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Construction of Optimal Designs for Mixture-of-Mixture Experiments with Inverse Terms

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Abstract-In agriculture and manufacturing allied industries there are many complex systems in which the use of polynomial models is not possible because of the presence of proportions having the value near to zero (almost all zero) with lower bound constraints. To simplify these types of complex helix system an attempt is made in which the components proportions are near to zero with lower bound constraints.

Keywords: Mixture Experiments, Mixture-of-Mixture Experiments, Optimal Designs, G-Efficiency etc.

1. INTRODUCTION

Experiment in which the response is a function of the proportions of the components present in the mixture and is not a function of the total amount of the mixture is called mixture experiment. Scheffe (1958, 1963) proposed mixture experiments by introducing simplex lattice and simplex centroid designs in which the n treatments are procured by splitting up the fixed amount of input for application in q stages and x_i denoted the proportions of i^{th} component under the following constraints

$$0 \le x_i \le 1 \quad \text{and} \quad \sum_{i=1}^{q} x_i = 1$$

Draper and John (1977) suggested the inverse terms with the Scheffe's polynomial models and also illustrated their use in fitting of the secondary data. However, Cornell (2002) portrays an extreme change in the behaviour of the components as the value of one or more components tends to a boundary of the simplex region that is $x_i \to 0$ in the Scheffe's polynomial models. He also proposed the following second degree model containing the inverse terms.

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

In addition to the mixture methodology, Verma (2017) proposed a second degree mixture-of-mixture model in which $c_i\ (i = 1,2)$ be the proportion of the i^{th} major component and this major component is composed of m_i minor components, whose proportions with respect to c_i are x_{ij}. He also constructed the designs for mixture-of-mixture experiments under the restricted regions using central composite for different number of major and minor components where upper or lower bound restrictions are imposed on one of the major components and one of the each minor component of each major component. The second degree mixture-of-mixture model as proposed by him is given as

$$Y = \sum_{i=1}^{M} \left[\sum_{j=1}^{m_i} \beta'_{ij} x_{ij} + \sum_{j<j'}^{m_i} \gamma'_{ijj'} x_{ij} x_{ij'} \right] c_i + \sum_{i=1}^{M} \sum_{j<j'}^{m_i} \left[\delta'_{ii'jj'} x_{ij} x_{i'j'} \right] c_i c_j + \varepsilon$$

Furthermore, Saini *et al.* (2018) constructed the optimal designs for mixture-of- mixture experiments using L- Pseudo and U- Pseudo components, to overcome from complexity on the component proportions in the form of both lower and upper bounds constituting the designs. In the present investigation, a slight modification is made to the mixture-of-mixture model proposed by the Verma (2017) with the inclusion of the terms that are reciprocals (i.e. inverse terms) of the component proportions.

2. METHODOLOGY

Let us assume that a system consists of M original major components and m_i respective original minor components and lower bound on these components then the L-Pseudo components proposed by Saini *et al.* (2018) are

for major components:	$c_i^* = \dfrac{c_i - L_i}{1 - L_c}$ where $L_c = \sum_{i=1}^{M} L_i$
for minor components:	$x_{ij}^* = \dfrac{x_{ij} - L_{ij}}{1 - L}$ where $L = \sum_{j=1}^{m_i} L_{ij}$

It is assumed that the value of any component never reaches zero but, it could be very close to zero, that is, $c_i \to \omega_i > 0$ and $x_{ij} \to \omega_{ij} > 0$, where ω_i and ω_{ij} are the respective arbitrary extremely small quantities that are defined for each respective application of mixture-of-mixture model, then if an extreme change in the response occurs as component proportion and it approaches the lower bound to the model under consideration, then

$$L_c' = L_i - \omega_i \text{ and } L' = L_{ij} - \omega_{ij}, \text{ where } L_i > \omega_i > 0;\ L_{ij} > \omega_{ij} > 0$$

In practice, some of the proportions of the components are zero then in order to include the inverse term in the model, it is adequate to add a small positive amount, say ω_i and ω_{ij}, to each value of major and minor component respectively. So, instead of above L-Pseudo components, the new L-Pseudo components are

for major components:	$c_i' = \dfrac{(c_i + \omega_i) - L_i'}{1 - L_c'}$ where $L_c' = \sum_{i=1}^{M} (L_i - \omega_i)$
for minor components:	$x_{ij}' = \dfrac{(x_{ij} + \omega_{ij}) - L_{ij}'}{1 - L'}$ where $L' = \sum_{j=1}^{m_i} (L_{ij} - \omega_{ij})$

For instance, consider the mixture-of-mixture system in which there are two major components each having the two-two minor components, then the respective Pseudo components with $\omega_i = \omega_{ij} = 0.002$ are given by

c_1'	c_2'	x_{11}'	x_{12}'	x_{21}'	x_{22}'
0.216	0.784	0.216	0.784	0.216	0.784
0.216	0.784	0.216	0.784	0.787	0.213
0.216	0.784	0.787	0.213	0.216	0.784
0.216	0.784	0.787	0.213	0.787	0.213
0.787	0.213	0.216	0.784	0.216	0.784
0.787	0.213	0.216	0.784	0.787	0.213
0.787	0.213	0.787	0.213	0.216	0.784
0.787	0.213	0.787	0.213	0.787	0.213
0.021	0.979	0.501	0.499	0.501	0.499
0.981	0.019	0.501	0.499	0.501	0.499
0.501	0.499	0.021	0.979	0.501	0.499
0.501	0.499	0.981	0.019	0.501	0.499
0.501	0.499	0.501	0.499	0.021	0.979
0.501	0.499	0.501	0.499	0.981	0.019
0.501	0.499	0.501	0.499	0.501	0.499

Figure 1(a) & (b) shows the response nomenclature at the point of the three original major components each having three original minor components and components after the inclusion of inverse terms respectively.

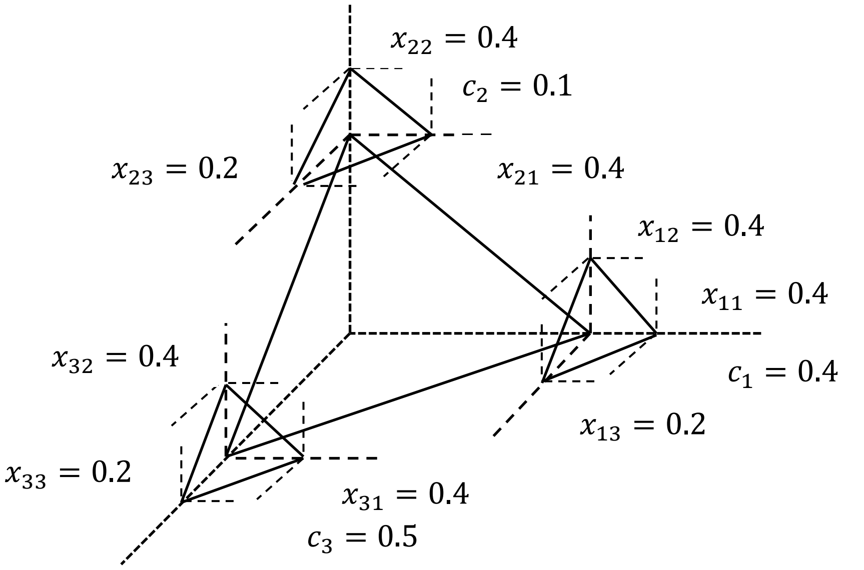

Figure 1(a): Original Components

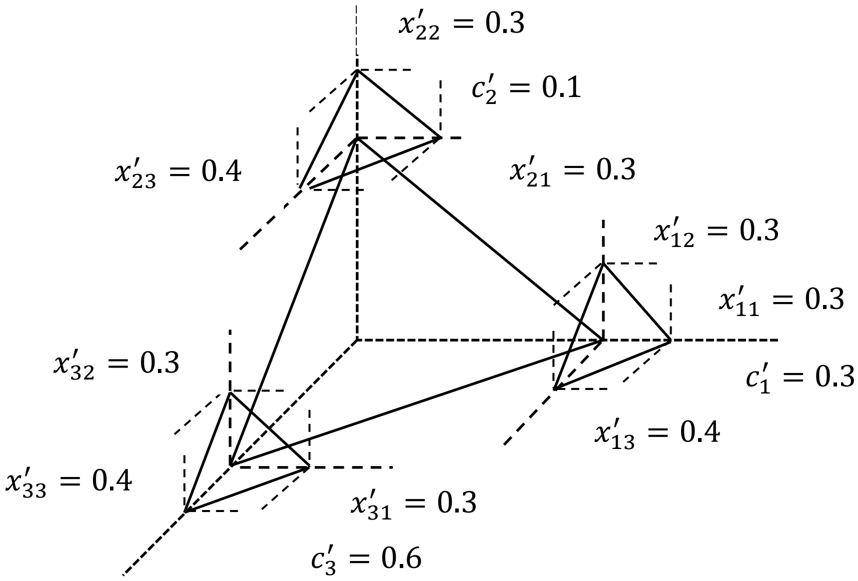

Figure 1(b): Components after inclusion of Inverse Terms

Here, G- efficiency criteria has been adopted for such type of response surface study to compare different designs having n number of design points, p number of parameters in the model and $d = max\{v = \boldsymbol{x}(\boldsymbol{x}'\boldsymbol{x})^{-1}\boldsymbol{x}'\}$ over a specified set of design points $\boldsymbol{x}$ in $\boldsymbol{X}$, where $\boldsymbol{X}$ is the extended design matrix depending on model to be fitted.

Table: G-efficiency for different number of major and minor components under various lower bound restrictions.

Major components	**Minor component for each major component**	**Lower Bound Restriction**	**G-efficiency**
2	2,2	$c'_1, c'_2, x'_{11}, x'_{12}, x'_{21}, x'_{22} \leq 0.86$	0.674
	2,3	$c'_1, x'_{11} \leq 0.2; c'_2, x'_{12}, x'_{23} \leq 0; x'_{21}, x'_{22} \leq 0.12$	0.646

	3,3	$c'_1 \leq 0.2;\ c'_2, x'_{13}, x'_{23} \leq 0; x'_{11}, x'_{12}, x'_{21}, x'_{22} \leq 0.12$	0.651
3	2,2,2	$c'_1, c'_2 \leq 0.12;\ x'_{11}, x'_{21}, x'_{31} \leq 0.2;\ c'_3, x'_{12}, x'_{22}, x'_{32} \leq 0$	0.749
	2,2,3	$c'_1, c'_2, x'_{22}, x'_{31}, x'_{32} \leq 0.12;\ x'_{11}, x'_{21} \leq 0.2; c'_3, x'_{12}, x'_{22}, x'_{33} \leq 0$	0.539
	2,3,3	$c'_1, c'_2, x'_{21}, x'_{22}, x'_{31}, x'_{32} \leq 0.12;\ x'_{11} \leq 0.2; c'_3, x'_{12}, x'_{23}, x'_{33} \leq 0$	0.389
	3,3,3	$c'_1, c'_2, x'_{11}, x'_{12}, x'_{21}, x'_{22}, \leq 0.12;\ c'_3, x'_{13}, x'_{23}, x'_{3} \leq 0$	0.272

3. CONCLUSION AND DISCUSSION

In the literature, nearly all the techniques that have been suggested for analysing data from the mixture and mixture-of-mixture experiments were developed around the fitting of the polynomials proposed by the Scheffe (1958, 1963), Draper and John (1977) Cornell (2002), Verma (2017) and others. The use of the polynomial models was possible because the data evolved from the well behaved system in which the surface are expressible with a functional form and within the range of experimental data. In practice, generally, there are other complex type of system in which the use of the polynomial models was not possible because some of the proportions of the components in the system are near to zero and also have lower bound constraints on them. In such situations, it is assumed that the value of the component never reaches zero but, the value could be very close to zero, that is, $c_i \rightarrow \omega_i > 0$ and $x_{ij} \rightarrow \omega_{ij} > 0$, where ω_i and ω_{ij} are the respective arbitrary extremely small quantities that is defined for each application of mixture-of-mixture model. In the present investigation an attempt is made to overcome from these types of complex situations in which the components proportions are near to zero by inclusion of the inverse term to the mixture-of-mixture model. The G-efficiencies for different number of major and minor components in the mixture-of-mixture model under the lower bound restrictions have also been evaluated.

REFERENCES

[1] Cornell, J.A. *Experiments with Mixtures: Designs, Models and the Analysis of Mixture Data*. 3rd Edition. John Wiley, New York, 2002.
[2] Draper, N. R. and John R. C. St. A mixture model with inverse terms. Technometrics, 19: 37-46, 1977.
[3] Saini Parul, Chetan and Laxmi Ratna Raj. Construction of Optimal Pseudo Designs for Mixture-of-Mixture Experiments, 6(7): 1772-1776, 2018.
[4] Scheffé, H. "Experiments with mixtures". Journal of the Royal Statistical Society, B20 (2): 344-360, 1958.
[5] Scheffé, H. "Simplex-centroid design for experiments with mixtures". Journal of the Royal Statistical Society, B25 (2): 235-263, 1963.
[6] Verma Chetan. "*Optimality and Analysis of Designs with Mixture Experiments"*. Author's Ink Publication, ISBN 978-93-85137-79-2, 2017.