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T-Optimal Designs for Discrimination between Rational and Polynomial Models

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This paper considers the problem of the analytical construction of T-optimal experimental designs for discrimination between the simplest rational and polynomial regression models. It is shown how the classical results from approximation theory can be used to derive explicit formulas describing the behavior of support points and weights of T-optimal designs for different fixed parameter values. The problem of discrimination between Michaelis–Menten model and quadratic model is considered as an example. The text is based on the paper [1].

Let experimental results $\{y_i\}$ be described by the equation:

$$y_i = \eta(x_i, \theta) + \varepsilon_i, \qquad i = 1, \dots, n,$$

where $x_1, \dots, x_n$ are experimental conditions that belong to a certain compact set $\mathcal{X}$ and are such that $x_i \neq x_j$ if $i \neq j$, $\theta = (\theta_1, \dots, \theta_d)^T \in \Theta$ is the vector of unknown parameters, $\eta(x, \theta)$ is a real-valued regression function, and $\{\varepsilon_i\}$ are independent normally distributed random errors with zero mean and fixed variance.

Suppose that we have two competing regression functions for $\eta(x, \theta)$: $\eta_1(x, \theta_1)$ and $\eta_2(x, \theta_2)$ that are both continuous over x. Besides we know a certain approximate value of $\overline{\theta}_1$ for the first model parameters θ_1 a priori and we also assume that η_2 is continuously differentiable over θ_2 on compact Θ_2. The discrete probability measure ξ^*, which maximizes the criterion

$$T_{1,2}(\xi, \overline{\theta}_1) = \inf_{\theta_2 \in \Theta_2} \int_{\mathcal{X}} \left[\eta_1(x, \overline{\theta}_1) - \eta_2(x, \theta_2)\right]^2 \xi(dx),$$

is called T-optimal experimental design (see [2]).

It is known that the problem of finding T-optimal designs is related to the best Chebyshev approximation problem (see, e.g., [3]) in the sense that the equality

$$\sup_{\xi} \inf_{\theta_2 \in \Theta_2} \int_{\mathcal{X}} \left[\eta_1(x, \overline{\theta}_1) - \eta_2(x, \theta_2)\right]^2 \xi(dx) = \inf_{\theta_2 \in \Theta_2} \sup_{x \in \mathcal{X}} \left|\eta_1(x, \overline{\theta}_1) - \eta_2(x, \theta_2)\right|, \quad (1)$$

holds, and the support points of a T-optimal design for discrimination between $\eta_1(x, \theta_1)$ and $\eta_2(x, \theta_2)$ coincide with the alternance points for the problem of the best Chebyshev approximation of the function $\eta_1(x, \overline{\theta}_1)$ with function $\eta_2(x, \theta_2)$.

Let us consider the following pair of regression models:

$$\eta_1(x, \theta_1) = \sum_{i=0}^{m} \theta_{1,i} x^i + \frac{1}{x - a}, \qquad \eta_2(x, \theta_2) = \sum_{i=0}^{m} \theta_{2,i} x^i, \quad (2)$$

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that are defined for $x \in [-1,1]$. Due to (1) the problem of finding the T-optimal design for discrimination between this models is reduced to the classical problem of Chebyshev approximation theory, i.e., the search for a polynomial providing the best fit to the function $1/(x-a)$. It is natural to assume that $a \notin [-1,1]$. Without loss of generality, we will assume that $a > 1$.

In the paper we prove that T-optimal design for discrimination between models (2) is concentrated at $(m+2)$ points from the interval $[-1,1]$, becides the points ± 1 always belong to this design's support for every m and the support points from the interval $(-1,1)$ are the roots of polynomials

$$\Psi_1(x) = U_m(x) - 2\alpha U_{m-1}(x) + \alpha^2 U_{m-2}(x), \qquad m \geq 2,$$
$$\Psi_2(x) = \left(\alpha^2 - 1\right) T_m(x) + \left(2\alpha - x - \alpha^2 x\right) U_{m-1}(x), \qquad m \geq 1,$$

where $\alpha = a - \sqrt{a^2 - 1}$. For $m \leq 4$ the roots of this polynomials can be easily found.

The similar result also holds for the following pairs of competing models:

$$\eta_1(x, \theta_1) = \sum_{i=0}^{m} \theta_{1,i} x^i + \frac{1}{x^2 - a}, \qquad \eta_2(x, \theta_2) = \sum_{i=0}^{m} \theta_{2,i} x^i; \tag{3}$$
$$\eta_1(x, \theta_1) = \sum_{i=0}^{m} \theta_{1,i} x^i + \frac{x}{x^2 - a}, \qquad \eta_2(x, \theta_2) = \sum_{i=0}^{m} \theta_{2,i} x^i; \tag{4}$$

on the interval $x \in [-1,1]$ with $a > 1$.

It is shown that T-optimal designs for models (3) and (4) are concentrated at $(m+2)$ points. If m is odd, the support points from the interval $(-1,1)$ of the design for pair (3) coincide with the roots of polynomials

$$\Psi_1(x) = U_m(x) - 2\alpha^2 U_{m-2}(x) + \alpha^4 U_{m-4}(x), \qquad m \geq 4,$$
$$\Psi_2(x) = 2x\left(\alpha^4 - 1\right) T_{m-1}(x) + \left(\alpha^4 + 2\alpha^2 + 1 - 2x^2[\alpha^4 + 1]\right) U_{m-2}(x), \quad m \geq 2,$$

and if m is even, this is true for pair (4). The points ± 1 always belong to an optimal designs support for every m. As earlier, $\alpha = a - \sqrt{a^2 - 1}$ here.

References

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