Splines in Statistics

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Splines in Statistics

ABSTRACT. Spline functions are particularly appropriate in fitting a smooth non-parametric model to noisy data. The use of spline functions in non-parametric density estimation and spectral estimation is surveyed. The requisite spline theory background is also developed.

Key Words and Phrases. Spline, Cubic Spline, Interpolating Spline, Smoothing Spline, Density Estimation, Spectral Density Estimation

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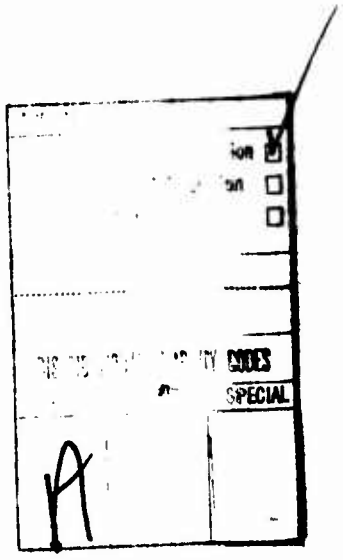

Splines in Statistics

§1 General Introduction

Statistics (as we know it) began with fitting parametric models to data. Various principles for making estimates and inferences were developed and refined until their efficiencies reached their (asymptotic) limits with methods such as maximum likelihood, minimum variance, and likelihood ratio. Attention returned to the basic models and there appeared a growing realization that not all of the parametric structure was needed to make inferences. From this idea arose the techniques variously known as distribution free or non-parametric. At the cost of some loss of efficiency in certain instances, these methods prevented model violations from being reflected in false inferences. Although non-parametric methods have had some remarkable success (for example, the theory of rank tests) they all too often ignore useful non-statistical information that may be present, and as a result lose efficiency.

The classical method of incorporating non-statistical information is by means of the Bayesian framework. In the absence of any canonical methods of determining and assessing priors, this has to be regarded with suspicion. Happily, there are at least three ways to incorporate validly non-statistical knowledge in inference procedures. We discuss each in turn.

The first occurs when it is realized that the predominantly normal data contains a certain amount of contamination, i.e. the normal model is roughly correct. This knowledge may come from central limit type considerations. The robustness methods of Huber (1964) and Hampel (1974) exploit this knowledge.

If a system is known to have an order structure, this knowledge may be exploited by methods known as isotonic inference. The book by Barlow, et al (1972) reviews most of these techniques. Knowledge of order often follows from elementary consideration of the structure of the system being modelled.

The third sort of non-statistical knowledge we can use is knowledge of smoothness. The least action principle of dynamics suggests that nature makes things change as smoothly as possible. Our main concern in this article will be with a certain measure of smoothness and the consequences of making the underlying function as smooth as possible. A function which optimizes a smoothness criterion is a spline. Perhaps a little ironically spline methods also provide a sound route for Bayesians to re-enter the scene, as Kimeldorf and Wahba (1970 and 1971) show there often exist a Bayesian model which gives a smoothing spline as the posterior mean in that model, given the data. Models which require an order structure as well as smoothness lead us to consider isotonic splines. Some original results in this area are presented in Wright (1977).

The present account is organized as follows: We begin from first principles and develop those parts of spline theory which have proved most relevant to the recent applications in statistics. We then review the literature associated with the main applications of splines to statistical problems, ending with some general remarks on isotonic splines.

We shall reserve the symbol D for the differentiation operator and the symbol L_2 for the set of measurable square integrable functions on the interval [0,1]. The symbol W_m will denote the set of functions f on [0,1] for which $D^j f$ is absolutely continuous for $j = 0,1,\ldots,m-1$ and $D^m f$ is in L_2. When we occasionally consider functions with domain other than [0,1] the relevant domain will be shown after the function space symbol above, e.g. $W_m(-\infty,\infty)$.

§2 Classical Spline Theory

The spline is the engineer's solution to a problem frequently concerning engineers. The problem is to fit a curve through points (t_i,y_i) $i = 1,2,\ldots,n$

in the plane. However, the engineer often needs to obtain values of the first and second derivatives of the underlying function from this fitted curve. The spline, an optimal solution of this problem, uses the analogy with weightless beams, part of the engineer's stock in trade. A precise account of the engineer's spline follows.

Let $\{(t_i,y_i): i = 1,\ldots,n\}$ be the (error-free) points in the plane for which we seek an interpolant. Call $\Delta = \{\xi_1 (= t_1) < \xi_2 < \xi_3 < \ldots < \xi_N (= t_n)\}$ a *mesh*. For computational considerations the mesh will normally just be the numbers $\{t_i: i = 1,\ldots,n\}$.

A (cubic) spline with mesh Δ, written $S_\Delta(t)$, is a function with continuous derivatives up to (and including) order 2 which coincides exactly with a (possibly different) cubic function on each interval $[\xi_i,\xi_{i+1}]$ $i = 1,\ldots,N-1$. The points $\{\xi_i: i = 2,\ldots,N-1\}$ are called the *knots* of the spline. A spline $S_\Delta(t)$ which in addition satisfies $S_\Delta(t_i) = y_i$, $i = 1,2,\ldots,n$ is an interpolant for the data. Some further restriction is needed in order to make this interpolant unique on $[t_1,t_n]$. Although for certain applications, other end conditions are more convenient, the most natural condition is $S''_\Delta(t_1) = S''_\Delta(t_n) = 0$. This corresponds to giving the analogous beam cantilevered ends (protruding beyond the end points) and also minimizes the "energy of flexion" of the beam (i.e. the mean square curvature). The proofs of these various properties are established in a more general context by various contributors to the theory of L-splines. See Ahlberg, Nilson and Walsh (1967). Notice that if the spline between (t_i,y_i) and (t_{i+1},y_{i+1}) has equation $y = a_i t^3 + b_i t^2 + c_i t + d_i$, the continuity of the lower derivatives ensures that b_i, c_i, d_i are constants, independent of i.

Since curve fitting is a very practical task, it is against numerical considerations that a curve fitting method must be judged. The ease with which a cubic spline is fitted must have contributed to its popularity.

We now sketch the main steps in fitting a cubic spline to data. Suppose data is $\{(t_i,y_i),\ i = 1,2,\ldots,n\}$. Let $h_i = t_{i+1} - t_i$ and take M_i = value of second derivative of interpolating spline S_Δ at t_i, $i = 1,2,\ldots,n$.

Suppose the polynomial interpolating (t_i,y_i) and (t_{i+1},y_{i+1}) is

$$y = a_i(t-t_i)^3 + b_i(t-t_i)^2 + c_i(t-t_i) + d_i \tag{2.1}$$

then

$$\begin{cases} b_i = M_i/2 \\ a_i = (M_{i+1} - M_i)/6h_i \\ c_i = \dfrac{y_{i+1} - y_i}{h_i} - \dfrac{2(h_iM_i + h_iM_{i+1})}{6} \\ d_i = y_i \end{cases} \tag{2.2}$$

Thus our curve fitting problem reduces to that of finding the values of M_i. The equations relating the M_i are obtained by using the continuity of the first derivative of the spline, along with the relations 2.2 to give

$$h_{i-1}\,M_{i=1} + (2h_{i-1} + 2h_i)M_i + h_iM_{i+1} = 6\left(\frac{y_{i+1}-y_i}{h_i} - \frac{y_i-y_{i-1}}{h_{i-1}}\right)$$

$$\text{for } i = 2,3,\ldots,n-1.$$

Our demand that $M_1 = M_n = 0$ leads immediately to a tridiagonal system of linear equations for $M_2,\ldots,M_{n-1}$. This system can be easily solved by Gaussian elimination. So eaily in fact, that fitting an interpolating spline to 40 points is feasible with only a simple calculator.

It was soon realized that the cubic spline was the solution of an optimizing problem which could be easily generalized. Let L be a differential operator with constant coefficients of order m (usually D^m) and let $\{(t_i,y_i)\colon i = 1,\ldots,n\}$ be data points. The problem

$$\begin{array}{lll} \text{minimize} & \int_{-\infty}^{\infty} (Lf)^2 dt & \\ \text{subject to} & f^{(j)} \in L_2(-\infty,\infty) & j = 0,1,\ldots,m \\ \text{and} & f(t_i) = y_i & i = 1,\ldots,n \end{array}$$

has a solution f(t) which satisfies $L^*Lf(t) = 0$ in the intervals between knot points, where L^* is the adjoint operator to L. We call such a solution an "*Interpolating L-Spline*". There are accounts of such splines in the books by Ahlberg, Nilson and Walsh (1967) and T. N. E. Greville (1969). However, for statistical purposes another type of spline turns out to be more useful.

§3 Smoothing Spline Theory

For most applications in statistics the smoothing spline is much more useful than the interpolating spline. This is because most real-life data is subject to error be it from sampling, measurement or other sources. There are two main spline fitting methods in common use corresponding to different ways of dealing with the "noise" in the data. Because this data does not constrain the fitted function nearly as firmly as in the interpolating spline case, the fitting requires a genuine optimization routine, not just the simple solution of a linear system of equations as with the cubic interpolating spline.

The first, more frequently used method, parallels the least squares curve fitting procedure by minimizing a criterion depending on squares of deviations from data points and on the "roughness" of the fitted curve. When we have little or no knowledge of the magnitude of possible errors in our data this method is the appropriate one to use.

On the other hand when the data points are, for example, direct readings from a calibrated instrument, we may be able to set fairly narrow 100% confidence limits for each data point. The second method is used in these circumstances. For this we need to replace the ordinate y in the two dimensional data with a 100% confidence interval, and constrain the fitted spline function to pass through all of these intervals. This is accomplished in practice by using an optimization routine to minimize the (convex) roughness criterion, subject to the linear constraints. It will be noticed that this method attaches considerable importance to outliers, rather than largely ignoring them.

First Method of Fitting Smoothing Splines

Suppose the t values of the data lie in a finite interval say [0,1] and we have $0 < t_1 < t_2 < \ldots < t_n < 1$. Fitting the spline leads us to solving the following problem.

$$\text{Minimize} \quad \sum_{i=1}^{n} (f(t_i)-y_i)^2 + \lambda \int_0^1 (f^{(m)})^2 \, dt$$

3.1

$$\text{Subject to } f \in W_m, \ \lambda \text{ fixed} > 0.$$

The solution is given explicitly in the paper of Kimeldorf and Wahba (1970) and as expected turns out to be a polynomial spline of degree 2m-1 with possible knots at the data points. As so often happens, this theoretical solution

cannot be used as an algorithm in any realistic practical case. When the t values are evenly spaced throughout [0,1], and f is periodic, Cogburn and Davis (1974) show how to do the fitting more easily. Apart from this one happy instance, a heavy ortimization is invariably required.

Notice that the number $\lambda > 0$ in 3.1 controls the amount of smoothing; λ too small results in overfitting and insufficient removal of noise, whereas λ too large results in underfitting and removal of much of the wanted signal with the noise. Clearly the correct choice of λ is of the greatest importance. A satisfactory solution to this problem is given by Wahba and Wold (1975), although not all theoretical consequences are yet developed.

Second Method of Fitting Smoothing Splines

From what was written in the preamble of this section, the reader will have seen that this spline is a cross between the interpolating spline and our first smoothing spline. For this reason the fitting technique is also known as (the solution procedure for) the Generalized Hermite-Birkhoff Interpolation Problem- (GHB problem).

Let $[\alpha_i, \beta_i]$ be the 100% confidence interval for the ordinate at t_i (with $\alpha_i < \beta_i$). The GHB problem is

$$\text{Minimize} \qquad \int_0^1 (f^{(m)})^2 \, dt$$

3.2 $$\text{subject to the constraints} \quad f \in W_m, \ \alpha_i \leq f(t_i) \leq \beta_i$$

$$\text{for } i = 1,2,\ldots,n.$$

Various recent contributions to the theory of such splines have been made by M. Attéia (1968), P. J. Laurent (1969), and K. Ritter (1969). Because Hilbert space methods are directly applicable, this spline has been more thoroughly theoretically analyzed than the first smoothing spline.

For the record, the solution of 3.2 is a spline of degree 2m-1 with knots at those data points where the constraints are active..

§4 Some Simplifications

For most practical applications a slightly sub-optimum solution may be preferable to the optimum if it involves a great deal less computation effort. We have already seen that not all of the data points are knot points for the smoothing spline. By using the following guidelines the old statistical virtue of eyeballing the data can be converted to considerable computational advantage.

Knot Point Selection (Cubic smoothing spline).

1) Knot points should be at data points.

2) Try to have at least 4 or 5 data points between knots.

3) Have not more than one extremum and one inflexion point between knots.

4) Have extrema centered in intervals and inflexion point near knots.

For more details see Wold (1974).

The form of the optimal spline function f.

Suppose data points $\{t_{i_1}, t_{i_2}, \ldots, t_{i_J}\}$ have been chosen as knots. Then the optimal spline function will be f such that $f(t) = a_0 + a_1 t + a_2 t^2 + \sum_{j=1}^{J} d_j (t - t_{i_j})_+^3$

where $(t - c)_+^3 = 0$ $t < c$

$= (t - c)^3$ $t \geq c$.

§5 Bayesian Estimation Again

We are now in a position to make our remarks about the equivalence of smoothness and Bayesian posterior means precise.

Let $L = \sum_{j=0}^{m} a_j D^j$ be a differential operator and let $B = [b_{jk}]$ be a positive definite matrix. Suppose $B^{-1} = [b^{jk}]$.

Problem I

Find $f \in W_m(-\infty,\infty)$ which minimizes

$$\sum_{j,k} (f(t_j) - y_j) b^{jk} (f(t_k) - y_k) + \int_{-\infty}^{\infty} (Lf)^2 \, dt$$

Problem II

Find $f(t)$ with $f(t) = E(x(t) | y(t_1), y(t_2), \ldots, y(t_n))$ where $y_j = x(t_j) + e_j$ with $e_j \sim N(0,B)$ and $x(t)$ is a stationary Gaussian process with mean zero and spectral density $f(\lambda) = \frac{1}{2\pi} \frac{1}{|P(\lambda)|^2}$ where $P(\lambda) = \sum_{j=0}^{m} a_j (i\lambda)^j$.

In their paper of 1970, Kimeldorf and Wahba show that the solution f of Problems I and II is the same function.

When the errors in our observations are independent, this theorem tells us nothing new about fitting the spline. However, if we are forced to effect an estimation from a non-independent sample where the errors have known auto-correlation, this result provides the solution. Since this question is peripheral to the main objective of our account we now let the matter rest.

§6 Some General Remarks

(a) A little reflection will convince the reader that smoothing spline methods will be the most useful when

(i) An appropriate parametric model is not known and

(ii) High accuracy is needed and

(iii) A considerable amount of (noisy) data is available.

When these conditions are satisfied, spline methods will give very good value for the computational effort invested.

(b) The (smoothing) spline is very much the child of its age - the 1960's - depending as it does on optimization theory and the medium/large computer for its implementation.

§7 Introduction to the Literature

In the introduction we tried to place spline methods in the statistical scheme of things. Splines will be seen to be a departure from the most general non-parametric model back a little towards the (structure rich) parametric situation. The reward for the changed position is improved efficiency coupled still with non-parametric integrity.

Although spline functions were available in a highly refined form by the mid 1960's they were for some years largely ignored by statisticians. This situation was dramatically changed by the appearance of the paper by Kimeldorf and Wahba (1970). Although the authors' intention was to show the equivalence of smoothing by splines with the finding of a posterior mean, the real effect was to convince statisticians that splines were effective and not as difficult as they had thought.

When all is said and done, spline methods are just a way of fitting a smooth curve to some data. The curve estimates most studied in the statistical spline literature are for non-parametric density estimation from an independent, identically distributed sample and for the estimation of the spectral density of a stationary time series. Splines have also been used in other areas, but are at present more a curiosity than a serious practical tool.

§8 Non-Parametric Density Estimation

Our account will be confined exclusively to density estimation based on an independent identically distributed sample. There are two main routes we may follow: we may use the empirical distribution function in some way or we may use an appropriate analogue of maximum likelihood adapted to the infinite dimensional (non-parametric) situation.

The empirical density is very easily obtained from the empirical distribution when we use the Sobolev spaces W_m because of the following:

Lemma: The solution f of the problem

$$(A)\quad \text{Minimize } \int_0^1 (f^{(m)})^2\,dt \text{ with } f \in W_m \text{ and } f(t_i) = y_i,\ i = 1,\ldots,n$$

and the solution g of the problem

$$(B)\quad \text{Minimize } \int_0^1 (g^{(m-1)})^2\,dt \text{ with } g \in W_{m-1} \text{ and } (D^{-1}g)(t_i) = y_i,\ i = 1,\ldots,n$$

are related by $Df = g$. This means the empirical spline fitted density is obtained by differentiating the spline fitted distribution function.

The histosplines described by Boneva, Kendall, and Stefanov (1971) are empirical densities, in the nature of a smooth analogue of a histogram, with pleasant mathematical features. To make their analysis feasible, the authors are prepared to allow densities which sometimes take small negative values in a small region.

Let $W_1(-\infty,\infty)$ denote the set of functions on the real line which are, along with their first derivatives, in $L_2(-\infty,\infty)$. Let ℓ_2 denote the set of square summable (double ended) real sequences with inner product $(h,k) = \sum_{i=-\infty}^{\infty} h_i k_i$. Define $\theta: W_1 \to \ell_2$ by $(\theta u)_j = \int_j^{j+1} u(t)dt$. Now define an inner product $[u,v]$ on W_1 by $[u,v] = (\theta u, \theta v)_{\ell_2} + \int_{-\infty}^{\infty} u'v'\,dt$. Write $Z = \{u \in W_1: \theta u = 0\}$ and $S = \{s \in W_1: [s,u] = 0 \text{ for all } u \in Z\}$. Each $\sigma \in W_1$ has unique decomposition $\sigma = s + z$, $s \in S$, $z \in Z$. Thus we obtain the projection $P: W_1 \to S$ where $P\sigma = s$. Then the authors show

1) θ is a 1-1 bicontinuous map $S \to \ell_2$
2) S consists of all $s \in W_1$: $\int_{-\infty}^{\infty} s'z'dt = 0$ for all $z \in Z$
3) For given $h \in \ell_2$, $\theta^{-1}h$ is the unique solution of $\theta\sigma = h$ which minimizes $\int_{-\infty}^{\infty} (\sigma')^2 dt$
4) S consists of those functions continuous and continuously differentiable such that
   i) $s(t)$ is quadratic in each cell
   ii) $\int (s^2 + s'^2)dt < \infty$.

The delta-spline is that function $s_0 \in S$ which has $(\theta s_0)_0 = 1$, $(\theta s_0)_i = 0$, $i \neq 0$. This function is tabulated explicitly in the paper. The maneuvering with Z and the unusual choice of the inner product [ ] is rewarded with the following result.

Proposition: Take $h \in \ell_2$, $h = (h_j)$. For any integer j, let s_j be the translated delta-spline with $(\theta s_j)_j = 1$, $(\theta s_j)_i = 0$, $i \neq j$. Then the unique histospline $\sigma \in W_1$ which has $\theta\sigma = h$ and which minimizes $\int (\sigma')^2 dt$ is given by $\sigma = \sum_{j=-\infty}^{\infty} s_j$. The paper of Boneva, Kendall and Stefanov (1971) also describes another histospline and includes much empirical material on histospline behavior.

Some Remarks on Histosplines

1. Once the tabulated form of the delta-spline is stored in the computer (requiring 39 parameters) there is no explicit optimization required - just the grouping of the data into classes. Consequently this method is well suited to programmable calculators and mini-computers without optimization routines.

2. Boneva, Kendall and Stefanov (1971) and Schoenberg (1972a and b) also consider the variant histospline defined as the derivative of that function G in $W_2[0,1]$ which solves:

$$\text{Minimize } \int_0^1 (G'')^2 dt$$

8.1 $$\text{Subject to } G(0) = 0 \text{ and } G(ih) = \sum_{i=0}^{i-1} h_j \quad i = 1,2,\ldots,\ell$$

$$\text{where } (\ell+1)h = 1 \text{ and } G'(0) = G'(1) = 0 .$$

Yet another variant of this problem is considered by Wahba (1975b). This involves replacing the final constraints in 8.1 by

$$G'(0) = \hat{a}_1 \text{ and } G'(1) = \hat{b}_1 \text{ where } \hat{a}_1, \hat{b}_1$$

are calculated from the empirical distribution function. This variant gives better accuracy near 0 and 1 than 8.1. When the criterion is minimum mean square error at a point, Wahba (1975b) also shows how to choose h optimally.

Finally we note that if the problem 8.1 has the further constraint $G'(t) \geq 0$ for all $t \in [0,1]$ the solution will be isotonic with respect to a natural order on W_2 and will give a more acceptable density function.

3. It must be emphasized that histosplines are interpolating splines based on the sample histogram, and not a smoothing spline. Consequently in the presence of noise (sampling error) we cannot expect this method to be much better at filtering the noise than the histogram it is derived from.

This assertion is supported by the results of Wahba (1975b) who shows for her variant of the histospline that for the true density $f \in W_m$ and f_n the histospline corresponding to a sample of size n

$$E(f_n(t) - f(t))^2 = 0 \quad (n^{-(2m-1)/2m}).$$

In a companion paper Wahba (1975a) shows that the expected mean square error at a point t has that same order of magnitude for all of the following estimation methods: the polynomial algorithm (Wahba), kernel type estimator (Parzen), certain orthogonal series estimates (Kronmal-Tatar), and the ordinary histogram. However, the constants covered by the 0 may be larger in these latter cases.

§9 Densities by Maximum Penalized Likelihood

This area is realtively unexplored to date. The analogy with parametric maximum likelihood estimation gives rise to the hope that Maximum Penalized Likelihood Estimators (MPLEs) may be optimal in some fundamental sense. We now look at some of the details.

Let Ω be an interval (a,b) and let $H(\Omega)$ be a manifold in $L_1(\Omega)$. (Manifold = Set of "reasonably similar" functions). Suppose $(t_1, t_2, \ldots, t_n)$ is a i.i.d. sample from an unknown density $f \in L_1(\Omega)$. Unfortunately the problem

$$9.1 \qquad \begin{aligned} &\text{Maximize } L(v) = \prod_{i=1}^{n} v(t_i) \text{ subject to } v \in H(\Omega), \\ &\int_\Omega v(t)dt = 1, \; v(t) \geq 0 \quad \forall t \in \Omega \end{aligned}$$

will not have a solution for most manifolds of interest (the unimodal or monotone functions are an exception). Specifically, any manifold which contains an approximating sequence to any linear combination of δ-functions, admits no maximum likelihood estimator for the density f.

From heuristic Bayesian considerations, Good and Gaskins (1971) suggested adding a penalty term to the likelihood which would penalize unsmooth estimates. They chose a manifold and penalty function that lead inevitably to polynomial splines. Good's and Gaskin's results were refined and made rigorous by de Montricher, Tapia and Thompson (1975). We can now describe the current state of the art.

It will normally be the case that the manifold $H(\Omega)$ is contained in $W_m(\Omega)$ and the penalty function $\Phi(v) = \int_\Omega (D^m v)^2 dt$. Let

$$\hat{L}(v) = \prod_{i=1}^{n} v(t_i) \exp(-\Phi(v))$$

and consider the optimization problem

9.2

$$\text{Maximize } \hat{L}(v) \text{ subject to}$$

$$\text{(i)} \quad v \in H(\Omega)$$

$$\text{(ii)} \quad \int_\Omega v \, dt = 1$$

$$\text{(iii)} \quad v(t) \geq 0, \quad \forall t \in \Omega$$

The solution v is the MPLE of the underlying density, f.

The task of computing the MPL Estimate of the density is greatly simplified by knowing the form the optimum must take. The following existence theorem is proved in the paper by de Montricher, Tapia and Thompson (1975).

Theorem: For $m \geq 1$, the MPLE corresponding to W_m exists, is unique, and is a polynomial spline of degree 2m-1. Moreover, if the estimate is positive in the interior of an interval, then in this interval it is of degree 2m-1 and of continuity class 2m-2 with knots at the sample points.

From (Fisher) information-theoretic considerations, as well as a desire to avoid the awkward non-negativity constraint $v(t) \geq 0$, Good and Gaskins (1971) also considered the MPLE problem with manifold

9.3
$$H_1(\Omega) = \{v: v^{\frac{1}{2}} \in W_1\ (-\infty,\infty)\} \quad \text{and}$$
$$\Phi_1(v) = \alpha \int_{-\infty}^{\infty} \frac{(v')^2}{v}\, dt = 4\alpha \int_{-\infty}^{\infty} (Dv^{\frac{1}{2}})^2\, dt \quad \alpha > 0$$

where $v = (v^{\frac{1}{2}})^2$ is to be the (necessarily positive) density.

After noting that the reformulation trick (9.3) is standard in the literature, deMontricher, Tapia and Thompson (1975) record conditions for its valid use with the following lemma.

Lemma: Let H be a subset of $L_2(\Omega)$ and J a functional on H. Consider

Problem I
$$\text{Maximize } J(v^{\frac{1}{2}}) \text{ subject to}$$
$$v^{\frac{1}{2}} \in H,\ \int v\, dt = 1,\ v(t) \geq 0 \quad \forall t$$

and Problem II
$$\text{Maximize } J(u) \text{ subject to } u \in H$$
$$\text{and } \int u^2 dt = 1$$

Let u^* be a solution of II. Then $v^* = (u^*)^2$ solves I if and only if $|u^*| \in H$ and $J(u^*) = J(|u^*|)$.

The authors (deMontricher, Tapia and Thompson) go on to establish that the price of using the non-negativity trick is to lose the polynomial spline form of solution - the solution is an exponential spline instead, with knots at the sample points.

The paper of Good and Gaskins (1971) shows how one might prove that MPLEs are weakly consistent and also gives algorithms and some empirical material.

We regretfully record that on the two most important aspects - how effectively noise is filtered out, and the asymptotic (large n) performance - the literature on MPLEs is quite silent.

§10 Noise Filtering by Smoothing Splines

Statisticians and applied mathematicians are continually faced with the problem of recovering a smooth function when only noisy measurements of it are available. In fitting a parametric model the residuals are made up of the noise as well as the deviations of the model from the true function. Smoothing splines are admirably placed to estimate this true function (known only to be smooth) for two reasons. First, they are flexible enough to respond to any real local variation, without allowing pathological behavior, and second, the actual degree of smoothing (= filtering of noise together with rapid variation) is controllable. Even when the correct degree of smoothing is unknown, these features, in conjunction with a technique called cross-validation (to determine the correct degree of smoothing) allow us to remove most of the model deviation component from the residuals, leaving virtually only the (real) noise. We presently give an account of the main features of fitting smoothing spline functions by cross validation - full details are given by Wahba and Wold (1975a and b).

The model we are fitting is

$$Y(t) = f(t) + e(t) \quad t \in [0,1] \text{ where}$$

10.1 $$f \in W_m \text{ and } Ee(t) = 0 \text{ all } t \text{ and}$$

$$Ee(s)e(t) = \sigma^2 \quad s = t$$
$$= 0 \quad s \neq t$$

The noise variance σ^2 is generally unknown and Y(t) is observed at (an increasing set of points) $t_1, t_2, \ldots, t_n$.

Consider the problem: Find $f \in W_m$ to

$$\text{Minimize } \left(\frac{1}{n} \Sigma(Y(t_j) - f(t_j))^2 + \lambda \int_0^1 (f^{(m)})^2 dt\right) \qquad 10.2$$

where $\lambda > 0$ is a fixed real number.

The first term is a measure of the fidelity to the data, the second is λ times the "smoothness" of f. The optimum solution is known (Greville (1969), Reinsch (1967)) to be a cubic spline with knots at the t_i, $i = 1,2,\ldots,n$. As $\lambda \to \infty$, the solution $f_{n,\lambda}$ approaches its smoothest possible form - the least squares straight line through the data. As $\lambda \to 0$, $f_{n,\lambda}$ approaches the interpolating spline through all of the data points. Thus we call λ *the degree of smoothing*. It is shown in Wahba (1973 and 1974) that in order to have $f_{n,\lambda} \overset{W_m}{\to} f$ as $n \to \infty$ we must also have $\lambda \to 0$.

If (from previous experience of our particular problem) the correct value of λ is known, we have only to solve 10.2 using that λ. Unless the problem 10.1 can be converted to the periodic smoothing spline form of Cogburn and Davis (1974) there is no simple way of solving 10.2 other than the usual optimization routine.

When λ is not known we can (with much labor) use the Cross Validation Mean Square Error (minimizing) technique to estimate the appropriate degree of smoothing *from the data alone*. The method has been used successfully in various applications by Feinberg and Holland (1972), Hocking (1972), Mosteller and Wallace (1963) and others. In effect the CVMSE method gives the value of parameter which maximizes the internal consistency of the data set with regard to the applied model.

Wahba and Wold find it useful to recast problem 10.2 into a form used by Reinsch (1967).

10.3 Find $f \in W_2$ to minimize $\int_0^1 (f'')^2 dt$ subject to $\frac{1}{n} \sum_{j=1}^{n} (Y(t_j) - f(t_j))^2 \leq S$, where S is given.

It is well known that if

$$n S \leq \inf_{a,b} \sum (Y(t_j) - a + b\, t_j)^2$$

then there exists a unique $\lambda = \lambda(S)$ such that $f_{n,\lambda}$ is the solution to 10.2 and

$$\frac{1}{n} \sum (Y(t_j) - f_{n,\lambda}(t_j))^2 = S.$$

Armed with the appropriate tools from the last paragraph, we now give an account of Wahba and Wold's Cross Validation procedure (1975a).

1) Divide the data set into p groups

Group 1: $t_1, t_{1+p}, t_{1+2p}, \cdots$

Group 2: $t_2, t_{2+p}, t_{2+2p}, \cdots$

...

Group p: $t_p, t_{2p}, t_{3p}, \cdots$

2) Guess a starting value for S (Amost invariably $S = k\sigma^2$ with $0.7 \leq k \leq 1$. A reasonable starting point might be $k = 0.8$).

3) Delete the first group of data. Fit a smoothing spline to the rest of the data using the method of Reinsch with the S of step 2. Compute the sum of squared deviations of this smoothing spline from the deleted data points.

4) Delete instead the second group of data. Fit a smoothing spline with the S of step 2. Compute the sum of squared deviations of the spline from the data points.

5) Repeat Step 4 for the 3rd, 4th, ..., p^{th} group of data.

6) Add the sums of squared deviation from steps 3-5, and divide by n. This is the CVMSE for S and is written CV(S).

7) Determine the $S = S_1$ making CV(S) a minimum.

The smoothing problem 10.3 can now be solved with $S = S_1$.

Empirical studies by Wahba and Wold (1975a) indicate that when σ^2 is extremely small, the CVMSE estimate for k in $S = k\sigma^2$ has positive bias, resulting in very slight undersmoothing. This effect is negligible for realistic sized σ^2, although the authors do not present a proof.

§11 Periodic Smoothing Splines

The work of Cogburn and Davis (1974) has been referred to several times already. We now describe their results in detail.

Let G be the group of real numbers modulo 2Π with the usual topology and measure. The model to be fitted is

$$
\begin{aligned}
& h(t) = f(t) + e(t) \qquad \forall t \in G \\
11.1 \qquad & \text{with } f \in W_m(G) \text{ and } Ee(t) = 0, \quad \forall t \in G \\
& \text{and } Ee(s)\,e(t) = \sigma^2 \quad s = t \\
& \qquad\qquad\qquad\quad = 0 \quad s \neq t
\end{aligned}
$$

where h is observed either on a lattice of points or continuously and the noise variance σ^2 is unknown. The asymptotic solution for large n devised by Cogburn and Davis is very convenient to handle, and easy to compute since it avoids explicit optimization.

§12 Estimating Spectral Densities

Determining spectral densities gives spline theory not only a great opportunity but also a severe test. When the spectrum is absolutely continuous, spline methods are extremely effective. However, when the spectrum has a discrete component, i.e. δ-function spikes, spline methods based on L_2 have little chance of sharply resolving the spike without a great deal of data in the vicinity of the spike. The heart of the difficulty is that every sequence of functions approximating a δ-function must be unbounded in L_2 norm and so also in W_m norm, and thus the smoothing spline is duty bound to flatten these real spikes out. However, before abandoning the L_2 based W_m spaces, we need to see the problem in perspective. Because of the superficial similarity between a δ-spike and a noisy observation, any attempt to transfer the problem to a space where δ-function approximants are bounded seems doomed to failure because we would be unable to filter out the noise in such a space.

Thus reconciled to remaining in W_m with its pleasant inner product and Fourier Transform structure we may yet be able to find a way out. One strategy may be to proceed as follows. Since further data points are easily obtained from the periodogram, it might be feasible to use repeated applications of the CVMSE method coupled with a procedure to introduce extra data points in regions where the rate of change (of fitted function) is large.

First let us examine the current state of the art for estimating spectral densities with spline methods.

Estimating the Spectral Density of a Stationary Stochastic Process

Let $X_1, X_2, X_3, \ldots$ be a second order stationary stochastic process with $EX_k = 0$, $EX_jX_{j+k} = \rho_k$.

The ρ_k are Fourier coefficients of a symmetric distribution function F on $[-\Pi,\Pi]$, $\rho_k = \frac{1}{\Pi} \int_0^{\Pi} \text{Cos kw d } F(w)$. When F is absolutely continuous, it is completely determined by the spectral density

$$f(s) = (DF)(w)$$

$$f(w) = \sum_{-\infty}^{\infty} \rho_k \, e^{ikw} .$$

The statistical problem is to estimate f(w) on the basis of observations $X_1, X_2, \ldots, X_n$. Let $\hat{f}(w)$ denote the periodogram

12.1
$$\hat{f}(w) = \sum_{-n+1}^{n-1} \hat{\rho}_k \, e^{ikw} = \hat{\rho}_o + \sum_{k=1}^{n-1} \hat{\rho}_k \text{ Cos kw where}$$

$$\hat{\rho}_k = \frac{1}{n} \sum_{j=1}^{n-k} X_j X_{j+k}, \quad k = 0,\ldots,n-1.$$

When the process is Gaussian it is shown in Walker (1965) that

12.2
$$\hat{f}(w) = f(w) \, U_{\varepsilon}(w) + \eta_n(w)$$

where $\eta_n \to 0$ in probability as $n \to \infty$ and $U_{\varepsilon}(j\Pi/n)$ are uncorrelated exponential random variables with a mean and variance of 1 for $j = 0,\ldots,\pm\, n-1$.
Since the periodogram is an inconsistent estimator of f, some modification is required. Smoothed (consistent) estimators of f(w) are obtained either by smoothing the periodogram

$$f^*(w) = \int_{-\Pi}^{\Pi} \hat{f}(\lambda) \, K(w - \lambda) \, d\lambda$$

or by weighting the covariances by a "lag window" $k_M(r)$ giving

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or by weighting the covariances by a "lag window" $k_M(r)$ giving

$$f^*(w) = \frac{1}{2\Pi} \sum_{r=-M}^{M} k_M(r) e^{-irw} \hat{\rho}_r$$

where

$$K(w) = \frac{1}{2\Pi} \sum_{-M}^{M} e^{-irw} k_M(r) .$$

Cogburn and Davis (1974) consider estimating f by a CSS or LSS to $\hat{f}$: i.e. $\hat{f} * {}^{n} S_{n,\lambda}$ or $\hat{f} * \hat{t}_{\lambda}$. They take $L = D^m$ and obtain an estimate of the integrated mean square error for n large. It is $\int_{-\Pi}^{\Pi} MSE(\hat{f}(t))dt \cong \frac{\lambda}{2n} \sigma_m^2 \int_{-\Pi}^{\Pi} f^2 dt + \frac{1}{\lambda^{4m}} \int_{-\Pi}^{\Pi} (f^{(2m)})^2 dt$. The value of λ minimizing the RHS is

$$\lambda_0 = \left(\frac{4nm}{\sigma_m^2} \int (f^{(2m)})^2 dt / \int f^2 dt \right)^{\frac{1}{4m+1}}$$

and the resulting MSE is $0(\frac{1}{n})$.

Wahba and Wold (1975b) are concerned with estimating log f(w) for spectral densities f which are bounded below. Taking the logarithm of equation 12.2 converts the curve fitting problem to that of §11.

We have

$$Y(j) = \log f\left(\frac{j\Pi}{N}\right) + \gamma + e_j, \quad j = \pm 1, \pm 2, \ldots, \pm n-1$$

with $Ee_j = 0$, $Ee_j^2 = \frac{\Pi^2}{6}$, $\gamma = 0.5772\ldots$. Euler's constant, and a reasonably symmetric distribution of e_j about 0 with constant variance. In their paper (1975b) Wahba and Wold use various results from Cogburn and Davis (1974) en route to their objective which is to show (in principle) that the smoothing parameter chosen by CVMSE converges to the parameter minimizing the mean squared error.

Wegman (1977) records the various advantages and disadvantages of using log f(w) rather than f(w) for the spline fitting model. Although the fit to log f(w) is improved, the kernel interpretation and the attendant results on consistency are lost. For multiple time series (with which Wegman was concerned) various functions such as transfer function, multiple coherence and coherency fit the spline model directly via log $f_{XX}(w)$, log $f_{XY}(w)$, etc. and each of the above functions may be estimated directly with a spline, rather than as products and quotients of spline estimates.

§13 Isotonic Splines

There are many model fitting problems where we either have some prior knowledge of the form the solution must take, or else have some insight into the laws governing the system. This knowledge may be equivalent to the requirement that the fitted function preserve some order on the data points - and obvious example is a fitted distribution function - this must satisfy $F(x) \geq F(y)$ whenever $x \geq y$. Functions which preserve (in some sense) an order relation of their requirements are called isotone. Knowledge of isotonicity may follow from very elementary considerations.

Some important isotone families of functions are the monotone functions, the convex functions, the positive functions and the unimodal functions.

The main virtues of isotonic splines are that they are locally very flexible in one direction for following the true underlying function and exceedingly stiff in the other direction so as to filter out the noise. The convex functions for example can easily bend upwards but not down. Preliminary studies suggest this filtering is spectacularly effective when the noise variance is large. A general account of isotonic splines is given in Wright (1977) and a more statistically oriented account in the paper by Wright and Wegman (1977).

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