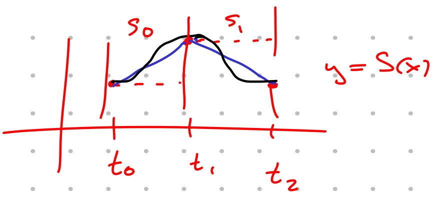
Cubic Splines $(k=3)$



x	$t_0 < t_1 < \cdots < t_n$
y	$y_0 \quad y_1 \quad \cdots \quad y_n$

let $S_i = S|_{[t_i, t_{i+1}]}$. Each S_i is a cubic polynomial.

$$\boxed{S(x) = \begin{cases} S_0(x) & \text{if } t_0 \le x < t_1 \\ S_1(x) & \text{if } t_1 \le x < t_2 \\ \vdots & \\ S_{n-1}(x) & \text{if } t_{n-1} \le x \le t_n \end{cases}}$$

$\{1, x, x^2, x^3\}$

$S_i(x) = a_i x^3 + b_i x^2 + c_i x + d_i \qquad 0 \le i \le n-1$ (We won't be using this form later)

$\Rightarrow$ $4n$ variables a_i, b_i, c_i, d_i

$S \in C^2[t_0, t_n] \Rightarrow$
$S_{i-1}(t_i) = S_i(t_i) = y_i \qquad 1 \le i \le n-1$
$S'_{i-1}(t_i) = S'_i(t_i)$ — $4(n-1)$ equations
$S''_{i-1}(t_i) = S''_i(t_i)$

& $S_0(t_0) = y_0$ & $S_{n-1}(t_n) = y_n$ $\Rightarrow$ Total of $4(n-1)+2 = 4n-2$ equations.

$(4n \text{ variables}) - (4n-2 \text{ equations}) = (2 \text{ degrees of freedom})$

Natural Cubic Spline:

Consider $S(t_i) = y_i$ and $S''(t_i) = z_i \qquad 0 \le i \le n$

Set $h_i = t_{i+1} - t_i \qquad 0 \le i < n$

$S_i \to$ cubic $\qquad S_i''$ is linear

Since $S_i''(t_i) = z_i$, $S_i''(t_{i+1}) = z_{i+1}$ and S_i'' is linear,

Clearly linear in x.

$$S_i''(x) = \frac{z_i}{h_i}(t_{i+1} - x) + \frac{z_{i+1}}{h_i}(x - t_i)$$

$S_i''(t_i) = \frac{z_i}{h_i} h_i + 0 = z_i$

$S_i''(t_{i+1}) = 0 + \frac{z_{i+1}}{h_i} h_i = z_{i+1}$

$$\Rightarrow S_i(x) = \frac{z_i}{6h_i}(t_{i+1}-x)^3 + \frac{z_{i+1}}{6h_i}(x-t_i)^3 + Ax + B$$

or
$$S_i(x) = \frac{z_i}{6h_i}(t_{i+1}-x)^3 + \frac{z_{i+1}}{6h_i}(x-t_i)^3 + C(x-t_i) + D(t_{i+1}-x)$$

since $\text{span}(1, x) = \text{span}(x - t_i, t_{i+1} - x)$.

$S(t_i) = S_i(t_i) = y_i$

$$\Rightarrow y_i = \frac{z_i}{6\cancel{h_i}} h_i^{\cancel{3}\,2} + 0 + 0 + D h_i$$

$$\Rightarrow D h_i = y_i - \frac{z_i h_i^2}{6} \Rightarrow D = \frac{y_i}{h_i} - \frac{z_i h_i}{6}$$

$S(t_{i+1}) = S_i(t_{i+1}) = y_{i+1}$

$$\Rightarrow y_{i+1} = 0 + \frac{z_{i+1}}{6\cancel{h_i}} h_i^{\cancel{3}\,2} + C h_i + 0$$

$$\Rightarrow C h_i = y_{i+1} - \frac{z_{i+1}}{6} h_i^2 \Rightarrow C = \frac{y_{i+1}}{h_i} - \frac{z_{i+1} h_i}{6}$$

Thus,
$$S_i(x) = \frac{z_i}{6h_i}(t_{i+1}-x)^3 + \frac{z_{i+1}}{6h_i}(x-t_i)^3 + \left(\frac{y_{i+1}}{h_i} - \frac{z_{i+1}h_i}{6}\right)(x-t_i) + \left(\frac{y_i}{h_i} - \frac{z_i h_i}{6}\right)(t_{i+1}-x)$$

Note that all the constants are in terms of t_i, y_i, z_i's so once we determine the values of $z_0, z_1, \ldots, z_n$; we get $S(x)$.

In fact, $z_1, z_2, \ldots, z_{n-1}$ can be determined from z_0 and z_n using $S'_{i-1}(t_i) = S'_i(t_i)$.

$$S_i'(x) = -\frac{z_i}{2h_i}(t_{i+1}-x)^2 + \frac{z_{i+1}}{2h_i}(x-t_i)^2 + \left(\frac{y_{i+1}}{h_i} - \frac{z_{i+1}h_i}{6}\right) - \left(\frac{y_i}{h_i} - \frac{z_i h_i}{6}\right)$$

Thus,
$$S_i'(t_i) = -\frac{z_i h_i}{2} + \frac{y_{i+1}}{h_i} - \frac{z_{i+1} h_i}{6} - \frac{y_i}{h_i} + \frac{z_i h_i}{6}$$

$$= -\frac{z_i h_i}{3} - \frac{z_{i+1} h_i}{6} + \frac{y_{i+1}}{h_i} - \frac{y_i}{h_i}$$

$$S_{i-1}'(t_i) = 0 + \frac{z_i}{2\cancel{h_{i-1}}}(h_{i-1})^{\cancel{2}} + \frac{y_i}{h_{i-1}} - \frac{z_i h_{i-1}}{6} - \frac{y_{i-1}}{h_{i-1}} + \frac{z_{i-1} h_{i-1}}{6}$$

$$= \frac{z_i h_{i-1}}{3} + \frac{z_{i-1} h_{i-1}}{6} + \frac{y_i}{h_{i-1}} - \frac{y_{i-1}}{h_{i-1}}$$

Now, $S_i'(t_i) = S_{i-1}'(t_i)$

$$\Rightarrow \frac{h_{i-1}}{6} z_{i-1} + \left(\frac{h_{i-1} + h_i}{3}\right) z_i + \frac{h_i}{6} z_{i+1} = \frac{y_{i+1} - y_i}{h_i} - \frac{y_i - y_{i-1}}{h_{i-1}}$$

or
$$h_{i-1} z_{i-1} + 2(h_{i-1} + h_i) z_i + h_i z_{i+1} = 6\left(\frac{y_{i+1} - y_i}{h_i}\right) - 6\left(\frac{y_i - y_{i-1}}{h_{i-1}}\right)$$

Choosing $z_0 = z_n = 0$ and solving these equations, we get the natural cubic spline.

Set $u_i = 2(h_{i-1}+h_i)$, $b_i = \dfrac{6(y_{i+1}-y_i)}{h_i}$, and $v_i = b_i - b_{i-1}$

Then the equations we want to solve are given by

$$\begin{pmatrix} u_1 & h_1 & & & 0 \\ h_1 & u_2 & h_2 & & \\ & h_2 & u_3 & h_3 & \\ & & h_3 & \ddots & \ddots \\ & & & \ddots & u_{n-2} & h_{n-2} \\ 0 & & & & h_{n-2} & u_{n-1} \end{pmatrix} \begin{pmatrix} z_1 \\ \vdots \\ \vdots \\ z_{n-1} \end{pmatrix} = \begin{pmatrix} v_1 \\ \vdots \\ \vdots \\ v_{n-1} \end{pmatrix}$$

(diagonally dominant: $|A_{ii}| > \sum_{j=1, j\neq i}^{n} |A_{ij}|$

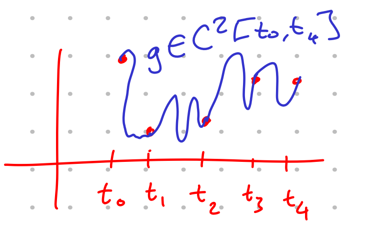
Since $h_i > 0$ and $u_i = 2(h_{i-1}+h_i)$ the tridiagonal system is diagonally dominant and can be solved using Gaussian elim. without scaled row pivoting. (In fact, because of this special form you can come up with a more efficient algorithm.)

Thm Theorem on Optimallity of Natural Cubic Splines

Let f'' be continuous in $[a,b]$ and let $a = t_0 < t_1 < \cdots < t_n = b$. If S is the natural cubic spline interpolating f at the knots t_i, then

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

$$\boxed{\|g\|_2^2 = \int_a^b (g(x))^2\,dx}$$



Pf let $g = f - S$ then $g(t_i) = 0$ and

$$\int_a^b (f'')^2\,dx = \int_a^b (S'')^2\,dx + \underbrace{\int_a^b (g'')^2\,dx}_{\geq 0} + \underbrace{2\int_a^b S''g''\,dx}_{\geq 0}$$

If $\int_a^b S''g''\,dx \geq 0$ we are done.

$$\int_a^b S''g''\,dx = \sum_{i=1}^{n} \int_{t_{i-1}}^{t_i} S''g''\,dx$$

$$\boxed{\begin{matrix} u = S'' & dv = g''dx \\ du = S'''dx & v = g' \end{matrix}}$$

$$= \sum_{i=1}^{n} \left[S''g' \Big|_{t_{i-1}}^{t_i} - \int_{t_{i-1}}^{t_i} S_i'''g'\,dx \right]$$

$S''(t_n) = S''(t_0) = 0$ because S is the natural cubic spline.

$$= \underbrace{S''(t_1)g'(t_1) - \boxed{\cancel{S''(t_0)}g'(t_0)}}_{i=1} + \underbrace{S''(t_2)g'(t_2) - S''(t_1)g'(t_1)}_{i=2} + \cdots$$

$$\cdots + \underbrace{\boxed{\cancel{S''(t_n)}g'(t_n)} - S''(t_{n-1})g'(t_{n-1})}_{i=n}$$

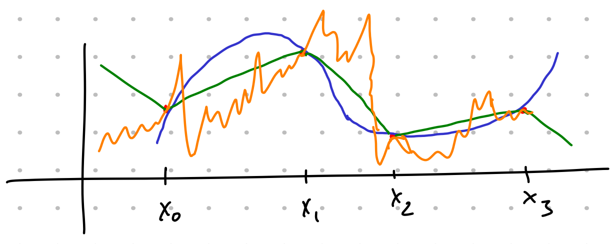
$$- \sum_{i=1}^{n} \int_{t_{i-1}}^{t_i} c_i\, g'\,dx \qquad \text{where } S_i'''(x) = c_i$$

$$= -\sum_{i=1}^{n} c_i \int_{t_{i-1}}^{t_i} g'\,dx = -\sum_{i=1}^{n} c_i\,(\overset{0}{g(t_i)} - \overset{0}{g(t_{i-1})}) = 0 \qquad (g = f - S)$$

Chp 7 Numerical Differentiation and Integration

7.1 Numerical Differentiation and Richardson Extrapolation

Say we know that f passes through $(x_0,y_0), \ldots, (x_n,y_n)$. What can we say about $f'(x)$ or $\int_a^b f(x)\,dx$?



If f can be any continuous function, we cannot say much. However, if f is a polynomial of degree $\leq n$, then we can compute $f'(x)$ and $\int_a^b f(x)\,dx$ exactly (up to roundoff errors).

In general, if we should be skeptical of any numerical estimate of f' or $\int_a^b f\,dx$ unless we also have bounds on the errors involved.

Numerical Differentiation

Since $f'(x) = \lim_{h\to 0} \dfrac{f(x+h) - f(x)}{h}$, we can approximate

$$f'(x) \approx \frac{f(x+h) - f(x)}{h} \qquad \text{Error?}$$

$$\rightarrow f(x+h) = f(x) + f'(x)h + \frac{f''(y)}{2}h^2 \qquad \text{for some } y \text{ between } x \text{ and } x+h.$$

(Assuming f'' exist and cont)

$$\Rightarrow f'(x) = \underbrace{\frac{f(x+h) - f(x)}{h}}_{\text{"formula" estimate}} - \frac{h}{2} f''(y)$$

Error term applies to $f \in C^2(I)$

Error $\rightarrow 0$ linearly as $h \rightarrow 0$

Example For $f(x) = \cos x$, approximate $f'(\frac{\pi}{4})$ with $h = 0.01$

$$f'\left(\frac{\pi}{4}\right) \simeq \frac{\cos(\frac{\pi}{4} + 0.01) - \cos(\frac{\pi}{4})}{0.01} \overset{\text{calculator}}{=} \frac{1}{0.01}(0.70000476 - 0.70710678)$$

$$= -0.71063051$$

$$|\text{Error}| = \left|\frac{h}{2} f''(y)\right| = 0.005\,|\cos(y)| \leq 0.005$$

Since $\frac{\pi}{4} < y < \frac{\pi}{4} + 0.01$, $|\cos y| < 0.707107$

$\Rightarrow |\text{Error}| \leq 0.0035355$

Error $= -\frac{h}{2} f''(y)$ is called the truncation error "because" it is the error obtained from a "truncated Taylor series."

Taylor series:

$$f(x+h) = f(x) + h f'(x) + \boxed{\frac{h^2}{2} f''(x)} + \frac{h^3}{3!} f'''(x) + \cdots$$

Example For $f(x) = \tan^{-1} x$, estimate $f'(\sqrt{2})$ using a sequence of $h \to 0$. $\left(f'(x) = \frac{1}{1+x^2} \text{ so } f'(\sqrt{2}) = \frac{1}{3} \right)$

Using $h = 2^{-k}$, set $r = \frac{f(\sqrt{2}+h) - f(\sqrt{2})}{h}$

k	h	r
4	$0.62 \cdot 10^{-1}$	0.32374
12	$0.24 \cdot 10^{-3}$	0.33325 $\approx 1/3$
20	$0.95 \cdot 10^{-6}$	0.31250
24	$0.60 \cdot 10^{-7}$	1.00000
26	$0.15 \cdot 10^{-7}$	0.00000

(Why do we see $r = 0$?)

Error $= O(h)$!