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ON OPTIMALITY OF THE ORTHOGONAL BLOCK DESIGN

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Abstract

In the paper a usual block design with treatment effects fixed and block effects random is considered. To compare experimental design the asymptotic covariance matrix of a robust estimator proposed by Bednarski and Zontek (1996) for simultaneous estimation of shift and scale parameters is used. Asymptotically A - and D - optimal block designs in the class of designs with bounded block sizes are characterized.

Keywords: Experimental design, orthogonal block design, robust estimator, maximum likelihood estimator, A -optimality, D -optimality.

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1. INTRODUCTION

Consider an experiment with $v \geq 1$ treatments arranged in $b \geq 2$ blocks according to the $v \times b$ incidence matrix \mathbf{N} with entries $n_{ij} \geq 0$. We assume that an observed

random variable y_{ijl} for $i = 1, \dots, v$, $j = 1, \dots, b$ and $l = 1, \dots, n_{ij}$ have the following additive structure

$$(1) \quad y_{ijl} = \mu_i + \lambda_j + e_{ijl},$$

where μ_1, \dots, μ_v – fixed (treatment) effects, $\lambda_1, \dots, \lambda_b$ – independent unobservable random (block) effects normally distributed $N(0, \sigma_\lambda^2)$, while $e_{111}, \dots, e_{vbn_{vb}}$ – independent random errors with $N(0, \sigma_e^2)$ distribution (σ_λ and σ_e are scale parameters). Moreover, we assume that λ 's and e 's are independent. Denote by μ the vector $(\mu_1, \dots, \mu_v)'$ of fixed effects and by σ the vector $(\sigma_\lambda, \sigma_e)'$ of scale parameters. Throughout the paper we assume that the parameter $\theta = (\mu', \sigma)'$ is identifiable in the model, that is we assume that every row and every column in \mathbf{N} have a nonzero element, and that there is a column in \mathbf{N} for which the sum of its components exceeds 1.

For the model (1) there are different approaches to the problem of comparison of experimental designs. Usually a comparison of designs is based on the covariance matrix of a given estimator of μ and only equiblock-sized designs was considered. One of used estimators is the best linear unbiased estimator (BLUE) of μ in interblock model i.e. BLUE among linear unbiased estimators based on block totals (Gaffke and Kraft, 1980, and Christof and Pukelsheim, 1985). Another proposition is BLUE of μ in the original model under restriction to such designs for which BLUE exists (Kageyama and Zmysłony, 1993). In both cases the orthogonal block design is A - and D - optimal. Somewhat different approach has been proposed by Zmysłony and Zontek (1994). They have used a robust estimator for θ given by Fisher consistent and Fréchet differentiable functional (see Bednarski and Zontek, 1994, 1996). Since the exact covariance matrix of the estimator is not known, the asymptotic covariance matrix has been used to define criteria of optimality.

In this paper we extend and generalize results of Zmysłony and Zontek (1994). We characterize block designs which are A - as well as D - optimal separately for estimation of μ , σ and θ in the class of designs with bounded block sizes. For estimation μ as well as θ only the orthogonal block design is optimal in the considered class of designs. Moreover, it belongs to the class of A - as well as D - optimal experimental designs for estimation of σ . Since robust estimators are here considered, optimal properties of the orthogonal design are valid for small departures from the model distribution. In the last section, values of considered type of criterion functionals at the scaled asymptotic covariance matrix are compared with the corresponding values of them at the sample covariance matrix resulting from estimates of θ computed from generated data. Calculations was made for selected experimental designs, parameters of the model and a type of contamination of the model distribution, using the maximum likelihood estimator and a robust estimator.

Throughout the paper w' stands for the transpose of a vector w and $\text{diag}(w)$ for a diagonal matrix with i -th diagonal element equal to the i -th component of w . The a -dimensional vector with all entries unity and the identity $a \times a$ matrix are denoted by $\mathbf{1}_a$ and I_a , respectively. For any $a \times a$ matrix M , the symbol $\det M$ denotes the determinant of M and $\text{tr } M$ the trace of M . We write $M_1 \geq M_2$ ($M_1 > M_2$) when M_1 and M_2 are nonnegative definite (we mean also symmetric) matrices such that $M_1 - M_2$ is nonnegative (positive) definite matrix. A block diagonal matrix with blocks B_1, \dots, B_a is written as $\text{diag}(B_1, \dots, B_a)$. Finally, let $\mathcal{R}_+^a = \{(u_1, \dots, u_a)' : u_1 > 0, \dots, u_a > 0\}$, $\mathcal{S}_+^a = \{u \in \mathcal{R}_+^a : u' \mathbf{1}_a = 1\}$ and let $\mathcal{N}^a = \{(n_1, \dots, n_a)' : n_1, \dots, n_a \text{ are natural numbers}\}$.

2. ASYMPTOTIC COVARIANCE MATRIX OF ROBUST ESTIMATORS

As in Zmyślony and Zontek (1994) optimal properties of experimental designs are derived by using an asymptotic covariance matrix (see also Müller, 1992) of a robust estimator of $\theta = (\mu', \sigma')'$ proposed by Bednarski and Zontek (1994). For convenience of the reader we briefly describe their results needed in this paper.

For $j = 1, \dots, b$ let Y_j be a vector of random variables in the j -th block ordered in the following way

$$Y_j = (y_{1j1}, \dots, y_{1jn_{1j}}, y_{2j1}, \dots, y_{2jn_{2j}}, \dots, y_{vj1}, \dots, y_{vjn_{vj}})'$$

Under model assumptions, the random vector Y_j , $j = 1, \dots, b$, is normally distributed with expectation $EY_j = X_j \mu$, where $X_j = \text{diag}(\mathbf{1}_{n_{1j}}, \dots, \mathbf{1}_{n_{vj}})$, and with covariance matrix $\text{cov}(Y_j) = \sigma_\lambda^2 \mathbf{1}_{n_j} \mathbf{1}_{n_j}' + \sigma_e^2 I_{n_j}$, where $n_j = \sum_{i=1}^v n_{ij}$. It is easy to see that Y_1, \dots, Y_b are independent random vectors and that the distributions of, say, Y_j and Y_s coincide for each θ in the parameter space $\Theta = \mathcal{R}^v \times \mathcal{R}_+^2$ iff $n_{ij} = n_{is}$ for $i = 1, \dots, v$, i.e., when corresponding columns of the incidence matrices are equal.

We divide random vectors Y_1, \dots, Y_b on the minimal number of subgroups in such a way that in each subgroup there are identically distributed random vectors. Let N_1, \dots, N_p stand for different columns of the incidence matrix \mathbf{N} , and let b_i , $i = 1, \dots, p$, be the number of repetitions of N_i ($\sum_{i=1}^p b_i = b$). Then without loss of generality we can assume that the incidence matrix \mathbf{N} has the following form

$$\mathbf{N} = (N_1 \mathbf{1}_{b_1}', \dots, N_p \mathbf{1}_{b_p}').$$

So $Y_{c_{i-1}+1}, \dots, Y_{c_i}$, where $c_i = \sum_{s=1}^i b_s$, $c_0 = 0$, constitute the i -th subgroup.

Denoting by $\hat{F}_{b_i}^i$, $i = 1, \dots, p$, the empirical distribution function resulting

from $Y_{c_{i-1}+1}, \dots, Y_{c_i}$, define an estimator of θ as the parameter $\hat{\theta}_b$ in Θ for which

$$(2) \quad \int \sum_{i=1}^p \Phi_i(y_i|\theta) d(\hat{F}_{b_1}^1(y_1) \times \dots \times \hat{F}_{b_p}^p(y_p))$$

attains the minimum value, where $\Phi_i(\cdot, \cdot)$ is a real function on $\mathcal{R}^{n_i} \times \Theta$, while $n_i = N_i' \mathbf{1}_a$. Under some assumptions imposed on Φ_1, \dots, Φ_p , Bednarski and Zontek (1996) have shown that the functional corresponding to (2) is Fisher consistent and Fréchet differentiable at the model for the supremum norm. This imply that the estimator is consistent and is robust for small departures from the model distribution. Moreover, for fixed matrix $\tilde{\mathbf{N}} = (N_1, \dots, N_p)$ and under the assumption $\lim_{b \rightarrow \infty} (b_i/b) = q_i > 0$ for $i = 1, \dots, p$, the estimator $\hat{\theta}_b$ is asymptotically normal with expectation θ (at the model) and with covariance matrix $(1/b)\Sigma$ under whole infinitesimal model. The matrix Σ depends on $\tilde{\mathbf{N}}$, $q = (q_1, \dots, q_p)'$ and σ , and is given by

$$(3) \quad \Sigma = \Sigma(\tilde{\mathbf{N}}, q; \sigma) = \text{diag}(w_1 V_1(\tilde{\mathbf{N}}, q; \sigma), w_2 V_2(\tilde{\mathbf{N}}, q; \sigma)),$$

where for $j = 1, 2$

$$(4) \quad V_j(\tilde{\mathbf{N}}, q; \sigma) = \left[\sum_{i=1}^p M_j(N_i; \sigma) \right]^{-1} \left[\sum_{i=1}^p \frac{1}{q_i} M_j(N_i; \sigma) \right] \left[\sum_{i=1}^p M_j(N_i; \sigma) \right]^{-1},$$

while for $K \in \mathcal{N}^v$, $k = K' \mathbf{1}_v$ and $\alpha = (\alpha_1, \alpha_2)' \in \mathcal{R}_+^2$

$$(5) \quad M_1(K; \alpha) = \frac{1}{\alpha_2^2} \left(\text{diag}(K) - \frac{\alpha_1^2}{k\alpha_1^2 + \alpha_2^2} K K' \right),$$

$$(6) \quad M_2(K; \alpha) = \frac{2}{(k\alpha_1^2 + \alpha_2^2)^2} \begin{bmatrix} k^2 \alpha_1^2 & k\alpha_1 \alpha_2 \\ k\alpha_1 \alpha_2 & \alpha_2^2 \end{bmatrix} + 2 \frac{k-1}{\alpha_2^2} \begin{bmatrix} 0 & 0 \\ 0 & 1 \end{bmatrix}.$$

The constants $w_1 \geq 1$ and $w_2 \geq 1$, which can be interpreted as efficiency coefficients with respect to the maximum likelihood estimator of μ and σ , respectively, depend on chosen functions Φ_1, \dots, Φ_p . For more details see Bednarski and Zontek (1996).

3. MAIN RESULTS

For our considerations it is convenient to identify an experimental design with pair $(\tilde{\mathbf{N}}, \tilde{q})$, where $\tilde{q} = (b_1/b, \dots, b_p/b)'$, instead of the original incidence matrix

N (throughout the paper we assume that b is fixed). Assume we have defined an estimator $\hat{\theta}_E$ (we omitte subscript b) of θ for the model associated with an experimental design E in a class \mathcal{E} and suppose we are interesting in estimation of parametric function $C'\theta$, where C is $(v+2) \times r$ matrix. Take $C'\hat{\theta}_E$ as an estimator of $C'\theta$. Usually for a given criterion functional f defined on $\{\text{cov}_\theta(C'\hat{\theta}_E) : E \in \mathcal{E}\}$, an experimental design E_o is said to be optimal in \mathcal{E} for estimation of $C'\theta$, if $f(\text{cov}_\theta(C'\hat{\theta}_{E_o}))$ is minimum in \mathcal{E} for each $\theta \in \Theta$. However, when the covariance matrix cannot be explicitly calculated, such definition induce some difficulties. This is the case when the robust estimator is used. Therefore Zmysłony and Zontek (1994) have proposed a modification of the above definition, by exchange $\text{cov}_\theta(C'\hat{\theta}_E)$ for its approximation given by $\frac{1}{b}C'\Sigma(\tilde{N}, \tilde{q}; \sigma)C$, where $E = (\tilde{N}, \tilde{q})$. Since the approximation is based on the asymptotic covariance matrix, an optimal experimental design will be called asymptotically optimal.

We are interested in two types of criterion functional, the first one is associated with the trace operation and the second one is based on the matrix determinant.

Definition 1. An experimental design (\tilde{N}, \tilde{q}) in a class \mathcal{E} of experimental designs is called asymptotically A - (D -) optimal in \mathcal{E} for a function $C'\theta$, if

$$\text{tr}[C'\Sigma(\tilde{N}, \tilde{q}; \sigma)C] \quad (\det[C'\Sigma(\tilde{N}, \tilde{q}; \sigma)C])$$

is minimum in \mathcal{E} for every $\sigma \in \mathcal{R}_+^2$.

In this paper, we are concentrated only with three cases, namely $C'\theta = \mu$, $C'\theta = \sigma$ and $C'\theta = \theta$.

For fixed v , b and k let us consider the following classes of experimental designs

$$\mathcal{E}_o = \{(\tilde{N}, \tilde{q}) : \tilde{N} \in \mathcal{M}_k(p), \tilde{q} \in \mathcal{S}_+^p, p = 1, \dots, b\},$$

$$\mathcal{E}_o^* = \{(\tilde{N}, \tilde{q}) : \tilde{N} \in \mathcal{M}_k^*(p), \tilde{q} \in \mathcal{S}_+^p, p = 1, \dots, b\},$$

$$\mathcal{E}_1 = \{(\tilde{N}, (1/b)\mathbf{1}_p) : \tilde{N} \in \mathcal{M}_k^*(p), p = 1, \dots, b\}$$

and

$$\mathcal{E}_2 = \{(\tilde{N}, 1) : \tilde{N} \in \mathcal{M}_k^*(1)\},$$

where

$$\mathcal{M}_k(p) = \{(K_1, K_2, \dots, K_p) : K_j \in \mathcal{N}^v, K_j'\mathbf{1}_v \leq k, j = 1, \dots, p\},$$

while

$$\mathcal{M}_k^*(p) = \{K \in \mathcal{M}_k(p) : K'\mathbf{1}_v = k\mathbf{1}_p\}.$$

Zmysłony and Zontek (1994) have characterized experimental designs which are asymptotically A - as well as D -optimal in \mathcal{E}_o^* for σ . Moreover, they have proved that the orthogonal design is asymptotically A - as well as D -optimal in \mathcal{E}_1 for μ . In this paper we extend these results by considering A - and D -optimality in a broader class of designs for μ and σ , and we generalize them to the case of the function $C'\theta = \theta$.

It is intuitively clear that when we give in addition observations in some subgroup of blocks, then we should get better experimental design. For $p = 1$ this is stated in the following lemma.

Lemma 2. *For any $K_1, K_2 \in \mathcal{N}^v$ and for any $\alpha = (\alpha_1, \alpha_2)' \in \mathcal{R}_+^2$ we have*

$$(i) \text{ if } K_1 - K_2 \in \mathcal{N}^v, \text{ then } M_1(K_1; \alpha) \geq M_1(K_2; \alpha),$$

$$(ii) \text{ if } (K_1 - K_2)'\mathbf{1}_v > 0, \text{ then } M_2(K_1; \alpha) > M_2(K_2; \alpha).$$

Proof. To prove the first part of the lemma, it is sufficient to consider a case when $K_1 = K_2 + T$, where $T \in \mathcal{N}^v$ and $T'\mathbf{1}_v = 1$. Using $\text{diag}(T) = TT'$, simple algebra shows that

$$M_1(K_1; \alpha) - M_1(K_2; \alpha) = \frac{1}{\alpha_2^2[(\kappa + 1)\alpha_1^2 + \alpha_2^2](\kappa\alpha_1^2 + \alpha_2^2)} BB',$$

where $\kappa = K_2'\mathbf{1}_v$, while $B = \alpha_1^2 K_2 - (\kappa\alpha_1^2 + \alpha_2^2)T$, which terminates the proof of part (i).

The second implication we show for K_1 and K_2 such that $K_1'\mathbf{1}_v = K_2'\mathbf{1}_v + 1$. It follows easily for general $K_1'\mathbf{1}_v$ and $K_2'\mathbf{1}_v$ by induction. In the considered case one can verify that

$$M_2(K_1; \alpha) - M_2(K_2; \alpha) = \frac{2}{((\kappa + 1)\alpha_1^2 + \alpha_2^2)^2(\kappa\alpha_1^2 + \alpha_2^2)^2} (BB' + 2\kappa\alpha_1^2 D),$$

where $\kappa = K_2'\mathbf{1}_v$, $B = \frac{1}{\alpha_2}(\alpha_1\alpha_2^3, -\kappa(\kappa + 1)\alpha_1^4 + \alpha_2^4)'$, while

$$D = \begin{bmatrix} (\kappa + 1)\alpha_1^2\alpha_2^2 + \alpha_2^4 & 0 \\ 0 & (\kappa + 1)(2\kappa + 1)\alpha_1^4 + (4\kappa + 3)\alpha_1^2\alpha_2^2 + 2\alpha_2^4 \end{bmatrix}.$$

This finishes the proof. ■

The second lemma will be used on a step of construction of an experimental design better than a given block design in $\mathcal{E}_o \setminus \mathcal{E}_o^*$.

Lemma 3. Let W_1, \dots, W_p be n.n.d. $m \times m$ matrices such that $W_1 + \dots + W_p > 0$ and let $u = (u_1, \dots, u_p)' \in \mathcal{S}_+^p$. Then

$$(7) \quad \sum_{i=1}^p u_i W_i \geq \left(\sum_{i=1}^p W_i \right) \left(\sum_{i=1}^p \frac{1}{u_i} W_i \right)^{-1} \left(\sum_{i=1}^p W_i \right).$$

Proof. It is sufficient to prove that for $u \in \mathcal{S}_+^p$

$$(8) \quad \sum_{i=1}^p u_i W_i \geq \left(\sum_{i=1}^p \frac{1}{u_i} W_i \right)^{-1},$$

where W_1, \dots, W_p satisfy an additional condition that $W_1 + \dots + W_p = I_m$. First we show this inequality for $p = 2$.

Let $W_1 = \sum_{j=1}^m \lambda_j T_j T_j'$ be a spectral decomposition of W_1 , where $\lambda_j \in [0, 1]$ is an eigenvalue corresponding to an eigenvector T_j of W_1 , $j = 1, \dots, m$. Since $W_2 = I_m - W_1 = \sum_{j=1}^m (1 - \lambda_j) T_j T_j'$ we get that

$$u_1 W_1 + (1 - u_1) W_2 - \left(\frac{1}{u_1} W_1 + \frac{1}{1 - u_1} W_2 \right)^{-1} = \sum_{j=1}^m \frac{(2u_1 - 1)^2 \lambda_j (1 - \lambda_j)}{u_1 (1 - \lambda_j) + (1 - u_1) \lambda_j} T_j T_j'$$

is n.n.d. for $u_1 \in (0, 1)$, which shows (8) for $p = 2$.

Using this we easily see that for $p > 2$

$$\begin{aligned} \sum_{i=1}^p u_i W_i &= u_1 W_1 + (1 - u_1) \sum_{i=2}^p \frac{u_i}{1 - u_1} W_i \\ &\geq \left(\frac{1}{u_1} W_1 + \frac{1}{1 - u_1} \sum_{i=2}^p \frac{u_i}{1 - u_1} W_i \right)^{-1}. \end{aligned}$$

According to $0 < u_i / (1 - u_1) < 1$, $i = 2, \dots, p$, it may be concluded that

$$\sum_{i=2}^p \frac{1}{u_i} W_i \geq \frac{1}{1 - u_1} \sum_{i=2}^p \frac{u_i}{1 - u_1} W_i,$$

which terminates the proof. ■

Under additional assumption that $W_1 > 0, \dots, W_p > 0$, inequality (7) follows from inequality due to Kiefer (Lemma 3.2, 1959).

Using above two lemmas we can get the following characterization of asymptotically A - as well D - optimal designs for σ

Theorem 4. *An experimental design (\tilde{N}, \tilde{q}) is asymptotically A - (D -) optimal in \mathcal{E}_o for σ if and only if (\tilde{N}, \tilde{q}) belongs to \mathcal{E}_1 .*

Proof. Let $\tilde{N} = (N_1, \dots, N_p)$ be a matrix in $\mathcal{M}_k(p) \setminus \mathcal{M}_k^*(p)$ and let $\tilde{q} = (\tilde{q}_1, \dots, \tilde{q}_p)' \in \mathcal{S}_+^p$. We have for each σ in \mathcal{R}_+^2

$$V_2(\tilde{N}, \tilde{q}; \sigma) \geq \left[\sum_{i=1}^p \tilde{q}_i M_2(N_i; \sigma) \right]^{-1} > V_2(\tilde{N}^*, 1; \sigma),$$

where \tilde{N}^* is a vector in \mathcal{N}^v such that $\tilde{N}^* \mathbf{1}'_v = k$. The first inequality follows from Lemma 3 and the second one from Lemma 2. This imply that no experimental design in $\mathcal{E}_o \setminus \mathcal{E}_o^*$ is asymptotically A - as well as D -optimal in \mathcal{E}_o for σ . Since, as it is shown in Zmysłony and Zontek (Theorem 1, 1994), an experimental design (\tilde{N}, \tilde{q}) is asymptotically A - as well as D - optimal in \mathcal{E}_o^* for σ if and only if $(\tilde{N}, \tilde{q}) \in \mathcal{E}_1$, the assertion follows. ■

Note that the matrix $M_2(K, \alpha)$ given by (6) depends on K through $K' \mathbf{1}_v$. So arrangement of treatments in blocks is not important, if we are interested in choosing of asymptotically optimal experimental design for σ .

Lemma 5. *Let $K = (K_1, \dots, K_p)$ be an element of $\mathcal{M}_k(p)$. If (K_1^*, \dots, K_p^*) in $\mathcal{M}_k^*(p)$ satisfies*

$$(9) \quad K_i^* - K_i \in \mathcal{N}^v, \quad i = 1, \dots, p,$$

then for every $u = (u_1, \dots, u_p)' \in \mathcal{S}_+^p$ and $\alpha \in \mathcal{R}_+^2$

$$V_1(K, u; \alpha) \geq V_1(K_u^*, 1; \alpha),$$

where $K_u^* = \sum_{i=1}^p u_i K_i^*$.

Proof. Using assumption (9) and Lemma 2 we get that for $\alpha \in \mathcal{R}_+^2$

$$M_1(K_i^*; \alpha) \geq M_1(K_i; \alpha), \quad i = 1, \dots, p.$$

Lemma 3 and the above inequality imply now that

$$(10) \quad \sum_{i=1}^p u_i M_1(K_i^*; \alpha) \geq V_1^{-1}(K, u; \alpha).$$

Since $\sum_{i=1}^p u_i K_i^* (K_i^*)' \geq K_u^* (K_u^*)'$, it follows that

$$V_1^{-1}(K_u^*, 1; \alpha) \geq \sum_{i=1}^p u_i M_1(K_i^*, \alpha),$$

which proves the assertion by (10). ■

As a consequence of the above lemma we can obtain the following theorem.

Theorem 6. *An experimental design $(\tilde{\mathbf{N}}, \tilde{q})$ is asymptotically A - (D -) optimal in \mathcal{E}_o for μ if and only if $(\tilde{\mathbf{N}}, \tilde{q}) = ((k/v)\mathbf{1}_v, 1)$, i.e. $(\tilde{\mathbf{N}}, \tilde{q})$ is the orthogonal design $(\mathbf{N} = (k/v)\mathbf{1}_v\mathbf{1}'_b)$.*

Proof. Zmysłony and Zontek (Lemma 3, 1994) have proved that for every vector $K \in \mathcal{R}_+^a$ such that $K'\mathbf{1}_a = k$ and for every σ in \mathcal{R}_+^2 the following inequalities hold

$$\text{tr}V_1((k/v)\mathbf{1}_v, 1; \sigma) \leq \text{tr}V_1(K, 1; \sigma)$$

and

$$\det V_1((k/v)\mathbf{1}_v, 1; \sigma) \leq \det V_1(K, 1; \sigma)$$

with equality if and only if $K = (k/v)\mathbf{1}_v$. Combining this with Lemma 5 we get the statement. ■

Since only the orthogonal design is asymptotically A - as well as D - optimal in \mathcal{E}_o both for μ and for σ we get the following characterization.

Remark 7. A block design $(\tilde{\mathbf{N}}, \tilde{q})$ is asymptotically A - (D -) optimal in \mathcal{E}_o for θ if and only if $(\tilde{\mathbf{N}}, \tilde{q}) = ((k/v)\mathbf{1}_v, 1)$.

It is known that the orthogonal block design has a number of good properties under normality assumptions. We showed another optimal properties of it. The starting point here is a robust estimator resulting from Fréchet differentiable functional, which implies asymptotic normality with covariance matrix given by (3) under whole infinitesimal model. So the optimality of the orthogonal design are valid also when the distribution of Y_j , $j = 1, \dots, b$, comes from a neighbourhood, induced by the supremum norm, of model (normal) distribution.

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