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Testing the (Parametric) Null Model Hypothesis  
in (Semiparametric) Partial and Generalized Spline Models

by

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Testing the (Parametric) Null Model Hypothesis in (Semiparametric)  
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ABSTRACT

Cox and Koh (August 1986) considered the model  $y_i = f(x(i)) + \varepsilon_i$ ,  $\varepsilon_i$  i.i.d.  $N(0, \sigma^2)$ , with the (parametric) null hypothesis  $f(x)$ ,  $x \in [0, 1]$  a polynomial of degree  $m-1$  or less, versus the alternative  $f$  is "smooth", based on the Bayesian model for  $f$  which leads to polynomial smoothing spline estimates for  $f$ . They showed that there was no uniformly most powerful test, and found the locally most powerful (LMP) test. We extend their result to the generalized smoothing spline models of Wahba (1985) and to the partial spline models proposed and studied by Engle et al. (1986), Shiller (1984), Green, Jennison, and Seheult (1985), Wahba (1984), Heckman (to appear) and others. We also show that the test statistic has an intimate relationship with the behavior of the generalized cross validation (GCV) function at  $\lambda = \infty$ . If the GCV function has a minimum at  $\lambda = \infty$ , then GCV has chosen the (parametric) model corresponding to the null hypothesis; we show that if the LMP test statistic is no larger than a certain multiple of the residual sum of squares after (parametric) regression, then the GCV function will have a (possibly local) minimum at  $\lambda = \infty$ .

*key words: partial splines, hypothesis testing in spline models, parametric vs smooth models*

## 1. Introduction.

Cox and Koh (August 1986) considered the model

$$y_i = f(x(i)) + \varepsilon_i, \quad i=1, \dots, n \quad (1.1)$$

where  $x \in [0,1]$ ,  $\varepsilon = (\varepsilon_1, \dots, \varepsilon_n)' \sim N(0, \sigma^2 I)$ ,  $\sigma^2$  known, and  $f(x)$ ,  $x \in [0,1]$  is a Gaussian stochastic process independent of  $\varepsilon$  satisfying

$$f(x) \sim \sum_{v=1}^m \alpha_v \Phi_v(x) + b^{1/2} Z(x), \quad (1.2)$$

where here  $\Phi_1, \dots, \Phi_m$  span the polynomials of degree  $\leq m-1$  and  $Z$  is an  $m-1$ -fold integrated Wiener process (Shepp (1966)). The parameter vector  $\alpha = (\alpha_1, \dots, \alpha_m)'$  may be considered as a fixed vector of unknown parameters or as a random vector having the improper prior distribution  $N(0, \xi I)$  with  $\xi \rightarrow \infty$ . This model is called the (special) spline model because the Bayes estimate of  $f$  is a polynomial spline. Cox and Koh were interested in the (parametric) null hypothesis  $H_0: b = 0$  vs  $H_1: b > 0$ , equivalently,  $H_0: f$  is a polynomial of degree at most  $m-1$  vs  $H_1: f$  is "smooth", i.e. (1.2) holds. They showed that there is no uniformly most powerful (UMP) test, and they constructed the locally most powerful (LMP) test. They observed that the test statistic is a certain quadratic form in  $y$  which is related to the polynomial spline penalty functional  $J_m(f) = \int_0^1 (f^{(m)}(x))^2 dx$ .

It is the purpose of this note to show that the Cox-Koh results extend easily to the univariate and multivariate partial spline models proposed by Engle et al. (1986), Shiller (1984), Green, Jennison, and Seheult (1985), Wahba (1984), Heckman (to appear) and others, and to the generalized spline models considered in Wahba (1985), and to note an intimate relationship between the LMP test statistic and the GCV estimate of  $\lambda = \sigma^2/nb$ .

## 2. Generalized and Partial Spline Models.

To make clear the relationship between the special spline model and the generalizations we will be interested in, we review a few facts. Let the set  $\{x(1), \dots, x(n)\}$  contain at least  $m$  distinct points, and let  $f_\lambda$  be the unique minimizer, in the Sobolev space  $W_2^m[0,1]$ , of

$$\frac{1}{n} \sum_{i=1}^n (y_i - f(x(i)))^2 + \lambda J_m(f). \quad (2.1)$$

Then it is known that

$$f_{\lambda}(x) = E(f(x) | y_1, \dots, y_n), \quad (2.2)$$

if  $\lambda = \sigma^2/nb$ . (See Kimeldorf and Wahba (1971) for  $\alpha$  an unknown parameter and Wahba (1978) for  $\alpha$  having an improper prior.)

The general smoothing spline model (see Wahba (1985) for more details) begins with a reproducing kernel Hilbert space  $H_Q$  of real valued functions of  $x$  for  $x$  in some domain  $I$  ( $= E^d$  for example), an  $M$ -dimensional subspace of  $H_Q$  spanned by  $\Phi_1, \dots, \Phi_M$ , and  $L_1, \dots, L_n$ ,  $n$  bounded linear functionals on  $H_Q$ . The model is

$$y_i = L_i f + \varepsilon_i, \quad i=1, \dots, n, \quad (2.3)$$

where the  $\varepsilon_i$ 's are as before. Let  $T$  be the  $n \times M$  matrix with  $(i, v)$ th entry  $L_i \Phi_v$ . We shall always assume that  $T$  is of full column rank, that is, the least squares regression of  $y$  onto span  $\{\Phi_1, \dots, \Phi_M\}$  is unique. Then the generalized spline estimate  $f_{\lambda}$  of  $f$  is the unique minimizer in  $H_Q$  of

$$\frac{1}{n} \sum_{i=1}^n (y_i - L_i f)^2 + \lambda \|P_1 f\|_Q^2 \quad (2.4)$$

where  $P_1$  is the orthogonal projection of  $f$  onto  $H_{Q_1}$ , the orthocomplement in  $H_Q$  of span  $\{\Phi_1, \dots, \Phi_M\}$ . Equation (2.2) holds here, with the Bayes model

$$f(x) \sim \sum_{v=1}^M \alpha_v \Phi_v(x) + b^{1/2} Z(x) \quad (2.5)$$

where now  $Z(x)$ ,  $x \in I$  is a family of zero mean Gaussian random variables with the (prior) covariance

$$EZ(x)Z(x') = Q_1(x, x'), \quad (2.6)$$

where  $Q_1$  is the reproducing kernel for  $H_{Q_1}$ . This prior differs from the one considered by Cox and Koh for the setting of Section 1, but only on the space of polynomials of degree  $\leq m-1$ . The test derived in the next section will be the same, and the prior covariance (2.6) is more convenient.

A popular example is the thin plate spline case, where  $I = E^d$ , the  $\Phi_1, \dots, \Phi_M$  are the  $M = \binom{d+m-1}{d}$  polynomials of total degree less than  $m$  in  $d$  variables  $(x_1, \dots, x_d)$  with  $2m-d > 0$ , and  $\|P_1 f\|^2 = J_m^d(f)$  given by

$$J_m^d(f) = \sum_{\alpha_1 + \dots + \alpha_d = m} \frac{m!}{\alpha_1! \cdots \alpha_d!} \quad (2.7)$$



$$\times \int_{-\infty}^{\infty} \cdots \int_{-\infty}^{\infty} \left[ \frac{\partial^m f}{\partial x_1^{\alpha_1} \cdots \partial x_d^{\alpha_d}} \right]^2 dx_1 \cdots dx_d.$$

In the thin plate spline case, the hypothesis that  $b = 0$  can be viewed as the hypothesis that  $f$  is a polynomial in  $d$  variables of total degree less than  $m$  vs the alternative that  $f$  is a fairly arbitrary "smooth" function. The partial spline model (which is really a special case of the general spline model) allows a response which is the sum of a "smooth" function of  $x = (x_1, \dots, x_d)$  and a parametric function of  $x$  and some other concomitant variables  $s$ , that is,

$$y_i = L_i g(\cdot; s_i) + \epsilon_i \quad (2.8)$$

where

$$g(x; s) = f(x) + \sum_{j=1}^p \beta_j \Psi_j(x; s), \quad (2.9)$$

here  $f$  is as in Eq.(2.5) and the  $\Psi_j$ 's are  $p$  linearly independent functions such that  $L_i \Psi_j(\cdot; s_i)$  is well defined for each  $i, j$ . The vector  $\beta = (\beta_1, \dots, \beta_p)'$  may be considered as a nuisance parameter or as  $N(0, \xi I_p)$  with  $\xi \rightarrow \infty$ , similar to  $\alpha$ . Let  $T$  be as before, let  $S$  be the  $n \times p$  matrix with  $ij$ th entry  $L_i \Psi_j \equiv L_i \Psi_j(\cdot; s_i)$  and suppose  $X = (T : S)$  has rank  $(M+p)$ . Then an estimate  $g_\lambda$  of  $g$  is obtained by finding  $f_\lambda \in H_Q$  and  $\beta_\lambda \in E^p$  as the unique minimizer of

$$\frac{1}{n} \sum_{i=1}^n (y_i - L_i f - \sum_{j=1}^p \beta_j L_i \Psi_j)^2 + \lambda \|P_1 f\|_Q^2. \quad (2.10)$$

Then

$$g_\lambda(x; s) = f_\lambda(x) + \sum_{j=1}^p \beta_{j,\lambda} \Psi_j(x; s) = E(g(x; s) | y_1, \dots, y_n). \quad (2.11)$$

with  $\lambda = \sigma^2/nb$ . We have in fact just relabeled the domain in the general spline model and adjoined  $\text{span}\{\Psi_1, \dots, \Psi_p\}$  to  $H_Q$  and called the generic element of this enlarged space  $g$ . Now, the hypothesis that  $b = 0$  is the "null model" hypothesis that  $g$  is of the parametric form

$$g(x; s) = \sum_{v=1}^M \alpha_v \Phi_v(x) + \sum_{j=1}^p \beta_j \Psi_j(x; s), \quad (2.12)$$

vs the alternative that  $g$  is a "smooth" function of  $f$  plus a parametric function of  $x$  and  $s$  of the form (2.9).

### 3. Results.

We are now in a position to reduce the problem of testing that  $g$  is of the special parametric form (2.12) in the model (2.9) to the Cox-Koh setup. We always assume that the "parametric design matrix"  $X$  defined following (2.9) is of full column rank. Let  $\Sigma$  be the  $n \times n$  matrix with

$ij$ th entry

$$EL_i ZL_j Z = L_{i(x)} L_{j(x')} Q_1(x, x'), \quad (3.1)$$

where  $L_{i(x)}$  means the linear functional applied to what follows considered as a function of  $x$ . Let  $\theta = (\alpha': \beta')'$ . Then if we look at  $\theta$  as a fixed, unknown parameter we have

$$y \sim N(X\theta, b\Sigma + \sigma^2 I) \quad (3.2)$$

and if we adopt the improper prior  $\theta \sim N(0, \xi I)$  with  $\xi \rightarrow \infty$  we have

$$y \sim N(0, \xi XX' + b\Sigma + \sigma^2 I). \quad (3.3)$$

Now, let  $R$  be any  $n - (M+p) \times n$  matrix with  $RR' = I$  and  $RX = 0$ , and let

$$u = Ry. \quad (3.4)$$

Then

$$u \sim N(0, bR\Sigma R' + \sigma^2 I) \quad (3.5)$$

for either model (3.2) or (3.3). Let  $\Gamma D \Gamma'$  be the eigenvalue-eigenvector decomposition of  $R\Sigma R'$ , with  $\lambda_v, v=1, \dots, n - (M+p)$  the diagonal elements of  $D$ . Let

$$\bar{y} = \Gamma' u, \quad (3.6)$$

then the  $\bar{y}_v$  are independent with

$$\bar{y}_v \sim N(0, b\lambda_v + \sigma^2), \quad v = 1, \dots, \bar{n} \quad (3.7)$$

where  $\bar{n} = n - (M+p)$ .

Theorem:

Let  $y_1, \dots, y_n$  be given by (2.8) where  $g$  is given by (2.9). Consider the problem of testing  $H_0: g$  given by (2.12) vs  $H_1: g$  given by (2.9) with  $b > 0$  in (2.5). Let  $\lambda_1, \dots, \lambda_{\bar{n}}$  be the eigenvalues above. Let  $Y$  denote the family of tests invariant under translations by vectors in  $\text{span}\{(L_1 \Phi_v, \dots, L_n \Phi_v): 1 \leq v \leq M \cup (L_1 \Psi_j(\cdot; s_1), \dots, L_n \Psi_j(\cdot; s_n)): 1 \leq j \leq p\}$ .

(a) If there are at least two distinct eigenvalues  $\lambda_i \neq \lambda_k$ , then no UMP test exists in  $Y$ .

(b) There exists an LMP test in  $Y$  (at  $b=0$ ). It rejects when

$$\bar{T}(\bar{y}) = \sum_{v=1}^{\bar{n}} \lambda_v \bar{y}_v^2 \quad (3.8)$$

is too large.

*Proof.* Observe that  $\bar{y}$  is a maximal invariant under the group of translations, so tests in  $Y$  are functions of  $\bar{y}$ . The rest of the proof follows as in Cox and Koh (August 1986) using the distributional results (3.7).

Substituting (3.4) and (3.6) into (3.5) gives our main result:

Theorem:

$$\tilde{T}(\tilde{y}) = T(y) = y'R'R\Sigma R'Ry \quad (3.9)$$

is the LMP test statistic for  $H_0$ :  $g$  has the parametric form (2.12), vs the alternative,  $g$  has the (semiparametric) form (2.9).

We remark that if  $R\Sigma R'$  is not of full rank then the  $\tilde{y}_v$ 's which correspond to  $\lambda_v=0$  do not appear in (3.8), nevertheless, the right hand side of (3.9) may be used to compute  $T(y)$ .

We also remark that there is an interesting relationship between  $J(f_\lambda)$  and  $T(y)$  (also noticed by Cox and Koh). Let  $\hat{f}_\lambda = (L_1 f_\lambda, \dots, L_n f_\lambda)'$ . It can be shown using the usual spline calculations (see e. g. Wahba (1985)), that

$$J(f_\lambda) = \hat{f}_\lambda' R' (R\Sigma R')^+ R \hat{f}_\lambda. \quad (3.10)$$

Thus, setting  $T(y) = y'Sy$ , we have  $J(f_\lambda) = \hat{f}_\lambda' S^+ \hat{f}_\lambda$ , where  $^+$  denotes the Moore-Penrose generalized inverse.

#### 4. A connection between the LMP test and the GCV estimate of $\lambda$ .

There is an interesting relationship between the test statistic  $\tilde{T}(\tilde{y})$  of (3.8), and the GCV estimate  $\hat{\lambda}$  of  $\lambda$ . If  $\hat{\lambda}$  is infinity, then GCV has chosen the null model.  $\hat{\lambda}$  is the minimizer of  $V(\lambda)$  given (see Wahba (1985)) by

$$V(\lambda) = \frac{\sum_{v=1}^{\tilde{n}} \left[ \frac{n\lambda}{n\lambda + \lambda_v} \right]^2 \tilde{y}_v^2}{\left[ \sum_{v=1}^{\tilde{n}} \left[ \frac{n\lambda}{n\lambda + \lambda_v} \right] \right]^2}. \quad (4.1)$$

Theorem:

$V(\lambda)$  has a (possibly local) minimum at  $\lambda = \infty$  whenever

$$T(y) = \sum_{v=1}^{\tilde{n}} \lambda_v \tilde{y}_v^2 \leq \frac{1}{\tilde{n}} \left[ \sum_{v=1}^{\tilde{n}} \lambda_v \right] \left[ \sum_{v=1}^{\tilde{n}} \tilde{y}_v^2 \right]. \quad (4.2)$$

Note that  $\sum_{v=1}^{\tilde{n}} \tilde{y}_v^2$  is the residual sum of squares after least squares regression on the (parametric) null model.

*Proof* : Let  $\gamma = 1/n\lambda$  and let

$$\bar{V}(\gamma) = \frac{\sum_{v=1}^{\bar{n}} \left[ \frac{1}{1+\gamma\lambda_v} \right]^2 \bar{y}_v^2}{\left[ \sum_{v=1}^{\bar{n}} \left[ \frac{1}{1+\gamma\lambda_v} \right] \right]^2} = \frac{N(\gamma)}{D(\gamma)}, \text{ say.} \quad (4.3)$$

Then  $V(\lambda)$  has a minimum at  $\lambda = \infty$  if and only if  $\bar{V}(\gamma)$  has a minimum at  $\gamma = 0$ , and this occurs when  $\bar{V}'(0) \geq 0$ , equivalently, when

$$D(0)N'(0) \geq N(0)D'(0), \text{ or} \quad (4.4)$$

$$(\bar{n})^2 (-2 \sum_{v=1}^{\bar{n}} \lambda_v \bar{y}_v^2) \geq (\sum_{v=1}^{\bar{n}} \bar{y}_v^2) (-2\bar{n} \sum_{v=1}^{\bar{n}} \lambda_v).$$

Note that under the null hypothesis the right and left sides of (4.2) have the same expectation. Hence there is about a 50% chance that GCV will pick the null model when it is true, whereas the LMP test will pick the null model 95% of the time in such circumstances, assuming the usual .05 level of significance. Thus the test of hypothesis is more conservative in rejection of the null hypothesis, as one would expect. Nonetheless, we conjecture that the model selected by GCV will probably be not far from the null model when it is true.

We remark that, intuitively, if  $Q_1$  behaves like a Green's function, then the  $\bar{y}_v$ 's that correspond to large  $\lambda_v$ 's generally are measures of the "low frequency" components of  $y$  (perpendicular to the null model) whereas the  $\bar{y}_v$ 's corresponding to small  $\lambda_v$ 's are measuring the "high frequency" components. We conjecture that roughly similar (approximate, asymptotic) results as these can be obtained for the penalized likelihood estimates with GCV of O'Sullivan (1983), O'Sullivan, Yandell, and Raynor (1986), Green (1985), and O'Sullivan and Wahba (1985).

## 5. Some remarks concerning the computation of T.

Let  $F:G$  be the QR decomposition of  $X$ ,

$$X = F:G = (F_1:F_2) \begin{bmatrix} G_1 \\ 0 \end{bmatrix} \quad (5.1)$$

where  $F$  is orthogonal and  $G_1$  is lower triangular. Then  $R$  can be taken as  $F_2'$ . Let the Cholesky factorization of  $F_2' \Sigma F_2$  be  $LL'$ . Then

$$T(y) = \|L'F_2'y\|^2. \quad (5.2)$$

Cox and Koh discuss some approximations to the distribution of  $T(y)$ , which depends on the non zero values of  $\lambda_v \sigma^2, v=1, \dots, \bar{n}$ . The  $\lambda_v$ 's can be computed as the squares of the singular values



of  $L'F_2'$  by using the singular value decomposition in LINPACK (Dongarra et al. (1979)). The subroutine library GCVPACK (Bates et al. (November 1985)) can be used to compute  $f_\lambda, g_\lambda$  and the GCV estimate of  $\lambda$  and with slight modifications can return  $T(y)$ , both in the partial thin plate spline case with evaluation data, and in general.

## 6. More on thin plate splines.

In the thin plate spline (TPS) case a reproducing kernel is known, (see for example, Wahba and Wendelberger (1980)), but it is much easier to work with the so called "semi-kernel"  $E_m(x, x')$ , given, up to a multiplicative constant, by

$$\begin{aligned} E_m(x, x') &= \text{const } \|x - x'\|^{2m-d} \log \|x - x'\|, \quad 2m-d \text{ an even integer} \\ &= \text{const } \|x - x'\|^{2m-d}, \quad \text{otherwise} \end{aligned} \quad (6.1)$$

where  $\|x\|^2 = \sum_{i=1}^d x_i^2$ . The semi-kernel  $E_m$  (also called a "variogram" in the kriging literature) has the property that it gives the covariances of generalized divided differences. Specifically, we call  $(c_1^l, \dots, c_n^l : x(1), \dots, x(n))$  a generalized divided difference of order  $m$  if it annihilates polynomials of total degree less than  $m-1$ , that is,  $T'c^l = 0$ . Then in the Bayes model corresponding to  $J_m^d$  of (2.7)

$$E\left(\sum_{j=1}^n c_j^1 f(x(j))\right)\left(\sum_{k=1}^n c_k^2 f(x(k))\right) = \sum_{j,k} c_j^1 c_k^2 E_m(x(j), x(k)).$$

It can be shown, using the reproducing kernel  $Q_1$  in Wahba and Wendelberger (1980) that the matrix  $K$  with  $i, j$ th entry  $L_{i(x)} L_{j(x')} E_m(x, x')$  satisfies  $K = \Sigma + B$  where  $F_2' B F_2 = 0$  so that  $K$  may be used instead of  $\Sigma$  in (3.9) and elsewhere.

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## ABSTRACT

Cox and Koh (August 1986) considered the model  $y_i = f(x(i)) + \varepsilon_i$ ,  $\varepsilon_i$  i.i.d.  $N(0, \sigma^2)$ , with the (parametric) null hypothesis  $f(x)$ ,  $x \in [0, 1]$  a polynomial of degree  $m-1$  or less, versus the alternative  $f$  is "smooth", based on the Bayesian model for  $f$  which leads to polynomial smoothing spline estimates for  $f$ . They showed that there was no uniformly most powerful test, and found the locally most powerful (LMP) test. We extend their result to the generalized smoothing spline models of Wahba (1985) and to the partial spline models proposed and studied by Engle et al. (1986), Shiller (1984), Green, Jennison, and Scheult (1985), Wahba (1984), Heckman (to appear) and others. We also show that the test statistic has an intimate relationship with the behavior of the generalized cross validation (GCV) function at  $\lambda = \infty$ . If the GCV function has a minimum at  $\lambda = \infty$ , then GCV has chosen the (parametric) model corresponding to the null hypothesis; we show that if the LMP test statistic is no larger than a certain multiple of the residual sum of squares after (parametric) regression, then the GCV function will have a (possibly local) minimum at  $\lambda = \infty$ .

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