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T-optimal discriminating designs for Fourier regression models

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ABSTRACT

The problem of constructing T-optimal discriminating designs for Fourier regression models is considered. Explicit solutions of the optimal design problem for discriminating between two Fourier regression models, which differ by at most three trigonometric functions, are provided. In general, the T-optimal discriminating design depends in a complicated way on the parameters of the larger model, and for special configurations of the parameters T-optimal discriminating designs can be found analytically. Moreover, in the remaining cases this dependence is studied by calculating the optimal designs numerically. In particular, it is demonstrated that D- and D_s-optimal designs have rather low efficiencies with respect to the T-optimality criterion.

1. Introduction

The problem of identifying an appropriate regression model in a class of competing candidate models is one of the most important problems in applied regression analysis. Nowadays, it is well known that a well designed experiment can improve the performance of model discrimination substantially, and several authors have addressed the problem of constructing optimal designs for this purpose. The literature on designs for model discrimination can roughly be divided into two parts. Hunter and Reiner (1965) and Stigler (1971) considered two nested models, where the extended model reduces to the "smaller" model for a specific choice of a subset of the parameters. The optimal discriminating designs are then constructed such that these parameters are estimated most precisely. Since these fundamental papers several authors have investigated this approach in various regression models (see Hill, 1978; Studden, 1982; Spruill, 1990; Dette, 1994, 1995; Dette and Haller, 1998, Song and Wong, 1999; Zen and Tsai, 2004; Biedermann et al., 2009 among many others). The second line of research was initialized in a fundamental paper of Atkinson and Fedorov (1975a), who introduced the T-optimality criterion for discriminating between two competing regression models. Since the introduction of this criterion, the problem of determining T-optimal discriminating designs has been considered by numerous authors (see Atkinson and Fedorov, 1975b; Ucinski and Bogacka, 2005; Dette and Titoff, 2009; Atkinson, 2010; Tommasi and López-Fidalgo, 2010 or Wiens, 2009, 2010 among others). The T-optimal design problem is essentially a minimax problem, and – except for very simple models – the corresponding optimal designs are not easy to find and have to be determined numerically in most cases of practical interest. On the other hand, analytical solutions are helpful for a better understanding of the optimization problem and can also be used to validate numerical procedures for the construction of optimal designs. Some explicit solutions of

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the T-optimal design problem for discriminating between two polynomial regression models can be found in Dette et al. (2012), but to our best knowledge no other analytical solutions are available in the literature.

In the present paper, we consider the problem of constructing T-optimal discriminating designs for Fourier regression models, which are widely used to describe periodic phenomena (see for example Lestrel, 1997). Optimal designs for estimating all parameters of the Fourier regression model have been discussed by numerous authors (see e.g. Karlin and Studden, 1966, page 347, Lau and Studden, 1985; Kitsos et al., 1988; Riccomagno et al., 1997 and Dette and Melas, 2003 among others). Discriminating design problems in the spirit of Hunter and Reiner (1965) and Stigler (1971) have been discussed by Biedermann et al. (2009) and Zen and Tsai (2004) among others, but T-optimal designs for Fourier regression models, have not been investigated in the literature so far. In Section 2, we introduce the problem and provide a characterization of T-optimal discriminating designs in terms of a classical approximation problem. Explicit solutions of the T-optimal design problem for Fourier regression models are discussed in Section 3. Finally, in Section 4, we provide some numerical results of these challenging optimization problems. In particular, we demonstrate that the structure (more precisely the number of support points) of the T-optimal discriminating design depends sensitively on the location of the parameters.

2. *T*-optimal discriminating designs

Consider the classical regression model

$$y = \eta(x) + \varepsilon, \tag{2.1}$$

where the explanatory variable x varies in a compact design space, say $\mathcal{X}$, and observations at different locations, say x and x', are assumed to be independent. In (2.1), the quantity ε denotes a random variable with mean 0 and variance σ^2, and $\eta(x)$ is a function, which is called regression function in the literature (see Seber and Wild, 1989). We assume that the experimenter has two parametric models, say $\eta_1(x, \boldsymbol{\theta_1})$ and $\eta_2(x, \boldsymbol{\theta_2})$, for this function in mind to describe the relation between predictor and response, and that the first goal of the experiment is to identify the appropriate model from these two candidates. In order to find "good" designs for discriminating between the models η_1 and η_2, we consider approximate designs in the sense of Kiefer (1974), which are probability measures on the design space $\mathcal{X}$ with finite support. The support points, say $x_1, \ldots, x_s$, of an (approximate) design ξ define the locations where observations are taken, while the weights denote the corresponding relative proportions of total observations to be taken at these points. If the design ξ has masses $\omega_i > 0$ at the different points $x_i (i = 1, \ldots, s)$ and n observations can be made, the quantities $\omega_i n$ are rounded to integers, say n_i, satisfying $\sum_{i=1}^{s} n_i = n$, and the experimenter takes n_i observations at each location $x_i (i = 1, \ldots, s)$ (see for example Pukelsheim and Rieder, 1992).

For the construction of a good design for discriminating between the models η_1 and η_2, Atkinson and Fedorov (1975a) proposed in a seminal paper to fix one model, say η_2, and to determine the discriminating design such that the minimal deviation between the model η_2 and the class of models defined by η_1 is maximized. More precisely, a T-optimal design is defined ξ^* by

$$\xi^* = \arg\max_{\xi} \int_{\mathcal{X}} \Big(\eta_2(x, \boldsymbol{\theta_2}) - \eta_1(x, \widehat{\boldsymbol{\theta}}_1)\Big)^2 \xi(dx),$$

where the parameter $\widehat{\boldsymbol{\theta}}_1$ minimizes the expression

$$\widehat{\boldsymbol{\theta}}_1 = \arg\min_{\boldsymbol{\theta_1}} \int_{\mathcal{X}} (\eta_2(x, \boldsymbol{\theta_2}) - \eta_1(x, \boldsymbol{\theta_1}))^2 \xi(dx).$$

Note that the T-optimality criterion is a local optimality criterion in the sense of Chernoff (1953), because it requires knowledge of the parameter $\boldsymbol{\theta_2}$. Bayesian versions of this criterion have recently been investigated by Dette et al. (2013, 2015).

Remark 2.1. Consider the case where the models η_1 and η_2 are linear and nested, say

$$\eta(x, \boldsymbol{\theta_1}) = \boldsymbol{\theta_1}^T f_1(x); \qquad \eta_2(x, \tilde{\boldsymbol{\theta}}_2, b) = \tilde{\boldsymbol{\theta}}_1^T f_1(x) + b^T f_2(x).$$

It was pointed out by Dette and Titoff (2009) that the function $\int_{\mathcal{X}} (\eta_2(x, \boldsymbol{\theta_2}) - \eta_1(x, \hat{\boldsymbol{\theta}}_1))^2 \xi(dx)$ has the representation

$$T(\xi, b) = \int_{\mathcal{X}} (\eta_2(x, \boldsymbol{\theta_2}) - \eta_1(x, \hat{\boldsymbol{\theta}}_1))^2 \xi(dx) = b^T (M_{22}(\xi) - M_{12}^T(\xi) M_{11}^{-}(\xi) M_{12}(\xi)) b$$

where

$$M_{ij}(\xi) = \int_{\mathcal{X}} f_i(x) f_j^T(x) \xi(dx) \quad (i, j = 1, 2)$$