On the study of maximin efficient designs by the functional approach

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Abstract

The aim of this paper is to construct and to study maximin efficient designs, introduced in (Muller, 1995) for some types of nonlinear regression models on the base of the functional approach developed in (Melas, 1978, 2005).

Preface

- Nonlinear regression models
- Maximin efficient designs
- The functional approach

The main difficulty is **the dependence of optimal (in a usual sense) designs on he true values**

Two approaches:

- locally optimal approach (Chernoff, 1953)
- maximin efficient (Muller, 1978)

Functional approach (Melas, 1978)

- the study of support points as **functions of initial values**
- represent of these functions by Taylor series (Melas, 2005)

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1.1 Nonlinear regression models

Let us consider the standard general homoscedastic regression model

$$y_j = \eta(x_j, \theta) + \varepsilon_j,\ j = 1, \dots, n$$

where $y_1, \dots, y_n$ are experimental results, $\varepsilon_1, \dots, \varepsilon_n$ are i.i.d. random values, $\eta(x, \theta)$ is a function given with parameters precision, $\theta = (\theta_1, \dots, \theta_n)^T$ is the vector of unknown parameters, $x_j \in [0, \infty)$.

We will consider regression function of the form

$$\eta(x, \theta) = \sum_{i=1}^{k} \theta_i \phi(x, \theta_{i+k})$$

where $\phi(x, \lambda)$ is a given function.

With $\phi(x, \lambda) = 1/(x + \lambda)$ we have $\eta(x, \theta) = \sum_{i=1}^{k} \theta_i/(x + \theta_{i+k})$

and with $\phi(x, \lambda) = e^{-\lambda x}$ we have $\eta(x, \theta) = \sum_{i=1}^{k} \theta_i e^{-x\theta_{i+k}}$.

Exponential models

Let us restrict attention by exponential models

$$\eta(x,\theta) = \sum_{i=1}^{k} A_i e^{-\lambda_i x},$$

where $A_i = \theta_i$, $\lambda_i = \theta_{i+k}$, $A_i \neq 0$, $\lambda_i > 0$, $i = 1, \ldots, k$, $\lambda_i \neq \lambda_j$, $(i \neq j)$. Let

$$\xi = \left(\begin{array}{ccc} x_1 & \ldots & x_n \\ \omega_1 & \ldots & \omega_n \end{array} \right), \ \omega_i > 0, \ \sum_{i=1}^{n} \omega_i = 1$$

be a discrete probability measure which is called approximate design.
The covariance matrix of the least square estimate tends to the matrix $\sigma^2 M^{-1}(\xi,\theta)$ with $\theta = \theta^*$ where θ^* is the true values of the parameters, where

$$M(\xi,\theta) = \left(\sum_{l=1}^{n} \frac{\partial \eta(x_l,\theta)}{\partial \theta_i} \frac{\partial \eta(x_l,\theta)}{\partial \theta_j} \omega_l \right)_{i,j=1}^{m}, \ m = 2k.$$

The matrix M is called the information matrix.

1.2 Locally D-optimal (LD) designs

Let us call a design locally D-optimal if it maximizes the value

$$\det M(\xi, \theta)$$

under fixed θ (the initial guess) among all approximate designs.
Such designs were constructed either explicitly (for simplest models with one nonlinear parameter) or numerically [See Box, Lucas, 1959; Han, Chaloner, 2003].
The functional approach allows to represent the support points of such designs by Taylor series [see Melas, 2005].
We will consider designs which are locally D-optimal among the designs with minimal support ($n = m$), briefly, $LDMS$ design. It can be proved that in many cases $LDMS$ designs are locally D-optimal among all approximate designs.
$LDMS$ designs depend only on nonlinear parameters $\Lambda = (\lambda_1, \dots, \lambda_k)$ and are of the form

$$\xi = \begin{pmatrix} 0 & x_2 & \dots & x_m \\ 1/m & 1/m & \dots & 1/m \end{pmatrix}.$$

We can fix the parameters A_i and consider

$$M(\xi, \Lambda) = M(\xi, \theta).$$

1.3 Maximin efficient (MME) designs

A design will be called maximin efficient D-optimal design (or, briefly, MME design) if it maximizes the value

$$\min_{\Lambda\in\Omega}\left[\frac{\det M(\xi,\Lambda)}{\det M(\xi^*(\Lambda),\Lambda)}\right]^{1/m},\ m=2k,$$

where $\xi^*(\Lambda)$ is a LD design, Ω is a given compact set.
Consider the following set

$$\Omega=\Omega(\delta)=\Omega(\delta,c)=\left\{\Lambda\,:\,(1-\delta)c_i\le\lambda_i\le(1+\delta)c_i,\ i=1,\dots,k\right\},$$

where $c=(c_1,\dots,c_k)$ is a given vector, $0<\delta<1$. Vector c can be considered as an approximation for θ^* and δ is a relative error of this approximation.
Up to now such designs were constructed only for models with one nonlinear parameter [see Dette, Haines, Imhof, 2003].

The concept of design with a minimal structure

Let us consider designs of the form

$$\xi_\tau = \begin{pmatrix} 0 & x_2 & \dots & x_m \\ 1/m & 1/m & \dots & 1/m \end{pmatrix}, \ \tau = (x_2, \dots, x_m).$$

and let $\tau = \hat{\tau}$ maximizes the value

$$\min\{\varphi(\tau, \Lambda_{(1)}), \varphi(\tau, \Lambda_{(2)})\} = \min_{0 \le \alpha \le 1} \alpha\varphi(\tau, \Lambda_{(1)}) + (1-\alpha)\varphi(\tau, \Lambda_{(2)}),$$

where

$$\varphi(\tau, \Lambda) = \left[\frac{\det M(\xi_\tau, \Lambda)}{\det M(\xi_{\tau^*(\Lambda)}, \Lambda)}\right]^{1/m}, \ \Lambda_{(1)} = (1-\delta)c, \ \Lambda_{(2)} = (1+\delta)c,$$

$\xi_{\tau^*(\Lambda)}$ is a LD design with minimal support.

Such designs will be called MME designs with minimal structure ($MMEMS$ designs).

It can be proved that for sufficiently small δ and arbitrary c such design are MME designs among all approximate designs.

Explicit solution for $c_1 = \ldots = c_k$

Let us denote

$$u = (\tau, \alpha) = (\tau_1, \ldots, \tau_{n-1}, \alpha), \;\; \Psi(u, \delta) = \alpha\varphi(\tau, (1-\delta)c) + (1-\alpha)\varphi(\tau, (1+\delta)c).$$

Denote by $\gamma_1, \ldots, \gamma_{m-1}$ zeros of the Laguerre's polynomial with associated parameters 1. Let

$$h = h(\delta) = 2\delta \Big/ \ln\left(\frac{1+\delta}{1-\delta}\right).$$

Theorem 1. *For exponential regression models with $c_1 = c_2 = \ldots = c_k$.*

(I) There exists a unique MMEMS design for any fixed $\delta \in (0,1)$. The support points of this design are

$$\hat{\tau}_i = \gamma_i/(c_1 h), \; i = 1, \ldots, m-1.$$

(II) This design is locally D-optimal for $\Lambda = hc$ for any $\delta \in (0,1)$.

(III) For arbitrary sufficiently small δ this design is MME design among all approximate designs.

Note that numerically we can verify that the part (III) is true for $\delta \leq 0.54$ $(k=1)$, $\delta \leq 0.22$ $(k=2)$, $\delta \leq 0.14$ $(k=3)$.

The basic equation of the functional approach

The idea of the approach consists of

1. considering the support points as implicitly given functions of δ
2. proving that these functions are real analytic, that is they can be expanding into convergent Taylor series
3. using the recurrent formulas for calculating Taylor coefficients [Dette, Melas, Pepelyshev, 2004 or Melas, 2005]

Consider the basic equation

$$\frac{\partial}{\partial u_i}\Psi(u,\delta) = 0,\ i = 1,\ldots,m,$$

$u = (u_1,\ldots,u_m) = (\tau_1,\ldots,\tau_{m-1},\alpha)$ and its Jacobi matrix

$$J(\delta) = \left(\frac{\partial^2\Psi(u,\delta)}{\partial u_i \partial u_j}\right)_{i,j=1}^{m}\Bigg|_{u=\hat{u}(\delta)}.$$

where $u = \hat{u}(\delta)$ is a solution of the basic equation.

The basic equation of the functional approach

Theorem 2. *For exponential regression models*

1. $\det J(\delta) \neq 0$, *the basic equation has a unique solution for arbitrary* c *and* $\delta \in (0,1)$. *The first* $m-1$ *coordinates of this solution generate support points of a unique* $MMEMS$ *design. The functions* $\hat{u}_i(\delta)$ *are real analytic for any* c *and* $\delta \in (0,1)$.

2. *If* $LDMS$ *design are* LD *design among all approximate designs in a vicinity of point* c *then for sufficiently small* δ *the* $MMEMS$ *design is* MME *design among all approximate designs.*

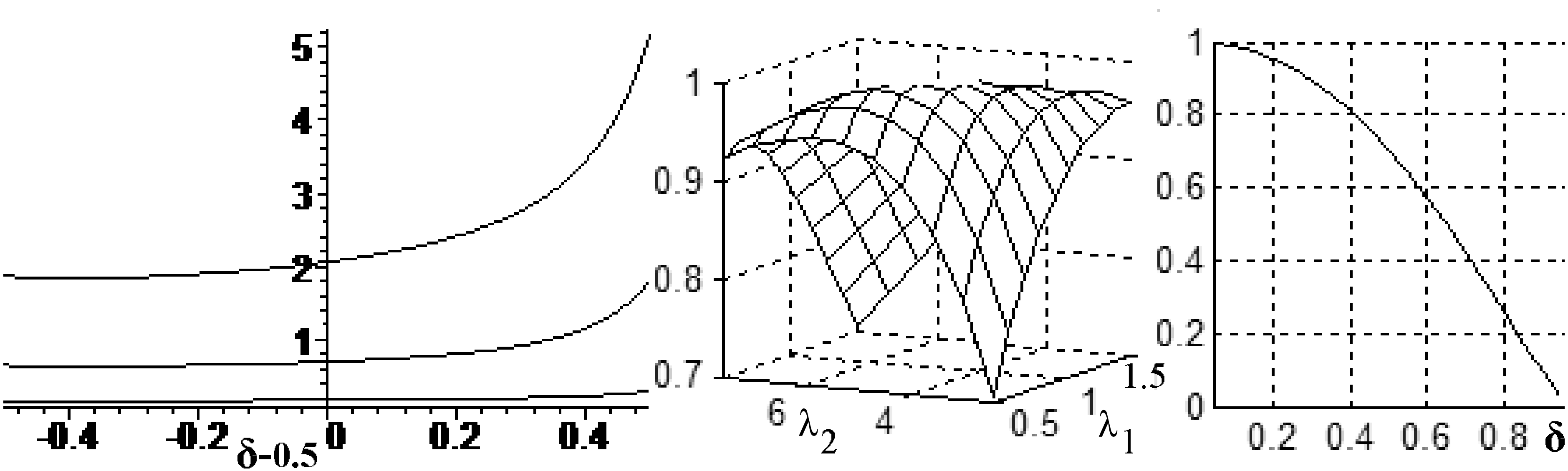
3.1 Algorithm of the numerical study

1. Find numerically $MMEMS$ design for $\delta = \delta_0 = 0.5$
2. By the recurrent formulas construct Taylor expansions for the functions $\hat{\tau}_1(\delta), \ldots, \hat{\tau}_{k-1}(\delta), \hat{\alpha}(\delta)$
3. Check whether the designs constructed are MME designs among all approximate designs for different values of δ by the equivalence theorem from [Dette, Haines, Imhof, 2003].

3.2 Numerical results

For $k = 1$ the explicit form of $MMEMS$ designs is given by Theorem 1.

Let $k = 2$. Set $c_1 = 1, c_2 = 5$ (for other cases we received similar results).



Functions $\hat{x}_2(\delta)$, $\hat{x}_3(\delta)$, $\hat{x}_4(\delta)$ (at left) and the minimal of efficiency of $MMEMS$ design (at right) with $\delta \in (0, 1)$. The efficiency of $MMEMS$ design with $\delta = 0.5$ over $\Omega(0.5)$ (at center).

3.2 Numerical results

Taylor coefficients for the functions $\hat{x}_2(\delta)$, $\hat{x}_3(\delta)$, $\hat{x}_4(\delta)$ and $\alpha(\delta)$.

j	$\hat{x}_2$	$\hat{x}_3$	$\hat{x}_4$	α
0	0.172	0.697	2.062	0.440
1	0.052	0.348	1.165	-0.145
2	0.090	0.673	2.131	-0.097
3	0.111	0.992	2.870	-0.144
4	0.178	1.737	4.768	-0.199
5	0.288	2.998	7.855	-0.325

j	$\hat{x}_2$	$\hat{x}_3$	$\hat{x}_4$	α
6	0.498	5.337	13.562	-0.543
7	0.883	9.556	23.805	-0.942
8	1.604	17.265	42.595	-1.662
9	2.954	31.352	77.194	-2.975
10	5.502	57.225	141.406	-5.370
11	10.321	104.911	261.170	-9.748

The minimal efficiencies of MME, $MMEMS$ and equidistant design $\{0, 0.2, 0.4, ..., 1.8; 1/10, \ldots, 1/10\}$.

δ	MME	$MMEMS$	equid.
0.1	0.9878	0.9878	0.7301
0.2	0.9530	0.9530	0.7092
0.3	0.8972	0.8941	0.6844
0.4	0.8699	0.8113	0.6323
0.5	0.8403	0.7045	0.5417

4. Concluding remarks

- The functional approach allows to construct $MMEMS$ designs with a high precision
- For realistic values of δ these designs proved to maximin efficient among all approximate designs
- The minimal efficiency of MME design is very high (more that 0.84 with $\delta \leq 0.5$)
- $MMEMS$ and MME designs are considerable more efficient than equidistant designs usually implemented in practice
- Similar results were obtained for rational models