitioned into t^2 equilateral triangles, where t is a positive integer. Centroids of these t^2 equilateral triangles are used as augmented points and they are included of the design.

For {3, 2} simplex-lattice design, while doing augmentation with centroid points of the smaller triangle, all the centroid points are included as augmented points. {3, 3} standard simplex-lattice design contains the overall centroid of the triangle in the design. It is seen that only for $t = 3$, we get all the nine centroid points as unique and they are included as augmented points in the design. For other cases one of the augmented centroid point becomes identical to the overall centroid. Hence, we get one less augmented points. For simplex-centroid design, only for $t = 3$ comes to be unique, other augmented designs are identical to the corresponding augmented {3, 2} simplex-lattice design.

The quantity $|X'X|^{1/p}$ increases by augmenting the standard designs with more number of points, which implies that more information are extracted from the design. But D-efficiency per point and G-efficiency are reduced as the number of augmenting points are increasing. This may be due to the presence of term “n” in the denominator for both the equations. Wheeler (1972) recommended that a design with G-efficiency more than or equal to 50% may be considered as “good” for practical purposes. It is seen that for augmented simplex-centroid design for Scheffé cubic model considering up to $t = 3$ can be called as “good”. And for all the other augmented designs, up to $t = 2$ can be considered as “good” form G-efficiency point of view.

D-efficiency per point of the design (Ref. No. 69(7)) used by Batra *et al*. (1999b) for Scheffé quadratic model is less than the proposed augmented ten-point design. But G-efficiency per point is more than the proposed augmented ten-point design. Other seven-point designs used by Batra *et al*. (1999b) (Ref. No. 66(196), 67(182), 65(191) and 71(28)) are always inferior to the proposed seven-point design.

In comparison with Yantram Designs (Khattree, 2015), it is seen that proposed ten-point augmented design is better both from the D-efficiency per point and G-efficiency per point of view.

Efforts need to be made to develop methods to augment mixture designs with $q > 3$. For example, mixture designs with $q = 4$ is a tetrahedron. Since it is not known how to equally partition a tetrahedron into equal volume areas, augmenting such designs using the proposed approach is not possible.

R codes for visualization of design points

R code visualization of augmented design points in the simplex region for {3, 2} simplex-lattice design when *t* = 2

```
library(Ternary)
TernaryPlot(grid.lines=2, grid.lwd = 2 )
 p1=c(1,0,0)
 p2=c(0,1,0)
 p3=c(0,0,1)
 p4=c(0.5,0.5,0)
 p5=c(0,0.5,0.5)
 p6=c(0.5,0,0.5)
 p7=c(0.6667,0.1667,0.1667)
 p8=c(0.1667,0.6667,0.1667)
 p9=c(0.3333,0.3333,0.3333)
 p10=c(0.1667,0.1667,0.6667)
TernaryPoints(p1,col = 'blue', pch = 19)
TernaryPoints(p2,col = 'blue', pch = 19)
TernaryPoints(p3,col = 'blue', pch = 19)
TernaryPoints(p4,col = 'blue', pch = 19)
TernaryPoints(p5,col = 'blue', pch = 19)
TernaryPoints(p6,col = 'blue', pch = 19)
TernaryPoints(p7,col = 'blue', pch = 19)
TernaryPoints(p8,col = 'blue', pch = 19)
```

```
TernaryPoints(p9,col = 'blue', pch = 19)
TernaryPoints(p10,col = 'blue', pch = 19)
```

R code visualization of augmented design points in the simplex region for {3, 3} simplex-lattice design when *t* = 3

```
library(Ternary)
TernaryPlot(grid.lines=3, grid.lwd = 2 )
 p1=c(1,0,0)
 p2=c(0,1,0)
 p3=c(0,0,1)
 p4=c(0.6667,0.3333,0)
 p5=c(0.3333,0.6667,0)
 p6=c(0,0.6667,0.3333)
p7=c(0,0.3333,0.6667)
 p8=c(0.3333,0,0.6667)
 p9=c(0.6666,0,0.3333)
 p10=c(0.3333,0.3333,0.3333)
p11=c(0.7778,0.1111,0.1111)
 p12=c(0.4444,0.4444,0.1111)
 p13=c(0.5556,0.2222,0.2222)
 p14=c(0.4444,0.1111,0.4444)
 p15=c(0.1111,0.7778,0.1111)
 p16=c(0.2222,0.5556,0.2222)
 p17=c(0.1111,0.4444,0.4444)
```

```
 p18=c(0.2222,0.2222,0.5556)
 p19=c(0.1111,0.1111,0.7778)
TernaryPoints(p1,col = 'blue', pch = 19)
TernaryPoints(p2,col = 'blue', pch = 19)
TernaryPoints(p3,col = 'blue', pch = 19)
TernaryPoints(p4,col = 'blue', pch = 19)
TernaryPoints(p5,col = 'blue', pch = 19)
TernaryPoints(p6,col = 'blue', pch = 19)
TernaryPoints(p7,col = 'blue', pch = 19)
TernaryPoints(p8,col = 'blue', pch = 19)
TernaryPoints(p9,col = 'blue', pch = 19)
TernaryPoints(p10,col = 'blue', pch = 19)
TernaryPoints(p11,col = 'blue', pch = 19)
TernaryPoints(p12,col = 'blue', pch = 19)
TernaryPoints(p13,col = 'blue', pch = 19)
TernaryPoints(p14,col = 'blue', pch = 19)
TernaryPoints(p15,col = 'blue', pch = 19)
TernaryPoints(p16,col = 'blue', pch = 19)
TernaryPoints(p17,col = 'blue', pch = 19)
TernaryPoints(p18,col = 'blue', pch = 19)
TernaryPoints(p19,col = 'blue', pch = 19)
```

R code visualization of augmented design points in the simplex region for simplex-centroid design when *t* = 4

```
library(Ternary)

TernaryPlot(grid.lines=4, grid.lwd = 2 )

 p1=c(1,0,0)

 p2=c(0,1,0)

 p3=c(0,0,1)

 p4=c(0.5,0.5,0)

 p5=c(0,0.5,0.5)

 p6=c(0.5,0,0.5)

p7=c(0.3333,0.3333,0.3333)

p8=c(0.8333,0.0833,0.0833)

 p9=c(0.5833,.03333,0.0833)

 p10=c(0.6667,0.1667,0.1667)

 p11=c(0.5833,0.0833,0.3333)

 p12=c(0.3333,0.5833,0.0833)

 p13=c(0.4167,0.4167,0.1667)

p14=c(0.4167,0.1667,0.4167)

 p15=c(0.3333,0.0833,0.5833)

 p16=c(0.0833,0.8333,0.0833)

 p17=c(0.1667,0.6667,0.1667)

 p18=c(0.0833,0.5833,0.3333)

 p19=c(0.1667,0.4167,0.4167)
```

```
 p20=c(0.0833,0.3333,0.5833)
 p21=c(0.1667,0.1667,0.6667)
 p22=c(0.0833,0.0833,0.8333)
TernaryPoints(p1,col = 'blue', pch = 19)
TernaryPoints(p2,col = 'blue', pch = 19)
TernaryPoints(p3,col = 'blue', pch = 19)
TernaryPoints(p4,col = 'blue', pch = 19)
TernaryPoints(p5,col = 'blue', pch = 19)
TernaryPoints(p6,col = 'blue', pch = 19)
TernaryPoints(p7,col = 'blue', pch = 19)
TernaryPoints(p8,col = 'blue', pch = 19)
TernaryPoints(p9,col = 'blue', pch = 19)
TernaryPoints(p10,col = 'blue', pch = 19)
TernaryPoints(p11,col = 'blue', pch = 19)
TernaryPoints(p12,col = 'blue', pch = 19)
TernaryPoints(p13,col = 'blue', pch = 19)
TernaryPoints(p14,col = 'blue', pch = 19)
TernaryPoints(p15,col = 'blue', pch = 19)
TernaryPoints(p16,col = 'blue', pch = 19)
TernaryPoints(p17,col = 'blue', pch = 19)
TernaryPoints(p18,col = 'blue', pch = 19)
TernaryPoints(p19,col = 'blue', pch = 19)
TernaryPoints(p20,col = 'blue', pch = 19)
```

```
TernaryPoints(p21,col = 'blue', pch = 19)
TernaryPoints(p22,col = 'blue', pch = 19)
```

R code visualization of augmented design points in the simplex region for simplex-centroid design when *t* = 5

```
library(Ternary)
TernaryPlot(grid.lines=5, grid.lwd = 2 )
 p1=c(1,0,0)
 p2=c(0,1,0)
 p3=c(0,0,1)
 p4=c(0.5,0.5,0)
 p5=c(0,0.5,0.5)
 p6=c(0.5,0,0.5)
p7=c(0.3333,0.3333,0.3333)
p8=c(0.8667,0.0667,0.0667)
 p9=c(0.6667,0.2667,0.0667)
 p10=c(0.7333,0.1333,0.1333)
 p11=c(0.6667,0.0667,0.2667)
 p12=c(0.4667,0.4667,0.0667)
 p13=c(0.5333,0.3333,0.1333)
 p14=c(0.4667,0.2667,0.2667)
 p15=c(0.5333,0.1333,0.3333)
 p16=c(0.4667,0.0667,0.4667)
 p17=c(0.2667,0.6667,0.0667)
```

```
 p18=c(0.3333,0.5333,0.1333)

 p19=c(0.2667,0.4667,0.2667)

 p20=c(0.2667,0.2667,0.4667)

 p21=c(0.3333,0.1333,0.5333)

 p22=c(0.2667,0.0667,0.6667)

 p23=c(0.0667,0.8667,0.0667)

 p24=c(0.1333,0.7333,0.1333)

 p25=c(0.0667,0.6667,0.2667)

 p26=c(0.1333,0.5333,0.3333)

 p27=c(0.0667,0.4667,0.4667)

 p28=c(0.1333,0.3333,0.5333)

 p29=c(0.0667,0.2667,0.6667)

 p30=c(0.1333,0.1333,0.7333)

 p31=c(0.0667,0.0667,0.8667)

TernaryPoints(p1,col = 'blue', pch = 19)

TernaryPoints(p2,col = 'blue', pch = 19)

TernaryPoints(p3,col = 'blue', pch = 19)

TernaryPoints(p4,col = 'blue', pch = 19)

TernaryPoints(p5,col = 'blue', pch = 19)

TernaryPoints(p6,col = 'blue', pch = 19)

TernaryPoints(p7,col = 'blue', pch = 19)

TernaryPoints(p8,col = 'blue', pch = 19)

TernaryPoints(p9,col = 'blue', pch = 19)
```

```
TernaryPoints(p10,col = 'blue', pch = 19)
TernaryPoints(p11,col = 'blue', pch = 19)
TernaryPoints(p12,col = 'blue', pch = 19)
TernaryPoints(p13,col = 'blue', pch = 19)
TernaryPoints(p14,col = 'blue', pch = 19)
TernaryPoints(p15,col = 'blue', pch = 19)
TernaryPoints(p16,col = 'blue', pch = 19)
TernaryPoints(p17,col = 'blue', pch = 19)
TernaryPoints(p18,col = 'blue', pch = 19)
TernaryPoints(p19,col = 'blue', pch = 19)
TernaryPoints(p20,col = 'blue', pch = 19)
TernaryPoints(p21,col = 'blue', pch = 19)
TernaryPoints(p22,col = 'blue', pch = 19)
TernaryPoints(p23,col = 'blue', pch = 19)
TernaryPoints(p24,col = 'blue', pch = 19)
TernaryPoints(p25,col = 'blue', pch = 19)
TernaryPoints(p26,col = 'blue', pch = 19)
TernaryPoints(p27,col = 'blue', pch = 19)
TernaryPoints(p28,col = 'blue', pch = 19)
TernaryPoints(p29,col = 'blue', pch = 19)
TernaryPoints(p30,col = 'blue', pch = 19)
TernaryPoints(p31,col = 'blue', pch = 19)
```

R code for computing D-efficiency

```
m=read.csv(file.choose(),header=T)
m
m1=as.matrix(m)
m1
z1=crossprod(m1,y=NULL)
z1
a=det(z1)
a
p=6
b=(a)^(1/p)
b
n=6

D=(b/n)*100

D
```

R code for computing G-efficiency

```
m=read.csv(file.choose(),header=T)
m
m1=as.matrix(m)
m1
z1=crossprod(m1,y=NULL)
z1
a=inv(z1)
a
b=t(m1)
b
h=m1%*%a%*%b
h
d=max(diag(h))
d
p=6
n=10
G=(p/(n*d))*100
G
```

SUMMARY AND CONCLUSIONS

In mixture experiments, the response is considered to be a function of the relative proportions of the ingredients constituting the mixture and it does not depend on the total amount of the mixture. Sum of these proportions is always unity. There are two important classes of mixture designs namely simplex-lattice designs introduced by Scheffé (1958, 1963) and simplex-centroid designs introduced by Scheffé (1963). For a three-component mixture experiment, the simplex design space is represented by an equilateral triangle. In both the designs, most of the design points are distributed on the perimeter of the equilateral triangle. When the response surface over the interior portion of the triangle is quite different than the perimeter, the standard design points are not capable of extracting much information from the design. Again, when only these standard points are considered in an experiment, there would be no degrees of freedom left out for the error and the significance of the parameters cannot be tested. Augmentation of the simplex space can be done to solve these problems (Cornell, 1986).

So the purpose of this thesis is to develop suitable methods for augmentation of standard simplex-lattice designs and simplex-centroid designs. The design evaluation criteria such that D-efficiency per point and G-efficiency per point of these augmented designs are studied. The summary of various chapters are given in sequel.

Chapter 1 gives introduction to mixture experiments along with an example of mixture experimental situation in agricultural research. A brief description of canonical polynomials used in mixture experiment is given. Detailed description of simplex-lattice designs, simplex-centroid designs, and motivation to undertake this topic as a research work are also provided.

Chapter 2 gives a brief review of the work done in the area of mixture experiment, simplex-lattice designs and simplex-centroid designs, Scheffé’s polynomial, restricted mixture designs, mixture experiments with process variable etc.

Chapter 3 includes material and methods for obtaining augmented simplex-lattice and simplex-centroid designs i.e. how the simplex region equilateral triangle is divided into smaller equilateral triangles and the centroids of these smaller equilateral triangles are included in the designs as augmented points. The concept of canonical polynomials and their derivations are discussed in this chapter. Design evaluation criteria D-efficiency per point and G-efficiency per point are also discussed in brief along with their calculation procedures.

Chapter 4 comprises of the results and discussions of this study. Augmented {3, 2} simplex-lattice designs, augmented {3, 3} simplex-lattice designs, and augmented simplex-centroid designs along with the co-ordinates of the augmented points are presented. D-efficiency per point and G-efficiency per point of all these augmented designs are calculated and presented in tabular form. D-efficiency per point and G-efficiency per point of these proposed augmented designs are also compared with the designs proposed by Batra *et al*. (1999b) and Yantram Designs (Khattree, 2015).

ABSTRACT

In mixture experiments, it is assumed that the response is a function of the relative proportions of the ingredients or components in the mixture and the response does not depend on the total amount of the mixture used in the experiment. Augmentation of the design points of the standard simplex-lattice and simplex-centroid designs are needed for better exploration of interior portion of the simplex space. A new method of obtaining more design points by augmenting the design points of simplex-lattice and simplex-centroid designs for mixture experiments with three components is developed in this study. For this purpose, a special property of equilateral triangles is used. From the geometry of triangle, it is known that any equilateral triangle can be partitioned into t^2 equilateral triangles, where t is a positive integer. Simplex space of standard simplex-lattice and simplex-centroid designs are divided into smaller equilateral triangles by this method. The centroid of these smaller equilateral triangles are included in the designs as augmented points. Design evaluation criteria namely D-efficiency per point and G-efficiency per point of these augmented designs are also studied to evaluate the efficiency of the obtained designs. These efficiencies are compared with previously used designs in agricultural experimentation with same number of design points.

सार

मिश्रण परीक्षणों में प्रतिक्रिया मिश्रण में सामग्रियों के सापेक्ष अनुपात का एक कार्य माना जाता है एवं ना की परीक्षण में उपयोग किया गया मिश्रण की कुल मात्रा का कार्य माना जाता है । सिम्पलेक्स विस्तार का आंतरिक भाग की बेहतर खोजके लिए सिम्पलेक्स सेंट्रोइड एवं सिम्पलेक्स लेटिस अभिकल्पनाओं के बिंदुओं का संवर्ध करना आवश्यक है । तीन घटक वाले मिश्रण परीक्षण के लिए मानक सिम्पलेक्स लेटिस एवं सिम्पलेक्स सेंट्रोइड अभिकल्पनाओं काबिंदुओं का संवर्धन करके अधिक संख्या में अभिकल्पना बिंदु पाने के लिए इस अध्यन में एक नई विधि विकसित किया गया है । इस उद्देश्य के लिये समबाहु त्रिकोण का एक विशेष गुण का उपयोग किया गया है । त्रिकोण की ज्यामिति से यह ज्ञात है की किसी भी समबाहु त्रिकोण को t^2 समबाहु त्रिकोण में विभाजन किया जा सकता है जहाँ t एक सकारात्मक पूर्णांक है । इस विधि से मानक सिम्पलेक्स लेटिस एवं सिम्पलेक्स सेंट्रोइड अभिकल्पनाओं का सिम्पलेक्स विस्तार को छोटे समबाहु त्रिकोन में विभाजित किया गया । इन छोटे समबाहु त्रिकोनो का केन्द्रकोको संवर्धित अभिकल्पना बिंदुओंके रूप में अभिकल्पना में शामिल किया गया । एसे प्राप्त अभिकल्पनाओं के दक्षता का मूल्यांकन के लिए इन संवर्धित अभिकल्पनाओं का अभिकल्पना के मूल्यांकन पैमाना यथा प्रति बिंदु D-दक्षता एवं G-दक्षता का अध्ययन किया गया । इन दक्षताओ को समसंख्यक अभिकल्पना बिंदु वाले पहले प्राप्त अभिकल्पनाओं के दक्षताओ के साथ तुलना किया गया ।

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