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Comparing the Intercept Mixture Model with the Slack-Variable Mixture Model

Comparación del modelo de mezclas con intercepto con el modelo de mezclas de variable de holgura

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Abstract

Mixture experiments are experiments performed using ingredients whose proportions are restricted. This restriction may result in extremely small range in terms of the mixtures, causing difficulties in model fitting arising from ill-conditioning. The choice of model form is a very important factor in the numerical stability of the information matrix. In this paper, the intercept model is compared against the slack-variable model for mixture experiments. We analyzed if it matter which component is replaced for the constant term in the intercept model, in the sense on numerical stability. We also show by numerical examples that the Correlation Criterion, presented in Kang *et al.* (2015), does not work for the intercept model. Next, as suggested in the literature, we use linear transformation to alleviate the numerical instability. In addition, we try four transformation methods and choose the best one for the intercept model and the slack-variable model. Finally, we compare the intercept model with the slack-variable model based mainly on the prediction accuracy and numerical stability.

Keywords:

- mixture experiments
- intercept model
- slack-variable model
- variable transformation
- condition number
- variance inflation factor

Resumen

Los diseños de experimentos para mezclas son diseños que se llevan a cabo usando ingredientes cuyas proporciones están sujetas a restricciones. Dichas restricciones pueden dar como resultado un rango extremadamente pequeño en términos de las mezclas, causando dificultades en el ajuste del modelo debido a problemas de colinealidad. La elección de la forma del modelo es un factor importante en la estabilidad numérica de la matriz de información. En este artículo, se compara el modelo intercepto contra el modelo de variable de holgura en experimentos para mezclas. Se analizó la importancia de cuál componente se remplaza por el término constante en el modelo intercepto, en el sentido de estabilidad numérica. Asimismo, se muestra mediante ejemplos numéricos que el Criterio de Correlación, presentado por Kang et al. (2015), no funciona para el modelo intercepto. Después, como se sugiere en la literatura, se emplearon transformaciones numéricas para mejorar la inestabilidad numérica. Adicionalmente, se probaron cuatro métodos de transformación y se seleccionó el mejor, tanto para el modelo intercepto como para el modelo de variable de holgura. Finalmente, se comparó el modelo intercepto contra el modelo de variable de holgura basado principalmente en la precisión de predicción y la estabilidad numérica.

Descriptores:

- *diseño de experimentos para mezclas*
- *modelo intercepto*
- *modelo de variable de holgura*
- *transformación de variables*
- *número condicional*
- *factor de inflación de la varianza*

Introduction

A mixture experiment is one in which the response depends only on the relative proportions of the ingredients, or components, present in the mixture, this proportions represent the design variables. In such experiments, by mixing different components, the product is developed. Mixture experiments frequently appear in fields such as chemical, pharmaceutical, food and plastic industries. There are certain type of mixture experiments where the total amount of the mixture, or process variables, are involve too as a design variables (Piepel and Cornell, 1985; Goldfarb *et al*., 2004). In this paper, we focus on the mixture experiments with the proportions of the components as the only input variables.

If x_i denotes the proportion of the *ith* of q components, then $xi \geq 0$ for $i = 1, 2, ..., q$, and

$$\sum_{i=1}^{q} x_i = 1 \qquad (1)$$

Commonly the design region (1) is subject to additional constraints of the form

$$a_i \leq x_i \leq b_i \qquad (2)$$

to one or several components. These additional restrictions may result in extremely small range in terms of the mixtures. Not only does the experimental design region become constrained, but the resulting model from a mixture experiment also has to satisfy the constraint. This can cause difficulties in model fitting arising from ill-conditioning. That is, the columns of the corresponding model matrix can be almost linearly dependent (Prescott *et al*., 2002). Some consequences of ill-conditioning are that the least squares estimators of the parameters have large standard errors and are highly correlated, and the estimates are highly dependent on the precise location of the design points.

Data from a mixture experiment are usually modelled using Scheffe´´s polynomial models (Sheffé, 1958). The quadratic Scheffe´´s model has the general form:

Scheffe´´s model

$$E(y) = \sum_{i=1}^{q} \beta_i x_i + \sum_{i=1}^{q-1} \sum_{j=i+1}^{q} \beta_{ij} x_i x_j$$

where β_i and β_{ij} are unknown parameters to be estimated.

Because of the mixture constraint Eq. (1), the quadratic form of Scheffe´´s model involves linear terms and cross-product terms only, but this could be re-parameterized to include square terms (Philip and Norman, 2009). In fact, there are a number of different ways of writing a polynomial model, of any specified order, obtained by re-parameterization using the mixture constraint (Prescott *et al*., 2002).

Alternative polynomial model forms include the intercept models, which are obtained by replacing one mixture component, for example x_q, for a constant term.