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# DESIGNS FOR SCHEFFÉ'S MIXTURE MODELS

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(Extended summary)

ABSTRACT. Models for mixtures of ingredients are typically fitted by Scheffé's canonical model forms. An alternative representation is discussed, which offers attractive symmetries, compact notation and homogeneous model functions. It is based on the Kronecker algebra of vectors and matrices, used successfully in previous response surface work. For this alternative approach, a complete class theorem for mixture designs relative to the Kiefer design ordering is given, for a second-degree model with three ingredients.

In joint work with N. R. Draper ([2], [3]) we have recently proposed a new approach to analyze Scheffé's ([6], [7]) mixture models. The emphasis is to represent the regression function as a polynomial that is homogeneous in the ingredients $t_1, \ldots, t_m$. The usual (Cornell, [1]) way of representing the expected response, for example in a second-degree model, is

$$\eta = \sum_{1 \le i \le m} \beta_i t_i + \sum_{1 \le i < j \le m} \beta_{ij} t_i t_j ,$$

where $\beta_i$ and $\beta_{ij}$ signify the unknown parameters (S-model).

However, we may multiply the linear terms $t_i$ by the constant $1 = t_1 + \cdots + t_m$ to obtain a model which contains exclusively second-degree terms. We prefer to collect these second degree terms by making use of the Kronecker product (K-model), in the form

$$\eta = (t \otimes t)'\theta = \sum_{1 \le i,j \le m} \theta_{ij} t_i t_j .$$

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A similar transition between the S- and the K-model is also available for the third-degree regression. For details see Draper and Pukelsheim ([2]).

In the K-model, the expected response is a homogeneous (of degree two) polynomial of the ingredients $t_i$. We contend that this advantage pays off, well beyond the minor complication that the K-model is overparameterized in that, of course, $\theta_{ji} = \theta_{ji}$ for all $i \neq j$.

For a parsimonious model fitting process, it is imperative to know under which conditions a model of higher degree simplifies to a model of lower degree. The identities (nullhypotheses), under which a third-degree model simplifies to a second-degree model, or a second-degree model simplifies to a first-degree model are derived in Draper and Pukelsheim ([2]).

We now apply this approach to the design problem, following Draper and Pukelsheim ([3]). Let $\tau$ be a mixture design, that is, a collection of points $t$ in the simplex indicating for which settings of the ingredients the experimenter is supposed to observe the response. Each support point $t$ is associated with a weight that defines the proportion of observations under these conditions. The properties of the design $\tau$ are studied, as usual, through its moment matrix

$$M(\tau) = \int (t \otimes t)(t \otimes t)' d\tau .$$

For the special case of two or three ingredients, these moment matrices are spelled out in full detail in Draper and Pukelsheim ([3]). These matrices are homogeneous of degree four, by our choice of the regression function in the K-models.

The moment matrices take a particularly simple form for designs that are *exchangeable*, that is, permutationally invariant. The transition from an arbitrary design to its exchangeable version, obtained by averaging over all permutations, entails an increase in symmetry. The two-stage improvement that consists of this increasing symmetry, followed by an increase of the moment matrices in the usual Loewner ordering is the *Kiefer design ordering*, introduced and discussed in detail in Pukelsheim ([5], Chapter 14). The notion originates with Kiefer's universal optimality which he originally discussed in a restricted setting of block designs. Here we meet a manifestation of the idea in a different setting, second-degree polynomial regression on the simplex.

To achieve an improvement in the Kiefer design ordering, the first step is symmetrization. The second step, improvement of an exchangeable moment matrix in the Loewner matrix ordering, is subdivided into three lemmas.

The *Comparison Lemma* gives a necessary and sufficient condition for the moment matrixes of two exchangeable designs $\eta$ and $\tau$ to be comparable in the Loewner matrix ordering, $M(\eta) \geq M(\tau)$. The condition is in terms of individual moments of the two designs and comes in two parts: (I) The two designs must have identical moments up to order three. (II) The fourth order moments of $\eta$ and $\tau$ must satisfy appropriate inequalities.

Following Galil and Kiefer ([4]) it is tempting to conjecture that the weighted centroid designs form a complete class. Hence the second step, the *Characterization Lemma*, characterizes weighted centroid designs through the moment condition that the (3,1)-moment equals the (2,2)-moment.

The third step then is the *Improvement Lemma*. Given an exchangeable design $\tau$, it provides closed form expressions for the quantities of an appropriate weighted centroid design $\eta$ to improve upon $\tau$ in the Loewner ordering sense, $M(\eta) \geq M(\tau)$. In summary, then, we conclude that in the three ingredients, second-degree model, the set of weighted centroid designs constitutes a complete class of designs for the Kiefer design ordering.

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