Journal of the Korean Statistical Society 41 (2012) 49–60

Contents lists available at SciVerse ScienceDirect

Journal of the Korean Statistical Society

journal homepage: www.elsevier.com/locate/jkss

Orthogonally blocked mixture component–amount designs via projections of F-squares

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ARTICLE INFO

Article history:
Received 21 October 2010
Accepted 16 May 2011
Available online 15 June 2011

AMS 2000 subject classifications:
primary 62K20
secondary 62K10

Keywords:
Mixture–amount experiments
Orthogonal blocking
Scheffé's quadratic model
Latin squares
F-squares
D-optimality
A-optimality
E-optimality

ABSTRACT

Orthogonal block designs for Scheffé's quadratic model have been considered previously by Draper et al. (1993), John (1984), Lewis et al. (1994) and Prescott, Draper, Dean, and Lewis (1993). Prescott and Draper (2004) obtained mixture component–amount designs via projections of standard mixture designs, *viz.*, the simplex-lattice, the simplex-centroid and the orthogonally blocked mixture designs based on latin squares. Aggarwal, Singh, Sarin, and Husain (2009) considered the case of components assuming equal volume fractions and obtained mixture designs in orthogonal blocks using F-squares. In this paper, we construct orthogonal blocks of two and three mixture component–amount blends by projecting the class of four component mixture designs presented by Aggarwal et al. (2009).

1. Introduction

The response to mixture experiments is usually assumed to depend only on the respective proportions of the q (≥ 2) components present in the mixture and not on the total amount of the mixture. The proportions of a mixture of q (≥ 2) components may be expressed as a q-vector $\boldsymbol{x} = (x_1, x_2, \ldots, x_q)'$ in the $(q-1)$ dimensional simplex S_{q-1}.

$$S_{q-1} = \left\{ \boldsymbol{x} : (x_1, x_2, \ldots, x_q) \middle| \sum_{i=1}^{q} x_i = 1, x_i \geq 0 \right\}. \tag{1.1}$$

Scheffé (1958, 1963) introduced models and designs for experiments with mixtures. Scheffé's second order model including the block effect γ is

$$E(y) = \sum_{i=1}^{q} \beta_i x_i + \sum_{1 \leq i < j \leq q} \beta_{ij} x_i x_j + \gamma Z_u + e_u. \tag{1.2}$$

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doi:10.1016/j.jkss.2011.05.007

John (1984) simplified conditions presented by Nigam (1970, 1976) for the orthogonal blocking of blends for Scheffé's quadratic model and constructed designs using latin squares. Conditions given by John (1984) when the blocks are of the same size are:

$$\sum_{u=1}^{n_w} x_{ui} = k_i \text{ (constant) for each block;} \quad i = 1, 2, \ldots, q$$
$$\sum_{u=1}^{n_w} x_{ui}x_{uj} = k_{ij} \text{ (constant) for each block;} \quad 1 \le i < j \le q. \tag{1.3}$$

In particular, it is necessary that in each block the total of the volume fractions for the first component shall be k_1 and the total for the second component shall be k_2; it is not necessary that $k_1 = k_2$. In addition, the considered orthogonal block designs are made non-singular by a suitable choice of the mixture component levels and by the addition of runs common to all the blocks. For instance, the centroid could serve as one additional common run to make $\mathbf{X}^{/}\mathbf{X}$ non-singular.

There are several investigations dealing with drugs, fertilizers, chemicals, nutrition and agriculture, etc. where the response is expected to depend not only on the relative proportions of the mixture ingredients but also on the total amount of the ingredients used. A mixture–amount experiment is a mixture experiment that is performed at two or more levels of the total amount. For example, the variable of interest could be the effect of varying the amount as well as the composition of food flavorings (composed of two or more flavor constituents) on the taste of the food product.

Piepel and Cornell (1985) considered models for mixture experiments when the response depends on the total amount and presented mixture–amount models appropriate for such situations. For q ingredients, the following mixture–amount model consists of three second-order Scheffé polynomial forms in q ingredients, each multiplied by powers of the total amount $\mathcal{A}$, *viz.*, $\mathcal{A}^0$, $\mathcal{A}^1$ and $\mathcal{A}^2$.

$$E(y) = \sum_{i=1}^{q} \gamma_i^0 x_i + \sum_{i<j}^{q} \gamma_{ij}^0 x_i x_j + \sum_{k=1}^{2} \left(\sum_{i=1}^{q} \gamma_i^k x_i + \sum_{i<j}^{q} \gamma_{ij}^k x_i x_j \right) \mathcal{A}^k. \tag{1.4}$$

Piepel and Cornell's (1985) alternative model to the mixture–amount model involves defining the individual component amounts as $a_i = x_i\mathcal{A}$, $i = 1, 2, \ldots, q$ for each level of the total amount $\mathcal{A}$, so that $a_1 + a_2 + \cdots + a_q = \mathcal{A}$. For a mixture–amount experiment when $\mathcal{A}$ is not fixed for all compositions, the component amounts a_i $(i = 1, 2, \ldots, q)$ are mathematically independent variables. Hence standard methods for modeling and analyzing mathematically independent variables may be used to study mixture–amount experiments. For a second degree fit, this alternative polynomial model in the a_i, called a component–amount model is as given in (1.5).

$$E(y) = \alpha_0 + \sum_{i=1}^{q} \alpha_i a_i + \sum_{i=1}^{q} \alpha_{ii} a_i^2 + \sum \sum_{i<j}^{q} \alpha_{ij} a_i a_j. \tag{1.5}$$

Designs for fitting mixture–amount models called mixture–amount designs were considered by Piepel and Cornell (1987). Some mixture–amount experiments involve "control tests" for which the total amount of the experiment is set to zero. Piepel (1988) referred to such experiments as mixture–amount-zero (MAZ) experiments. For example, MAZ experiments include drugs (some patients do not receive any of the formulations being tested). Such experiments allow the study of how the response behaves as the amount of the mixture changes from zero to positive values. Hilgers and Bauer (1995) studied optimal designs for mixture–amount experiments. Clayton, Goldberg, and Potter (1997) employed mixture–amount models and MAZ models to design and analyze an experiment for assessing cyanide in gold mining wastes.

Prescott and Draper (2004) projected standard designs of the simplex-lattice and simplex-centroid and obtained sets of points at various levels of the total amount for two or more ingredients. Moreover, for second order mixture models, they projected known D-optimal orthogonal block designs in two blocks for three and four ingredients based on latin squares and obtained the corresponding D-optimal orthogonal block designs in two blocks for two and three ingredients, respectively.

In this paper, we consider mixture experiments in which some of the component proportions are equal and achieve orthogonal blocking of blends using F-squares. There are several applications in the field of pharmaceutical industry, drugs, metallurgical processes, chemical industry, food and beverages, etc. where certain mixtures require the use of two or more components with negligible or no difference among their volume fractions. For example, each ml of Testosterone Complex INJ 250 mg/1 ml AMP contains:

Testosterone propionate	30 mg
Testosterone phenyl-propionate	60 mg
Testosterone isocaproate	60 mg
Testosterone decanoate	100 mg

In these situations, we may use F-squares instead of using latin squares. Equal volume fractions have previously been considered by John (1984) for the case $q = 5$. The specific design of Cornell (1990) involving six blocks each of $5 + n$ blends, where n is the number of common runs added so as to make the designs non-singular, is considered further by Prescott et al.