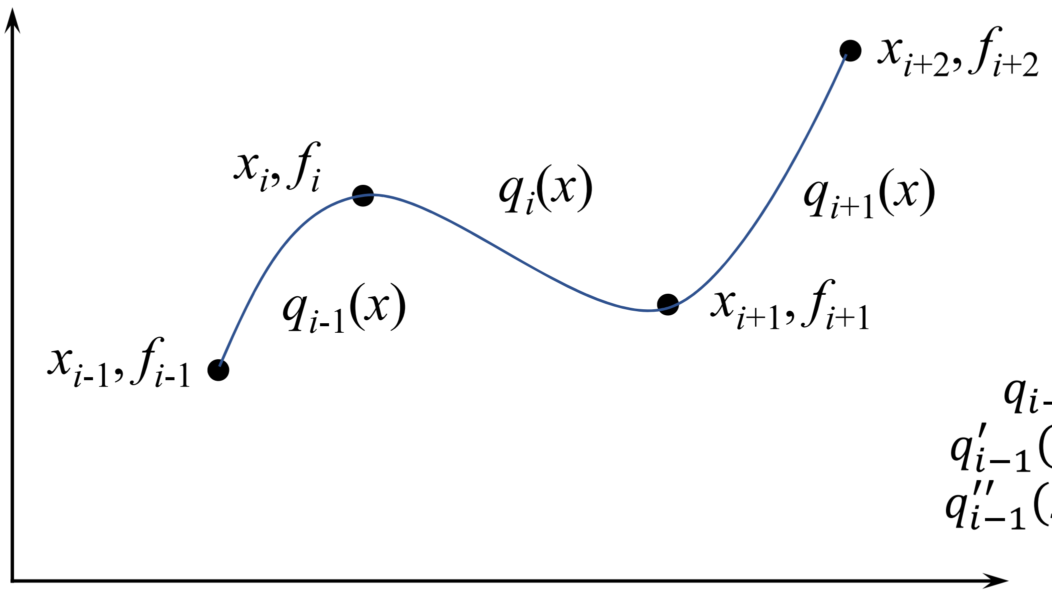
Spline Interpolation

- ✓ Given: $(n + 1)$ observations or data pairs $[(x_0, f_0), (x_1, f_1), (x_2, f_2) \ldots (x_n, f_n)]$
- ✓ This gives a mesh of *nodes* $\{x_0, x_1, x_2, \cdots x_n\}$ on the independent variable and the corresponding function values as $\{f_0, f_1, f_2, \cdots f_n\}$
- ✓ Goal: fit an independent polynomial in each interval (between two points) with certain continuity requirements at the nodes.
  - ✓ *Linear spline*: continuity in function values, C^0 continuity
  - ✓ *Quadratic spline*: continuity in function values and 1st derivatives, C^1 continuity
  - ✓ *Cubic spline:* continuity in function values, 1st and 2nd derivatives, C^2 continuity
- ✓ Denote for node i or at x_i: functional value f_i, first derivative u_i, second derivative v_i

Spline Interpolation: Cubic



$$q_i(x_i) = f_i$$
$$q_{i-1}(x_i) = q_i(x_i)$$
$$q'_{i-1}(x_i) = u_i = q'_i(x_i)$$
$$q''_{i-1}(x_i) = v_i = q''_i(x_i)$$

- ✓ A cubic polynomial in each interval: $(n+1)$ points, n cubic polynomials, $4n$ unknowns
- ✓ Available conditions: $(n + 1)$ function values, $(n - 1)$ function continuity, $(n - 1)$ 1st derivative continuity conditions and $(n - 1)$ 2nd derivative continuity conditions, total $4n - 2$ conditions.
- ✓ **2 free conditions to be chosen by the user!**

Spline Interpolation: Cubic

- ✓ Cubic Spline in the interval $\{x_i, x_{i+1}\}$: $q_i(x)$
- ✓ $q_i''(x)$ is a set of linear splines.
- ✓ Let us denote the 2nd derivative (v) of the function at the ith node as

$$f''(x_i) = v(x_i) = v_i$$

- ✓ Therefore: $q_i''(x_i) = v(x_i) = v_i$ and $q_i''(x_{i+1}) = v(x_{i+1}) = v_{i+1}$
- ✓ We may write:

$$q_i''(x) = \frac{v_{i+1}}{h_i}(x - x_i) - \frac{v_i}{h_i}(x - x_{i+1})$$

$$q_i(x) = \frac{v_{i+1}}{6h_i}(x - x_i)^3 - \frac{v_i}{6h_i}(x - x_{i+1})^3 + c_1 x + c_2$$

$$q_i(x_i) = f_i = \frac{v_i h_i^2}{6} + c_1 x_i + c_2$$

$$q_i(x_{i+1}) = f_{i+1} = \frac{v_{i+1} h_i^2}{6} + c_1 x_{i+1} + c_2$$

Spline Interpolation: Cubic

$$q_i(x) = \frac{v_{i+1}}{6h_i}(x - x_i)^3 - \frac{v_i}{6h_i}(x - x_{i+1})^3 + c_1 x + c_2$$

$$q_i(x_i) = f_i = \frac{v_i h_i^2}{6} + c_1 x_i + c_2; \quad q_i(x_{i+1}) = f_{i+1} = \frac{v_{i+1} h_i^2}{6} + c_1 x_{i+1} + c_2$$

$$c_1 = f[x_{i+1}, x_i] - \frac{h_i}{6}(v_{i+1} - v_i) = \frac{f_{i+1}}{h_i} - \frac{f_i}{h_i} + \frac{h_i}{6} v_i - \frac{h_i}{6} v_{i+1}$$

$$c_2 = -\frac{f_{i+1}}{h_i} x_i + \frac{f_i}{h_i} x_{i+1} - \frac{h_i}{6} v_i x_{i+1} + \frac{h_i}{6} v_{i+1} x_i$$

$$\begin{aligned} q_i(x) \\ &= \frac{v_{i+1}}{6}\left[\frac{(x - x_i)^3}{h_i} - h_i(x - x_i)\right] + \frac{v_i}{6}\left[-\frac{(x - x_{i+1})^3}{h_i} + h_i(x - x_{i+1})\right] \\ &+ \frac{f_{i+1}}{h_i}(x - x_i) - \frac{f_i}{h_i}(x - x_{i+1}) \end{aligned}$$

We need to estimate $(n + 1)$ unknown v_i. We have $(n - 1)$ conditions from the continuity of the first derivative.

Spline Interpolation: Cubic

$$q_i'(x_i) = q_{i-1}'(x_i); \qquad i = 1, 2, 3, \cdots n-1 \qquad \ldots (eq. 1)$$

$$q_i(x) = \frac{v_{i+1}}{6}\left[\frac{(x-x_i)^3}{h_i} - h_i(x-x_i)\right] + \frac{v_i}{6}\left[-\frac{(x-x_{i+1})^3}{h_i} + h_i(x-x_{i+1})\right] + \frac{f_{i+1}}{h_i}(x-x_i) - \frac{f_i}{h_i}(x-x_{i+1})$$

$$q_i'(x) = \frac{v_{i+1}}{6}\left[\frac{3(x-x_i)^2}{h_i} - h_i\right] + \frac{v_i}{6}\left[-\frac{3(x-x_{i+1})^2}{h_i} + h_i\right] + f[x_{i+1}, x_i]$$

$$q_{i-1}'(x) = \frac{v_i}{6}\left[\frac{3(x-x_{i-1})^2}{h_{i-1}} - h_{i-1}\right] + \frac{v_{i-1}}{6}\left[-\frac{3(x-x_i)^2}{h_{i-1}} + h_{i-1}\right] + f[x_i, x_{i-1}]$$

In eq. (1),

$$-\frac{h_i}{6}v_{i+1} - \frac{h_i}{3}v_i + f[x_{i+1}, x_i] = \frac{h_{i-1}}{3}v_i + \frac{h_{i-1}}{6}v_{i-1} + f[x_i, x_{i-1}]$$

$$-\frac{h_{i-1}}{6}v_{i-1} - \left(\frac{h_i + h_{i-1}}{3}\right)v_i - \frac{h_i}{6}v_{i+1} = f[x_i, x_{i-1}] - f[x_{i+1}, x_i]$$

$$\boldsymbol{\frac{h_{i-1}}{6}v_{i-1} + \left(\frac{h_i + h_{i-1}}{3}\right)v_i + \frac{h_i}{6}v_{i+1} = f[x_{i+1}, x_i] - f[x_i, x_{i-1}]}$$

✓ $\mathbf{h_{i-1}v_{i-1} + 2(h_i + h_{i-1})v_i + h_i v_{i+1} = 6f[x_{i+1}, x_i] - 6f[x_i, x_{i-1}]}$

$$\sigma_{i-1} h_i + 2\sigma_i (h_i + h_{i+1}) + \sigma_{i+1} h_{i+1}$$
$$= 6 (g_{i+1} - g_i) \longrightarrow i = 1, 2, \ldots n$$

$$\begin{bmatrix} \boxed{\quad BCs \quad} & & & & \\ h_1 & 2(h_1+h_2) & h_2 & - - & - - \\ & h_2 & 2(h_2+h_3) & h_3 & - - - \\ & & \ddots & & \\ & & h_{n-1} & 2(h_{n-1}+h_n) & h_n \\ \boxed{\quad BCs \quad} & & & & \end{bmatrix} \begin{bmatrix} \sigma_0 \\ \sigma_1 \\ \vdots \\ \sigma_n \end{bmatrix} = 6 \begin{bmatrix} g_2 - g_1 \\ g_3 - g_2 \\ \vdots \\ g_n - g_{n-1} \end{bmatrix}$$

n-1 equation

Natural spline

Spline Interpolation: Cubic

$$\boldsymbol{h_{i-1}v_{i-1} + 2(h_i + h_{i-1})v_i + h_i v_{i+1} = 6f[x_{i+1}, x_i] - 6f[x_i, x_{i-1}]}$$

$$i = 1, 2, 3, \cdots n - 1.$$

- ✓ So, $(n - 1)$ equations, $(n + 1)$ unknowns, two conditions have to be provided by the users. They decide the type of cubic splines
- ✓ *Natural Spline:*

$$v_0 = v_n = 0$$

- ✓ *Parabolic Runout:*

$$v_0 = v_1 \qquad \text{and} \qquad v_{n-1} = v_n$$

- ✓ *Not-a-knot:*

$$q_0(x) = q_1(x) \qquad \Longrightarrow \qquad \frac{v_1 - v_0}{h_0} = \frac{v_2 - v_1}{h_1}$$

$$q_{n-2}(x) = q_{n-1}(x) \qquad \Longrightarrow \qquad \frac{v_{n-1} - v_{n-2}}{h_{n-2}} = \frac{v_n - v_{n-1}}{h_{n-1}}$$

- ✓ *Periodic:*

$$f_0 = f_n; \qquad u_0 = u_n \qquad \text{and} \qquad v_0 = v_n$$

First one comes from the data (if not satisfied, the periodic spline is not appropriate); the next two give the other two equations.

Spline Interpolation: Cubic

$$\boldsymbol{h_{i-1}v_{i-1} + 2(h_i + h_{i-1})v_i + h_i v_{i+1} = 6f[x_{i+1}, x_i] - 6f[x_i, x_{i-1}]}$$

- ✓ $i = 1, 2, 3, \cdots n-1.$ So, $(n-1)$ equations, $(n+1)$ unknowns, two conditions have to be provided by the users. They decide the type of cubic splines

- ✓ *Clamped Spline:*

$$u_0 = q_0'(x_0) = \alpha \qquad \text{and} \qquad u_n = q_{n-1}'(x_n) = \beta$$

$$q_0'(x) = \frac{v_1}{6}\left[\frac{3(x-x_0)^2}{h_0} - h_0\right] + \frac{v_0}{6}\left[-\frac{3(x-x_1)^2}{h_0} + h_0\right] + f[x_1, x_0]$$

$$q_0'(x_0) = -\frac{v_1 h_0}{6} - \frac{v_0 h_0}{3} + f[x_1, x_0] = \alpha \quad \Longrightarrow \quad \boldsymbol{2v_0 + v_1 = \frac{6}{h_0}(f[x_1, x_0] - \alpha)}$$

$$q_{n-1}'(x) = \frac{v_n}{6}\left[\frac{3(x-x_{n-1})^2}{h_{n-1}} - h_{n-1}\right] + \frac{v_{n-1}}{6}\left[-\frac{3(x-x_n)^2}{h_{n-1}} + h_{n-1}\right] + f[x_n, x_{n-1}]$$

$$q_{n-1}'(x_n) = \frac{v_n h_{n-1}}{3} + \frac{v_{n-1} h_{n-1}}{6} + f[x_n, x_{n-1}] = \beta$$

$$\Longrightarrow \quad \boldsymbol{2v_n + v_{n-1} = \frac{6}{h_{n-1}}(\beta - f[x_n, x_{n-1}])}$$

Example Problem: Q4 of Tutorial 9

Consider the function exp(x) sampled at points

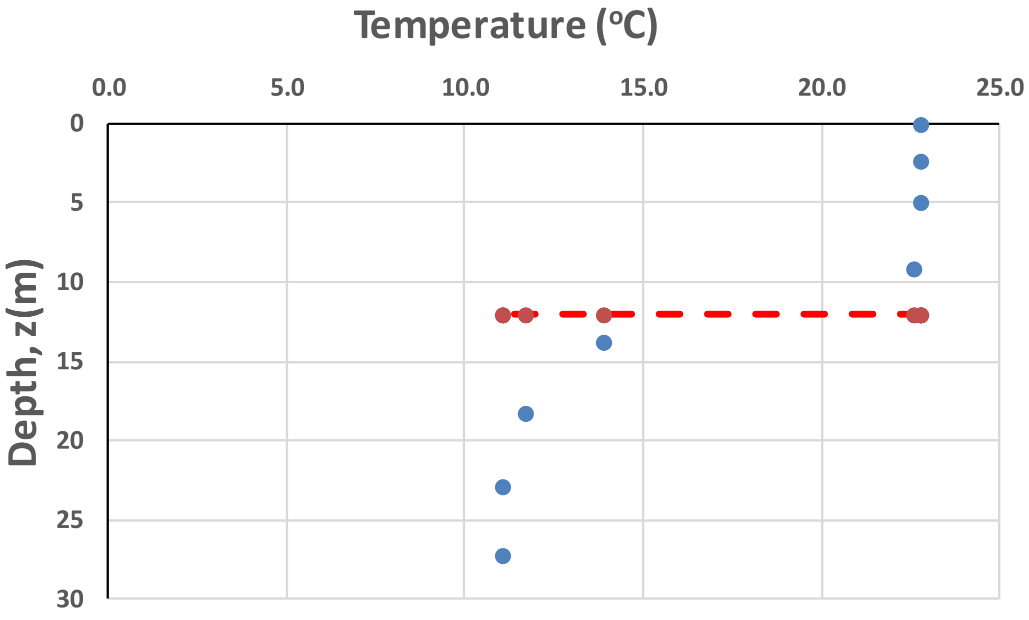
$x = 0,\ 0.5,\ 1.0,\ 1.5$ and 2

Estimate the function value at x = 1.80 by interpolating the function using - (a) natural cubic spline and (b) not-a-knot cubic spline. Calculate the true percentage error for both the splines. Which is the better spline for this problem and why?

Solution: Posted online along with Tutorial 9 solutions

Example Problem: Heat Transfer in Lake

Lakes in temperate zone can become thermally stratified during the summer. As depicted below, warm, buoyant water near the surface overlies colder, denser bottom water. Such stratification effectively divides the lake into two layers: the *epilimnion* and the *hypolimnion* separated by a plane called the *thermocline.*



z (m)	T(°C)
0	22.8
2.3	22.8
4.9	22.8
9.1	22.6
13.7	13.9
18.3	11.7
22.9	11.1
27.2	11.1

Example Problem: Heat Transfer in Lake

The location of the thermocline can be defined as the inflection point of the T-z curve; i.e. where $\frac{d^2T}{dx^2}$= 0. It is also the point at which the absolute value of the first derivative or gradient is maximum. Use cubic splines to determine the thermocline depth of this lake. Also use splines to determine the value of the gradient at the thermocline.

Spline Interpolation: Using Local Coordinate

$$x \in [x_i, x_{i+1}] \quad \rightarrow \quad t \in [0,1]$$
$$q_i(x) \text{ in } [x_i, x_{i+1}] \quad \rightarrow p_i(t) \text{ in } [0,1]$$

- ✓ At each *node i*, we denote the following:
  - ✓ Location: x_i
  - ✓ Functional value: f_i
  - ✓ Intervals: $h_i = x_{i+1} - x_i$ and $h_{i-1} = x_i - x_{i-1}$
  - ✓ Derivatives: First derivative u_i and the 2nd derivative v_i
- ✓ Transformations:

$$t = \frac{x - x_i}{x_{i+1} - x_i} = \frac{1}{h_i}(x - x_i) \quad \Longrightarrow \quad \frac{dt}{dx} = \frac{1}{h_i}$$

$$q_i'(x) = p_i'(t)\frac{dt}{dx} = \frac{1}{h_i}p_i'(t) \qquad q_i''(x) = \frac{1}{h_i^2}p_i''(t)$$

Spline Interpolation: Using Local Coordinate

- ✓ C^0 – Continuity:

$$p_{i-1}(1) = q_{i-1}(x_i) = q_i(x_i) = p_i(0) = f_i$$

- ✓ C^1 – Continuity:

$$\frac{1}{h_{i-1}} p'_{i-1}(1) = q'_{i-1}(x_i) = q'_i(x_i) = \frac{1}{h_i} p'_i(0) = u_i$$

- ✓ C^2 – Continuity:

$$\frac{1}{h_{i-1}^2} p''_{i-1}(1) = q''_{i-1}(x_i) = q''_i(x_i) = \frac{1}{h_i^2} p''_i(0) = v_i$$

Linear and Quadratic Splines: Local Coordinate

✓ Linear Spline: C^0 – Continuous

$$p_i(t) = a_i t + b_i \quad \Rightarrow \quad p_i(0) = b_i = f_i, \qquad p_i(1) = a_i + b_i = f_{i+1}$$

$$p_i(t) = (f_{i+1} - f_i)t + f_i \quad \Longrightarrow \quad q_i(x) = f[x_{i+1}, x_i](x - x_i) + f_i$$

✓ Quadratic Spline: C^1 – Continuous

$$p_i(t) = a_i t^2 + b_i t + c_i \Rightarrow p_i(0) = c_i = f_i, \qquad p_i(1) = a_i + b_i + c_i = f_{i+1}$$

Using the definition of u_i:

$$\frac{1}{h_i} p_i'(0) = \frac{b_i}{h_i} = u_i \quad \Rightarrow \quad a_i = h_i(f[x_{i+1}, x_i] - u_i)$$

$$p_i(t) = h_i(f[x_{i+1}, x_i] - u_i)t^2 + h_i u_i t + f_i$$

Using C^1 – Continuity:

$$\frac{1}{h_{i-1}} p_{i-1}'(1) = \frac{1}{h_i} p_i'(0) \quad \Rightarrow \quad u_i = 2f[x_i, x_{i-1}] - u_{i-1}$$

Cubic Spline: Using Local Coordinate

✓ Cubic Spline: C^2 – Continuous

$$p_i(t) = a_i t^3 + b_i t^2 + c_i t + d_i$$

Using C^0 – Continuity:

$$p_i(0) = d_i = f_i, \qquad p_i(1) = a_i + b_i + c_i + d_i = f_{i+1}$$

Now we have two options:

- ✓ Option 1: Using the 1st derivative u_i as unknown and C^2 – Continuity to estimate them
- ✓ Option 2: Using the 2nd derivative v_i as unknown and C^1 – Continuity to estimate them

Cubic Spline: Using Local Coordinates

Option 1: Using the 1st derivative u_i as unknown and C^2 – Continuity to estimate them

$$p_i(t) = a_i t^3 + b_i t^2 + c_i t + d_i$$

$$d_i = f_i, \qquad a_i + b_i + c_i + d_i = f_{i+1}$$

$$\frac{1}{h_i} p_i'(0) = \frac{c_i}{h_i} = u_i; \quad \frac{1}{h_i} p_i'(1) = \frac{3a_i + 2b_i + c_i}{h_i} = u_{i+1}$$

$$a_i = h_i(u_{i+1} + u_i - 2f[x_{i+1}, x_i])$$

$$b_i = h_i(3f[x_{i+1}, x_i] - u_{i+1} - 2u_i)$$

Using C^2 – Continuity:

$$\frac{1}{h_{i-1}^2} p_{i-1}''(1) = \frac{1}{h_i^2} p_i''(0) \Rightarrow \frac{6a_{i-1} + 2b_{i-1}}{h_{i-1}^2} = \frac{2b_i}{h_i^2}$$

$$h_i u_{i-1} + 2(h_{i-1} + h_i)u_i + h_{i-1} u_{i+1} = 3h_{i-1} f[x_{i+1}, x_i] + 3h_i f[x_i, x_{i-1}]$$

$$i = 1, 2, 3, \cdots n - 1$$

Using the two other conditions, one may obtain similar splines of different types!

Cubic Spline: Using Local Coordinates

- ✓ *Natural Spline:*

$$v_0 = v_n = 0$$

$$v_0 = \frac{p_0''(0)}{h_0^2} = \frac{2b_0}{h_0^2} = 0; \qquad b_0 = h_0(3f[x_1, x_0] - u_1 - 2u_0) = 0$$

$$v_n = \frac{p_{n-1}''(1)}{h_{n-1}^2} = \frac{6a_{n-1} + 2b_{n-1}}{h_{n-1}^2} = 0$$

$$6h_{n-1}(u_n + u_{n-1} - 2f[x_n, x_{n-1}]) + 2h_{n-1}(3f[x_n, x_{n-1}] - u_n - 2u_{n-1}) = 0$$

$$2u_0 + u_1 = 3f[x_1, x_0] \qquad\qquad 2u_n + u_{n-1} = 3f[x_n, x_{n-1}]$$

- ✓ *Clamped Spline:*

$$u_0 = \alpha \qquad \text{and} \qquad u_n = \beta$$

- ✓ *Parabolic Runout:*

$$v_0 = v_1 \qquad \text{and} \qquad v_{n-1} = v_n$$

$$\frac{p_0''(0)}{h_0^2} = \frac{p_0''(1)}{h_0^2} \implies \frac{2b_0}{h_0^2} = \frac{6a_0 + 2b_0}{h_0^2} \implies u_0 + u_1 = 2f[x_1, x_0]$$

$$\frac{p_{n-1}''(0)}{h_{n-1}^2} = \frac{p_{n-1}''(1)}{h_{n-1}^2} \implies \frac{2b_{n-1}}{h_{n-1}^2} = \frac{6a_{n-1} + 2b_{n-1}}{h_{n-1}^2} \implies u_{n-1} + u_n = 2f[x_n, x_{n-1}]$$

Cubic Spline: Using Local Coordinates

✓ *Not-a-knot:*

$$q_0(x) = q_1(x) \qquad \Longrightarrow \qquad \frac{v_1 - v_0}{h_0} = \frac{v_2 - v_1}{h_1}$$

$$q_{n-2}(x) = q_{n-1}(x) \qquad \Longrightarrow \qquad \frac{v_{n-1} - v_{n-2}}{h_{n-2}} = \frac{v_n - v_{n-1}}{h_{n-1}}$$

✓ *Periodic:*

$$f_0 = f_n; \qquad u_0 = u_n \qquad \text{and} \qquad v_0 = v_n$$

First one comes from the data (if not satisfied, the periodic spline is not appropriate); the next two give the other two equations.

Formulation of these two is left as homework!

Cubic Spline: Using Local Coordinates

Option 2: Using the 2nd derivative v_i as unknown and C^1 – Continuity to estimate them

$$p_i(t) = a_i t^3 + b_i t^2 + c_i t + d_i$$

$$d_i = f_i, \qquad a_i + b_i + c_i + d_i = f_{i+1}$$

$$\frac{1}{h_i^2} p_i''(0) = \frac{2b_i}{h_i^2} = v_i; \qquad \frac{1}{h_i^2} p_i''(1) = \frac{6a_i + 2b_i}{h_i^2} = v_{i+1}$$

$$a_i = \frac{h_i^2}{6}(v_{i+1} - v_i); \qquad c_i = h_i f[x_{i+1}, x_i] - \frac{h_i^2}{6}(v_{i+1} + 2v_i)$$

Using C^1 – Continuity:

$$\frac{1}{h_{i-1}} p_{i-1}'(1) = \frac{1}{h_i} p_i'(0) \quad \Rightarrow \quad \frac{3a_{i-1} + 2b_{i-1} + c_{i-1}}{h_{i-1}} = \frac{c_i}{h_i}$$

$$h_{i-1} v_{i-1} + 2(h_{i-1} + h_i) v_i + h_i v_{i+1} = 6f[x_{i+1}, x_i] - 6f[x_i, x_{i-1}]$$

$$i = 1, 2, 3, \cdots n - 1$$

This is the same equation that was obtained using Lagrange polynomials!

Boundary conditions are also the same!

ESO 208A: Computational Methods in Engineering

Numerical Differentiation

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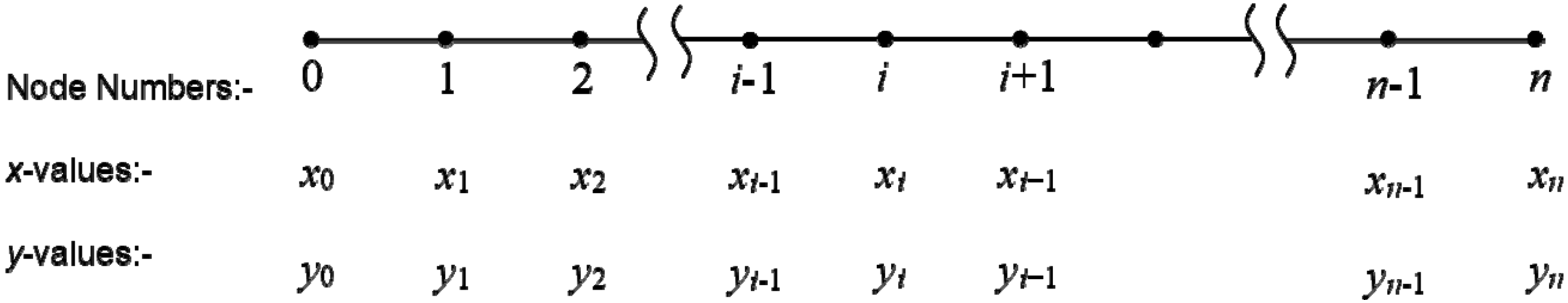
Acknowledgements: Profs. Saumyen Guha and Shivam Tripathi (CE)

Numerical Differentiation



Let us compute *dy/dx* or *df/dx* at node *i*

Denote the difference operators:

$\Delta x = x_{i+1} - x_i \qquad \nabla x = x_i - x_{i-1} \qquad \delta x = x_{i+1/2} - x_{i-1/2}$

Numerical Differentiation: Finite Difference

Approximate the function between $\{x_i, x_{i+1}\}$ as:

$$f(x) = \frac{x - x_i}{x_{i+1} - x_i} f_{i+1} + \frac{x - x_{i+1}}{x_i - x_{i+1}} f_i = \frac{f_{i+1}}{\Delta x}(x - x_i) - \frac{f_i}{\Delta x}(x - x_{i+1})$$

Forward Difference:

$$\frac{df}{dx} = \frac{f_{i+1} - f_i}{\Delta x} = \frac{\Delta f}{\Delta x}$$

Approximate the function between $\{x_{i-1}, x_i\}$ as:

$$f(x) = \frac{x - x_i}{x_{i-1} - x_i} f_{i-1} + \frac{x - x_{i-1}}{x_i - x_{i-1}} f_i = -\frac{f_{i-1}}{\nabla x}(x - x_i) + \frac{f_i}{\nabla x}(x - x_{i-1})$$

Backward Difference:

$$\frac{df}{dx} = \frac{f_i - f_{i-1}}{\nabla x} = \frac{\nabla f}{\nabla x}$$

Numerical Differentiation: Finite Difference

Approximate the function between three points: $\{x_{i-1}, x_i, x_{i+1}\}$

$$f(x)$$

$$= \frac{(x - x_i)(x - x_{i+1})}{(x_{i-1} - x_i)(x_{i-1} - x_{i+1})} f_{i-1} + \frac{(x - x_{i-1})(x - x_{i+1})}{(x_i - x_{i-1})(x_i - x_{i+1})} f_i$$

$$+ \frac{(x - x_{i-1})(x - x_i)}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)} f_{i+1}$$

$$= \frac{f_{i-1}}{\nabla x(\Delta x + \nabla x)}(x - x_i)(x - x_{i+1}) - \frac{f_i}{\nabla x \Delta x}(x - x_{i-1})(x - x_{i+1})$$

$$+ \frac{f_{i+1}}{(\Delta x + \nabla x)\Delta x}(x - x_{i-1})(x - x_i)$$

Now, evaluate *df/dx* at $x = x_i$:

$$\left.\frac{df}{dx}\right|_{x_i} = \frac{f_{i-1}}{\nabla x(\Delta x + \nabla x)}(-\Delta x) - \frac{f_i}{\nabla x \Delta x}(\nabla x - \Delta x) + \frac{f_{i+1}}{(\Delta x + \nabla x)\Delta x}(\nabla x)$$

Numerical Differentiation: Finite Difference

Central Difference:

$$\left.\frac{df}{dx}\right|_{x_i}$$

$$= \frac{f_{i-1}}{\nabla x(\Delta x + \nabla x)}(-\Delta x) - \frac{f_i}{\nabla x \Delta x}(\nabla x - \Delta x) + \frac{f_{i+1}}{(\Delta x + \nabla x)\Delta x}(\nabla x)$$

For regular or uniform grid: $\Delta x = \nabla x = h$

$$\left.\frac{df}{dx}\right|_{x_i} = \frac{f_{i+1} - f_{i-1}}{2h} = \frac{\delta f}{\delta x}$$

Let us assume regular grid with a mesh size of h

Numerical Differentiation: Finite Difference

Approximate the function between three points: $\{x_{i-1}, x_i, x_{i+1}\}$

$$f(x) = \frac{(x - x_i)(x - x_{i+1})}{(x_{i-1} - x_i)(x_{i-1} - x_{i+1})} f_{i-1} + \frac{(x - x_{i-1})(x - x_{i+1})}{(x_i - x_{i-1})(x_i - x_{i+1})} f_i + \frac{(x - x_{i-1})(x - x_i)}{(x_{i+1} - x_{i-1})(x_{i+1} - x_i)} f_{i+1}$$

$$f(x) = \frac{f_{i-1}}{2h^2}(x - x_i)(x - x_{i+1}) - \frac{f_i}{h^2}(x - x_{i-1})(x - x_{i+1}) + \frac{f_{i+1}}{2h^2}(x - x_{i-1})(x - x_i)$$

Now, evaluate central difference approximations of df/dx and d^2f/dx^2 at $x = x_i$:

$$\frac{df}{dx} = \frac{f_{i-1}}{2h^2}[(x - x_i) + (x - x_{i+1})] - \frac{f_i}{h^2}[(x - x_{i-1}) + (x - x_{i+1})] + \frac{f_{i+1}}{2h^2}[(x - x_{i-1}) + (x - x_i)]$$

$$\left.\frac{df}{dx}\right|_{x_i} = \frac{f_{i+1} - f_{i-1}}{2h}$$

$$\left.\frac{d^2f}{dx^2}\right|_{x_i} = \frac{f_{i-1} - 2f_i + f_{i+1}}{h^2}$$

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✓ Similarly, one can approximate the function between three points $\{x_i, x_{i+1}, x_{i+2}\}$ and obtain the *forward difference* expressions of the first and second derivatives at $x = x_i$ as follows:

$$\left.\frac{df}{dx}\right|_{x_i} = \frac{-3f_i + 4f_{i+1} - f_{i+2}}{2h}$$

$$\left.\frac{d^2f}{dx^2}\right|_{x_i} = \frac{f_i - 2f_{i+1} + f_{i+2}}{h^2}$$

This is left for homework practice!

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✓ Similarly, one can approximate the function between three points $\{x_{i-2}, x_{i-1}, x_i\}$ and obtain the *backward difference* expressions of the first and second derivatives at $x = x_i$ as follows:

$$\left.\frac{df}{dx}\right|_{x_i} = \frac{3f_i - 4f_{i-1} + f_{i-2}}{2h}$$

$$\left.\frac{d^2f}{dx^2}\right|_{x_i} = \frac{f_{i-2} - 2f_{i-1} + f_i}{h^2}$$

This is left for homework practice!

Numerical Differentiation: Finite Difference

- ✓ *Accuracy:* How accurate is the numerical differentiation scheme with respect to the TRUE differentiation?
  - ✓ **Truncation Error** analysis
  - ✓ **Modified Wave Number, Amplitude Error and Phase Error** analysis for periodic functions
- ✓ Recall: True Value (a) = Approximate Value ($\tilde{a}$) + Error (ε)
- ✓ *Consistency:* A numerical expression for differentiation or a numerical differentiation scheme is consistent if it converges to the TRUE differentiation as $h \longrightarrow 0$.