
DEPARTMENT OF STATISTICS

University of Wisconsin
Madison, Wisconsin 53706

TECHNICAL REPORT NO. 420

August 1975

A CANONICAL FORM FOR THE PROBLEM
OF ESTIMATING SMOOTH SURFACES

by

Grace Wahba

Department of Statistics
University of Wisconsin-Madison

This work was supported by the U.S. Air Force Office of Scientific
Research under Grant AF-AFOSR-2363-B

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MOS (1970) Subject classification 41A15, 41A63, 41A65 65D10.

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ABSTRACT

We show how the problem of estimating a smooth surface on a rectangle in Euclidean p -space, which is measured discretely and with normally distributed errors, reduces to the problem of estimating the mean of a multivariate normal vector.

Two empirical Bayes type estimators are noted, and it is observed that cross-validation is useful in certain cases.

1. The Problem of Estimating a Smooth Surface

Our model is

$$y(t) = f(t) + \epsilon(t), \quad t \in T$$

where T is a rectangle in Euclidean p -space^{1/} and

$$i) \quad \epsilon(t) \sim \mathcal{N}(0, \sigma^2), \text{ i.i.d., } t \in T.$$

σ^2 may be known or unknown. $f(t)$ is either a smooth function in a given reproducing kernel Hilbert space \mathcal{H}_Q with reproducing kernel $Q(s, t)$ or a stochastic process with $Ef(t) = 0$, $Ef(s)f(t) = bQ(s, t)$, b unknown. It is instructive to compare the two situations.

$Q(s, t)$ is given by

$$Q(s, t) = \sum_{v=1}^{\infty} \lambda_v \phi_v(s) \phi_v(t)$$

where $\{\phi_v\}_{v=1}^{\infty}$ is an orthonormal set of continuous functions on $\mathcal{L}_2[T]$, $\lambda_v > 0$ and

$$\lambda_v = O(v^{-2m})$$

for some fixed $m \geq 2$.^{2/} $f \in \mathcal{H}_Q$ iff $f \in \text{span}\{\phi_v\}$ and

$$\sum_{v=1}^{\infty} f_v^2 / \lambda_v < \infty, \text{ where the generalized Fourier coefficients } f_v \text{ are}$$

given by

^{1/} T can be much more general, specifically any compact metric space on which can be defined an infinite sequence of continuous \mathcal{L}_2 -orthonormal functions.

^{2/} Our analysis can be carried out for other decay rates of λ_v , e.g., $\lambda_v = O(e^{-\alpha v})$.

$$f_v = \int_T \phi_v(s) f(s) ds . \quad (1)$$

We consider the two (distinct) cases

$$\text{ii)} \quad f \in \mathcal{H}_Q \quad \text{and} \quad \sum_{v=1}^{\infty} \frac{f_v^2}{\lambda_v^2} < \infty$$

$$\text{ii')} \quad f(t) = \sum_{v=1}^{\infty} f_v \phi_v(t) , \quad f_v \sim \mathcal{N}(0, b\lambda_v) \text{ independent.}$$

The smoothing problem is to recover an estimate $\hat{f}(t)$ of $f(t)$, $t \in T$, given observations $y(t)$, $t \in T_n$, where T_n is an n -point subset of T . The loss when \hat{f} is used is $\int_T (f(t) - \hat{f}(t))^2 dt$. In this note we demonstrate how this problem can (large n) be reduced to the problem of estimating the mean of a multivariate normal, thus the extensive literature on this latter problem (see Efron and Morris [5] and Hudson [7] and the bibliographies there) can be brought to bear on the problem. We suggest a simple estimate for the σ^2 known case which looks reasonable for both ii) and ii'). When σ^2 is unknown, we note that an estimator derived from cross validation as in Wahba and Wold [12] is good for ii). An idea of Anderson and Bloomfield [1] [2] applies to ii').

2. The Estimates

We define a one-parameter family of estimates, $f_{n,\lambda}$, $\lambda \geq 0$ for f as follows:

$$f_{n,\lambda}(t) = \sum_{v=1}^n \frac{\hat{f}_v}{(1 + \lambda/\lambda_v)} \phi_v(t), \quad t \in T$$

where

$$\hat{f}_v = \lambda_v(\phi_v(t_1), \dots, \phi_v(t_n)) Q_n^{-1} \begin{pmatrix} y(t_1) \\ \vdots \\ y(t_n) \end{pmatrix}$$

and Q_n is the $n \times n$ matrix with i, j th entry $Q(t_i, t_j)$. The $\{\hat{f}_v\}$ should be viewed as the sample generalized Fourier coefficients and the formula for \hat{f}_v as a quadrature formula for the integral

$$\int_0^1 \phi_v(s) g(s) ds$$

given $g(t_1), g(t_2), \dots, g(t_n)$.

We have

$$E\hat{f}_v \equiv f_{vn} = \lambda_v(\phi_v(t_1), \dots, \phi_v(t_n)) Q_n^{-1} \begin{pmatrix} f(t_1) \\ \vdots \\ f(t_n) \end{pmatrix} \quad v = 1, 2, \dots, n.$$

It can be shown that

$$f_{vn} = \int_0^1 \phi_v(t) (P_{T_n} f)(t) dt, \quad v = 1, 2, \dots$$

where $P_{T_n} f$ is the orthogonal projection in \mathcal{H}_Q of f onto the

subspace $V_n = \text{span}\{Q_{t_i}(\cdot)\}_{i=1}^n$, where $Q_{t_i}(\cdot) \equiv Q(t_i, \cdot)$. (For calculations of this type see [9] [11] and references cited there.) Sometimes

$$\hat{f}_v \approx \frac{1}{n} \sum_{v=1}^n \phi_v(t_i) y(t_i).$$

Furthermore, by Parseval's theorem,

$$\sum_{v=1}^{\infty} (f_v - f_{vn})^2 = \int_T [f(t) - (P_{T_n} f)(t)]^2 dt. \quad (1)$$

Convergence properties of $f - P_{T_n} f$ when $T = [0,1]$ may be found in [9,10,11], the quantity (1) is $O(n^{-(4m-1)})$ when ii) holds if the maximum distance between two neighboring points is $O(1/n)$. Under the model ii'), $(1+\lambda/\lambda_v)^{-1}$. \hat{f}_v can be viewed as a good approximation to the posterior mean of f_v and $f_{n,\lambda}(t)$ as a good approximation to the posterior mean of $f(t)$ when $\lambda = \sigma^2/nb$.

Letting Γ be the $n \times n$ matrix with i th entry $\phi_v(t_i)$, and D be the $n \times n$ diagonal matrix with v th entry λ_v , we have that the covariance matrix Σ of $(\hat{f}_1, \dots, \hat{f}_n)$ is

$$\Sigma = \sigma^2 D \Gamma' (\Gamma D \Gamma' + B)^{-2} \Gamma D$$

where the i, j th entry of B is $\sum_{v=n+1}^{\infty} \lambda_v \phi_v(t_i) \phi_v(t_j)$. If

$\frac{1}{n} \sum_{v=1}^n \phi_v^2(t_i)$ is uniformly bounded, then $\text{Trace } B = O(n^{-(2m-2)})$. Then, ^{3/} to a good approximation,

^{3/} This is the only place $m \geq 2$ is used. Elsewhere we only use $m \geq 1$.

$$\Sigma \simeq \sigma^2 D\Gamma'(\Gamma D\Gamma')^{-2} \Gamma D = \sigma^2(\Gamma'\Gamma)^{-1}$$

The loss when $f_{n,\lambda}(t)$ is used is given by

$$\int_T (f(t) - f_{n,\lambda}(t))^2 dt ,$$

and the expected loss, $R(\lambda)$ is given by

$$\begin{aligned} R(\lambda) &= \sum_{v=n+1}^{\infty} f_v^2 + E \sum_{v=1}^n \left(f_v - \frac{\lambda_v \hat{f}_v}{(\lambda_v + \lambda)} \right)^2 \\ &= \sum_{v=n+1}^{\infty} f_v^2 + \sum_{v=1}^n \left(f_v - \frac{\lambda_v f_{vn}}{(\lambda_v + \lambda)} \right)^2 + \sum_{v=1}^n \frac{\lambda_v^2 \text{var } \hat{f}_v}{(\lambda_v + \lambda)^2} \\ &= \left\{ \sum_{v=n+1}^{\infty} f_v^2 + \sum_{v=1}^n \frac{\lambda_v^2 (f_v - f_{vn})^2}{(\lambda_v + \lambda)^2} + 2 \sum_{v=1}^n \frac{\lambda \lambda_v f_v (f_v - f_{vn})}{(\lambda_v + \lambda)^2} \right\} \\ &\quad + \left\{ \lambda^2 \sum_{v=1}^n \frac{f_v^2}{(\lambda + \lambda_v)^2} + \sum_{v=1}^n \frac{\lambda_v^2 \text{var } \hat{f}_v}{(\lambda_v + \lambda)^2} \right\} . \end{aligned}$$

The first term in brackets is bounded in absolute value by

$$\sum_{v=n+1}^{\infty} f_v^2 + \sum_{v=n+1}^{\infty} f_{vn}^2 + \int_T (f(t) - P_{T_n} f(t))^2 dt + 2\lambda \left(\sum_{v=1}^n \frac{f_v^2}{\lambda_v} \right)^{1/2} \left(\sum_{v=1}^n \lambda_v^2 (f_v - f_{vn})^2 \right)^{1/2}$$

and we shall suppose that it is negligible compared to the second term in brackets as $n \rightarrow \infty$. This is true in all the examples we know of whenever the points in T_n become dense in T .

Suppose further, that the $\{t_i\}$ are regularly enough spaced so that

$$\begin{aligned} \frac{1}{n} \sum_{i=1}^n \phi_v(t_i) \phi_\mu(t_i) &\simeq \int_T \phi_v(t) \phi_\mu(t) dt \\ &= 1, \quad \mu = v \\ &= 0, \quad \mu \neq v. \end{aligned} \quad (2)$$

Regularity conditions on the distribution of the t_i 's would be required for this. Then

$$\Gamma' \Gamma \simeq nI, \quad \text{var } \hat{f}_v \simeq \frac{\sigma^2}{n}.$$

Thus whenever (1) is very small, and (2) holds approximately, we have reduced the problem to the "canonical" form

$$\hat{f}_v \sim \mathcal{N}(f_v, \sigma^2/n), \quad \text{independent}$$

with either

$$\text{ii)} \quad \sum_{v=1}^{\infty} \frac{f_v^2}{\lambda_v^2} < \infty$$

or

$$\text{ii')} \quad f_v \sim \mathcal{N}(0, b\lambda_v).$$

In either case ii) or ii'), we estimate f_v by $\hat{f}_v(1 + \lambda/\lambda_v)^{-1}$, with expected loss

$$R(\lambda) = E \sum_{v=1}^n \left(f_v - \frac{\hat{f}_v}{(1 + \lambda/\lambda_v)} \right)^2 \approx \lambda^2 \sum_{v=1}^n \frac{f_v^2}{(\lambda_v + \lambda)^2} + \frac{\sigma^2}{n} \sum_{v=1}^n \frac{\lambda_v^2}{(\lambda_v + \lambda)^2} \quad (3)$$

(An argument resulting in an expression similar to (3) can be found in Cogburn and Davis [3].)

If σ^2 is known, and $\sum_{v=1}^n (f_v - f_{vn})^2$ negligible, then an unbiased estimate of $R(\lambda)$ of (3) is $\hat{R}(\lambda)$ given by

$$\hat{R}(\lambda) = \lambda^2 \sum_{v=1}^n \frac{\hat{f}_v^2}{(\lambda_v + \lambda)^2} + \frac{\sigma^2}{n} \sum_{v=1}^n \frac{\lambda_v^2 - \lambda^2}{(\lambda_v + \lambda)^2},$$

and it is reasonable to suppose that the minimizer of $\hat{R}(\lambda)$ would provide a good choice of λ for either model ii) or ii'). If (2) does not hold, then $\text{var } \hat{f}_v = \sigma^2/n$ must be replaced by $\text{var } \hat{f}_v = \sigma^2 \gamma^{vv}$ where γ^{vv} is the vv th entry of $(\Gamma' \Gamma)^{-1}$, and $\hat{R}(\lambda)$ becomes

$$\hat{R}(\lambda) = \lambda^2 \sum_{v=1}^n \frac{\hat{f}_v^2}{(\lambda_v + \lambda)^2} + \sigma^2 \sum_{v=1}^n \frac{\lambda_v^2 - \lambda^2 \gamma^{vv}}{(\lambda_v + \lambda)^2}.$$

Suppose ii') holds along with (2) and σ^2 and b are unknown. Then a maximum likelihood estimate for $\lambda = \sigma^2/nb$ can be obtained using in the likelihood function the distribution

$$\hat{f}_v \sim \mathcal{N}(0, b(\lambda_v + \sigma^2/nb)) \equiv \mathcal{N}(0, b(\lambda_v + \lambda)), \text{ independent.}$$

The estimate for λ is the minimizer of

$$\frac{\lambda \sum_{v=1}^n (\hat{f}_v^2 / (\lambda_v + \lambda))}{[\prod_{v=1}^n (\lambda / (\lambda_v + \lambda))]^{1/n}}$$

This idea is to be found in Anderssen and Bloomfield [1] [2].

Suppose ii) and (2) holds. If $\lambda_v = h^{-1}(v) v^{-2m}$ where $a \leq h \leq b$, then

$$\sum_{v=1}^n \frac{\lambda_v^2}{(\lambda_v + \lambda)^2} = \sum_{v=1}^n \frac{1}{(1 + \lambda h(v) v^{2m})} \approx \frac{c}{\lambda^{1/2m}} \int_0^\infty \frac{dx}{(1 + x^{2m})^2}$$

where $b^{-1/2m} \leq c \leq a^{-1/2m}$. It is then not hard to show (see [14] for details) that the minimizer λ^* of $R(\lambda)$ of (3) satisfies

$$\lambda^* = \left[\frac{\sigma^2}{\sum_{v=1}^n \frac{f_v^2}{\lambda_v^2}} \frac{\frac{k}{4m} \frac{1}{n}}{\frac{1}{n}} \right]^{2m/(4m+1)} (1 + o(1)),$$

with $o(1) \rightarrow 0$ as $n \rightarrow \infty$, and so

$$R(\lambda^*) = O(n^{-4m/(4m+1)}).$$

Let

$$V(\lambda) = \frac{\lambda^2 \sum_{v=1}^n (f_v^2 / (\lambda_v + \lambda)^2)}{(\frac{1}{n} \sum_{v=1}^n (\lambda / (\lambda_v + \lambda))^2)}.$$

It is shown in [12][13] that

$$V(\lambda) \approx \sum_{k=1}^n (f_{n,\lambda}^{(k)}(t_k) - y(t_k))^2 \omega_{kk}(\lambda)$$

where $f_{n,\lambda}^{(k)}$ is $f_{n-1,\lambda}$ where the k th data point $y(t_k)$ has been omitted, and

$$\omega_{kk}(\lambda) = m_{kk}(\lambda) / \frac{1}{n} \sum_{j=1}^n m_{jj}(\lambda)$$

where $m_{jj}(\lambda)$ is the jj th entry of $(Q_n + n\lambda I)^{-1}$. The minimizer of $V(\lambda)$ may thus be viewed as a cross-validation estimate of λ . It is shown in [12][13] that, if $\tilde{\lambda}$ is the minimizer of $EV(\lambda)$, then $\tilde{\lambda} = \lambda^*(1 + o(1))$, where $o(1) \rightarrow 0$ as $n \rightarrow \infty$.

4. Remarks on Tensor Product Spaces and Reduction to Regression Models.

For computational purposes, when T is the unit cube in Euclidean p -space, it may be convenient to let $\mathcal{H}_Q = \mathcal{H}_R \times \mathcal{H}_R \times \cdots \mathcal{H}_R$ where \mathcal{H}_R is a reproducing kernel Hilbert space of functions on $[0,1]$. When $p = 2$ and $\underline{s} = (s_1, s_2)$, $\underline{t} = (t_1, t_2)$, then

$$Q(\underline{s}, \underline{t}) \equiv Q(s_1, s_2; t_1, t_2) = R(s_1, t_1) R(s_2, t_2) .$$

where $R(s_1, t_1)$ is the reproducing kernel for \mathcal{H}_R . If $R(s, t) = \sum_{v=1}^{\infty} \lambda_v \phi_v(s) \phi_v(t)$, then the eigenfunctions and eigenvalues of Q are given by

$$\lambda_{\mu\nu} = \lambda_{\mu} \lambda_{\nu} ,$$

$$\mu, \nu = 1, 2, \dots .$$

$$\phi_{\mu\nu}(\underline{s}) = \phi_{\mu}(s_1) \phi_{\nu}(s_2) ,$$

See Cogburn and Davis [3], Golomb [6] for handy reproducing kernels for spaces of periodic functions on $[0,1]$. If $R(s_1, \cdot)$ is a spline function (see, e.g. [4] [8]) then $Q(\underline{s}, \cdot)$ will be a tensor product spline.

Under model ii'), the exact posterior mean $f_{n,\lambda}^0(\underline{t})$, say, of $f(\underline{t})$ when $\lambda = \sigma^2/nb$ is given by

$$f_{n,\lambda}^0(\underline{t}) = (Q_{\underline{t}_{\underline{1}}}(\underline{t}), \dots, Q_{\underline{t}_n}(\underline{t})) (Q_n + n\lambda I)^{-1} \begin{pmatrix} y(\underline{t}_{\underline{1}}) \\ \vdots \\ y(\underline{t}_n) \end{pmatrix}$$

of which $f_{n,\lambda}$ is a good approximation. $f_{n,\lambda}^0$ is in the subspace V_n . If the $\underline{t}_{\underline{1}}$ are irregularly spaced and n is very large the following procedure ($p = 2$), which reduces to the model to a regression model, may be computationally simpler without much loss in accuracy. Let

$$V_{kk} = \text{span}\{Q_{\underline{t}}(\cdot), \underline{t} \in T_{kk}\} \quad \text{where } T_{kk} = \left(\frac{i}{k}, \frac{j}{k}\right),$$

$i, j = 0, 1, \dots, k, (k+1)^2 = q < n$. If, e.g., $R(s_1, \cdot)$ is a cubic spline, then V_{kk} is a space of bi-cubic (tensor product) splines. Choose any convenient basis, say $\{\omega_v(\underline{t})\}_{v=1}^q$ for V_{kk} . Then

$$f(\underline{t}) = \sum_{v=1}^q \omega_v(\underline{t}) \beta_v + (f - P_{T_{kk}} f)(\underline{t}),$$

for some $\{\beta_v\}$ where $P_{T_{kk}} f$ is the projection of f onto V_{kk} . If $R(s, t)$ "behaves like" a Green's function for a $2m_0$ th order linear differential operator, ^{4/} (which happens for $R(s_1, \cdot)$ a polynomial spline of degree $2m_0 - 1$) then it can be shown for model ii) that

$$|f(\underline{t}) - P_{V_{kk}} f(\underline{t})| \leq O(k^{-(2m_0 - \frac{1}{2})}).$$

^{4/} Then the eigenvalues for $R(s, t)$ are $O(v^{-2m_0})$.

(See [10] for some of the details.) Thus a good approximation to the original model ii) is the regression model,

$$y(\underline{t}) = \sum_{v=1}^q \omega_v(\underline{t}) \beta_v + \epsilon(\underline{t}), \quad t \in T \quad (4)$$

If X is the $n \times q$ matrix with i th entry $\omega_v(\underline{t}_i)$ and (4) is a good approximation to the original model, then the prior ii') is approximately equivalent to a zero mean Gaussian prior on the $\{\beta_v\}$ with covariance $b\Sigma_{\beta\beta}$ approximately satisfying $bQ_n \approx bX\Sigma_{\beta\beta}X'$. Under model ii'), then, the posterior mean of $\beta = (\beta_1, \dots, \beta_q)$ is β_λ given by

$$\beta_\lambda = (X'X + \lambda\Sigma_{\beta\beta}^{-1})^{-1}X'y$$

where $\lambda = \sigma^2/b$. $\Sigma_{\beta\beta}^{-1}$ can be approximated e.g. by

$$\Sigma_{\beta\beta}^{-1} \simeq X' \Gamma_q \begin{pmatrix} \lambda_1 & & 0 \\ & \ddots & \\ 0 & & \lambda_q \end{pmatrix}^{-1} \Gamma_q' X$$

where Γ_q' is the $q \times n$ dimensional matrix whose rows are the first q eigenvectors of Q_n , and $\lambda_1, \dots, \lambda_q$ are the first (largest) q eigenvalues of Q_n .

Acknowledgment

We wish to thank the Department of Statistics, Stanford University, for their generous hospitality while this was being written, and Professor Ingram Olkin for stimulating the author's interest in the problem of smoothing surfaces.

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Numerische Mathematik, to appear.

REPORT DOCUMENTATION PAGE		READ INSTRUCTIONS BEFORE COMPLETING FORM
1. REPORT NUMBER Technical Report #420	2. GOVT ACCESSION NO.	3. RECIPIENT'S CATALOG NUMBER
4. TITLE (and Subtitle) A CANONICAL FORM FOR THE PROBLEM OF ESTIMATING SMOOTH SURFACES		5. TYPE OF REPORT & PERIOD COVERED Scientific Interim
		6. PERFORMING ORG. REPORT NUMBER
7. AUTHOR(s) Grace Wahba		8. CONTRACT OR GRANT NUMBER(s) AFOSR 72-2363 B
9. PERFORMING ORGANIZATION NAME AND ADDRESS Department of Statistics University of Wisconsin 1210 W. Dayton Street		10. PROGRAM ELEMENT, PROJECT, TASK AREA & WORK UNIT NUMBERS
11. CONTROLLING OFFICE NAME AND ADDRESS Air Force Office of Scientific Research 1400 Wilson Blvd. Arlington, VA		12. REPORT DATE August 1975
		13. NUMBER OF PAGES 14
14. MONITORING AGENCY NAME & ADDRESS (if different from Controlling Office)		15. SECURITY CLASS. (of this report)
		15a. DECLASSIFICATION/DOWNGRADING SCHEDULE
16. DISTRIBUTION STATEMENT (of this Report) This document has been approved for public release and sale; its distribution is unlimited.		
17. DISTRIBUTION STATEMENT (of the abstract entered in Block 20, if different from Report)		
18. SUPPLEMENTARY NOTES		
19. KEY WORDS (Continue on reverse side if necessary and identify by block number) estimating surfaces splines cross-validation		
20. ABSTRACT (Continue on reverse side if necessary and identify by block number) We show how the problem of estimating a smooth surface on a rectangle in Euclidean p-space, which is measured discretely and with normally distributed errors, reduces to the problem of estimating the mean of a multivariate normal vector. Two empirical Bayes type estimators are noted, and it is observed that cross-validation is useful in certain cases.		