AD-A109 545 SOUTHERN METHODIST UNIV DALLAS TEX DEPT OF STATISTICS F/G 12/1
UNIQUENESS AND EVENTUAL UNIQUENESS OF OPTIMAL DESIGNS IN SOME T--ETC(U)
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UNIQUENESS AND EVENTUAL UNIQUENESS OF OPTIMAL DESIGNS IN SOME TIME SERIES MODELS, II

by

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Technical Report No. 150
Department of Statistics ONR Contract

November, 1981

Research sponsored by the Office of Naval Research
Contract N00014-75-C-0439

DEPARTMENT OF STATISTICS
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Uniqueness and Eventual Uniqueness of Optimal Designs in Some Time Series Models, II

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Short Title: Optimal Designs in Time Series

Summary. Earlier results on the uniqueness and eventual uniqueness of optimal designs for certain time series models are extended to a wider class of processes which includes those with covariance structures such as that of multiple integrals of Brownian motion and Brownian bridge processes. The relationship between the problems of regression design for time series and piecewise polynomial approximation with free breakpoints is discussed and, consequently, asymptotic results obtained by Sacks and Ylvisaker (1970) are seen to hold under weaker assumptions for these processes.

1. Introduction. Consider the linear regression model in which a stochastic process, Y, is observed having the form

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

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 exactly k-1 quadratic mean derivatives.

When the Y process is observed, for instance, overall of [0,1], the reproducing kernel Hilbert space (RKHS) techniques developed by Parzen (1961a, 1961b), may be utilized to obtain a linear unbiased estimator of the unknown parameter β. When, instead, the process is to be sampled at only a finite number of points the regression design problem has been considered by Sacks and Ylvisaker (1966, 1968, 1970), Wahba (1971, 1974), and Eubank, Smith and Smith (1981a, 1981b). Under a variety of assumptions on the covariance kernel R, and the amount of information available on the Y process these authors consider the problem of selecting an element, T, from the set of all n+1 point designs

(1.2) $$D_n := \{(t_0, t_1, \ldots, t_n) \mid 0 = t_0 < t_1 < \cdots < t_n = 1\}$$

(where := means " is defined as") so as to minimize the variance of the best linear unbiased estimator (BLUE) of β obtained by sampling according to T.

Of particular importance for this paper is the case when the Y process as well as its derivatives may be sampled at each of the design points. Then, for a given $T \in D_n$, one may consider the estimation of β from the observation set

$$Y_{k,T} := \{Y^{(j)}(t) \mid t \in T,\ j = 0, \ldots, k-1\} .$$

We denote by $\hat{\beta}_{k,T}$ the BLUE of β based on the observations $Y_{k,T}$. The regression design problem, in this setting, may be summarized as follows: Find $T^* \in D_n$ such that

(1.3) $$\mathrm{Var}(\hat{\beta}_{k,T^*}) = \inf_{T \in D_n} \mathrm{Var}(\hat{\beta}_{k,T}) .$$

In general such a T* may not be unique and for this and other reasons may be quite difficult to construct. The computational difficulties associated with optimal designs led Sacks and Ylvisaker (1970) and Wahba (1971, 1974) to develop an asymptotic solution to problem (1.3) for several types of covariance kernels.

In a previous paper [5] we addressed the question of uniqueness for optimal designs. It was found that for covariance kernels of a certain form and under certain conditions on the regression function, f, problem (1.3) had a unique solution for each n. In addition, under weaker assumptions on f, the regression design problem was shown to eventually (for all n greater than some finite n_0) have unique optimal solutions. It is the objective of the present paper to extend these uniqueness and eventual uniqueness results to a wider class of processes. The class of processes considered includes those having covariance structures such as that of multiple integrals of Brownian motion and Brownian bridge processes. It is of interest to note that an algorithm for optimal design computation developed by Eubank, Smith and Smith (1981b) will also now be applicable to this class of processes, and, consequently, may be utilized along with the unicity results of this paper to develop a computationally feasible scheme for optimal design construction.

In Section 2 we discuss the class of processes to be considered and present our principal results. The proofs of these findings are provided in Section 3. The techniques utilized in the proofs make it possible to draw certain conclusions regarding the asymptotic equivalence of variable breakpoint piecewise polynomial approximation and the regression design problem considered by Sacks and Ylvisaker (1970). This point is discussed in Section 4.

2. Results and notation. It is well known (c.f. Parzen (1961a, 1961b)) that the covariance kernel R generates a RKHS which is isometrically isomorphic to the Hilbert space spanned by the X process. We denote this RKHS by H(R) and its associated norm by $||\cdot||_R$. Under the assumption that $f \in H(R)$, the regression design problem may be reformulated as a

minimum norm approximation problem. Let

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

and for $T \varepsilon D_n$ set

$$(2.2) \quad R_{k,T} := \text{span } \{R^{(0,j)}(\cdot,t) \mid t \varepsilon T,\ j = 0,\ldots,k-1\}.$$

Then, Sacks and Ylvisaker (1970) have shown that

$$\text{Var}(\hat{\beta}_{k,T}) = ||\mathcal{R}_{k,T} f||_R^{-2}$$

where $\mathcal{R}_{k,T}$ denotes the H(R) orthogonal projector for the subspace $R_{k,T}$. As $||\mathcal{R}_{k,T} f||_R^2 = ||f||_R^2 - ||f - \mathcal{R}_{k,T} f||_R^2$, it follows that the optimal design problem is equivalent to finding a $T^* \varepsilon D_n$ such that

$$(2.3) \quad ||f - \mathcal{R}_{k,T^*} f||_R = \inf_{T \varepsilon D_n} ||f - \mathcal{R}_{k,T} f||_R \quad .$$

In general, very little is known about the properties of T* for finite n. However, for the type of processes studied in this paper several positive statements can be made.

We now restrict our attention to a specific class of processes and their corresponding covariance kernels. Let

$$(2.4) \quad K(s,t) = \int_0^1 \frac{(s-u)_+^{k-1} (t-u)_+^{k-1}}{(k-1)!^2} du$$

and let $Z(\cdot)$ denote the corresponding normal process, i.e., a (k-1)-fold multiple integral of Brownian motion. Define a new process, W, by

$$(2.5) \quad W(t) = \begin{cases} Z(t) - E[Z(t) \mid Z^{(j)}(1),\ j=k-q,\ldots,k-1], & 0 < q \leq k, \\ Z(t) & , q = 0 \quad . \end{cases}$$

Unless noted to the contrary, it will be assumed in subsequent discussions that R is given by

(2.6) $R(s,t) = \mathrm{Cov}(W(s),W(t))$.

More specifically, for $0 < q \leq k$, R can be shown to have the form

(2.7) $R(s,t) = K(s,t) - \nu(s)'B^{-1}\nu(t)$

where $\nu(s)$ is a vector whose ith component is

(2.8) $$\nu_i(s) := K^{(0,k-q+i)}(s,1) = \int_0^1 \frac{(s-u)_+^{k-1}}{(k-1)!} \frac{(1-u)^{q-i-1}}{(q-i-1)!} du, \quad i=0,\ldots,q-1,$$

and B is a $q \times q$ matrix with ijth element

(2.9) $$b_{ij} := K^{(k-q+i,k-q+j)}(1,1) = \int_0^1 \frac{(1-u)^{q-i-1}}{(q-i-1)!} \frac{(1-u)^{q-j-1}}{(q-j-1)!} du, \quad i,j = 0,\ldots,q-1.$$

When $q = 0$, R is the covariance kernel corresponding to a $(k-1)$-fold multiple integral of Brownian motion whereas the case $q=1$ corresponds to a multiple integral of the Brownian bridge process. The case $q = k$ was considered by Eubank, Smith and Smith (1981a, 1981b).

For processes with covariance kernels of the form (2.7), it is possible to prove the following theorem regarding the unicity and eventual unicity of optimal designs for the linear estimation of β.

Theorem 2.1 . Let k be a fixed positive integer and let $f \in H(R) \cap C^{2k}[0,1]$ with $f^{(2k)} > 0$ on $[0,1]$ and $\log f^{(2k)}$ concave on $(0,1)$. Then, for each positive integer n there exists a unique optimal solution to the regression design problem (2.3). If, instead, we assume that $f \in H(R)$ with both $f^{(2k)} > 0$ and $f^{(2k+3)}$ continuous on $[0,1]$ then there is a positive integer n_0 such that for all n larger than n_0 problem (2.3) has a unique solution.

In addition, it is possible to prove, for general k, a finite sample analog of an asymptotic result given by Sacks and Ylvisaker (1970) for the special case of $k = 2$.

Theorem 2.2. If k is even and $f \in H(R)$ with $f^{(2k)} > 0$ then if $T^* \in D_n$ is an optimal design $\mathrm{Var}(\hat{\beta}_{k-1,T^*}) = \mathrm{Var}(\hat{\beta}_{k,T^*})$.

Theorem 2.2 has the consequence that through the use of optimal designs one can obtain equivalent resolution using $(k-1)(n+1)$ rather than $k(n+1)$ observations for k even. A result similar to Theorem 2.2 has been given by Wahba (1971) for a certain class of covariance kernels and specific types of regression functions.

The principal difficulties associated with the use of optimal designs have been their possible duplicity and computational infeasibility. However, in some cases it is possible to use an algorithm developed by Chow (1978) and adapted to the regression design problem by Eubank, Smith, and Smith (1981b) for optimal design computation. As a result of our proofs in the next section it follows that this algorithm is applicable for covariance kernels of the form (2.7). Consequently, through use of this algorithm in conjunction with Theorem 2.1 the utilization of optimal regression designs may now be considered as a viable estimation technique for the type of processes studied in this paper. In addition, this entails that Theorem 2.2 has both practical and theoretical implications for these processes.

3. Proofs of theorems. In this section we analyze the structure of the optimal design problem for covariance kernels of the form (2.7). In particular, we prove Theorems 2.1 and 2.2. First, however, it will be useful to consider certain recent results regarding piecewise polynomial approximation which will be required in the proofs.

For $1 \leq q \leq k$ denote the set of polynomials of order q (degree < q) by P_q and for a given $T = (t_0, t_1, \ldots, t_n) \varepsilon D_n$ let $P_{k,T}$ represent the set of piecewise polynomials on [0,1] with breakpoints at $t_1, \ldots, t_{n-1}$. Also, denote by $P_{k,n} := \bigcup_{T\varepsilon D_n} P_{k,T}$ the set of all piecewise polynomials of order k with n-1 distinct breakpoints in [0,1]. As most of the work which follows will involve approximation in the $L_2[0,1]$ norm we make the identifications for f, g ε $L_2[0,1]$,

$$\langle f,g \rangle = \int_0^1 f(x)g(x)dx$$

and

$$||f|| = \{\int_0^1 f(x)^2 dx\}^{\frac{1}{2}} \quad .$$

Given f ε $L^2[0,1]$ it is frequently of interest to consider finding a best approximation to f from $P_{k,n}$. Thus, one attempts to find a $T_n^* \varepsilon D_n$ such that

(3.1) $$||f - \mathcal{P}_{k,T_n^*} f|| = \inf_{T\varepsilon D_n} ||f - \mathcal{P}_{k,T} f||$$

where $\mathcal{P}_{k,T}$ denotes the $L_2[0,1]$ orthogonal projector for $P_{k,T}$. Several recent results due to Barrow, et al. (1978), Barrow and Smith (1978) and Chow (1978) are available regarding the properties of T_n^*. These results were discussed in Eubank, Smith and Smith (1981) and are stated again here for completeness.

<u>Theorem 3.1.</u> Let f ε $C^k[0,1]$ with $f^{(k)} > 0$ on [0,1] and log $f^{(k)}$ concave on (0,1). Then, for each positive integer n, T_n^* in (3.1) is unique. If, instead, it is assumed that f ε $C^{k+3}[0,1]$ with $f^{(k)} > 0$ on [0,1] then there is a particular integer, n_0, such that for all $n > n_0$ T_n^* is unique.

<u>Proposition.</u> Let $f^{(k)} > 0$ and let p^* be a best $L_2[0,1]$ approximation to f from $P_{k,n}$. Then, if k is even, $p^* \varepsilon C[0,1]$.

We now consider the structure of the optimal design problem for covariance kernels of the form (2.7). For fixed values of k and q, H(R) is seen to consist of functions with k-1 absolutely continuous derivatives and is given by

$$(3.2)\quad H(R) = \begin{cases} \{f|f^{(j)}(0)=0, j=0,\ldots,k-1, f^{(j)}(1)=0, j=k-q,\ldots,k-1, f^{(k)} \varepsilon L_2[0,1]\}, & 1 \le q \le k, \\ \{f|f^{(j)}(0)=0,\ j = 0,\ldots,k-1, f^{(k)}\ \varepsilon\ L_2[0,1]\}, & q=0. \end{cases}$$

where the norm for $f\ \varepsilon\ H(R)$ is

$$(3.3)\qquad ||f||_R = ||f^{(k)}|| \ .$$

Now let $r_{t,j}(s) = R^{(k,j)}(s,t)$, $j = 0,\ldots,k-1$, and define the corresponding $(L_2[0,1])$subspace

$$(3.4)\qquad R^k_{k,T} := \text{span}\{R^{(k,j)}(\cdot,t)|t\varepsilon T, j = 0,\ldots,k-1\}$$

$$= \text{span}\{r_{t,j}|t\ \varepsilon\ T,\ j = 0,\ldots,k-1\} \ .$$

Then, in view of (3.3), we have

$$(3.5)\quad ||f - \mathcal{R}_{k,T}f||_R = ||f^{(k)} - (\mathcal{R}_{k,T}f)^{(k)}|| = ||f^{(k)} - \mathcal{R}^k_{k,T}f^{(k)}||$$

where $\mathcal{R}^k_{k,T}$ is the $L_2[0,1]$ orthogonal projector for $R^k_{k,T}$. Consequently, the optimal design problem is equivalent to finding the best $L_2[0,1]$ approximation to $f^{(k)}$ from the functions in $R^k_{k,T}$.

The preceding discussion serves to motivate further study of the form of $R^k_{k,T}$. Therefore, let $K(s,t)$, $\nu_i(s)$ and b_{ij} be as given in Section 2 and for $0 \le j \le k$ let

$$(3.6)\qquad \nu^{(j)}(s) = (\nu_0^{(j)}(s),\ldots,\nu_{q-1}^{(j)}(s))' .$$

Then, the elements of $R^k_{k,T}$ are

(3.7) $$r_{t,j}(s) = K^{(k,j)}(s,t) - \nu^{(k)}(s)'B^{-1}\nu^{(j)}(t),\ 0 \le j \le k-1 .$$

Now set

(3.8) $$p^i_t(s) = \frac{(t-s)_+^{i-1}}{(i-1)!}, \quad i = 1,\dots,k ,$$

with

(3.9) $$p^i(s) := p^i_1(s) = \frac{(1-s)^{i-1}}{(i-1)!}$$

and note that this implies that

(3.10) $$K^{(k,j)}(s,t) = p^{k-j}_t(s),\ j = 0,\dots,k-1,$$

and

(3.11) $$\nu^{(k)}_i(s) = p^{q-i}(s),\ i = 0,\dots,q-1 .$$

Upon observing that

(3.12) $$\nu^{(j)}_i(t) = \left\langle p^{k-j}_t, p^{q-i} \right\rangle, \quad i = 0,\dots,q-1,\ j = 0,\dots,k-1$$

and

(3.13) $$b_{ij} = \left\langle p^{q-i}, p^{q-j} \right\rangle,\ i,j = 0,\dots,q-1,$$

it is readily seen that $r_{t,j}$ is the error function resulting from the $L_2[0,1]$ approximation of p^{k-j}_t from P_q. Using $\mathcal{P}_q$ to denote the orthogonal projector for P_q, the basis elements for $R^k_{k,T}$ are succinctly summarized in the following array.

(3.14)

	$t_0 = 0$	t_1	...	t_{n-1}	$t_n = 1$
$r_{t_i,0}$	0	$p^k_{t_1} - \mathcal{P}_q p^k_{t_1}$	...	$p^k_{t_{n-1}} - \mathcal{P}_q p^k_{t_{n-1}}$	$p^k - \mathcal{P}_q p^k$
$\vdots$	$\vdots$	$\vdots$		$\vdots$	$\vdots$
$r_{t_i,k-q-1}$	0	$p^{q+1}_{t_1} - \mathcal{P}_q p^{q+1}_{t_1}$	...	$p^{q+1}_{t_{n-1}} - \mathcal{P}_q p^{q+1}_{t_{n-1}}$	$p^{q+1} - \mathcal{P}_q p^{q+1}$
$r_{t_i,k-q}$	0	$p^q_{t_1} - \mathcal{P}_q p^q_{t_1}$	...	$p^q_{t_{n-1}} - \mathcal{P}_q p^q_{t_{n-1}}$	0
$\vdots$	$\vdots$	$\vdots$		$\vdots$	$\vdots$
$r_{t_i,k-1}$	0	$p^1_{t_1} - \mathcal{P}_q p^1_{t_1}$	...	$p^1_{t_{n-1}} - \mathcal{P}_q p^1_{t_{n-1}}$	0

The zeros in (3.14) which occur at $t_0 = 0$ and $t_n = 1$ arise from the fact that $p_0^j(s)$ vanishes identically and that $p^{k-j} \in P_q$ for $j = k-q,\ldots,k-1$. This may be interpreted as indicating that observations taken on the corresponding derivatives of the Y process at these points will provide no information about β. This, of course, is otherwise clear from the boundary conditions that functions in H(R) must satisfy.

It follows from (3.14) that, for $T \in D_n$, $R^k_{k,T} \subset P_{k,T}$. Thus, in view of (3.5), it is now apparent that the problem of optimal design unicity is similar to the problem addressed by Theorem 3.1. The only obstacle preventing the immediate proof of Theorem 2.1 is that $R^k_{k,T}$ is properly contained in $P_{k,T}$. To resolve this difficulty we prove the following lemma.

<u>Lemma.</u> Let $f \in H(R)$ and $T \in D_n$. Then the best $L_2[0,1]$ approximation to $f^{(k)}$ from $P_{k,T}$ is $\mathcal{R}^k_{k,T} f^{(k)}$.

<u>Proof</u>. From (3.14), we may write

$$P_{k,T} = P_q \oplus R^k_{k,T} \quad .$$

Using the boundary conditions in (3.2) and integration by parts it can also be shown that for any $g \in H(R)$ and $p \in P_q$,

$$\int_0^1 g^{(k)}(x)p(x)dx = 0 \ .$$

In particular, as $f - \mathcal{R}_{k,T} f$ is in H(R), this entails that $f^{(k)} - \mathcal{R}^k_{k,T} f^{(k)}$ is orthogonal in L_2 to both $R^k_{k,T}$ and P_q. Hence $f^{(k)} - \mathcal{R}^k_{k,T} f^{(k)}$ is orthogonal to $P_{k,T}$ and the lemma is proved.

Theorem 2.1 now follows directly, through use of the lemma, from Theorem 3.1 upon replacing f by $f^{(k)}$. To obtain Theorem 2.2 we use the Proposition to see that when k is even and T* is an optimal design

$$R^k_{k,T^*}f^{(k)} \in R^k_{k,T^*} \cap C[0,1] = \{r_{t,j} | t \in T^*, j = 0,\ldots,k-2\} .$$

4. Piecewise polynomials and regression design. Sacks and Ylvisaker (1970) have considered the asymptotic behaviour of optimal regression designs for a particular class of covariance kernels. Under the assumption that Q is a covariance kernel satisfying certain assumptions (see Assumptions A, B and C in Section 2 of Sacks and Ylvisaker (1968)) R is assumed to have the form

$$(4.1) \qquad R(s,t) = \int_0^1\int_0^1 \frac{(s-u)_+^{k-1}(t-v)_+^{k-1}}{(k-1)!^2} Q(u,v)\,du\,dv .$$

It is then shown that for this type of covariance kernel when f admits the representation

$$(4.2) \qquad f(t) = \int_0^1 \phi(s)R(s,t)\,ds$$

for some $\phi \in C[0,1]$ then

$$(4.3) \qquad \lim_{n\to\infty} n^{2k} \inf_{T\in D_n} ||f - R_{k,T}f||_R^2 = \frac{(k!)^2}{(2k)!(2k+1)!} \left\{\int_0^1 \phi(x)^{2/2k+1} dx\right\}^{2k+1} .$$

The technique utilized in the proof of this result was to first show that (4.3) held in the special case when Q has the form $Q_o(s,t) = \min(s,t)$ and then extend this outcome to general Q through the use of a mapping from H(Q) onto $H(Q_o)$.

Results similar to (4.3) have been obtained by several authors for the asymptotic behaviour of the error from the best $L_2[0,1]$ approximation of a function from $P_{k,n}$. For instance, Burchard and Hale (1975) have shown that if $f \in L_1^k[0,1]$, where

$$(4.4) \qquad L_1^k[0,1] = \{f | f^{(j)} \text{absolutely continuous}, j=0,\ldots,k-1, \int_0^1 |f^{(k)}(x)|\,dx < \infty\},$$

then

$$(4.5)\quad \lim_{n\to\infty} n^{2k} \inf_{T\varepsilon D_n} ||f - P_{k,T}f||^2 = \frac{k!}{(2k)!(2k+1)!} \left\{ \int_0^1 (f^{(k)}(x))^{2/2k+1} dx \right\}^{2k+1}.$$

We now indicate the connection between these two bodies of theory.

The case of $Q(s,t) = \min(s,t)$ corresponds to the event when R is given by (2.4) and $\phi = (-1)^k f^{(2k)}$. As this entails $q = 0$ in our work it now follows from (3.14) that in this case $R^k_{k,T} = P_{k,T}$ and, therefore, in this instance, the optimal design problem corresponds precisely to the problem of best approximating $f^{(k)}$ from $P_{k,n}$. This clearly indicates the reasons underlying the similarity between the asymptotic behaviour of best piecewise polynomial approximations and optimal designs (for other remarks on this relationship see, e.g. McClure (1975)). We now utilize the duality between these two areas of study and note that, for the processes considered in this paper, the work of Burchard and Hale (1975) has the consequence that (4.3) still holds under the weaker assumption that $f^{(k)} \varepsilon L^k_1[0,1]$.

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SECURITY CLASSIFICATION OF THIS PAGE (When Data Entered)

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER 150	2. GOVT ACCESSION NO. AD-A109545	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) Uniqueness and Eventual Uniqueness of Optimal Designs in Some Time Series Models, II		5. TYPE OF REPORT & PERIOD COVERED TECHNICAL REPORT
		6. PERFORMING ORG. REPORT NUMBER 150
7. AUTHOR(s) R. L. Eubank, P. L. Smith and P. W. Smith		8. CONTRACT OR GRANT NUMBER(s) N00014-75-C-0439
9. PERFORMING ORGANIZATION NAME AND ADDRESS Southern Methodist University Dallas, Texas 75275		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS
11. CONTROLLING OFFICE NAME AND ADDRESS Office of Naval Research Arlington, VA 22217		12. REPORT DATE November 1981
		13. NUMBER OF PAGES 14
14. MONITORING AGENCY NAME & ADDRESS(If different from Controlling Office)		15. SECURITY CLASS. (of this report)
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE

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18. SUPPLEMENTARY NOTES

19. KEY WORDS (Continue on reverse side if necessary and identify by block number)

Approximation, optimal designs, piecewise polynomials, time series.

20. ABSTRACT (Continue on reverse side if necessary and identify by block number) Earlier results on the uniqueness and eventual uniqueness of optimal designs for certain time series models are extended to a wider class of processes which includes those with covariance structures such as that of multiple integrals of Brownian motion and Brownian bridge processes. The relationship between the problems of regression design for time series and piecewise approximation with free break-points is discussed and, consequently, asymptotic results obtained by Sacks and Ylvisaker (1970) are seen to hold under weaker assumptions for these processes.

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S/N 0102-014-6601 |

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