Numerical Analysis
Grinshpan

**Natural Cubic Spline**

Let $x_1, \ldots, x_n$ be given nodes (strictly increasing) and let $y_1, \ldots, y_n$ be given values (arbitrary). Our goal is to produce a function $s(x)$ with the following properties:

1. $s(x_k) = y_k$, $k = 1, \ldots, n$,
2. $s(x)$ is twice continuously differentiable on $[x_1, x_n]$,
3. $\int_{x_1}^{x_n} s''(x)^2 \, dx$ 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, $k = 1, \ldots, n - 1$,
5. $s(x)$ is almost linear at the endpoints, $s''(x_1) = s''(x_n) = 0$.

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

a) $s'(x_k)$ exists ($s'(x_{k-}) = s'(x_{k+})$), $k = 2, \ldots, n - 1$,

b) $s''(x_k)$ exists ($s''(x_{k-}) = s''(x_{k+})$), $k = 2, \ldots, n - 1$.

**Construction of $s(x)$**

We will first construct a unique function $s(x)$ that satisfies properties 1, 2, 4, 5, and then show that it also satisfies property 3.

An auxiliary formula is needed.

**Lemma.** Let $u(x)$ be a cubic polynomial on $[0, 1]$, and let $u(0) = a$, $u(1) = b$, $u''(0) = A$, and $u''(1) = B$. Then $u(x)$ has the form

$$u(x) = \frac{A}{6} (1 - x)^3 + \left( a - \frac{A}{6} \right) (1 - x) + \frac{B}{6} x^3 + \left( b - \frac{B}{6} \right) x.$$

**Proof of lemma.** It is straightforward to check that the formula works. Alternatively, the second derivative $u''(x)$ is a linear function with $u''(0) = A$ and $u''(1) = B$. Hence $u''(x) = A(1 - x) + Bx$. Integrating $u''(x)$ twice, we obtain $u(x) = \frac{A}{6} (1 - x)^3 + \frac{B}{6} x^3 + c(1 - x) + dx$. To satisfy $u(0) = a$ and $u(1) = b$ we must take $c = a - \frac{A}{6}$ and $d = b - \frac{B}{6}$. □

If the interval $[0, 1]$ is replaced by $[x_k, x_{k+1}]$, with $\delta_k = x_{k+1} - x_k$, the formula changes as follows:

$$u(x) = \frac{A}{6\delta_k} (x_{k+1} - x)^3 + \left( \frac{a}{\delta_k} - \frac{A\delta_k}{6} \right) (x_{k+1} - x) + \frac{B}{6\delta_k} (x - x_k)^3 + \left( \frac{b}{\delta_k} - \frac{B\delta_k}{6} \right) (x - x_k).$$
For each $k = 1, \ldots, n - 1$, define

$$s(x) \bigg|_{[x_k, x_{k+1}]} = \frac{M_k}{6\delta_k} (x_{k+1} - x)^3 + \left( \frac{y_k}{\delta_k} - \frac{M_k\delta_k}{6} \right) (x_{k+1} - x) + \frac{M_{k+1}}{6\delta_k} (x - x_k)^3 + \left( \frac{y_{k+1}}{\delta_k} - \frac{M_{k+1}\delta_k}{6} \right) (x - x_k),$$

where $M_1 = M_n = 0$ and parameters $M_2, \ldots, M_{n-1}$ are to be determined.

By construction, $s(x)$ restricted to $[x_k, x_{k+1}]$ is a cubic polynomial and $s(x_k) = y_k$, $k = 1, \ldots, n$, which makes it continuous.

The first derivative $s'(x)$ restricted to $(x_k, x_{k+1})$ is a quadratic polynomial,

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

We are going to choose $M_k$ to make $s'(x)$ continuous at each interior joint.

The second derivative $s''(x)$ restricted to $(x_k, x_{k+1})$ is linear,

$$s''(x) \bigg|_{(x_k, x_{k+1})} = \frac{M_k}{\delta_k} (x_{k+1} - x) + \frac{M_{k+1}}{\delta_k} (x - x_k).$$

Since $s''(x_k^-) = s''(x_k^+) = M_k$, $k = 2, \ldots, n - 1$, the line segments connect continuously. Hence $s''(x)$ is continuous as long as $s'(x)$ is.

To make sure that $s'(x)$ is continuous, i.e., that condition a) holds, examine two abutting intervals $[x_{k-1}, x_k]$, $[x_k, x_{k+1}]$ and equate one-sided derivatives

$$s'(x_k^+) = -\frac{\delta_k}{3} M_k - \frac{\delta_k}{6} M_{k+1} + \frac{y_{k+1} - y_k}{x_{k+1} - x_k},$$

$$s'(x_k^-) = \frac{\delta_{k-1}}{6} M_{k-1} + \frac{\delta_k}{3} M_k + \frac{y_k - y_{k-1}}{x_k - x_{k-1}}.$$

This gives

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

Multiplying by 6 and dividing by $\delta_k + \delta_{k-1} = x_{k+1} - x_k$, we have

$$\frac{\delta_{k-1}}{\delta_k + \delta_{k-1}} M_{k-1} + 2M_k + \frac{\delta_k}{\delta_k + \delta_{k-1}} M_{k+1} = 6 \Delta_k^{(2)}, \quad k = 2, \ldots, n - 1,$$

where $\Delta_k^{(2)}$ are the second divided differences

$$\Delta_k^{(2)} = \frac{y_{k+1} - y_k}{x_{k+1} - x_k} - \frac{y_k - y_{k-1}}{x_k - x_{k-1}}.$$
We thus obtain a linear system of \((n - 2)\) equations in \((n - 2)\) unknowns \(M_2, \ldots, M_{n-1}\). In matrix form,

\[
\begin{pmatrix}
\frac{2}{\delta_1 + \delta_2} & \frac{\delta_2}{\delta_2 + \delta_3} & \frac{\delta_3}{\delta_3 + \delta_4} & \cdots & \frac{\delta_{n-2}}{\delta_{n-2} + \delta_{n-1}} \\
\frac{\delta_1}{\delta_2 + \delta_3} & \frac{2}{\delta_2 + \delta_3} & \frac{\delta_3}{\delta_3 + \delta_4} & \cdots & \frac{\delta_{n-2}}{\delta_{n-2} + \delta_{n-1}} \\
\frac{\delta_2}{\delta_3 + \delta_4} & \frac{\delta_3}{\delta_3 + \delta_4} & \frac{2}{\delta_3 + \delta_4} & \cdots & \frac{\delta_{n-2}}{\delta_{n-2} + \delta_{n-1}} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\frac{\delta_{n-2}}{\delta_{n-2} + \delta_{n-1}} & \frac{\delta_{n-2}}{\delta_{n-2} + \delta_{n-1}} & \frac{\delta_{n-2}}{\delta_{n-2} + \delta_{n-1}} & \cdots & \frac{2}{\delta_{n-2} + \delta_{n-1}}
\end{pmatrix}
\begin{pmatrix}
M_2 \\
M_3 \\
M_4 \\
\vdots \\
M_{n-2} \\
M_{n-1}
\end{pmatrix}
= 6
\begin{pmatrix}
\Delta_2^{(2)} \\
\Delta_3^{(2)} \\
\Delta_4^{(2)} \\
\vdots \\
\Delta_{n-2}^{(2)} \\
\Delta_{n-1}^{(2)}
\end{pmatrix}.
\]

The values of \(M_2, \ldots, M_{n-1}\) are uniquely determined by these equations: the tridiagonal coefficient matrix is invertible because it is diagonally dominant,

\[
\frac{\delta_{k-1}}{\delta_k + \delta_{k-1}} + \frac{\delta_k}{\delta_k + \delta_{k-1}} = 1 < 2.
\]

\(M_k = s''(x_k)\) are sometimes called moments.

If all subintervals \([x_k, x_{k+1}]\) are of equal length \(\delta\), we have simplification:

\[
M_{k+1} + 4M_k + M_{k-1} = \frac{6}{\delta^2} (y_{k+1} - 2y_k + y_{k-1}), \quad k = 2, \ldots, n-1,
\]
or

\[
\begin{pmatrix}
\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\
\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\
\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} \\
\vdots & \vdots & \vdots & \ddots & \vdots \\
\frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2} & \frac{1}{2}
\end{pmatrix}
\begin{pmatrix}
M_2 \\
M_3 \\
M_4 \\
\vdots \\
M_{n-2} \\
M_{n-1}
\end{pmatrix}
= 6
\begin{pmatrix}
\Delta_2^{(2)} \\
\Delta_3^{(2)} \\
\Delta_4^{(2)} \\
\vdots \\
\Delta_{n-2}^{(2)} \\
\Delta_{n-1}^{(2)}
\end{pmatrix}.
\]

**Extremum Property**

Let \(f(x)\) be an interpolant to the values of \(y_k\) at points \(x_k\), and let \(f''(x)\) exist and be continuous. The difference \(\Delta(x) = s(x) - f(x)\) is then zero at each \(x_k\).

Examine the following integration:

\[
\int_{x_1}^{x_n} s''(x) \Delta''(x) dx = s''(x) \Delta'(x)|_{x_1}^{x_n} - \int_{x_1}^{x_n} s'''(x) \Delta'(x) dx
\]

\[
= - \int_{x_1}^{x_n} s'''(x) \Delta'(x) dx \quad \text{(because \(s''(x_1) = s''(x_n) = 0\))}
\]

\[
= - \sum_{k=1}^{n-1} c_k \int_{x_k}^{x_{k+1}} \Delta'(x) dx \quad \text{(because \(s'''(x)|_{[x_k, x_{k+1}]}\) is constant)}
\]

\[
= - \sum_{k=1}^{n-1} c_k [\Delta(x_{k+1}) - \Delta(x_k)]
\]

\[
= 0 \quad \text{(because \(\Delta(x_k) = 0\)).}
\]
It follows that
\[
\int_{x_1}^{x_n} f''(x)^2 \, dx = \int_{x_1}^{x_n} (s''(x) - \Delta''(x))^2 \, dx \\
= \int_{x_1}^{x_n} s''(x)^2 \, dx - 2s''(x)\Delta''(x) + \Delta''(x)^2 \, dx \\
= \int_{x_1}^{x_n} s''(x)^2 \, dx + \int_{x_1}^{x_2} \Delta''(x)^2 \, dx \\
\geq \int_{x_1}^{x_n} s''(x)^2 \, dx.
\]
Thus \( s(x) \) minimizes the integral \( \int_{x_1}^{x_n} f''(x)^2 \, dx \) over all twice continuously differentiable functions \( f(x) \) with \( f(x_k) = y_k \). Equality in
\[
\int_{x_1}^{x_n} f''(x)^2 \, dx \geq \int_{x_1}^{x_n} s''(x)^2 \, dx
\]
holds if and only if \( \Delta''(x) = 0 \) on \([x_1, x_n]\), i.e., \( \Delta(x) \) is linear on \([x_1, x_n]\). But, since \( \Delta(x_k) = 0 \), this can only happen if \( \Delta(x) = 0 \) or \( f(x) = s(x) \).

We have proved:

**THEOREM.** Among all twice continuously differentiable functions \( f(x) \) satisfying the interpolation conditions \( f(x_k) = y_k, \ k = 1, \ldots, n \), the minimum value of the integral
\[
\int_{x_1}^{x_n} f''(x)^2 \, dx
\]
is realized by the natural cubic spline \( s(x) \) and only by \( s(x) \).

**ERROR ESTIMATE**

Let \( f(x) \) be a four times continuously differentiable function on \([x_1, x_n]\) with \( f(x_k) = y_k \) and \( f''(x_1) = f''(x_n) = 0 \). Let \( \delta_{\max} \) be the maximum of \( \delta_k \) and \( \delta_{\min} \) be the minimum of \( \delta_k \). Then
\[
|f(x) - s(x)| \leq C \max_{[x_1, x_n]} |f^{(4)}(x)| \delta_{\max}^4,
\]
where \( C = \delta_{\max}/\delta_{\min} \). In particular, if all subintervals \([x_k, x_{k+1}]\) are of equal length \( \delta \), we have:
\[
|f(x) - s(x)| \leq \max_{[x_1, x_n]} |f^{(4)}(x)| \delta^4.
\]

I’m leaving out a proof of the error estimate. We may later come back to this topic and supply justification.
APPENDIX: DIAGONAL DOMINANCE

A matrix $A = (a_{ij})$ is diagonally dominant if $|a_{ii}| > \sum_{j \neq i} |a_{ij}|$ for each $i$.

LEMMA. Diagonal dominance implies invertibility.

Proof. If $v = (v_i) \neq 0$ but $Av = 0$, choose $v_m$ of maximum modulus. Then
$0 = \sum_j a_{mj} v_j$ and so
$|a_{mm} v_m| \leq \sum_{j \neq m} |a_{mj} v_j| \leq \sum_{j \neq m} |a_{mj}| |v_m|$, a contradiction. □