

A NOTE ON OPTIMAL AND ASYMPTOTICALLY OPTIMAL DESIGNS FOR CERTAIN TIME SERIES MODELS

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The problem of regression design in the presence of correlated errors is considered. Under the assumption that derivative information is available on the response process, uniqueness results for optimal designs given in Eubank, Smith and Smith (1981) for the BLUE of the regression coefficient are extended to a wider class of processes. In the event that derivatives cannot be sampled, an asymptotic solution is developed and extended to the multiparameter setting.

1. Introduction. Consider the linear regression model in which one observes a stochastic process, Y , of the form

$$(1.1) \quad Y(t) = \beta f(t) + X(t), \quad t \in [0, 1],$$

where β is an unknown parameter, f is a known regression function and X is a zero mean process with known covariance kernel R . The X process is assumed to admit $k - 1$ quadratic mean derivatives.

If the Y process is sampled at only a finite number of noncoincident design points, then the best linear unbiased estimator (BLUE) of β is obtained by generalized least squares. In this paper we consider the problem of optimal design selection for the BLUE. More precisely, we consider the selection of an element from the set of all $(n + 2)$ -point designs, $D_n = \{(t_0, t_1, \dots, t_n, t_{n+1}): 0 = t_0 < t_1 < \dots < t_n < t_{n+1} = 1\}$, which provides minimal variance for the BLUE.

For model (1.1) two types of BLUE's have been studied in the literature. If information is available on the Y process alone then, given $T \in D_n$, the BLUE is computed using $\{Y(t): t \in T\}$. Let $\hat{\beta}_T$ denote this estimator of β . The properties of optimal designs for $\hat{\beta}_T$ have been studied by Sacks and Ylvisaker (1966, 1968, 1970) for $k = 1, 2$ and certain types of covariance kernels. As optimal designs are difficult to construct, they develop an asymptotic (approximate) solution based on design sequences. If h is a continuous density on $[0, 1]$ then h generates a sequence of designs, $\{T_n\}$ with $T_n \in D_n$, whose n th element consists of the $(n + 1)$ -tiles of h . This sequence is termed the *regular sequence* (RS) *generated by* h which we abbreviate by $\{T_n\}$ is RS(h). Their approximate solution is obtained by deriving a density h^* for which the corresponding RS, $\{T_n^*\}$, is *asymptotically optimal* in the sense that

$$(1.2) \quad \lim_{n \rightarrow \infty} \{\inf_{T \in D_n} \text{Var}(\hat{\beta}_T) - \text{Var}(\hat{\beta})\} \{\text{Var}(\hat{\beta}_{T_n^*}) - \text{Var}(\hat{\beta})\}^{-1} = 1,$$

where $\hat{\beta}$ is the linear estimator of β based on Y information from all of $[0, 1]$ (c.f. Parzen, 1961a, b). One then samples according to T_n^* for n sufficiently large.

If, in addition to the Y process, its first $k - 1$ derivatives can also be sampled, this results in a different BLUE constructed from the observations $\{Y^{(i)}(t): i = 0, \dots, k - 1,$

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$t \in T$), which we denote as $\hat{\beta}_{k,T}$. Approximate solutions to the optimal design problem for $\hat{\beta}_{k,T}$, similar to those for $\hat{\beta}_T$, have been developed by Sacks and Ylvisaker (1970), Wahba (1971, 1974) and Hajek and Kimeldorf (1974); see also Speckman (1982) for some closely related work.

In this paper the design problems for both $\hat{\beta}_T$ and $\hat{\beta}_{k,T}$ will be considered for a specific class of X processes. Define the covariance kernel

$$(1.3) \quad K(s, t) = \{(k - 1)!\}^{-2} \int_0^1 (s - u)_+^{k-1} (t - u)_+^{k-1} du$$

where $(x)_+^k = x^k$ for $x \geq 0$ and is zero otherwise. Let $Z(t)$ denote the corresponding normal process and define a new process by

$$(1.4) \quad W(t) = \begin{cases} Z(t) - E[Z(t) | Z^{(j)}(1), j = k - q, \dots, k - 1], & 0 < q \leq k, \\ Z(t), & q = 0. \end{cases}$$

Now, and in subsequent discussions, we restrict R to the form

$$(1.5) \quad R(s, t) = \text{Cov}\{W(s), W(t)\}.$$

The case $q = 0$ corresponds to the covariance kernel for a $(k - 1)$ -fold multiple integral of a Brownian motion process and has played an important role in previous work on this design problem (cf. Sacks and Ylvisaker, 1970). When $q = 1$, (1.4) is the covariance kernel for a $(k - 1)$ -fold multiple integral of a Brownian bridge process. Although not discussed here, the results of this paper, in this instance, have applications to data compression for location and/or scale parameter estimation using sample quantiles; see Eubank (1981) as an illustration for $k = 1$. The case of $q = k$ was studied in Eubank, Smith and Smith (1981) which is hereafter referred to as ESS (1981).

For $\hat{\beta}_{k,T}$ our primary concern is with optimal designs, as an asymptotic solution follows from Sacks and Ylvisaker (1970). In Section 2 it is shown that the uniqueness results for optimal designs given by ESS (1981) in the case $q = k$ for kernel (1.5) extend to all values $0 \leq q \leq k$. As we will frequently draw from results in ESS (1981) the reader is referred to that paper for notation or results not explicitly mentioned here.

The design problem for $\hat{\beta}_T$ is more complicated and only asymptotically optimal designs are considered. In contrast to previous studies, however, such designs are constructed for general k , not just $k = 1$ or 2. These results are also extended to the multiparameter or multiple regression setting.

2. Optimal designs for $\hat{\beta}_{k,T}$. The optimal design problem for $\hat{\beta}_{k,T}$ consists of finding a $T^* \in D_n$ that satisfies $\text{Var}(\hat{\beta}_{k,T^*}) = \inf_{T \in D_n} \text{Var}(\hat{\beta}_{k,T})$. This may be reformulated as a best approximation problem involving f , the regression function, through use of the reproducing kernel Hilbert space (RKHS) that is generated by R and is congruent to the X process (see Parzen, 1961a, b). Denote this RKHS by $H(R)$ and its norm by $\|\cdot\|_R$. Also, for $T \in D_n$, let $R_{k,T}$ denote the $H(R)$ subspace spanned by $\{R^{(0,j)}(\cdot, t): j = 0, \dots, k - 1, t \in T\}$, where

$$(2.1) \quad R^{(i,j)}(s, t) = \frac{\partial^{i+j}}{\partial s^i \partial t^j} R(s, t),$$

with associated orthogonal projection operator $\mathcal{R}_{k,T}$. It can then be shown that $\|\mathcal{R}_{k,T} f\|_R^{-2} = V(\hat{\beta}_{k,T})$. As $\|\mathcal{R}_{k,T} f\|_R^2 = \|f\|_R^2 - \|f - \mathcal{R}_{k,T} f\|_R^2$ the optimal design problem is now seen as equivalent to finding a $T^* \in D_n$ such that

$$(2.2) \quad \|f - \mathcal{R}_{k,T^*} f\|_R = \inf_{T \in D_n} \|f - \mathcal{R}_{k,T} f\|_R.$$

For covariance kernels of the form (1.5), it can be verified that a function $f \in H(R)$ admits $k - 1$ absolutely continuous derivatives with $f^{(k)} \in L_2[0, 1]$ and will satisfy the boundary conditions $f^{(j)}(0) = 0, j = 0, \dots, k - 1$ and $f^{(j)}(1) = 0, j = k - q, \dots, k - 1$ for $1 \leq q \leq k$ or just $f^{(j)}(0) = 0, j = 0, \dots, k - 1$ for $q = 0$. The norm for $f \in H(R)$ is

$$(2.3) \quad \|f\|_R = \|f^{(k)}\|$$

where $\|\cdot\|$ is the usual $L_2[0, 1]$ norm. If we now let $R_{k,T}^k$ denote the $L_2[0, 1]$ linear span of $\{R^{(k,j)}(\cdot, t): j = 0, \dots, k - 1, t \in T\}$ with associated orthogonal projector $\mathcal{R}_{k,T}^k$ then, from (2.3), the optimal design problem is also equivalent to: Find $T^* \in D_n$ such that

$$(2.4) \quad \|f^{(k)} - \mathcal{R}_{k,T^*}^k f^{(k)}\| = \inf_{T \in D_n} \|f^{(k)} - \mathcal{R}_{k,T}^k f^{(k)}\|.$$

To study the properties of optimal designs a connection will be established between problem (2.4) and the best $L_2[0, 1]$ approximation of $f^{(k)}$ by piecewise polynomials with variable breakpoints. The results we require, subsequently, regarding this latter problem can be found in Section 3 of ESS (1981). However, slightly different notation is employed here that is now summarized. For $(t_0, t_1, \dots, t_n, t_{n+1}) \in D_n$ we will use $P_{k,T}$ to denote the set of all piecewise polynomials of order k with breakpoints at t_1, \dots, t_n and $\mathcal{P}_{k,T}$ to represent its associated $L_2[0, 1]$ orthogonal projection operator. We also define

$$(2.5) \quad p_i^i(s) = (t - s)_+^{i-1} / (i - 1)!, \quad i = 1, \dots, k,$$

with the convention that

$$(2.6) \quad p^i(s) = p_1^i(s) = (1 - s)^{i-1} / (i - 1)!, \quad i = 1, \dots, k.$$

It is well known that $\{p_i^i: i = 1, \dots, k, t \in T\}$ provides a basis for $P_{k,T}$ and that the subspace of polynomials of order q , denoted P_q , is spanned by $\{p^i: i = 1, \dots, q\}$. We now proceed to examine the form of $R_{k,T}^k$.

Define $v^{(j)}(t)$ as the $q \times 1$ vector having i th element

$$(2.7) \quad v_i^{(j)}(t) = \begin{cases} \int_0^1 p_i^{k-j}(s)p^{q-i}(s) ds, & i = 0, \dots, q - 1, j = 0, \dots, k - 1, \\ p^{q-i}(t), & i = 0, \dots, q - 1, j = k. \end{cases}$$

Also, let B denote the $q \times q$ matrix whose elements are

$$(2.8) \quad b_{ij} = \int_0^1 p^{q-i}(s)p^{q-j}(s) ds, \quad i, j = 0, \dots, q - 1.$$

Straightforward calculations then show that

$$(2.9) \quad R^{(k,j)}(s, t) = p_i^{k-j}(s) - \{v^{(k)}(s)\}' B^{-1} \{v^{(j)}(t)\},$$

which is recognized as the error function from the $L_2[0, 1]$ approximation of p_i^{k-j} from P_q . Thus, from (2.9) and a dimensionality argument, we see that $P_{k,T} = R_{k,T}^k \oplus P_q$. Consequently, problem (2.4) is a form of variable breakpoint $L_2[0, 1]$ piecewise polynomial approximation problem for $f^{(k)}$. However, to apply available results on piecewise polynomial approximation it is first necessary to show that $\mathcal{P}_{k,T} f^{(k)} = \mathcal{R}_{k,T}^k f^{(k)}$. This can be accomplished as in ESS (1981) through integration by parts and application of the $H(R)$ boundary conditions. A shorter statistical proof has been supplied by a referee who notes that $f \in H(R)$ is isomorphic to some Z in the Hilbert space spanned by $\{Z(t): 0 \leq t \leq 1\}$ and, due to f 's membership in $H(R)$, $Z \perp Z^{(i)}(1)$, $i = k - q, \dots, k - 1$. The result now follows from

$$\begin{aligned} E[Z | W^{(i)}(t), 0 \leq i < k, t \in T] &= E[Z | W^{(i)}(t), 0 \leq i < k, t \in T, Z^{(j)}(1), k - q \leq j < k] \\ &= E[Z | Z^{(i)}(t), 0 \leq i < k, t \in T, Z^{(j)}(1), k - q \leq j < k] \end{aligned}$$

upon noting that the k th derivative for the first term is $\mathcal{R}_{k,T}^k f^{(k)}$ and $\mathcal{P}_{k,T} f^{(k)}$ for the last.

We can now apply Theorems 3.1 and 3.2 of ESS (1981) to problem (2.4) and conclude, therefore, that Theorems 2.1-2.3 of ESS (1981) hold for processes with covariance kernels of the form (1.5) for all values $0 \leq q \leq k$. Thus, in particular, if $f \in H(R) \cap C^{2k}[0, 1]$ and

$f^{(2k)}$ is of one sign on $[0, 1]$ with $\log f^{(2k)}$ (or $\log -f^{(2k)}$ as appropriate) concave on $(0, 1)$ then $\hat{\beta}_{k,T}$ has unique optimal designs for each n .

REMARK 2.1. The work in this section has the consequence that optimal designs for model (1.1) with R as in (1.5) can be constructed using the algorithm in Eubank, Smith and Smith (1982). These processes, therefore, provide some of the few instances where optimal designs can be readily computed.

REMARK 2.2. It follows from Sacks and Ylvisaker (1970) that if $f \in H(R) \cap C^{2k} [0, 1]$ then the asymptotic behaviour of optimal designs for $\hat{\beta}_{k,T}$ is characterized by

$$(2.10) \quad \lim_{n \rightarrow \infty} n^{2k} \inf_{T \in D_n} \|f^{(k)} - \mathcal{R}_{k,T}^k f^{(k)}\|^2 = \frac{(k!)^2}{(2k)!(2k+1)!} \left\{ \int_0^1 |f^{(2k)}(x)|^{2/2k+1} dx \right\}^{2k+1}.$$

One can, however, exploit the connection between the design problem for these processes and piecewise polynomial approximation to obtain (2.10) under weaker conditions such as $f \in H(R)$ with $f \in C^{2k-1}[0, 1]$ and $f^{(2k)} \in L_1[0, 1]$ (see Burchard and Hale, 1975). Similar comments can be made for other asymptotic results about designs for $\hat{\beta}_{k,T}$.

3. Asymptotically optimal designs for $\hat{\beta}_T$. In this section, we consider the problem of design selection for $\hat{\beta}_T$. An optimal design, in this setting, is a $T^* \in D_n$ that satisfies

$$(3.1) \quad \text{Var}(\hat{\beta}_{T^*}) = \inf_{T \in D_n} \text{Var}(\hat{\beta}_T).$$

It has been noted by Sacks and Ylvisaker (1966) that for processes which are differentiable in quadratic mean the optimal designs may lie on the boundary of D_n and, hence, require the use of derivative information. We will, however, develop an approximate solution to (3.1) that does not involve the use of derivatives of the Y process.

To devise our approximate solution, problem (3.1) will be reformulated as an $L_2[0, 1]$ variable knot spline approximation problem for $f^{(k)}$. In the process we will have occasion to use several spline subspaces and, since all projections are in $L_2[0, 1]$, adopt the notational convention that the projection operators for subspaces are denoted through the use of script symbols. For example, given $T = \{t_0, t_1, \dots, t_n, t_{n+1}\} \in D_n$, define the set of all splines of order k with knots at t_1, \dots, t_n by $S_{k,T} = P_{k,T} \cap C^{k-2}[0, 1]$. The $L_2[0, 1]$ projection operator for $S_{k,T}$ is then denoted $\mathcal{S}_{k,T}$.

Problem (3.1) can also be formulated as a best approximation problem in $L_2[0, 1]$. For $T \in D_n$, let R_T^k denote the $L_2[0, 1]$ linear span of $\{R^{(k,0)}(\cdot, t) : t \in T\}$; then by arguments such as those in Section 2, it follows that selecting an optimal design for $\hat{\beta}_T$ is equivalent to finding a $T^* \in D_n$ that satisfies

$$(3.2) \quad \|f^{(k)} - \mathcal{R}_T^k \cdot f^{(k)}\| = \inf_{T \in D_n} \|f^{(k)} - \mathcal{R}_T^k f^{(k)}\|.$$

Upon examination of (2.9), we see that $R_{k,T} \subset S_{k,T}$ and, hence, (3.2) is a form of free knot spline approximation problem for $f^{(k)}$. In fact, when $q = k$, it follows from Section 2 that $S_{k,T} = R_T^k \oplus P_k$ with $f^{(k)} \perp P_k$. Therefore, $\mathcal{S}_{k,T} f^{(k)} = \mathcal{R}_T^k f^{(k)}$ and results from the theory of spline approximation may be applied directly. This fact was used to obtain Theorems 5.1 and 5.2 in ESS (1981). We now concentrate on extending these results to $q < k$.

For $q < k$ assume that $f \in C^{2k}[0, 1]$ and admits the representation

$$(3.3) \quad f(t) = (-1)^k \int_0^1 f^{(2k)}(s) R(s, t) ds.$$

This has the consequence that f satisfies the additional boundary conditions

$$(3.4) \quad f^{(k+j)}(1) = 0, \quad j = q, \dots, k - 1.$$

Also, observe, from (2.9), that $R^{(k,0)}(\cdot, t)$ satisfies (3.4) except for $t = 1$ when $R^{(k,0)}(1, 1) =$

1. Thus, for $T \in D_n$, let T' denote the set obtained by deleting the element $t_{n+1} = 1$ and consider the subspace $R_{T'}^k$, spanned by $\{R^{(k,0)}(\cdot, t) : t \in T'\}$. This latter subspace is properly contained in $S_{k,T}^q$, the set of all splines in $S_{k,T}$ satisfying (3.4). A dimensionality argument and results from Section 2 show these two subspaces are related by $S_{k,T}^q = R_{T'}^k \oplus P_q$. Problem (3.2) is then very nearly a variable knot spline approximation problem where both the splines and function being approximated are subject to boundary constraints.

The asymptotic properties of free knot approximation by splines and splines subject to boundary conditions have been studied by Barrow and Smith (1978, 1979). For the problem at hand their results have the consequence that

$$\lim_{n \rightarrow \infty} n^k \inf_{T \in D_n} \|f^{(k)} - \mathcal{S}_{k,T}^q f^{(k)}\| = \lim_{n \rightarrow \infty} n^k \inf_{T \in D_n} \|f^{(k)} - \mathcal{S}_{k,T} f^{(k)}\|.$$

They have also shown that an asymptotically optimal design (knot) sequence is generated by the density proportional to $|f^{(2k)}|^{2/2k+1}$. To apply these results to problem (3.2), we need only observe that

$$(3.5) \quad \|f^{(k)} - \mathcal{S}_{k,T}^q f^{(k)}\| = \|f^{(k)} - \mathcal{R}_{T'}^k f^{(k)}\| \geq \|f^{(k)} - \mathcal{R}_T^k f^{(k)}\| \geq \|f^{(k)} - \mathcal{S}_{k,T} f^{(k)}\|$$

which, in view of Theorems 3.3 and 3.4 of ESS (1981) and previous comments, allows us to state the following theorem.

THEOREM 1. *Suppose f satisfies (3.3) with $f^{(2k)} \in C[0, 1]$. If h is a continuous density on $[0, 1]$ and $\{T_n\}$ is RS(h) then*

$$(3.6) \quad \lim_{n \rightarrow \infty} n^{2k} \|f^{(k)} - \mathcal{R}_{T_n}^k f^{(k)}\|^2 = C_k^2 \int_0^1 [\{f^{(2k)}(x)\}^2 / h^2(x)] dx,$$

where $C_k = |B_{2k}|/2k!$ and B_{2k} is the $2k$ th Bernoulli number. An optimal density is

$$(3.7) \quad h^*(x) = |f^{(2k)}(x)|^{2/2k+1} / \int_0^1 |f^{(2k)}(s)|^{2/2k+1} ds$$

for which the corresponding RS, $\{T_n^*\}$, satisfies

$$(3.8) \quad \begin{aligned} \lim_{n \rightarrow \infty} n^{2k} \|f^{(k)} - \mathcal{R}_{T_n^*}^k f^{(k)}\|^2 &= \lim_{n \rightarrow \infty} n^{2k} \inf_{T \in D_n} \|f^{(k)} - \mathcal{R}_T^k f^{(k)}\|^2 \\ &= C_k^2 \left\{ \int_0^1 \left| f^{(2k)}(x) \right|^{2/(2k+1)} dx \right\}^{2k+1}. \end{aligned}$$

REMARK 1. Theorem 1 provides the first result of its kind, of which we are aware, for general k . By reference to Sacks and Ylvisaker (1970), $\{T_n^*\}$ is found to also provide asymptotically optimal designs for $\hat{\beta}_{k,T}$. The only difference in the limits of $n^{2k} \|f^{(k)} - \mathcal{R}_{T_n}^k f^{(k)}\|^2$ and $n^{2k} \|f^{(k)} - \mathcal{R}_{k,T_n^*}^k f^{(k)}\|^2$ is their respective asymptotic constants C_k^2 and $(k!)^2 / \{(2k)!(2k+1)!\}$. We conjecture that this type of result holds for more general processes such as those considered by Sacks and Ylvisaker (1970).

REMARK 2. It should be noted that the best spline approximant to $f^{(k)}$ may have interior knots (design points) with multiplicities. This means, as noted previously, that optimal designs may require derivative information. However, as a result of Theorem 1, we can do as well asymptotically without derivatives by using $\hat{\beta}_{T_n^*}$.

To conclude this section we consider the extension of Theorem 1 to the multiparameter setting where Y has the form

$$(3.9) \quad Y(t) = \sum_{j=1}^J \beta_j f_j(t) + X(t), \quad t \in [0, 1].$$

The objective now is to obtain asymptotically optimal designs for $\hat{\beta}_T$ the BLUE of $\beta = (\beta_1, \dots, \beta_J)'$. Let A_T^{-1} denote the variance-covariance matrix for $\hat{\beta}_T$ and let $\hat{\beta}$ denote the

linear estimator of β , with $\text{Var}(\hat{\beta}) = A^{-1}$ say, obtained using information over all of $[0, 1]$. To accomplish our objective it suffices to prove the following analog of Theorem 3.2 of Sacks and Ylvisaker (1968).

THEOREM 2. For $j = 1, \dots, J$ assume that f_j satisfies (3.3) with $f_j^{(2k)} \in C[0, 1]$ and for any set of positive constants a_1, \dots, a_J define the density

$$(3.10) \quad h^*(x) = [\sum_{j=1}^J a_j \{f_j^{(2k)}(x)\}^2]^{1/(2k+1)} \bigg/ \int_0^1 [\sum_{j=1}^J a_j \{f_j^{(2k)}(s)\}^2]^{1/(2k+1)} ds.$$

If $\{T_n\}$ is any design sequence and $\{T_n^*\}$ is RS(h^*) then

$$(3.11) \quad \begin{aligned} & \liminf_{n \rightarrow \infty} n^{2k} \sum_{j=1}^J a_j \|f_j^{(k)} - \mathcal{A}_{T_n}^k f^{(k)}\|^2 \\ & \geq \lim_{n \rightarrow \infty} n^{2k} \sum_{j=1}^J a_j \|f_j^{(k)} - \mathcal{A}_{T_n^*}^k f^{(k)}\|^2 = C_k^2 \left(\int_0^1 [\sum_{j=1}^J a_j \{f_j^{(2k)}(x)\}^2]^{1/(2k+1)} dx \right)^{2k+1}. \end{aligned}$$

PROOF. It suffices to prove the inequality in (3.11) as the remainder follows from Theorem 1. This can be accomplished by modifying the proof to Theorem 2 in Barrow and Smith (1978). We highlight the differences here and refer the reader to the latter paper for more details.

First note from (3.5) that the result will follow upon showing that

$$(3.12) \quad \sum_{j=1}^J a_j \|f_j^{(k)} - \mathcal{S}_{k, T_n} f^{(k)}\|^2 \geq C_k^2 \left(\int_0^1 [\sum_{j=1}^J a_j \{f_j^{(2k)}(x)\}^2]^{1/(2k+1)} dx \right)^{2k+1}.$$

The proof now proceeds by showing that (3.12) holds first when $f_j^{(k)}(t) = c_j t^k/k!$ where c_j is a constant and then when $f_j^{(k)}(t) \in C^k[0, 1]$ with $\sum_{j=1}^J a_j \{f_j^{(2k)}(t)\}^2 \geq \delta > 0$ before finally considering the general case of $f_j^{(k)} \in C^k[0, 1]$. The details involved in verifying (3.12) for these cases can be deduced from Barrow and Smith (1978).

Using Theorem 2 it is now possible to obtain analogs of the theorems given in Section 4 of Sacks and Ylvisaker (1968) using similar methods of proof. For example it follows from Theorem 2 that if $\phi(x) = (f_1^{(2k)}(x), \dots, f_J^{(2k)}(x))$, the density proportional to $\{\phi(x)' A^{-1} \phi(x)\}^{1/(2k+1)}$ generates an asymptotically D -optimal design sequence, $\{T_n^*\}$, in the sense that

$$\lim_{n \rightarrow \infty} \{\det(A) - \sup_{T \in D_n} \det(A_T)\} \{\det(A) - \det(A_{T_n^*})\}^{-1} = 1.$$

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