Smoothing Splines: Hilbert Space Approach

This document provides a proof for Lorimier's theorem on smoothing splines.

Theorem (Lorimier)**.** *The unique solution f of*

$$\min_{f \in H} \int_0^{T_*} (f'(u))^2 \, du + \alpha \sum_{i=1}^{N} \left(T_i y_i - \int_0^{T_i} f(u) \, du \right)^2, \quad \alpha > 0,$$

is a quadratic spline characterized by

$$f(u) = \beta_0 + \sum_{i=1}^{N} \beta_i h_i(u), \tag{1}$$

where $h_i \in C^1[0, T_*]$ is a quadratic basis spline with

$$h_i'(u) = (T_i - u)^+, \quad h_i(0) = T_i, \tag{2}$$

and $\beta_0, \dots, \beta_N$ solve the linear system of equations

$$\sum_{i=1}^{N} \beta_i T_i = 0, \quad \alpha \left(y_i T_i - \beta_0 T_i - \sum_{l=1}^{N} \beta_l \langle h_l, h_i \rangle_H \right) = \beta_i, \quad i = 1, \dots, N. \tag{3}$$

Proof. Integration by parts yields

$$\begin{aligned}
\int_0^{T_i} g(u) \, du &= T_i g(T_i) - \int_0^{T_i} u g'(u) \, du \\
&= T_i g(0) + T_i \int_0^{T_i} g'(u) \, du - \int_0^{T_i} u g'(u) \, du \\
&= T_i g(0) + \int_0^{T_*} (T_i - u)^+ g'(u) \, du = \langle h_i, g \rangle_H,
\end{aligned}$$

for all $g \in H$. In particular,

$$\int_0^{T_i} h_l \, du = \langle h_l, h_i \rangle_H.$$

Define the nonlinear functional F on H:

$$F(f) = \int_0^{T_*} (f'(u))^2 \, du + \alpha \sum_{i=1}^{N} \left(T_i y_i - \int_0^{T_i} f(u) \, du \right)^2.$$

A local minimizer f of F satisfies, for any $g \in H$, the first-order condition

$$\frac{d}{d\epsilon} F(f + \epsilon g)|_{\epsilon=0} = 0$$

or equivalently

$$\int_0^{T_*} f' g' \, du = \alpha \sum_{i=1}^N \left(y_i T_i - \int_0^{T_i} f \, du \right) \int_0^{T_i} g \, du. \tag{4}$$

In particular, for all $g \in H$ with $\langle g, h_i \rangle_H = 0$ we obtain

$$\langle f - f(0), g \rangle_H = \int_0^{T_*} f'(u) g'(u) \, du = 0.$$

Hence

$$f - f(0) \in span\{h_1, \ldots, h_N\},$$

which proves that we can write f as:

$$f(u) = \beta_0 + \sum_{i=1}^N \beta_i h_i(u), \quad \text{with} \quad \beta_0 = f(0) \quad \text{and} \quad \sum_{i=1}^N \beta_i T_i = 0.$$

Hence we have

$$\begin{aligned}
\int_0^{T_*} f' g' \, du &= \sum_{i=1}^N \beta_i \int_0^{T_*} (T_i - u)^+ g'(u) \, du \\
&= \sum_{i=1}^N \beta_i \left(-T_i g(0) + \int_0^{T_i} g(u) \, du \right) = \sum_{i=1}^N \beta_i \int_0^{T_i} g(u) \, du,
\end{aligned}$$

and (4) can be rewritten as

$$\sum_{i=1}^N \left(\beta_i - \alpha \left(y_i T_i - \beta_0 T_i - \sum_{l=1}^N \beta_l \langle h_l, h_i \rangle_H \right) \right) \int_0^{T_i} g(u) \, du = 0$$

for all $g \in H$. This is true if and only if the following holds:

$$\alpha \left(y_i T_i - \beta_0 T_i - \sum_{l=1}^N \beta_l \langle h_l, h_i \rangle_H \right) = \beta_i, \quad i = 1, \ldots, N.$$

Thus we have shown that (4) is equivalent to (1)–(3).

Next we show that (4) is a sufficient condition for f to be a global minimizer of F. Let $g \in H$, then

$$
\begin{aligned}
F(g) &= \int_0^{T_*} \left((g' - f') + f'\right)^2 \, du + \alpha \sum_{i=1}^{N} \left(y_i T_i - \int_0^{T_i} g \, du \right)^2 \\
&\overset{(4)}{=} F(f) + \int_0^{T_*} (g' - f')^2 \, du + \alpha \sum_{i=1}^{N} \left(\int_0^{T_i} f \, du - \int_0^{T_i} g \, du \right)^2 \\
&\geq F(f),
\end{aligned}
$$

where we used (4) with g replaced by $g - f$.

It remains to show that f exists and is unique; that is, the linear system (3) has a unique solution $(\beta_0, \beta_1, \ldots, \beta_N)^\top$. The corresponding $(N+1) \times (N+1)$ matrix is

$$
A = \begin{pmatrix}
0 & T_1 & T_2 & \cdots & T_N \\
\alpha T_1 & \alpha\langle h_1, h_1\rangle_H + 1 & \alpha\langle h_1, h_2\rangle_H & \cdots & \alpha\langle h_1, h_N\rangle_H \\
\vdots & \vdots & \ddots & \ddots & \vdots \\
\alpha T_N & \alpha\langle h_N, h_1\rangle_H & \alpha\langle h_N, h_2\rangle_H & \cdots & \alpha\langle h_N, h_N\rangle_H + 1
\end{pmatrix}. \tag{5}
$$

That is, the system (3) reads

$$
A\,\beta = \begin{pmatrix} 0 \\ Z \end{pmatrix} \tag{6}
$$

where $\beta = (\beta_0, \ldots, \beta_N)^\top$ and $Z = \alpha(y_1 T_1, \ldots, y_N T_N)^\top$. Let $\lambda = (\lambda_0, \ldots, \lambda_N)^\top \in \mathbb{R}^{N+1}$ such that $A\lambda = 0$, that is,

$$
\sum_{i=1}^{N} T_i \lambda_i = 0
$$

$$
\alpha T_i \lambda_0 + \alpha \sum_{l=1}^{N} \langle h_i, h_l\rangle_H \lambda_l + \lambda_i = 0, \quad i = 1, \ldots, N.
$$

Multiplying the latter equation with λ_i and summing up over i yields

$$
\alpha \left\| \sum_{i=1}^{N} \lambda_i h_i \right\|_H^2 + \sum_{i=1}^{N} \lambda_i^2 = 0
$$

where we write $\|g\|_H = \sqrt{\langle g, g\rangle_H}$ for the corresponding norm on H. Hence $\lambda = 0$, whence A is non-singular, and the theorem is proved. □