Optimal designs for linear mixture models

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by

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The Netherlands

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Summary

In a recent paper Snee and Marquardt (1974) considered designs for linear mixture models, where the components are subject to individual lower and/or upper bounds. When the number of components is large their algorithm XVERT yields designs far too extensive for practical purposes. The purpose of this paper is to describe a numerical procedure resulting in a design of fixed size N, which is approximately D-optimal, and where the components may be subject to linear constraints (f.e. upper or lower bounds). The proposed method is more general(ly) applicable for models linear in the independent variables and the parameters and the convex hull of the experimental region is a polyhedron whose vertices are known.

1. Introduction

In a recent paper Snee and Marquardt (1974) considered designs for linear mixture models, where the m components c_i in a mixture have to satisfy individual constraints:

$$(1.1) \quad 0 \leq a_i \leq c_i \leq b_i \leq 1 \quad (i = 1, \dots, m) .$$

Because we are dealing with mixtures the condition

$$(1.2) \quad \sum_{i=1}^m c_i = 1$$

will have to hold as well.

The problem is to design experiments from which a linear response function

$$(1.3) \quad \underline{E}y = \beta_1 c_1 + \dots + \beta_m c_m$$

can be estimated with optimal precision. A survey of possible criteria for optimality has been given in this journal by van Oorschot (1974).

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There is a class of practical problems where the experimental region is bounded not only by constraints as (1.1) but also by more general linear restrictions of the type

$$(1.4) \quad \ell_k \leq \alpha_{k1} c_1 + \dots + \alpha_{km} c_m \leq u_k \quad (k = 1, \dots, s) .$$

This occurs for instance when the estimated response function is subsequently used in a linear programming model. The response variable y may correspond to a property of the mixture which must lie between certain bounds: In that case preliminary estimates, if available from earlier experiments, can be used to obtain restrictions of type (1.4).

2. Definitions and notations

Denote by x the mixture with m components c_i . Then $x \in \mathbb{R}^m$ and the response function equals:

$$E\mathbf{y} = \mathbf{x}^T \boldsymbol{\beta} .$$

The experimental region X defined by (1.1), (1.2) and (1.4) is a convex polyhedron. Note that (1.1) and (1.2) are special cases of (1.4).

A continuous design ϵ is a probability measure on X . The information matrix of ϵ , denoted M_ϵ , is defined by:

$$M_\epsilon = \int_X \mathbf{x} \mathbf{x}^T d\epsilon(\mathbf{x}) .$$

A design is called D-optimal if it minimizes $|M_\epsilon^{-1}|$. Define:

$$d_\epsilon(\mathbf{x}) = \mathbf{x}^T M_\epsilon^{-1} \mathbf{x} .$$

A design is called G-optimal if it minimizes $\max_{\mathbf{x} \in X} d_\epsilon(\mathbf{x})$.

Kiefer and Wolfowitz (1961) proved the following three statements to be equivalent:

- 1) ϵ is D-optimal
- 2) ϵ is G-optimal
- 3) $\max_{\mathbf{x} \in X} d_\epsilon(\mathbf{x}) = m$.

If ϵ assigns to n points $\mathbf{x}_1, \dots, \mathbf{x}_n$ weights p_i adding up to one ϵ will be called a n -point continuous design. The information matrix then equals:

$$M_\epsilon = \sum_{i=1}^n p_i \mathbf{x}_i \mathbf{x}_i^T .$$

A discrete design assigns weight one to N points $x_1, \dots, x_N$ (some perhaps equal). The corresponding N -point continuous design gives weight $1/N$ to $x_1, \dots, x_N$ and may be called normalized discrete.

If the observational errors are independent with common variance σ^2 , the covariance matrix of the best linear unbiased estimator $\hat{\beta}$ of β equals:

$$\sigma^2 N^{-1} M_{\epsilon}^{-1}.$$

The determinant of this matrix is called the generalized variance of $\hat{\beta}$. The variance of the best linear unbiased estimator of $E y = x^T \beta$ equals

$$\sigma^2 N^{-1} d_{\epsilon}(x).$$

The D-efficiency of ϵ is defined to be:

$$(2.1) \quad [|M_{\epsilon}| / \max_{\epsilon'} |M_{\epsilon'}|]^{1/m}.$$

To justify this definition, suppose we take n_1 observations using ϵ and n_2 observations using an optimal design. The corresponding best linear unbiased estimators will have equal generalized variances if and only if the ratio of sample sizes n_2/n_1 equals (2.1).

Likewise we define the G-efficiency of ϵ to be:

$$m / \max_{x \in X} d_{\epsilon}(x).$$

Atwood (1969) proved that for all ϵ holds:

$$D\text{-efficiency} \geq G\text{-efficiency}.$$

This is of practical value since D-efficiency usually is impossible to compute when no optimal design is known. The optimal continuous design is not likely to be normalized discrete, so the D-efficiency of the optimal discrete design may be smaller than one.

3. Problem reduction

In this section we prove that there exists a D-optimal discrete design of fixed size N , consisting only of vertices of the simplex. We consider a discrete design with a regular information matrix:

$$M := \sum_{i=1}^N x_i x_i^T.$$

Then the predictor variance is:

$$\text{var}(\mathbf{x}^T \hat{\beta}) = \mathbf{x}^T \mathbf{M}^{-1} \mathbf{x} \sigma^2 .$$

Replacing the design point $\mathbf{x}_j$ by $\mathbf{x} \in X$ yields a design with information matrix:

$$\tilde{\mathbf{M}} := \left(\sum_{i=1}^N \mathbf{x}_i \mathbf{x}_i^T - \mathbf{x}_j \mathbf{x}_j^T + \mathbf{x} \mathbf{x}^T \right) .$$

Now define the $m \times 2$ matrix:

$$\mathbf{F} := (i \mathbf{x}_j, \mathbf{x})$$

where $i = \sqrt{-1}$ then:

$$\tilde{\mathbf{M}} = \mathbf{M} + \mathbf{F} \mathbf{F}^T .$$

Using the well-known identity:

$$\begin{vmatrix} \mathbf{A} & \mathbf{B} \\ \mathbf{C} & \mathbf{D} \end{vmatrix} = |\mathbf{A}| |\mathbf{D} - \mathbf{C} \mathbf{A}^{-1} \mathbf{B}| = |\mathbf{D}| |\mathbf{A} - \mathbf{B} \mathbf{D}^{-1} \mathbf{C}| ,$$

($\mathbf{A}$ and $\mathbf{D}$ regular) with $\mathbf{A} = \mathbf{M}$, $\mathbf{B} = \mathbf{F}$, $\mathbf{C} = -\mathbf{F}^T$ and $\mathbf{D} = \mathbf{I}$ results in:

$$\begin{aligned} |\tilde{\mathbf{M}}| &= |\mathbf{M} + \mathbf{F} \mathbf{F}^T| = |\mathbf{M}| |\mathbf{I} + \mathbf{F}^T \mathbf{M}^{-1} \mathbf{F}| = |\mathbf{M}| \begin{vmatrix} 1 - \mathbf{x}_j^T \mathbf{M}^{-1} \mathbf{x}_j & i \mathbf{x}_j^T \mathbf{M}^{-1} \mathbf{x} \\ i \mathbf{x}^T \mathbf{M}^{-1} \mathbf{x}_j & 1 + \mathbf{x}^T \mathbf{M}^{-1} \mathbf{x} \end{vmatrix} = \\ &= |\mathbf{M}| \{ (1 - \mathbf{x}_j^T \mathbf{M}^{-1} \mathbf{x}_j) (1 + \mathbf{x}^T \mathbf{M}^{-1} \mathbf{x}) + (\mathbf{x}_j^T \mathbf{M}^{-1} \mathbf{x})^2 \} \\ &:= |\mathbf{M}| \Delta_j(\mathbf{x}) \quad (\text{cf. Fedorov (1972), pag. 167}) . \end{aligned}$$

$\Delta_j(\mathbf{x})$ is a positive semi-definite quadratic form in $\mathbf{x}$ provided:

$$1 - \mathbf{x}_j^T \mathbf{M}^{-1} \mathbf{x}_j \geq 0 .$$

To prove the latter inequality select $\mathbf{x}_{i_k}$ ($i_k \in (1, \dots, N)$, $k = 1, \dots, m$) such that $\mathbf{x}_{i_1} = \mathbf{x}_j$ and $X := (\mathbf{x}_{i_1}, \dots, \mathbf{x}_{i_m})$ regular.
Then:

$$\begin{aligned} x_j^T M^{-1} x_j &= x_j^T \left(\sum_{i=1}^N x_i x_i^T \right)^{-1} x_j \leq x_j^T \left(\sum_{k=1}^m x_{i_k} x_{i_k}^T \right)^{-1} x_j = x_j^T (X X^T)^{-1} x_j = \\ &= x_{i_1}^T X^{-T} X^{-1} x_{i_1} = (1 \ 0 \ \dots \ 0) \begin{pmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{pmatrix} = 1, \end{aligned}$$

according to the definition of the inverse of a matrix.

The inequality says that the predictor variance in x_j does not decrease when measurements are deleted. A positive semi-definite quadratic form is constant on ellipsoids and therefore $\Delta_j(x)$ attains its maximum value in a vertex of the simplex. One can improve a given design by replacing the design point x_j by $x \in X$ if $\Delta_j(x) > 1$ for some j and x . In that case a maximum improvement can be obtained if x_j is replaced by one of the vertices of the simplex. D-optimality evidently implies:

$$\max_{x \in X} \Delta_j(x) = 1 \quad \text{for all } j.$$

In that case the maximum is attained in x_j , because we have always $\Delta_j(x_j) = 1$. If the ellipsoids of constant $\Delta_j(x)$ are degenerate x_j may not be a vertex but in that case it can be replaced by a vertex without changing the generalized variance.

Therefore there is a D-optimal discrete design on the vertices of the simplex.

4. The algorithm

We now formulate an algorithm (based on Fedorov (1972)) for the construction of a D-optimal discrete design of fixed size N for mixture models, where the experimental region is a simplex.

First. Determine all vertices of the simplex.

This is done by means of an algorithm, implemented in ALGOL for a BURROUGHS computer by Keulemans (1974).

Second. Determine a good starting design. An ad-hoc method by Dirkx (1974) is used for this purpose.

Compute the information matrix and its inverse.

Third. Determine

$$\max_{j,i} \Delta_j(x_{i_1}) \text{ where } j = 1, \dots, N; i = 1, \dots, d \text{ (number of vertices)}$$

replace the corresponding design point x_j by the vertex x_{i_1} and update the information matrix and its inverse.

Fourth. Repeat the third step until

a) a prescribed G-efficiency level has been reached or

b) $\max_{j,i} \Delta_j(x_i) = 1$ ($j = 1, \dots, N$; $i = 1, \dots, d$).

Note. Stopcriterion b) causes some trouble because it means either that the optimal discrete design has G-efficiency smaller than the prescribed one or the design is only locally optimal, meaning that the design is not optimal though $\max_j \Delta_j(x) = 1$ all j . That such locally optimal designs exist can be demonstrated by the following example:

$$E\mathbf{y} = \mathbf{x}^T \beta; \mathbf{X} = \{\mathbf{x}_1, \dots, \mathbf{x}_6\}$$

where

$$\mathbf{x}_1^T = (1, 0, 0); \mathbf{x}_2^T = (0, 1, 0); \mathbf{x}_3^T = (0, 0, 1); \mathbf{x}_4^T = (0, .9, .9);$$

$$\mathbf{x}_5^T = (.9, 0, .9) \text{ and } \mathbf{x}_6^T = (.9, .9, 0).$$

The 3-point discrete design on $\mathbf{x}_4$, $\mathbf{x}_5$ and $\mathbf{x}_6$ is optimal while the design on $\mathbf{x}_1$, $\mathbf{x}_2$ and $\mathbf{x}_3$ is locally optimal. A way out of local optimality is starting from another starting design.

5. Application

To save computing time the algorithm was modified in the third step: The vertices were divided into subgroups of prescribed size and maximum design improvement was searched for in that subgroup. Computing times were substantially reduced in that way.

The modified algorithm was applied in 2 cases with 11 components in a mixture. In one case there were 11 constraints of type (1.1). The corresponding simplex had 1089 vertices. A design of prescribed size 50 and G-efficiency 92% was constructed. As stated in section 2 the D-efficiency is never less than the G-efficiency.

In the other case there were 4 constraints of type (1.4) which resulted in a simplex of 607 vertices. A 70-points design with D-efficiency at least 93% was constructed. In these and other cases these designs were far better than the ones, constructed with the aid of heuristic methods. For more details see Mendieta (1974).

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