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Optimal designs for probability-based optimality, parameter estimation and model discrimination

N.M. Kilany

Faculty of Science, Menoufia University, Shebin El Koom, Egypt

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ABSTRACT

In this paper, a new compound optimality criterion will be introduced. This criterion called PDKL-optimality. The proposed criterion aimed to introduce designs satisfy maximum probability of success, efficient parameter estimation and true model. An equivalence theorem is stated and proved for PDKL-optimality criterion.

1. Introduction

The D-optimality criterion is the common criterion for achieving efficient parameter estimation. For more details about D-optimality, see [1–3]. D-optimal designs are conventional optimizations based on a chosen optimality criterion and the model that will be suitable.

In the literature, there are several optimality criteria for discriminate between models (Ds -, T- and KL-criteria). Each of these criteria becomes applicable under certain condition and situation. In the case of the experimenter want to discriminate between nested models, the Ds-criterion can be applied. Thus, for two nested regression models which differ by $s > 1$ parameters. T-optimality criterion introduced in [4,5] is a different method for discriminating between models. This criterion is useful for two or more regression models and applied on linear or nonlinear models. However, T-criterion must be used to discrimination homoscedastic models with Gaussian errors. Uciński and Bogacka [6] introduced an extension of T-criterion for non-homoscedastic errors. For discriminating between more generalized models with random errors following any distribution [7, 8] introduced the KL-criterion, which depends on the Kullback–Liebler distance. Moreover, the T-criterion is a special case of the KL-criterion in the homoscedastic case and the generalization provided by Uciński and Bogacka [6] (in the heteroscedastic case), when the error distribution is normal. Finally, the KL-criterion can be used when the rival models are nested or not, homoscedastic or heteroscedastic, and in the case of the distribution has normal error.

Sometimes, experimenters wish to maximize the probability of an outcome. To this aim, McGree and Eccleston [9] have proposed a P-optimality criterion, which provide a maximum probability of observing outcome. Moreover, there are situation when an experimenter may be interested to achieve multiple objectives. For this aim, a PDKL-optimality criterion will be derived in this paper. This criterion proposed a method of compound criteria to achieve designs to hold an efficient parameter estimation, true model and a high probability of favorite outcome.

The paper is organized as follows: Section 2 introduced a simple review for D-, KL-, P- optimum designs. Compound design criteria DKL- and DP-optimum designs are presented Section 3. Finally, a new criterion called PDKL-optimality will be derived and an equivalence theorem is proved in Section 4.

E-mail address: neveenkilany@hotmail.com

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2. D-, KL-, P-optimum designs

2.1. KL-optimum designs

López-Fidalgo et al. [8] introduced a criterion for discrimination between two models, which consider a generalization of T-criterion for the case of non-normal models. This criterion called KL-criterion and it is definition depend on the Kullback–Leibler distance between two statistical models.

Let y be a random variable and let $f_1(y, \mathrm{x}, \theta_1)$ and $f_2(y, \mathrm{x}, \theta_2)$ be two rival probability density functions of y, $\mathrm{x} \in \chi$ and on a vector of unknown parameters, $\theta_i \in \Theta_i, i = 1, 2$. Assuming that $f_1(y, \mathrm{x}, \theta_1)$ is the "true" model, then the KL distance between the true model $f_1(y, \mathrm{x}, \theta_1)$ and other model $f_2(y, \mathrm{x}, \theta_2)$ is

$$\mathcal{I}(f_1, f_2, \mathrm{x}, \theta_2) = \int_\chi f_1(y, \mathrm{x}; \theta_1) log \frac{f_1(y, \mathrm{x}; \theta_1)}{f_2(y, \mathrm{x}; \theta_2)} dy, \qquad \mathrm{x} \in \chi$$

where, an experimental condition x generated by the experimenter from a design ξ is a random variable (or a random vector) belongs to an experimental domain $\chi \subset \mathbb{R}^m, m \geq 1$.

The KL-optimality criterion is given by

$$I_{21}(\xi) = \min_{\theta_2 \in \Theta_2} \int_\chi \mathcal{I}(f_1, f_2, \mathrm{x}, \theta_2) \xi(d\mathrm{x}) \tag{1}$$

The KL-optimum design is the design maximizes $\mathrm{I}_{21}(\xi)$ and denoted by ξ^*_{KL}.

For regular design ξ^*_{21}, López-Fidalgo et al. [8] prove that $\xi^*_{21}$is a KL-optimum design if f $\psi_{21}(x, \xi^*_{21}) \leq 0$, $x \in \chi$, where,

$$\psi_{21}(x, \xi) = \mathcal{I}\left(f_1, f_2, \mathrm{x}, \hat{\theta}_2\right) - \int_\chi \mathcal{I}\left(f_1, f_2, \mathrm{x}, \hat{\theta}_2\right) \xi(dx)$$

is the directional derivative of $I_{21}(\xi)$. The KL-efficiency of a design ξ relative to the optimum design $\xi^*_{21}$is

$$Eff_{21}(\xi) = \frac{\mathrm{I}_{21}(\xi)}{\mathrm{I}_{21}\left(\xi^*_{21}\right)} \tag{2}$$

2.2. D-optimum designs

D-optimality is the vital design criterion, introduced by [10], which interested of the quality of the parameter estimates. The idea of D-optimality depends on maximization of logarithm the determinant of the information matrix $M(\xi, \theta)$,$log|M(\xi, \theta)|$, or equivalently, minimizes logarithm determinant of the inverse of information matrix, $log|M^1(\xi, \theta)|$. In the general context for D-optimality [11] redefined the D-optimality criterion as follows:

$$\Phi_{D_i}[M_i(\xi, \theta_i)] = \begin{cases} log|M_i(\xi, \theta_i)| & \text{if } |M_i(\xi, \theta_i)| \text{ is nonsingular,} \\ -\infty & \text{if } |M_i(\xi, \theta_i)| \text{ is singular} \end{cases} \tag{3}$$

where $|M_i((\xi, \theta_i), \xi)| = \sum_{\mathrm{x} \in \chi} J_i(\mathrm{x}, \theta_i) \xi(\mathrm{x})$ is the information matrix corresponding to the probability density function $f_i(y, \mathrm{x}; \theta_i)$, $i = 1, 2$ and $J_i(\mathrm{x}, \theta_i)$ is the Fisher's information matrix for a single observation on y at x.

A design $\xi^*_{D_i}$ is a D-optimum design iff $\psi_{D_i}(\mathrm{x}, \xi^*_{D_i}) \leq 0$, $x \in \chi$, where

$$\psi_{D_i}(\mathrm{x}, \xi) = tr\left[M_i^{-1}(\xi, \theta_i) J_i(\mathrm{x}, \theta_i)\right] - q_i, \ \ i = 1, 2$$

is the directional derivative of the D-criterion function. The D-efficiency of any design ξ is given by

$$Eff_{D_i}(\xi) = \left(\frac{|M(\xi, \theta_i)|}{\left|M\left(\xi^*_{D_i}, \theta_i\right)\right|}\right)^{1/q_i} \quad i = 1, 2. \tag{4}$$

where q_i is the number of parameters for each model.

2.3. P-optimum designs

Often, experimenters request to obtain a maximum probability of an outcome. To this aim, McGree and Eccleston [9] have proposed a P-optimality criterion. P-optimality criterion is a criterion aimed to maximize a function of the probability of observing a particular outcome.

One of the forms of P-optimality which defined as a maximization of a weighted sum of the probabilities of success, which is defined as follows:

$$\Phi_P(\xi) = \sum_{j=1}^n \pi_j(\boldsymbol{\theta}, \xi_j) w_j, \quad \text{for} \quad j = 1, 2, \ldots\ldots, n$$

where, $\pi_j(\boldsymbol{\theta}, \xi_j)$ is the j-th probability of success given by ξ_j and w_j is the experimental effort relating to the j-th support point. In this criterion, design weights have been included and will play a role in maximizing the probabilities.

For two rival models $f_1(y, x, \theta_1)$ and $f_2(y, x, \theta_2)$, we can defined the P-optimality criterion by the following function

$$\Phi_{P_i}(\xi) = \sum_{j=1}^n \pi_{ij}(\theta_i, \xi_j) w_j, \ \ i = 1, 2 \tag{5}$$

where $\pi_{ij}(\theta_i, \xi_j)$ is the j-th probability of success in the model $f_i(y, x; \theta_i)$ and θ_i are the parameters for the two possible models. A design $\xi^*_{P_i}$ is a P-optimum design for high probability of success for the model $f_i(y, x; \theta_i)$ iff $\psi_{P_i}(x, \xi^*_{P_i}) \leq 0$, $x \in \chi$, where

$$\psi_{P_i}\left(x, \xi^*_{P_i}\right) = \frac{\Phi_{P_i}(x) - \Phi_{P_i}\left(\xi^*_{P_i}\right)}{\Phi_{P_i}\left(\xi^*_{P_i}\right)}$$

is the directional derivative of $\Phi_{P_i}(\xi)$. The P- efficiency of a design ξ relative to the optimum design ξ^*_P is

$$Eff_{P_i}(\xi) = \frac{\sum_{j=1}^n \pi_{ij}(\theta_i, \xi_j) w_j}{\sum_{j=1}^n \pi_{ij}\left(\theta_i, \xi^*_{P_i}\right) w_j}, \ \ i = 1, 2 \tag{6}$$

3. Compound design criteria

There are situations when a practitioner may be interested in a multiple objectives. To achieve the possible objectives, compound criteria can be used. A compound criterion optimizes a combination of multiple objective functions molded by maximizing a weighted product of efficiencies. In this Section, the DKL- and DP-compound criteria will be presented. The aim of DKL-optimality is to obtain an efficient parameter estimation and true model and DP-optimality aimed to obtain an efficient parameter estimation with probability based optimality.

3.1. DKL-optimum designs

Tommasi [12] introduced the DKL-optimality criterion for dual objective; discrimination between two rival models and efficient estimation for their parameters. For discrimination between $f_1(y, \mathrm{x}; \theta_1)$ and $f_2(y, \mathrm{x}; \theta_2)$ models, two possible KL-criteria have been considered, namely $I_{21}(\xi)$ and $I_{12}(\xi)$, excepting the case of nested models, where the largest model must be considered as the true model.

The DKL-optimality defined as follows

$$\Phi_{DKL}(\xi) = \left(\frac{\mathrm{I}_{21}(\xi)}{\mathrm{I}_{21}\left(\xi^*_{21}\right)}\right)^{\alpha_1} \left(\frac{\mathrm{I}_{12}(\xi)}{\mathrm{I}_{12}\left(\xi^*_{12}\right)}\right)^{\alpha_2} \left(\frac{\left|M_1(\boldsymbol{\theta}, \xi)\right|}{\left|M_1\left(\boldsymbol{\theta}, \xi^*_{D_1}\right)\right|}\right)^{\alpha_3/q_1} \times \left(\frac{\left|M_2(\boldsymbol{\theta}, \xi)\right|}{\left|M_2\left(\boldsymbol{\theta}, \xi^*_{D_2}\right)\right|}\right)^{1-\alpha_1-\alpha_2-\alpha_3/q_2} \tag{7}$$

where the coefficients $\sum_{i=1}^{3}\alpha_i = 1,\ 0 \le \alpha_i \le 1$. These coefficients illustrates the importance of the parts of the design criterion. Taking the logarithm of (7) yields,

$$\log \Phi_{DKL}(\xi) = \alpha_1 \log \mathrm{I}_{21}(\xi) + \alpha_2 \log \mathrm{I}_{12}(\xi) + \frac{\alpha_3}{q_1} \log\left|M_1(\boldsymbol{\theta}, \xi)\right| + \frac{1-\alpha_1-\alpha_2-\alpha_3}{q_2} \log\left|M_2(\boldsymbol{\theta}, \xi)\right| \tag{8}$$

The terms involving ξ^*_{21}, ξ^*_{12}, $\xi^*_{D_1}$ and $\xi^*_{D_2}$ must be ignored, when the maximization will be taken over ξ. A DKL-optimum design, ξ^*_{DKL}, maximizes $\log \Phi_{DKL}(\xi)$.

The equivalence theorem for DKL-optimum designs is state that the directional derivative function, $\psi_{DKL}(\mathrm{x}, \xi^*_{\mathrm{DKL}}) \le 0$, where,

$$\psi_{DKL}(\mathrm{x}, \xi) = \alpha_1 \frac{\psi_{21}(\mathrm{x}, \xi)}{\mathrm{I}_{21}(\xi)} + \alpha_2 \frac{\psi_{12}(\mathrm{x}, \xi)}{\mathrm{I}_{12}(\xi)} + \frac{\alpha_3}{q_1} \psi_{\mathrm{D}_1}(\mathrm{x}, \xi) + \frac{1-\alpha_1-\alpha_2-\alpha_3}{q_2} \psi_{\mathrm{D}_2}(\mathrm{x}, \xi)$$

3.2. DP-optimum designs

For the aim of parameter estimation and probability based-optimality, McGree and Eccleston [9] have proposed DP-optimality criterion. From the definition of the compound design criterion, DP-optimality defined a weighted geometric mean of efficiencies design ξ with respect to *D*- and *P*- optimality. That is

$$\Phi_{DP}(\xi) = \left(\frac{\left|M_1(\boldsymbol{\theta}, \xi)\right|}{\left|M_1(\boldsymbol{\theta}, \xi^*_D)\right|}\right)^{\alpha/q_1} \left(\frac{\sum_{i=1}^{n} \pi_i(\boldsymbol{\theta}, \xi_i) w_i}{\sum_{i=1}^{n} \pi_i(\boldsymbol{\theta}, \xi^*_P) w_i}\right)^{1-\alpha} \tag{9}$$

Taking the logarithm of (9) yields,

$$\log \Phi_{DP}(\xi) = \frac{\alpha}{q_1} \log\left|M_1(\boldsymbol{\theta}, \xi)\right| + (1-\alpha) \log \sum_{i=1}^{n} \pi_i(\boldsymbol{\theta}, \xi_i) w_i \quad (10))$$

The terms containing ξ^*_D and ξ^*_P have been ignored, since they are constants when a maximum is taken over ξ. A *DP*-optimum design, ξ^*_{DP}, maximizes $\log \Phi_{DP}(\xi)$. The equivalence theorem for *DP*-optimum design states that the derivative function, $\psi_{DP}(x, \xi^*_{DP}) \le \alpha$, where

$$\psi_{DP}(\mathrm{x}, \xi^*_{DP}) = \frac{\alpha}{q_1} f^{\mathrm{T}}(\mathrm{x}) M^{-1}(\boldsymbol{\theta}, \xi^*_{DP}) f(\mathrm{x}) + (1-\alpha)\left(\frac{\Phi_P(\mathrm{x}) - \Phi_P(\xi^*_{DP})}{\Phi_P(\xi^*_{DP})}\right)$$

where, $f(\mathrm{x})^T$is arrow of the design matrix X=$\{f(\mathrm{x}_1)^T, \ldots . f(\mathrm{x}_n)^T\}$.

4. PDKL-optimum designs

In this section, we will introduce a new compound criterion; called PDKL-optimality. The PDKL- optimality criterion aimed to obtain the maximum joint efficiency for parameter estimation, model discrimination and probability based- optimality.

The new criterion is useful for different generalized linear models GLMs with binary data. GLMs extend normal theory of regression to any distribution belonging to the one-parameter exponential family. As well as the normal, this includes the gamma, Poisson, and binomial distributions, all of which are important in the analysis of data. GLMs relates the random term (the independent response Y) to the systematic term to the linear predictor $(X\beta)$ via a link function g(.). Consider the generalized linear model GLMs

$$E(Y) = \mu = \eta = g^{-1}(X\beta)$$

which is defined by the distribution of the response, Y, a linear predictor η and two functions:

- A link function g(.) that describes how the mean, $E(Y_i) = \mu_i$ depends on the linear predictor $g(\mu_i) = Y_i$.
- A variance function that describes how the variance, $Var(Y_i)$ depends on the mean

  $$Var(Y_i) = \phi(V(\mu))$$

  where the dispersion parameter ϕ is a constant.

In GLMs, the errors or noise ϵ_i have relaxed assumptions where it may or may not have normal distribution. Some common link functions are used such that the identity, logit, log and probit link to induce the traditional linear regression, logistic regression, Poisson regression models.

The formula of PDKL-optimality can be derived using the weighted geometric mean of efficiencies design for P-, D-, and KL-optimum design. That is

$$\left(\frac{\mathrm{I}_{21}(\xi)}{\mathrm{I}_{21}(\xi^*_{21})}\right)^{\alpha_1} \left(\frac{\mathrm{I}_{12}(\xi)}{\mathrm{I}_{12}(\xi^*_{12})}\right)^{\alpha_2} \left(\frac{\left|M_1(\boldsymbol{\theta}, \xi)\right|}{\left|M_1(\boldsymbol{\theta}, \xi^*_{D_1})\right|}\right)^{\frac{\alpha_3}{q_1}} \left(\frac{\left|M_2(\boldsymbol{\theta}, \xi)\right|}{\left|M_2(\boldsymbol{\theta}, \xi^*_{D_2})\right|}\right)^{\frac{\alpha_4}{q_2}} \times \left(\frac{\sum_{j=1}^{n} \pi_{1j}(\boldsymbol{\theta}_1, \xi_j) w_j}{\sum_{j=1}^{n} \pi_{1j}(\boldsymbol{\theta}_1, \xi^*_{P_1}) w_j}\right)^{\alpha_5} \left(\frac{\sum_{j=1}^{n} \pi_{2j}(\boldsymbol{\theta}_2, \xi_j) w_j}{\sum_{j=1}^{n} \pi_{2j}(\boldsymbol{\theta}_2, \xi^*_{P_2}) w_j}\right)^{\alpha_6} \tag{11}$$

where the coefficients $\sum_{i=1}^{6}\alpha_i = 1$ and $0 \le \alpha_i \le 1,\ i = 1, 2, \ldots, 6$.

To interpret the structure of the design criterion, take logarithm of Eq. (11). Except for some constant terms, the criterion to be maximized will be

$$\Phi_{PDKL}(\xi) = \alpha_1 \log \mathrm{I}_{21}(\xi) + \alpha_2 \log \mathrm{I}_{12}(\xi) + \frac{\alpha_3}{q_1} \log\left|M_1(\boldsymbol{\theta}, \xi)\right| + \frac{\alpha_4}{q_2} \log\left|M_2(\boldsymbol{\theta}, \xi)\right| + \alpha_5 \log \sum_{j=1}^{n} \pi_{1j}(\boldsymbol{\theta}_1, \xi_j) w_j + \alpha_6 \log \sum_{j=1}^{n} \pi_{2j}(\boldsymbol{\theta}_2, \xi_j) w_j \tag{12}$$

A PDKL-optimum design, ξ^*_{PDKL}, maximizes $\Phi_{PDKL}(\xi)$. The directional derivative function for Eq. (12) is given by:

$$\psi_{PDKL}(\mathrm{x}, \xi_{PDKL}) = \alpha_1 \frac{\psi_{21}(\mathrm{x}, \xi_{21})}{\mathrm{I}_{21}(\xi)} + \alpha_2 \frac{\psi_{12}(\mathrm{x}, \xi)}{\mathrm{I}_{12}(\xi)} + \frac{\alpha_3}{q_1} \psi_{D_1}(\mathrm{x}, \xi) + \frac{\alpha_4}{q_2} \psi_{D_2}(\mathrm{x}, \xi) + \alpha_5 \frac{\psi_{P_1}(\mathrm{x}, \xi)}{\sum_{j=1}^{n} \pi_{1j}(\theta_1, \xi_j) w_j} + \alpha_6 \frac{\psi_{P_2}(\mathrm{x}, \xi)}{\sum_{j=1}^{n} \pi_{2j}(\theta_2, \xi_j) w_j} \tag{13}$$

The general equivalence theorem for *PDKL*-optimality may be stated as follows,

Theorem. *For PDKL-optimal design, ξ^*_{PDKL}, the following three conditions are equivalent.*

(i) A necessary and sufficient condition for a design ξ^*_{PDKL} to be *PDKL*-optimum is fulfillment of the inequality, $\psi_{PDKL}(\mathrm{x}, \xi^*_{PDKL}) \le 0,\ \mathrm{x} \in \chi$, where the directional derivative ψ_{PDKL} is given in Eq. (13).

(ii) The upper bound of $\psi_{PDKL}(\mathrm{x}, \xi^*_{PDKL})$ is attained at the points of the optimum design.

(iii) For any non-optimum design ξ, that is a design for which $\Phi_{PDKL}(\xi) < \Phi_{PDKL}(\xi^*_{PDKL})$, $\sup_{x \in \chi} \psi_{PDKL}(\mathrm{x}, \xi^*_{PDKL}) > 1$

Proof. Let ξ_1 and ξ_2 be any two designs and $0 < \lambda < 1$ be a constant. From the definition of the KL- criterion function it follows that

$$I_{12}[\lambda\xi_1 + (1-\lambda)\xi_2]$$

$$= \min_{\theta_1 \in \Theta_1} \left\{ \lambda \int_{\chi} \mathcal{J}[(f_2, \mathrm{x}, \ \theta_2), (f_1, \mathrm{x}, \ \theta_1)] \xi_1(d\mathrm{x}) \right.$$
$$\left. +(1-\lambda) \int_{\chi} \mathcal{J}[(f_2, \mathrm{x}, \ \theta_2), (f_1, \mathrm{x}, \ \theta_1)] \xi_2(d\mathrm{x}) \right\}$$
$$\geq \lambda I_{12}(\xi_1) + (1-\lambda) I_{12}(\xi_2)$$

where the last inequality follows immediately by replacing each term

$$\int_{\chi} \mathcal{J}[(f_2, \mathrm{x}, \ \theta_2), (f_1, \mathrm{x}, \ \theta_1)] \xi_j(d\mathrm{x}), \ \ j = 1, 2$$

with its minimum $I_{12}(\xi_j), \ \ j = 1, 2$. Thus the KL-criterion function is concave function and hence the tow first terms in Eq. (12) are concave functions. The third and fourth terms of Eq. (12) is D-optimality for two rival models $f_1(y$, x, $\theta_1)$ and $f_2(y$, x, $\theta_2)$, respectively, which are concave optimality criterion. Also, since $\sum_{j=1}^{n} \pi_{1j}(\boldsymbol{\theta}_1, \xi_j) w_j \geq 0$ and $\sum_{j=1}^{n} \pi_{2j}(\boldsymbol{\theta}_2, \xi_j) w_j \geq 0$, so that $log \sum_{j=1}^{n} \pi_{1j}(\boldsymbol{\theta}_1, \xi_j) w_j$ and $log \sum_{j=1}^{n} \pi_{2j}(\boldsymbol{\theta}_2, \xi_j) w_j$ are concave functions. Thus Eq. (12) is a convex combination of concave functions, since the coefficients $\alpha_i, \ \ i = 1, 2, 3, 4, 5, 6$ satisfy the conditions $\sum_{i=1}^{6} \alpha_i = 1, \ \ 0 \leq \alpha_i \leq 1$. Consequently, the PDKL-design criterion defined in Eq. (12) is concave function. Thus, the PDKL-criterion satisfies the conditions of convex optimum design theory and therefore an equivalence theorem has been proved.

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