Numerical Analysis

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Natural Cubic Spline: an example.

Let x_1, x_2, x_3, x_4 be given nodes (strictly increasing) and let y_1, y_2, y_3, y_4 be given values (arbitrary). Our goal is to produce a function $s(x)$ with the following properties:

1. $s(x_k) = y_k$, $k = 1, 2, 3, 4$,
2. $s(x)$ is two times continuously differentiable on $[x_1, x_4]$,
3. $\int_{x_1}^{x_4} s''(x)^2 dx$ is as small as possible.

There is a unique function $s(x)$ that has the required properties. It turns out to also satisfy

4. $s(x)$ restricted to $[x_k, x_{k+1}]$ is a cubic, $k = 1, 2, 3$,
5. $s''(x_1) = s''(x_4) = 0$.

This function is called the natural cubic spline. It is arbitrarily smooth on every open subinterval (x_k, x_{k+1}) and

a) $s'(x_k)$ exists $(s'(x_k-) = s'(x_k+))$, $k = 2, 3$,
b) $s''(x_k)$ exists $(s''(x_k-) = s''(x_k+))$, $k = 2, 3$.

Construction. Introduce the parameters $M_1 = s''(x_1)$, $M_2 = s''(x_2)$, $M_3 = s''(x_3)$, $M_4 = s''(x_4)$. M_2, M_3 are to be specified and M_1, M_4 are zero. Write

$$s''(x)\Big|_{[x_k, x_{k+1}]} = \frac{(x_{k+1} - x)M_k + (x - x_k)M_{k+1}}{x_{k+1} - x_k}, \quad k = 1, 2, 3,$$

so that $s''(x)$ is a piecewise linear continuous function. Integrate $s''(x)$ twice and write the result in the form

$$s(x)\Big|_{[x_k, x_{k+1}]} = \frac{(x_{k+1} - x)^3 M_k + (x - x_k)^3 M_{k+1}}{6(x_{k+1} - x_k)} + \frac{(x_{k+1} - x)y_k + (x - x_k)y_{k+1}}{x_{k+1} - x_k}$$
$$- \frac{1}{6}(x_{k+1} - x_k)((x_{k+1} - x)M_k + (x - x_k)M_{k+1}), \quad k = 1, 2, 3.$$

Thus $s(x)$ is piecewise cubic, $s''(x)$ is piecewise linear and continuous, and it is easy to check that $s(x_k) = y_k$, $k = 1, 2, 3, 4$. We only need to make sure that property a) holds.

We have:

$$s'(x)\Big|_{(x_k, x_{k+1})} = \frac{-(x_{k+1} - x)^2 M_k + (x - x_k)^2 M_{k+1}}{2(x_{k+1} - x_k)} + \frac{y_{k+1} - y_k}{x_{k+1} - x_k} - \frac{x_{k+1} - x_k}{6}(M_{k+1} - M_k).$$

Examine two abutting intervals $[x_{k-1}, x_k]$, $[x_k, x_{k+1}]$ $(k = 2, 3)$ and compute $s'(x_k-)$ and $s'(x_k+)$:

$$\begin{aligned} s'(x_k+) &= -\frac{1}{2}(x_{k+1} - x_k)M_k + \frac{y_{k+1} - y_k}{x_{k+1} - x_k} - \frac{x_{k+1} - x_k}{6}(M_{k+1} - M_k) \\ &= -\frac{x_{k+1} - x_k}{3}\ M_k - \frac{x_{k+1} - x_k}{6}\ M_{k+1} + \frac{y_{k+1} - y_k}{x_{k+1} - x_k}\ , \\ s'(x_k-) &= \frac{x_k - x_{k-1}}{3}\ M_k + \frac{x_k - x_{k-1}}{6}\ M_{k-1} + \frac{y_k - y_{k-1}}{x_k - x_{k-1}}\ . \end{aligned}$$

Equate one-sided derivatives:

$$\frac{x_k - x_{k-1}}{6}\ M_{k-1} + \frac{x_k - x_{k-1}}{3}\ M_k + \frac{y_k - y_{k-1}}{x_k - x_{k-1}} = -\frac{x_{k+1} - x_k}{3}\ M_k - \frac{x_{k+1} - x_k}{6}\ M_{k+1} + \frac{y_{k+1} - y_k}{x_{k+1} - x_k}$$

or

$$\frac{x_k - x_{k-1}}{6}\ M_{k-1} + \frac{x_{k+1} - x_{k-1}}{3}\ M_k + \frac{x_{k+1} - x_k}{6}\ M_{k+1} = \frac{y_{k+1} - y_k}{x_{k+1} - x_k} - \frac{y_k - y_{k-1}}{x_k - x_{k-1}}.$$

In general, this is a tridiagonal linear system of $(n-2)$ equations in $(n-2)$ unknowns $M_2, \ldots, M_{n-1}$. But for $n = 4$ we just have

$$\begin{cases} \dfrac{x_3 - x_1}{3}\ M_2 + \dfrac{x_3 - x_2}{6}\ M_3 = \dfrac{y_3 - y_2}{x_3 - x_2} - \dfrac{y_2 - y_1}{x_2 - x_1} \\ \dfrac{x_3 - x_2}{6}\ M_2 + \dfrac{x_4 - x_2}{3}\ M_3 = \dfrac{y_4 - y_3}{x_4 - x_3} - \dfrac{y_3 - y_2}{x_3 - x_2}\ . \end{cases}$$

The values of M_2, M_3 are uniquely determined by these equations.

If the nodes are equispaced, say $h = x_{k+1} - x_k$, we have

$$\begin{cases} 4M_2 + M_3 = \dfrac{6}{h^2}\ (y_1 - 2y_2 + y_3) \\ M_2 + 4M_3 = \dfrac{6}{h^2}\ (y_2 - 2y_3 + y_4)\ . \end{cases}$$

In this case,

$$M_2 = \frac{2}{5h^2}\ (4y_1 - 9y_2 + 6y_3 - y_4), \quad M_3 = \frac{2}{5h^2}\ (-y_1 + 6y_2 - 9y_3 + 4y_4).$$

Remark. A direct calculation gives

$$\begin{aligned} \int_{x_1}^{x_4} s''(x)^2 dx =& \frac{1}{3}\Big((x_2 - x_1)M_1^2 + (x_2 - x_1)M_1M_2 + (x_3 - x_1)M_2^2 \\ &+ (x_3 - x_2)M_2M_3 + (x_4 - x_2)M_3^2 + (x_4 - x_3)M_3M_4 + (x_4 - x_3)M_4^2 \Big) \\ =& \frac{1}{3}\Big((x_3 - x_1)M_2^2 + (x_3 - x_2)M_2M_3 + (x_4 - x_2)M_3^2 \Big). \end{aligned}$$