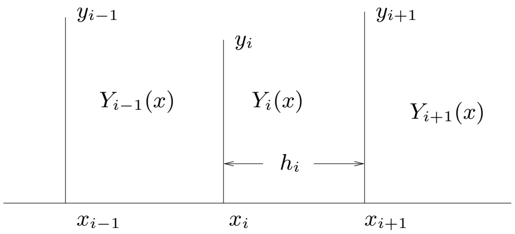
**Another spline formulation with $s_i''$ as primary variables.**




$$\begin{aligned}
\text{Let } Y_i(x) &= a_i(x-x_i)^3 + b_i(x-x_i)^2 + c_i(x-x_i) + d_i \\
Y_i'(x) &= 3a_i(x-x_i)^2 + 2b_i(x-x_i) + c_i \\
Y_i''(x) &= 6a_i(x-x_i) + 2b_i \\
\textbf{at } x_i: \quad y_i &= Y_i(x_i) = d_i \qquad \leftarrow \text{ interpolates the function at } x_i \qquad (1) \\
y_{i+1} &= Y_i(x_{i+1}) = a_i h_i^3 + b_i h_i^2 + c_i h_i + y_i \leftarrow \text{ enforce continuity} \qquad (2)
\end{aligned}$$

$$\text{Introduce primary variable}: s_i'' = Y_i''(x_i) = 2b_i \Rightarrow \boxed{b_i = s_i''/2} \qquad (3)$$

$$\text{Build in continuity of } Y'' \Rightarrow s_{i+1}'' = Y_i''(x_{i+1}) = 6a_i h_i + s_i'' \Rightarrow \boxed{a_i = \frac{s_{i+1}''-s_i''}{6h_i}} \qquad (4)$$

$$\begin{aligned}
\therefore Y_i(x) &= \left(\frac{s_{i+1}''-s_i''}{6h_i}\right)(x-x_i)^3 + \frac{s''}{2}(x-x_i)^2 + c_i(x-x_i) + y_i \\
(2) \Rightarrow \quad y_{i+1} &= \left(\frac{s_{i+1}''-s_i''}{6h_i}\right)h_i^3 + \frac{s_i''}{2}h_i^2 + c_i h_i + y_i \\
c_i &= \left(\frac{y_{i+1}-y_i}{h_i}\right) - \left(\frac{s_{i+1}''-s_i''}{6}\right)h_i - \frac{s_i''}{2}hi \\
&= \frac{\Delta y_i}{h_i} - \left(\frac{s_{i+1}''+2s_i''}{6}\right)h_i
\end{aligned}$$

Impose continuity of first derivatives:

$$\begin{aligned}
Y_i'(x_i) &= 3a_i(x_i-x_i)^2 + 2b_i(x_i-x_i) + c_i = c_i \\
Y_{i-1}'(x_i) &= 3a_{i-1}h_{i-1}^2 + 2b_{i-1}h_{i-1} + c_{i-1} \\
\therefore c_i = \frac{\Delta y_i}{h_i} - \left(\frac{s_{i+1}''+2s_i''}{6}\right)h_i &= 3\left(\frac{s_i''-s_{i-1}''}{6h_{i-1}}\right)h_{i-1}^2 + s_{i-1}''h_{i-1} + \left\{\frac{\Delta y_{i-1}}{h_{i-1}} - \left(\frac{s_i''+2s_{i-1}''}{6}\right)h_{i-1}\right\}
\end{aligned}$$

$$\boxed{h_{i-1}s_{i-1}''(-3+6-2) + (2h_i+2h_{i-1})s_i'' + h_i s_{i+1}'' \qquad = 6\left(\frac{\Delta y_i}{h_i} - \frac{\Delta y_{i-1}}{h_{i-1}}\right)}$$

or

$$\boxed{h_{i-1}s_{i-1}'' + (2h_i+2h_{i-1})s_i'' + h_i s_{i+1}'' \qquad = 6\left(\frac{\Delta y_i}{h_i} - \frac{\Delta y_{i-1}}{h_{i-1}}\right)}$$

$i = 1, \ldots N-1 \qquad N-1$ EQ

2 EXTRA CONDITIONS

**Boundary Conditions**


(1) **Natural Spline:** $s''_0 = 0 = s''_N$ two extra condtions

$$\begin{bmatrix} (2h_0+2h_1) & h_1 & & \\ h_1 & (2h_1+2h_2) & h_2 & \\ \vdots & \vdots & \vdots & \\ & & & h_{N-2} \\ & & h_{N-2} & (2h_{N-2}+2h_{N-1}) \end{bmatrix} \begin{bmatrix} s''_1 \\ s''_2 \\ \vdots \\ \vdots \\ s''_{N-1} \end{bmatrix} = 6 \begin{bmatrix} \frac{y_2-y_1}{h_1} - \frac{y_1-y_0}{h_0} \\ \frac{y_3-y_2}{h_2} - \frac{y_2-y_1}{h_1} \\ \vdots \\ \vdots \\ \frac{y_N-y_{N-1}}{h_{N-1}} - \frac{y_{N-1}-y_{N-2}}{h_{N-2}} \end{bmatrix}$$

(2) **Clamped Spline:** Specified first derivatives

Given $f'(x_0) = A$ and $f'(x_n) = B$.

$$\begin{aligned} \mathrm{A} = \mathrm{Y}'_0(x_0) &= c_0 = \frac{y_1-y_0}{h_0} - \frac{2h_0 s''_0 + h_0 s''_1}{6} = \mathrm{A} \Rightarrow \boxed{2h_0 s''_0 + h_0 s''_1 = 6\left(\tfrac{y_1-y_0}{h_0} - \mathrm{A}\right)} \\ \mathrm{B} = \mathrm{Y}'_{N-1}(x_n) &= 3a_{n-1}h_{n-1}^2 + 2b_{n-1}h_{n-1} + c_{n-1} \\ &= 3\left(\frac{s_n - s_{n-1}}{6h_{n-1}}\right) h_{n-1}^2 + s_{n-1}h_{n-1} + \frac{y_n - y_{n-1}}{h_{n-1}} - \left(\frac{2h_{n-1}s''_{n-1} + h_{n-1}s''_n}{6}\right) \\ 6\left(B - \frac{y_n - y_{n-1}}{h_{n-1}}\right) &= 3h_{n-1}s''_n - 3h_{n-1}s''_{n-1} + 6h_{n-1}s''_{n-1} - 2h_{n-1}s''_{n-1} - h_{n-1}s''_n \end{aligned}$$

$$\boxed{6\left(B - \tfrac{y_n - y_{n-1}}{h_{n-1}}\right) = 2h_{n-1}s''_{n-1} + 2h_{n-1}s''_n}$$

But $h_0 s''_0 + (2h_0 + 2h_1)s''_1 + h_1 s''_2 = 6\{[f[x_1,x_2] - f[x_0,x_1]\}$

$$\begin{bmatrix} 2h_0 & h_0 & & & \\ h_0 & (2h_0+2h_1) & h_1 & & \\ & & & & \\ & h_{n-2} & (2h_{n-2}+2h_{n-1}) & h_{n-1} \\ & & h_{n-1} & 2h_{n-1} \end{bmatrix} \begin{bmatrix} s''_0 \\ s''_1 \\ \\ s''_{N-1} \\ s''_N \end{bmatrix} = 6 \begin{bmatrix} (y_1-y_0)/h_0 - \mathrm{A} \\ (y_2-y_1)/h_1 - \frac{y_1-y_0}{h_0} \\ \vdots \\ \vdots \\ (y_n - y_{n-1})/h_{n-1} - (y_{n-1}-y_{n-2})/h_{n-2} \\ \mathrm{B} - \frac{y_n - y_{n-1}}{y\,h_{n-1}} \end{bmatrix}$$

3. **Quadratic boundary interval representation**

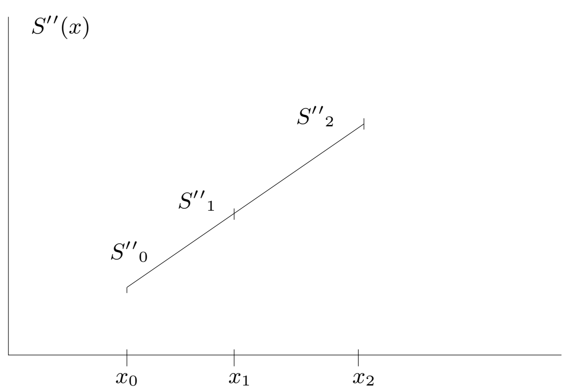
$$s_0'' = s_1'' \qquad s_{N-1}'' = s_N''$$

$$a_0 = \left(\frac{s_1''-s_0''}{6h_0}\right) = 0 \qquad\qquad a_{n-1} = \frac{s_N''-s_{N-1}''}{6h_{N-1}}$$

$\therefore$ a quadratic $\qquad\qquad$ a quadratic

$$\begin{bmatrix} (3h_0+2h_1) & h_1 & 0 & & \\ h_1 & (2h_1+2h_2) & h_2 & 0 & 0 \\ & & & & \\ & & & (2h_{N-3}+2h_{N-2})h_{N-2} & \\ & & & h_{N-2}(2h_{N-2}+3h_{N-1}) & \end{bmatrix} \begin{bmatrix} s_1'' \\ s_2'' \\ \vdots \\ \\ s_{N-1}'' \end{bmatrix} = 6 \begin{bmatrix} f[x_1,x_2]-f[x_0,x_1] \\ \\ \\ \\ f[x_{N-1},x_N)-f[x_{N-2},x_{N-1}] \end{bmatrix}$$

4. **Linear extrapolation**




$$\frac{s_1''-s_0''}{h_0} = \frac{s_2''-s_1''}{h_1} \Rightarrow s_0'' = s_1'' - (s_2''-s_1'')\frac{h_0}{h_1} = s_1''\frac{(h_1+h_0)}{h_1} - s_2''\frac{h_0}{h_1}$$

$$h_0 s_0'' + (2h_0+2h_1)s_1'' + h_1 s_1'' = 6(f[x_1,x_2]-f[x_0,x_1])$$

$$h_0\frac{(h_0+h_1)}{h_1}s_1'' - s_2''\frac{h_0^2}{h_1} + \frac{h_1}{h_1}2(h_0+h_1)s_1'' + h_1 s_2'' = \text{ RHS}$$

$$\therefore \qquad \frac{(h_0+h_1)}{h_1}(h_0+2h_1)s_1'' + \left(\frac{h_1^2-h_0^2}{h_1}\right)s_2'' = \text{ RHS}$$

$$\begin{bmatrix} \frac{(h_0+h_1)}{h_1}(h_0+2h_1) & \frac{(h_0^2-h_0^2)}{h_1} & 0 & \dots \\ h_1 & (2h_1+2h_2) & h_2 & 0 \\ 0 & & & \end{bmatrix} \begin{bmatrix} s_1'' \\ s_2'' \\ \vdots \end{bmatrix}$$

5. **Not-a-knot condition**

$Y_0(x) \equiv Y_1(x) \qquad Y_{N-2}(x) \equiv Y_{N-1}(x)$

Unknowns $= 4(N-2)$
Constraints $= 3(N-3)$

$4(N-2) - 3(N-3) = N+1 \qquad$ unknowns $\longleftrightarrow$ the values at $x_0, \ldots, x_N$.

$$
\begin{aligned}
s''_{i-1}h_{i-1} &+ 2(h_{i-1}+h_i)s''_i + h_i s''_{i+1} \quad = \quad 6(f[x_1,x_2] - f[x_0,x_1]) \\
Y_1(x) &= a_1(x-x_1)^3 + b_1(x-x_1)^2 + c_1(x-x_1) + d_1 \\
Y'_1(x) &= 3a_1(x-x_1)^2 + b_1(x-x_1) + c_1 \\
Y''_1(x) &= 6a_1(x-x_1) + 2b_1, \qquad\qquad x_1 - x_0 = h_0 \\
s''_0 &= Y''_1(x_0) = 6\left(\frac{s''_2 - s''_1}{6h_1}\right)(x_0 - x_1) + 2(s''_1/2) \\
&\qquad = -(s''_2 - s''_1)\frac{h_0}{h_1} + s''_1 \\
\therefore &\quad s''_0 = s''_1\frac{(h_1+h_0)}{h_1} - s''_2\frac{h_0}{h_1} \\
\text{But } h_0 s''_0 &+ 2(h_0+h_1)s''_1 + h_1 s''_2 = 6(f[x_1,x_2] - f[x_0,x_1]) \\
\therefore &\quad \left(2 + \frac{h_0}{h_1}\right)(h_0+h_1)s''_1 + \left(1 - \frac{h_0}{h_1}\right)(h_0+h_1)s''_2 = 6(f[x_1,x_2] - f[x_0,x_1])
\end{aligned}
$$

$$
\text{Also} \left(2 + \frac{h_{N-1}}{h_{N-2}}\right)(h_{N-2} + h_{N-1})s''_{N-1} + \left(1 - \frac{h_{N-1}}{h_{N-2}}\right)(h_{N-2}+h_{N-1})s''_{N-2} = 6(f[x_{N-1},x_N] - f[x_{N-2},x_{N-1}])
$$

$$
\begin{bmatrix}
(2+\frac{h_0}{h_1})(h_0+h_1) & (1-\frac{h_0}{h_1})(h_1+h_0) & 0 & \ldots & 0 & \\
h_1 & 2(h_1+h_2) & h_2 & 0 & \ldots & 0 \\
0 & & & & & \\
& & & & & \\
& & & h_{N-2} & & \\
& & (1-\frac{h_{N-1}}{h_{N-2}})(h_{N-2}+h_{N-1}) & (2+\frac{h_{N-1}}{h_{N-2}})(h_{N-2}+h_{N-1}) & &
\end{bmatrix}
\begin{bmatrix}
s''_1 \\ s''_2 \\ \vdots \\ s''_{N-2} \\ s''_{N-1}
\end{bmatrix}
$$

6. **A periodic spline**:

$$
\begin{aligned}
s''(x_{0^+}) &= s''(x_{N^-}) \\
s''(x_{0^+}) &= s''(x_{N^-}).
\end{aligned}
$$

(III) **Smoothness property of a natural spline** $\quad s''(x_0) = 0 = s''(x_N)$

In order to impose this condition it is convenient to consider the $s''_k$ as unknowns in which case the equations become:

$$\Delta x_k s''_{k-1} + 2(\Delta x_k + \Delta x_{k+1})s''_k + \Delta x_{k+1}s''_{k+1} = 6(f[x_k, x_{k+1}] - f[x_{k-1}, x_k]) \qquad k = 1, \ldots, N-1.$$

Important identity: $(y'' - s'')[(y'' - s'') + 2s''] = (y'' - s'')(y'' + s'') = (y'')^2 - (s'')^2$

**NOTE**:

1. Let $y(x)$ be any other interpolant of $f(x)$ at $(x_0, \ldots, x_N)$ then

$$\int_a^b (y'')^2 dx - \int_a^b (s''^2) dx = \int_a^b (y'' - s'')^2 dx + 2\int_a^b s''(y'' - s'')dx.$$

$$\begin{aligned} \text{Now} \int_a^b s''(y'' - s'')dx &= s''(y' - s')\Big|_a^b - \sum_{k=1}^{N} \int_{x_{k-1}}^{x_k} s'''(y' - s')dx \qquad s''' = \text{ const on each subinterval} \\ &= s''(y' - s')\Big|_a^b - \sum_{k=1}^{N} c_k(y - s)\Big|_{x_{k-1}}^{x_k} \quad \text{both interpolants} \\ &= s''(y' - s')\Big|_a^b \end{aligned}$$

If we choose $s : s''(a) = 0 = s''(b)$ for example or if $y$ and $s$ both interpolate $f'$ at $a$ and $b$ then $\int_a^b s''(y'' - s'')dx = 0$.

$$\therefore \int_a^b y''^2 dx = \int_a^b (y'' - s'')^2 dx + \int_a^b (s'')^2 dx \geq \int_a^b s''^2 dx.$$

Thus $s$ is the interpolant with the **MINIMUM CURVATURE** (i.e. smoothest)

2. **Error involved in spline interpolation**:

$$\begin{aligned} |f(x) = s(x)| &\leq ||f^{(4)}||_\infty 5\frac{\Delta\bar{x}^4}{384} \qquad \Delta\bar{x} = \max \Delta x : \\ |f'(x) - s'(x)| &\leq ||f^{(4)}||_\infty \frac{\Delta\bar{x}^3}{24} \qquad \text{for nonuniform points} \\ &\leq ||f^{(5)}||_\infty \frac{\Delta x^4}{60} \qquad \text{for uniform points} \end{aligned}$$

$\therefore$ cubic spline provides an excellent technique for **NUMERICAL DIFFERENTIATION**.

**How do we solve for the $\{s_k''\}$?**

$$\begin{bmatrix} d_1 & c_1 & & & & \\ a_2 & d_2 & c_2 & & 0 & \\ 0 & a_3 & d_3 & & & \\ & & & \ddots & \ddots & \\ & & 0 & & d_{n-1} & c_{n-1} \\ & & & \ddots & & \\ & & & & a_n & d_n \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \\ \\ \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ \\ \\ \\ \\ b_n \end{bmatrix}$$

$$\begin{aligned} d_1 \neq 0 \qquad d_1x_1 + c_1x_2 &= b_1 && (1) \\ a_2x_1 + d_2x_2 + c_2x_3 &= b_2 && (2) \\ (2) - \frac{a_2}{d_1}(1) \Rightarrow \qquad \left(d_2 - \frac{a_2}{d_1}c_1\right)x_2 + c_2x_3 &= b_2 - \frac{a_2}{d_1}b_1 \\ d_2'x_2 + c_2x_3 &= b_2' \qquad d_2' = d_2 - \frac{a_2}{d_1}c_1 \\ & \qquad b_2' = b_2 - \frac{a_2}{d_1}b_1 \end{aligned}$$

Similarly

$$\boxed{\begin{aligned} & d_{k+1}'x_{k+1} + c_{k+1}x_{k+2} = b_{k+1}' \\ \text{where} \quad & d_{k+1}' = d_{k+1} - \frac{a_{k+1}}{d_k'}c_k \qquad b_{k+1}' = b_{k+1} - \frac{a_{k+1}}{d_k'}b_k' \end{aligned}}$$

$$\begin{bmatrix} d_1' & c_1 & & & \\ & d_2' & c_2 & & \\ & & & & \\ & & & d_{n-1}' & c_{n-1} \\ & & & & d_n' \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1' \\ b_2' \\ \\ b_n' \end{bmatrix}$$

**Back Substitution**

$$\begin{aligned} x_n &= b_n'/d_n' \\ x_{n-1} &= (b_{n-1}' - c_{n-1}x)/d_{n-1}' \end{aligned}$$

$$\boxed{\begin{aligned} x_n &= b_n'/d_n' \\ x_k &= (b_k' - c_kx_{k+1})/d_k' \qquad k = n-1, \ldots, 1 \end{aligned}}$$

Note, if we let $m_k = \frac{a_k}{d_{k-1}'}$ then

$$A = \begin{bmatrix} 1 & \ddots & 0 \\ m_2 & \ddots & \\ 0 & & \\ & & m_n 1 \end{bmatrix} \begin{bmatrix} d_1' & c_1 & 0 \\ & \ddots & \\ 0 & \ddots & c_{n-1} \\ & & d_n' \end{bmatrix} = LU \begin{bmatrix} & LU & \\ \text{Forward} & Ly = b & y = L^{-1}b \\ \text{Back} & Ux = y & \\ \text{Substitution} & & \end{bmatrix}$$