Splines

Let $a = x_0 < x_1 < \ldots < x_{n-1} < x_n = b$. A <u>spline of degree m</u> is a function $S(x)$ which satisfies the following conditions:

1. For $x \in [x_i, x_{i+1}]$, $S(x) = S_i(x)$: polynomial of degree $\leq m$
2. $S^{(m-1)}$ exists and continuous at the interior points $x_1, \ldots, x_{n-1}$, i.e. $\lim_{x \to x_i^-} S_{i-1}^{(m-1)}(x) = \lim_{x \to x_i^+} S_i^{(m-1)}(x)$

`EXAMPLE`

$$S(x) = \begin{cases} 0, \ -1 \leq x \leq 0 \\ x^2, \ 0 \leq x \leq 1 \end{cases}$$

$$x_0 = -1, \ x_1 = 0, \ x_2 = 1$$

$S(x)$ <u>is</u> a spline of degree $m = 2$ (<u>quadratic spline</u>).

`EXAMPLE`

$$S(x) = \begin{cases} 0, \ -1 \leq x \leq 0 \\ 1 - (x-1)^2, \ 0 \leq x \leq 1 \end{cases}$$

$S(x)$ <u>is not</u> a quadratic spline because $\lim_{x \to 0^-} S'(x) \neq \lim_{x \to 0+} S'(x)$.

Cubic Spline Interpolation

Given f, $x_0, \ldots, x_n$ as above, find a cubic spline S such that $S(x_i) = f(x_i)$, $i = 0, \ldots, n$.

$n+1$ points $\Rightarrow$ n intervals $\Rightarrow$ $4n$ coefficients

$2n$ conditions needed to interpolate $f(x_0), \ldots, f(x_n)$

$2(n-1)$ conditions needed to ensure S', S'' are continuous at the interior points

This leaves 2 free conditions. Popular choices are:

(i) $S''(x_0) = S''(x_n) = 0$: the <u>natural cubic spline interpolant</u>

(ii) $S'(x_0) = f'(x_0)$, $S'(x_n) = f'(x_n)$: the <u>clamped cubic spline interpolant</u>

Given $f(x)$; $x_0, \ldots, x_n$, how to find $S(x)$?

<u>`EXAMPLE`</u>

$$x_i = ih, \quad h = 1/n, \quad x_0 = 0, \quad x_n = 1$$

<u>`STEP 1`</u> (2nd derivative conditions)

Since $S_i(x)$ is a cubic polynomial, $S_i''(x)$ is linear for x

$$S_i''(x) = a_i \left(\frac{x_{i+1} - x}{h} \right) + a_{i+1} \left(\frac{x - x_i}{h} \right), \quad i = 0, \ldots, n-1$$

(using Lagrange 1st order interpolating polynomial).

Then

$$\left.\begin{array}{l} S_i''(x_i) = a_i \\ S_i''(x_{i+1}) = a_{i+1} \end{array}\right\} \quad \Rightarrow \quad S_{i-1}''(x_i) = a_i = S_i''(x_i)$$

Thus, $S''(x)$ is continuous at the interior nodes.

<u>`STEP 2`</u> (function values)

Integrate twice

$$S_i(x) = \frac{a_i (x_{i+1} - x)^3}{6h} + \frac{a_{i+1} (x - x_i)^3}{6h} + b_i (x_{i+1} - x) + c_i (x - x_i)$$

the last two terms are written in this special form just for convenience

$$\left.\begin{array}{l} S_i(x_i) = a_i \frac{h^2}{6} + b_i h = f_i \\ S_i(x_{i+1}) = a_{i+1} \frac{h^2}{6} + c_i h = f_{i+1} \end{array}\right\} \begin{array}{l} b_i h = f_i - a_i \frac{h^2}{6} \\ c_i h = f_{i+1} - a_{i+1} \frac{h^2}{6} \end{array}$$

Substitute

$$\begin{aligned} S_i(x) = & \frac{a_i (x_{i+1} - x)^3}{6h} + \frac{a_{i+1} (x - x_i)^3}{6h} \\ & + \left(f_i - a_i \frac{h^2}{6} \right) \left(\frac{x_{i+1} - x}{h} \right) + \left(f_{i+1} - a_{i+1} \frac{h^2}{6} \right) \left(\frac{x - x_i}{h} \right) \end{aligned}$$

<u>`STEP 3`</u> (1st derivative conditions).

$$S_i'(x) = -\frac{a_i (x_{i+1} - x)^2}{2h} + \frac{a_{i+1} (x - x_i)^2}{2h} - \left(\frac{f_i}{h} - a_i \frac{h}{6} \right) + \left(\frac{f_{i+1}}{h} - a_{i+1} \frac{h}{6} \right)$$

$$S_i'(x_i) = -a_i\frac{h}{2} - \left(\frac{f_i}{h} - a_i\frac{h}{6}\right) + \left(\frac{f_{i+1}}{h} - a_{i+1}\frac{h}{6}\right)$$

$$S_i'(x_{i+1}) = a_{i+1}\frac{h}{2} - \left(\frac{f_i}{h} - a_i\frac{h}{6}\right) + \left(\frac{f_{i+1}}{h} - a_{i+1}\frac{h}{6}\right)$$

We require, $S_{i-1}'(x_i) = S_i'(x_i)$, so (shifting $i \to i-1$ in $S_i'(x_{i+1})$)

$$\begin{aligned} a_i\frac{h}{2} &- \left(\frac{f_{i-1}}{h} - a_{i-1}\frac{h}{6}\right) + \left(\frac{f_i}{h} - a_i\frac{h}{6}\right) \\ &= -a_i\frac{h}{2} - \left(\frac{f_i}{h} - a_i\frac{h}{6}\right) + \left(\frac{f_{i+1}}{h} - a_{i+1}\frac{h}{6}\right) \end{aligned}$$

Collect like terms

$$a_{i-1}\frac{h}{6} + a_i\left(\frac{h}{2} - \frac{h}{6} + \frac{h}{2} - \frac{h}{6}\right) + a_{i+1}\frac{h}{6} = \left(f_{i-1} - 2f_i + f_{i+1}\right)/h$$

Multiply both sides by $\frac{6}{h}$

$$a_{i-1} + 4a_i + a_{i+1} = \frac{6}{h^2}\left(f_{i-1} - 2f_i + f_{i+1}\right)$$

This holds for $i = 1, \ldots, n-1$.

<u>STEP 4</u> (boundary conditions)

$$\begin{aligned} S_0''(x_0) = 0 \;&\Rightarrow\; a_0 = 0 \\ S_{n-1}''(x_n) = 0 \;&\Rightarrow\; a_n = 0 \end{aligned} \qquad (*)$$

$$\begin{pmatrix} 4 & 1 & 0 & 0 & \ldots & 0 \\ 1 & 4 & 1 & 0 & \ldots & 0 \\ & \ddots & \ddots & \ddots & & \\ & & \ddots & \ddots & \ddots & \\ & & & \ddots & \ddots & 1 \\ 0 & & & & 1 & 4 \end{pmatrix} \begin{pmatrix} a_1 \\ \\ \vdots \\ \vdots \\ \\ a_{n-1} \end{pmatrix} = \frac{6}{h^2} \begin{pmatrix} f_0 - 2f_1 + f_2 \\ \\ \vdots \\ \vdots \\ \\ f_{n-2} - 2f_{n-1} + f_n \end{pmatrix}$$

The coefficient matrix is

- tridiagonal
- symmetric

- positive definite
- strictly diagonally dominant

<u>`Notes`</u>:

1. For clamped splines, there are two additional equations that involve a_0 and a_n.
2. Condition (*) explains why the spline has additional inflection points. See the handout about natural cubic spline interpolation.

Recall
$A = (a_{ij})$ is <u>strictly diagonally dominant</u> if

$$|a_{ii}| > \sum_{\substack{j=1 \\ j \neq i}}^{n} |a_{ij}| \quad \text{for all} \quad i = 1, \ldots, n$$

Theorem *If A is strictly diagonally dominant, then A is invertible.*

`Proof`. Suppose A is not invertible. Then there exists a vector $x \neq 0$ such that $Ax = 0$. Choose index i such that $|x_i| = ||x||_\infty = \max_j |x_j|$. Then

$$0 = (Ax)_i = \sum_{j=1}^{n} a_{ij} x_j = a_{ii} x_i + \sum_{\substack{j=1 \\ j \neq i}}^{n} a_{ij} x_j$$

$$\Rightarrow \quad |a_{ii} x_i| = \left| - \sum_{\substack{j=1 \\ j \neq i}}^{n} a_{ij} x_j \right| \leq \sum_{\substack{j=1 \\ j \neq i}}^{n} |a_{ij}||x_j|$$

$$\Rightarrow \quad |a_{ii}| \leq \sum_{\substack{j=1 \\ j \neq i}}^{n} |a_{ij}| \frac{|x_j|}{|x_i|} \leq \sum_{\substack{j=1 \\ j \neq i}}^{n} |a_{ij}|$$

This contradicts the assumption that A is strictly diagonally dominant.

<u>`Note`</u>
In practice, the values $a_i = S''(x_i)$ are found by Gaussian elimination for a tridiagonal system.

Theorem *Let f be defined on $[a,b]$, $a = x_0 < x_1 < \ldots < x_{n-1} < x_n = b$ and let S be the natural cubic spline interpolant of f (or clamped cubic spline).*

$$1. \quad |f(x) - S(x)| \leq \frac{5}{384} \max_{a \leq x \leq b} |f^{(4)}(x)| \cdot h^4$$

where $h = \max_i |x_{i+1} - x_i|$

$$\int_a^b [S''(x)]^2 dx \leq \int_a^b [f''(x)]^2 dx \quad \textit{Minimum curvature property of cubic splines}$$

Note

1. Cubic spline interpolation is 4^{th} order accurate.
2. Condition (2) is optimality property: spline $S(x)$ "oscillates least" of all smooth functions satisfying interpolation condition + BC (natural BC or clamped spline $S'(x_0) = y_0'$, $S'(x_n) = y_n'$).

   Curvature

   $$\kappa(x) = \frac{|f''(x)|}{(1 + [f'(x)]^2)^{3/2}} \approx |f''(x)|$$

   $\Rightarrow$ $\int_a^b [f''(x)]^2 dx$ is a crude measure of the total curvature over an interval.

   $$\int_a^b [S''(x)]^2 dx \leq \int_a^b [f''(x)]^2 dx :$$

   any smooth interpolating function must have a total curvature at least as large as that of the cubic spline (natural or clamped)

`Proof of (2) for natural splines`

algebraic identity: $F^2 - S^2 = (F - S)^2 - 2S(S - F)$
Let $F = f''(x)$, $S = S''(x)$, integrate over $[a,b]$.

$$\int_a^b [f''(x)]^2 dx - \int_a^b [S''(x)]^2 dx = \int_a^b [f''(x) - S''(x)]^2 dx$$

$$- 2 \int_a^b S''(x)(S''(x) - f''(x)) dx$$

The first term is ≥ 0. We will show that the second term is 0.

<u>`Integration by parts`</u>:

$$\int_a^b u(x)v'(x)dx = u(x)v(x)|_a^b - \int_a^b u'(x)v(x)dx$$

$$\int_a^b S''(x)(S''(x) - f''(x))dx = \sum_{i=0}^{n-1} \int_{x_i}^{x_{i+1}} S''(x)(S''(x) - f''(x))dx$$

$$= \sum_{i=0}^{n-1} \left(S''(x)(S'(x) - f'(x))|_{x_i}^{x_{i+1}} - \int_{x_i}^{x_{i+1}} S'''(x)(S'(x) - f'(x))dx \right)$$

$$= -\sum_{i=0}^{n-1} S'''(x_i) \int_{x_i}^{x_{i+1}} (S'(x) - f'(x))dx$$

using $S''(x_0) = S''(x_n) = 0$; telescoping sum and $S_i'''(x)$ is constant

$$-\sum_{i=0}^{n-1} S'''(x_i)(S(x) - f(x))|_{x_i}^{x_{i+1}} = 0$$

using $S(x_i) = f(x_i)$, $i = 0, \ldots, n$.