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A NOTE ON THE REGRESSION DESIGN

PROBLEM OF SACKS AND YLVISAKER

by

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# A Note on the Regression Design Problem of Sacks and Ylvisaker

By

Grace Wahba

## 0. Summary

We consider the experimental design problem of Sacks and Ylvisaker. We first consider the case of the (noise) stochastic process  $X$  satisfying a stochastic differential equation of the form

$$L_m X(t) = dW(t)/dt \quad 0 \leq t \leq 1 \quad (0.1)$$

where  $L_m$  is an  $m$ th order differential operator whose null space is spanned by an ECT system and  $W(t)$  is a Wiener process. We show that the non degeneracy of the covariance matrix of  $\{X^{(\nu)}(t_i), \nu=0, 1, 2, \dots, m-1, t_i \in [0, 1], i=1, 2, \dots, n\}$  is equivalent to the total positivity properties of the Green's function for  $L_m^* L_m$  with appropriate boundary conditions. An asymptotically optimal sequence of designs is found for this case and its dependence on the characteristic discontinuity of the above mentioned Green's function is exhibited. We next show how an entire class of experimental design-regression problems reduces to the experimental design problem in question, for general  $X$ . Returning to  $X$  of (0.1), we finally show that a special case of the problem is equivalent to the problem of the optimal approximation of a monomial by Spline function in the  $L_2$  norm. Some recent results are available on this latter problem which provide some information concerning existence and uniqueness of optimal designs with distinct points.

# 1. Introduction

Consider the linear regression model in which one may observe a stochastic process  $Y$  having the form

$$Y(t) = \theta f(t) + X(t) \quad 0 \leq t \leq 1. \quad (1.1)$$

$\theta$  is an unknown constant,  $f(t)$  is a known function and  $X$  is assumed to have mean value function 0 and known continuous covariance kernel  $Q(t, t') = EX(t) X(t')$ . Let  $T$  be a subset of  $[0, 1]$  and let  $\hat{\theta}_T$  be the best linear estimate (if it exists) of  $\theta$  based on observing  $\{Y(t), t \in T\}$ . Let  $\sigma_T^2$  be  $E(\theta - \hat{\theta}_T)^2$ . Let  $\mathcal{D}_n = \{T_n \mid T_n = t_0, t_1, \dots, t_n, 0 \leq t_0 < \dots < t_n \leq 1\}$ . Sacks and Ylvisaker, in a series of papers [8], [9], [10], Consider the problem of finding a member  $T_n^*$  of  $\mathcal{D}_n$  for which

$$\sigma_{T_n^*}^2 = \inf_{T_n \in \mathcal{D}_n} \sigma_{T_n}^2. \quad (1.2)$$

In [8], [9] they consider processes  $X(t)$  which are assumed to have no quadratic mean derivatives and satisfy a number of other conditions. [10] considered situations where  $X(t)$  has exactly  $m-1$  quadratic mean derivatives. It is assumed there that  $X(t)$  has a representation

$$X(t) = \int_0^t dt_{m-1} \int_0^{t_{m-1}} dt_{m-2} \dots \int_0^{t_2} X_0(t_1) dt_1 \quad (1.3)$$

where

$$EX_0(t) = 0$$

(1.4)

$$EX_0(s)X_0(t) = K(s,t)$$

with

$$\lim_{s \downarrow t} \frac{\partial}{\partial s} K(s,t) - \lim_{s \uparrow t} \frac{\partial}{\partial s} K(s,t) = \alpha(t) = \text{const} > 0 \quad (1.5)$$

and  $K(s,t)$  satisfies some other conditions.

Throughout [8], [9], [10] it is assumed that  $f(t)$  is of the form

$$f(t) = \int_0^1 Q(t,t') \rho(t') dt', \quad \rho \text{ continuous} \quad (1.6)$$

where

$$Q(t,t') = E X(t) X(t'),$$

and  $f$  satisfies some other conditions.

A sequence  $T_n^*$ ,  $n=1,2,\dots$  of designs  $T_n^* \in \mathcal{D}_n$ , is said by Sacks and Ylvisaker to be asymptotically optimum if

$$\lim_{n \rightarrow \infty} \frac{\sigma_{T_n^*}^2 - \sigma^2}{\inf_{T_n \in \mathcal{D}_n} \sigma_{T_n}^2 - \sigma^2} = 1 \quad (1.7)$$

where  $\sigma^2 = \sigma_T^2$  with  $T = [0,1]$ . It is well known that  $\sigma^2 > 0$  if

$f \in \mathcal{H}_Q$ , where  $\mathcal{H}_Q$  is the reproducing kernel Hilbert space associated with the kernel  $Q$ , and that (1.6) insures that  $f \in \mathcal{H}_Q$ . (See [7] for details).

$\mathcal{H}_Q$ , for any  $Q$  positive definite on  $[0,1] \times [0,1]$ , has the following properties (see [1]):



$$1) \quad Q_t(\cdot) \in \mathcal{H}_Q \quad \forall t \in [0, 1]$$

where  $Q_t(\cdot) = Q(t, \cdot)$

$$2) \quad (Q_t, h)_Q = h(t) \quad , \quad \forall h \in \mathcal{H}_Q \quad , \\ t \in [0, 1] \quad .$$

We are using the symbol  $\langle \cdot, \cdot \rangle_Q$  for the inner product in  $\mathcal{H}_Q$ .

Let  $\mathcal{H}_X$  be the Hilbert space spanned by the random variables  $\{X(t), t \in [0, 1]\}$ , with inner product

$$\langle Z_1, Z_2 \rangle = E Z_1 Z_2 \quad Z_1, Z_2 \in \mathcal{H}_X .$$

There is an isometric isomorphism between  $\mathcal{H}_Q$  and  $\mathcal{H}_X$  generated by the correspondence

$$X(t) \sim Q_t(\cdot) \quad , \quad \forall t \in [0, 1]$$

which follows from the fact that

$$E X(t) X(t') = Q(t, t') = \langle Q_t, Q_{t'} \rangle_Q \quad , \quad t, t' \in [0, 1] \quad .$$

It is well known that if  $Z \in \mathcal{H}_X$  and  $f(\cdot) \in \mathcal{H}_Q$ , then

$$Z \sim f \iff EZX(t) = f(t)$$

and it is easy to check that  $f$  of (1.6) satisfies

$$\int_0^1 X(t') \rho(t') dt' \sim f(\cdot) \quad .$$

If  $Z \in \mathcal{H}_Q$  and  $Z \sim f$ , it will be convenient to use the symbol

$$\langle f, X \rangle_{\sim}$$

to represent the random variable  $Z$ , which corresponds to the element  $f$  of  $\mathcal{H}_Q$  under this congruence. It is well known that if  $\hat{\theta}_T$  is a best linear estimate for  $\theta$  given  $\{Y(t), t \in T\}$  it satisfies

$$\hat{\theta}_T - \theta = \langle P_T f, X \rangle_{\sim} / \langle P_T f, P_T f \rangle_Q \quad (1.8)$$

where  $P_T$  is the projection operator on the subspace of  $\mathcal{H}_Q$  spanned by  $\{Q_t(\cdot), t \in T\}$ . Hence, using the fact that  $E \langle \rho_1, X \rangle_{\sim} \langle \rho_2, X \rangle_{\sim} = \langle \rho_1, \rho_2 \rangle_Q$

we have

$$\text{Var } \hat{\theta}_T = [ \|P_T f\|_Q^2 ]^{-1} \quad (1.9)$$

where  $\|\cdot\|_Q$  denotes the norm in  $\mathcal{H}_Q$ . Thus (1.7) is equivalent to

$$\lim_{n \rightarrow \infty} \frac{\|f\|_Q^2 - \|P_{T_n^*} f\|_Q^2}{\|f\|_Q^2 - \sup_{T_n \in \mathcal{D}_n} \|P_{T_n} f\|_Q^2} = 1 \quad (1.10)$$

Suppose that  $X(t)$  has  $m-1$  quadratic mean derivatives (which entails that  $f$  of the form (1.6) has  $2m$  continuous derivatives). Let  $\hat{\theta}_{m, T_n}$  be the best linear estimate, if it exists, of  $\theta$ , based on observing  $\{Y^{(\nu)}(t), \nu=0, 1, 2, \dots, m-1, t \in T_n\}$ . Allowing  $m-1$  (quadratic mean) derivatives to be observable at the design points  $T_n$ , the

definition of asymptotically optimal may be revised to read:  $T_n^* \in \mathcal{T}_n$  is asymptotically optimal if

$$\lim_{n \rightarrow \infty} \frac{\sigma_{m, T_n^*}^2 - \sigma^2}{\inf_{T_n \in \mathcal{T}_n} \sigma_{m, T_n}^2 - \sigma^2} = 1 \quad (1.11)$$

where

$$\sigma_{m, T_n}^2 = E(\hat{\theta}_{m, T_n} - \theta)^2 \quad (1.12)$$

In this case we have

$$\hat{\theta}_{m, T_n} - \theta = \langle P_{m, T_n} f, X \rangle_{\sim} / \langle P_{m, T_n} f, P_{m, T_n} f \rangle_Q \quad (1.13)$$

where  $P_{m, T_n}$  is the projection operator in  $\mathcal{H}_Q$  onto the subspace of  $\mathcal{H}_Q$  spanned by

$$\{Q_t^{(\nu)}(\cdot), t \in T_n, \nu = 0, 1, 2, \dots, m-1\} \quad (1.14)$$

where

$$Q_t^{(\nu)}(\cdot) = \frac{\partial^\nu}{\partial s^\nu} Q(s, \cdot) \Big|_{s=t}$$

since

$$Q_t^{(\nu)}(\cdot) \sim X^{(\nu)}(t) .$$

Hence,

$$\text{Var } \hat{\theta}_{m, T_n} = \left[ \|P_{m, T_n} f\|_Q^2 \right]^{-1} .$$

If  $X(t)$  and its first  $m-1$  derivatives are continuous in quadratic mean, then  $X^{(\nu)}(t)$ ,  $\nu \leq m-1$  may be approximated arbitrarily closely by  $\{X(t + \delta_i(t))\}_{i=1}^{\nu+1}$  if we are allowed to choose  $\{\delta_i(t)\}_{i=1}^{\nu+1}$  arbitrarily close to  $t$ , and

$$\inf_{T_{nm} \in \mathcal{A}_{nm}} \|f - P_{T_{nm}} f\|_Q \leq \inf_{T_n \in \mathcal{A}_n} \|f - P_{m, T_n}\|_Q \leq \inf_{T_n \in \mathcal{A}_n} \|f - P_{T_n} f\|_Q. \quad (1.15)$$

Suppose that the  $mn$  elements in brackets in (1.14) are linearly independent for every  $T_n$  in  $\mathcal{A}_n$  and every finite  $n$ . Then it is easy to see that if  $f$  has a representation of the form (1.6) then  $f$  cannot be in the range of  $P_{m, T_n}$ , for any  $T_n \in \mathcal{A}_n$ ,  $n < \infty$ , that is  $f$  cannot have a representation of the form

$$f(\cdot) = \sum_{\nu=0}^{m-1} \sum_{i=0}^n c_{\nu i} Q_{t_i}^{(\nu)}(\cdot), \quad t_i \in T_n, \quad (1.16)$$

and conversely. Thus it becomes apparent that different analyses are required according as some condition like (1.6) holds or not.

In this note we consider only  $f$  of the form (1.6) and primarily the situation where derivatives are allowed. Sacks and Ylvisaker prove the following

Theorem (Sacks and Ylvisaker). Under some assumptions on  $Q$  and  $f$  stated in [10] and including (1.3), (1.5) and (1.6),  $T_n^* = \{t_{in}^*\}_{i=0}^n$  given by

$$\int_0^{t_{in}^*} \rho^{2/(2m+1)}(u) du = \frac{1}{n} \int_0^1 \rho^{2/(2m+1)}(u) du, \quad i = 1, 2, \dots, n \quad (1.16)$$

is an asymptotically optimal sequence, and

$$n^{2m} \|f - P_m, T_n^* f\|_Q^2 = \frac{m!^2}{(2m)!(2m+1)!} \left[ \int_0^1 \rho^{2/(2m+1)}(u) du \right]^{2m+1} + o(1) \quad (1.17)$$

In this note we first consider a special class of stochastic processes.  $X(t)$  is assumed to (formally) satisfy the stochastic differential equation

$$L_m X(t) = \frac{dW(t)}{dt} \quad (1.18)$$

with random (left) boundary conditions where  $W(t)$  is the Wiener process and  $L_m$  is an  $m$ th order linear differential operator whose null space is spanned by an extended complete Tchebychev (ECT) system, of continuity class  $C^{2m}$ . For these processes we will have

$$\lim_{s \downarrow t} \frac{\partial^{2m-1}}{\partial s^{2m-1}} Q(s, t) - \lim_{s \uparrow t} \frac{\partial^{2m-1}}{\partial s^{2m-1}} Q(s, t) = (-1)^m \alpha(t) \quad (1.19)$$

where  $\alpha(t) > 0$  but may not be a constant. Thus this class is not covered by [10].  $Q$  is a Green's function for  $L_m^* L_m$ , with appropriate self adjoint boundary conditions, where  $L_m^*$  is the adjoint operator to  $L_m$  and  $\alpha(t)$  is the characteristic discontinuity of the Green's function. These processes are  $m$ -ple Markov processes in the sense of Hida [3]. In Section 2, we define the class of processes under consideration and point out that it is an immediate consequence of the total positivity properties of Green's functions for certain self-adjoint differential operators that the dimension of the subspace spanned by the set (1.14) is  $nm$ . In Section 3, by writing down an appropriate representation of the Green's function for  $L_m$  we obtain

Theorem 2. Let  $E X(s)X(t) = Q(s, t)$ ,  $s, t \in [0, 1]$ , where  $X(t)$  satisfies

$$L_m X(t) = d W(t) / dt$$

$$X^{(\nu)}(0) = \xi_{\nu+1}, \quad \nu = 0, 1, 2, \dots, m-1$$

where  $W(t)$  is a Wiener process,  $\{\xi_\nu\}_{\nu=1}^m$  are  $m$  linearly independent normal, zero mean random variables independent of  $W(t)$ , and  $L_m$  is an  $m$ th order differential operator with null space spanned by an ECT system of continuity class  $C^{2m}$

Let

$$f(s) = \int_0^1 Q(s, t) \rho(t) dt \quad (1.20)$$

and

$$\lim_{s \downarrow t} \frac{\partial^{2m-1}}{\partial s^{2m-1}} Q(s, t) - \lim_{s \uparrow t} \frac{\partial^{2m-1}}{\partial s^{2m-1}} Q(s, t) = (-1)^m \alpha(t)$$

Suppose  $\rho$  is strictly positive and has a bounded first derivative on  $[0, 1]$ .

Then  $T_n^* = \{t_{in}^*\}_{i=0}^n$  with  $t_{in}^*$  given by

$$\int_0^{t_{in}^*} [\rho^2(u)\alpha(u)]^{\frac{1}{2m+1}} du = \frac{1}{n} \int_0^1 [\rho^2(u)\alpha(u)]^{\frac{1}{2m+1}} du, \quad i=1, 2, \dots, n \quad (1.21)$$

$$t_{on}^* = 0$$

is an asymptotically optimal sequence, and

$$\|f - P_{m, T_n^*} f\|_Q^2 = \frac{1}{n^{2m}} \frac{(m!)^2}{(2m)!(2m+1)!} \left[ \int_0^1 [\rho^2(u)\alpha(u)]^{\frac{1}{2m+1}} du \right]^{2m+1} + o\left(\frac{1}{n^{2m}}\right)$$

(1.22)

In Section 4, we go back to general  $Q(s, t)$ . We show how a family of other experimental design problems reduce to the one under consideration, and use Hermite interpolation to show more generally that  $\|f - P_{m, T_n} f\|_Q^2 = O(\Delta^{2m})$ , where  $\Delta = \max_i |t_{i+1} - t_i|$ .

We conclude by noting that, in the case of processes of the type considered in Section 2, the experimental design problem is equivalent to the problem of optimally approximating a monomial or related function by Spline functions, in the  $L_2$  norm. This problem is discussed by Karlin [5] and Schoenberg [11] for which some interesting results have become recently available.

## 2. Extended Complete Tchebychev Systems and Associated Stochastic Processes

In this section we quote some basic definitions and Theorems which will be used in the sequel. They may be found in [4].

Let  $\{\Phi_i(t)\}_{i=1}^m$  be a set of  $m$  functions. The set is said to be a Tchebychev system if the determinant

$$\begin{vmatrix} \Phi_1(t_1) & \dots & \Phi_m(t_1) \\ \vdots & & \vdots \\ \Phi_1(t_m) & \dots & \Phi_m(t_m) \end{vmatrix}$$

is strictly positive whenever  $0 < t_1 < t_2 < \dots < t_m < 1$ , and a complete Tchebychev system if  $\{\Phi_i\}_{i=1}^v$  is a Tchebychev system for each  $v=1, 2, \dots, m$ . Suppose  $\Phi_i(t)$  has  $m-1$  continuous derivatives on  $(0, 1)$ . The domain of definition of the determinant may be extended to  $0 < t_1 \leq t_2 \leq \dots \leq t_{m-1} \leq t_m < 1$ , where, whenever we have an  $r$  tuple coincidence  $t_v = t_{v+1} = \dots = t_{v+r-1}$ ,

the  $v+j$ th column of the determinant is replaced by

$$\begin{pmatrix} \Phi_1^{(j)} & (t_\nu) \\ \vdots & \\ \Phi_m^{(j)} & (t_\nu) \end{pmatrix}$$

for  $j = 1, 2, \dots, r-1$ .

(See [4], p. 48 for details). If the determinant is always strictly positive, with this interpretation then  $\{\Phi_\nu\}_{\nu=1}^m$  is called an extended Tchebychev (ET) system, and if  $\{\Phi_\nu\}_{\nu=1}^m$  is an ET system for each  $\nu=1, 2, \dots, m$  then it is called an extended complete Tchebychev (ECT) system. The following theorem will be useful to motivate our requirement that  $L_m$  have a null space spanned by an ECT system.

Theorem ([4], p. 276). Let  $\{\Phi_i\}_{i=1}^m$  be of class  $C^{m-1}$  on  $[0, 1]$  obeying the initial conditions

$$\Phi_k^{(p)}(0) = 0 \quad p = 0, 1, 2, \dots, k-2, \quad k = 2, 3, \dots, m.$$

Then the following three assertions are equivalent:

a)  $\{\Phi_i\}_{i=1}^m$  has a representation of the form

$$\begin{aligned} \Phi_1(t) &= \omega_1(t) \\ \Phi_2(t) &= \omega_1(t) \int_0^t \omega_2(\xi_1) d\xi_1 \\ &\vdots \\ \Phi_m(t) &= \omega_1(t) \int_0^t \omega_2(\xi_1) d\xi_1 \int_0^{\xi_1} \omega_3(\xi_2) d\xi_2 \dots \int_0^{\xi_{m-2}} \omega_m(\xi_{m-1}) d\xi_{m-1} \end{aligned} \quad (2.2)$$

where  $\{\omega_i\}_{i=1}^m$  are  $m$  strictly positive functions with  $\omega_k$  of continuity class  $C^{m-k}[0, 1]$



b)  $\{\Phi_i\}_{i=1}^m$  is an ECT system

c) The Wronskian of  $\{\Phi_i\}_{i=1}^{\nu}$  is strictly positive on  $[0, 1]$ , for  $\nu=1, 2, \dots, m$ .

Now let the first order differential operator  $D_i$  be defined by

$$(D_i \Phi)(t) = \frac{d}{dt} \frac{1}{\omega_i(t)} \Phi(t) \quad i=1, 2, \dots, m \quad (2.3)$$

and the  $m$ th order differential operator  $L_m$  be defined by

$$L_m \Phi = D_m D_{m-1} \dots D_1 \Phi \quad (2.4)$$

It may be verified that  $\{\Phi_\nu\}_{\nu=1}^m$  given by (2.2) are the solutions of

$$L_m \Phi = 0$$

satisfying the initial conditions

$$M_\nu \Phi_k(0) = \delta_{k, \nu+1} \omega_k(0), \quad \nu = 0, 1, 2, \dots, m-1,$$

where

$$M_\nu = D_\nu D_{\nu-1} \dots D_1, \quad \nu = 1, 2, \dots, m-1 \quad (2.5)$$

$$M_0 = I.$$

Let

$$G_m(t, s) = \omega_1(t) \int_s^t \omega_2(\xi_1) d\xi_1 \int_s^{\xi_1} \omega_3(\xi_2) d\xi_2 \dots \int_s^{\xi_{m-2}} \omega_m(\xi_{m-1}) d\xi_{m-1} \quad (2.6)$$

$$t \geq s$$

$$= 0 \quad t \leq s.$$

$G_m(t, s)$  is well known to be the Green's function for the differential operator  $L_m$  with boundary conditions  $\mathcal{B}$ :

$$\mathcal{B}: \{(M_\nu f)(0) = 0, \quad \nu = 0, 1, 2, \dots, m-1\} \quad (2.7)$$

That is, the solution to the equation

$$L_m f = g, \quad f \in \mathcal{B} \quad (2.8)$$

is given by

$$f(t) = \int_0^1 G_m(t, u) g(u) du \quad (2.9)$$

Let now

$$X(t) = \sum_{i=1}^m \xi_i \Phi_i(t) + \int_0^t G_m(t, u) dW(u) \quad (2.10)$$

where  $W(t)$  is a Wiener process and  $\{\xi_i\}_{i=1}^m$  are  $m$  zero mean normal random variables with non-degenerate covariance matrix  $S = \{s_{ij}\}$ , independent of  $W(t)$ . We say that a stochastic process  $X(t)$  constructed as in (2.10) formally satisfies the stochastic differential equation

$$L_m X = \frac{dW}{dt}$$

with (random) boundary conditions

$$M_\nu X(0) = \xi_{\nu+1}, \quad \nu = 0, 1, 2, \dots, m-1.$$

We have

$$E X(s) X(t) = Q_O(s, t) + Q(s, t) = \widetilde{Q}(s, t) \quad (2.11)$$

where

$$Q_O(s, t) = \sum_{\mu=1}^m \sum_{\nu=1}^m s_{\mu\nu} \Phi_{\mu}(s) \Phi_{\nu}(t) \quad (2.12)$$

and

$$Q(s, t) = \int_0^{\min(s, t)} G_m(s, u) G_m(t, u) du \quad (2.13)$$

To insure that  $Q(s, t)$  has the usual continuity properties for Green's functions (see e.g. [6], p.29) we now further assume that  $\Phi_{\nu}$  is of continuity class  $C^{2m}$ ,  $\nu=1, 2, \dots, m$ .

It can be shown that  $Q(s, t)$  is the Greens function for the differential operator  $L_m^* L_m$  with boundary conditions  $B \cap B^*$ , where

$$B^*: L_m \Phi(1) = 0 \quad (2.14)$$

$$\begin{aligned} D_m^* L_m \Phi(1) &= 0 \\ &\vdots \\ D_2^* \dots D_m^* L_m \Phi(1) &= 0 \end{aligned}$$

where

$$D_i^* \Phi(t) = -\frac{1}{\omega_i(t)} \frac{d\Phi(t)}{dt} \quad (2.15)$$

We will later on use the properties of the characteristic discontinuity of Greens functions for differential equations, (see [6]) namely

$$\lim_{s \downarrow t} \frac{\partial^{2m-1}}{\partial s^{2m-1}} Q(s, t) - \lim_{s \uparrow t} \frac{\partial^{2m-1}}{\partial s^{2m-1}} Q(s, t) = (-1)^m \alpha(t) \quad (2.16)$$

where  $[(-1)^m \alpha(t)]^{-1}$  is the coefficient of  $\frac{\partial^{2m}}{\partial t^{2m}}$  in the expansion of

$L_m^* L_m$ . Here we have

$$\alpha(t) = \prod_{i=1}^m \omega_i^2(t). \quad (2.17)$$

Let

$$\widetilde{X}(t) = \int_0^t G_m(t, u) dW(u) \quad (2.18)$$

We have

$$E \widetilde{X}^{(\mu)}(t_i) \widetilde{X}^{(\nu)}(t_j) = \frac{\partial^{\mu+\nu}}{\partial r^\mu \partial s^\nu} Q(r, s) \Big|_{\substack{r=t_i \\ s=t_j}} \quad (2.19)$$

Let  $\widetilde{\Sigma}$  be the  $mn \times mn$  covariance matrix of the  $mn$  random variables

$$\{\widetilde{X}^{(\mu)}(t_i), \mu = 0, 1, 2, \dots, m-1, i = 1, 2, \dots, n\}$$

with entries given by (2.19). We have the following.

Theorem 1.

$$\det \widetilde{\Sigma} > 0$$

Proof: The remarkable fact that  $\widetilde{\Sigma} > 0$  is a direct consequence of Theorem (8.1) p. 547, [4] concerning the strict total positivity of Greens functions for differential operators of the form  $L_m^* L_m$  with (self-adjoint) boundary conditions  $B \cap B^*$ .

Corollary. Let  $\Sigma$  be the  $(n+1)m \times (n+1)m$  covariance matrix of the  $(n+1)m$  random variables  $X^{(\mu)}(t_i)$ ,  $\left\{ \begin{array}{l} \mu = 0, 1, 2, \dots, m-1 \\ i = 0, 1, 2, \dots, n, t_0 = 0 \end{array} \right\}$  then

$$\det \Sigma > 0 .$$

The reproducing kernel Hilbert space  $\mathcal{H}_{\tilde{Q}}$  with  $\tilde{Q}$  given by (2.11), corresponding to the stochastic process  $X$ , consists of all functions  $f$  for which  $M_{m-1}f$  is absolutely continuous and  $L_m f \in L_2[0,1]$ , with inner product

$$\begin{aligned} \langle f_1, f_2 \rangle &= \sum_{\mu=1}^m \sum_{\nu=1}^m s^{\mu\nu} (M_{\mu-1} f_1)(0) (M_{\nu-1} f_2)(0) \\ &+ \int_0^1 (L_m f_1)(u) (L_m f_2)(u) du \end{aligned} \quad (2.20)$$

where  $S^{-1} = \{s^{\mu\nu}\}$ .

If  $X(t)$ ,  $0 \leq t \leq 1$  is a segment of a stationary stochastic process with spectral density

$$f(\lambda) = \left| \sum_{\nu=0}^m \alpha_{\nu} (i\lambda)^{\nu} \right|^{-2}$$

where the polynomial  $\sum_{\nu=0}^m \alpha_{\nu} z^{\nu}$  has no real zeroes, then  $X(t)$ ,  $0 \leq t \leq 1$  is an example of (2.10) with  $L_m \Phi = \sum_{\nu=0}^m \alpha_{\nu} \Phi^{(\nu)}$  (compare (2.20) and equation (5.24) of [7]). The simplest example is the unpinned, integrated

Wiener process (see [12]),  $L_m \Phi = \frac{d^m}{dt^m} \Phi$ ,

$$G_m(t, u) = \frac{(t-u)^{m-1}}{(m-1)!}, \quad (x)_+ = x, x > 0 \quad (2.21)$$

$$= 0 \text{ otherwise}$$

and  $\Phi_i(t) = \frac{t^{i-1}}{(i-1)!}$ . (In both these examples,  $\alpha(t)$  is a constant).

We may always add a fixed finite number of points to each member of an asymptotically optimum sequence of designs without modifying the asymptotic optimality. Thus we may without loss of generality restrict ourselves to processes of the form

$$X(t) = \int_0^t G_m(t, u) dW(u), \quad (2.22)$$

since the random variables  $\{\xi_i\}_{i=1}^m$  are known arbitrarily accurately if we may observe  $X(s_i)$ ,  $i=1, 2, \dots, m$  for  $s_i$  arbitrarily near 0, or exactly if we observe  $X^{(\nu)}(0)$ ,  $\nu=0, 1, 2, \dots, m-1$ .

### 3. An Asymptotically Optimal Sequence of Designs.

The main goal of this section is to prove Theorem 2. This is done via several lemmas which study the behavior of  $\|f - P_{m, T_n} f\|_Q^2$ .

Lemma 1

Let  $X(t)$  be given by (2.10) and let

$$f(t) = \int_0^1 Q(t, u) \rho(u) du, \text{ where } \rho \in L_2[0, 1]. \quad (3.1)$$

and let  $t_0 = 0, t_n = 1$ .

Then

$$\begin{aligned} & \|f - P_{m, T_n} f\|_Q^2 \\ &= \sum_{i=0}^{n-1} \int_{t_i}^{t_{i+1}} \int_{t_i}^{t_{i+1}} \rho(s) B_i(s, t) \rho(t) ds dt \end{aligned} \quad (3.2a)$$

where

$$\begin{aligned} B_i(s, t) &= \int_{t_i}^{\min(s, t)} G_m(s, u) G_m(t, u) du - \\ &\sum_{\mu, \nu=0}^{m-1} \int_{t_i}^s G_m(s, u) G_{m, \mu}(t_{i+1}, u) du s_i^{\mu\nu} \int_{t_i}^t G_m(t, v) G_{m, \nu}(t_{i+1}, v) dv, \\ & \quad s, t \in [t_i, t_{i+1}] \quad (3.2b) \\ &= 0 \quad \text{otherwise,} \end{aligned}$$

with

$$G_{m, \mu}(s, u) = M_{\mu}(s) G_m(s, u), \quad \mu = 1, 2, \dots, m-1 \quad (3.2c)$$

$$G_{m, 0}(s, u) = G_m(s, u),$$

$M_{\mu}(s)$  is the operator  $M_{\mu}$  defined by (2.5), applied to the variable  $s$ ,  
and  $\{s_i^{\mu\nu}\}_{\mu, \nu=0}^{m-1}$  are defined by

$$S_i^{-1} = \{s_i^{\mu\nu}\}_{\mu, \nu=0}^{m-1}, \quad S_i = \{s_{i, \mu\nu}\}_{\mu, \nu=0}^{m-1} \quad (3.2d)$$

with

$$s_{i, \mu\nu} = \int_{t_i}^{t_{i+1}} G_{m, \mu}(t_{i+1}, u) G_{m, \nu}(t_{i+1}, u) du. \quad (3.2e)$$

Proof:

Let

$$P_{m, T_n} X(u) = E \{X(u) | X^{(\nu)}(t_i), \nu=0, 1, 2, \dots, m-1, t_i \in T_n\} \quad (3.3)$$

Then, since

$$f(t) = EX(t) \int_0^1 X(u) \rho(u) du \quad (3.4a)$$

and

$$P_{m, T_n} f(t) = EX(t) \int_0^1 P_{m, T_n} X(u) du \quad (3.4b)$$

we have

$$f(\cdot) \sim \int_0^1 X(u) \rho(u) du \quad (3.4c)$$

$$P_{m, T_n} f(\cdot) \sim \int_0^1 P_{m, T_n} X(u) \rho(u) du \quad (3.4d)$$

and

$$\|f - P_{m, T_n} f\|_Q^2 = \int_0^1 \int_0^1 \rho(s) \rho(t) E(X(s) - P_{m, T_n} X(s))(X(t) - P_{m, T_n} X(t)) ds dt. \quad (3.5)$$

We will evaluate the right hand side of (3.5).

Since  $t_0 = 0 \in T_n$ , it is only necessary to carry out the proof for  $X(t)$  of the form (2.21), that is,  $X \in \mathcal{B}$ . This follows, since, in



calculating  $X(t) - P_{m, T_n} X(t)$ , it makes no difference whether  $X^{(\nu)}(0)$ ,  $\nu=0, 1, 2, \dots, m-1$  are observed, or known to be zero. Now, for

$$L_m X(t) = dW(t)/dt, \quad (3.6)$$

$$X^{(\nu)}(0) = 0, \quad \nu=0, 1, 2, \dots, m-1$$

$X(t)$  has the representation.

$$X(t) = \omega_1(t) \int_0^t \omega_2(t_1) dt_1 \int_0^{t_1} \omega_3(t_2) \dots \int_0^{t_{m-2}} \omega_m(t_{m-1}) W(t_{m-1}) dt_{m-1}. \quad (3.7)$$

It will be convenient to work with so-called generalized derivatives,  $M_\nu X(t)$ ,  $\nu=0, 1, 2, \dots, m-1$ . We have the representations

$$M_\nu X(t) = \omega_{\nu+1}(t) \int_0^t \omega_{\nu+2}(t_{\nu+1}) dt_{\nu+1} \dots \int_0^{t_{m-2}} \omega_m(t_{m-1}) W(t_{m-1}) dt_{m-1} \quad \nu = 0, 1, 2, \dots, m-2 \quad (3.8)$$

$$M_{m-1} X(t) = \omega_m(t) W(t),$$

and

$$M_\nu X(t) = M_\nu(t) \int_0^t G_m(t, s) dW(s) \quad (3.9a)$$

$$\nu = 0, 1, 2, \dots, m-1$$

$$= \int_0^t G_{m, \nu}(t, s) dW(s). \quad (3.9b)$$

$G_{m, \nu}(t, s)$  is the Green's function for the operator  $L_{m, \nu}$  given by

$$L_{m, \nu} \Phi = D_m D_{m-1} \dots D_{\nu+1} \Phi, \quad \nu = 1, 2, \dots, m-1 \quad (3.10)$$

with boundary conditions

$$\mathcal{B}_{m,\nu} : \{ \Phi^{(\mu)}(0) = 0, \mu=0,1,2,\dots,m-\nu \}. \quad .$$

We will use another representation for  $G_{m,\nu}(t,s)$ ,  $\nu=1,2,\dots,m-1$ .

Let

$$\begin{aligned} \Phi_{1,\nu}(s) &= \omega_{m-\nu+1}(s) & (3.11) \\ \Phi_{2,\nu}(s) &= \omega_{m-\nu+1}(s) \int_0^s \omega_{m-\nu+2}(\xi_1) d\xi_1 \\ &\vdots \\ \Phi_{\nu,\nu}(s) &= \omega_{m-\nu+1}(s) \int_0^s \omega_{m-\nu+2}(\xi_1) d\xi_1 \int_0^{\xi_1} \omega_{m-\nu+3}(\xi_2) d\xi_2 \dots \\ &\quad \int_0^{\xi_{\nu-2}} \omega_m(\xi_{\nu-1}) d\xi_{\nu-1}, \quad \nu = 1, 2, \dots, m. \end{aligned}$$

and let

$$\begin{aligned} \Phi_1(s) &= \Phi_{1,m}(s) = \omega_1(s) & (3.12) \\ \Phi_2(s) &= \Phi_{2,m}(s) = \omega_1(s) \int_0^s \omega_2(\xi_1) d\xi_1 \\ &\vdots \\ \Phi_m(s) &= \Phi_{m,m}(s) = \omega_1(s) \int_0^s \omega_2(\xi_1) d\xi_1 \int_0^{\xi_1} \omega_3(\xi_2) d\xi_2 \dots \\ &\quad \int_0^{\xi_{m-2}} \omega_m(\xi_{m-1}) d\xi_{m-1} \end{aligned}$$

as before.

Also let

$$\begin{aligned}
 \Phi_1^*(s) &= (-1)^2 \\
 \Phi_2^*(s) &= (-1)^3 \int_0^s \omega_m(\xi_{m-1}) d\xi_{m-1} \\
 &\vdots \\
 \Phi_m^*(s) &= (-1)^{m+1} \int_0^s \omega_m(\xi_{m-1}) d\xi_{m-1} \int_0^{\xi_{m-1}} \omega_{m-1}(\xi_{m-2}) d\xi_{m-2} \cdots \int_0^{\xi_2} \omega_2(\xi_1) d\xi_1
 \end{aligned} \tag{3.13}$$

Algebraic manipulations on the representation of the Greens function in the form of (2.6) give the Green's function, in another, familiar form:

$$\begin{aligned}
 G_{m,\nu}(t,s) &= \sum_{\mu=1}^{m-\nu} \Phi_{m-\nu-\mu+1, m-\nu}(t) \Phi_{\mu}^*(s) & t \geq s, \\
 &= 0 & t < s.
 \end{aligned} \tag{3.14}$$

$\nu = 0, 1, 2, \dots, m-1$

Substituting (3.14) into (3.9b), we have that the random variables  $M_{\nu}X(t_i)$ , have the representation

$$M_{\nu}X(t_i) = \sum_{\mu=1}^{m-\nu} \Phi_{m-\nu-\mu+1, m-\nu}(t_i) \int_0^{t_i} \Phi_{\mu}^*(u) dW(u), \quad \nu=0, 1, 2, \dots, m-1 \tag{3.15}$$

and that the  $m$ -dimensional space  $\mathcal{H}_{t_i}$  spanned by  $\{M_{\nu}X(t_i)\}_{\nu=0}^{m-1}$  is also spanned by  $\{\int_0^{t_i} \Phi_{\mu}^*(u) dW(u)\}_{\mu=1}^m$ . (We are using the fact that the 3 systems of (3.11), (3.12), and (3.13) are each ECT).

Now we have, for  $t \geq t_i$

$$X(t) - E \{X(t) | M_\nu X(t_i), \nu=0, 1, 2, \dots, m-1\} = \int_{t_i}^t G_m(t, u) dW(u) \quad (3.16)$$

This (well known) result follows by writing

$$\begin{aligned} X(t) &= \int_0^{t_i} G_m(t, u) dW(u) + \int_{t_i}^t G_m(t, u) dW(u) \\ &= \left\{ \sum_{\mu=1}^m \Phi_{m-\mu+1, m}(t) \int_0^{t_i} \Phi_\mu^*(u) dW(u) \right\} + \left\{ \int_{t_i}^t G_m(t, u) dW(u) \right\} \end{aligned} \quad (3.17)$$

and the first term in brackets is in  $\mathcal{H}_{t_i}$ , while the second term is perpendicular to it. Using (3.15) and the remarks following, it follows that  $\mathcal{H}_{t_i} \cup \mathcal{H}_{t_{i+1}}$  is also spanned by

$$\{M_\nu X(t_i), \int_{t_i}^{t_{i+1}} G_{m, \nu}(t_{i+1}, u) dW(u), \nu=0, 1, 2, \dots, m-1\}.$$

It may then be calculated, for  $t_i \leq t \leq t_{i+1}$ , that

$$\begin{aligned} X(t) - E \{X(t) | M_\nu X(t_i), M_\nu X(t_{i+1}), \nu=0, 1, 2, \dots, m-1\} \\ = \int_{t_i}^t G_m(t, u) dW(u) - \sum_{\mu} \sum_{\nu=0}^{m-1} \int_{t_i}^t G_m(t, u) G_{m, \mu}(t_{i+1}, u) du s_i^{\mu \nu} \int_{t_i}^{t_{i+1}} G_{m, \nu}(t_{i+1}, v) dW(v) \end{aligned} \quad (3.18)$$

where  $S_i^{-1} = \{s_i^{\mu\nu}\}$  is given by

$$S_i = \{s_{i,\mu\nu}\}, \quad s_{i,\mu\nu} = \int_{t_i}^{t_{i+1}} G_{m,\mu}(t_{i+1},u)G_{m,\nu}(t_{i+1},u)du \quad (3.19)$$

$$\mu, \nu = 0, 1, 2, \dots, m-1$$

Finally, we have that, for  $t_i \leq t \leq t_{i+1}$

$$X(t) - P_{m, T_n} X(t) = X(t) - E \{X(t) | M_\nu X(t_j), \nu = 0, 1, 2, \dots, m-1, t_j \in T_n\}$$

$$= X(t) - E \{X(t) | M_\nu X(t_i), M_\nu X(t_{i+1}), \nu = 0, 1, 2, \dots, m-1\} \quad (3.20)$$

since a direct check shows that this last random variable, as given by (3.18) is already orthogonal to each random variable of the form

$$\int_{t_j}^{t_{j+1}} G_{m,\mu}(t_{j+1},u)dW(u), \quad \mu = 0, 1, 2, \dots, m-1$$

$$j = 0, 1, 2, \dots, n-1$$

Finally, it also follows that

$$E(X(s) - P_{m, T_n} X(s)) (X(t) - P_{m, T_n} X(t)) = 0, \quad (3.21)$$

$$s \in [t_j, t_{j+1}]$$

$$t \in [t_i, t_{i+1}], \quad i \neq j$$

A quick calculation from (3.18) shows

$$E(X(s) - P_{m, T_n} X(s)) (X(t) - P_{m, T_n} X(t)) =$$

$$B_i(s, t), \quad s, t \in [t_i, t_{i+1}], \quad (3.22)$$

and the Lemma is proved.

Lemma 2

Let  $b_s(t)$ , for fixed  $s \in [t_i, t_{i+1}]$  satisfy

$$b_s(t) \in C^{2m}, t \in [t_i, s) \cup (s, t_{i+1}], \quad b_s(t) \in C^{2m-2}, t \in [t_i, t_{i+1}],$$

$$\lim_{t \downarrow s} b_s^{(2m-1)}(t) - \lim_{t \uparrow s} b_s^{(2m-1)}(t) = (-1)^m \alpha(s) \text{ and } b_s^{(\nu)}(t_i) = b_s^{(\nu)}(t_{i+1}) = 0, \nu = 0, 1, \dots, m-1$$

Then

$$\int_{t_i}^{t_{i+1}} b_s(t) dt = \alpha(s) \frac{(t_{i+1}-s)^m (s-t_i)^m}{(2m)!} + (-1)^m \int_{t_i}^{t_{i+1}} b_s^{(2m)}(t) \frac{(t_{i+1}-t)^m (t-t_i)^m}{(2m)!} dt$$

(3.23)

Proof:

Let

$$\frac{(t_{i+1}-t)^m (t-t_i)^m}{(2m)!} = \delta_i(t) \quad t \in [t_i, t_{i+1}] \quad (3.24)$$

and note that

$$\delta_i^{(\nu)}(t_i) = \delta_i^{(\nu)}(t_{i+1}) = 0, \quad \nu = 0, 1, 2, \dots, m-1 \quad (3.25)$$

$$\delta_i^{(2m)}(t) = (-1)^m \quad (3.26)$$

By successive integration by parts, we have

$$\int_{t_i}^{s-} b_s^{(2m)}(t) \delta_i(t) dt + \int_{s+}^{t_{i+1}} b_s^{(2m)}(t) \delta_i(t) dt \quad (3.27.1)$$

$$= \int_{t_i}^{s-} b_s^{(2m-1)}(t) \delta_i(t) + \int_{s-}^{t_{i+1}} b_s^{(2m-1)}(t) \delta_i(t) - \int_{t_i}^{t_{i+1}} b_s^{(2m-1)}(t) \delta_i'(t) dt$$

$$= (-1)^{m+1} \alpha(s) \delta_i(s) - \int_{t_i}^{t_{i+1}} b_s^{(2m-2)}(t) \delta_i'(t) + \int_{t_i}^{t_{i+1}} b_s^{(2m-2)}(t) \delta_i^{(2)}(t) dt \quad (3.27.2)$$

⋮

$$= (-1)^{m+1} \alpha(s) \delta_i(s) + (-1)^{\ell-1} \int_{t_i}^{t_{i+1}} b_s^{(2m-\ell)}(t) \delta_i^{(\ell-1)}(t) + (-1)^\ell \int_{t_i}^{t_{i+1}} b_s^{(2m-\ell)}(t) \delta_i^{(\ell)}(t) dt \quad (3.27.\ell)$$

⋮

$$= (-1)^{m+1} \alpha(s) \delta_i(s) + (-1)^{2m} \int_{t_i}^{t_{i+1}} b_s^{(2m)}(t) \delta_i^{(2m)}(t) dt \quad (3.27.2m)$$

$$= (-1)^{m+1} \alpha(s) \delta_i(s) + (-1)^m \int_{t_i}^{t_{i+1}} b_s^{(m)}(t) dt ,$$

thus proving the Lemma.

### Lemma 3.

Suppose  $\rho(t) > 0$ , and  $\rho$  has a bounded derivative on  $[0, 1]$ ,<sup>†</sup>

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<sup>†</sup>Recall that since  $\Phi_\nu \in C^{2m}$ ,  $\omega_\nu \in C^{2m-(\nu-1)}$  and hence  $\alpha(t)$  has at least a bounded first derivative,  $m \geq 1$ .

and  $t_0 = 0, t_n = 1$ .

Then

$$\|f - P_{m, T_n} f\|_Q^2 = \frac{(m!)^2}{(2m)!(2m+1)!} \sum_{i=0}^{n-1} \rho^2(t_i) \alpha(t_i) \left[ (t_{i+1} - t_i)^{2m+1} (1 + O(\Delta_i)) \right] \quad (3.28)$$

where

$$\Delta_i = |t_{i+1} - t_i|. \quad (3.29)$$

Proof: By the assumptions on  $\rho$ , the mean value theorem and

Lemma 1,

$$\begin{aligned} \|f - P_{m, T_n} f\|_Q^2 &= \sum_{i=0}^{n-1} \rho(\theta_{i1}) \rho(\theta_{i2}) \int_{t_i}^{t_{i+1}} \int_{t_i}^{t_{i+1}} B_i(s, t) ds dt \\ &= \sum_{i=0}^{n-1} \rho^2(t_i) (1 + O(\Delta_i)) \int_{t_i}^{t_{i+1}} \int_{t_i}^{t_{i+1}} B_i(s, t) ds dt \end{aligned} \quad (3.30)$$

where  $\theta_{i1}, \theta_{i2}$  are some numbers in  $[t_i, t_{i+1}]$ . Hence it remains to show that

$$\int_{t_i}^{t_{i+1}} ds \int_{t_i}^{t_{i+1}} B_i(s, t) dt = \frac{(m!)^2}{(2m)!(2m+1)!} \alpha(t_i) \left[ (t_{i+1} - t_i)^{2m+1} (1 + O(\Delta_i)) \right] \quad (3.31)$$

Now,  $B_i(s, t), s, t \in [t_i, t_{i+1}]$  can be shown to be the Green's function for the operator  $L_m^* L_m$  with boundary conditions  $\mathcal{B}_i \cap \mathcal{B}_{i+1}$ , where

$$\mathcal{B}_j: \{ (M_\nu f)(t_j) = 0, \nu = 0, 1, 2, \dots, m-1 \}, \quad j = 0, 1, 2, \dots, n. \quad (3.32)$$



( $B_i(s, t)$  satisfies the hypotheses of Theorem (8.1), [4], with the appropriate changes in domain.)

We now evaluate  $\int_{t_i}^{t_{i+1}} B_i(s, t) dt$ . For fixed  $i$ , and fixed  $s \in [t_i, t_{i+1}]$ , it will be convenient to write

$$b_{is}(t) = B_i(s, t). \quad (3.33)$$

The properties of  $b_{is}$  given below, up to and including (3.36) are the properties of Green's functions.

$$(M_\nu b_{is})(t_i) = (M_\nu b_{is})(t_{i+1}) = 0, \quad \nu=0, 1, 2, \dots, m-1. \quad (3.34)$$

Also,  $b_{is}(t)$  is of continuity class  $C^{2m-2}$  for  $t \in [t_i, t_{i+1}]$  and of continuity class  $C^{2m}$  on the set  $[t_i, s) \cup (s, t_{i+1}]$ , and has the same characteristic jump in the  $2m-1$  st derivative as does  $Q(s, t)$ , that is

$$\lim_{t \downarrow s} \frac{\partial^{2m-1}}{\partial t^{2m-1}} b_{is}(t) - \lim_{t \uparrow s} \frac{\partial^{2m-1}}{\partial t^{2m-1}} b_{is}(t) = (-1)^m \alpha(s), \quad t \in [t_i, t_{i+1}]. \quad (3.35)$$

Furthermore,  $b_{is}(t)$  satisfies

$$\begin{aligned} L_m^* L_m b_{is}(t) &= 0, & t_i \leq t < s \\ L_m^* L_m b_{is}(t) &= 0, & s < t \leq t_{i+1} \end{aligned} \quad (3.36)$$

Note that the set of conditions (3.34) is equivalent to

$$b_{is}^{(\nu)}(t_i) = b_{is}^{(\nu)}(t_{i+1}) = 0, \quad \nu = 0, 1, 2, \dots, m-1. \quad (3.37)$$

Therefore, by Lemma 2,

$$\int_{t_i}^{t_{i+1}} B_i(s, t) dt = \alpha(s) \frac{(t_{i+1}-s)^m (s-t_i)^m}{(2m)!} + (-1)^m \int_{\substack{t_i \\ t \neq s}}^{t_{i+1}} b_{is}^{(2m)}(t) \frac{(t_{i+1}-t)^m (t-t_i)^m}{(2m)!} dt \quad (3.38)$$

The proof would be nearly finished if it were shown, for example that,  $b_{is}^{(2m)}$  is bounded independent of  $\Delta_i$ . A simple proof was not found, so a somewhat roundabout argument is given. For the special case of  $L_m^* L_m f = f^{(2m)}$ ,  $G_m(t, u) = \frac{(t-u)_+^{m-1}}{(m-1)!}$ , we have  $b_{is}^{(2m)}(t) = 0$ ,  $t \in [t_i, s) \cup (s, t_{i+1}]$ , and since, in this case  $\alpha(t) \equiv (-1)^m$  we have

$$\int_{t_i}^{t_{i+1}} \int_{t_i}^{t_{i+1}} B_i(s, t) ds dt = \int_{t_i}^{t_{i+1}} \frac{(t_{i+1}-s)^m (s-t_i)^m}{(2m)!} ds = \frac{(m!)^2}{(2m)! (2m+1)!} (t_{i+1}-t_i)^{2m+1}. \quad (3.39)$$

We proceed by relating the general case to this special case.

By analogy with (2.6), and the mean value theorem

$$\begin{aligned} G_{m, \nu}(t, s) &= \omega_{\nu+1}(t) \int_s^t \omega_{\nu+2}(\xi_{\nu+1}) d\xi_{\nu+1} \dots \int_s^{\xi_{m-2}} \omega_m(\xi_{m-1}) d\xi_{m-1}, \quad t > s \\ &= 0 \quad t \leq s \\ &= \prod_{i=\nu+1}^m \omega_i(\theta_{i\nu}) \frac{(t-s)_+^{m-\nu-1}}{(m-\nu-1)!}, \quad \nu = 0, 1, 2, \dots, m-1 \end{aligned} \quad (3.40)$$

where  $\theta_{i\nu} \in [s, t]$ .

Thus, for  $s, t \in [t_i, t_{i+1}]$  we may write

$$\begin{aligned}
 & \int_{t_i}^{\min(s, t)} G_m(s, u) G_m(t, u) - \sum_{\mu, \nu=0}^{m-1} \sum_{t_i}^s G_m(s, u) G_{m, \mu}(t_{i+1}, u) du s_i^{\mu \nu} \times \\
 & \int_{t_i}^t G_m(t, v) G_{m, \nu}(t_{i+1}, v) dv \\
 & = \prod_{j=1}^m \prod_{k=1}^m \omega_j(\theta_{j1}) \omega_k(\theta_{k2}) \int_{t_i}^{\min(s, t)} \frac{(s-u)_+^{m-1} (t-u)_+^{m-1}}{(m-1)! (m-1)!} du - \\
 & \left[ \sum_{\mu, \nu=0}^{m-1} \prod_{j=1}^m \prod_{k=\mu+1}^m \omega_j(\theta_{j3}) \omega_k(\theta_{k4}) \int_{t_i}^s \frac{(s-u)_+^{m-1}}{(m-1)!} \frac{(t_{i+1}-u)_+^{m-\mu-1}}{(m-\mu-1)!} du \cdot s_i^{\mu \nu} \times \right. \\
 & \left. \prod_{j=1}^m \prod_{k=\nu+1}^m \omega_j(\theta_{j5}) \omega_k(\theta_{k6}) \int_{t_i}^t \frac{(t-v)_+^{m-1}}{(m-1)!} \frac{(t_{i+1}-v)_+^{m-\nu-1}}{(m-\nu-1)!} dv \right] \quad (3.41)
 \end{aligned}$$

where

$$S_i^{-1} = \{s_i^{\mu \nu}\}, S_i = \{s_{i, \mu \nu}\},$$

and

$$s_{i, \mu \nu} = \prod_{j=\mu+1}^m \prod_{k=\nu+1}^m \omega_j(\theta_{j7}) \omega_k(\theta_{k8}) \int_{t_i}^{t_{i+1}} \frac{(t_{i+1}-u)_+^{2m-\mu-\nu-2}}{(m-\mu-1)! (m-\nu-1)!} du \quad (3.42)$$

and where  $\{\theta_{j\ell}, \theta_{k\ell}, j, k = 1, 2, \dots, m, \ell = 1, 2, \dots, 8\}$  are all in the interval  $[t_i, t_{i+1}]$ .

Then, by the continuity and strict positivity properties of the  $\{\omega_i\}_{i=1}^m$ ,

$$\prod_{j=\nu+1}^m \omega_j(\theta_{j\ell}) = \prod_{j=\nu+1}^m \omega_j(t_i)(1 + O(\Delta_i)) \quad \nu = 0, 1, 2, \dots, m-1 \quad (3.43)$$

$$\ell = 1, 2, \dots, 8$$

In particular

$$s_{i,\mu\nu} = \prod_{j=\mu+1}^m \prod_{k=\nu+1}^m \omega_j(t_i) \omega_k(t_i) (1 + O(\Delta_i)) \tilde{s}_{i,\mu\nu} \quad (3.44)$$

where

$$\tilde{s}_{i,\mu\nu} = \int_{t_i}^{t_{i+1}} \frac{(t_{i+1}-u)_+^{2m-\mu-\nu-2}}{(m-\mu-1)! (m-\nu-1)!} du \quad (3.45)$$

The matrix  $\tilde{S}_i$ ,  $\tilde{S}_i = \{\tilde{s}_{i,\mu\nu}\}$ , is strictly positive definite. We have by (3.42) and the continuity properties of the matrix inverse transformation

$$s_i^{\mu\nu} = \left[ \prod_{j=\mu+1}^m \prod_{k=\mu+1}^m \omega_j(t_i) \omega_k(t_i) \right]^{-1} \tilde{s}_i^{\mu\nu} (1 + O(\Delta_i)) \quad (3.46)$$

where  $\tilde{s}_i^{\mu\nu}$  is defined by  $\tilde{S}_i^{-1} = \{\tilde{s}_i^{\mu\nu}\}$ . We therefore have the right hand side of (3.41) is given by

(r.h.s.) (3.41) =

$$\prod_{k=1}^m \omega_k^2(t_i) (1 + O(\Delta_i)) \int_{t_i}^{\min(s,t)} \frac{(s-u)_+^{m-1} (t-u)_+^{m-1}}{(m-1)! (m-1)!} du - \prod_{k=1}^m \omega_k^2(t_i) (1 + O(\Delta_i)) \times$$

$$\sum_{\mu, \nu=0}^{m-1} \int_{t_i}^s \frac{(s-u)_+^{m-1} (t_{i+1}-u)_+^{m-\mu-1}}{(m-1)! (m-\mu-1)!} du \quad \tilde{s}_i^{\mu\nu} \int_{t_i}^t \frac{(t-v)_+^{m-1} (t_{i+1}-v)_+^{m-\nu-1}}{(m-1)! (m-\nu-1)!} dv \quad (3.47)$$

From (3.39) and (3.47) we obtain

$$\begin{aligned}
 & \int_{t_i}^{t_{i+1}} \int_{t_i}^{t_{i+1}} B_i(s, t) ds dt \\
 &= \frac{(m!)^2}{(2m)! (2m+1)!} \alpha(t_i)(t_{i+1}-t_i)^{2m+1} + \\
 & \quad O(\Delta_i) \left\{ \int_{t_i}^{t_{i+1}} \int_{t_i}^{t_{i+1}} ds dt \int_{t_i}^{\min(s, t)} \frac{(s-u)_+^{m-1} (t-u)_+^{m-1}}{(m-1)! (m-1)!} du \right\} + \\
 & \quad O(\Delta_i) \left\{ \int_{t_i}^{t_{i+1}} \int_{t_i}^{t_{i+1}} ds dt \sum_{\mu, \nu=0}^{m-1} \left[ \int_{t_i}^s \frac{(s-u)_+^{m-1}}{(m-1)!} \frac{(t_{i+1}-u)_+^{m-\mu-1}}{(m-\mu-1)!} du \widetilde{s}_i^{\mu\nu} \times \right. \right. \\
 & \quad \left. \left. \int_{t_i}^t \frac{(t-v)_+^{m-1}}{(m-1)!} \frac{(t_{i+1}-v)_+^{m-\nu-1}}{(m-\nu-1)!} dv \right] \right\} \quad (3.48)
 \end{aligned}$$

Since the first term in curly brackets in (3.48) is greater than the second term in curly brackets (which is non-negative), we have, upon evaluating the first term in curly brackets

$$\begin{aligned}
 & \int_{t_i}^{t_{i+1}} \int_{t_i}^{t_{i+1}} B_i(s, t) ds dt \\
 &= \frac{(m!)^2}{(2m)!(2m+1)!} \alpha(t_i)(t_{i+1}-t_i)^{2m+1} + O(\Delta_i)(t_{i+1}-t_i)^{2m+1} \\
 &= \frac{(m!)^2}{(2m)!(2m+1)!} \alpha(t_i)(t_{i+1}-t_i)^{2m+1} (1+O(\Delta_i)). \quad (3.49)
 \end{aligned}$$

and the Lemma is proved.

Theorem 2 Let  $E X(s) X(t) = Q(s, t)$ ,  $s, t \in [0, 1]$ , where  $X(t)$  satisfies

$$L_m X(t) = d W(t)/dt$$

$$X^{(v)}(0) = \xi_{v+1}, \quad v = 0, 1, 2, \dots, m-1$$

where  $W(t)$  is a Wiener process,  $\{\xi_v\}_{v=1}^m$  are  $m$  linearly independent, normal, zero mean random variables independent of  $W(t)$ , and  $L_m$  is an  $m$ th order differential operator with null space spanned by an ECT system of continuity class  $C^{2m}$ .

Let

$$f(s) = \int_0^1 Q(s, t) \rho(t) dt$$

and

$$\lim_{s \downarrow t} \frac{\partial^{2m-1}}{\partial s^{2m-1}} Q(s, t) - \lim_{s \uparrow t} \frac{\partial^{2m-1}}{\partial s^{2m-1}} Q(s, t) = (-1)^m \alpha(t)$$

Suppose  $\rho$  is strictly positive and has a bounded first derivative on

$[0,1]$ . Let  $T_n^* = \{t_{in}^*\}_{i=0}^n$  with  $t_{in}^*$  given by

$$\int_0^{t_{in}^*} [\rho^2(u)\alpha(u)]^{\frac{1}{2m+1}} du = \frac{1}{n} \int_0^1 [\rho^2(u)\alpha(u)]^{\frac{1}{2m+1}} du \quad i = 1, 2, \dots, n$$

$$t_{0n}^* = 0 \quad (3.50)$$

Then  $T_n^*$  is an asymptotically optimal sequence, and

$$\|f - P_{m, T_n^*} f\|_Q^2 = \frac{1}{n^{2m}} \frac{(m!)^2}{(2m)!(2m+1)!} \left[ \int_0^1 [\rho^2(\theta)\alpha(\theta)]^{\frac{1}{2m+1}} d\theta \right]^{2m+1} + o\left(\frac{1}{n^{2m}}\right)$$

(3.51)

Proof: Let  $\Delta = \max_i |t_{i+1} - t_i|$ . We know that for any asymptotically optimal sequence,  $\lim_{n \rightarrow \infty} \Delta = 0$ , since otherwise  $\|f - P_{m, T_n} f\|_Q^2$  will not tend to 0.

Using a Holder inequality on (3.28), gives, for any  $T_n$  that includes  $t_0 = 0, t_n = 1$ ,

$$\|f - P_{m, T_n} f\|_Q^2 \geq \frac{1}{n^{2m}} \frac{(m!)^2}{(2m)!(2m+1)!} \left[ \sum_{i=0}^{n-1} \rho^{\frac{2}{2m+1}}(t_i) \alpha^{\frac{1}{2m+1}}(t_i) (1+O(\Delta_i))(t_{i+1} - t_i) \right]^{2m+1}$$

$$= \frac{1}{n^{2m}} \frac{(m!)^2}{(2m)!(2m+1)!} \left[ \int_0^1 [\rho^2(t)\alpha(t)]^{\frac{1}{2m+1}} dt \right]^{2m+1} + \frac{O(\Delta)}{n^{2m}} \quad (3.52)$$

Now, using (3.50) and the mean value theorem,

$$\begin{aligned} \frac{2}{\rho^{2m+1}} (\theta_i^*)^{\frac{1}{2m+1}} (\theta_i^*)^{\frac{1}{2m+1}} (t_{i+1,n}^* - t_{in}^*) &= \int_{t_{in}^*}^{t_{i+1,n}^*} [\rho^2(u) \alpha(u)]^{\frac{1}{2m+1}} du \\ &= \frac{1}{n} \int_0^1 [\rho^2(u) \alpha(u)]^{\frac{1}{2m+1}} du. \end{aligned} \quad (3.53)$$

where  $\theta_i^*$  is some number in  $[t_{in}^*, t_{i+1,n}^*]$ .

If, in Lemma 3 we use that

$$\rho^2(t_i) \alpha(t_i) (1+O(\Delta_i)) = \rho^2(\theta_i) \alpha(\theta_i) (1+O(\Delta_i)) \quad (3.54)$$

we have

$$\begin{aligned} \|f - P_{m, T_n^*} f\|_Q^2 &= \frac{1}{n^{2m+1}} \frac{(m!)^2}{(2m)!(2m+1)!} \left[ \int_0^1 [\rho^2(u) \alpha(u)]^{\frac{1}{2m+1}} du \right]^{2m+1} \sum_{i=0}^{n-1} (1+O(\Delta_i)) \\ &= \frac{1}{n^{2m}} \frac{(m!)^2}{(2m)!(2m+1)!} \left[ \int_0^1 [\rho^2(u) \alpha(u)]^{\frac{1}{2m+1}} du \right]^{2m+1} + o\left(\frac{1}{n^{2m}}\right) \end{aligned} \quad (3.55)$$

Since  $\|f - P_{m, T_n^*} f\|_Q^2$  achieves the lower bound (3.52) up to a vanishingly small term,  $T_n^*$  is an asymptotically optimal sequence. This completes the proof of Theorem 2.

It appears that the theorem can be proved under weaker conditions on  $\rho$ , similar to those considered in [10]. We do not carry this out.



#### 4. Other Design Problems

Let  $T, S$  be two index sets, let  $\mathcal{H}_X$  be the Hilbert space spanned by  $X(s)$ ,  $s \in S$ , and let  $U(t) \in \mathcal{H}_X$  every  $t \in T$ . The problem of choosing an optimal index set  $T_n^* = \{t_0, t_1, \dots, t_n\}$  to estimate a random variable  $\langle f, X \rangle_\sim$ ,  $f \in \mathcal{H}_Q$  of a certain form, from the random variables  $U(t)$ ,  $t \in T$  is immediately reduced to the problem considered previously by the following two theorems.

Theorem 3. Let  $Q(s, s')$  be a given covariance kernel, on  $S \times S$ , let  $a(t, s)$  have the property that

$$a_t(\cdot) = a(t, s) \in \mathcal{H}_Q, \quad \forall t \in T,$$

Let

$$R(t, t') = \langle a_t(\cdot), a_{t'}(\cdot) \rangle_Q \quad t, t' \in T \times T$$

and let  $\mathcal{H}_R$  be the reproducing kernel space associated with  $R$ . Let  $V$  be the subspace of  $\mathcal{H}_Q$  spanned by  $\{a_t(\cdot), t \in T\}$  and let  $V_n$  be the subspace of  $V$  spanned by  $\{a_t(\cdot), t \in T_n\}$ . Then

$$\|P_V f - P_{V_n} f\|_Q^2 = \|g - P_{T_n} g\|_R^2 \quad (4.1)$$

where  $\|\cdot\|_R$  is the inner product in  $\mathcal{H}_R$ ,  $g$  is defined by

$$g(t) = \langle a_t, f \rangle_Q \in \mathcal{H}_R \quad (4.2)$$

and  $P_V, P_{V_n}$  are the projection operators in  $\mathcal{H}_Q$  onto  $V$  and  $V_n$

respectively, and  $P_{T_n}$  is the projection operator in  $\mathcal{H}_R$  onto the subspace spanned by  $\{R_t(\cdot), t \in T_n\}$ ,  $R_t(\cdot) = R(t, \cdot)$ .

Proof: Since  $R(t, t') = \langle a_t, a_{t'} \rangle_Q$  there is an isometric isomorphism between  $\mathcal{H}_R$  and  $V$  generated by the correspondence

$$R_t(\cdot) \in \mathcal{H}_R \sim a_t(\cdot) \in \mathcal{H}_Q \quad (4.3)$$

since

$$\langle R_t, R_{t'} \rangle_R = R(t, t') = \langle a_t, a_{t'} \rangle_Q \quad .$$

Furthermore

$$\langle a_t, f \rangle_Q = \langle a_t, P_V f \rangle_Q = g(t) = \langle R_t, g \rangle_R \quad (4.4)$$

Hence, since  $\{a_t, t \in T\}$  spans  $V$ ,  $\{R_t, t \in T\}$  spans  $\mathcal{H}_R$ ,  $V_n \sim \mathcal{H}_{T_n}$ , where  $\mathcal{H}_{T_n}$  is spanned by  $\{R_t, t \in T_n\}$ , we have

$$P_V f \sim g$$

$$P_{V_n} f \sim P_{T_n} g$$

and

$$\|P_V f - P_{V_n} f\|_Q = \|g - P_{T_n} g\|_R^2 \quad .$$

Theorem 4. Let  $T$  be a closed interval,  $\rho(t)$  continuous on  $T$ , and  $R(t, t')$  continuous on  $T \times T$ . Then (i) any  $f(s)$  of the form

$$f(s) = \int_T a(t, s) \rho(t) dt \quad (4.5)$$

is in  $V$  and (ii)

$$f \sim g$$

under the correspondance (4.3) where

$$g(t) = \int_T R(t, t') \rho(t') dt'$$

and hence (iii)

$$\langle f, X \rangle_{\sim} = \int_T U(t') \rho(t') dt' \quad (4.6)$$

where  $U(t) = \langle a_t, X \rangle_{\sim}$ .

Proof: Let  $\pi_\ell = \{t_{1\ell}, t_{2\ell}, \dots, t_{1\ell}\}$ ,  $\ell=1, 2, \dots$  be a sequence of partitions of  $[0, 1]$ , such that for every  $t$ , the Riemann sums for  $\pi_\ell$  for the integral

$$\int_0^1 R(t, t') \rho(t') dt'$$

converge.

Then

$$f_\ell(\cdot) = \sum_{j=1}^{\ell-1} a(t_{j\ell}, \cdot) \rho(t_{j\ell})(t_{j+1\ell} - t_{j\ell}), \quad \ell=1, 2, \dots$$

is a Cauchy sequence in  $V$  whose limit must be representable as  $f(\cdot)$  and the sequence of functions  $g_\ell(\cdot)$ ,  $\ell=1, 2, \dots$  defined by

$$g_\ell(t) = \langle a_t, f_\ell \rangle_Q = \langle a_t(\cdot), \sum_{j=1}^{\ell-1} a_{t_{j\ell}}(\cdot) \rho(t_{j\ell})(t_{j+1, \ell} - t_{j\ell}) \rangle_Q$$

is a Cauchy sequence in  $\mathcal{H}_{T_n}$  with

$$g_\ell(t) \longrightarrow \int_0^1 R(t, t') \rho(t') dt'.$$

Assertion (iii) follows by noting that

$$\begin{aligned} E X(s) \int_0^1 U(t) \rho(t) dt &= \int_0^1 \langle Q_s, a_t \rangle_Q \rho(t) dt \\ &= \int_0^1 a(t, s) \rho(t) dt = f(s) \end{aligned} \quad (4.7)$$

This completes the proof of Theorem 4.

The next theorem shows that  $\|f - P_{m, T_n} f\|_Q^2 = O(\Delta^{2m})$  under more general conditions on the covariance than those in Section 3.

#### Theorem 5

Suppose  $Q(s, t)$ ,  $s, t \in [0, 1]$  has continuous mixed partial derivatives up to order  $2m$  for  $s \neq t$ , and

$$\lim_{s \downarrow t} \frac{\partial^{2m-1}}{\partial s^{2m-1}} Q(s, t) - \lim_{s \uparrow t} \frac{\partial^{2m-1}}{\partial s^{2m-1}} Q(s, t) = (-1)^m \alpha(t) \quad (4.8)$$

Let

$$f(s) = \int_0^1 Q(s, t) \rho(s) ds \quad (4.9)$$

and suppose  $\alpha$  and  $\rho$  are continuous on  $[0,1]$  and  $\frac{\partial^{2m}}{\partial t^{2m}} Q(s,t)$  is bounded for  $t \neq s$ .

Then

$$\|f - P_{m, T_n} f\|_Q^2 \leq O(\Delta^{2m}) \quad (4.10)$$

Proof:

$$\|f - P_{m, T_n} f\|_Q^2 \leq \int_0^1 \int_0^1 \rho(s) \rho(t) E (X(s) - \widetilde{X}(s))(X(t) - \widetilde{X}(t)) ds dt \quad (4.11)$$

Where for each  $s$ ,  $\widetilde{X}(s)$  is any random variable in the subspace spanned by  $\{X^{(\nu)}(t_i), t_i \in T_n, \nu = 0, 1, 2, \dots, m-1\}$ .

We construct  $\widetilde{X}(s)$  for  $t_i \leq s \leq t_{i+1}$  as follows. (To avoid trivial details we let  $t_0$  and  $t_n$  be the boundaries of  $T$ .)

Let  $p_{i\nu}(t)$ ,  $q_{i\nu}(t)$  be the unique  $(2m-1)$ st degree polynomials satisfying

$$p_{i\nu}^{(\mu)}(t_i) = \delta_{\mu\nu}, \quad p_{i\nu}^{(\mu)}(t_{i+1}) = 0, \quad \mu, \nu = 0, 1, 2, \dots, m-1 \quad (4.12)$$

$$q_{i\nu}^{(\mu)}(t_i) = 0, \quad q_{i\nu}^{(\mu)}(t_{i+1}) = \delta_{\mu\nu} \quad (4.13)$$

where  $\delta_{\mu\nu} = 1, \mu = \nu, \delta_{\mu\nu} = 0$  otherwise.

Let

$$\widetilde{X}(s) = \sum_{\nu=0}^{m-1} p_{i\nu}(s) X^{(\nu)}(t_i) + q_{i\nu}(s) X^{(\nu)}(t_{i+1}), \quad t_i \leq s \leq t_{i+1}. \quad (4.14)$$

$\widetilde{X}(s)$ ,  $s \in [t_i, t_{i+1}]$  is the  $2m-1$  st degree polynomial which satisfies

$$X^{(\nu)}(t_i) - \widetilde{X}^{(\nu)}(t_i) = X^{(\nu)}(t_{i+1}) - \widetilde{X}^{(\nu)}(t_{i+1}) = 0, \quad \nu = 0, 1, 2, \dots, m-1. \quad (4.15)$$

This is the classical Hermite interpolation procedure, (see [11]). It is also the correct interpolation procedure if

$$Q(s, t) = \int_0^1 \frac{(s-u)_+^{m-1}}{(m-1)!} \frac{(t-u)_+^{m-1}}{(m-1)!} du \quad (4.16)$$

In this case  $P_{m, T_n} X(s) = \widetilde{X}(s)$ ,  $s \in [t_i, t_{i+1}]$ , since  $\widetilde{X}(s)$  is the unique  $(2m-1)$ st degree polynomial in  $s$  satisfying (4.15), and these conditions determine  $P_{m, T_n} X(s)$ .

Let

$$\widetilde{Q}_{si}(\cdot) = \sum_{\nu=0}^{m-1} (p_{i\nu}(s) Q_{t_i}^{(\nu)}(\cdot) + q_{i\nu}(s) Q_{t_{i+1}}^{(\nu)}(\cdot)) \quad (4.17)$$

We have, from (4.11)

$$\begin{aligned} \|f - P_{m, T_n} f\|_Q^2 &\leq \sum_{i,j=0}^{n-1} \int_{t_i}^{t_{i+1}} \int_{t_j}^{t_{j+1}} dt \, \rho(s) \rho(t) \times \\ &\quad \langle Q_s - \widetilde{Q}_{si}, Q_t - \widetilde{Q}_{tj} \rangle_R \, ds dt \\ &\leq \sum_{i,j=0}^{n-1} \rho(\theta_{i1}) \rho(\theta_{j2}) \int_{t_i}^{t_{i+1}} ds \int_{t_j}^{t_{j+1}} dt \langle Q_s - \widetilde{Q}_{si}, Q_t - \widetilde{Q}_{tj} \rangle_Q \end{aligned} \quad (4.18)$$

for some  $\{\theta_{i\ell}\}$  satisfying  $t_i \leq \theta_i \leq t_{i+1}$ .

By the assumptions on  $Q$ ,  $g \in \mathcal{H}_Q$  implies that  $g$  has at least  $m$  square integrable derivatives. Furthermore, for any  $g \in \mathcal{H}_Q$ , if we define  $\tilde{g}(s)$ ,  $s \in [t_i, t_{i+1}]$  by

$$\langle Q_s - \tilde{Q}_{si}, g \rangle_Q = \tilde{g}(s), \quad (4.19)$$

then

$$\tilde{g}^{(\nu)}(t_i) = \tilde{g}^{(\nu)}(t_{i+1}) = 0, \quad \nu = 0, 1, 2, \dots, m-1. \quad (4.20)$$

Then by use of (3.27m), we have

$$\int_{t_i}^{t_{i+1}} ds \langle Q_s - \tilde{Q}_{si}, g \rangle_Q = \int_{t_i}^{t_{i+1}} \frac{d^m}{du^m} \delta_i(u) \frac{d^m}{du^m} g(u) du \quad (4.21)$$

$$g \in \mathcal{H}_Q.$$

where  $\delta_i$  is given by (3.24).

Now letting  $g(u) = Q_t(u) - \tilde{Q}_{tj}(u)$ ,

we have

$$\begin{aligned} & \int_{t_j}^{t_{j+1}} dt \int_{t_i}^{t_{i+1}} ds \langle Q_s - \tilde{Q}_{si}, Q_t - \tilde{Q}_{tj} \rangle_Q \\ &= \int_{t_j}^{t_{j+1}} dt \int_{t_i}^{t_{i+1}} \frac{d^m}{du^m} \delta_i(u) \frac{d^m}{du^m} (Q_t(u) - \tilde{Q}_{tj}(u)) du \\ &= \int_{t_i}^{t_{i+1}} du \frac{d^m}{du^m} \delta_i(u) \frac{d^m}{du^m} \int_{t_j}^{t_{j+1}} \langle Q_t - \tilde{Q}_{tj}, Q_u \rangle_Q dt. \end{aligned} \quad (4.22)$$

For  $i \neq j$ ,  $t \neq u$  all the appropriate derivatives exist and are continuous by assumption, and (4.22) becomes, by another application of (4.21), equal to

$$\int_{t_i}^{t_{i+1}} \int_{t_j}^{t_{j+1}} \frac{d^m}{du^m} \delta_i(u) \frac{d^m}{dt^m} \delta_j(t) \frac{\partial^{2m}}{\partial u \partial t} Q(u, t) du dt. \quad (4.23)$$

We have that (4.23) is  $O(\Delta^{2m+2})$ , since  $\frac{d^m}{du^m} \delta_i(u) = O(t_{i+1} - t_i)^m$ .

For  $i=j$ , the left hand side of (4.22) becomes

$$\int_{t_i}^{t_{i+1}} dt \int_{t_i}^{t_{i+1}} ds \langle Q_s - \tilde{Q}_{si}, Q_t \rangle_Q + \int_{t_i}^{t_{i+1}} ds \int_{t_i}^{t_{i+1}} \langle Q_t - \tilde{Q}_{ti}, \tilde{Q}_{si} \rangle_Q dt \quad (4.24)$$

The first term in (4.24) is

$$\int_{t_i}^{t_{i+1}} dt \int_{t_i}^{t_{i+1}} \frac{d^m}{du^m} \delta_i(u) \frac{d^m}{du^m} Q_t(u) du. \quad (4.25)$$

Integrating by parts  $m$  times in the inner integral in (4.25) results in

$$\begin{aligned} & \int_{t_i}^{t_{i+1}} dt \left[ \delta_i(t) \alpha(t) + \int_{t_i}^{t_{i+1}} \frac{d^{2m}}{du^{2m}} Q_t(u) du \right] \\ & \quad u \neq t \\ & = \alpha(\theta_{i3})(t_{i+1} - t_i)^{2m+1} \frac{(m)!}{(2m)!(2m+1)!} + O((t_{i+1} - t_i)^{2m+2}) \end{aligned} \quad (4.26)$$

for some  $t_i \leq \theta_{i3} \leq t_{i+1}$ .



The second term in (4.24) becomes

$$\begin{aligned}
 & \int_{t_i}^{t_{i+1}} ds \int_{t_i}^{t_{i+1}} \delta_i^{(m)}(u) \frac{d^m}{du^m} \tilde{Q}_{si}(u) du \\
 &= \int_{t_i}^{t_{i+1}} ds \int_{t_i}^{t_{i+1}} \delta_i^{(m)}(u) \times \\
 & \left\{ \sum_{\nu=0}^{m-1} p_{i\nu}(s) \frac{\partial^{\nu+m}}{\partial r^\nu \partial u^m} \Big|_{r=t_i} Q(r, u) + \sum_{\nu=0}^{m-1} q_{i\nu}(s) \frac{\partial^{\nu+m}}{\partial r^\nu \partial u^m} \Big|_{r=t_{i+1}} Q(r, u) \right\} du \\
 &= \int_{t_i}^{t_{i+1}} ds \int_{t_i}^{t_{i+1}} \sum_{\nu=0}^{m-1} \delta_i^{(\nu)}(u) \times \\
 & \left\{ p_{i\nu}(s) \frac{\partial^{2m}}{\partial r^\nu \partial u^{2m-\nu}} \Big|_{r=t_i} Q(r, u) + q_{i\nu}(s) \frac{\partial^{2m}}{\partial r^\nu \partial u^{2m-\nu}} \Big|_{r=t_{i+1}} Q(r, u) \right\} du \quad (4.27)
 \end{aligned}$$

Now  $\delta_i^{(\nu)}(u) = O(t_{i+1} - t_i)^{2m-\nu}$ , and it can be shown by using the representation for  $p_{i\nu}(s)$ ,  $q_{i\nu}(s)$  given in [2] that

$$p_{i\nu}(s), q_{i\nu}(s) = O((t_{i+1} - t_i)^\nu)$$

Thus (4.27) is  $O((t_{i+1} - t_i)^{2m+2})$ , and we have

$$\begin{aligned}
 \|f - P_{m, T_n} f\|_Q^2 &\leq \frac{(m!)^2}{(2m)!(2m+1)!} \sum_{i=0}^{n-1} \alpha(\theta_{i3}) \rho(\theta_{i1}) \rho(\theta_{i2}) (t_{i+1} - t_i)^{2m+1} \\
 &+ \sum_{\substack{i, j=0 \\ i \neq j}}^{n-1} \rho(\theta_{i1}) \rho(\theta_{i2}) \int_{t_i}^{t_{i+1}} \int_{t_j}^{t_{j+1}} \frac{d^m}{du^m} \delta_i(u) \frac{d^m}{dv^m} \delta_j(v) \frac{\partial^{2m}}{\partial u^m \partial v^m} Q(u, v) du dv \\
 &+ O(\Delta^{2m+1}) \\
 &= O(\Delta^{2m})
 \end{aligned}$$

where  $\theta_{i1}, \theta_{i2}, \theta_{i3} \in [t_i, t_{i+1}]$ . This completes the proof of Theorem 5.

Suppose now we have available  $X(t_i)$ ,  $t_i \in T_{2mn}$  instead of derivatives. Group the design points into successive groups of  $2m$  points  $(t_{i+1}, t_{i+2}, \dots, t_{i+2m})$ , having common end members, and let now  $\tilde{X}(s)$  be given, for  $t_{i+1} \leq s \leq t_{i+2m}$  by the  $2m$ -1st degree polynomial which interpolates to  $X(t_\ell)$ ,  $\ell=i+1, \dots, i+2m$ . (Lagrange interpolation). By using the remainder theorem for Lagrange interpolation, it may be shown in a similar manner that  $\|f - P_{T_{2mn}} f\|_Q \leq O(\Delta)^{2m}$ .

5. Other Related Results

Suppose that a square root  $G$  of  $Q$  is known of the form

$$Q(t, t') = \int_0^1 G(t, u)G(t', u)du \quad (5.1)$$

where only  $G(t, \cdot) \in L_2[0, 1]$ , for every  $t \in [0, 1]$ . Then  $X(t)$  has a representation

$$X(t) = \int_0^1 G(t, u)dW(u)$$

and

$$f(t) = \int_0^1 Q(t, t') \rho(t') dt' \quad (5.2)$$

$$\begin{aligned} f(\cdot) &\sim \int_0^1 \rho(t)X(t)dt \\ &= \int_0^1 \int_0^1 \rho(t')G(t', u)dt'dW(u) \\ &= \int_0^1 h(u)dW(u) \end{aligned}$$

where

$$h(u) = \int_0^1 G(t, u)\rho(t)dt \quad (5.3)$$

If  $X(t)$  has  $m-1$  quadratic mean derivatives, then for any constants  $\{c_{i\nu}\}$ ,

$$\begin{aligned} \left\| f - \sum_{i=0}^n \sum_{v=0}^{m-1} c_{iv} Q_{t_i}^{(v)} \right\|_Q^2 &= E \left\{ \int_0^1 \rho(t) X(t) dt - \sum_{i=1}^n \sum_{v=0}^{m-1} c_{iv} X^{(v)}(t_i) \right\}^2 \\ &= \int_0^1 (h(u) - \sum_{i=0}^n \sum_{v=0}^{m-1} c_{iv} G^{(v)}(t_i, u))^2 du \end{aligned} \quad (5.4)$$

where

$$G^{(v)}(t_i, u) = \frac{\partial^v}{\partial t^v} G(t, u) \Big|_{t=t_i}.$$

Hence the design problems we have considered are equivalent to the problem of best approximation of  $h(u)$  by linear combinations of

$$\{G(t_i, u)\}_{i=1}^n \quad \text{or} \quad \{G^{(v)}(t_i, u)\}_{v=0}^{m-1}, i=0$$

in the  $L_2$  norm.

Let  $g \in \mathcal{H}_Q$ , then a quadrature formula for  $\int_0^1 \rho(t)g(t)dt$  is given by  $\int_0^1 \rho(t)P_{T_n} g(t)dt$ , since this latter expression is a linear combination of the values of  $g(t)$  at  $t=t_i \in T_n$ .

Then

$$\left| \int_0^1 \rho(t)g(t)dt - \int_0^1 \rho(t)P_{T_n} g(t) dt \right|^2 \quad (5.5)$$

$$= | \langle f, g - P_{T_n} g \rangle_Q |^2$$

$$= | \langle f - P_{T_n} f, g \rangle_Q |^2 \leq \|g\|_Q \|f - P_{T_n} f\|_Q$$

$$\leq \|g\|_Q \cdot \int_0^1 (h(u) - \sum_{i=1}^n c_i G(t_i, u))^2 du$$

In the case  $G(t, u) = \frac{(t-u)_+^{m-1}}{(m-1)!}$ ,  $\rho(t) = 1$ , we have

$$h(u) = \frac{(1-u)_+^m}{m!} \quad (5.6)$$

By making the change of variable  $x = 1-u$  in (5.5) the problem of minimizing  $\|f - P_{T_n} f\|_Q^2$  is equivalent to that of optimally approximating the monomial  $\frac{x^m}{m!}$  by linear combinations of the functions

$$\left\{ \frac{(x-\xi_i)_+^{m-1}}{(m-1)!} \right\}_{i=0}^n, \quad (\xi_i = 1-t_i), \text{ in the } L_2[0,1] \text{ norm.}$$

Similarly, it is

clear that the problem of minimizing  $\|f - P_{m, T_n} f\|_Q^2$  is equivalent to optimally approximating  $\frac{x^m}{m!}$  by linear combination of the functions

$\left\{ \frac{(x-\xi_i)_+^{m-1-\nu}}{(m-1-\nu)!} \right\}_{\nu=0, i=0}^{m-1, n}$  in the  $L_2[0,1]$  norm. Such linear combina-

tions are known as spline functions. (See e.g. the volume in [11]).

Functions of the form

$$s(x) = \frac{x^m}{m!} + \sum_{i=1}^n \sum_{\nu=0}^{m-1} c_{i\nu} \frac{(x-\xi_i)_+^{m-1-\nu}}{(m-1-\nu)!} \quad (5.7)$$

for some constants  $\{c_{i\nu}\}$  are known in the approximation theory literature (see [5] [11] as monosplines).

Monosplines of smallest  $L_2$  norm have recently attracted attention in the context of establishing optimal quadrature formulae via minimizing the error bound of (5.5). Some of the results are relevant to the experimental design problem. These results are available when  $\frac{(t_1-u)_+^{m-1-\nu}}{(m-1-\nu)!}$  is replaced by  $G_{m,\nu}(t_1, u)$  of (2.6),  $\nu=0, 1, 2, \dots, m-1$ .<sup>1</sup> We state two relevant theorems, in our notation.

Theorem. (Karlin, [5], following Theorem 5). Let  $Q$  be of the form (2.13),  $f$  given by (5.2) with  $\rho(t) = 1$ . Then, for every  $T_n \in \mathcal{D}_n$ , there exists a  $\tilde{T}_{mn} \in \mathcal{A}_{mn}$  such that

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<sup>1</sup>

Linear combinations of the functions  $\{G_{m-\nu}(t_i, u)\}_{\nu=0, i=1}^{m-1, n}$  are so called Tchebychev splines with respect to  $L^*$ , compare [4], Chapter 10, section 3.

$$\|f - P_{\tilde{T}_{mn}} f\|_Q^2 \leq \|f - P_{m, T_n} f\|_Q^2.$$

Professor Karlin informs us that it is sufficient for this Theorem that only  $\rho(t) > 0$ .

Theorem. (Karlin, [5], Theorem 5). Let  $Q$  satisfy the hypotheses of the preceding Theorem. Then

$$\inf_{T_n \in \mathcal{D}_n} \|f - P_{T_n} f\|_Q^2 = \|f - P_{T_n^*} f\|_Q^2$$

where

- (i)  $T_n^*$  is unique
- (ii)  $T_n^*$  consists of  $n$  distinct points
- (iii)  $\langle f - P_{T_n^*} f, Q_{t_i^*}^{(1)} \rangle_Q = 0, \quad t_i^* \in T_n^*, \quad (m > 1)$

The statement (iii) is the remarkable result that, at the optimal design  $T_n^*$  for data without derivatives, the addition of first derivatives to the data set provides no new information.

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