Optimal Designs for the Multiresponse Polynomial Regression Models in Symmetric Domains

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Abstract—The multiresponse polynomial regression models are deal with by a linear combination to the responses for getting a manageable single-response model. Based on this method, prove that the symmetric design is optimal in the case of multiresponse polynomial regression models in symmetric domains.

Keywords-optimal designs; multiresponse polynomial regression models; symmetric design

I. INTRODUCTION

The polynomial regression model is widely used. It has been proved that the symmetric design is optimal in the case of singleresponse polynomial regression models in symmetric domains. But the construction of optimal designs for the multiresponse models is difficultly. However, the multiresponse polynomial regression models can be dealt with by a linear combination to the responses for getting a singleresponse model. Based on this method, it can be proved that the symmetric design is also optimal in the case of multiresponse polynomial regression models.

II. MODEL TRANSFORMATION

Consider the following linear models with r responses

$$Ey_i(x) = f_i'(x)\beta_i, \quad i = 1, 2, \cdots r, \qquad (1)$$

where y_i is an observation on the ith responses, f_i is a $k_i \times 1$ vector of the regression functions, β_i is a $k_i \times 1$ vector of unknown constant parameters. A multivariate formulation of the models given in (1) is

$$Ey(x) = f'(x)\beta, \qquad (2)$$

where $y = (y_1, \cdots, y_r)$ is the r-dimensional vector from the multivariate normal populations with the mean $f'(x)\beta$ and a variance-covariance matrix $\Sigma = (\sigma_{ij})_{r \times r}$, $f' = (f_1', \cdots, f_2')$ is the k-dimensional vector and $k = \sum_{i=1}^r k_i$, $\beta = \text{diag}(\beta_1, \cdots, \beta_r)$ is the block diagonal matrix of the parameters.

Let $c = (c_1, \cdots, c_r)'$ be an arbitrary nonzero $r \times 1$ vector. From (2) we obtain the single-response model

$$Ey_c(x) = f'(x)\beta_c = \sum_{i=1}^r c_i f_i'(x)\beta_i, \qquad (3)$$

where $y_c = yc = \sum_{i=1}^r c_i y_i$, $\beta_c = \beta c$

$= (c_1\beta_1', \cdots, c_r\beta_r')'$ is a $k \times 1$ vector of parameters. Note that y_c, being a linear combination of normally distributed random variable, has the normal distribution with a variance σ_c^2, and

$$\sigma_c^2 = \text{var}(y_c) = \text{var}(yc) = c'\Sigma c$$
$$= \sum_{i=1}^r c_i^2 \sigma_{ii} + 2\sum_{i \neq j} c_{ij} c_{ji} \sigma_{ij}.$$

The combination coefficients vector c can be determined according to criteria. For example, Khuri(1985) developed a multivariate test for lack of fit test and let c^* be the eigenvector of $G_2^{-1}G_1$ associated with its largest eigenvalue. But in this paper, it does not change the result that c is an arbitrary nonzero $r \times 1$ vector.

III. SYMMETRIC POLYNOMIAL DESIGNS

Consider the multiresponse polynomial regression models

$$Ey_i(x) = f_i'(x)\beta_i$$
$$= \beta_{i0} + \beta_{i1}x + \beta_{i2}x^2 + \cdots + \beta_{ik}x^k \qquad (4)$$
$$i = 1, 2, \cdots r,$$

where $f_i(x) = (1, x, x^2, \cdots, x^k)'$ is a $(k+1) \times 1$ vector of the regression functions, $\beta_i = (\beta_{i0}, \beta_{i1}, \cdots, \beta_{ik})'$ is a $(k+1) \times 1$ vector of unknown constant parameters.

Let $c = (c_1, \cdots, c_r)'$ be an arbitrary nonzero $r \times 1$ vector. From (4) we obtain the single-response polynomial regression model

$$Ey_c(x) = f'(x)\beta$$
$$= \sum_{i=1}^r c_i f_i'(x)\beta_i = \sum_{j=0}^k \sum_{i=1}^r c_i \beta_{ij} x^j, \qquad (5)$$

where $f(x) = (1, x, x^2, \cdots, x^k)'$ is a $(k+1) \times 1$ vector of the regression functions, $\beta = (\sum_{i=1}^{r} c_i \beta_{i0}, \sum_{i=1}^{r} c_i \beta_{i1}, \cdots, \sum_{i=1}^{r} c_i \beta_{ik})'$ is a $(k+1) \times 1$ vector of unknown constant parameters.

For the model (5), the experimental conditions $x_1, x_2, \cdots, x_n$ are assumed to lie in $[-1,1]$ and the experiment design is $\xi = \begin{pmatrix} x_1 & x_2 & \cdots & x_n \\ p_1 & p_2 & \cdots & p_n \end{pmatrix}$,

where $p_i = \dfrac{N_i}{N}$, $\sum_{i=1}^{n} p_i = 1$. $N = \sum_{i=1}^{n} N_i$ is the total number of observations, and the information matrix

$$M(\xi) = \int_{[-1,1]} f(x) f'(x) d\xi = \sum_{i=1}^{n} p_i f(x_i) f'(x_i).$$

An information matrix M_1 is at least as good as another information matrix M_2, relative to the criterion ϕ, when $\phi(M_1) \geq \phi(M_2)$. It is essential that a reasonable criterion conforms:

$$M_1 \geq M_2 \geq 0 \Rightarrow \phi(M_1) \geq \phi(M_2),$$

$\phi(M_1 + M_2) \geq \phi(M_1) + \phi(M_2)$, for all nonnegative definite M_1 and M_2.

The most prominent optimality criteria are the matrix means ϕ_t, for $t \in (-\infty, 2]$, which enjoy many desired properties. The classical $A-$, $D-$ and $E-$ optimality criteria are special cases of ϕ_t. Let $\lambda_1, \lambda_2, \cdots, \lambda_p$ denote the eigenvalues of a positive definite information matrix M. Then the matrix means ϕ_t is defined by $\phi_t = \left(\dfrac{1}{p} \sum_{i=1}^{p} \lambda_i^t \right)^{\frac{1}{t}}$.

Because of the formula $V[\hat{\beta}(\xi)] = M(\xi)^{-1}$, the matrix mean criteria can be expressed in terms of dispersion matrices as well. Criterion ϕ_{-1} is the $A-$ optimality criteria. Maximizing $\phi_{-1}(M)$ is equivalent to minimizing the trace of the corresponding dispersion matrix. The determinant criterion ($D-$ optimality criteria) $\phi_0(M)$ is equal to $|M|$, and hence it induces the same preordering among information matrices as $|M|$. The extreme member of ϕ_t for $t \to -\infty$ yields the smallest-eigenvalue criterion ($E-$ optimality criteria) $\phi_{-\infty}(M) = \lambda_{\min}(M)$.

According to the well known de la Garza phenomenon, let $\xi_n = \begin{pmatrix} x_1 & x_2 & \cdots & x_n \\ p_1 & p_2 & \cdots & p_n \end{pmatrix}$ with $n > k+1$ be an n-point design for the LSE of β in the polynomial model (5) of degree k. Then there exists a $(k+1)$-point design $\xi_{k+1}^* = \begin{pmatrix} x_1^* & x_2^* & \cdots & x_{k+1}^* \\ p_1^* & p_2^* & \cdots & p_{k+1}^* \end{pmatrix}$ for the LSE of β in model (5) such that $M(\xi_{k+1}^*) = M(\xi_n)$.

First we consider the reflection operation. Let ξ be a design for the LSE of β on $\chi = [-1,1]$ in the polynomial model (5). The reflected design ξ^R is given by $\xi^R = \begin{pmatrix} -x_1 & -x_2 & \cdots & -x_n \\ p_1 & p_2 & \cdots & p_n \end{pmatrix}$, then

$$M(\xi^R) = Q M(\xi) Q, \qquad (6)$$

where $Q = Diag(1, -1, 1, -1, \cdots, \pm 1)$.

The symmetrised design

$$\bar{\xi} = \frac{1}{2}(\xi + \xi^R)$$

$$\equiv \begin{pmatrix} x_1 & -x_1 & x_2 & -x_2 & \cdots & x_n & -x_n \\ \dfrac{p_1}{2} & \dfrac{p_1}{2} & \dfrac{p_2}{2} & \dfrac{p_2}{2} & \cdots & \dfrac{p_n}{2} & \dfrac{p_n}{2} \end{pmatrix},$$

Assigns the weight $\dfrac{p_i}{2}$ to x_i and $-x_i$ for each i. The information matrix of $\bar{\xi}$ is

$$M(\bar{\xi}) = \frac{1}{2}(M(\xi) + Q M(\xi) Q),$$

where all odd moments are zero and the even moments are equal to the corresponding moments of the original design ξ. Hence the averaging operation simplifies information matrices by letting all odd moments vanish. Since $M(\xi^R)$ is obtained from $M(\xi)$ by the similarity transformation (6), $M(\xi^R)$ and $M(\xi)$ have the same eigenvalues.

From the above, it follows that any optimality criterion which is a function of the eigenvalues of the information matrices will be invariant with respect to the reflection operation and superadditive of ϕ (with respect to the reflection) imply

$$\phi\left[M\left(\overline{\xi}\right)\right]=\phi\left\{\frac{1}{2}\left[M\left(\xi\right)+M\left(\xi^{R}\right)\right]\right\}$$
$$\geq\frac{1}{2}\left\{\phi\left[M\left(\xi\right)\right]+\phi\left[M\left(\xi^{R}\right)\right]\right\}$$
$$=\phi\left[M\left(\xi\right)\right].$$

Thus symmetrization improves the value of the criterion ϕ, or at least maintains the same value, provided that ϕ is superadditive and invariant with respect to the reflection. Therefore, for such criteria, we may confine ourselves to the class of symmetric designs.

IV. SYMMETRIC DESIGNS FOR QUADRATIC REGRESSION

Let ξ_3 be a symmetric 3-point design on $\chi=[-1,1]$ for the LSE of $\beta=(\sum_{i=1}^{r}c_i\beta_{i0},\sum_{i=1}^{r}c_i\beta_{i1},\sum_{i=1}^{r}c_i\beta_{i2})'$ in the quadratic model

$$EY_c=\sum_{i=1}^{r}c_i\beta_{i0}+\sum_{i=1}^{r}c_i\beta_{i1}x+\sum_{i=1}^{r}c_i\beta_{i2}x^2. \quad (7)$$

According to the E.P. Liski(2002) result, there exists a symmetric 3-point design $\xi_3^*=\begin{pmatrix}-1 & 0 & 1 \\ \dfrac{p}{2} & 1-p & \dfrac{p}{2}\end{pmatrix}$ with $p<1$ such that $M\left(\xi_3^*\right)\geq M\left(\xi_3\right)$.

The characteristic function of $M\left(\xi_3^*\right)$ is

$$F\left(\lambda\right)=\left(p-\lambda\right)\left[\left(1-\lambda\right)\left(p-\lambda\right)-p\right],$$

which yields the eigenvalues of $M\left(\xi_3^*\right)$:

$$\lambda_1=\frac{1}{2}\left(p+1\right)+\frac{1}{2}\sqrt{5p^2-2p+1},$$
$$\lambda_2=p,$$
$$\lambda_3=\frac{1}{2}\left(p+1\right)-\frac{1}{2}\sqrt{5p^2-2p+1}.$$

The optimal designs are as follows:

$A-$optimal design: $\begin{pmatrix}-1 & 0 & 1 \\ \dfrac{1}{4} & \dfrac{1}{2} & \dfrac{1}{4}\end{pmatrix},$

$D-$optimal design: $\begin{pmatrix}-1 & 0 & 1 \\ \dfrac{1}{3} & \dfrac{1}{3} & \dfrac{1}{3}\end{pmatrix},$

$E-$optimal design: $\begin{pmatrix}-1 & 0 & 1 \\ \dfrac{1}{5} & \dfrac{3}{5} & \dfrac{1}{5}\end{pmatrix}.$

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