A B S T R A C T

A Study In Mixture Designs: Method Of Multi-stage Fitting

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One of the problems in fitting a response surface in a mixture experiment is the suitable choice of terms. The mathematical complexities greatly restrict this choice. It is possible to have a new and very general approach and use it for many situations in mixture experiments.

In this dissertation, a new method is developed for fitting a response surface at points in the simplex space of a mixture by certain regression techniques. The multi-stage method, as it is called, generally starts with grouping, partitioning and ordering points in the simplex space in a certain fashion finally obtaining a sequence of sets S_1, S_2 ..... S_r, Chapter 2. The general model representing the response surface is a sum of functions $f_1 + f_2 + \ldots + f_r$ in variables x_1, x_2 .... x_n representing variable mixture component proportions. Each function f_i vanishes at points in the subsequence S_1, S_2 .... S_{i-1} and has parameters estimated from responses in S_i by the method of least squares. The method proceeds in a stage-wise manner estimating parameters of all functions in the general model. It encompasses the usual approach to fitting a mixture response model which, under the new scheme, is called the classical approach.

Functions f_1, f_2, ... f_r are considered in the first instance as polynomials in x_1, x_2 .... x_n, Chapter 3. Because general polynomials,

when used for mixture response surfaces, present computational and other difficulties, some special polynomials are defined for f_1, f_2 .... f_r.

A wide range of mixture response surfaces may not be covered by polynomials in x_1 .... x_n. Multi-stage methods considering surfaces in which the reciprocal of one or more of the functions f_1, f_2 .... f_r is a polynomial in the reciprocals $\frac{1}{x_1}$, ... $\frac{1}{x_n}$ are developed for dealing with some of these, Chapter 4. Every stage of the approach is regarded as a seperate regression problem in which seperate analysis is carried out, Chapter 5. An overall analysis at all points in the simplex space is based on analysis within each stage and between all stages.

A brief review of relevant material and incentive for a multi-stage method of fitting a mixture response surface is given in Chapter 1.