$\Rightarrow \boxed{|e_n(x)| \le \frac{M}{8} h^2}$ note: $M = \max_{x \in [a,b]} |f''(x)|$

Note: This result says: If the nodes $x_0, x_1, \dots, x_n$ are very close, then h is small, and error can be small

Problems with Linear Splines

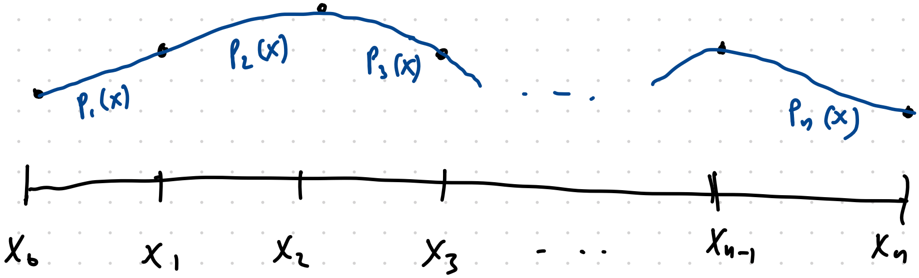
- They are NOT smooth. That is, although $s(x)$ is continuous for all x, $s'(x)$ is NOT continuous at breakpoints (think of solutions of ODEs/PDEs)

High-degree Splines – properties of degree m spline

1) Domain is a closed interval $[\alpha, \beta]$
2) $s(x), s'(x), \dots, s^{(m-1)}(x)$ are continuous on $[\alpha, \beta]$
3) $[\alpha, \beta]$ is partioned s.t.

$$\alpha = x_0 < x_1 < x_2 < \dots < x_n = \beta$$

where $s(x)$ is a polynomial of degree at most m on $[x_{i-1}, x_i]$



Terminology

Knots = break points That is, points where you switch from one poly. to another

Nodes = points where spline interpolates data

Often knots = nodes

Cubic Splines : Used often in applications.

How do we construct these?

Basic Idea:

- Suppose we are given interpolation data $\{(x_i, f_i)\}_{i=0}^{n}$
- Find $S(x)$ satisfying

$$S(x) = \begin{cases} P_1(x) & x_0 \le x < x_1 \\ P_2(x) & x_1 \le x < x_2 \\ \vdots & \vdots \\ P_n(x) & x_{n-1} \le x \le x_n \end{cases}$$

where $P_i(x) = a_i + b_i(x - x_i) + c_i(x - x_i)^2 + d_i(x - x_i)^3$

and $S(x_i) = f(x_i)$.

To find $S(x)$, we need to find

a_i, b_i, c_i, d_i, $i = 1, 2, \ldots, n$ $\Rightarrow$ have $4n$ unknowns $\Rightarrow$ need $4n$ equations.

Conditions to be satisfied

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1) **Interpolation** : $s(x_i) = f_i \quad , \quad i = 0, 1, \dots, n$

Note $p_i(x) = a_i + b_i(x - x_i) + c_i(x - x_i)^2 + d_i(x - x_i)^3$

$$\left.\begin{aligned} p_1(x_0) &= f_0 \\ p_1(x_1) &= f_1 \\ p_2(x_2) &= f_2 \\ &\vdots \\ p_n(x_n) &= f_n \end{aligned}\right\} \quad \boxed{\begin{aligned} a_1 + b_1(x_0 - x_1) + c_1(x_0 - x_1)^2 + d_1(x_0 - x_1)^3 &= f_0 \\ a_1 &= f_1 \\ a_2 &= f_2 \\ &\vdots \\ a_n &= f_n \end{aligned}}$$

This gives $n+1$ equations

2) **Continuity of $s(x)$** : $p_{i+1}(x_i) = p_i(x_i) \quad , \quad i = 1, 2, \dots, n-1$

$$\left.\begin{aligned} p_2(x_1) &= p_1(x_1) \\ p_3(x_2) &= p_2(x_2) \\ &\vdots \\ p_n(x_{n-1}) &= p_{n-1}(x_{n-1}) \end{aligned}\right\} \quad \boxed{\begin{aligned} a_2 + b_2(x_1 - x_2) + c_2(x_1 - x_2)^2 + d_2(x_1 - x_2)^3 &= a_1 \\ a_3 + b_3(x_2 - x_3) + c_3(x_2 - x_3)^2 + d_3(x_2 - x_3)^3 &= a_2 \\ &\vdots \\ a_n + b_n(x_{n-1} - x_n) + c_n(x_{n-1} - x_n)^2 + d_n(x_{n-1} - x_n)^3 &= a_{n-1} \end{aligned}}$$

This gives $n-1$ equations

3) Continuity of $s'(x)$: $P_{i+1}'(x_i) = P_i'(x_i)$, $i=1,\dots,n-1$

Note: $P_i'(x) = b_i + 2c_i(x-x_i) + 3d_i(x-x_i)^2$

$$\left.\begin{aligned} P_2'(x_1) &= P_1'(x_1) \\ P_3'(x_2) &= P_2'(x_2) \\ &\vdots \\ P_n'(x_{n-1}) &= P_{n-1}'(x_{n-1}) \end{aligned}\right\} \quad \boxed{\begin{aligned} b_2 + 2c_2(x_1-x_2) + 3d_2(x_1-x_2)^2 &= b_1 \\ b_3 + 2c_3(x_2-x_3) + 3d_3(x_2-x_3)^2 &= b_2 \\ &\vdots \\ b_n + 2c_n(x_{n-1}-x_n) + 3d_n(x_{n-1}-x_n)^2 &= b_{n-1} \end{aligned}}$$

this gives $n-1$ equations.

4) Continuity of $s''(x)$: $P_{i+1}''(x_i) = P_i''(x_i)$, $i=1,2,\dots,n-1$

Note: $P_i''(x) = 2c_i + 6d_i(x-x_i)$

$$\left.\begin{aligned} P_2''(x_1) &= P_1''(x_1) \\ P_3''(x_2) &= P_2''(x_2) \\ &\vdots \\ P_n''(x_{n-1}) &= P_{n-1}''(x_{n-1}) \end{aligned}\right\} \quad \boxed{\begin{aligned} 2c_2 + 6d_2(x_1-x_2) &= 2c_1 \\ 2c_3 + 6d_3(x_2-x_3) &= 2c_2 \\ &\vdots \\ 2c_n + 6d_n(x_{n-1}-x_n) &= 2c_{n-1} \end{aligned}}$$

This gives $n-1$ equations

Note: So far, we have $(n+1)+(n-1)+(n-1)+(n-1)$
$= 4n-2$ equations

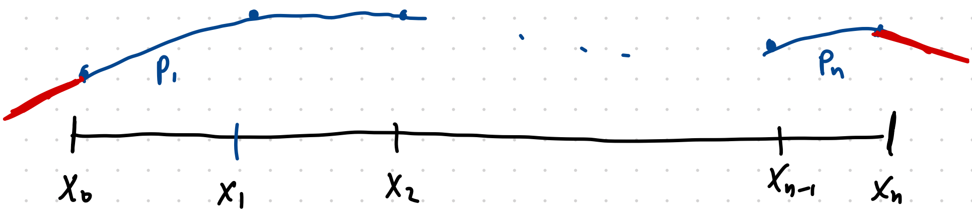
- But we have $4n$ unknowns $\Rightarrow$ we need two more equations. Where to get these?

we specify extra boundary conditions.

5) End Conditions (Several Options)

a) Natural (or Free) boundary conditions

Assume $s(x)$ is a linear polynomial (line) for $x < x_0$ and $x > x_n$



This means:

$s''(x_0) = 0 \quad \Rightarrow \quad p_1''(x_0) = 0$

$s''(x_n) = 0 \quad \Rightarrow \quad p_n''(x_n) = 0$

Recall

$$\boxed{p_i''(x) = 2c_i + 6\,d_i\,(x - x_i)}$$

$$\Rightarrow \boxed{\begin{aligned} 2c_1 + 6\,d_1\,(x_0 - x_1) &= 0 \\ 2c_n &= 0 \end{aligned}}$$

b) Clamped End conditions (1st deriv. condition)

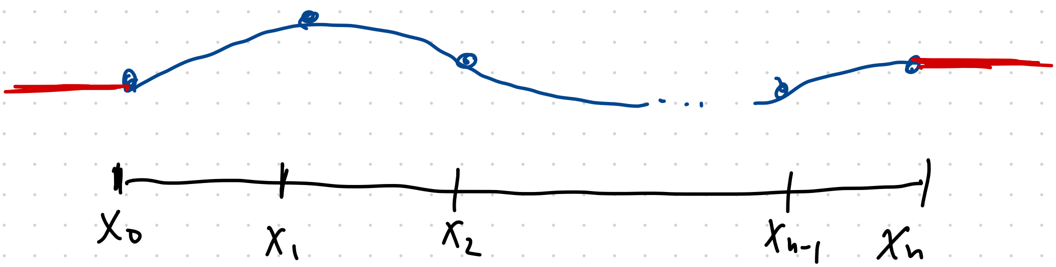
Here, we specify slope at endpoints. That is, we suppose we want the slope at x_0 to be δ_0 and slope at x_n to be δ_n.

Then

$$s'(x_0) = \delta_0 \qquad \Rightarrow \qquad p_1'(x_0) = \delta_0$$
$$s'(x_n) = \delta_n \qquad \qquad p_n'(x_n) = \delta_n$$

$$\Rightarrow \boxed{\begin{aligned} b_1 + 2c_1(x_0 - x_1) + 3d_1(x_0 - x_1)^2 &= \delta_0 \\ b_n &= \delta_n \end{aligned}}$$

For example, if we choose $\delta_0 = \delta_n = 0$, then our spline might look like:



c) Can similarly clamp 2^{nd} derivative

Cubic B-Splines ("Basis" Splines)

Recall from polynomial interpolation, we find

- $p(x)$ s.t. $p(x_i) = f_i$
- $p(x)$ is unique, but can write in different ways (different bases).

- Power Series Basis (Monomial basis)

$$\{1, x, x^2, \dots, x^n\} \qquad p(x) = \sum_{i=0}^{n} a_i x^i$$

- Newton Basis

$$\{1, (x-x_0), (x-x_0)(x-x_1), \dots, (x-x_0)(x-x_1)\cdots(x-x_{n-1})\}$$

$$p(x) = \sum_{i=0}^{n} \left[b_i \prod_{j=0}^{i-1} (x-x_j) \right]$$

- Lagrange Basis

$$\{L_{n,0}(x), L_{n,1}(x), \dots, L_{n,n}(x)\} \qquad p(x) = \sum_{i=0}^{n} f_i L_{n,i}(x)$$

<u>Question:</u> Can we find a basis for cubic splines?

That is, instead of writing

$$S_{3,n}(x) = \begin{cases} P_1(x) \\ P_2(x) \\ \vdots \\ P_n(x) \end{cases}$$

We want to find basis function

$$\{ B_{-1}(x), B_0(x), \ldots, B_n(x), B_{n+1}(x) \}$$

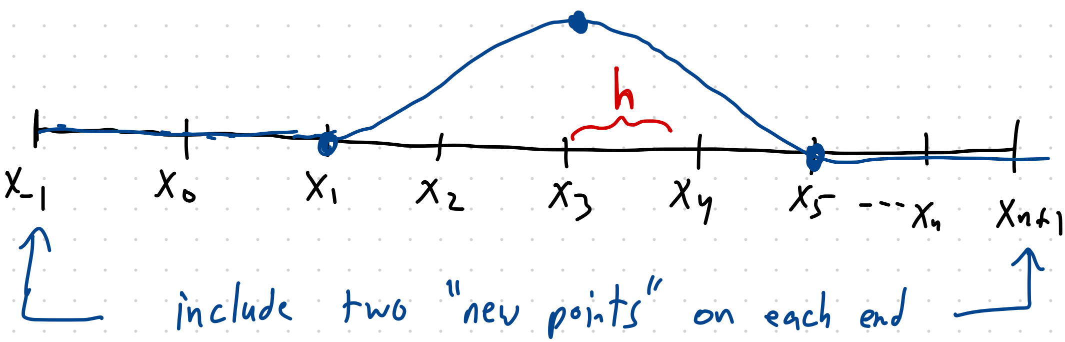
s.t.

$$\boxed{S_{3,n}(x) = \sum_{i=-1}^{n+1} a_i B_i(x)}$$

← called B-Spline

Basic Idea:

- Use equally-spaced points



- Define cubic polynomials on

$[x_{i-2}, x_{i+2}] = [x_i - 2h, x_i + 2h]$ (consider $x_i = x_3$)

with properties:

$B_i(x) = 0$ for $x \notin [x_i - 2h, x_i + 2h]$

$B_i(x)$ is cubic spline interpolating

$(x_i - 2h, 0)$, $(x_i, 1)$, $(x_i + 2h, 0)$

After some algebra, we get:

$$\boxed{B_i(x) = \begin{cases} \frac{1}{4h^3}(x - x_{i-2})^3 & x_{i-2} \le x < x_{i-1} \\ \frac{1}{4h^3}(x - x_{i-2})^3 - \frac{1}{h^3}(x - x_{i-1})^3 & x_{i-1} \le x < x_i \\ \frac{-1}{4h^3}(x - x_{i+2})^3 + \frac{1}{h^3}(x - x_{i+1})^3 & x_i \le x < x_{i+1} \\ -\frac{1}{4h^3}(x - x_{i+2})^3 & x_{i+1} \le x \le x_{i+2} \\ 0 & \text{else} \end{cases}}$$

- Then, we find a_i s.t.

$$\sum_{i-1}^{i+1} a_i \, B_i(x_j) = f_j \,, \qquad j = 0, 1, \dots, n$$

Note: B_i, $i = -1, \dots, n+1$, are the set of all B-spline basis which are <u>non-zero</u> in interval $[x_i - 2h, x_i + 2h]$

Observe

$$\vdots$$

$$B_{j-2}(x_j) = 0$$

$$B_{j-1}(x_j) = 1/4$$

$$B_j(x_j) = 1 \quad \Rightarrow \quad a_{j-1} B_{j-1}(x_j) + a_j B_j(x_j) + a_{j+1} B_{j+1}(x_j) = f_j$$

$$B_{j+1}(x_j) = 1/4 \qquad\qquad j = 0, 1, \dots, n$$

$$B_{j+2}(x_j) = 0$$

$$\vdots$$

Or $\frac{1}{4} a_{j-1} + a_j + \frac{1}{4} a_{j+1} = f_j$, $j = 0, 1, \dots, n$

This gives $n+1$ eqns but have $n+3$ unknowns:

$a_{-1}, a_0, a_1, \ldots, a_n, a_{n+1}$

Need two more equations

In the case of natural end (Free boundary) conditions

$$s''(x_0) = s''(x_n) = 0$$

Note that $\frac{d}{dx}\left(\frac{1}{4h^3}(x-x_{i-2})^3\right) = \frac{3}{4h^3}(x-x_{i-2})^2$

$$\Rightarrow \frac{d^2}{dx^2}\left(\frac{1}{4h^3}(x-x_{i-2})^3\right) = \frac{3}{2h^3}(x-x_{i-2})$$

$$\Rightarrow \begin{array}{ll} s''(x_0)=0 \Rightarrow & \frac{3}{2h^2}a_{-1} - \frac{3}{h^2}a_0 + \frac{3}{2h^2}a_1 = 0 \\ s''(x_n)=0 \Rightarrow & \frac{3}{2h^2}a_{n-1} - \frac{3}{h^2}a_n + \frac{3}{2h^2}a_{n+1} = 0 \end{array} \quad (*)$$

$n+3$ linear eqn can be solved using Gaussian Elim.

But we can simplify the eqns.

Adding first two equations:

$$\begin{array}{l} \frac{3}{2}a_{-1} - 3a_0 + \frac{3}{2}a_1 = 0 \\ \frac{1}{4}a_{-1} + a_0 + \frac{1}{4}a_1 = f_0 \end{array} \Rightarrow \boxed{a_0 = \frac{2}{3}f_0}$$

Similarly, adding last two eqns : $\boxed{a_n = \frac{2}{3} f_n}$ (9)

So we have (recall $\frac{1}{4} a_0 + a_1 + \frac{1}{4} a_2 = f_1$)

$$a_1 + \frac{1}{4} a_2 = f_1 - \frac{1}{6} f_0$$

$$\frac{1}{4} a_1 + a_2 + \frac{1}{4} a_3 = f_2$$

$$\frac{1}{4} a_2 + a_3 + \frac{1}{4} a_4 = f_3$$

$$\vdots$$

$$\frac{1}{4} a_{n-3} + a_{n-2} + \frac{1}{4} a_{n-1} = f_{n-2}$$

$$\frac{1}{4} a_{n-2} + a_{n-1} = f_{n-1} - \frac{1}{6} f_n$$

$\Rightarrow$ To find coeffs. $a_1, \dots, a_{n-1}$, we solve

$$\begin{bmatrix} 1 & \frac{1}{4} & & & \\ \frac{1}{4} & 1 & \frac{1}{4} & & \\ & \frac{1}{4} & 1 & \frac{1}{4} & \\ & & \ddots & \ddots & \frac{1}{4} \\ & & & \frac{1}{4} & 1 \end{bmatrix} \begin{bmatrix} a_1 \\ a_2 \\ \vdots \\ a_{n-2} \\ a_{n-1} \end{bmatrix} = \begin{bmatrix} f_1 - \frac{1}{6} f_0 \\ f_2 \\ \vdots \\ f_{n-2} \\ f_{n-1} - \frac{1}{6} f_n \end{bmatrix}$$

Tridiagonal system can be efficiently computed using, e.g., Thomas Algorithm ($O(n)$ instead of $\underbrace{O(n^3)}_{\text{Gaussian Elimination}}$ FLOPs)

Finally, compute the values of a_{-1} and a_{n+1} from (*)

Chapter 4: Numerical Differentiation and Integration

Differentiation:

Calculus Definition: $f'(x) = \lim\limits_{h \to 0} \dfrac{f(x+h) - f(x)}{h}$

Idea: approximate numerically using small h.

Finite Difference Approximation

Consider Taylor series centered at x

A $\quad f(x+h) = f(x) + f'(x) \cdot h + \dfrac{f''(x)}{2!} h^2 + \dfrac{f'''(x)}{3!} h^3 + \cdots$

B $\quad f(x-h) = f(x) - f'(x) \cdot h + \dfrac{f''(x)}{2!} h^2 - \dfrac{f'''(x)}{3!} h^3 + \cdots$

Forward Difference Approximation

Use series A:

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

$$\Rightarrow \frac{f(x+h)-f(x)}{h} = f'(x) + \underbrace{\frac{f''(x)}{2!}h + \frac{f'''(x)}{3!}h^2 + \cdots}_{\text{If } h \text{ is small, truncate}}$$

$$\Rightarrow \boxed{f'(x) \approx \frac{f(x+h)-f(x)}{h} \quad \text{with approximation error } O(h)}$$