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OPTIMAL STATISTICAL DESIGNS WITH CIRCULAR STRING PROPERTY

Rahul Mukerjee
Stat.-Math. Division
Indian Statistical Institute
Calcutta - 700035, India

and

S. Huda
Department of Statistics
King Saud University
Riyadh 11451, Saudi Arabia

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ABSTRACT

This paper develops an approximate theory for D- and A-optimal statistical designs with a circular string property. It is shown how the problems of deriving optimal designs can be reduced to non-linear programming problems involving small numbers of decision variables. The results are seen to be helpful in dealing with the exact design problem with a finite number of observations.

1. INTRODUCTION

A statistical design is said to have the string property if the design matrix be a (0,1)- matrix having exactly one run of 1's in each row. The problem of finding optimal designs with string property has been considered recently by Sinha and Saha (1983), Mukerjee and Huda (1985) and Mukerjee and Saharay (1985). Sinha and Saha (1983) indicate various applications of such designs in a number of fields. The present paper deals with a variant of the string property, namely the circular string property.

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Consider the standard linear model

$$\underline{Y} = X\underline{\beta} + \varepsilon,\ E(\underline{\varepsilon}) = \underline{0},\ \text{Disp}\ (\underline{\varepsilon}) = \sigma^2 I, \tag{1.1}$$

where $\underline{Y}$ is the observational vector, X is the design matrix, $\underline{\beta}(p\times 1)$ is the vector of parameters and $\sigma^2 > 0$. Let the p positions in each row of X be labeled $0,1,\ldots,p-1$. Then a design will be defined to have the circular string property (CSP) if (i) the entries of X are 0 or 1, and (ii) for $i = 1,2,\ldots$, in the ith row of X, 1's occur in positions labeled $u_i, u_i+1, \ldots, u_i+v_i$ for some u_i, v_i, where $0 \le u_i, v_i \le p-1$ and addition is reduced mod p. The condition (ii) essentially means that there is exactly one 'circular' run of 1's in each row of X. As an example if

$$X = \begin{bmatrix} 0 & 0 & 1 & 1 \\ 1 & 1 & 0 & 1 \\ 1 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 \end{bmatrix}$$

then the design has CSP with $p=4$, $u_1=2$, $v_1=1$, $u_2=3$, $v_2=2$, $u_3=3$, $v_3=1$, $u_4=1$, $v_4=0$ and $u_5=1$, $v_5=1$.

Designs with CSP may arise naturally in many practical situations. For example, suppose interest lies in measuring the consecutive distances, along the circumference, between p objects fixed along a ring. Since the measurement of the distance between any two objects automatically takes account of the intermediate objects, the resulting design matrix has CSP. Yet another example arises considering the problem of measuring the lengths of the sides of a convex polygon. These examples are quite general in nature and cover many particular practical situations especially in the fields of biometry and industry.

Under the model (1.1), this paper derives D- and A-optimal designs with CSP for estimating $\underline{\beta}$. An approximate theory, following the line of Fedorov (1972) and Silvey (1980), has been developed which is seen to be helpful in dealing with the more intractable design problem with a finite number of observations. It may be noted that the designs considered here have a close link with spring balance weighing designs (see Raghavarao (1971), Banerjee (1975) for a comprehensive list of references).

2. PRELIMINARIES

Let $S = \{(u,v): 0 \le u \le p-1,\ 0 \le v \le p-2\} \cup \{(0,p-1)\}$. For $(u,v) \in S$, let $\underline{h}_{uv}$ be a p-component (0,1)-vector with 1 at the uth, (u+1)th,..., (u+v)th (mod p) positions. In particular, $\underline{h}_{0,p-1}$ is the p-component vector with all elements unity. With p parameters and CSP, each row of the design matrix must be the transpose of one of the vectors $\underline{h}_{uv}$. Let $\mathcal{X}$, the design space, be the set of vectors $\underline{h}_{uv}$, $(u,v) \in S$.

Following Silvey (1980, p. 15), let H be the class of probability distributions on the Borel sets of $\mathcal{X}$. Any $\eta \in H$ will be called a design measure. The finiteness of $\mathcal{X}$ implies that any such η defines a discrete distribution over $\mathcal{X}$ assigning a mass π_{uv}, say, at $\underline{h}_{uv}$, $(u,v) \in S$. For $\eta \in H$, define the p×p information matrix $M(\eta) = E(\underline{x}\ \underline{x}')$, $\underline{x}$ being a random vector with distribution η. Let $\Gamma = \{M(\eta): \eta \in H\}$ and ϕ be an extended real-valued function defined over the class of p×p non-negative definite matrices and bounded above on Γ. A design measure that maximizes $\phi\{M(\eta)\}$ over H will be called ϕ-optimal. In particular, for D- and A-optimality one takes

$$\begin{aligned} \phi\{M(\eta)\} &= \log\det M(\eta) \text{ and} \\ \phi\{M(\eta)\} &= -\operatorname{tr}[\{M(\eta)\}^{-1}] \text{ if } M(\eta) \text{ is positive definite,} \\ &= -\infty \text{ otherwise} \end{aligned} \tag{2.1}$$

respectively.

In a similar setting, Mukerjee and Saharay (1985) and Mukerjee and Huda (1985) applied the technique of Fréchet derivative (cf. Silvey (1980, p. 19)) in obtaining optimal designs. But a successful application of this technique requires some guess about the optimal design which appears to be extremely difficult for the present problem. Therefore, as an alternative approach, we first reduce H to a much smaller subclass containing the D- and A-optimal designs. This subclass will be seen to be much simpler to deal with. The reduction is achieved through a number of theorems as follows.

Theorem 2.1. Let H_1 be a subclass of H containing only the design measures for which

$$\pi_{0v} = \pi_{1v} = \ldots = \pi_{p-1,v} \quad (0 \le v \le p-2).$$

Then a ϕ-optimal design measure in H_1 is also ϕ-optimal in H provided ϕ is concave and permutation invariant.

Proof. Take any $\eta_o \in H$ such that the probability masses distributed by η_o are π^o_{uv}, $(u,v) \in S$. Let $\bar{\eta}_o$ be a design measure for which

$$\pi_{uv} = p^{-1}\sum_{u=0}^{p-1} \pi^o_{uv} \quad (0 \le u \le p-1,\ 0 \le v \le p-2),\quad \pi_{0,p-1} = \pi^o_{0,p-1}.$$

Then $\bar{\eta}_o \in H_1$ and

$$M(\bar{\eta}_o) = p^{-1}\sum_{u=0}^{p-1} R_u M(\eta_o) R_u' , \tag{2.2}$$

where $R_0 = I_p$ and $R_1,\ldots,R_{p-1}$ are cyclic permutation matrices of order p. If ϕ is concave and permutation invariant then proceeding along the line of proof of Proposition 1 in Kiefer (1975), it follows from (2.2) that $\phi\{M(\eta_o)\} \le \phi\{M(\bar{\eta}_o)\}$, completing the proof.

Since by (2.1) the function ϕ is concave and permutation invariant for D- and A-optimality, attention will hereafter be restricted only to the class H_1 in view of Theorem 2.1.

3. FURTHER REDUCTION

For any design measure in H_1 let α_{v+1} be the common value of $\pi_{0v}, \pi_{1v}, \ldots, \pi_{p-1,v}$ $(0 \le v \le p-2)$ and $\alpha_p = \pi_{0,p-1}$. Clearly,

$$p(\alpha_1+\ldots+\alpha_{p-1}) + \alpha_p = 1. \tag{3.1}$$

To achieve a further reduction of the problem, the cases of odd and even p are considered separately. In the sequel, the p×p circulant

$$\begin{bmatrix} b_0 & b_1 & \cdots & b_{p-1} \\ b_{p-1} & b_0 & \cdots & b_{p-2} \\ & & \vdots & \\ b_1 & b_2 & \cdots & b_0 \end{bmatrix}$$

will be denoted by $\{b_0, b_1, \ldots, b_{p-1}\}$.

Considering first the case of odd p, let $p = 2m+1$. Then for $\eta \in H_1$ it may be seen, after some simplification, that

$$M(\eta) = \{a_0, a_1, \ldots, a_m, a_m, \ldots, a_1\} ,$$

where

$$a_0 = \sum_{u=1}^{2m} u\alpha_u + \alpha_{2m+1},$$

$$a_j = \sum_{u=j+1}^{2m-j} (u-j)\alpha_u + \sum_{u=2m-j+1}^{2m} (2u-2m-1)\alpha_u + \alpha_{2m+1} \quad (1 \le j \le m-1) \tag{3.2}$$

$$a_m = \sum_{u=m+1}^{2m} (2u-2m-1)\alpha_u + \alpha_{2m+1}.$$

Hence the eigenvalues of $M(\eta)$ turn out (cf. Rao (1973, p. 68)) as linear functions of $\alpha_1, \ldots, \alpha_{2m+1}$ as

$$\lambda_0 = \sum_{u=1}^{2m} u^2\alpha_u + (2m+1)\alpha_{2m+1},$$

$$\lambda_j = \sum_{u=1}^{m} [u+2\sum_{r=1}^{u-1} (u-r)\cos\{2r\pi j/(2m+1)\}](\alpha_u+\alpha_{2m+1-u}) \quad (1 \le j \le 2m). \tag{3.3}$$

<u>Theorem 3.1</u>. For $p = 2m+1$, let H_0 be a subclass of H_1 containing only those design measures for which $\alpha_1 = \ldots = \alpha_m = \alpha_{2m+1} = 0$. Then a D-(A-)optimal design in H_0 is also D-(A-)optimal in H_1 and hence in H.

<u>Proof</u>. Consider any $\eta_1 \in H_1$ such that the probability

masses associated with η_1 are $\alpha_u^{(1)}$ $(1 \le u \le 2m+1)$. To avoid trivialities, let $\alpha_{2m+1}^{(1)} < 1$, for otherwise $M(\eta_1)$ becomes singular and one can easily identify designs in H_o dominating η_1 in terms of D- and A-optimality. Define $\eta_2 \in H_o$ such that the probability masses associated with η_2 are $\alpha_u^{(2)}$ where

$$\alpha_1^{(2)}=\ldots=\alpha_m^{(2)}=\alpha_{2m+1}^{(2)}=0,$$
$$\alpha_u^{(2)}=(\alpha_u^{(1)}+\alpha_{2m+1-u}^{(1)})/(1-\alpha_{2m+1}^{(1)}) \quad (m+1 \le u \le 2m). \tag{3.4}$$

For notational simplicity, let $a = \alpha_{2m+1}^{(1)}$ and

$$c = \sum_{u=m+1}^{2m} u^2(\alpha_u^{(1)}+\alpha_{2m+1-u}^{(1)}).$$

Since the $\alpha_u^{(1)}$'s satisfy (3.1),

$$c \ge (2m+1) \sum_{u=m+1}^{2m} (\alpha_u^{(1)}+\alpha_{2m+1-u}^{(1)}) = 1-a. \tag{3.5}$$

Denoting the eigenvalues of $M(\eta_1)$ and $M(\eta_2)$ by λ_{j1} and λ_{j2} $(0 \le j \le 2m)$ respectively, it follows from (3.3), (3.4) that

$$\lambda_{01} = \sum_{u=1}^{2m} u^2\alpha_u^{(1)} + (2m+1)a \le c + (2m+1)a,$$
$$\lambda_{02} = (1-a)^{-1}c, \quad \lambda_{j1} = (1-a)\lambda_{j2} \quad (1 \le j \le 2m). \tag{3.6}$$

Hence by (3.5),

$$\det M(\eta_2)/\det M(\eta_1) \ge [c/\{c+(2m+1)a\}](1-a)^{-(2m+1)}$$
$$\ge (1+2ma)^{-1}(1-a)^{-2m} \ge 1,$$

proving the assertion regarding D-optimality.

Considering now the proof for A-optimality, which is slightly more involved, note that for $\eta \in H_1$, $\mathrm{tr}\{M(\eta)\} = (2m+1)a_0$ and hence by (3.2), (3.3),

$$\sum_{j=1}^{2m} \lambda_{j1} = \mathrm{tr}\{M(\eta_1)\} - \lambda_{01} = \sum_{u=1}^{2m} u(2m+1-u)\alpha_u^{(1)}$$
$$= \sum_{u=m+1}^{2m} u(2m+1-u)(\alpha_u^{(1)}+\alpha_{2m+1-u}^{(1)})$$

$$\leq \sum_{u=m+1}^{2m} u^2(\alpha_u^{(1)}+\alpha_{2m+1-u}^{(1)}) = c.$$

Hence

$$\sum_{j=1}^{2m} \lambda_{j1}^{-1} \geq (2m)^2(\sum_{j=1}^{2m} \lambda_{j1})^{-1} \geq (2m)^2 c^{-1} \qquad (3.7)$$

By (3.6),

$$\mathrm{tr}[\{M(\eta_2)\}^{-1}]/\mathrm{tr}[\{M(\eta_1)\}^{-1}]$$

$$\leq (1-a)(c^{-1}+\sum_{j=1}^{2m}\lambda_{j1}^{-1})/[\{c+(2m+1)a\}^{-1}+\sum_{j=1}^{2m}\lambda_{j1}^{-1}]$$

Since the right-hand member in the above is non-increasing in $\Sigma_{j=1}^{2m} \lambda_{j1}^{-1}$, it follows from (3.7) and then (3.5) that

$$\mathrm{tr}[\{M(\eta_2)\}^{-1}]/\mathrm{tr}[\{M(\eta_1)\}^{-1}]$$

$$\leq (1-a)(c^{-1}+4m^2c^{-1})/[\{c+(2m+1)a\}^{-1} + 4m^2c^{-1}]$$

$$= (1-a)(1+4m^2)/[\{1+(2m+1)ac^{-1}\}^{-1} + 4m^2]$$

$$\leq (1-a)(1+4m^2)/[\{1+(2m+1)a(1-a)^{-1}\}^{-1} + 4m^2] \leq 1,$$

after some simplification, proving the assertion regarding A-optimality.

In view of Theorem 3.1, for odd p (=2m+1) it is enough to consider the class H_0. By (3.3), for $\eta \in H_0$, the eigenvalues of $M(\eta)$ are

$$\lambda_0 = \sum_{u=m+1}^{2m} u^2\alpha_u, \qquad (3.8)$$

$$\lambda_j = \sum_{u=1}^{m} [u+2\sum_{r=1}^{u-1}(u-r)\cos\{2r\pi j/(2m+1)\}]\alpha_{2m+1-u} \quad (1\leq j\leq 2m),$$

where by (3.1),

$$(2m+1)\sum_{u=m+1}^{2m}\alpha_u = 1;\ \alpha_{m+1},\ldots,\alpha_{2m} \geq 0. \qquad (3.9)$$

Note that $\lambda_j = \lambda_{2m+1-j}$ $(1\leq j\leq m)$. Hence by (2.1), the problems of finding D- or A-optimal designs reduce to non-linear programming problems involving the selection of $\alpha_{m+1},\ldots,\alpha_{2m}$, subject to (3.9) so as to maximize $\lambda_0\Pi\lambda_j^2$ or minimize $\lambda_0^{-1}+2\Sigma\lambda_j^{-1}$ respectively, where the product and the summation extend over $j = 1,\ldots,m$, and $\lambda_0,\lambda_1,\ldots,\lambda_m$ are as in (3.8). The number of decision variables m $(=(p+1)/2)$ is small for moderate values of p and, although one cannot hope to obtain compact algebraic expressions for optimal values of $\alpha_{m+1},\ldots,\alpha_{2m}$, the underlying non-linear programming problems may be tackled by standard numerical methods. Table I presents the values of $\alpha_{m+1},\ldots,\alpha_{2m}$ yielding D- or A-optimal designs for $p = 3,5,\ldots,19$. As one can see, in the optimal solutions each of $\alpha_{m+1},\ldots,\alpha_{2m}$ is positive which suggests that no further reduction of the class H_o, along the line of Theorem 3.1, is possible.

Turning to the case of even p $(=2m)$ the following result holds along the line of Theorem 3.1.

Theorem 3.2. For $p = 2m$, let H_e be a subclass of H_1 containing those design measures for which $\alpha_1=\ldots=\alpha_{m-1}=\alpha_{2m} = 0$. Then a D-(A-)optimal design in H_e is also D-(A-) optimal in H_1 and hence in H.

Analogously to (3.8), (3.9), for $\eta \in H_e$ the eigenvalues of $M(\eta)$ are

$$\lambda_0 = \sum_{u=m}^{2m-1} u^2\alpha_u,$$

$$\lambda_j = \sum_{u=1}^{m}[u+2\sum_{r=1}^{u-1}(u-r)\cos(r\pi j/m)]\alpha_{2m-u} \quad (1\le j\le 2m-1).$$

where $2m(\alpha_m+\ldots+\alpha_{2m-1}) = 1$; $\alpha_m,\ldots,\alpha_{2m-1} \ge 0$. Note that $\lambda_j = \lambda_{2m-j}(1\le j\le m-1)$. As before, the problems of finding D- or A-optimal designs reduce to non-linear programming problems in m variables and the optimal choices of $\alpha_m,\ldots,\alpha_{2m-1}$, obtained numerically for $p = 4,6,\ldots,18$, have been presented in Table I. Just as in the case of odd p, in the optimal solutions each of $\alpha_m,\ldots,\alpha_{2m-1}$ is positive and hence no further reduction of the class H_e is possible.

Table I: Optimal designs for $3 \leq p \leq 19$

p	D-optimal design	A-optimal design
3	$\alpha_2 = 0.3333$	$\alpha_2 = 0.3333$
4	$\alpha_2 = 0.0342$, $\alpha_3 = 0.2158$	$\alpha_2 = 0.0398$, $\alpha_3 = 0.2102$
5	$\alpha_3 = 0.0685$, $\alpha_4 = 0.1315$	$\alpha_3 = 0.0462$, $\alpha_4 = 0.1538$
6	$\alpha_3 = 0.0159$, $\alpha_4 = 0.0595$, $\alpha_5 = 0.0913$	$\alpha_3 = 0.0116$, $\alpha_4 = 0.0325$, $\alpha_5 = 0.1225$
7	$\alpha_4 = 0.0304$, $\alpha_5 = 0.0465$, $\alpha_6 = 0.0660$	$\alpha_4 = 0.0155$, $\alpha_5 = 0.0252$, $\alpha_6 = 0.1022$
8	$\alpha_4 = 0.0090$, $\alpha_5 = 0.0277$, $\alpha_6 = 0.0378$, $\alpha_7 = 0.0505$	$\alpha_4 = 0.0049$, $\alpha_5 = 0.0116$, $\alpha_6 = 0.0206$, $\alpha_7 = 0.0879$
9	$\alpha_5 = 0.0172$, $\alpha_6 = 0.0236$, $\alpha_7 = 0.0307$, $\alpha_8 = 0.0396$	$\alpha_5 = 0.0071$, $\alpha_6 = 0.0093$, $\alpha_7 = 0.0175$, $\alpha_8 = 0.0772$
10	$\alpha_5 = 0.0058$, $\alpha_6 = 0.0160$, $\alpha_7 = 0.0205$, $\alpha_8 = 0.0257$, $\alpha_9 = 0.0320$	$\alpha_5 = 0.0025$, $\alpha_6 = 0.0055$, $\alpha_7 = 0.0078$, $\alpha_8 = 0.0153$ $\alpha_9 = 0.0689$
11	$\alpha_6 = 0.0110$, $\alpha_7 = 0.0143$, $\alpha_8 = 0.0177$, $\alpha_9 = 0.0216$ $\alpha_{10} = 0.0263$	$\alpha_6 = 0.0038$, $\alpha_7 = 0.0046$, $\alpha_8 = 0.0067$, $\alpha_9 = 0.0135$ $\alpha_{10} = 0.0623$
12	$\alpha_6 = 0.0039$, $\alpha_7 = 0.0104$, $\alpha_8 = 0.0129$ $\alpha_9 = 0.0155$ $\alpha_{10} = 0.0185$, $\alpha_{11} = 0.0221$	$\alpha_6 = 0.0013$, $\alpha_7 = 0.0031$, $\alpha_8 = 0.0039$, $\alpha_9 = 0.0059$ $\alpha_{10} = 0.0122$, $\alpha_{11} = 0.0569$
13	$\alpha_7 = 0.0077$, $\alpha_8 = 0.0096$, $\alpha_9 = 0.0114$, $\alpha_{10} = 0.0135$ $\alpha_{11} = 0.0159$, $\alpha_{12} = 0.0188$	$\alpha_7 = 0.0022$, $\alpha_8 = 0.0026$, $\alpha_9 = 0.0034$, $\alpha_{10} = 0.0053$ $\alpha_{11} = 0.0111$, $\alpha_{12} = 0.0523$

(continued)

Table I (continued): Optimal designs for $3 \leq p \leq 19$

p	D-optimal design	A-optimal design
14	α_7= 0.0029, α_8= 0.0074, α_9= 0.0088, α_{10}= 0.0103 α_{11}= 0.0120, α_{12}= 0.0139, α_{13}= 0.0162	α_7= 0.0009, α_8= 0.0019, α_9= 0.0022, α_{10}= 0.0030 α_{11}= 0.0048, α_{12}= 0.0102, α_{13}= 0.0484
15	α_8= 0.0057, α_9= 0.0068, α_{10}= 0.0080, α_{11}= 0.0092 α_{12}= 0.0106, α_{13}= 0.0122, α_{14}= 0.0141	α_8= 0.0014, α_9= 0.0016, α_{10}= 0.0020, α_{11}= 0.0028 α_{12}= 0.0044 α_{13}= 0.0094, α_{14}= 0.0451
16	α_8= 0.0023, α_9= 0.0054, α_{10}= 0.0064, α_{11}= 0.0073 α_{12}= 0.0084, α_{13}= 0.0095, α_{14}= 0.0108, α_{15}= 0.0124	α_8= 0.0006, α_9= 0.0013, α_{10}= 0.0014, α_{11}= 0.0018 α_{12}= 0.0024, α_{13}= 0.0040, α_{14}= 0.0088, α_{15}= 0.0422
17	α_9= 0.0044, α_{10}= 0.0051, α_{11}= 0.0059, α_{12}= 0.0067, α_{13}= 0.0076, α_{14}= 0.0085, α_{15}= 0.0097, α_{16}= 0.0109	α_9= 0.0010, α_{10}= 0.0011, α_{11}= 0.0013, α_{12}= 0.0016, α_{13}= 0.0022, α_{14}= 0.0037 α_{15}= 0.0082, α_{16}= 0.0397
18	α_9= 0.0018, α_{10}= 0.0042, α_{11}= 0.0048, α_{12}= 0.0055, α_{13}= 0.0062, α_{14}= 0.0069, α_{15}= 0.0077, α_{16}= 0.0087, α_{17}= 0.0097	α_9= 0.0004, α_{10}= 0.0009, α_{11}= 0.0010 α_{12}= 0.0011, α_{13}= 0.0015, α_{14}= 0.0021, α_{15}= 0.0035, α_{16}= 0.0077, α_{17}= 0.0374
19	α_{10}= 0.0035, α_{11}= 0.0040, α_{12}= 0.0045, α_{13}= 0.0051, α_{14}= 0.0057, α_{15}= 0.0063, α_{16}= 0.0070, α_{17}= 0.0078, α_{18}= 0.0087	α_{10}= 0.0007, α_{11}= 0.0008, α_{12}= 0.0009, α_{13}= 0.0010, α_{14}= 0.0013, α_{15}= 0.0019, α_{16}= 0.0033, α_{17}= 0.0073, α_{18}= 0.0354

4. CONCLUDING REMARKS

A major object of developing the approximate theory is to help with the more intractable n observation design problem. Starting from the results presented in this paper one can construct n observation designs which are quite close to optimality unless n is very small (see e.g. Fedorov (1972, Ch. 3), Silvey (1980, p. 37)). This is of importance when the available resources allow a moderately large number of observations and interest lies in taking these observations efficiently. In fact, it is seen that very often the simple rule of rounding off to the nearest integer leads to highly satisfactory designs. The following example serves as an illustration.

Example 4.1. Let $p=5$, $n=20$. From Table I, the D- and A-optimal design measures, say η' and η'', are members of H_o with $\alpha_3= 0.0685$, $\alpha_4= 0.1315$ and $\alpha_3= 0.0462$, $\alpha_4= 0.1538$ respectively. With $n=20$, under the rule of rounding off to the nearest integer, both η' and η'' yield the design measure $\hat{\eta}$, also a member of H_o, with $\alpha_3= 1/20$, $\alpha_4= 2/20$. The D-efficiency of $\hat{\eta}$, measured as $[\det M(\hat{\eta})/\det M(\eta')]^{1/p}$, is 0.9968, while the A-efficiency of $\hat{\eta}$, measured as $[\mathrm{tr}\{M(\eta'')\}^{-1}/\mathrm{tr}\{M(\hat{\eta})\}^{-1}]$, is 0.9997.

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