Statistics and Probability Letters 137 (2018) 201–208

Contents lists available at ScienceDirect

Statistics and Probability Letters

journal homepage: www.elsevier.com/locate/stapro

Optimal designs for multi-factor nonlinear models based on the second-order least squares estimator☆

Lei He

Department of Mathematics, Shanghai Normal University, Shanghai, 200234, China

ARTICLE INFO

Article history:
Received 30 November 2017
Received in revised form 9 January 2018
Accepted 10 January 2018
Available online 8 February 2018

MSC:
62K05

Keywords:
Additive models
Locally *D*-optimality
Standardized maximin *D*-optimality
Second-order least squares estimator
Exponential models

ABSTRACT

In this paper, we investigate the locally and maximin optimal design problems for multi-factor nonlinear models based on the second-order least squares estimator (SLSE), it is shown that the product-type designs are optimal based on the SLSE for the multi-factor nonlinear models without constant term when the sufficient conditions are satisfied. Some examples are presented to illustrate the theoretical results. Several by-products on locally and maximin optimal designs for uni-factor exponential decay models are also obtained.

1. Introduction

In subject areas, such as biology, chemistry, agriculture and pharmacokinetics, nonlinear regression models are commonly used to characterize an adequate functional relationship between a response of interest, say y, and the associated input variables. With a careful choice of design, as we known, the efficiency of the statistical analysis for these models can be improved substantially. In this respect, mention may be made of the monograph by Fedorov and Leonov (2014).

Most experiments may involve several different factors and are described by multi-factor models. In this direction Schwabe (1996) made an excellent study of optimal designs for multi-factor linear models with homoscedastic errors. The linear heteroscedastic case has also been discussed by numerous authors, see, for example, Wong (1994), Rodríguez and Ortiz (2005) and He and Yue (2017) among others. However, little attention has been paid to the multi-factor nonlinear models. Biedermann, et al. (2011) developed optimal design theory for additive partially nonlinear regression models and applied for least-squares regression splines. Recently, Rodríguez et al. (2015) studied the construction of locally and maximin optimal designs for multi-factor nonlinear models from optimal designs in one dimension.

Note that the aforementioned references mainly focused on finding optimal designs based on the ordinary least squares estimator (OLSE). For the OLSE that is most efficient if the random errors in the model are assumed to have normally distributed. When the random error distribution is not normal or asymmetric, however, the second-order least squares estimator (SLSE) proposed in Wang and Leblanc (2008) is more efficient than the OLSE. Under the framework of the SLSE, Gao and Zhou (2014) formulated a new class of D- and A-optimality criteria and investigated the transformation invariance and symmetry of the design, and subsequently, Bose and Mukerjee (2015) and Gao and Zhou (2017) made further developments,

☆ This work was supported by NSFC Grant 11471216.
E-mail address: lhstat@163.com.

https://doi.org/10.1016/j.spl.2018.01.005
0167-7152/

including the convexity results for the criteria and numerical algorithms. Moreover, mention may be made to Yin and Zhou (2017) who derived a characterization of the A-optimality criterion based on the SLSE.

These literatures under the SLSE are only concerned with locally optimal designs. This approach is however not necessarily robust with respect to a misspecification and may lead to an inefficient design. A more flexible strategy to obtain robust designs is to incorporate some prior information into an appropriate criterion, that is Bayesian optimality (see Chaloner and Verdinelli (1995)). While the Bayesian methodology has also somewhat restrictive in the sense that requires a pre-specified prior for the nonlinear parameters in the models. Alternatively, and less stringently, we consider in this paper a maximin approach based on the D-optimality criterion proposed by Gao and Zhou (2014), which only requires to specify a range of the unknown parameters (see Silvey (1980)). It is the purpose of the present paper to construct locally and standardized maximin D-optimal designs under the SLSE for multi-factor nonlinear models without constant term. In addition, as by-products of this paper, we also investigate the locally and maximin optimal design problems under the SLSE for the single variable exponential decay models that are widely used in applications.

The rest of this paper is structured as follows. In Section 2, a brief introduction of the D-optimality criterion based on the SLSE and a general definition of the standardized maximin D-optimality criterion are given. The main results about the construction of locally and standardized maximin D-optimal designs for the multi-factor models are derived in Section 3. Some concluding remarks are given in Section 4. Finally, an available result of maximin optimal design based on the SLSE in applications is addressed in the Appendix for uni-factor exponential decay models.

2. Preliminaries

Consider a multi-factor nonlinear regression model

$$y = \eta(x, \theta) + \epsilon, \quad x \in \mathcal{X} \subset \mathbb{R}^p, \tag{1}$$

where y is the response observed at $x = (x_1, \ldots, x_p)$ of p independent variables $x_1, \ldots, x_p$ with values in a compact subset $\mathcal{X}$, $\theta = (\theta_1, \ldots, \theta_q)^T \in \Theta \subset \mathbb{R}^q$ is a vector of unknown parameters, ϵ is the random error satisfying $E(\epsilon|x) = 0$ and $E(\epsilon^2|x) = \sigma^2$, and $\eta(x, \theta)$ is a nonlinear function of both arguments (x, θ) and differentiable with respect to the variable θ. In addition, we assume here that y and ϵ have finite fourth moments.

Assume that there are N independent observations on the response variable at the points $x^{(1)}, \ldots, x^{(N)} \in \mathcal{X}$. Then the SLSE $\hat{\gamma}_{SLS}$ of $\gamma = (\theta^T, \sigma^2)^T$ for the multi-factor nonlinear model (1) can be obtained by minimizing

$$Q(\gamma) = \sum_{i=1}^{N} \rho_i^T(\gamma) W_i \rho_i(\gamma),$$

where $\rho_i(\gamma) = (y_i - \eta(x^{(i)}, \theta), y_i^2 - \eta^2(x^{(i)}, \theta) - \sigma^2)^T$, and $W_i = W(x^{(i)})$ is a 2×2 nonnegative definite matrix which may depend on $x^{(i)}$. Throughout this paper we consider approximate designs in sense of Kiefer (1974) which are defined as probability measures on the design space $\mathcal{X}$ with n support points $x^{(1)}, \ldots, x^{(n)}$ replicated, respectively, $r_1, \ldots, r_n$ times, where $\sum_{i=1}^{n} r_i = N$. Using the following limiting relation

$$\lim_{r_i \to \infty} \frac{r_i}{N} = \omega_i, \quad i = 1, \ldots, n,$$

an approximate design is of the form

$$\xi = \begin{Bmatrix} x^{(1)} & x^{(2)} & \cdots & x^{(n)} \\ \omega_1 & \omega_2 & \cdots & \omega_n \end{Bmatrix}, \quad x^{(i)} = (x_1^{(i)}, \ldots, x_p^{(i)}) \in \mathcal{X}, \; 0 < \omega_i \le 1, \; \sum_{i=1}^{n} \omega_i = 1.$$

Following Wang and Leblanc (2008) and Gao and Zhou (2014), the information matrix for a design ξ based on the SLSE that allow a precise estimation for the parameter vector θ is given by

$$\begin{aligned} M(\xi, \vartheta) &= G_2(\xi, \theta) - t g_1(\xi, \theta) g_1^T(\xi, \theta) \\ &= \int_{\mathcal{X}} \nabla\eta(x, \theta) \nabla\eta(x, \theta)^T d\xi - t \int_{\mathcal{X}} \nabla\eta(x, \theta) d\xi \left(\int_{\mathcal{X}} \nabla\eta(x, \theta) d\xi \right)^T, \end{aligned} \tag{2}$$

where $\vartheta = (\theta^T, t)^T \in \Theta \subset \mathbb{R}^q \times [0, 1)$, $t = \mu_3^2 / \{\sigma^2(\mu_4 - \sigma^4)\}$ with $E(\varepsilon^3|x) = \mu_3$ and $E(\varepsilon^4|x) = \mu_4$, and

$$\nabla\eta(x, \theta) = \frac{\partial \eta(x, \theta)}{\partial \theta} = \left(\frac{\partial \eta(x, \theta)}{\partial \theta_1}, \ldots, \frac{\partial \eta(x, \theta)}{\partial \theta_q} \right)^T.$$

Note that the information matrices of the design ξ based on the SLSE and OLSE are the same when $\mu_3 = 0$ which means the error distribution is symmetric and $t = 0$.

An optimal design minimizes some convex function of the inverse of the information matrix and numerous criteria have been proposed in the literature to find optimal designs in the entire class of competing designs (see, for example, Fedorov (1972), Pukelsheim (1993) and Dette (1997) among others). Based on the most efficient SLSE, Gao and Zhou (2014) proposed