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Robust designs for probability estimation in binary response experiments ☆

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A R T I C L E I N F O

In memory of a great mentor
Professor William J. Studden
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A B S T R A C T

The purpose of this work is to investigate robust design problems for estimation of the response probability curve under binary response experiments with model uncertainty consideration. A minimax type of model robust design criterion, called *WB*-optimum in short is proposed, based on minimization of the maximum of the weighted squared probability bias function under two rival models. The corresponding design issues are investigated and results under the above design criterion for given rival models with several commonly seen symmetric links are presented.

1. Introduction

Binary response experiments occur in many scientific investigations, such as sensitivity and safety analysis for the pyrotechnics experiments discussed in Chao and Fuh (2001). Optimal design problems for accurate parameter estimations of a given model in binary response experiments have been discussed in various works. See for example, Abdelbasit and Plackett (1983), Minkin (1987), Wu (1988) Sitter and Wu (1993) and Sitter and Fainaru (1997). In practice, estimation of quantiles is of great interest, see for example, Biedermann et al. (2006, 2007). Fuh et al. (2003) argue that proper estimation of the pth quantile for p close to one depends on the correct choice of the parametric model, say, logit, probit, or otherwise. Hence, model discrimination is an important issue, especially for accurate estimation of extreme quantiles. There are lots of investigations devoted to design problems on how to discriminate between models including Chambers and Cox (1967), Atkinson and Fedorov (1975), Yanagisawa (1988, 1990), Müller and Ponce de Leon (1996) and Uciński and Bogacka (2004). However, lots of trials are usually needed for discriminating binary models. For example, Yanagisawa (1988) and Müller and Ponce de Leon (1996) show that approximately 1000 or more trials are needed to discriminate between probit and logit models with 50% power at a significant level 5%. On the other hand, Atkinson (2008) also indicates that optimal designs for discrimination between models often have poor properties for estimation of the parameters. Thus, when the number of trials is limited, estimation of quantiles after making model discrimination may not be feasible with good accuracy.

In this work, we propose a new design criterion for estimation of quantiles from a different perspective, that is, the probability biases of quantiles are considered instead of the location biases of them. Our main objective is to find a locally optimal design under a minimax type of design criterion, which is more robust to model misspecification while estimating

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the quantiles of interest. Minimax type of design criteria has been used in design of experiments, see for example, Dette and Studden (1994) and Dette and Sahm (1998). The idea of this kind of criterion is to try to control the damage in the worst case, and the experimenters may have confidence to avoid serious mistakes. The robustness here refers to the choice of different models, such as that in Huang and Studden (1988). The binary model is usually constructed through the link function and linear predictor, and our robustness focuses on the choice of link functions. The linear predictor considered is a first-order model with respect to the explanatory variable. In what follows, we will propose first a minimax type of design criterion called *WB*-optimum, which seeks designs minimizing the maximum value of a certain loss function related to the weighted probability bias on quantiles with respect to two rival models. Next, a compound *D*-criterion or a compound c_p-criterion can be adopted for choosing one of the above designs with a reasonably good efficiency with respect to the variation of the parameter estimator or with respect to the variation of the locations of quantile estimators.

This paper is organized as follows. In the following two sections, some preliminaries about the binary response models and designs are presented, and the minimax criterion is introduced. In Section 4, main theoretical results for the *WB*-optimal design are presented. Some simulation and computation results about the performances of *WB*-optimal designs compared with those of *D*- and *T*-optimal designs are shown in Section 5. The final section ends with some discussions and conclusions.

2. Preliminaries

A realization of a binary response model $F(\mathbf{x}^T\theta)$ at a certain explanatory variable level x is a Bernoulli trial with response probability $p(x)=F(\mathbf{x}^T\theta)$, where F is called the link function and $\mathbf{x}^T\theta$ is the linear predictor containing design vector $\mathbf{x}=(1,x)^T$ and parameter vector $\theta=(\alpha,\beta)^T$. The link function is usually assumed to be a continuous cumulative distribution function (cdf), like logistic (logit model) or normal (probit model) distribution, and to be point-symmetric at $F(0)=0.5$, i.e., $F(t)=1-F(-t)$. The sign of β only influences that the response probability increases or decreases as x increases, and $\mu=-\alpha/\beta$ indicates the location of the median (with response probability one half) when $\beta\neq 0$. Without loss of generality, it is assumed that $\alpha\in\mathbb{R}$ and $\beta>0$, i.e., $\theta\in\mathbb{R}\times\mathbb{R}^+$.

An exact design ξ_N denoted by

$$\xi_N=\begin{Bmatrix} x_1 & \dots & x_m \\ w_1 & \dots & w_m \end{Bmatrix},$$

includes n_i independent observations obtained at distinct experimental level x_i for $i=1$ to m, where N is the total number of trials, $\sum_{i=1}^m w_i=1$, and $w_iN=n_i$ is a positive integer. Let r_i be the number of responses in n_i trials at x_i, then the log-likelihood function with link F is proportional to

$$L_F(\theta)=\sum_{i=1}^m w_i\left[\frac{r_i}{n_i}\log\left(F\left(\mathbf{x}_i^T\theta\right)\right)+\left(1-\frac{r_i}{n_i}\right)\log\left(1-F\left(\mathbf{x}_i^T\theta\right)\right)\right],$$

and the maximum likelihood estimate (mle) of θ is obtained through maximizing the above function. An approximate design ξ removes the restriction that $w_iN=n_i$ is a positive integer, and the limit of the mle of θ, denoted by $\theta^{(M)}$, can be obtained through maximizing

$$L_F^{(M)}(\theta)=\sum_{i=1}^m w_i[p(x_i)\log(F(\mathbf{x}_i^T\theta))+(1-p(x_i))\log(1-F(\mathbf{x}_i^T\theta))], \tag{1}$$

where $p(x)$ is the true response probability at x. Note that here $\theta^{(M)}$ is a real value vector which is not random, and is determined by $p(x)$, the given design ξ, and the working link F might be misspecified.

When F is the correct link, $\theta^{(M)}$ exists and it is the true parameter vector. On the other hand, even if F is incorrect, White (1982) shows that $\theta^{(M)}$ exists under some regular conditions, and Czado and Santner (1992) give some regular conditions for feasible designs with binary response, where "feasible" means that $\theta^{(M)}$ exists. Optimal designs considered here are assumed to be from a class, denoted by Ξ, of feasible approximate designs for all candidate links.

3. *WB*-optimum criterion

In this work, the fitness of a binary response model is judged by how far the estimated probability curve from the true one, and the importance of the probability bias may vary on different places. Roughly speaking, the loss function for a given model $F(\mathbf{x}^T\theta)$ with respect to the true response probability $p(x)$ can be defined as the weighted squared probability bias function as

$$\lambda(x)(F(\mathbf{x}^T\theta)-p(x))^2,$$

where $\lambda(x)$ is a given weight function indicating the importance of probability bias at x.

Following the idea above, when the working link is F_1 and the true link is F_2, the loss function for a design $\xi\in\Xi$ is defined by

$$\lambda_1(x)(F_1(\mathbf{x}^T\theta_{1,\xi}^{(M)})-F_2(\mathbf{x}^T\theta_{2,\xi}^{(M)}))^2, \tag{2}$$