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Multiplicative algorithms for computing optimum designs

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ABSTRACT

We study a new approach to determine optimal designs, exact or approximate, both for the uncorrelated case and when the responses may be correlated. A simple version of this method is based on transforming design points on a finite interval to proportions of the interval. Methods for determining optimal design weights can therefore be used to determine optimal values of these proportions. We explore the potential of this method in a range of examples encompassing linear and non-linear models, some assuming a correlation structure and some with more than one design variable.

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1. Optimal design problems

Consider the linear model

$$y(\underline{x}) = \underline{\eta}^T(\underline{x})\underline{\theta} + \varepsilon(\underline{x}),$$

where the components of $\underline{\eta}^T(\underline{x}) = (\eta_1(\underline{x}), \ldots, \eta_k(\underline{x}))$ are k linearly independent continuous functions on some compact space χ, $\underline{\theta} = (\theta_1, \ldots, \theta_k)$ is a vector of unknown parameters to be estimated and the error terms $\varepsilon(\underline{x})$ are assumed uncorrelated and homoscedastic.

1.1. Exact design problem

An *exact design* is defined by a set of experimental conditions $\underline{\widetilde{x}}_1, \ldots, \underline{\widetilde{x}}_N$, which are not necessarily distinct at which observations are to be taken.

If the $\underline{\widetilde{x}}_i$'s are taken on J distinct values $\underline{x}_j, j = 1, \ldots, J$ and if the point $\underline{x}_j$ appears n_j times in the design, $j = 1, \ldots, J$, we denote the design by

$$\lambda = \begin{Bmatrix} \underline{x}_1 & \underline{x}_2 & \cdots & \underline{x}_J \\ n_1 & n_2 & \ldots & n_J \end{Bmatrix}.$$

Clearly $g_j = n_j/N$ will be the proportion of experimental runs at $\underline{x}_j$. Conversely given a probability measure $\xi(\underline{x})$ on χ an exact design of N runs can be approximately defined by $\lambda(\underline{x}) = N\xi(\underline{x})$. Rounding will be necessary to convert $\lambda(\underline{x})$ to a non-negative integer vector $\forall \underline{x} \in \chi$. The exact design problem can be viewed as one of determining these proportions optimally subject to them being rational. In contrast the approximate or continuous optimal design problem relaxes this condition. The calculus of the general equivalence theorem (see Whittle, 1973) can then be brought to bear in determining conditions of optimality; in particular conditions defining optimal weights. In this paper we use an idea presented by Torsney (2007) to deal with the problem of constructing both types of design. One aspect is the transformation of the exact design problem to one of determining optimally a different set of namely proportions of the design space. We first outline the approximate design problem.

1.2. Approximate design problem

Following Kiefer (1971) any probability measure, ξ on χ with finite support is called an approximate design; e.g.

$$\xi = \begin{Bmatrix} \underline{x}_1 & \underline{x}_2 & \cdots & \underline{x}_J \\ p_1 & p_2 & \ldots & p_J \end{Bmatrix},$$

where $\xi(\underline{x}_j) = p_j$ define design weights and satisfy the conditions $p_j \geq 0, j = 1, \ldots, J$ and $\sum p_j = 1$. The $x_i's$ now are said to be the design or support points. The per observation information matrix is defined by

$$M(\xi) = \sum_{j=1}^{J} \eta(\underline{x}_j)\eta^T(\underline{x}_j)p_j = VPV^T,$$

where $P = \mathrm{diag}(p_1, p_2, \ldots, p_J)$ and the ith column of the matrix V is $\eta(\underline{x}_i)$ denoted by $\underline{v}_i = \underline{v}(\underline{x}_i)$. That is $M(\xi) = \sum_j I(\underline{\theta}, x_j)p_j$, where $I(\underline{\theta}, \underline{x})$ is the expected information matrix of a single observations under the linear model, $I(\underline{\theta}, \underline{x}) = \underline{\eta}(\underline{x})\underline{\eta}^T(\underline{x})$.

We note that non-linear models of the form, $y(\underline{x}) = \eta^T(\underline{x}, \underline{\theta}) + \varepsilon(\underline{x})$ can be subsumed here with $\varepsilon(\underline{x})$ as above. These models depend non-linearly on the values of the parameters $\underline{\theta}$. It is common to replace them by their linear approximations in terms of a Taylor expansion about a prior point estimate $\underline{\theta}^0$. In this way the corresponding information matrix is $M(\xi) = \sum_{j=1}^{N} g(\underline{x}_j)g^T(\underline{x})_j p_j$ where $g(\underline{x}) = (\partial\eta(\underline{x}, \underline{\theta})/\partial\underline{\theta})_{\underline{\theta}=\underline{\theta}^0}$. If we have heteroscedastic errors with variances known up to a constant, then $M(\xi)$ has the form $M(\xi) = \sum_{j=1}^{N} g(\underline{x}_j)g^T(\underline{x})_j \omega_j p_j$. Also for a class of generalized linear models the information matrix has the same form with weights ω_j depending on the linear predictor; see Ford et al. (1992).

For an N-point exact design ξ_N we can without loss of generality assume, $J = N, p_j = 1/N$, so

$$M(\xi_N) = \frac{1}{N} V V^T \propto V V^T.$$

An optimal design maximizes an appropriate function of the information matrix, say $\phi(\xi) = \Psi[M(\xi)]$; these functions are homogeneous and concave. Standard criteria are D-optimality, c-optimality and A-optimality which, respectively, maximize

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