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CDT-optimum designs for model discrimination, parameter estimation and estimation of a parametric function

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ABSTRACT

After initiating the theory of optimal design by Smith (1918), many optimality criteria were introduced. Atkinson et al. (2007) used the definition of compound design criteria to combine two optimality criteria and introduced the DT- and CD-optimalities criteria. This paper introduces the CDT-optimum design that provides a specified balance between model discrimination, parameter estimation and estimation of a parametric function such as the area under curve in models for drug absorbance. An equivalence theorem is presented for the case of two models.

1. Introduction

Optimum designs for discrimination between models introduced by Atkinson and Fedorov (1975) consider discrimination between two linear polynomial regression models: a constant and a quadratic. There is a long history of papers that seek to find a balance between model discrimination and parameter estimation, at least from Hill et al. (1968) to Biswas and Chaudhuri (2002) and Waterhouse et al. (2004).

Atkinson et al. (2007) discussed C-optimum designs for three features of a three-parameter compartmental model for the concentration of theophylline in the blood of a horse. The C-optimum designs, for example that for estimation of the area under curve, all had either two or one points of support and so provided no information on the values of the parameters in the model. Here, we use optimum design theory to provide designs of known properties with a specified balance between parameter estimation, discrimination and estimation of a parametric function such as the area under curve. To check the validity of the derived criterion, an equivalence theorem will be introduced.

The paper is organized as follows: in the section the D-, T- and C-optimum designs are introduced. Compound design criteria which include DT- and CD-optimum designs are explored in the section. Finally, in the section, a new criterion namely CDT-optimality will be derived.

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2. C-, D-, T-optimum designs

2.1. T-optimum designs

T-optimality arises in discrimination between two or more models, one of which is true. Atkinson and Fedorov (1975) describe designs for discrimination between two rival regression models $\eta_1(x,\theta_1)$ and $\eta_2(x,\theta_2)$. The models may be linear or nonlinear in the parameters, which are estimated by least squares. Suppose that the first model is true, so that the observations

$$y_i=\eta_t(x)+\varepsilon_i=\eta_t(x,\theta_1)+\varepsilon_i. \quad (1)$$

For classical linear models, the T-optimal design assumes that the true model is known and maximizes the residual sum of squares arising from the fit of the competing model, which equivalently maximizes the non-centrality parameter of the χ^2 distribution of the residual sum of squares for the competing model. Thus, the T-optimal design provides the most powerful lack-of-fit test for the competing model, and it is in this sense that the T-optimal design is optimal in discriminating the true model from the competing model.

The lack-of-fit sum of squares for model 2 is made as large as possible by maximizing

$$\Delta_1(\xi)=\sum_{i=1}^{k} w_i\left\{\eta_t(x_i)-\eta_2(x_i,\hat{\theta}_{t2})\right\}^2, \quad (2)$$

where

$$\sum_{i=1}^{k} w_i\left\{\eta_t(x_i)-\eta_2(x_i,\hat{\theta}_{t2})\right\}^2=\inf_{\theta_2\in\Theta_2}\sum_{i=1}^{k} w_i\{\eta_t(x_i)-\eta_2(x_i,\theta_2)\}^2. \quad (3)$$

A design ξ puts weights w_i at k support points x_i in the experimental region χ.

Let ξ_T^* be the design maximizing Eq. (2). Under some regularity conditions, Atkinson and Fedorov (1975) prove an equivalence theorem for T-optimum designs, in which the derivative function

$$\psi_1^T(x,\xi_T^*)\le\Delta_1(\xi_T^*),\quad x\in\chi, \quad (4)$$

where the directional derivative

$$\psi_1^T(x,\xi)=\left\{\eta_t(x)-\eta_2(x,\hat{\theta}_{t2})\right\}^2.$$

The T-efficiency of any design ξ relative to the T-optimum design ξ_T^* is given by

$$E^T(\xi)=\frac{\Delta_1(\xi)}{\Delta_1(\xi_T^*)} \quad (5)$$

2.2. D-optimum designs

D-optimality is the most important and popular design criterion, introduced by Wald (1943), which puts the emphasis on the quality of the parameter estimates. D-optimum designs maximize $\log|M(\xi)|$, where $M(\xi)$ is the information matrix. The original equivalence theorem for D-optimum designs for linear models, due to Kiefer and Wolfowitz (1960), states that the derivative function

$$\psi^D(x,\xi_D^*)=d(x,\xi_D^*)\le p,\quad x\in\chi,$$

where

$$d(x,\xi_D^*)=f^T(x)M^{-1}(\xi_D^*)f(x)$$

and ξ_D^* is the D-optimum design. The D-efficiency of any design ξ relative to the D-optimum design ξ_D^* is given by

$$E^D(\xi)=\{|M(\xi)|/|M(\xi_D^*)|\}^{1/p}, \quad (6)$$

where p is the number of parameters in the model.

2.3. C-optimum designs

In C-optimality, the interest is in estimating the linear combination of the parameters $c^T\beta$ with minimum variance, where c is $m\times 1$ vector of constants. It was introduced by Elfving (1952) who provided a geometrical interpretation for finding C-optimal designs, developed by Silvey and Titterington (1973) and Titterington (1975). Pukelsheim and Torsney (1991) give a method for computing C-optimal weights given the support points. Fellman (1974) justifies that at most m linearly independent support points are needed for a C-optimal design. The design criterion to be minimized is thus

$$\text{var}\, c^T\hat{\beta}\propto c^TM^{-1}(\xi)c.$$