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STOCHASTIC INTERPRETATIONS AND RECURSIVE ALGORITHMS FOR SPLINE FUNCTIONS

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Spline functions, which are solutions to certain deterministic optimization problems, can also be regarded as solutions to certain stochastic optimization problems; in particular, certain linear least-squares estimation problems. Such an interpretation leads to simple recursive algorithms for interpolating and smoothing splines. These algorithms compute the spline using one data point at a time, and are useful in real-time calculations when data are acquired sequentially.

1. Introduction. Spline functions are natural generalizations of polynomials. The simplest type of spline function, a polynomial spline, is in fact a piecewise polynomial that satisfies certain continuity requirements over its range of definition. Whereas polynomials have long been used as approximating and interpolating functions because of their simple mathematical properties, splines are almost as easy to work with and actually provide a closer approximation to functions and smoother interpolation of data than do polynomials. These properties follow from the fact that the solutions of certain deterministic optimization problems are (natural) splines.

Kimeldorf and Wahba [6], [7], [8] have recently shown that splines could also be regarded as solutions of certain stochastic optimization problems; in particular, certain minimum-variance unbiased linear estimation problems. These results suggested to us that it should be possible to find recursive algorithms for calculating spline functions similar to the recursive algorithms that have been extensively used by control engineers for calculating least-squares estimates. Existing algorithms for calculating splines cannot be easily updated: the relevant equations have to be re-solved if new data are added. A recursive algorithm, which can compute the spline using one data point at a time, is particularly useful in real-time computations when data are acquired sequentially.

However, we found that the form of the solution given by Kimeldorf and Wahba was not amenable to recursive calculation. The difficulty lay in their choice of a norm for the underlying Hilbert space. By choosing a different norm, one can obtain a solution whose form lends itself to recursive computation.

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The paper is organized as follows. In Section 2 a very general type of interpolating spline, the so-called *Lg*-spline, is defined as the solution of a certain deterministic optimization problem in a Sobolev space H. We then show that H can be made into a reproducing kernel Hilbert space (rkhs). This can be done in many ways depending on the norm that is chosen. Our choice, which differs from that of Kimeldorf and Wahba, permits a reformulation of the original optimization problem as a minimum norm problem in H. Several characterizations of the solution of this problem are given.

In Section 3, a recursive solution of the minimum norm interpolation problem is given. Section 4 presents a stochastic interpretation for the spline interpolation problem in terms of linear least-squares estimation. The recursive solution of this estimation problem provides a recursive solution to the spline problem that is equivalent to the algorithm of Section 3. The spline smoothing problem is treated in an analogous fashion in Section 5.

2. Interpolation with *Lg*-splines. We shall first give the basic definition of an *Lg*-spline and then describe some existence and uniqueness results.

Let H denote the linear space of real-valued functions defined on the interval $I = [0, T]$, such that $f \in H$ if and only if $f \in C^{m-1}(I)$, $f^{(m-1)}$ is absolutely continuous, and $Lf \in \mathscr{L}_2(I)$, where L is an ordinary differential operator of the form

$$L = D^m + a_{m-1}(t)D^{m-1} + \cdots + a_1(t)D + a_0(t)$$
$$D \equiv d/dt\,, \qquad a_j \in C^j(I)\,, \qquad 0 \leqq j \leqq m-1\,.$$

Suppose

$\{\lambda_j\}_1^n$, $n \geqq m$, is a set of linear functionals that are linearly independent on H

and

$\{r_j\}_1^n$ is a set of real numbers.

H can be shown to be a Hilbert space under a variety of equivalent norms, two of which will be considered in the sequel. We assume that $\{\lambda_j\}_1^n$ are continuous with respect to these norms.

DEFINITION 1. A function $s \in H$ is an *Lg-spline* interpolating $\{r_j\}_1^n$ with respect to $\{\lambda_j\}_1^n$ if and only if it solves the following minimization problem:

$$\int_I (Ls)^2 = \min_{f \in U(\mathbf{r})} \int_I (Lf)^2 \tag{1}$$

where

$$U(\mathbf{r}) = \{f \in H\colon \lambda_j f = r_j,\ 1 \leqq j \leqq n\}\,.$$

If $\lambda_j f \equiv f(t_j)$ and $0 \leqq t_1 < \cdots < t_n \leqq T$, then s is an *L-spline*, and the points $t_1, \cdots, t_n$ are called knots. If $L = D^m$, then s is a *polynomial spline*.

Now let

$$N = \text{null space of } L\,.$$

Since L is of order m, N is an m-dimensional linear subspace of H. Also let

$$\{z_j\}_1^m = \text{basis for } N\,.$$

The following results on existence and uniqueness of solutions to (1) were first proved by Jerome and Schumaker [3].

THEOREM 1. *A solution to* (1) *always exists*; *it is unique if and only if* $N \cap U(0) = \{0\}$, *where*

$$U(0) = \{f \in H\colon \lambda_j f = 0,\ 1 \leqq j \leqq n\}\,. \tag{2}$$

An alternative uniqueness criterion is provided by the following theorem.

THEOREM 2. $N \cap U(0) = \{0\}$ *if and only if there exists a subset* $\{\tilde{\lambda}_j\}_1^m$ *of* $\{\lambda_j\}_1^n$ *that is linearly independent on* N.

In the remainder of this paper we shall assume that (1) has a unique solution for arbitrary L and $\{\lambda_j\}_1^n$. Consequently, by Theorem 2, we can assume that

$$\{\lambda_j\}_1^m \quad \text{are linearly independent on} \quad N\,.$$

A. *Introduction of a reproducing kernel.* H can be made into a reproducing kernel Hilbert space with respect to a certain inner product. First, let $\{z_j\}_1^m$ be the basis for N that is dual to $\{\lambda_j\}_1^m$; i.e.,

$$\begin{aligned} Lz_j &= 0\,, & 1 \leqq j \leqq m \\ \lambda_j z_i &= \delta_{ij}\,, & 1 \leqq i, j \leqq m\,. \end{aligned}$$

Our uniqueness assumption guarantees that $\{z_j\}_1^m$ can be chosen in this manner. Also let

$$G(t, u) = \text{the Green's function}$$

for the boundary value problem

$$Lp = w\,, \qquad \lambda_j p = 0\,, \qquad 1 \leqq j \leqq m\,.$$

Define a (kernel) function

$$K(t, u) = \textstyle\sum_{j=1}^m z_j(t) z_j(u) + \int_I G(t, v) G(u, v)\, dv\,. \tag{3}$$

The following theorem was first proved by deBoor and Lynch [2]. A shorter and more direct proof is given by Weinert [12].

THEOREM 3. *H is a reproducing kernel Hilbert space with inner product*

$$\langle e, f\rangle = \textstyle\sum_{j=1}^m (\lambda_j e)(\lambda_j f) + \int_I (Le)(Lf)\,, \tag{4}$$

and with reproducing kernel $K(t, u)$.

The reproducing kernel has the following two properties:

$$K(\cdot, t) \in H$$
$$\langle f(\cdot), K(\cdot, t)\rangle = f(t)$$

for every $t \in I$ and every $f \in H$. A full discussion of these spaces can be found in Aronszajn [1].

The Riesz representation theorem guarantees that corresponding to each λ_j there exists a unique function $h_j \in H$ that satisfies for all $f \in H$

$$\lambda_j f = \langle f, h_j \rangle .$$

The function h_j is called the *representer* of the continuous linear functional λ_j.

THEOREM 4. *The representers $\{h_j\}_1^n$ are linearly independent and are given by*

$$h_j(u) = \lambda_{j(t)} K(t, u) , \qquad 1 \leqq j \leqq n .$$

PROOF. The reproducing property and the definition of h_j show that $h_j(u) = \langle K(\cdot, u), h_j(\cdot)\rangle = \lambda_{j(t)} K(t, u)$. Now suppose $\sum_{j=1}^n c_j h_j(u) = 0$. Then $\sum_{j=1}^n c_j \lambda_{j(t)} K(t, u) = 0$, which implies that $c_j = 0$, $1 \leqq j \leqq n$, since $\{\lambda_j\}_1^n$ are linearly independent. □

THEOREM 5. *Let $\mathscr{S}$ denote the n-dimensional linear subspace of H spanned by $\{h_j\}_1^n$. Then*

$$H = \mathscr{S} \oplus U(0)$$

where $U(0)$ is defined in Equation (2).

PROOF. Since $\mathscr{S}$ is finite-dimensional it suffices to show that $U(0) = \mathscr{S}^\perp$ (the orthogonal complement of $\mathscr{S}$). Let $f \in \mathscr{S}^\perp$. Then $0 = \langle f, h_j\rangle = \lambda_j f$, $1 \leqq j \leqq n$. Therefore, $\mathscr{S}^\perp \subset U(0)$. Now let $g \in U(0)$. Then $0 = \lambda_j g = \langle g, h_j\rangle$, $1 \leqq j \leqq n$, which means that $U(0) \subset \mathscr{S}^\perp$. □

B. *Minimum-norm formulation of the spline problem.* If we want to solve for the interpolating spline directly in H, it turns out that we must somehow reformulate (1) as a minimum norm problem in H. As it stands now, the integral on the right-hand-side of (1) represents the norm of Lf in $\mathscr{L}_2(I)$, and the projection theorem can be used in $\mathscr{L}_2(I)$ to find Ls. (In fact, as we shall discuss later, several authors have used this indirect method.) However, the integral in (1) is only a pseudo-norm in H since it is not strictly positive. We now show how to reformulate (1) as a minimum norm problem in H, and we give various characterizations of the spline solution.

THEOREM 6. *A function $s \in H$ is the Lg-spline interpolating $\{r_j\}_1^n$ with respect to $\{\lambda_j\}_1^n$ if and only if it solves the following minimization problem*:

$$||s||^2 = \min_{f \in U(\mathbf{r})} ||f||^2 . \tag{5}$$

PROOF. From (4), $||f||^2 = \sum_{j=1}^m (\lambda_j f)^2 + \int_I (Lf)^2$. Since the minimization is carried out for $f \in U(\mathbf{r})$, $\lambda_j f = r_j$ and is fixed. Therefore, minimizing $\int_I (Lf)^2$ over $U(\mathbf{r})$ is equivalent to minimizing $||f||^2$ over $U(\mathbf{r})$. □

The solution to (5) is established in the following theorem.

THEOREM 7. *The unique Lg-spline interpolating $\{r_j\}_1^n$ with respect to $\{\lambda_j\}_1^n$ is given by*

$$s(t) = \mathbf{h}'(t)\mathbf{R}^{-1}\mathbf{r} \tag{6}$$

where

$$\mathbf{h}' = \text{row}\,(h_1, \cdots, h_n)\,,$$
$$\mathbf{r} = \text{col}\,(r_1, \cdots, r_n)\,,$$
$\mathbf{R} =$ *the symmetric* $n \times n$ *matrix whose* i, jth *element equals* $\langle h_i, h_j \rangle$.

PROOF. A slight modification of the projection theorem ([9], page 64) shows that (5) has a unique solution, and that this solution is in $\mathscr{S}$. Therefore, $s = \sum_{j=1}^{n} c_j h_j$. The coefficients are found by using the interpolation conditions. □

Equation (5) shows that the spline is the minimum-norm interpolating function. Several other equivalent characterizations of the spline are possible. We give some here and refer to Weinert [12] for others. Thus it can be shown that the solution to (5)

(a) is the only function in $\mathscr{S} \cap U(\mathbf{r})$

(b) is the projection onto $\mathscr{S}$ of *any* function in $U(\mathbf{r})$

(c) can be written as $s(t) = \langle g(\cdot), K_{\mathscr{S}}(\cdot, t)\rangle$ where g is any function in $U(\mathbf{r})$ and $K_{\mathscr{S}}$ is the reproducing kernel of $\mathscr{S}$.

3. A recursive algorithm. All existing algorithms for calculating Lg-splines have one feature in common: if an extra data point (interpolation constraint) is added to the problem, the relevant equations have to be re-solved. The reformulation that leads to (6) permits us to calculate the spline interpolating $n + 1$ points by adding a correction term to the spline that interpolates the first n points. To do this, we find an orthonormal basis for $\mathscr{S}$.

THEOREM 8. *The spline solution to* (5) *can be written as*

$$s(t) = \sum_{j=1}^{n} \hat{r}_j \hat{h}_j(t) \tag{7}$$

where $\{\hat{h}_j\}_1^n$ *is obtained from* $\{h_j\}_1^n$ *by the Gram–Schmidt orthonormalization procedure, and* $\{\hat{r}_j\}_1^n$ *is obtained from* $\{r_j\}_1^n$ *using the same linear operations by which* $\{\hat{h}_j\}_1^n$ *is obtained from* $\{h_j\}_1^n$.

PROOF. Equation (7) follows immediately from (6) since $\langle \hat{h}_i, \hat{h}_j \rangle = \delta_{ij}$. Let $\hat{r}_j \equiv \langle g, \hat{h}_j \rangle$ for $g \in U(\mathbf{r})$. The Gram–Schmidt procedure determines coefficients d_{ij}, $i \geqq j$, such that $\hat{h}_i = \sum_{j=1}^{i} d_{ij} h_j$. Thus $\hat{r}_i = \sum_{j=1}^{i} d_{ij} \langle g, h_j \rangle = \sum_{j=1}^{i} d_{ij} r_j$. □

The topology of H permits various simplifications in the Gram–Schmidt procedure. For details, see Weinert [12].

An example. Let $L = D^2 + 1$, $\lambda_1 f \equiv f(0)$, $\lambda_2 f \equiv \dot{f}(0)$, $\lambda_3 f \equiv f(T)$ and $\lambda_4 f \equiv \dot{f}(T)$ with $T = 2\pi$. Thus $m = 2$ and $n = 4$. H consists of functions f with absolutely continuous first derivatives such that $\int_0^{2\pi} (\ddot{f} + f)^2 < \infty$, and with inner product

$$\langle e, f \rangle = e(0)f(0) + \dot{e}(0)\dot{f}(0) + \int_0^{2\pi} (\ddot{e} + e)(\ddot{f} + f)\,.$$

We have

$$z_1(t) = \cos t\,, \qquad z_2(t) = \sin t\,,$$
$$G(t, u) = \sin(t - u)\,, \qquad t > u$$
$$= 0\,, \qquad \text{other}$$

$$K(t, u) = \tfrac{1}{2}(t \wedge u)\cos(t-u) + \tfrac{1}{4}\sin(|t-u|) - \tfrac{1}{4}\sin(t+u) + \cos(t-u),$$

$$\hat{h}_1(t) = z_1(t), \qquad \hat{h}_2(t) = z_2(t),$$

$$\hat{h}_3(t) = (t\cos t - \sin t)/2\pi^{\frac{1}{2}}, \qquad \hat{h}_4(t) = t\sin t/2\pi^{\frac{1}{2}},$$

$$\hat{r}_1 = r_1, \qquad \hat{r}_2 = r_2, \qquad \hat{r}_3 = (r_3 - r_1)/\pi^{\frac{1}{2}}, \qquad \hat{r}_4 = (r_4 - r_2)/\pi^{\frac{1}{2}},$$

$$s(t) = r_1 \cos t + r_2 \sin t + (r_3 - r_1)(t\cos t - \sin t)/2\pi + (r_4 - r_2)t\sin t/2\pi. \quad \square$$

Many algorithms have been developed for calculating interpolating splines. Jerome and Schumaker [4] and Lyche and Schumaker [10] use a local-support basis for $\mathcal{S}$ to find polynomial splines. However, though both algorithms have good numerical properties, they are conceptually quite a bit more complicated than ours. Moreover, preliminary numerical results indicate that if sequential computation of the spline is necessary or desirable, the recursive algorithm will require less computation time and less storage than the Lyche–Schumaker algo-algorithm, while giving results of comparable accuracy. There are many problems in nonlinear trajectory estimation and seismic data processing, for example, in which the recursive algorithm can be useful.

4. Splines and stochastic interpretations. The search for a recursive spline algorithm was motivated by the work of Kimeldorf and Wahba [7], [8] who showed that splines could be found by solving certain minimum-variance estimation problems. It seemed that with the proper stochastic interpretation of the spline problem, knowledge of recursive estimation methods could be used to compute the spline recursively. We will now show how this can be done.

Let y be a real-valued random process with zero mean and covariance equal to the reproducing kernel K, and let $\hat{y}(t)$ be the linear least-squares estimate of $y(t)$ given data random variables $\{\lambda_j y\}_1^n$, with $\{\lambda_j\}_1^n$ as before. Then if we make the identification $\lambda_j y = r_j$, $1 \leqq j \leqq n$, it is easy to see that

$$\hat{y}(t) = \mathbf{h}'(t)\mathbf{R}^{-1}\mathbf{r} = s(t).$$

The estimate $\hat{y}$ can be found recursively by using the Gram–Schmidt procedure on the data $\{\lambda_j y\}_1^n$. Since $s = \hat{y}$, we have a recursive algorithm for the spline, which is identical to that given in Theorem 8.

The stochastic model developed by Kimeldorf and Wahba [7], [8] uses a different inner product and reproducing kernel; namely,

$$(e, f) = \textstyle\sum_{j=0}^{m-1} e^{(j)}(0)f^{(j)}(0) + \int_I (Le)(Lf)$$

and

$$\tilde{K}(t, u) = \tilde{K}_0(t, u) + \tilde{K}_1(t, u) = \textstyle\sum_{j=1}^{m} \tilde{z}_j(t)\tilde{z}_j(u) + \int_I g(t, v)g(u, v)\,dv$$

where $\{\tilde{z}_j\}_1^m$ span N and are chosen so that

$$\tilde{z}_i^{(j-1)}(0) = \delta_{ij}, \qquad 1 \leqq i, j \leqq m,$$

and $g(t, u)$ is the Green's function for the initial value problem

$$Lp = q, \qquad p^{(i)}(0) = 0, \qquad 0 \leqq i \leqq m-1.$$

With this inner product, (1) cannot be reformulated as a minimum norm problem in H because $\sum_{j=0}^{m-1} (f^{(j)}(0))^2$ is not constant for all $f \in U(\mathbf{r})$. In their stochastic model y is a random process with *unknown* mean value in N, and with covariance equal to $\tilde{K}_1$. It is shown that if $\hat{y}(t)$ is the minimum-variance unbiased linear estimate of $y(t)$ given data $\{\lambda_j y\}_1^n$, then $\hat{y}(t) = s(t)$ under the correspondence $\lambda_j y = r_j$. The formula for $\hat{y}$ does not seem to lend itself to recursive computation. For the special case in which L has constant coefficients and functions in H are defined on $(-\infty, \infty)$, Kimeldorf and Wahba [6] developed a correspondence between L-splines and least-squares estimates of zero-mean, stationary, autoregressive random processes with spectral densities $(2\pi)^{-1}|P(\omega)|^{-2}$ where $P(\omega) = \sum_{j=0}^{m} a_j(i\omega)^j$ and $L = \sum_{j=0}^{m} a_j D^j$.

Two equivalent detection problems. The information preserving property of splines will now be illustrated by showing the equivalence of two signal detection problems. First let $H(\mathbf{R})$ be the reproducing kernel Hilbert space determined by $\mathbf{R}$. The elements of $H(\mathbf{R})$ are n-vectors and the inner product is given by

$$\langle \mathbf{r}_1, \mathbf{r}_2 \rangle_{H(\mathbf{R})} = \mathbf{r}_1'\mathbf{R}^{-1}\mathbf{r}_2 .$$

It can be shown [12] that $\mathscr{S}$ and $H(\mathbf{R})$ are congruent, and that under this congruence, $s \in \mathscr{S}$ corresponds to $\mathbf{r} \in H(\mathbf{R})$. Therefore,

$$\|s\|^2 = \|\mathbf{r}\|^2_{H(\mathbf{R})} . \tag{8}$$

Now consider the two detection problems:

$$H_1: \chi(t) = s(t) + w(t) , \qquad H_0: \chi(t) = w(t) , \qquad t \in I$$
$$H_1': \boldsymbol{\chi} = \mathbf{r} + \mathbf{w} , \qquad H_0': \boldsymbol{\chi} = \mathbf{w}$$

where $w(\cdot)$ is a zero-mean Gaussian random process with covariance K given by (3), $\mathbf{w}$ is a n-vector of zero-mean Gausian random variables with covariance matrix $\mathbf{R}$, and $s(\cdot)$ is the spline that interpolates $\{r_j\}_1^n$ with respect to $\{\lambda_j\}_1^n$. Equation (8) shows that the two detection problems have the same detectability [5] and therefore the same probability of error. In other words, s and $\{r_j\}_1^n$ $(= \{\lambda_j s\}_1^n)$ contain the same information.

5. Smoothing with Lg-splines. In the spline interpolation problem (5) we are essentially assuming that the data $\{r_j\}_1^n$ are perfect. If the data contain errors, it makes sense to consider a spline smoothing problem. The usual formulation of the smoothing problem is

$$\min_{f \in H} \{\textstyle\int_I (Lf)^2 + \boldsymbol{\xi}'\mathbf{Q}^{-1}\boldsymbol{\xi}\} \tag{9}$$

where $\boldsymbol{\xi} = \operatorname{col}(\xi_1, \cdots, \xi_n)$, $\xi_j = r_j - \lambda_j f$, and $\mathbf{Q}$ is a symmetric, positive-definite weighting matrix with jth column $\mathbf{q}_j$. However, it does not seem that (9) can be solved recursively. Therefore, the following modified smoothing problem will be considered:

$$\min_{f \in H} \{\|f\|^2 + \boldsymbol{\xi}'\mathbf{Q}^{-1}\boldsymbol{\xi}\} . \tag{10}$$

Let $H(\mathbf{Q})$ be the reproducing kernel Hilbert space determined by $\mathbf{Q}$, and let $H^+ = H \oplus H(\mathbf{Q})$, $f^+ = f + \boldsymbol{\xi}$, $h_j^+ = h_j + \mathbf{q}_j$. Then $||f^+||_{H^+}^2 = ||f||^2 + \boldsymbol{\xi}'\mathbf{Q}^{-1}\boldsymbol{\xi}$ and $\langle f^+, h_j^+\rangle_{H^+} = r_j$. Thus the smoothing problem (10) can be solved by considering

$$(11) \qquad \min_{f^+ \in U(\mathbf{r})^+} ||f^+||_{H^+}^2 , \qquad U(\mathbf{r})^+ = \{f^+ \in H^+ : \langle f^+, h_j^+\rangle_{H^+} = r_j,\ 1 \leqq j \leqq n\} .$$

This augmented interpolation problem is in the same form as (5) and can be solved recursively as in Section 3, If $\tilde{s}^+$ is the solution to (11), then the solution $\tilde{s}$ to (10) is just the component of $\tilde{s}^+$ in H; namely,

$$(12) \qquad \tilde{s}(t) = \mathbf{h}'(t)(\mathbf{R} + \mathbf{Q})^{-1}\mathbf{r} .$$

As pointed out by a referee, (12) can also be obtained by first showing that $s \in \mathscr{S}$ and then writing $\tilde{s} = \mathbf{h}'\mathbf{R}^{-1}\tilde{\mathbf{r}}$ and $||\tilde{s}||^2 = \tilde{\mathbf{r}}'\mathbf{R}^{-1}\tilde{\mathbf{r}}$. Then (10) becomes an n-dimensional optimization problem and can be solved in the usual way to obtain $\tilde{\mathbf{r}} = \mathbf{R}(\mathbf{R} + \mathbf{Q})^{-1}\mathbf{r}$.

The smoothing problem (10) has a stochastic interpretation in terms of a signal-plus-noise least-squares estimation problem in which the noise has covariance $\mathbf{Q}$.

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