The theory and application of penalized methods

or

Reproducing Kernel Hilbert Spaces

made easy

Nancy Heckman

Department of Statistics
The University of British Columbia
Vancouver BC Canada
e-mail: nancy@stat.ubc.ca

Abstract: The popular cubic smoothing spline estimate of a regression function arises as the minimizer of the penalized sum of squares $\sum_j (Y_j - \mu(t_j))^2 + \lambda \int_a^b [\mu''(t)]^2 \, dt$, where the data are $t_j, Y_j, j = 1, \ldots, n$. The minimization is taken over an infinite-dimensional function space, the space of all functions with square integrable second derivatives. But the calculations can be carried out in a finite-dimensional space. The reduction from minimizing over an infinite dimensional space to minimizing over a finite dimensional space occurs for more general objective functions: the data may be related to the function $\mu$ in another way, the sum of squares may be replaced by a more suitable expression, or the penalty, $\int_a^b [\mu''(t)]^2 \, dt$, might take a different form. This paper reviews the Reproducing Kernel Hilbert Space structure that provides a finite-dimensional solution for a general minimization problem. Particular attention is paid to penalties based on linear differential operators. In this case, one can sometimes easily calculate the minimizer explicitly, using Green’s functions.

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1. Introduction

A Reproducing Kernel Hilbert Space (RKHS) provides a practical and elegant structure to solve optimization problems in function spaces. This article considers the use of an RKHS to analyze the data $Y_1, \ldots, Y_n \in \mathbb{R}$ and $t_1, \ldots, t_n \in \mathbb{R}^p$. The distribution of the $Y_i$'s depends on $\mu$, a function of $t \in \mathbb{R}^p$, which is usually assumed to be smooth. The goal is to find $\mu$ in a specified function space $\mathcal{H}$ to minimize

$$G(t_1, \ldots, t_n, Y_1, \ldots, Y_n, F_1(\mu), \ldots, F_n(\mu)) + \lambda P(\mu)$$

where $G$ and the $F_j$'s are known, $P$ is a known penalty on $\mu$, and $\lambda$ serves to balance the importance between $G$ and $P$. Typically, $F_j(\mu) = \mu(t_j)$ and $P(\mu)$ is based on derivatives of $\mu$. Some results here will concern general $P$ and $t_j \in \mathbb{R}^p$, $p \geq 1$, and some more extensive results will concern $t_j \in [a, b] \subset \mathbb{R}$ and $P$ generated from a differential operator $L$:

$$P(\mu) = \int_a^b [(L\mu)(t)]^2 dt$$

where $(L\mu)(t) = \mu^{(m)}(t) + \sum_{j=0}^{m-1} w_j(t)\mu^{(j)}(t)$

with $w_j$ real-valued and continuous. For this type of penalty, we restrict $\mu$ to lie in the space

$$\mathcal{H}^m[a, b] = \{ f : [a; b] \to \mathbb{R} : \mu^{(j)}; j = 0; \ldots, m - 1 \text{ are absolutely continuous and} \int_a^b [\mu^{(m)}(t)]^2 dt < \infty \}.$$ 

Note that, for all $\mu \in \mathcal{H}^m[a, b]$, $\int_a^b [ (L\mu)(t) ]^2 dt$ is well defined: $L\mu(t)$ exists almost everywhere $t$ and $L\mu$ is square integrable, since the $\omega_j$'s are continuous and $[a, b]$ is finite.
The most well-known case of (1.1) occurs in regression analysis, when we seek the regression function \( \mu \in H^2[a, b] \) to minimize

\[
\sum_j [Y_j - \mu(t_j)]^2 + \lambda \int_a^b [\mu''(t)]^2 dt. \tag{1.3}
\]

The minimizing \( \mu \) is a cubic smoothing spline, a popular regression function estimate. The non-negative smoothing parameter \( \lambda \) balances the minimizing \( \mu \)'s fit to the data (via minimizing \( \sum_j [Y_j - \mu(t_j)]^2 \)) with its closeness to a straight line (achieved when \( \int_a^b [\mu''(t)]^2 \, dt = 0 \)). The value of \( \lambda \) is typically chosen “by eye” – by examining the resulting estimates of \( \mu \), or by some automatic data-driven method such as cross-validation. See, for instance, Wahba [23], Eubank [7] or Green and Silverman [8].

To extend (1.3) to (1.1), we can consider a first term other than a sum of squares, functionals other than \( F_j(\mu) = \mu(t_j) \) and a differential operator other than the second derivative operator. Examples of these variations are given in Section 2. Section 3 contains the reduction of (1.1) to a finite dimensional optimization problem. Section 4 relates the minimizer of (1.1) to a Bayes estimate. Sections 5 and 6 contain results and algorithms for minimizing (1.1) with \( P \) as in (1.2), with Section 5 containing the “warm-up” of the cubic smoothing spline result for minimizing (1.3) and Section 6 containing the general case. The Appendix contains pertinent results from the theory of solutions of differential equations.

The material contained here is, for the most part, not original. The material is drawn from many sources: from statistical and machine learning literature, from the theory of differential equations, from numerical analysis, and from functional analysis. The purpose of this paper is to collect this diverse material in one article and to present it in an easily accessible form, to show the richness of statistical problems that involve minimizing (1.1) and to explain the theory and provide easy to follow algorithms for minimizing (1.1). A briefer review of RKHS’s can be found in Wahba [24].

2. Examples

2.1. Penalized likelihoods with \( F_j(f) = f(t_j) \)

Most statistical applications that lead to minimizing (1.1) have the first term in (1.1) equal to a negative log likelihood. In these cases, the \( \mu \) that minimizes (1.1) is called a penalized likelihood estimate of \( \mu \). Indeed, (1.3) yields a penalized likelihood estimator: the sum of squares arises from a likelihood by assuming that \( Y_1, \ldots, Y_n \) are independent normally distributed with the mean of \( Y_j \) equal to \( \mu(t_j) \) and the variance equal to \( \sigma^2 \). Then \(-2\times\) the log likelihood is simply

\[
n \log(\sigma^2) + \frac{1}{\sigma^2} \sum (Y_j - \mu(t_j))^2.
\]
A penalized likelihood estimate of $\mu$ with penalty $P(\mu)$ minimizes
\[
n \log(\sigma^2) + \frac{1}{\sigma^2} \sum (Y_j - \mu(t_j))^2 + \lambda^* P(\mu)
\]
\[= \frac{1}{\sigma^2} \left[ \sigma^2 n \log(\sigma^2) + \sum (Y_j - \mu(t_j))^2 + \lambda^* \sigma^2 P(\mu) \right].\]

Thus, for a given $\sigma^2$, the penalized likelihood estimate of $\mu$ minimizes (1.1) with $\lambda = \lambda^* \sigma^2$. If the $Y_j$’s are not independent but the vector $(Y_1, \ldots, Y_n)'$ has covariance matrix $\sigma^2 \Sigma$, then we would replace the sum of squares with $\sum_{j,k} (Y_j - \mu(t_j)) \Sigma^{-1}[j, k] (Y_k - \mu(t_k))$.

Another likelihood, important in classification, is based on data $Y_j = 1$ or $-1$ with probabilities $p(t_j)$ and $1 - p(t_j)$, respectively. Thus
\[
\text{the log likelihood} = \sum_j \frac{1 + Y_j}{2} \log p(t_j) + \frac{1 - Y_j}{2} \log[1 - p(t_j)].
\]

To avoid placing inequality constraints on the function of interest, we reparameterize by setting $\mu(t) = \log[p(t)/(1 - p(t))]$ or equivalently $p(t) = \exp(\mu(t))/(1 + \exp(\mu(t)))$. This reparameterization yields
\[
\text{the log likelihood} = \sum_j \frac{1 + Y_j}{2} \log \frac{\exp(\mu(t_j))}{1 + \exp(\mu(t_j))} + \frac{1 - Y_j}{2} \log \frac{1}{1 + \exp(\mu(t_j))}.
\]

(2.1)

2.2. $F_j$’s based on integrals

While $F_j(\mu) = \mu(t_j)$ is common, $F_j(\mu)$ is sometimes chosen to involve an integral of $\mu$, specifically, $F_j(\mu) = \int_a^b H(s, t_j) \mu(s) ds$, with $H$ known. See Wahba [23].

Li [15] and Bacchetti et al. [5] used (1.1) to estimate $\mu(t)$, the HIV infection rate at time $t$, based on data, $Y_j$, the number of new AIDS cases diagnosed in time period $(t_{j-1}, t_j]$. The expected value of $Y_j$ depends not only on $\mu(t_j)$, but also on $\mu(t)$ for values of $t \leq t_j$. This dependence involves the distribution of the time of progress from HIV infection to AIDS diagnosis, which is estimated from cohort studies. Letting $F(t|s)$ denote the probability that AIDS has developed by time $t$ given HIV infection occurred at time $s$,
\[
\mathbb{E} \left( \sum_{j=1}^n Y_j \right) = \int_{s=0}^{t_j} \mu(s) F(t_j|s) \, ds \equiv F_j(\mu).
\]

Thus we could define the first term in (1.1) as a negative log likelihood assuming the $Y_j$’s are independent Poisson counts with $\mathbb{E}(Y_j) = F_j(\mu) - F_{j-1}(\mu)$. Or we could take the computationally simpler approach by setting the first term in (1.1) equal to
\[
\sum_{j=1}^n \left( Y_j - [F_j(\mu) - F_{j-1}(\mu)] \right)^2.
\]
Both Li [15] and Bacchetti et al. [5] use this simpler approach, with the former using penalty $P(\mu) = \int (\mu'')^2$ while the latter used a discretized version of $\int (\mu'')^2$.

In a non-regression setting, Nychka et al. [16] estimated the distribution of the volumes of tumours in livers by using data from cross-sectional slices of the livers. The authors modelled tumours as spheres and so cross-sections were circles. They estimated $\mu$, the probability density of the spheres’ radii, using an integral to relate the radius of a sphere to the radius of a random slice of the sphere. Their estimation criterion was the minimization of an expression of the form (1.1) with $F_j$ using that integral and with $P(\mu) = \int (\mu'')^2$.

2.3. Support vector machines

Support vector machines are a classification tool, with classification rules built from data $Y_i \in \{-1, 1\}$, $t_i \in \mathbb{R}^p$ (see, for instance, Hastie et al. [9]). The goal is to find a function $\mu$ for classifying: classify $Y_i$ as 1 if and only if $\mu(t_i) > 0$. We see that $Y_i$ is misclassified by this rule if and only if $Y_i \mu(t_i)$ is positive. Thus, it is common to find $\mu$ to minimize $\sum_i \text{sign}[Y_i \mu(t_i)]$ subject to some penalty for rough $\mu$: that is, to find $\mu$ to minimize

$$\sum \text{sign}[Y_i \mu(t_i)] + \lambda P(\mu).$$

This can be made more general by minimizing

$$\sum_j H[Y_j \mu(t_j)] + \lambda P(\mu)$$

for a known non-decreasing function $H$. The function $H(x) = \text{sign}(x)$ is not continuous at 0, which can make minimization challenging. To avoid this problem, Wahba [22] proposed using “softer” $H$ functions, such as $H(x) = \ln[1+\exp(-x)]$. This function is not only continuous, but is differentiable and convex. Wahba [22] showed that this $H$ corresponds to a negative log likelihood. Specifically, she showed that the log likelihood in (2.1) is equal to $- \sum \log\{1 + \exp[-Y_j \mu(t_j)]\}$. 

2.4. Using different differential operators in the penalty

Ansley, Kohn, and Wong [3] and Heckman and Ramsay [10] demonstrated the usefulness of appropriate choices of $L$ in the penalty $P(\mu) = \int (L\mu)^2$. For instance, Heckman and Ramsay compared two estimates of a regression function for the incidence of melanoma in males. The data, described in Andrews and Herzberg [1], are from the Connecticut Tumour Registry, for the years 1936 to 1972. The data show a roughly periodic trend superimposed on an increasing trend. A cubic smoothing spline, the minimizer of (1.3), tracks the data fairly well, but slightly dampens the periodic component. This dampening does not
occur with Heckman and Ramsay’s preferred estimate, the estimate that minimizes a modified version of (1.3) but with the penalty \( \int |\mu''(t)|^2 \, dt \) replaced by the penalty \( \int (\mu''(t) + \omega^2 \mu''(t))^2 \, dt \) with \( \omega = 0.58 \). The differential operator \( L = D^4 + \omega^2 D^2 \) was chosen since it places no penalty on functions of the form \( \mu(t) = \alpha_1 + \alpha_2 t + \alpha_3 \cos \omega t + \alpha_4 \sin \omega t \): such functions are exactly the functions satisfying \( L \mu \equiv 0 \) and form a popular parametric model for fitting melanoma data. The value of \( \omega \) was chosen by a nonlinear least squares fit to this parametric model.

The use of appropriate differential operators in the penalty has been further developed in the field of Dynamic Analysis. See, for instance, Ramsay et al. [17]. These authors use differential operators equal to those used by subject area researchers, who typically work in the finite dimensional space defined by solutions of \( L \mu \equiv 0 \).

3. Results for the general minimization problem

This section contains some background on Reproducing Kernel Hilbert Spaces and shows how to use Reproducing Kernel Hilbert Space structure to reduce the minimization of (1.1) to minimization over a finite-dimensional function space (see Theorem 3.1). Whether or not the minimizer exists can be determined by studying the finite-dimensional version. While a complete review of Hilbert spaces is beyond the scope of this article, a few definitions may help the reader. Further background on Hilbert spaces can be found in any standard functional analysis textbook, such as Kolmogorov and Fomin [13] or Kreyszig [14]. For a condensed exposition of the necessary Hilbert space theory, see, for instance, Wahba [23], [24] or the appendix of Thompson and Tapia [21]. We will only consider Hilbert spaces over \( \mathbb{R} \).

Consider \( \mathcal{H} \), a collection of functions from \( T \subseteq \mathbb{R}^p \) to \( \mathbb{R} \). Suppose that \( \mathcal{H} \) is a vector space over \( \mathbb{R} \) with inner product \( \langle \cdot, \cdot \rangle \). The inner product induces a norm on \( \mathcal{H} \), namely \( ||f|| = \langle f, f \rangle^{1/2} \). The existence of a norm allows us to define limits of sequences in \( \mathcal{H} \) and continuity of functions with arguments in \( \mathcal{H} \). The vector space \( \mathcal{H} \) is a Hilbert space if it is complete with respect to this norm, that is, if any Cauchy sequence in \( \mathcal{H} \) converges to an element of \( \mathcal{H} \).

A linear functional \( F \) is a function from a Hilbert space \( \mathcal{H} \) to the reals satisfying \( F(\alpha f + \beta g) = \alpha F(f) + \beta F(g) \) for all \( \alpha, \beta \in \mathbb{R} \) and all \( f, g \in \mathcal{H} \). The Riesz Representation Theorem states that a linear functional \( F \) is continuous on \( \mathcal{H} \) if and only if there exists \( \eta \in \mathcal{H} \) such that \( \langle \eta, f \rangle = F(f) \) for all \( f \in \mathcal{H} \). The function \( \eta \) is called the representer of \( F \).

The Hilbert space \( \mathcal{H} \) is a Reproducing Kernel Hilbert Space if and only if, for all \( t \in T \), the linear functional \( F_t(f) \equiv f(t) \) is continuous, that is, if and only if, for all \( t \in T \), there exists \( R_t \in \mathcal{H} \) such that \( \langle R_t, f \rangle = f(t) \) for all \( f \in \mathcal{H} \). Noting that the collection of \( R_t \)'s, \( t \in T \), defines a bivariate function \( R \), namely \( R(s, t) \equiv R_t(s) \), we see that \( \mathcal{H} \) is a Reproducing Kernel Hilbert Space if and only if there exists a bivariate function \( R \) defined on \( T \times T \) such that \( \langle R(\cdot, t), f \rangle = f(t) \) for all \( f \in \mathcal{H} \) and all \( t \in T \). The function \( R \) is called the reproducing kernel of \( \mathcal{H} \).
One can show that the reproducing kernel is symmetric in its arguments, as follows. To aid the proof, use the notation that $R_t(s) = R(s, t)$ and $R_s(t) = R(t, s)$. By the reproducing properties of $R_t$ and $R_s$, $< R_t, R_s >= R_s(t)$ and $< R_t, R_t >= R_t(s)$. But the inner product is symmetric, that is $< R_t, R_s >= < R_s, R_t >$. So $R_s(t) = R_t(s)$.

To give the form of the finite-dimensional minimizer of (1.1), we assume that the following conditions hold.

(C.1) There are $\mathcal{H}_0$ and $\mathcal{H}_1$, linear subspaces of $\mathcal{H}$, with $\mathcal{H}_1$ the orthogonal complement of $\mathcal{H}_0$.
(C.2) $\mathcal{H}_0$ is of dimension $m < \infty$, with basis $u_1, \ldots, u_m$. If $m = 0$, take $\mathcal{H}_0$ equal to the empty set and $\mathcal{H}_1 = \mathcal{H}$.
(C.3) There exists $R_0 \in \mathcal{H}_0$ and $R_1 \in \mathcal{H}_1$ such that $R_i$ is a reproducing kernel for $\mathcal{H}_i$, in the sense that $< R_i(\cdot, t), \mu > = \mu(t)$ for all $\mu \in \mathcal{H}_i$, $i = 0, 1$.

Since $\mathcal{H}_0$ is finite dimensional, it is closed. The orthogonal complement of a subspace is always closed. Thus Condition (C.1) implies that any $\mu \in \mathcal{H}$ can be written as $\mu = \mu_0 + \mu_1$ for some $\mu_0 \in \mathcal{H}_0$ and $\mu_1 \in \mathcal{H}_1$ and that $< \mu_0, \mu_1 > = 0$. This is often written as $\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_1$. Note that Conditions (C.1), (C.2) and (C.3) imply that $R \equiv R_0 + R_1$ is a reproducing kernel for $\mathcal{H}$.

We require one more condition, relating the penalty $P$ to the partition of $\mathcal{H}$.

(C.4) Write $\mu = \mu_0 + \mu_1$, with $\mu_1 \in \mathcal{H}_1$. Then $P(\mu) = < \mu_1, \mu_1 >$.

**Theorem 3.1.** Suppose that conditions (C.1) through (C.4) hold and that $F_1, \ldots, F_n$ are continuous linear functionals on $\mathcal{H}$. Let $\eta_j(t) = F_j(R_1(\cdot, t))$, that is, $F_j$ applied to the function $R_1$ considered as a function of $s$, with $t$ fixed. Then to minimize (1.1), it is necessary and sufficient to find

$$
\mu(t) = \mu_0(t) + \mu_1(t) = \sum_{j=1}^m \alpha_j u_j(t) + \sum_{j=1}^n \beta_j \eta_j(t)
$$

where the $\alpha_j$’s and $\beta_j$’s minimize

$$
G(t_1, \ldots, t_n, Y_1, \ldots, Y_n, F_1(\mu_0 + \mu_1), \ldots, F_n(\mu_0 + \mu_1)) + \lambda \beta^T K \beta.
$$

Here $\beta = (\beta_1, \ldots, \beta_n)^T$ and the matrix $K$ is symmetric and non-negative definite, with $K[j, k] = F_j(\eta_k)$. If $F_j(f) = f(t_j)$ and $F_k(f) = f(t_k)$, then $\eta_j(t) = R_1(t_j, t_1), \eta_k(t) = R_1(t_k, t_1)$ and $K[j, k] = R_1(t_j, t_k)$.

**Proof.** By the Riesz Representation Theorem, there exists a representer $\eta_j \in \mathcal{H}$ such that $< \eta_j, \mu >= F_j(\mu)$ for all $\mu \in \mathcal{H}$. Applying the Riesz Representation Theorem to the subspaces $\mathcal{H}_0$ and $\mathcal{H}_1$, which can be considered as Hilbert spaces in their own rights, there exists $\eta_{0j} \in \mathcal{H}_0$ and $\eta_{1j} \in \mathcal{H}_1$, representers of $F_j$ in the sense that $< \eta_{0j}, \mu >= F_j(\mu)$ for all $\mu \in \mathcal{H}_0$ and $< \eta_{1j}, \mu >= F_j(\mu)$ for all $\mu \in \mathcal{H}_1$. One easily shows that this $\eta_{1j}$ is equal to $\eta_{1j}$, as defined in the statement of the Theorem: by the definition of the representer of $F_j$, $\eta_{1j}$ must define...
satisfy $F_j(R_1(\cdot,t)) = <\eta_{j1}^*, R_1(\cdot,t)>$. But, by the reproducing quality of $R_1$, $<\eta_{j1}^*, R_1(\cdot,t)> = \eta_{j1}(t)$. So $\eta_{j1} = \eta_{j1}$. One also easily shows that
\[ \eta_j = \eta_{j0} + \eta_{j1}. \]

We use the $\eta_{j1}$’s to partition $\mathcal{H}_1$ as follows. Let $\mathcal{H}_{11}$ be the finite dimensional subspace of $\mathcal{H}_1$ spanned by $\eta_{j1}, j = 1, \cdots, n$, and let $\mathcal{H}_{12}$ be the orthogonal complement of $\mathcal{H}_{11}$ in $\mathcal{H}_1$. Then $\mathcal{H} = \mathcal{H}_0 \oplus \mathcal{H}_{11} \oplus \mathcal{H}_{12}$ and so any $\mu \in \mathcal{H}$ can be written as
\[ \mu = \mu_0 + \mu_{11} + \mu_{12} \quad \text{with} \quad \mu_0 \in \mathcal{H}_0 \quad \text{and} \quad \mu_{1k} \in \mathcal{H}_{1k}, k = 1, 2. \]

We now show that any minimizer of (1.1) must have $\mu_{12} \equiv 0$. Let $\mu$ be any element of $\mathcal{H}$. Since $\eta_j$ is the representor of $F_j$ and $\mu_{12}$ is orthogonal to $\eta_j$,
\[ F_j(\mu) = <\eta_j, \mu> = <\eta_j, \mu_0 + \mu_{11} + \mu_{12}> = <\eta_j, \mu_0 + \mu_{11}> = F_j(\mu_0 + \mu_{11}). \]
Therefore, $\mu_{12}$ is irrelevant in computing the first term in (1.1). To study the second term in (1.1), by (C.4) and the orthogonality of $\mu_{11}$ and $\mu_{12}$,
\[ P(\mu) = <\mu_1, \mu_1> = <\mu_{11}, \mu_{11}> + <\mu_{12}, \mu_{12}>. \]

Therefore, we want to find $\mu_0 \in \mathcal{H}_0$, $\mu_{11} \in \mathcal{H}_{11}$ and $\mu_{12} \in \mathcal{H}_{12}$ to minimize
\[ G(t_1, \ldots, t_n, Y_1, \ldots, Y_n, F_1(\mu_0 + \mu_{11}), \ldots, F_n(\mu_0 + \mu_{11}))+\lambda[<\mu_{11}, \mu_{11}> + <\mu_{12}, \mu_{12}>]. \]
Clearly, we should take $\mu_{12}$ to be the zero function and so any minimizer of (1.1) is of the form
\[ \mu(t) = \mu_0(t) + \mu_{11}(t) = \sum_{j=1}^{m} \alpha_j u_j(t) + \sum_{i=1}^{n} \beta_i \eta_{j1}(t). \]

Now consider rewriting $P(\mu)$ as $\beta^T K \beta$: $P(\mu) = <\mu_{11}, \mu_{11}> = \sum_{j,k} \beta_j \beta_k <\eta_{j1}, \eta_{k1}> = \beta^T K \beta$ for $K$ symmetric and non-negative definite. To show that $K[j, k] = F_j(\eta_{k1})$, use the fact that $\eta_{j1}$ is the representor of $F_j$ in $\mathcal{H}_1$, that is, that $<\eta_{j1}, f> = F_j(f)$ for all $f \in \mathcal{H}_1$. Applying this to $f = \eta_{k1}$ yields the desired result, that $<\eta_{j1}, \eta_{k1}> = F_j(\eta_{k1})$.

Consider the case that $F_j(f) = f(t_j)$ and $F_k(f) = f(t_k)$. Then $\eta_{j1}(t) = F_j(R_1(\cdot,t)) = R_1(t_j, t)$, $\eta_{k1}(t) = R_1(t_k, t)$, and $K[j, k] = F_j(\eta_{k1}) = R_1(t_k, t_j) = R_1(t_j, t_k)$ by symmetry of $R_1$.

The proof of the following Corollary is immediate, by taking $m = 0$ in (C.2).

**Corollary 3.1.** Suppose that $\mathcal{H}$ is an RKHS with inner product $<\cdot, \cdot>$ and reproducing kernel $R$. In (1.1), suppose that $P(\mu) = <\mu, \mu>$ and assume that the $F_j$’s are continuous linear functionals. Then the minimizer of (1.1) is of the form
\[ \mu(t) = \sum_{j=1}^{n} \beta_j F_j(R_1(\cdot,t)). \]
4. A Bayesian connection

Sometimes, the minimizer of (1.1) is related to a Bayes estimate of \( \mu \). In the Bayes formulation, \( Y_j = \mu(t_j) + \epsilon_j \) where the \( \epsilon_j \)'s are independent normal random variables with zero means and variances equal to \( \sigma^2 \). The function \( \mu \) is the realization of a stochastic process and is independent of the \( \epsilon_j \)'s.

The connection between \( \hat{\mu} \), the minimizer of \( \sum_j (Y_j - \mu(t_j))^2 + \lambda \int (L \mu)^2 \), and a Bayes estimate of \( \mu \) was first given by Kimeldorf and Wahba \cite{kimeldorf1970} for the case that \( L \mu = \mu^{(m)} \). The result was generalized to \( L \)'s as in (1.2) by Kohn and Ansley \cite{ansley1980}. The function \( \mu \) is defined on \( \mathbb{R} \) and is generated by the stochastic differential equation \( L \mu(t) \, dt = \sigma \sqrt{X} \, dW(t) \) where \( W \) is a mean zero Wiener process on \([a, b]\) with \( \text{var}(W(t)) = t \). Assume that \( \mu \) satisfies the initial conditions: \( \mu(a), \mu'(a), \ldots, \mu^{(m-1)}(a) \) are independent normal random variables with zero means and variances equal to \( k \). Let \( \hat{\mu}_k(t) \) be the posterior mean of \( \mu(t) \) given \( Y_1, \ldots, Y_n \). Then Kimeldorf and Wahba \cite{kimeldorf1970} and Kohn and Ansley \cite{ansley1980} show that \( \hat{\mu}(t) = \lim_{k \to \infty} \hat{\mu}_k(t) \).

Another Bayes connection arises in Gaussian process regression, a tool of machine learning (see, for instance, Rasmussen and Williams \cite{rasmussen2006}). Consider \( \mu \) defined on \( A \subseteq \mathbb{R}^D \), with \( \mu \) the realization of a mean zero stochastic process with covariance function \( S \). Let \( \hat{\mu}_B \) be the pointwise Bayes estimate of \( \mu \):

\[
\hat{\mu}_B(t) = E(\mu(t)|Y_1, \ldots, Y_n) = S(t, t) \left[ \sigma^2 I + S(t, t) \right]^{-1} Y
\]

where \( S(t, t)' \) is an \( n \)-vector with \( j \)th entry \( S(t, t_j) \), \( S(t, t) \) is the \( n \times n \) matrix with \( j \)th entry \( S(t_j, t_k) \) and \( Y = (Y_1, \ldots, Y_n)' \). Then, as shown below, for an appropriately defined Reproducing Kernel Hilbert Space \( \mathcal{H}_S \) with reproducing kernel \( S \), the Bayes estimate of \( \mu \) is equal to

\[
\arg \min_{\mu \in \mathcal{H}_S} \sum_{j=1}^n (Y_j - \mu(t_j))^2 + \sigma^2 < \mu, \mu > .
\]  

The existence of the space \( \mathcal{H}_S \) with reproducing kernel \( S \) is given by the Moore-Atrensajn Theorem \cite{aronszajn1950}. The space is defined by constructing finite-dimensional spaces: fix \( J > 0 \) and \( t_1, \ldots, t_J \in A \) and consider the finite dimensional linear space of functions, \( \mathcal{H}_{(t_1, \ldots, t_J)} \), consisting of all linear combinations of \( S(t_1, \cdot), S(t_2, \cdot), \ldots, S(t_J, \cdot) \). Let \( \mathcal{H}^* \) be the union of these \( \mathcal{H}_{(t_1, \ldots, t_J)} \)'s over all \( J \) and all values of \( t_1, \ldots, t_J \). Let \( < \cdot, \cdot > \) be the inner product on \( \mathcal{H}^* \) generated by \( S(t_j, \cdot), S(t_k, \cdot) \), that is, \( < \sum_j a_j S(t_j, \cdot), \sum_k b_k S(t_k, \cdot) > = \sum_j a_j b_k S(t_j, t_k) \). Let \( \mathcal{H}_S \) be the completion of \( \mathcal{H}^* \) under the norm associated with this inner product. Then \( \mathcal{H}_S \) is a Reproducing Kernel Hilbert Space with reproducing kernel \( S \). So, by Theorem 3.1, the solution to (4.1) is of the form

\[
\mu(t) = \sum_{l=1}^n \beta_l S(t_l, t) = S(t, t)\beta, \quad \text{with the} \ \beta_l \text{'s chosen to minimize}
\]

\[
\sum_{j=1}^n \left[ Y_j - \sum_{l=1}^n \beta_l S(t_l, t_j) \right]^2 + \sigma^2 \sum_{l,k=1}^n \beta_l \beta_k S(t_l, t_k) = ||Y - S(t, t)\beta||^2 + \sigma^2 \beta' S(t, t)\beta
\]

where \( \beta = (\beta_1, \ldots, \beta_n)' \). The minimizing \( \hat{\beta} \) is \( [\sigma^2 I + S(t, t)]^{-1} Y \), and so the solution to (4.1) is equal to \( \hat{\mu}_B \).
5. Results for the cubic smoothing spline

Here, we minimize (1.3) using Theorem 3.1. The expressions for the reproducing kernels $R_0$ and $R_1$ are provided. The next section contains an algorithm for computing $R_0$ and $R_1$ for general $L$.

The first step to minimize (1.3) over $\mu \in \mathcal{H}^2[a,b]$ is to define the inner product on $\mathcal{H}^2[a,b]$:

$$<f, g> = f(a)g(a) + f'(a)g'(a) + \int_a^b f''(t) g''(t) \, dt.$$ 

Verifying that this is an inner product is straightforward, including showing that $<f, f> = 0$ if and only if $f \equiv 0$. The proof that $\mathcal{H}^2[a,b]$ is complete under this inner product uses the completeness of $L^2[a,b]$.

For (C.1) and (C.2) of Section 3, we partition $\mathcal{H}^2[a,b]$ into $\mathcal{H}_0$ and $\mathcal{H}_1$:

$$\mathcal{H}_0 = \{f : f''(t) \equiv 0\} = \text{the span of } \{1, t\}$$
and

$$\mathcal{H}_1 = \{f \in \mathcal{H}^2[a,b] : f(a) = f'(a) = 0\}.$$ 

$\mathcal{H}_1$ is the orthogonal complement of $\mathcal{H}_0$ and so $\mathcal{H}^2[a,b] = \mathcal{H}_0 \oplus \mathcal{H}_1$. (This is shown in Theorem 6.1 for $\mathcal{H}^m[a,b]$.)

For (C.3) let

$$R_0(s, t) = 1 + (s - a)(t - a)$$
and

$$R_1(s, t) = st (\min\{s, t\} - a) + \frac{s + t}{2} [(\min\{s, t\})^2 - a^2] + \frac{1}{3} [(\min\{s, t\})^3 - a^3].$$

Then direct calculations verify that $R_0$ and $R_1$ are the reproducing kernels of, respectively, $\mathcal{H}_0$ and $\mathcal{H}_1$, that is, that $R_i \in \mathcal{H}_i$ and that $<R_i(\cdot, t), f> = f(t)$ for all $f \in \mathcal{H}_i, i = 0, 1$.

To verify that condition (C.4) is satisfied, write $\mu = \mu_0 + \mu_1$, with $\mu_i \in \mathcal{H}_i, i = 0, 1$. Then $P(\mu) = \int (\mu'')^2 = \int (\mu_1'')^2 = <\mu_1, \mu_1>$.

We can show that $F_j(\mu) = \mu(\cdot j)$ is a continuous linear functional, either by using the definition of the inner product to verify continuity of $F_j$ or by noting that $R = R_0 + R_1$ is the reproducing kernel of $H^2[a,b]$. Thus, by Theorem 3.1, to minimize (1.3) we can restrict attention to

$$\mu(t) = \alpha_0 + \alpha_1 t + \sum_1^n \beta_j R_1(t_j, t)$$
and find $\alpha_0, \alpha_1$ and $\beta = (\beta_1, \ldots, \beta_n)'$ to minimize

$$\sum_j [Y_j - \alpha_0 - \alpha_1 t_j - \sum_k \beta_k R_1(t_j, t_k)]^2 + \beta' K \beta$$


where $K[j,k] = R_1(t_j,t_k)$. In matrix/vector form, we seek $\beta$ and $\alpha = (\alpha_0, \alpha_1)'$ to minimize

$$||Y - T\alpha - K\beta||^2 + \lambda \beta'K\beta$$

(5.1)

with $Y = (Y_1, \cdots, Y_n)'$, $T_{i1} = 1$ and $T_{i2} = t_i$, $i = 1, \cdots, n$. One can minimize (5.1) directly, using matrix calculus.

Unfortunately, solving the matrix equations resulting from the differentiation of (5.1) involves inverting matrices which are ill-conditioned and large. Thus, the calculations are subject to round-off errors that seriously affect the accuracy of the solution. In addition, the matrices to be inverted are not sparse, so that $O(n^3)$ operations are required. This can be a formidable task for, say, $n = 1000$. The problem is due to the fact that the bases functions $1$, $t$, and $R_1(t_j, \cdot)$ are almost dependent with supports equal to the entire interval $[a, b]$. There are two ways around this problem. One way is to replace this inconvenient basis with a more stable one, one in which the elements have close to non-overlapping support. The most popular stable basis for this problem is that made up of cubic B-splines (see, e.g., Eubank [7]). The $i$th B-spline basis function has support $[t_i; t_i+2]$ and thus the matrices involved in the minimization of (1.3) are banded, well-conditioned, and fast to invert. Another approach is that of Reinsch ([19], [20]). The Reinsch algorithm yields a minimizer in $O(n)$ calculations. The approach for the Reinsch algorithm is based on a paper of Anselone and Laurent [2]. Section 6.4 gives this technique for minimization of expressions like (5.1).

6. Results for penalties with differential operators

Now consider the problem of minimizing (1.1) with penalty $P$ based on a differential operator $L$, as in (1.2), that is, of minimizing

$$G(t_1, \ldots, t_n, Y_1, \ldots, Y_n, F_1(\mu), \ldots, F_n(\mu)) + \lambda \int (L\mu)^2$$

(6.1)

over $\mu \in H^m[a,b]$. We can apply Theorem 3.1 using the Reproducing Kernel Hilbert Space structure for $H^m[a,b]$ defined in Section 6.1 below. We can then explicitly calculate the form of $\mu$ provided we can calculate reproducing kernels. Theorem 6.1 states a method for explicitly calculating reproducing kernels. Section 6.2 summarizes the algorithm for calculating reproducing kernels and the form of the minimizing $\mu$, and contains three examples of calculations. Theorem 6.1 and the calculations of Section 6.2 require results from the theory of differential equations. The Appendix contains these results, including a constructive proof of the existence of $G(\cdot, \cdot)$, the Green’s function associated with the differential operator $L$. Section 6.4 contains a fast algorithm for minimizing (6.1) when $G$ is a sum of squares and $F_j(f) = f(t_j)$.

6.1. The form of the minimizer of (6.1)

Giving the form of the minimizing $\mu$ uses the result of Theorem A.1 in the Appendix, that there exist linearly independent $u_1, \cdots, u_m \in H^m[a,b]$ with $m$
derivatives and that these functions form a basis for the set of all $\mu$ with $L\mu(t) = 0$ almost everywhere $t$. Furthermore $W(t)$, the Wronskian matrix associated with $u_1, \ldots, u_m$, is invertible for all $t \in [a,b]$. The Wronskian matrix is defined as

$$[W(t)]_{ij} = u_i^{(j-1)}(t), \ i, j = 1, \ldots, m.$$ 

The following is an inner product under which $H^m[a,b]$ is a Reproducing Kernel Hilbert Space:

$$< f, g > = \sum_{j=0}^{m-1} f^{(j)}(a)g^{(j)}(a) + \int_a^b (Lf)(t) (Lg)(t) \, dt.$$  \hfill (6.2)

To show that this is, indeed, an inner product is straightforward, except to show that $< f, f > = 0$ implies that $f \equiv 0$. But this follows immediately from Theorem A.4 in the Appendix.

**Theorem 6.1.** Let $L$ be as in (1.2), let $\{u_1, \ldots, u_m\}$ be a basis for the set of $\mu$ with $L\mu(t) = 0$ and let $W(t)$ be the associated Wronskian matrix. Then, under the inner product (6.2), $H^m[a,b]$ is a Reproducing Kernel Hilbert Space with reproducing kernel $R(s, t) = R_0(s, t) + R_1(s, t)$ where

$$R_0(s, t) = \sum_{i,j=1}^m C_{ij}u_i(s)u_j(t)$$

with

$$C_{ij} = [(W(a)W'(a))^{-1}]_{ij},$$

$$R_1(s, t) = \int_a^b G(s, u) G(t, u) \, du$$

and $G(\cdot, \cdot)$ is the Green’s function associated with $L$, as given in equations (A.1), (A.2) and (A.3) in the Appendix. Furthermore, $H^m[a,b]$ can be partitioned into the direct sum of the two subspaces

$$H_0 = \text{the set of all } f \in H^m[a,b] \text{ with } Lf(t) = 0 \text{ almost everywhere } t$$

$$= \text{the span of } u_1, \ldots, u_m$$

and

$$H_1 = \text{the set of all } f \in H^m[a,b] \text{ with } f^{(j)}(a) = 0, j = 0, \cdots m - 1.$$ 

$H_1$ is the orthogonal complement of $H_0$. $H_0$ has reproducing kernel $R_0$ and $H_1$ has reproducing kernel $R_1$. 

**Proof.** To prove the Theorem, it suffices to show the following.

(a) Any $f$ in $H^m[a,b]$ can be written as $f = f_0 + f_1$, with $f_i \in H_i$ and $< f_0, f_1 > = 0$. 


(b) $R_0$ is the reproducing kernel for $\mathcal{H}_0$ and $R_1$ is the reproducing kernel for $\mathcal{H}_1$.

Consider (a). Obviously, for $f_i \in \mathcal{H}_i$, $i = 0, 1$, $< f_0, f_1 >$ is equal to zero, by the definition of the inner product in (6.2). To complete the proof of (a), fix $f \in \mathcal{H}^m[a, b]$ and find $c_1, \cdots, c_m$ such that, if $f_0 = \sum c_i u_i$, then $f_1 = f - f_0 \in \mathcal{H}_1$. That is, we find $c_1, \cdots, c_m$ such that, for $j = 0, \cdots, m - 1$, $f^{(j)}(a) = 0$, that is $f^{(j)}(a) - \sum c_i u_i^{(j)}(a) = 0$. Writing this in matrix notation and using the Wronskian matrix yields

$$(f(a), f'(a), \cdots, f^{(m-1)}(a)) = (c_1, \cdots, c_m)W(a)$$

and we can solve this for $(c_1, \cdots, c_m)$, since the Wronskian $W(a)$ is invertible.

Consider (b). To prove that $R_1$ is the reproducing kernel for $\mathcal{H}_1$, first simplify notation, fixing $t \in [a, b]$ and letting $r(s) = R_1(s, t)$. We must show that $r \in \mathcal{H}_1$ and that that $< r, f >= f(t)$ for all $f \in \mathcal{H}_1$. Again, to simplify notation, let $h(u) = G(t, u)$. By definition of $R_1$, $r(s) = \int_a^b G(s, u) h(u) du$. By Theorems A.5 and A.6, $r \in \mathcal{H}_1$ and $Lr(s) = h(s) = G(t, s)$ almost everywhere $s$. Therefore, for $f \in \mathcal{H}_1$,

$$< r, f > = 0 + \int_a^b (Lr)(s) (Lf)(s) \, ds = \int_a^b G(t, s) (Lf)(s) \, ds = f(t)$$

by the definition of the Green’s function. See equation (A.1).

Now consider $R_0$. Obviously, $R_0(\cdot, t) \in \mathcal{H}_0$, since it is a linear combination of the $u_i$’s. To show that $< R_0(\cdot, t), f > = f(t)$, it suffices to consider $f = u_l, l = 1, \cdots, m$. Noting that $Lu_l \equiv 0$, write

$$< R_0(\cdot, t), u_l > = \sum_{i,j=1}^m C_{ij} u_j(t) \, u_i, u_l >$$

$$= \sum_{i,j=1}^m C_{ij} u_j(t) \left[ \sum_{k=0}^{m-1} u_i^{(k)}(a) u_i^{(k)}(a) + 0 \right]$$

$$= \sum_{i,j=1}^m C_{ij} u_j(t) \sum_{k=0}^{m-1} [W(a)]_{i,k+1} [W(a)]_{l,k+1}$$

$$= \sum_{i,j=1}^m C_{ij} u_j(t) [W(a)W'(a)]_{li}$$

$$= \sum_{j=1}^m u_j(t) [W(a)W'(a)C]_{ij}$$

$$= u_l(t).$$

\[ \square \]

We can now use Theorems 3.1 and 6.1 to write the form of the minimizer of (6.1). The proof of the following Theorem is straightforward.
Suppose that \( L \) is as in (1.2). Let \( u_1, \ldots, u_m \) be a basis for the set of \( \mu \)'s with \( L\mu = 0 \) and let \( G \) be the corresponding Green's function, defined in equations (A.1), (A.2) and (A.3) in the Appendix. Let

\[
R_1(s, t) = \int_a^b G(s, u) \, G(t, u) \, du
\]

and \( \eta_1(t) = F_j(R_1(\cdot, t)) \). Then the minimizer of (6.1) must be of the form

\[
\mu(t) = \sum_{j=1}^m \alpha_j u_j(t) + \sum_{j=1}^n \beta_j \eta_j(t)
\]

where the \( \alpha_j \)'s and \( \beta \equiv (\beta_1, \ldots, \beta_n)' \) minimize

\[
G(t_1, \ldots, t_n, Y_1, \ldots, Y_n, F_1(\mu), \ldots, F_n(\mu)) + \lambda \beta' K \beta
\]

with \( K \) as defined in Theorem 3.1.

### 6.2. Algorithm and examples for calculating \( R_0, R_1 \) and the minimizing \( \mu \)

Suppose that we're given a linear differential operator \( L \) as in (1.2). The following steps summarize results so far, describing how to calculate \( R_0 \) and \( R_1 \), the required reproducing kernels associated with \( L \), and the \( \mu \) that minimizes (6.1).

1. Find \( u_1, \ldots, u_m \), a basis for the set of functions \( \mu \) with \( L\mu = 0 \).
2. Calculate \( W(\cdot) \), the Wronskian of the \( u_i \)'s: \( W_{ij}(t) = u_i^{(j-1)}(t) \).
3. Set \( R_0(s, t) = \sum_{i,j} [W(a)W'(a)]^{-1} w_i(s)w_j(t) \).
4. Calculate \( (u_1^*(t), \ldots, u_m^*(t)) \), the last row of the inverse of \( W(t) \).
5. Find \( G \), the associated Green's function: \( G(t, u) = \sum u_i(t)u_i^*(u) \) for \( u \leq t \), 0 else.
6. Set \( R_1(s, t) = \int_a^b G(s, u) \, G(t, u) \, du. \)
7. Find \( \eta_j: \eta_j(t) = F_j(R_1(\cdot, t)). \)
8. Calculate the symmetric matrix \( K \): \( K[j, k] = F_k(\eta_j) \). If \( F_j(\mu) = \mu(t_j) \) and \( F_k(\mu) = \mu(t_k) \) then \( K[j, k] = R_1(t_j, t_k) \).
9. Set \( \mu(t) = \sum \alpha_j u_j(t) + \sum \beta_j \eta_j(t) \) and minimize \( G(t_1, \ldots, t_n, Y_1, \ldots, Y_n, F_1(\mu), \ldots, F_n(\mu)) + \lambda \beta' K \beta \) with respect to \( \beta \) and the \( \alpha_j \)'s.

The first step is the most challenging, and for some \( L \)'s, it may in fact be impossible to find the \( u_j \)'s in closed form. However, if \( L \) is a linear differential operator with constant coefficients, then the first step is easy, using Theorem A.2. Alternatively, if one has an approximate model in mind defined in terms of known functions \( u_1, \ldots, u_m \), then one can find the corresponding \( L \) (see Example 3 below).

The reader can use these steps to derive the expressions in Section 5 for the cubic smoothing spline.
Although the calculation of the minimizing $\mu$ does not involve $R_0$, step 3 is included for completeness, to allow the reader to calculate the reproducing kernel, $R_0 + R_1$, for $\mathcal{H}^m[a,b]$ under the inner product (6.2).

**Example 1.** Suppose that $L\mu = \mu'$ and that the interval $[a,b]$ is equal to $[0,1]$. In Step 1, the basis for $L\mu \equiv 0$ is $u_1(t) = 1$. In Step 2, the Wronskian is the one by one matrix with element equal to 1. So in Step 3, $R_0(s,t) \equiv 1$. In Step 4, $u_1^*(s) = 1$ and so, in Step 5, $G(t,u) = 1$ if $u \leq t$, 0 else. Therefore

$$R_1(s,t) = \int_0^{\min\{s,t\}} 1 \, du = \min\{s,t\}.$$ 

Thus, we seek $\mu$ of the form

$$\mu(t) = \alpha + \sum_{j=1}^{n} \beta_j F_j(R_1(\cdot,t)).$$

If $F_j(\mu) = \mu(t_j)$, $j = 1, \ldots, n$, then we seek

$$\mu(t) = \alpha + \sum_{j=1}^{n} \beta_j \min\{t_j,t\},$$

that is, the minimizing $\mu$ is piecewise linear with pieces defined in terms of $t_1, \ldots, t_n$. In Step 8, $K[j,k] = \min\{t_j,t_k\}$.

If, instead, $F_j(\mu) = \int_0^1 f_j \mu$ for known $f_j$, as in Section 2.2, then

$$F_j(R_1(\cdot,t)) = \eta_j(t) = \int_0^1 f_j(s) R_1(s,t) \, ds = \int_0^1 f_j(s) \min\{s,t\} \, ds$$

$$= \int_0^t s f_j(s) \, ds + t \int_t^1 f_j(s) \, ds$$

and, in Step 8,

$$K[j,k] = \int_{t=0}^1 f_k(t) \eta_j(t) \, dt = \int_{s,t=0}^1 f_k(t) f_j(s) \min\{s,t\} \, ds \, dt.$$ 

**Example 2.** Suppose that $Lf = f'' + \gamma f'$, $\gamma$ a real number.

For Step 1, we can find $u_1$ and $u_2$ via Theorem A.2 in the Appendix. We first solve $x^2 + \gamma x = 0$ for the two roots, $r_1 = 0$ and $r_2 = -\gamma$. So $u_1(t) = 1$ and $u_2(t) = \exp(-\gamma t)$.

For Step 2, we compute the Wronskian

$$W(t) = \begin{bmatrix} 1 & 0 \\ \exp(-\gamma t) & -\gamma \exp(-\gamma t) \end{bmatrix}.$$
For Step 3 we have

\[ [W(a)W'(a)]^{-1} = \left[ \begin{array}{cc} 1 + \frac{1}{\gamma^2} \exp(\gamma a) & -\frac{1}{\gamma^2} \exp(\gamma a) \\ -\frac{1}{\gamma^2} \exp(\gamma a) & \frac{1}{\gamma^2} \exp(2\gamma a) \end{array} \right] . \]

So

\[ R_0(s, t) = C_{11} u_1(s) u_1(t) + C_{12} u_1(s) u_2(t) + C_{21} u_2(s) u_1(t) + C_{22} u_2(s) u_2(t) \]

\[ = 1 + \frac{1}{\gamma^2} - \frac{1}{\gamma^2} \exp(-\gamma t^*) - \frac{1}{\gamma^2} \exp(-\gamma s^*) + \frac{1}{\gamma^2} \exp(-\gamma (s^* + t^*)) . \]

with \( s^* = s - a \) and \( t^* = t - a \).

For Step 4, inverting \( W(t) \) we find that

\[ u_1^*(t) = \frac{1}{\gamma} \quad \text{and} \quad u_2^*(t) = -\frac{1}{\gamma} \exp(\gamma t) \]

and so, in Step 5, the Green's function is given by

\[ G(t, u) = \begin{cases} \frac{1}{\gamma} (1 - \exp(-\gamma(t - u))) & \text{for } u \leq t \\ 0 & \text{else} \end{cases} . \]

To find \( R_1(s, t) \) in Step 6, first suppose that \( s \leq t \). Then

\[ R_1(s, t) = \int_a^s \gamma^{-2} (1 - e^{-\gamma(s-u)}) (1 - e^{-\gamma(t-u)}) \, du \]

\[ = -\frac{1}{\gamma^2} + \frac{s^*}{\gamma^2} + \frac{1}{\gamma^3} \exp(-\gamma s^*) + \frac{1}{\gamma^3} \exp(-\gamma t^*) \]

\[ -\frac{1}{2\gamma^3} \exp[-\gamma(t^* - s^*)] - \frac{1}{2\gamma^3} \exp[-\gamma(s^* + t^*)] . \] (6.3)

Since \( R_1(s, t) = R_1(t, s) \), if \( t < s \), then \( R_1(s, t) \) is gotten by interchanging \( s^* \) and \( t^* \) in the above.

Therefore, to minimize (6.1) over \( \mu \in \mathcal{H}_4[a, b] \), we seek \( \mu \) of the form

\[ \mu(t) = \alpha_1 + \alpha_2 \exp(-\gamma t) + \sum_{1}^{n} \beta_j F_j(R_1(\cdot, t)) . \]

The calculations in Steps 7 and 8 for \( \eta_j(t) = F_j(R_1(\cdot, t)) \) and \( K \) are tedious except in the case that \( F_j(f) = f(t_j) \).

**Example 3.** Instead of specifying the operator \( L \), one might more easily specify basis functions \( u_1, \cdots, u_m \) for a preferred approximate parametric model. For instance, one might think that \( \mu \) is approximately a constant plus a damped sinusoid: \( \mu(t) \approx \alpha_1 + \alpha_2 \sin(t) \exp(-t) \). Given \( u_1, \cdots, u_m \), one can easily find the operator \( L \) so that \( Lu_i \equiv 0 \), \( i = 1, \cdots, m \), and thus one can define an estimate of \( \mu \) as the minimizer of (6.1). Assume that each \( u_i \) has \( m \) continuous
derivatives and that the associated Wronskian matrix $W(t)$ is invertible for all $t \in [a, b]$. To find $L$, we solve for the $\omega_j$'s in (1.2):

$$0 = (Lu_i)(t) = u_i^{(m)}(t) + \sum_{j=0}^{m-1} \omega_j(t)u_i^{(j)}(t),$$

that is

$$u_i^{(m)}(t) = -\sum_{j=0}^{m-1} \omega_j(t)u_i^{(j)}(t).$$

This can be written in matrix/vector form as

$$W(t) \begin{bmatrix} \omega_0(t) \\ \vdots \\ \omega_{m-1}(t) \end{bmatrix} = - \begin{bmatrix} u_1^{(m)}(t) \\ \vdots \\ u_m^{(m)}(t) \end{bmatrix},$$

yielding

$$\begin{bmatrix} \omega_0(t) \\ \vdots \\ \omega_{m-1}(t) \end{bmatrix} = -W(t)^{-1} \begin{bmatrix} u_1^{(m)}(t) \\ \vdots \\ u_m^{(m)}(t) \end{bmatrix}.$$ 

Obviously, the $\omega_j$'s are continuous, by our assumptions concerning the $u_i$'s and the invertibility of $W(t)$.

For the example with $u_1 \equiv 1$ and $u_2 = \sin(t)\exp(-t)$, we find that

$$W(t) = \begin{bmatrix} \sin(t)\exp(-t) & \exp(-t)[\cos(t) - \sin(t)] \\ \exp(-t)[\cos(t) - \sin(t)] & 1 \end{bmatrix},$$

which is invertible on $[a, b]$ provided $\cos(t) \neq \sin(t)$ for $t \in [a, b]$. In this case, $\omega_0(t) \equiv 0$, $\omega_1(t) = \frac{2\cos(t)}{[\cos(t) - \sin(t)]}$ and so the associated differential operator is $L(\mu)(t) = \mu''(t) + 2\mu'(t)\cos(t)/[\cos(t) - \sin(t)]$. Note that we do not need $L$ to proceed with the minimization of (6.1) – we only need $u_1, \ldots, u_m$ to calculate the required reproducing kernels. However, if we would like to cast the problem in the Bayesian model of Section 4, we require $L$.

### 6.3. Minimization of the penalized weighted sum of squares via matrix calculus

Consider minimizing a specific form of (6.1) over $\mu \in \mathcal{H}^m[a, b]$, namely minimizing

$$\sum_j d_j[Y_j - F_j(\mu)]^2 + \lambda \int (Lu)^2$$

for known and positive $d_j$'s. We can rewrite this as a minimization problem easily solved by matrix/vector calculations, provided we can find a basis $\{u_1, \ldots, u_m\}$ for the set of $\mu$ with $L\mu = 0$. 
Theorem 6.2 implies that, to minimize (6.4), we must find $\alpha = (\alpha_1, \ldots, \alpha_m)'$ and $\beta = (\beta_1, \ldots, \beta_n)'$ to minimize

$$(\mathbf{Y} - T\mathbf{\alpha} - K\mathbf{\beta})'D(\mathbf{Y} - T\mathbf{\alpha} - K\mathbf{\beta}) + \lambda\mathbf{\beta}'K\mathbf{\beta}$$

where $\mathbf{Y} = (Y_1, \ldots, Y_n)'$, $T$ is $n \times m$ with $T[i,j] = u_j(t_i)$, $K$ is $n \times n$ with $K[j,k] = F_j(\eta_k)$, and $D$ is an $n$ by $n$ diagonal matrix with $D[i,i] = d_i$. Assume, as is typically the case, that $T$ is of full rank and $K$ is invertible. Taking derivatives with respect to $\mathbf{\alpha}$ and $\mathbf{\beta}$ and setting equal to zero yields

$$T' D (\mathbf{Y} - K\hat{\mathbf{\beta}}) = T' D \hat{\mathbf{\alpha}}.$$  \hspace{1cm} (6.5)

and

$$-2K'D(\mathbf{Y} - T\hat{\mathbf{\alpha}} - K\hat{\mathbf{\beta}}) + 2\lambda K\hat{\mathbf{\beta}} = 0$$

which is equivalent to

$$\mathbf{Y} - T\hat{\mathbf{\alpha}} - (K + \lambda D^{-1})\hat{\mathbf{\beta}} = 0.$$  

Let

$$M = K + \lambda D^{-1}.$$  

Then

$$\hat{\mathbf{\beta}} = M^{-1}(\mathbf{Y} - T\hat{\mathbf{\alpha}}).$$  \hspace{1cm} (6.6)

Substituting this into (6.5) yields

$$T' D[I - KM^{-1}] \mathbf{Y} = T' D[I - KM^{-1}] T\hat{\mathbf{\alpha}},$$

that is

$$T' D[M - K]M^{-1} \mathbf{Y} = T' D[M - K]M^{-1} T\hat{\mathbf{\alpha}}$$

or $\lambda T' M^{-1} \mathbf{Y} = \lambda T' M^{-1} T\hat{\mathbf{\alpha}}$.

Therefore, provided $T$ is of full rank,

$$\hat{\mathbf{\alpha}} = (T' M^{-1} T)^{-1} T' M^{-1} \mathbf{Y}$$  \hspace{1cm} (6.7)

and

$$\hat{\mathbf{\beta}} = M^{-1}[I - T(T' M^{-1} T)^{-1} T' M^{-1}] \mathbf{Y}.$$  \hspace{1cm} (6.8)

Unfortunately, using equations (6.7) and (6.8) results in computational problems since typically $M$ is an ill-conditioned matrix and thus difficult to invert. Furthermore, $M$ is $n \times n$ and $n$ is typically large, making inversion expensive. Fortunately, when $F_j(f) = f(t_j)$, we can transform the problem to alleviate the difficulties and to speed computation. The details are given in the next section.
6.4. Algorithm for minimizing the penalized weighted sum of squares when \( F_j(f) = f(t_j) \)

Assume that \( F_j(f) = f(t_j) \), that \( a < t_1 < \cdots < t_n < b \), that \( T \) is of full rank \( n - m \) and that \( K \) is invertible. The goal is to re-write \( \hat{\alpha} \) in (6.7) and \( \hat{\beta} \) in (6.8) so that we only need to invert small or banded matrices. Meeting this goal involves defining a “good” matrix \( Q \) and showing that

\[
\hat{\beta} = Q(Q'MQ)^{-1}Q'Y
\]  

(6.9)

and

\[
\hat{\alpha} = (T'T)^{-1}T'(Y - M\hat{\beta}).
\]  

(6.10)

We will define \( Q \) so that \( Q'MQ \) is banded and thus easy to invert. To begin, let \( Q \) be an \( n \times (n - m) \) matrix of full column rank such that \( Q'T \) is an \( n - m \times m \) matrix of zeroes. \( Q \) isn’t unique, but later, further restrictions will be placed on \( Q \) so that \( Q'MQ \) is banded.

We first show that \( T'\hat{\beta} = 0 \). This will imply that there exists an \( n - m \) vector \( \gamma \) such that \( \hat{\beta} = Q\gamma \). From (6.6)

\[
Y = M\hat{\beta} + T\hat{\alpha}
\]  

(6.11)

Substituting this into (6.7) yields

\[
\hat{\alpha} = (T'M^{-1}T)^{-1}T'\hat{\beta} + \hat{\alpha}.
\]

Therefore

\[
(T'M^{-1}T)^{-1}T'\hat{\beta} = 0
\]

and so \( T'\hat{\beta} = 0 \) and \( \hat{\beta} = Q\gamma \) for some \( \gamma \). To find \( \gamma \), use (6.6):

\[
Q'M\hat{\beta} = Q'(Y - T\hat{\alpha}) = Q'Y
\]

since \( Q'T = 0 \). So \( Q'MQ\gamma = Q'Y \), yielding

\[
\gamma = (Q'MQ)^{-1}Q'Y.
\]

Therefore equation (6.9) holds. Equation (6.10) follows immediately from equation (6.11).

We can also find an easy-to-compute form for \( \hat{Y} = T\hat{\alpha} + K\hat{\beta} \) using (6.11):

\[
Y = (K + \lambda D^{-1})\hat{\beta} + T\hat{\alpha} = \hat{Y} + \lambda D^{-1}\hat{\beta}
\]

and so

\[
\hat{Y} = Y - \lambda D^{-1}\hat{\beta}.
\]

Note that we have not yet used the fact that \( F_j(f) = f(t_j) \). In the special case that \( F_j(f) = f(t_j) \), we can choose \( Q \) so that \( Q'MQ \) is banded. Specifically, in addition to requiring that \( Q'T = 0 \), we also seek \( Q \) with

\[
Q_{ij} = 0 \text{ unless } i = j, j + 1, \cdots, j + m.
\]  

(6.12)
So we want $Q$ with $[Q'T]_{ij} = \sum_{l=0}^{m} Q_{i+l,i} u_j(t_{i+l}) = 0$ for all $j = 1, \ldots, m, i = 1, \ldots, n-m$. That is, for each $i$, we seek an $(m+1)$-vector $q_i = (Q_{i,1}, \ldots, Q_{i+m,i})'$ satisfying $q_i' T_i = 0$, where $T_i$ is the $(m+1)$ by $m$ matrix with $l$th entry equal to $u_j(t_{i+l})$. This is easily done by a QR decomposition of $T_i$: the matrix $T_i$ can be written as $T_i = Q_i R_i$ for some $Q_i$, an $(m+1) \times (m+1)$ orthonormal matrix, and some $R_i$, $(m+1) \times m$ with last row equal to 0. Take $q_i$ to be the last column of $Q_i$.

We now show that $Q'MQ$ is banded, specifically, that $[Q'MQ]_{kl} = 0$ whenever $|k-l| > m$. Write $Q'MQ = Q'KQ + \lambda Q'D^{-1}Q$. Since $D$ is diagonal, one easily shows that $[QD^{-1}Q]_{kl} = 0$ for $|k-l| > m$. To show that the same is true for $Q'KQ$, write

$$K[i,j] = R_1(t_i, t_j) = \int G(t_i, \omega) G(t_j, \omega) d\omega = \sum_{r,s} u_r(t_i) u_s(t_j) \int_\omega \min\{t_i, t_j\} u_r^*(\omega) u_s^*(\omega) d\omega = \sum_{r,s} u_r(t_i) u_s(t_j) F_{r,s}(\min\{t_i, t_j\}).$$

Since $Q'KQ$ is symmetric, it suffices to show that $[Q'KQ]_{kl} = 0$ for $k-l > m$. So fix $k$ and $l$ with $k-l > m$ and write

$$[Q'KQ]_{kl} = \sum_{i,j=1}^{n} Q_{ik} K_{ij} Q_{jl} = \sum_{i,j=0}^{m} Q_{k+i,k} K_{k+i,l+j} Q_{l+j,l} = \sum_{i,j=0}^{m} \sum_{r,s=1}^{m} Q_{k+i,k} F_{r,s}(\min\{t_{k+i}, t_{l+j}\}) T_{k+i,r} T_{l+j,s} Q_{l+j,l} = \sum_{j=0}^{m} \sum_{r,s=1}^{m} F_{r,s}(t_{l+j}) T_{l+j,s} Q_{l+j,l} \sum_{i=0}^{m} Q_{k+i,k} T_{k+i,r}.$$}

The last equality follows since $k > l + m$ and $0 \leq i, j \leq m$ imply that $k+i > l+j$ and so $t_{i+j} < t_{k+i}$. We immediately have that $[Q'KQ]_{kl} = 0$, since $\sum_{i=0}^{m} Q_{k+i,k} T_{k+i,r} = [Q'T]_{kr} = 0$.

Thus minimizing (6.4) when $F_j(f) = f(t_j)$ is easily and quickly done through the following steps.

1. Follow steps 1 through 8 of Section 6.2 to find $u_1, \ldots, u_m$, a basis for $\mathbb{L}_H = 0$, the reproducing kernel $R_1$ and the matrix $K$: $K[i,j] = R_1(t_i, t_j)$.
2. Calculate the matrix $T$: $T[i,j] = u_j(t_i)$.

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3. Find $Q_n$ by $(n - m)$ of full column rank satisfying equation (6.12) and $Q'T = 0$. One can find $Q$ directly or by the method outlined below equation (6.12).

4. Find $\hat{\beta}$ and $\hat{\alpha}$ using equations (6.9) and (6.10). Speed the matrix inversion by using the fact that $Q'MQ$ is banded.

Example 2 continued from Section 6.2. Suppose that we want to minimize

$$
\sum_{j=1}^{n} d_j (Y_j - u(t_j))^2 + \lambda \int_{0}^{1} (\mu''(t) + \gamma \mu'(t))^2 \, dt
$$

over $\mu \in \mathcal{H}^2[0,1]$. For simplicity, assume that $t_i = i/(n + 1)$. Using the calculations from Section 6.2, we set $T_{i1} = 1, T_{i2} = \exp(-\gamma t_i)$, and $K[i,j] = R_i(t_i, t_j)$, with $R_1$ as in (6.3).

For Step 3, we find $Q$ directly: we seek $Q_n$ by $(n - 2)$ with $Q_{ij} = 0$ unless $i = j, j + 1, j + 2$ and

$$
0 = [Q'T]_{ij} = Q_{ii}I_{ij} + Q_{i,i+1}T_{i+1,j} + Q_{i,i+2}T_{i+2,j}.
$$

Thus, for $j = 1$,

$$
0 = Q_{ii} + Q_{i,i+1} + Q_{i,i+2}
$$

and, for $j = 2$,

$$
0 = Q_{ii} \exp(-\gamma t_i) + Q_{i,i+1} \exp(-\gamma t_{i+1}) + Q_{i,i+2} \exp(-\gamma t_{i+2}).
$$

We take

$$
Q_{ii} = 1 - \exp\left(-\frac{\gamma}{n + 1}\right) \quad Q_{i,i+1} = -\exp\left(\frac{\gamma}{n + 1}\right) + \exp\left(-\frac{\gamma}{n + 1}\right)
$$

and

$$
Q_{i,i+2} = \exp\left(\frac{\gamma}{n + 1}\right) - 1.
$$

Continuing with the fourth step to find $\hat{\alpha}$ and $\hat{\beta}$ is straightforward.

Appendix A

The Appendix contains background on the solution of linear differential equations $L\mu = 0$ with $L$ as in (1.2). Section A.2 contains results about $G$, the Green’s function associated with $L$.

A.1. Differential Equations

Details of results in this section can be found in Coddington [6]. The main Theorem, stated without proof, follows.
Theorem A.1. Let $L$ be as in (1.2). Then there exists $u_1, \ldots, u_m$ a basis for the the set of all $\mu$ with $L\mu \equiv 0$, with each $u_i$ real-valued and having $m$ derivatives. Furthermore, any such basis will have an invertible Wronskian matrix $W(t)$ for all $t \in [a, b]$. The Wronskian matrix is defined as

$$\left[ W(t) \right]_{ij} = u_i^{(j)} \quad i, j = 1, \ldots, m.$$ 

The following Theorem, stated without proof, is useful for calculating the basis functions in the case that the $\omega_j$'s are constants.

Theorem A.2. Suppose that $L$ is as in (1.2), with the $\omega_j$'s real numbers. Denote the $s$ distinct roots of the polynomial $x^m + \sum_{j=0}^{m-1} \omega_j x^j$ as $r_1, \ldots, r_s$. Let $m_i$ denote the multiplicity of root $r_i$ (so $m = \sum_i m_i$). Then the following $m$ functions of $t$ form a basis for the set of all $\mu$ with $L\mu \equiv 0$:

$$\exp(r_i t), t \exp(r_i t), \ldots, t^{m_i-1} \exp(r_i t) \quad i = 1, \ldots, s.$$ 

The following result, stated without proof, is useful for checking that a set of functions does form a basis for the set of all $\mu$ with $L\mu \equiv 0$.

Theorem A.3. Suppose that $u_1, \ldots, u_m$ have $m$ derivatives on $[a, b]$ and that $Lu_i \equiv 0$. If $W(t_0)$ is invertible at some $t_0 \in [a, b]$, then the $u_i$'s are linearly independent, and thus a basis for the set of all $\mu$ with $L\mu \equiv 0$.

The following result was useful in defining the inner product in equation (6.2), where $t_0$ was taken to be $a$.

Theorem A.4. Suppose that $L$ is as in (1.2) and let $t_0 \in [a, b]$. Then the only function in $H^m[a, b]$ that satisfies $Lf = 0$ and $f^{(j)}(t_0) = 0, j = 0, \ldots, m - 1$, is the zero function.

Proof. By Theorem A.1, there exists $u_1, \ldots, u_m$ a basis for the set of all $\mu$ with $L\mu \equiv 0$, with $W(t)$ invertible for all $t \in [a, b]$. Suppose $Lf \equiv 0$. Then $f = \sum_i c_i u_i$ for some $c_i$'s. We see that the conditions $f^{(j)}(t_0) = 0, j = 0, \ldots, m - 1$ can be written in matrix/vector form as $(c_1, \cdots, c_m)W(t_0) = (0, \cdots, 0)$. Since $W(t_0)$ is invertible, $c_i = 0, i = 1, \cdots, m$. \hfill \Box

A.2. The Green’s Function Associated with the Differential Operator $L$

Suppose that $L$ is as in (1.2). The definition below gives the definition of $G(\cdot, \cdot)$, the Green’s function associated with $L$ with specified boundary conditions. Theorem A.5 gives an explicit form of $G$.

Definition. $G$ is a Green’s function for $L$ if and only if

$$f(t) = \int_{u=a}^{b} G(t, u) \left( Lf \right)(u) \, du$$

(A.1)
for all functions \( f \) in \( \mathcal{H}^m[a, b] \) satisfying the boundary conditions
\[
f^{(j)}(a) = 0, \quad j = 0, \cdots, m - 1. \tag{A.2}
\]

Of course, it’s not immediately clear that such a function \( G \) exists. However, \( G \) exists and is easily calculated using the Wronskian matrix associated with \( L \) (see Theorem A.5). Recall from Theorem A.1 of Section A.1 that there exists a basis for the set of all \( \mu \) with \( L\mu \equiv 0 \), \( u_1, \cdots, u_m \), with invertible Wronskian. Furthermore, each \( u_i \) has \( m \) derivatives.

**Lemma A.1.** Let \( u_1^*(t), \cdots, u_m^*(t) \) denote the entries in the last row of the inverse of \( W(t) \). Then \( u_j^* \) is continuous, \( j = 1, \ldots, m \).

**Proof.** The \( u_j^* \)'s are continuous, since \( u_j^* = (\det W(t))^{-1} \) times an expression involving sums and products of \( u_l^{(j)}, l = 1, \cdots, m, j = 0, \cdots, m - 1 \), and the \( u_l \)'s have \( m - 1 \) continuous derivatives. \( \square \)

**Theorem A.5.** Let \( u_1^*(t), \cdots, u_m^*(t) \) denote the entries in the last row of the inverse of \( W(t) \). Then
\[
G(t, u) = \begin{cases} 
\sum_{i=1}^m u_i(t)u_i^*(u) & \text{for } u \leq t \\
0 & \text{otherwise}
\end{cases} \tag{A.3}
\]
is a Green’s function for \( L \) and, for each fixed \( t \in [a, b] \), \( G(t, \cdot) \) is in \( L^2[a, b] \).

The following theorem will be useful in the proof of Theorem A.5.

**Theorem A.6.** Let \( G \) be as in (A.3) and suppose that \( h \in L_2 \). If
\[
r(t) = \int_a^b G(t, u) \, h(u) \, du
\]
Then
\[
r \in \mathcal{H}^m[a, b], \tag{A.4}
\]
\[
(Lr)(t) = h(t) \quad \text{almost everywhere } t \in [a, b] \tag{A.5}
\]
and
\[
r^{(j)}(a) = 0 \quad j = 0, \cdots, m - 1. \tag{A.6}
\]

**Proof.** Write
\[
r(t) = \sum_{i=1}^m u_i(t) \int_a^t u_i^*(u) \, h(u) \, du
\]
We’ll first show that
\[
r^{(j)}(t) = \sum_{i=1}^m u_i^{(j)}(t) \int_a^t u_i^*(u) \, h(u) \, du \quad j = 0, \cdots, m - 1 \tag{A.7}
\]
and

\[ r^{(m)}(t) = h(t) + \sum_{i=1}^{m} u_i^{(m)}(t) \int_a^t u_i^*(u) \, h(u) \, du \quad \text{almost everywhere } t \in [a, b]. \tag{A.8} \]

These equations follow easily by induction on \( j \). We only present the case \( j = 1 \). Then

\[ r'(t) = \sum_{i=1}^{m} u_i'(t) \int_a^t u_i^*(u) \, h(u) \, du + \sum_{i=1}^{m} u_i(t) \frac{d}{dt} \left[ \int_a^t u_i^*(u) \, h(u) \, du \right]. \]

Since \( u_i^* \) and \( h \) are in \( L_2 \),

\[ \sum_{i=1}^{m} u_i(t) \frac{d}{dt} \left[ \int_a^t u_i^*(u) \, h(u) \, du \right] = \sum_{i=1}^{m} u_i(t) u_i^*(t) h(t) \]

almost everywhere \( t \). But, by definition of \( W \) and the \( u_i^* \)'s, this is equal to

\[ h(t) \sum_i [W(t)]_{1i} [W(t)^{-1}]_{mi} = h(t) \ [W(t)^{-1}W(t)]_{m1} = h(t) \, 1 \{ m = 1 \}. \]

Therefore, for \( m = 1 \), (A.8) holds and for \( m > 1 \) (A.7) holds when \( j = 1 \). For \( m > 1 \) and \( j > 1 \), we can calculate derivatives of \( r \) up to order \( m - 1 \), and can calculate the \( m \)th derivative almost everywhere to prove (A.7) and (A.8). Clearly, the \( m \)th derivative in (A.8) is square-integrable. Therefore we’ve proven (A.4).

To prove (A.5), use (A.7) and (A.8) and write

\[(Lr)(t) = r^{(m)}(t) + \sum_{j=0}^{m-1} \omega_j(t)r^{(j)}(t)\]

\[= h(t) + \sum_{i=1}^{m} u_i^{(m)}(t) \int_a^t u_i^*(u) \, h(u) \, du + \sum_{j=0}^{m-1} \sum_{i=1}^{m} \omega_j(t) u_i^{(j)}(t) \int_a^t u_i^*(u) \, h(u) \, du \]

\[= h(t) + \sum_{i=1}^{m} \left[ u_i^{(m)}(t) + \sum_{j=0}^{m-1} \sum_{i=1}^{m} \omega_j(t) u_i^{(j)}(t) \right] \int_a^t u_i^*(u) \, h(u) \, du \]

\[= h(t) + \sum_{i=1}^{m} (Lu_i)(t) \int_a^t u_i^*(u) \, h(u) \, du = h(t) \]

since \( Lu_i \equiv 0 \).

Equation (A.6) follows directly from (A.7) by taking \( t = a \). \( \square \)
Proof of Theorem A.5. First consider the function in equation (A.3) as a function of \( u \) with \( t \) fixed. Since the \( u_i \)'s are continuous and \( W(u) \) is invertible for all \( u \), \( G(t, \cdot) \) is continuous on the finite closed interval \([a, b]\). Thus it is in \( L^2[a, b] \).

To show that equation (A.1) holds, let \( f \in H \) satisfy the boundary conditions (A.2). Define \( r(t) = \int_a^b G(t, u) (Lf)(u) \, du \). Then, by Theorem A.6, \( Lr = Lf \) almost everywhere and \( r^{(j)}(a) = 0, j = 0, \ldots, m - 1 \). Thus \( L(r - f) = 0 \) almost everywhere and \( (r - f)^{(j)}(a) = 0, j = 0, \ldots, m - 1 \). By Theorem A.4, \( r - f \) is the zero function, that is \( r = f \).

References

[1] Andrews, D. F. and Herzberg, A. M. (1985). Data: A Collection of Problems from Many Fields for the Student and Research Worker. Springer-Verlag, New York.
[2] Anselone, P. M. and Laurent, P. J. (1967). A general method for the construction of interpolating or smoothing spline-functions. Numerische Mathematik 12, 66–82.
[3] Ansley, C., Kohn, R., and Wong, C. (1993). Nonparametric spline regression with prior information. Biometrika 80, 75–88.
[4] Aronszain, N. (1950). Theory of reproducing kernels. Transactions of the American Mathematical Society 68, 337–404.
[5] Bacchetti, P., Segal, M.R., Hessol, N.A., and Jewell, N.P. (1993). Different AIDS incubation periods and their impacts on reconstructing human immunodeficiency virus epidemics and projecting AIDS incidence. Proceeding of the National Academy of Sciences, USA, 90, 2194-2196.
[6] Coddington, E. A. (1961). An Introduction to Ordinary Differential Equations. New Jersey: Prentice-Hall.
[7] Eubank, R. L. (1999). Spline Smoothing and Nonparametric Regression, Second Edition. New York: Marcel Dekker.
[8] Green, P. J. and Silverman, B. W. (1994). Nonparametric Regression and Generalized Linear Models: A Roughness Penalty Approach. London: Chapman and Hall.
[9] Hastie, T., Tibshirani, R, and Friedman, J. (2009). The Elements of Statistical Learning Data Mining, Inference, and Prediction, Second Edition. Springer Series in Statistics, Springer.
[10] Heckman, N. and Ramsay, J.O. (2000). Penalized regression with model based penalties. Canadian Journal of Statistics 28, 241–258.
[11] Kimeldorf, G. and Wahba, G. (1971). Some results on Tchebychefian spline functions. Journal of Mathematical Analysis and Applications 33, 8295.
[12] Kohn R. and Ansley, C.F. (1988). Equivalence between Bayesian smoothness priors and optimal smoothing for function estimation. Bayesian Analysis of Time Series and Dynamic Models 1, 393–430.
[13] Kolmogorov, A.N. and Fomin, S.V. (1999). Elements of the Theory of Functions and Functional Analysis. Dover Publications.
[14] Kreyszig, E. (1989). Introductory Functional Analysis with Applications. Wiley.
[15] Li, Xiaochun. (1996). Local Linear Regression versus Backcalculation in Forecasting. Ph.D. thesis, Statistics Department, University of British Columbia.
[16] Nychka, D., Wahba, G., Goldearb, S. and Pugh, T. (1984). Cross-validated spline methods for the estimation of three-dimensional tumor size distributions from observations on two-dimensional cross sections. Journal of the American Statistical Association 78, 832-846.
[17] Ramsay, J.O., Hooker, G., Campbell, D. and Cao, J. (2007). Parameter estimation for differential equations: a generalized smoothing approach. Journal of the Royal Statistical Society, Series B 69, 741-796.
[18] Rasmussen, C.E. and Williams, C.K.I. (2006). Gaussian Processes for Machine Learning. The MIT Press.
[19] Reinsch, C. (1967). Smoothing by spline functions. Numerische Mathematik, 10, 177-183.
[20] Reinsch, C. (1970). Smoothing by spline functions II. Numerische Mathematik, 16, 451-454.
[21] Thompson, J.R. and Tapia R.A. (1990). Nonparametric Function Estimation, Modeling, and Simulation. Society for Industrial Mathematics.
[22] Wahba, G. (1999). Support vector machines, Reproducing Kernel Hilbert Spaces, and randomized GCV. Advances in Kernel Methods: Support Vector Learning. Bernhard Schölkopf, Christopher J. C. Burges and Alexander J. Smola, Editors. MIT Press, Cambridge, MA, 69–88.
[23] Wahba, G. (1990). Spline Models for Observational Data. Philadelphia: Society for Industrial and Applied Mathematics.
[24] Wahba, G. (2003). An introduction to Reproducing Kernel Hilbert Spaces and why they are so useful. Proceedings Volume from the 13th IFAC Symposium on System Identification, 27–29. IPV-IFAC Proceedings Volume. Paul M.J. Van Den Hof, Bo Wahlberg and Siep Weiland, Editors.