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REGRESSION DESIGNS IN AUTOREGRESSIVE STOCHASTIC PROCESSES[1]

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This paper extends some recent results on asymptotically optimal sequences of experimental designs for regression problems in stochastic processes. In the regression model $Y(t) = \beta f(t) + X(t)$, $0 \leqq t \leqq 1$, the constant β is to be estimated based on observations of $Y(t)$ and its first $m-1$ derivatives at each of a set T_n of n distinct points. The function f is assumed known as is the covariance kernel of $X(t)$, a zero-mean mth order autoregressive process. Under certain conditions, we derive a sequence $\{T_n\}$ of experimental designs which are asymptotically optimal for estimating β.

1. Introduction and summary. Let $\{Y(t): 0 \leqq t \leqq 1\}$ be a stochastic process of the form

$$Y(t) = \beta f(t) + X(t) \tag{1.1}$$

where β is an unknown constant, $\{X(t)\}$ is a zero-mean, real stochastic process with known covariance kernel $k(s, t) = EX(s)X(t)$, and f is a known function of the form

$$f(t) = \textstyle\int_0^1 k(s, t)\phi(s)\, ds\,. \tag{1.2}$$

Given a subset T of $[0, 1]$, we observe $Y(t)$ and its first $m-1$ derivatives at each point $t \in T$. The parameter β is to be estimated by an unbiased estimator $\hat{\beta}_T$ which is linear in the observation set $\{Y^{(j)}(t): j = 0, 1, \cdots, m-1; t \in T\}$ and which has minimum variance among all such estimators. Given any n, let $\mathscr{T}_n$ be the class of all subsets T_n of $[0, 1]$ containing exactly n points. Then the problem of optimal design is to find a set $\hat{T}_n \in \mathscr{T}_n$ for which $\operatorname{Var} \hat{\beta}_{\hat{T}_n} \leqq \operatorname{Var} \hat{\beta}_{T_n}$ for all $T_n \in \mathscr{T}_n$. Because optimal designs when they exist are generally very difficult to compute, Sacks and Ylvisaker (1966) introduced the concept of an asymptotically optimal sequence of designs.

DEFINITION. A sequence $\{\hat{T}_n\}$ of designs is said to be asymptotically optimal (in the sense of Sacks and Ylvisaker) if

$$\lim_{n\to\infty} \frac{\operatorname{Var} \hat{\beta}_{\hat{T}_n} - \operatorname{Var} \hat{\beta}_T}{\inf \operatorname{Var} \hat{\beta}_{T_n} - \operatorname{Var} \hat{\beta}_T} = 1 \tag{1.3}$$

where $T = [0, 1]$ and the infimum is taken over all $T_n \in \mathscr{T}_n$.

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Sacks and Ylvisaker (1969) considered processes $\{X(t)\}$ of the form

$$X(t) = \int_0^t \int_0^{t_{m-1}} \cdots \int_0^{t_2} V(t_1)\, dt_1 \cdots dt_{m-1}$$

where

$$\lim_{s\to t^-} \frac{\partial}{\partial s} E[V(s)V(t)] - \lim_{s\to t^+} \frac{\partial}{\partial s} E[V(s)V(t)] = c ,$$

where c is a positive constant. Under certain assumptions, they showed that the designs $T_n = \{t_{in}: i = 1, 2, \cdots, n\}$ defined by

$$\int_0^{t_{in}} [\phi(t)]^{2/(2m+1)}\, dt = \frac{i}{n} \int_0^1 [\phi(t)]^{2/(2m+1)}\, dt$$

form an asymptotically optimal sequence. Wahba (1971) recently considered processes $\{X(t)\}$ satisfying the stochastic differential equation

$$LX(t) = dW(t)/dt \tag{1.4}$$

where $W(t)$ is Brownian motion and L is an mth order linear differential operator of the special form

$$L = D \frac{1}{\omega_m(t)} D \frac{1}{\omega_{m-1}(t)} \cdots D \frac{1}{\omega_1(t)} \tag{1.5}$$

where $\omega_j(t) > 0$ and $\omega_j(t) \in C^{m-j}$. (The symbol D denotes differentiation.) A differential operator L of the form (1.5) has the property that its null space is spanned by an extended complete Tchebycheff system.

The present paper considers a much broader class of processes $\{X(t)\}$, namely those processes which satisfy a linear stochastic differential equation (1.4) where L is *any* mth order linear differential operator of the form

$$L = \sum_{j=0}^m a_j(t) D^j , \qquad a_j(t) \in C^j,\ a_m(t) \neq 0 ; \tag{1.6}$$

thus, $\{X(t)\}$ is an mth order autoregressive process. The goal of this paper is to prove, under certain mild conditions, that an asymptotically optimal sequence of designs for estimating β in (1.1) is given by

$$\int_0^{t_{in}} [\phi(t)/a_m(t)]^{2/(2m+1)}\, dt = \frac{i}{n} \int_0^1 [\phi(t)/a_m(t)]^{2/(2m+1)}\, dt .$$

This result, with a form of error estimate, is stated precisely at the beginning of Section 3.

There are many examples of processes for which the results of Sacks and Ylvisaker (1966), (1968), (1969) and of Wahba (1971) are not applicable, but for which the present results are. One such process $\{X(t)\}$ is given by

$$X(t) = \frac{1}{2\pi} \int_0^t \frac{\sin 2\pi(t-s)}{1+s}\, dW(s) ,$$

which satisfies (1.4) when $L = (1+t)D^2 + 4\pi^2(1+t)$.

2. Some lemmas. We restrict our attention to an interval $[0, u]$, $0 < u \leqq 1$ where u is fixed. For any t, $0 \leqq t < u$, let $\psi(\cdot, t)$ be the unique solution on the interval $[t, u]$ of the differential equation $L\psi(\cdot, t) = 0$ subject to the initial conditions

$$\psi_{j0}(t^+, t) = \delta_{j,m-1}/a_m(t)\,, \qquad j = 0, 1, \cdots, m-1$$

where δ is the Kronecker delta and the notation $\psi_{pq}(a, b)$ means

$$\frac{\partial^{p+q}}{\partial s^p\, \partial t^q}\, \psi(s, t)\Big|_{s=a,t=b}\,.$$

Let $g(s, t) = \psi(s, t)$ if $s \geqq t$, and $g(s, t) = 0$ otherwise. Then g is the Green's function for the differential equation $Lf = h$ subject to the initial conditions $f^{(j)}(0) = 0$, $j = 0, 1, \cdots, m-1$. Thus, for fixed t, $g(\cdot, t) \in C^m$ on $(0, t)$ and on (t, u) while $g_{m-1,0}(t^+, t) - g_{m-1,0}(t^-, t) = 1/a_m(t)$. Similarly, if L^* is the operator $L^*f = \sum_{j=0}^m (-1)^j D^j[a_j f]$, which is adjoint to L, then the Green's function for the differential equation $L^*f = h$ subject to the initial conditions $f^{(j)}(u) = 0$, $j = 0, 1, \cdots, m-1$ is $g^*(s, t) = g(t, s)$.

Let $\{X(t)\}$ be the process defined by

$$X(t) = \textstyle\int_0^u g(t, s)\, dW(s)\,. \tag{2.1}$$

We state some well-known results about the process $\{X(t)\colon 0 \leqq t \leqq u\}$: The process $\{X(t)\}$ satisfies (1.4) and the initial conditions

$$X^{(j)}(0) = 0\,, \qquad j = 0, 1, \cdots, m-1\,. \tag{2.2}$$

Moreover, $\{X(t)\}$ is an mth order autoregressive process so that for $0 < s_1 < t < s_2 < u$, $X(s_1)$ and $X(s_2)$ are conditionally uncorrelated given the set $M = \{X^{(j)}(t)\colon j = 0, 1, \cdots, m-1\}$, and hence

$$E\{X(s_1) - E[X(s_1) \mid M]\}\{X(s_2) - E[X(s_2) \mid M]\} = 0\,. \tag{2.3}$$

We associate with the process $\{X(t)\}$ two Hilbert spaces. The first is the space $\mathscr{X}$ which is the closure of the vector space spanned by $\{X(t)\colon 0 \leqq t \leqq u\}$ with inner product determined by $\langle X(s), X(t)\rangle = EX(s)X(t) = k(s, t)$. The second is the space $\mathscr{H}$ of all real functions h on $[0, u]$ such that (i): For $j = 0, 1, \cdots, m-1$, $h^{(j)}$ is absolutely continuous and $h^{(j)}(0) = 0$, and (ii): Lh is square integrable. The inner product in $\mathscr{H}$ is given by $\langle h_1, h_2\rangle = \int (Lh_1)(Lh_2)$ and $\mathscr{H}$ is a reproducing kernel Hilbert space (RKHS) with kernel k. There is an isomorphism between $\mathscr{X}$ and $\mathscr{H}$ which preserves inner products. The image under this isomorphism of any random variable $Z \in \mathscr{X}$ is the function $h(t) = E[ZX(t)]$. For details on the above facts, the reader is referred to Hájek (1962), Parzen (1961) and Dolph and Woodbury (1952).

Using the foregoing theory with $u = 1$ it can be shown that for any design T, Var $\hat\beta_T = \|P_T f\|^{-2}$ where the norm is taken in $\mathscr{H}$ and P_T is the projection onto the subspace spanned by $\{k(\cdot, t)\colon t \in T\}$. Hence the definition (1.3) of asymptotic optimality is equivalent to

$$\lim_{n\to\infty} \frac{\|f - P_{\hat T_n} f\|^2}{\inf \|f - P_{T_n} f\|^2} = 1 \tag{2.4}$$

where the infimum is taken over all $T_n \in \mathscr{D}_n$.

For fixed u, $0 \leqq u \leqq 1$ let $\mathscr{U} = \{X^{(j)}(u): j = 0, 1, \cdots, m-1\}$ and P_u be the projection operator in $\mathscr{X}$ onto the subspace spanned by $\mathscr{U}$. Consider the stochastic process $\{\bar{X}(t): 0 \leqq t \leqq u\}$ where $\bar{X}(t) = X(t) - P_u X(t)$. The RKHS $\bar{\mathscr{H}}$ associated with the process $\{\bar{X}(t)\}$ can easily be shown to consist of the subspace of all functions $h \in \mathscr{H}$ for which $h^{(j)}(u) = 0$ for all $j = 0, 1, \cdots, m-1$.

LEMMA 1. *Let ϕ be a continuous function and let*

$$w(t) = E[\textstyle\int_0^u \phi(s)\bar{X}(s)\,ds]\bar{X}(t) \tag{2.5}$$
$$= E[\textstyle\int_0^u \phi(s)X(s)\,ds - P_u \int_0^u \phi(s)X(s)\,ds]X(t)\,.$$

Then $w(t)$ is the unique solution to the 2mth *order linear differential equation*:

$$L^*Lw(t) = \phi(t) \tag{2.6}$$

subject to the boundary conditions

$$w^{(j)}(0) = w^{(j)}(u) = 0\,, \qquad j = 0, 1, \cdots, m-1\,. \tag{2.7}$$

PROOF. To show that the solution to (2.6) and (2.7) is unique, we note that if $L^*Lv(t) = 0$, then $0 = \int (L^*Lv)v = \int (Lv)^2$ and hence $Lv = 0$ so that by (2.7) we have $v = 0$. Now $w(t)$ defined by (2.5) clearly satisfies (2.7). To show it satisfies (2.6) let $\bar{h}_t$ be the function in $\bar{\mathscr{H}}$ corresponding to $\bar{X}(t)$. For m suitable functions $\alpha_j(t)$,

$$\bar{X}(t) = X(t) - \textstyle\sum_{j=0}^{m-1} \alpha_j(t)X^{(j)}(u)$$
$$= \textstyle\int_0^u [g(t, s) - \sum \alpha_j(t)g_{j0}(u, s)]\,dW(s)\,.$$

Hence $L\bar{h}_t(s) = g(t, s) - \sum \alpha_j(t)g_{j0}(u, s)$ and

$$Lw(s) = \textstyle\int_0^u \phi(t)[g(t, s) - \sum \alpha_j(t)g_{j0}(u, s)]\,dt\,.$$

Now $L^*g_{j0}(u, s) = 0$ and $L^* \int_0^u \phi(t)g(t, s)\,dt = \phi(s)$; hence $L^*Lw(s) = \phi(s)$ and the lemma is proved.

LEMMA 2. Var $\int_0^u \phi(t)\bar{X}(t)\,dt = \int_0^u \phi(t)w(t)\,dt$ *where w is defined by* (2.5).

PROOF.

$$\text{Var} \textstyle\int_0^u \phi(t)\bar{X}(t)\,dt = E[\int_0^u \phi(t) \int_0^u \phi(s)\bar{X}(s)\bar{X}(t)\,ds\,dt]$$
$$= \textstyle\int_0^u \phi(t)E[\int_0^u \phi(s)\bar{X}(s)\bar{X}(t)\,ds]\,dt = \int_0^u \phi(t)w(t)\,dt\,.$$

In the preceding discussion u has been fixed. We now allow u to vary and indicate the dependence on u by a subscript.

LEMMA 3. *For $j = 0, 1, \cdots, m$,*

$$\lim_{u\to 0+} u^{j-m}w_u^{(m+j)}(0) = \frac{(-1)^j\binom{m}{j}(m+j)!}{(2m)!\,a_m^2(0)}\,\phi(0)\,. \tag{2.8}$$

PROOF. By (2.6) we have

$$w_u^{(2m)}(t) = (-1)^m a_m^{-2}(t)[\phi(t) - \textstyle\sum_{j=0}^{2m-1} b_j(t)w_u^{(j)}(t)]\,, \tag{2.9}$$

where the functions $b_j(t)$, which are expressible in terms of the coefficients $a_j(t)$, are of no present interest. Because of the boundary conditions at 0, the Taylor expansions for $w_u(t)$ and its first $m-1$ derivatives take the form

$$w_u^{(i)}(t) = \sum_{j=0}^{m} \frac{t^{m+j-i} w_u^{(m+j)}(0)}{(m+j-i)!} + o(t^{2m-i}), \tag{2.10}$$

which, by (2.9), equals

$$\sum_{j=0}^{m-1} \frac{t^{m+j-i} w_u^{(m+j)}(0)}{(m+j-i)!} + (-1)^m t^{2m-i} \frac{\phi(0) - \sum_{j=0}^{2m-1} b_j(0) w_u^{(j)}(0)}{a_m^2(0)(2m-i)!} + o(t^{2m-i}).$$

Hence the boundary conditions imply

$$0 = \sum_{j=0}^{m-1} \frac{u^{m+j-i} w_u^{(m+j)}(0)}{(m+j-i)!} + (-1)^m u^{2m-i} \frac{\phi(0) - \sum_{j=m}^{2m-1} b_j(0) w_u^{(j)}(0)}{a_m^2(0)(2m-i)!} + o(u^{2m-i}).$$

Multiplying by u^{i-2m} and denoting $u^{j-m} w_u^{(m+j)}(0)$ by $x_j(u)$, we derive

$$\frac{(-1)^{(m+1)}[\phi(0) - \sum_{j=0}^{m-1} u^{m-j} b_{m+j}(u) x_j(u)]}{(2m-i)!\, a_m^2(0)} = \sum_{j=0}^{m-1} \frac{x_j(u)}{(m+j-i)!} + o(1), \tag{2.11}$$

a system of m identities in u. The system (2.11) implies that for $j = 0, 1, \cdots, m-1$, $x_j = \lim_{u \to 0+} x_j(u)$ exist and satisfy

$$\frac{(-1)^{m+1}\phi(0)}{(2m-i)!\, a_m^2(0)} = \sum_{j=0}^{m-1} \frac{x_j}{(m+j-i)!}, \qquad i = 0, 1, \cdots, m-1. \tag{2.12}$$

But equation (8) of Riordan (1968, page 10) shows that the solution to the system (2.12) is

$$x_j = \frac{(-1)^j \binom{m}{j} (m+j)!\, \phi(0)}{(2m)!\, a_m^2(0)}. \tag{2.13}$$

The proof of the lemma is complete because (2.9) shows that (2.8) also holds for $j = m$.

LEMMA 4.

$$\lim_{u \to 0+} u^{-2m-1} \operatorname{Var} \int_0^u \phi(t) \bar{X}(t)\, dt = \frac{\phi^2(0)(m!)^2}{a_m^2(0)(2m)!\,(2m+1)!}.$$

PROOF. From (2.10) with $i = 0$, we get

$$\begin{aligned}
\lim_{u \to 0+} u^{-2m-1} \int_0^u \phi(t) w_u(t)\, dt
&= \lim_{u \to 0+} \sum_{j=0}^{m} \frac{u^{j-m} w_u^{(m+j)}(0) \phi(u_j)}{(m+j+1)!} \qquad \text{where } 0 \leqq u_j \leqq u \\
&= \frac{\phi^2(0)}{(2m)!\, a_m^2(0)} \sum_{j=0}^{m} \frac{(-1)^j \binom{m}{j}}{m+j+1} \\
&= \frac{\phi^2(0) B(m+1, m+1)}{(2m)!\, a_m^2(0)}
\end{aligned}$$

where B is the (complete) Beta function.

In the next section we shall need the following lemma, whose proof follows from Lemma 4 by letting $Z(t) = X(t - t_1)$.

LEMMA 5. *Suppose* $0 \leqq t_1 < t_2 \leqq 1$. *Let* $\Delta = t_2 - t_1$ *and* P *be the projection operator in* $\mathscr{H}$ *onto the subspace spanned by* $\{X^{(j)}(t_1), X^{(j)}(t_2): j = 0, 1, \cdots, m-1\}$. *Then*

$$\operatorname{Var} \int_{t_1}^{t_2} \phi(t)[X(t) - PX(t)]\, dt = \frac{(m!)^2 \Delta^{2m+1} \phi^2(t_1)}{a_m^2(t_1)(2m)!\,(2m+1)!} + o(\Delta^{2m+1}) .$$

3. The principal result. We shall prove the following theorem.

THEOREM. *Let* $\{X(t): 0 \leqq t \leqq 1\}$ *be a real stochastic process satisfying the stochastic differential equation* $LX(t) = dW(t)/dt$ *where* W *is the Wiener process and* L *is any* mth *order linear differential operator*,

$$L = \sum_{j=0}^{m} a_j(t) D^j , \qquad a_j \in C^j , \tag{3.1}$$

whose leading coefficient $a_m(t)$ *is never zero. Let* $f(t) = \int k(s, t)\phi(s)\, ds$ *where* ϕ *is non-vanishing and continuous on* $[0, 1]$ *and where* $k(s, t) = E[X(s)X(t)]$. *If, in the regression model* $Y(t) = \beta f(t) + X(t)$, β *is to be estimated based on observations* $\{Y^{(j)}(t_{in}): j = 0, 1, \cdots, m-1;\ t_{in} \in T_n\}$, *then an asymptotically optimal sequence of designs is* $\{\hat{T}_n\} = \{\{\hat{t}_{in}: i = 1, 2, \cdots, n\}\}$ *where*

$$\int_0^{\hat{t}_{in}} [\phi(t)/a_m(t)]^{2/(2m+1)}\, dt = \frac{i}{n} \int_0^1 [\phi(t)/a_m(t)]^{2/(2m+1)}\, dt . \tag{3.2}$$

Moreover,

$$\lim_{n\to\infty} n^{2m} \|f - \hat{P}f\|^2 = \frac{(m!)^2}{(2m)!\,(2m+1)!} \left[\int_0^1 [\phi(t)/a_m(t)]^{2/(2m+1)}\, dt\right]^{2m+1} , \tag{3.3}$$

where $\hat{P}$ *is the projection in* $\mathscr{H}$ *onto the space spanned by* $\{k^{(j)}(\hat{t}_{in}, \cdot)\}$.

PROOF. Without loss of generality we can assume $\{X(t)\}$ satisfies (2.2). (Otherwise we append the point $t_{0n} = 0$ to the design without affecting its asymptotic optimality.) Similarly, we can assume $t_{nn} = 1$ for every design. Also, we note that any candidate $\{T_n\}$ for an asymptotically optimal sequence must have

$$\lim_n \max_i (t_{i+1,n} - t_{in}) = 0 . \tag{3.4}$$

Now, let $\{T_n\} = \{\{t_{in}: i = 1, 2, \cdots, n\}\}$ be any sequence of designs satisfying (3.4) and $t_{nn} = 1$. For notational convenience we suppress the second subscript of t_{in}, we denote the function $[\phi(t)/a_m(t)]^2$ by $h(t)$, and we denote the constants $2m+1$, $(2m+1)/(2m)$ and $(m!)^2[(2m)!\,(2m+1)!]^{-1}$ by p, q, and c, respectively. By (2.3)

$$\begin{aligned} \|f - Pf\|^2 &= \operatorname{Var} \int_0^1 \phi(t)[X(t) - PX(t)]\, dt \\ &= \operatorname{Var} \sum_{i=0}^{n-1} \int_{t_i}^{t_{i+1}} \phi(t)[X(t) - PX(t)]\, dt \\ &= \sum_{i=0}^{n-1} \operatorname{Var} \int_{t_i}^{t_{i+1}} \phi(t)[X(t) - PX(t)]\, dt \end{aligned}$$

where $t_0 = 0$ and P is the projection in $\mathscr{H}$ onto the subspace spanned by $\{k^{(j)}(t_i, \cdot)\}$. Since (3.4) holds, Lemma 5 implies

$$\|f - Pf\|^2 = c \sum_{i=0}^{n-1} h(t_i)[(t_{i+1} - t_i)^p + o(t_{i+1} - t_i)^p] . \tag{3.5}$$

Having established (3.5) we complete the proof in a manner similar to that of Sacks and Ylvisaker (1966). Hölder's inequality implies

$$\|f - Pf\|^2 \geqq cn^{-p/q}[\textstyle\sum_{i=0}^{n-1} h^{1/p}(t_i)(t_{i+1} - t_i)]^p + o(n^{-2m}) \tag{3.6}$$
$$= cn^{-2m}[\textstyle\int_0^1 h^{1/p}(t)\,dt]^p + o(n^{-2m}) .$$

To evaluate $\|f - \hat{P}f\|^2$ we apply a mean value theorem to (3.2), which yields

$$(\hat{t}_{i+1} - \hat{t}_i)h^{1/p}(t_i) = n^{-1} \textstyle\int_0^1 h^{1/p}(t)\,dt + o(n^{-1}) ,$$

and apply (3.5) which yields

$$\|f - \hat{P}f\|^2 = c \textstyle\sum_{i=0}^{n-1} n^{-p}[\int_0^1 h^{1/p}(t)\,dt]^p + o(n^{-2m}) \tag{3.7}$$
$$= cn^{-2m}[\textstyle\int_0^1 h^{1/p}(t)\,dt]^p + o(n^{-2m}) .$$

This proves (3.3), and the asymptotic optimality of $\{\hat{T}_n\}$ follows from (3.6) and (3.7).

4. Remarks.

REMARK 1. The conditions of the theorem can be weakened somewhat. First, the condition that ϕ never vanish can be replaced by a condition which restricts the behavior of ϕ in the neighborhood of any zero. (For example, see Sacks and Ylvisaker (1969).) Second, although we assume that $\{X(t)\}$ satisfies the stochastic differential equation (1.4), we use only properties of the first two moments of $\{X(t)\}$, namely $EX(t) = 0$ and $E[X(s)X(t)] = k(s, t) = \int_0^1 g(t, \cdot)g(s, \cdot)$ where g is the Green's function corresponding to L. Hence the results of this paper are applicable to all processes of the form $X(t) = \int_0^1 g(t, s)\,dU(s)$ where $\{U(t)\}$ is a random orthogonal process with structural measure equal to Lebesgue measure.

REMARK 2. There is a close relation between the statistical design problem discussed here and certain integral approximation problems. The interested reader is referred to Sacks and Ylvisaker (1970). (Also, see Karlin (1972).)

REMARK 3. Many of the results of this paper can be extended to the more general regression model

$$Y(t) = \sum \beta_j f_j(t) + X(t)$$

where Var $\hat{\beta}$ is replaced by a suitable norm on the matrix **Var** $\hat{\boldsymbol{\beta}}$. (See Sacks and Ylvisaker (1968).)

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