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THE SAME OPTIMAL KNOTS IN SPLINE WITH
PIECEWISE POLYNOMIAL APPROXIMATION

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Running head. Functions with the same optimal knots.

Abstract. The relationship between functions with the same optimal knots for $L_2[0,1]$ approximation by k -th order splines or piecewise polynomials is investigated. It is shown that, if two functions have positive continuous k -th derivatives, they will have the same optimal knots if and only if they differ by a polynomial of order k . An application to design selection for continuous time regression is considered and extensions to L_p approximation are also provided.

1. Introduction Consider the $L_2[0,1]$ approximation of two functions by splines or piecewise polynomials with free knots. In this note we investigate the relationship between functions, f and g , having the same optimal knots.

Let P_N^k and S_N^k denote, respectively, the set of all k -th order piecewise polynomials and k -th order splines with $N-1$ distinct knots in the interior of $[0,1]$. For simplicity, a generic notation, f_N , will be used to indicate the best $L_2[0,1]$ approximation to f from either P_N^k or the closure of S_N^k , $\bar{S}_N^k$; its meaning will be clear from context. The properties of f_N for P_N^k have been studied by Chow [5] and Burchard and Hale [4]. Similar results for $\bar{S}_N^k$ can be found in Barrow, et al. [2] and Barrow and Smith [3]. All these papers, however, have focused on the behavior of f_N and its corresponding optimal knots for f in various function classes. For instance, Chow [5] has established conditions on f that insure unique optimal knots for each N whereas Barrow and Smith [3] have provided an asymptotic characterization of the behavior of the optimal knots in terms of f 's k -th derivative. In contrast, this paper focuses on what is, in a certain sense, an inverse of these problems. Rather than asking how f 's properties characterize the behavior of its optimal knots we ask, instead, to what extent the optimal knots characterize f . The answer is, essentially, that two functions with the same optimal knots for all N must differ by at most a k -th order polynomial. More specifically we show the following:

Theorem 1. Let $f, g \in L_2[0,1] \cap C^k[0,1]$ with $f^{(k)}$ and $g^{(k)}$ both positive on $[0,1]$. Then, f and g have the same optimal knots for $L_2[0,1]$ approximation from P_N^k (or from $\bar{S}_N^k$) for all N if and only if there exists constants $\alpha_0, \dots, \alpha_k$, ($\alpha_k \neq 0$) such that

$$f(t) = \sum_{i=0}^{k-1} \alpha_i t^i + \alpha_k g(t), \quad t \in [0,1]. \quad (1.1)$$

The proof of Theorem 1 is given in the next section. Although this

theorem is of interest in its own right it also has statistical applications, one of which is briefly discussed in Section 3. Another application is to the statistical problems of grouping, spacing and stratification considered by Adatia and Chan [1] who, when $k=1$, have obtained a special case of this result. It follows from Eubank [6] that Theorem 1 can be used to obtain their Theorem 5 under alternative conditions. Section 4 contains some concluding remarks and suggestions for future research. An extension of Theorem 1 to $L_p[0,1]$ approximation is also provided.

2. Proof of Theorem Let us first prove Theorem 1 for approximation from $\bar{S}_N^k$ as the case of P_N^k will follow similarly. Throughout this and the subsequent section we use $||\cdot||$ to denote the usual $L_2[0,1]$ norm and D_N for the set of 'all possible' knot choices, i.e.,

$$D_N = \{(t_0, t_1, \dots, t_N) : 0 = t_0 < t_1 < \dots < t_N = 1\}. \quad (2.1)$$

For $T \in D_N$ let S_T^k denote the $L_2[0,1]$ orthogonal projector for the set of all k -th order splines having knots at T . Then, a best approximation f_N is characterized by

$$||f - f_N|| = \inf_{T \in D_N} ||f - S_T^k f||. \quad (2.2)$$

Note that although $S_T^k f$ has noncoincident knots, the knots for f_N need not be distinct.

Now let $f(t) = \sum_{i=0}^{k-1} \alpha_i t^i + \alpha_k g(t)$ for some constants $\alpha_0, \dots, \alpha_k$ with $\alpha_k \neq 0$. Then $||f - S_T^k f|| = |\alpha_k| ||g - S_T^k g||$ for all $T \in D_N$. Consequently, f and g have the same optimal knots for all N and the direct implication has been verified.

To see the necessity of condition (1.1) let $\{f_N\}$ be a sequence of best approximations to f and $0 = t_0^N < t_1^N \leq \dots \leq t_{N-1}^N < t_N^N = 1$ the optimal knots corresponding to f_N . By assumption these will also be optimal knots for g . Define, as in Barrow and Smith [3], a piecewise linear function $\underline{T}^N \in [0,1]$ satisfying $\underline{T}^N(i/N) = t_i^N$, $i = 0, \dots, N$, and let $\underline{s}_N$ denote its right continuous inverse. It then follows from Theorem 3 of [3] that, since $f^{(k)} > 0$, as $N \rightarrow \infty$

$$s_N(\tau) \rightarrow \int_0^\tau \{f^{(k)}(t)\}^{2/2k+1} dt / \int_0^1 \{f^{(k)}(x)\}^{2/2k+1} dx, \text{ uniformly on } [0,1]. \quad (2.3)$$

But, since the $\{t_i^N\}_{i=0}^N$ are also optimal knots for g ,

$$s_N(\tau) \rightarrow \int_0^\tau \{g^{(k)}(t)\}^{2/2k+1} dt / \int_0^1 \{g^{(k)}(x)\}^{2/2k+1} dx. \quad (2.4)$$

The result now follows by equating (2.3) and (2.4) and differentiating.

To prove Theorem 1 for P_N^k we need only note that an analog of Theorem 3 in Barrow and Smith [3] can be shown to hold, in this case, by using their proof in conjunction with Theorem 1.1 of [4]. The required result can then be obtained as in the previous arguments.

3. An application to regression design for time series. In this section an application of Theorem 1 to the problem of optimal design for continuous time regression will be presented. The situation is as follows. A stochastic process, Y , is assumed to have the form

$$Y(t) = \beta f(t) + X(t), \quad t \in [0,1], \quad (3.1)$$

where f is a known regression function, β is an unknown parameter and X is a zero mean process with covariance kernel

$$R(s,t) = (k-1)! \int_0^1 (s-u)_+^{k-1} (t-u)_+^{k-1} du, \quad (3.2)$$

with $x_+^{k-1} = x^{k-1}$ if $x \geq 0$ and zero otherwise. The objective is to obtain an estimate of the unknown parameter β . However, suppose it is possible only to sample the Y process, as well as its $k-1$ quadratic mean derivatives, at some set of noncoincident time points $T \in D_N$. Thus an estimator must be based solely on the observations $Y_T^k = \{Y^{(i)}(t); t \in T, i=0, \dots, k-1\}$. For this purpose the best linear unbiased estimator of β can be obtained through the use of generalized least squares (c.f. Sacks and Ylvisaker [10].)

This estimator will be denoted by $\hat{\beta}_{k,T}$. Since the choice of T is usually at the discretion of the experimenter, the problem arises as to how T should be selected. Let $V(\hat{\beta}_{k,T})$ denote the variance of $\hat{\beta}_{k,T}$; then, an optimal

estimator can be obtained by choosing $T^* \in D_N$ to satisfy

$$V(\hat{\beta}_{k,T^*}) = \inf_{T \in D_N} V(\hat{\beta}_{k,T}). \quad (3.3)$$

Under the regularity condition that f admits the representation

$$f(t) = (k-1)! \int_0^1 f^{(k)}(u)(t-u)_+^{k-1} du \quad (3.4)$$

for some $f^{(k)} \in L_2[0,1]$ problem (3.3) is amenable to analysis and has been studied by Sacks and Ylvisaker [10], Wahba [11], Eubank, Smith and Smith [7] and others. We now investigate, with the aid of Theorem 1, the relationship between regression models having identical optimal designs for all N .

It follows from Eubank, Smith and Smith [7] that for R of the form (3.2), $T \in D_N$ and f satisfying (3.4) we may write $V(\hat{\beta}_{k,T}) = \|P_T^k f^{(k)}\|^{-2}$ where P_T^k is the $L_2[0,1]$ orthogonal projector for the set of all piecewise polynomials of order k with knots at T . As $\|P_T^k f^{(k)}\|^2 = \|f^{(k)}\|^2 - \|f^{(k)} - P_T^k f^{(k)}\|^2$ problem (3.3) can be restated as: find $(f^{(k)})_N$ such that

$$\|f^{(k)} - (f^{(k)})_N\| = \inf_{T \in D_N} \|f^{(k)} - P_T^k f^{(k)}\| \quad (3.5)$$

with T^* then provided by the knots for $(f^{(k)})_N$. In view of Theorem 1 this has the following immediate consequence.

Corollary. Let f_1 and f_2 be two regression functions satisfying (3.4) with $f_i^{(k)} \in C^k[0,1]$ and $f_i^{(2k)}$ positive on $[0,1]$ for $i=1,2$. Also let $\hat{\beta}_{k,T}^1$ and $\hat{\beta}_{k,T}^2$ denote the BLUE's of β corresponding to when f , in (3.1), is f_1 and f_2 respectively. Then, $\hat{\beta}_{k,T}^1$ and $\hat{\beta}_{k,T}^2$ have the same optimal designs for all N if and only if

$$f_1(t) = \sum_{i=0}^{k-1} \alpha_i t^{k+i} + \alpha_k f_2(t), \quad t \in [0,1].$$

Thus, not only does the regression function dictate the properties of the optimal designs but, conversely, the optimal designs also characterize the regression function up to a $2k$ -th order polynomial. The corollary can be extended to a wider class of processes through use of results in [8].

4. Concluding remarks. Theorem 1 has a straightforward extension to the case of best L_p $[0,1]$ approximation, $1 \leq p \leq \infty$, from P_N^k . Using the notation and results in Theorem 1.1 of [4] and the techniques of Section 2 it is possible to show the following:

Theorem 2. Assume that either $f, g \in W^{k,1}(0,1)$ or else $f, g \in W^{k,1,loc}(0,1) \cap L_p[0,1]$ and $|f^{(k)}|, |g^{(k)}|$ are monotone a.e. with $|f^{(k)}|^\sigma$ and $|g^{(k)}|^\sigma$ integrable for $\sigma = (k+p-1)^{-1}$. For $p = \infty$ also assume that $f, g \in C[0,1]$. If, in addition, $(f^{(k)} g^{(k)}) \geq 0$ (or $-(f^{(k)} g^{(k)}) \geq 0$, as appropriate) a.e., then f and g have the same optimal knots for all N if and only if (1.1) holds.

Note that when $p=2$ Theorem 2 implies Theorem 1 for P_N^k . An analog of Theorem 2 for $\bar{S}_N^k$ and $1 \leq p < \infty$ can be obtained using results in [9].

More general versions of Theorems 1 and 2 are desirable. In particular, relaxation of the conditions imposed on the sign change behavior of $f^{(k)}$ and $g^{(k)}$ would be of interest. Unfortunately, the asymptotic behavior of the optimal knots serves only to distinguish between functions whose k th derivatives are not proportional in absolute value. Thus, relaxation of these restrictions will require the use of information provided by the optimal knots for finite N . To illustrate the ideas involved consider the function $f(x)=x$, $x \in [0,1]$ and define $g(x)$ to be $f(x)$ on $[0,.5]$ and $1-f(x)$ on $[.5,1]$. Then, for $k=1$ and $p=2$, say, we have $|f'| = |g'|$ so that f and g are indistinguishable in terms of the asymptotic behavior of their optimal knots. However, the optimal knots can still be seen to separate these two functions by comparing the optimal knots for f when $N=2$, viz $1/3$ and $2/3$, to the breakpoints $1/4$ and $3/4$ for g .

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