MATH3701 Statistical Modelling
School of Mathematics, University of Leeds

Supplementary Proof: Optimality of Natural Splines

This note proves that among all sufficiently smooth functions interpolating prescribed values at a set of knots, the natural cubic spline has the smallest roughness. This result underpins Chapter 11 of the notes (Propositions 11.1 and 11.2).

Setup and statement

Let $t_1 < t_2 < \cdots < t_n$ be n distinct knots and let $y_1, \ldots, y_n$ be prescribed values. We consider functions f in the Sobolev space $W^{2,2}(\mathbb{R})$: functions that are twice differentiable with square-integrable second derivative. The *roughness* of f is

$$J(f) = \int_{-\infty}^{\infty} [f''(t)]^2 \, dt.$$

Theorem 1 (Optimality of the natural cubic spline)**.** *Let f^* be the natural cubic spline with knots at $t_1, \ldots, t_n$ satisfying $f^*(t_i) = y_i$ for $i = 1, \ldots, n$. Then, for any other function $g \in W^{2,2}(\mathbb{R})$ satisfying $g(t_i) = y_i$,*

$$J(g) \geq J(f^*),$$

with equality if and only if $g = f^*$.

Key property of the natural cubic spline

The proof rests on the following orthogonality lemma.

Lemma 1. *Let f^* be the natural cubic spline with $f^*(t_i) = y_i$. For any $h \in W^{2,2}(\mathbb{R})$ with $h(t_i) = 0$ for all i,*

$$\int_{-\infty}^{\infty} (f^*)''(t) \, h''(t) \, dt = 0.$$

Proof. Since f^* is a natural cubic spline, it is a piecewise cubic polynomial with the natural boundary conditions $(f^*)''(t) \to 0$ as $t \to \pm\infty$ (in fact $(f^*)'' = 0$ outside $[t_1, t_n]$). Integrate by parts twice:

$$\int_{-\infty}^{\infty} (f^*)''(t) \, h''(t) \, dt = \big[(f^*)''(t) \, h'(t)\big]_{-\infty}^{\infty} - \int_{-\infty}^{\infty} (f^*)'''(t) \, h'(t) \, dt.$$

The boundary term vanishes because $(f^*)'' = 0$ outside the knot range, so $(f^*)''(\pm\infty) = 0$. Integrate by parts again:

$$-\int_{-\infty}^{\infty} (f^*)'''(t) \, h'(t) \, dt = -\big[(f^*)'''(t) \, h(t)\big]_{-\infty}^{\infty} + \int_{-\infty}^{\infty} (f^*)''''(t) \, h(t) \, dt.$$

Since f^* is linear outside the knot range, $(f^*)''' = 0$ there, so the boundary term vanishes.

Inside the knot range, a cubic spline has $(f^*)''''(t) = 0$ on each open interval (t_{i-1}, t_i). Thus the integral reduces to a sum of contributions at the knots. Specifically, if we write the fourth derivative in the distributional sense, the jumps in $(f^*)'''$ at each knot t_i contribute a Dirac mass:

$$\int_{-\infty}^{\infty} (f^*)''''(t) \, h(t) \, dt = \sum_{i=1}^{n} \big[(f^*)'''(t_i^+) - (f^*)'''(t_i^-)\big] h(t_i) = 0,$$

since $h(t_i) = 0$ for all i. Hence $\int (f^*)'' h'' \, dt = 0$. $\square$

Proof of Theorem 1

Let g be any function in $W^{2,2}(\mathbb{R})$ with $g(t_i) = y_i$, and set $h = g - f^*$. Then $h(t_i) = 0$ for all i. We decompose:

$$\begin{aligned} J(g) &= \int_{-\infty}^{\infty} [g''(t)]^2 \, dt = \int_{-\infty}^{\infty} \big[(f^*)''(t) + h''(t)\big]^2 \, dt \\ &= J(f^*) + 2\int_{-\infty}^{\infty} (f^*)''(t)\, h''(t)\, dt + J(h). \end{aligned}$$

By Lemma 1, the cross-term vanishes, giving

$$J(g) = J(f^*) + J(h) \geq J(f^*),$$

since $J(h) = \int [h'']^2 \, dt \geq 0$.

Equality holds if and only if $J(h) = 0$, i.e., $h'' = 0$ everywhere, meaning h is a linear function. If $h(t_i) = 0$ for all $i \geq 2$ distinct knots, then $h \equiv 0$. Hence $g = f^*$, proving uniqueness. □

Representations of natural splines (Proposition 11.1)

The proof above also establishes that the natural cubic spline in $W^{2,2}(\mathbb{R})$ interpolating n points can be represented in the form

$$f^*(t) = a_0 + a_1 t + \sum_{i=1}^{n} b_i \, |t - t_i|^3,$$

subject to the constraints $\sum b_i = 0$ and $\sum b_i t_i = 0$ (which ensure $f'' = 0$ outside $[t_1, t_n]$). This gives $n + 2$ parameters with 2 constraints, leaving n free parameters to interpolate the n data values.

For the linear case ($\nu = 1$), the analogous representation is

$$f^*(t) = a_0 + \sum_{i=1}^{n} b_i \, |t - t_i|,$$

subject to $\sum b_i = 0$, and the optimality proof follows the same argument using $J(f) = \int [f'(t)]^2 dt$ and a single integration by parts.