Mixture-of-Mixture Design Using U-Pesdo Components

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ABSTRACT

A Mixture Experiment is defined as an experiment in which the outcome is a function of the proportions of its contents rather than the overall amount. In most of the experimental situations dealing with the mixture, its components are themselves consist of some other sub-components, in such situation it is important to study the individual effect of these sub-components on the response of the final product. The use of components are handled in a way in the experiments that it is important to have the restrictions on of proportions of sub-component in a predetermined way than the proportions themselves. Still there are many situations in which multiple restrictions on major and minor component proportions are imposed. For the development and improvement of product in agricultural and many more allied sectors, mixture experiments are generally used. To construct designs with the help of U-pseudo transformation for Mixture-of-Mixture experiments, upper bound restriction on each of the major and their minor components adopted on U-pseudo designs. For evaluation of the constructed designs, G-efficiencies under various upper restrictions on a number of majors and their minors components are(obtained, which are found) more than 50% which is good enough for the practical point of view.

Introduction

In agricultural experimentations several situations of dealing with mixture are embraced. Response is dependent on that how much quantity of components should be added a in blend for instance, the mileage from a gas mixture or the flavour of a fruit punch beverage. Mixture experiments are those experiments where the responses is determined by the proportions of the components in the mixture, not by the total quantity. Scheffe (1958, 1963) conducted groundbreaking work in the field of mixture experiment by developing “Simplex Lattice” and “Simplex Centroid designs” for experiments with mixture for single factor. Consider an experiment in which 'n' treatments are obtained by dividing the given dosage of fertilizer (mixture) to be applied at a number of times to a crop and x_i denotes the proportion of i^{th} component in the fixed dose (mixture), with the restrictions such as

$$\left.\begin{array}{c} 0 \le x_i \le 1, i = 1,2, \dots q \\ and \qquad \sum_{i=1}^{q} x_i = 1 \end{array}\right]$$

Lambrakis (1968a, 1968b) Multiple-Scheffé model and Multiple-Lattice design introduced the first. The Multiple-Scheffé model was then expanded by Cornell and Ramsey (1998) to the fluctuating main and minor components in the Multiple Factor model. Kang et al. (2011) presented the Major-Minor model, which addressed some of the shortcomings of the Multiple-Scheffé model. In some the experimental situations dealing with the mixture, any mixture's components are made up of a variety of sub-components (mixture), in such situation it is important to study the individual effect of these sub-components on the response of the final product. The experiment associated with such type of a situation is known as the Mixture-of-Mixture Experiment. In this paper, construction of design for Mixture-of-Mixture experiment is considered.

Let M be the number of major components of the experiment and let c_i is the proportion of the i^{th} major component then

$$\sum_{i=1}^{M} c_i = 1, \quad 0 \le c_i \le 1, \qquad i = 1,2,3, \dots\dots, M$$

Let each major component be further made up of m_i minor components, the proportions of which are x_{ij} with the restructions such as

$$\sum_{j=1}^{m_i} x_{ij} = 1, \quad 0 \le x_{ij} \le 1, \qquad \begin{array}{c} i = 1,2,3, \dots, M, \\ j = 1,2,3, \dots, m_i \end{array}$$

$$\sum_{i=1}^{M}\sum_{j=1}^{m_i} x_{ij} = 1$$

then the second order Mixture-of-Mixture model given by verma (2017) may be written as

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

Above designs were found to be very useful for the practical purposes on major and minor components. Furthermore, there are possibilities where these components are to be considered with restrictions on the upper bound of components. An attempt has been made to construct design for such type of situations, with the help of U-pseudo transformation for Mixture-of-Mixture experiments.

Methodology

Let U_i be the restriction on the percentage of the i^{th} major components, such that $c_i \leq U_i \leq 1$ and U_{ij} be the restruction on the percentage of the j^{th} minor component of the i^{th} major components with $x_{ij} \leq U_{ij} \leq 1$.

This upper bound constraints can be used to indicate the upper bound restrictions on the percentage of major and minor components.

$$c_i \leq U_i \leq 1\,, \quad U_c = \sum_{i=1}^{M} U_i > 1\,; \quad x_{ij} \leq U_{ij} \leq 1, \quad U = \sum_{i,j=1}^{M} U_{ij} > 1$$

where some of the U_i might be equal to one. Then the U-pseudo-component's proportion denoted by c_i^* for i^{th} major component the pseudo transformation will be

$$c_i^* = \frac{U_i - c_i}{U_c - 1}$$

From this transform minor components (x_{ij}) into U-pseudo-components $({x_{ij}}^*)$ imposing upper bound restriction on them as defined below

$$x_{ij}^{*} = \frac{U_{ij} - x_{ij}}{U - 1}$$

Therefor $x_{ij}'s$ and $c_i's$ can be expressed as

$$x_{ij} = U_{ij} - \quad x_{ij}^{*}(U - 1)$$

$$c_i = U_i - c_i^{*}(U_c - 1)$$

So the model (1) can be expressed in terms of the Pseudo proportions as

$$Y = \sum_{i=1}^{M}\left[\sum_{j=1}^{m_i}\beta'_{ij}U_{ij} - (U-1)\sum_{j=1}^{m_i}\beta'_{ij}\,x_{ij}^{*} + +(U-1)^2\sum_{j<j'}^{m_i}\gamma'_{ijj'}\,x_{ij}^{*}x_{ij'}^{*}\right.$$
$$\left. + (U-1)\sum_{j<j'}^{m_i}\gamma'_{ijj'}\left(-U_{ij}x_{ij'}^{*} - U_{ij'}x_{ij}^{*}\right) + \sum_{j<j'}^{m_i}\gamma'_{ijj'}\,U_{ij}U_{ij'}\right]\left(U_i - c_i^{*}(U_c - 1)\right)$$
$$+ \sum_{i=1}^{M}\sum_{j<j'}^{m_i}\left[\delta'_{ii'jj'}\left(U_{ij}U_{i'j'} - (U-1)\left(U_{ij}x_{i'j'}^{*} + U_{i'j'}x_{ij}^{*}\right)\right.\right.$$
$$\left.\left. + (U-1)^2x_{ij}^{*}x_{i'j'}^{*}\right)\right]\left(\left(U_i - c_i^{*}(U_c-1)\right)\left(U_j - c_j^{*}(U_c-1)\right)\right) + \varepsilon \ldots.(2)$$

To evaluate the design for the proposed experiments, G- efficiency criteria has been adopted to compare with another design

$$G - \; efficiency \; = \frac{p}{n * d}$$

having n being the total design points, p being total parameters and $d = max\{v = x(x'x)^{-1}x\}$ on a given set of design points x in extended design matrix X which depends on the model to be fitted.

This is an example of hypothetical situation. Let us consider the situation when a fertilizer is consisting of two chemicals c_1 *and* c_2 (major components) where first chemical itself is a mixture of two chemicals x_{11} *and* x_{12} (minor components) and second chemical is a mixture of x_{21} *and* x_{22}, with the restrictions:

$$\sum_{i} c_i = 1$$

$$\& \quad \sum_{j} x_{ij} = 1$$

c_1	c_2	x_{11}	x_{12}	x_{21}	x_{22}
0.272	0.728	0.272	0.728	0.272	0.728
0.272	0.728	0.272	0.728	0.815	0.185
0.272	0.728	0.815	0.185	0.272	0.728
0.272	0.728	0.815	0.185	0.815	0.185
0.815	0.185	0.272	0.728	0.272	0.728
0.815	0.185	0.272	0.728	0.815	0.185
0.815	0.185	0.815	0.185	0.272	0.728
0.815	0.185	0.815	0.185	0.815	0.185
0.086	0.914	0.543	0.457	0.543	0.457
1.000	0.000	0.543	0.457	0.543	0.457
0.543	0.457	0.086	0.914	0.543	0.457
0.543	0.457	1.000	0.000	0.543	0.457
0.543	0.457	0.543	0.457	0.086	0.914
0.543	0.457	0.543	0.457	1.000	0.000
0.543	0.457	0.543	0.457	0.543	0.457

Let the restrictions (with arbitrary value in this case) be imposed on the upper limits of major and minor components such as:

$$U_1 \leq 1;\ U_2 \leq 0.9;\ U_{11} \leq 1;\ U_{12} \leq 0.9;\ U_{21} \leq 1;\ U_{22} \leq 0.9$$

Now taking the proposed U-pseudo transformation for major components and minor components as

$$c_1^* = \frac{U_1 - c_1}{U_c - 1} \ and \ c_2^* = \frac{U_2 - c_2}{U_c - 1}$$

$$x_{ij}^* = \frac{U_{ij} - x_{ij}}{U - 1}$$

The transformed Mixture-of-Mixture design with above upper bound restrictions for the model (2) is given by

c_1^*	c_2^*	x_{11}^*	x_{12}^*	x_{21}^*	x_{22}^*
0.809	0.191	0.809	0.191	0.809	0.191
0.809	0.191	0.809	0.191	0.206	0.794
0.809	0.191	0.206	0.794	0.809	0.191
0.809	0.191	0.206	0.794	0.206	0.794
0.206	0.794	0.809	0.191	0.809	0.191
0.206	0.794	0.809	0.191	0.206	0.794
0.206	0.794	0.206	0.794	0.809	0.191
0.206	0.794	0.206	0.794	0.206	0.794
0.984	0.016	0.508	0.492	0.508	0.492
0.000	1.000	0.508	0.492	0.508	0.492
0.508	0.492	0.984	0.016	0.508	0.492
0.508	0.492	0.000	1.000	0.508	0.492
0.508	0.492	0.508	0.492	0.984	0.016
0.508	0.492	0.508	0.492	0.000	1.000
0.508	0.492	0.508	0.492	0.508	0.492

G-efficiency of the design with these components is 0.6741 which is more than 0.50 and so the design is good. Hence a recommendation for this design will result in a good experiment.

G-Efficiency with Upper Bound Restriction for Mixture–of-Mixture Experiments

After putting some restrictions on upper bounds, (an arbitrary value) designs with pseudo components for major and minor are obtained. G-efficiencies have been obtained for these designs and are summarized in the following tabular form:

Major Components	Minor component For each major component	Upper Bound Restriction	G- efficiency
2	2,2	$U_1 \leq 1;\ U_2 \leq 0.9;$ $U_{11} \leq 1; U_{12} \leq 0.9;$ $U_{21} \leq 1; U_{22} \leq 0.9$	0.6741
	2,3	$U_1 \leq 1;\ U_2 \leq 0.9;$ $U_{11} \leq 1; U_{12} \leq 0.9;$ $U_{21} \leq 0.625; U_{22} \leq 0.625;$ $U_{23} \leq 0.5$	0.6159

	3,3	$U_1 \leq 1;\ U_2 \leq 0.9;$ $U_{11} \leq 0.625; U_{12} \leq 0.625;$ $U_{13} \leq 0.5;$ $U_{21} \leq 0.625; U_{22} \leq 0.625;$ $U_{23} \leq 0.5$	0.6512
3	2,2,2	$U_1 \leq 0.625;\ U_2 \leq 0.625;$ $U_3 \leq 0.5;$ $U_{11} \leq 1; U_{12} \leq 0.9;$ $U_{21} \leq 1; U_{22} \leq 0.9;$ $U_{31} \leq 1; U_{32} \leq 0.9;$	0.6368
	2,2,3	$U_1 \leq 0.625;\ U_2 \leq 0.625;$ $U_3 \leq 0.5;$ $U_{11} \leq 1; U_{12} \leq 0.9;$ $U_{21} \leq 1; U_{22} \leq 0.9;$ $U_{31} \leq 0.625; U_{32} \leq 0.625;$ $U_{33} \leq 0.5$	0.4826
	2,3,3	$U_1 \leq 0.625;\ U_2 \leq 0.625;$ $U_3 \leq 0.5;$ $U_{11} \leq 1; U_{12} \leq 0.9;$ $U_{21} \leq 0.625; U_{22} \leq 0.625;$ $U_{22} \leq 0.5;$ $U_{31} \leq 0.625; U_{32} \leq 0.625;$ $U_{33} \leq 0.5$	0.377

Conclusion

The practical situtation involves the multifarious decision making based on the individual as well as the combined effect of different components proportions. To overcome from such complexity, the additional constraints on the component proportions of major as well as its minor in the form of upper bounds are considered in the present investigation. An attempt has also been made to construct the G-optimal designs for mixture-of-mixture experiments using U-Pseudo components, which simplifies the construction of designs in such types of situations. It is observed that the G- efficiencies under different upper restrictions on various majors and their minors components are more than 50% which is good enough for the practical point of view.

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