CDA-OPTIMUM DESIGN FOR PARAMETER ESTIMATION, MINIMIZING THE AVERAGE VARIANCE AND ESTIMATING THE AREA UNDER THE CURVE

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ABSTRACT

The aim of this paper is to introduce a new compound optimum design named*CDA*, by combining the C-optimality, D-optimality, and A-optimality together. The significance of the proposed compound gains from that it can be used for parameter estimation, minimizing the average variance and model estimation simultaneously.

KEYWORDS: optimum design; C-optimality; D-optimality; A-optimality; compound criteria.

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1. INTRODUCTION

Cook and Wong [2] considered a compound optimality criterion that is a convex combination of the two concave criteria and so we can find the optimal design directly as if this is a single objective optimal design problem. D-optimality focuses on the variances of the estimates of the coefficients in the model, which minimizing the determinant of $\left(X^T X\right)^{-1}$ which is equivalent to maximizing thedeterminant of $X^T X$. An exact design is called D-optimal, if it minimizes the determinant D of the covariance matrix. C-optimality interest is in estimating the linear combination of the parameters $c^T\beta$ with minimum variance, where c is a known vector of constants. In A-optimality $tr\, M^{-1}(\xi)$, the total variance of the parameter estimates, is minimized, equivalent to minimizing the average variance. This paper is organized as follows; the C -, D -, A – Optimum Designs were introduced in Section 2. The CDA-optimality was derived in section 3 and some of its properties were discussed. The generalized CDA- Optimum Design was introducedin Section 4.

2. C -, D -, A – OPTIMUM DESIGNS

C-optimality introduced by Elfving [2] which provided a geometrical interpretation for finding c-optimal designs and developed by Silvey and Titterington [10] and Titterington[11]. Fellman [4]justified that at most m linearly independent support points are needed for a c-optimal design. Pukelsheim and Torsney [9]introduced a method for computing c-optimal weights given the support points. C–optimality minimize the variance of the best linear unbiased estimate for a given linear combination of the model parameters $c^T \theta$, where *c* is $p \times 1$, a vector of a known constants. The c-optimaity criterion to be minimized is thus

$$\operatorname{var} c^T \hat{\theta} \propto c^T M^{-1}(\xi)\, c$$

The aim of c-optimality is to obtain the best design for estimating the linear combination of the parameters

$$c_1\theta_1 + \cdots + c_p\theta_p = c^T\theta$$

The efficiency of any design ξ relative to C-optimum design is defined as:

$$Eff^{\,c}(\xi) = \frac{c^T M^{-1}\left(\xi_c^*\right)c}{c^T M^{-1}(\xi)\,c}$$

C–optimality is defined as $\min \operatorname{var}\left(C^T\theta\right)$, which is proportional to $C^T M^{-1}(\xi)\,C$. A disadvantage of c-optimum designs is that they are often singular.

D- Optimum Design

D-optimum design is one of the most commonly used design criteria for linear regression model that is also known as the **D**eterminant criterion. This criterion introduced by Wald [12], and later was called D-optimality by Kiefer and Wolfowitz [5]. The D-Optimality is the most common criterion due to numerous applications found in the literature; see for example, Latif and Zafar Yab [6]and Poursina and Talebi [8]. D-optimality criterion is just to maximize the determinant of the Fisher information matrix, $|X^T X|$, this means that the optimal design matrixX^* contains the n experiments which maximizes the determinant of $X^T X$.

Mathematically, $$\left|X^{*T} X^*\right| = \max\left(\left|X^T X\right|\right)$$

Maximizing the determinant of the information matrix $X^T X$ is equivalent to minimizing the determinant of the dispersion matrix $\left(X^T X\right)^{-1}$. Using such an idea, the D-efficiency of an arbitrary design, *X*, is naturally defined as

$$Eff(D) = \left\{\frac{|M(\xi)|}{\left|M\left(\xi_D^*\right)\right|}\right\}^{1/P}$$

A-Optimum Design

A-optimality criterion introduced by Chernoff [1]; who showed that the employed criterion of optimality is the one that involves the use of Fisher's information matrix. Invariance under re-parameterization loses its appeal if the parameters of interest have a definite physical meaning. Then the average-variance criterion provides a reasonable alternative. If the coefficient matrix is partitioned into its columns, $K = (c_1, \ldots, c_s)$, then the inverse $1/\phi_{-1}$ can be represented as

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$$\frac{1}{\phi_{-1}(C_K(A))} = \frac{1}{s}tr\left(C_K(A)^{-1}\right) = \frac{1}{s}tr\left(K'A^{-}K\right) = \frac{1}{s}\sum_{j\le s} c_j^{'} A^{-} c_i$$

This is the average of the standardized variances of the optimal estimatorsfor the scalar parameter systems $c_1^{'}\theta,...,c_s^{'}\theta$ formed from the columns of K. From the point of view of computational complexity, the criterion ϕ_{-1} is particularly simple to evaluate since it only requires the computation of the *s* diagonal entries of the dispersion matrix $K'A^{-}K$.

3. CDA- OPTIMUM DESIGN

To obtainparameter estimation, minimizing the average variance and model estimation of the area under the curve, a new compound criteria called *CDA* is introduced.*CDA* is constructedby combing C, D and A-optimality. By maximizing a weighted product of the efficiencies

$$\left\{Eff^{(c)}\right\}^{k}.\left\{Eff^{(D)}\right\}^{k(1-k)}.\left\{Eff^{(A)}\right\}^{(k-1)^2}$$

Then taking the logarithm we get

$$k\log\left\{Eff^{(c)}\right\}+k(1-k)\left\{Eff^{(D)}\right\}+(k-1)^2\left\{Eff^{(A)}\right\}$$

$$=k\log\left\{\frac{c^T M^{-1}\left(\xi_c^*\right)c}{c^T M^{-1}(\xi)c}\right\}+k(1-k)\log\left\{\frac{|M(\xi)|}{\left|M\left(\xi_D^*\right)\right|}\right\}^{1/P}+(k-1)^2\log\left\{\frac{tr\,M^{-1}\left(\xi_A^*\right)}{tr\,M^{-1}(\xi)}\right\}$$

$$=-k\log\left\{c^T M^{-1}(\xi)c\right\}+k(1-k)\log\left\{|M(\xi)|\right\}^{1/P}+(k-1)^2\log\left\{tr\,M^{-1}(\xi)\right\}$$

The terms containing ξ_c^*, ξ_D^* and ξ_A^* are constants, a maximum is found over ξ. Hence, thecriterion that has to be maximized is given by

$$\Phi^{(CDA)}(\xi)=-k\log\left\{c^T M^{-1}(\xi)c\right\}+\frac{k(1-k)}{p}\log\left\{\left|M^{-1}(\xi)\right|\right\}+(k-1)^2\log\left\{tr\,M^{-1}(\xi)\right\}$$

and the derivative function for CDA-optimality is

$$\phi^{(CDA)}(x,\xi)=\frac{-k\left\{f^T(x)M^{-1}(\xi)c\right\}^2}{c^T M^{-1}(\xi)c}+\frac{(k-1)^2}{p}\left\{f^T(x)M^{-1}f(x)\right\}+(k-1)^2\left\{f^T(x)M^{-2}f(x)\right\}$$

A CDA-optimum design, ξ_{CDA}^*, maximizes $\Phi_{CDA}(\xi)$ or equivalently $\log\Phi_{CDA}(\xi)$. The equivalence theorem can now be stated as follows:

Theorem 1.

i. A necessary and sufficient condition for a design ξ_{CDA}^* to be CDA-optimum is fulfillment of the inequality $\phi^{(CDA)}\left(x,\xi_{CDA}^*\right)\le 1,\ x\in\chi$.

ii. The upper bound of $\phi^{(CDA)}(x,\xi_{CDA}^*)$ is achieved at the points of the optimum design.

iii. For any non-optimum design ξ_1 that is a design for which $\Phi^{(CDA)}(\xi)<\Phi^{(CDA)}\left(\xi_{CDA}^*\right)$ and $\sup_{x\in\chi}\phi^{(CDA)}\left(x,\xi_{CDA}^*\right)>1$.

A measure of efficiency of a design ξ relative to a CDA-optimum design is given by

$$Eff_{CDKL}(\xi)=\frac{\Phi_{CDA}(\xi)}{\Phi_{CDA}(\xi_{CDA}^*)}$$

The proof can be made directly, since $\Phi^{(CDA)}(\xi)$, $0\le k\le 1$ is a convex combination of three optimum design criteria, so the CDA-criterion is also convex and satisfying convexity conditions.

Properties of CDA-Optimality

A good design should give a small variance matrix, therefore the function Φ is related to the variance matrix, and should have following properties:

i. **Non-negativity:**$\Phi_{CDA}(M) \geq 0$,

ii. **Isotonicity:** if $(M^* - M)$ is a positive semi-definite matrix, then $\Phi[M^*] \geq \Phi[M]$.

iii. **Positive homogeneity:** $\Phi[kM] = \mathrm{k}\,\Phi[M]$; $k > 0$,

iv. **Superadditivity:** $\Phi[M + M^*] \geq \Phi[M] + \Phi[M^*]$.

The previous properties are important to define with a proper scaling the relative efficiency of an experiment (or a design with the matrix *M*) with respect to another reference experiment withM^*. Pazman [7]discussed some other optimality properties for small samples.

4. THE GENERALIZED CDA-OPTIMALITY:

A generalized CDA-criterion will be introduced as:

$$\Phi^{(GCDA)}(\xi) = -\sum_{j=1}^{m} a_j \log\left\{A_j^T c^T M^{-1}(\xi) c A_j\right\} + \sum_{i=1}^{n} \frac{s_i}{b_i} \log\left\{\left|A_i^T M^{-1}(\xi) A_i\right|\right\}$$
$$+ \sum_{l=1}^{k} c_l \log tr\left\{A_l^T M^{-1}(\xi) A_l\right\}$$

where, a_j, s_i, b_i *and* c_l are sets of non-negative coefficients reflecting the importance of the parts of the design criteria.

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