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A GRAPHICAL METHOD FOR ASSESSMENT OF THE PREDICTION CAPABILITY OF MIXTURE DESIGNS

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ABSTRACT

A measure for evaluating prediction capability in mixture designs is proposed. This measure is used to form variance dispersion graph evaluating capability of a mixture experimental design throughout the region of interest. This graph allows for an any comparison of competing mixture desings.

1. INTRODUCTION

In mixture experimental design, variance-minimizing design criteria are usaually considered. Unfortunately,these criteia are single-valued criteria. We should not look just at overall measures of a design; rather we should consider how well the design performs over every part of the design region.

The purpose of this paper is to propose a measure for evaluating prediction capability in mixture designs. This measure is used to form a graphical method evaluating prediction capability of an mixture experimental design throughout the region of interest.

2. ALPHABETIC CRITERIA

In the mixture experiment, let q represent the number of ingredients and we represent the proportion of the ith constituent in the mixture by x_i. Then,

$$x_i \geq 0,\ i = 1,\ 2,\ \cdots,\ q$$

and

$$\sum_{i=1}^{q} x_i = x_1 + x_2 + \cdots + x_q = 1.0 \qquad (2.1)$$

The general second-degree polynomial in q variable is

$$\eta(\underline{x}) = \sum_{i=1}^{q} \beta_i x_i + \sum_{\substack{i=1 \\ i<j}}^{q} \sum_{j=1}^{q} \beta_{ij} x_i x_j$$

which may be written on matrix notation as

$$\eta(\underline{x}) = \underline{x}_s' \underline{\beta}$$

in which the 1 x p vector $\underline{x}_s' = (x_1, x_2, \cdots, x_q, x_1 x_2, \cdots, x_{q-1} x_q)$ and $\underline{\beta}$ is the p x 1

column vector of the corresponding coefficients. Here $p = q + \binom{q}{2}$ is the number of parameters in the model. By the method of least squares, the fitted equation $\hat{y}(x) = \underline{x}_s' b$ is to be used to estimate $\eta(\underline{x})$, where

$$\underline{b} = (\mathbf{X}'\mathbf{X})^{-1}\mathbf{X}'\underline{y}$$

and $\mathbf{X}$ in an $\mathbf{N}$ x p model matrix which reflects the experimental design, and $\underline{y}$ is the observation vector.

The variance-covariance matrix of the estimated coefficient the assumption that $\underline{\varepsilon} \sim (\underline{0}, \sigma^2 I)$ is

$$var(\underline{b}) = (\mathbf{X}'\mathbf{X})^{-1}\sigma^2$$

where the p x p matrix $\mathbf{X}'\mathbf{X}$ is taken to be of full rank. The predicted respone at some point of composition $\underline{x}_s$ is $\hat{y}(\underline{x}_s)$ and

$$var[\hat{y}(\underline{x}_s)] = \underline{x}_s' (\mathbf{X}'\mathbf{X})^{-1} \underline{x}_s \sigma^2$$

where on the right-hand side of the equality in (2.3), the 1 x p vecter $\underline{x}_s'$ contains the values of the q component proportions and the p-q cross product terms at the point of composition.

The design optimality criteria $\mathbf{A}-$, $\mathbf{D}-$, $\mathbf{G}-$, and $\mathbf{V}-$ optimality are each concerned with the choice of the elements in the first q columns of $\mathbf{X}$,(which of course carries over to the remaining p-q

The matrix $\mathbf{W}_A$ is the matrix $\mathbf{W}$ with the qth column removed and augmented on the left side with an $\mathbf{N}$ column of 1's and on the right side with columns whose elements represent terms in the model equation of degree higher than 1. The vector of parameter estimates is

$$\underline{g} = (\mathbf{W}_A' \mathbf{W}_A)^{-1} \mathbf{W}'_A \underline{y}$$

and the variance of the estimate of the response in the w_i, $i = 1,2,\cdots,q-1$ is

$$Var(\hat{y}(\underline{w})) = \underline{w}'_s (\mathbf{W}_A' \mathbf{W}_A)^{-1} \underline{w}_s \sigma^2$$

where $\underline{w}_s'$ is a row of the matrix $\mathbf{W}_A$ in Eq. (3.4).

One needs to capture in a graphical way a sense of the distribution of $Var(\hat{y}(\underline{w})) / \sigma^2$ as a function of r, the radius from centroid. Consider a measure of the variability in $Var(y(\underline{w})) / \sigma^2$ where $\underline{w}$ takes values in $S_r = \{\underline{w} | \sum_{i=1}^{q-1} w_i^2 = r^2 \text{ and } \underline{w} \in \text{simplex}\}$.

We define the variance depersion measure, the range of $Var(\hat{y}(\underline{w})) / \sigma^2$ on the restricted sphere of radius r, as

$$RV(r) = \mathbf{V}\max(r) - \mathbf{V}\min(r)$$

where $\mathbf{V}\max(r) = \max_{x \in S_r} \frac{Var(y(\underline{w}))}{\sigma^2}$ and $\mathbf{V}\min(r) = \min_{x \in S_r} \frac{Var(\hat{y}(\underline{w}))}{\sigma^2}$.

Since the form of $Var(\hat{y}(\underline{w})) / \sigma^2$ depends on the chosen model, the form of the range will also depend on the model.

For the illustration of the range in the variance function, it is required that the function $Var(\hat{y}(\underline{w})) / \sigma^2$ be maximized and minimized over locations on the surface of a restricted hypersphere.

This is the problem of optimizing a nonlinear function subject to a nonlinear equality constraint on the variables. For the illustrations presented here, the computation was accomplished with ALM-BFGS algorithm(Seo,Ryu, ad Ryu(1992)). ALM-BFGS algorithm combines argumented Lagrange multiplier algorithm and Broydon-Fletcher -Goldfarb-Shanno algorithm.

4. COMPARISON OF MIXTURE DESIGN-ILLUSTRATIONS

For fitting the quadratic model

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

where the number of experimental runs is **N** = 9. Figure 4.1 are designs (a), (b), and (c). with claringbold's transformation, the w_i represent contrasts among the component proportions, that is, $w_1 = 6(2x_1 - x_2 - x_3)$, $w_2 = 18(x_2 - x_3)$. Figure 4.2 shows the variance dispersion graphs of three designs.

5. CONCLUDING REMARKS

Often, mixture designs are chosen on the basis of a single-valued criteria such as D− or G−optimality. While such criteria provide a useful basis for selecting designs, they often fail to convey the true nature of the design's support of the fitted model in terms of prediction properties over a region of interest. As an alternative to a single-valued criterion, we propose variance dispersion graphs to compare mixture designs. Futher study is as follows;

(1) VDG in restricted mixture models

(2) graphical method for assessment of slope estimation capability in mixture designs.

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