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:*

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

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

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

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:*

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

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 same!

ESO 208A: Computational Methods in Engineering

Numerical Differentiation

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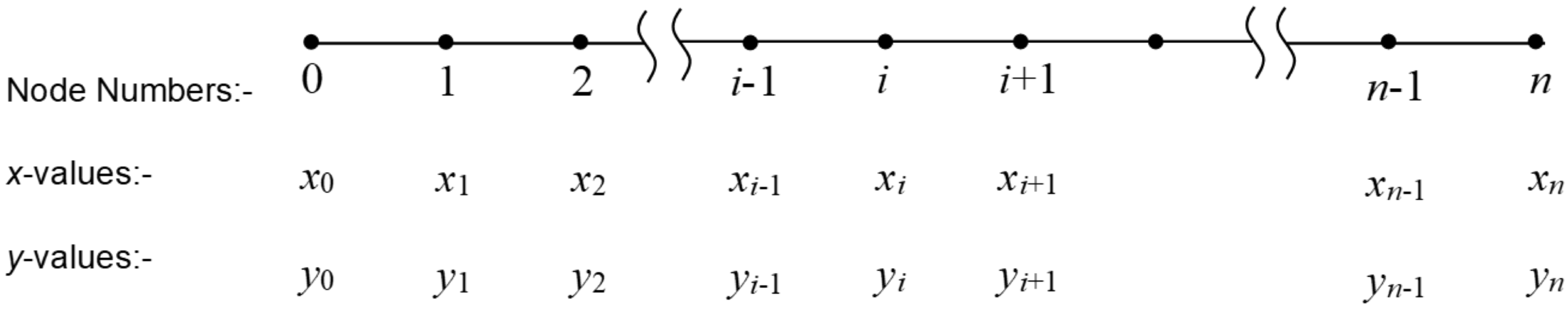
Numerical Differentiation



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: $\{x_{i-1}, x_i, x_{i+1}\}$

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

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

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 $x = x_i$:

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

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

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

Numerical Differentiation: Finite Difference

✓ 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!

Numerical Differentiation: Finite Difference

✓ 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 $h \rightarrow 0$.

Numerical Differentiation: Finite Difference

$$f_{i+1} = f_i + hf_i' + \frac{h^2}{2!}f_i'' + \frac{h^3}{3!}f_i''' + \frac{h^4}{4!}f_i^{IV} + \frac{h^5}{5!}f_i^{V} + \frac{h^6}{6!}f_i^{VI} \cdots$$

$$\frac{f_{i+1} - f_i}{h} = f_i' + \frac{h}{2!}f_i'' + \frac{h^2}{3!}f_i''' + \frac{h^3}{4!}f_i^{IV} + \frac{h^4}{5!}f_i^{V} \cdots$$

$$f_i' = \frac{f_{i+1} - f_i}{h} - \frac{h}{2!}f_i'' - \frac{h^2}{3!}f_i''' - \frac{h^3}{4!}f_i^{IV} - \frac{h^4}{5!}f_i^{V} \cdots$$

Truncation error for this forward difference scheme for the 1st Derivative is: $O(h)$

$$f_{i-1} = f_i - hf_i' + \frac{h^2}{2!}f_i'' - \frac{h^3}{3!}f_i''' + \frac{h^4}{4!}f_i^{IV} - \frac{h^5}{5!}f_i^{V} + \frac{h^6}{6!}f_i^{VI} \cdots$$

$$f_i' = \frac{f_i - f_{i-1}}{h} + \frac{h}{2!}f_i'' - \frac{h^2}{3!}f_i''' + \frac{h^3}{4!}f_i^{IV} - \frac{h^4}{5!}f_i^{V} \cdots$$

Truncation error for this backward difference scheme for the 1st Derivative is: $O(h)$

Numerical Differentiation: Finite Difference

$$f_{i+1} = f_i + hf_i' + \frac{h^2}{2!}f_i'' + \frac{h^3}{3!}f_i''' + \frac{h^4}{4!}f_i^{IV} + \frac{h^5}{5!}f_i^{V} + \frac{h^6}{6!}f_i^{VI} \cdots$$

$$f_{i-1} = f_i - hf_i' + \frac{h^2}{2!}f_i'' - \frac{h^3}{3!}f_i''' + \frac{h^4}{4!}f_i^{IV} - \frac{h^5}{5!}f_i^{V} + \frac{h^6}{6!}f_i^{VI} \cdots$$

$$\frac{f_{i+1} - f_{i-1}}{2h} = f_i' + \frac{h^2}{3!}f_i''' + \frac{h^4}{5!}f_i^{V} \cdots$$

$$f_i' = \frac{f_{i+1} - f_{i-1}}{2h} - \frac{h^2}{3!}f_i''' - \frac{h^4}{5!}f_i^{V} \cdots$$

Truncation error for this central difference scheme for the 1st Derivative is: $O(h^2)$

Numerical Differentiation: Finite Difference

$$f_{i+1} = f_i + hf_i' + \frac{h^2}{2!}f_i'' + \frac{h^3}{3!}f_i''' + \frac{h^4}{4!}f_i^{IV} + \frac{h^5}{5!}f_i^{V} + \frac{h^6}{6!}f_i^{VI} \cdots$$

$$f_{i-1} = f_i - hf_i' + \frac{h^2}{2!}f_i'' - \frac{h^3}{3!}f_i''' + \frac{h^4}{4!}f_i^{IV} - \frac{h^5}{5!}f_i^{V} + \frac{h^6}{6!}f_i^{VI} \cdots$$

$$\frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} = f_i'' + \frac{h^2}{12}f_i^{IV} + \frac{h^4}{360}f_i^{VI} \cdots$$

$$f_i'' = \frac{f_{i+1} - 2f_i + f_{i-1}}{h^2} - \frac{h^2}{12}f_i^{IV} - \frac{h^4}{360}f_i^{VI} \cdots$$

Truncation error for this central difference scheme for the 2nd Derivative is: $O(h^2)$

Numerical Differentiation: Finite Difference

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

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

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

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

Truncation error analysis for this forward and backward difference schemes are left as homework!

Numerical Differentiation: Finite Difference

$$f_{i+1} = f_i + \Delta x f_i' + \frac{\Delta x^2}{2!} f_i'' + \frac{\Delta x^3}{3!} f_i''' + \frac{\Delta x^4}{4!} f_i^{IV} + \frac{\Delta x^5}{5!} f_i^{V} + \cdots$$

$$f_{i-1} = f_i - \nabla x f_i' + \frac{\nabla x^2}{2!} f_i'' - \frac{\nabla x^3}{3!} f_i''' + \frac{\nabla x^4}{4!} f_i^{IV} - \frac{\nabla x^5}{5!} f_i^{V} + \cdots$$

$$\frac{f_{i+1} - f_{i-1}}{(\Delta x + \nabla x)} = f_i' + \frac{(\Delta x - \nabla x)}{2!} f_i'' + \frac{(\Delta x^2 - \Delta x \nabla x + \nabla x^2)}{3!} f_i''' \cdots$$

$$f_i' = \frac{f_{i+1} - f_{i-1}}{(\Delta x + \nabla x)} - \frac{(\Delta x - \nabla x)}{2!} f_i'' - \frac{(\Delta x^2 - \Delta x \nabla x + \nabla x^2)}{3!} f_i''' \cdots$$

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

$$f_i' = \frac{f_{i+1} - f_{i-1}}{2h} - \frac{h^2}{3!} f_i''' - \frac{h^4}{5!} f_i^{V} \cdots$$

Truncation error for this central difference scheme for the 1st Derivative is $O(h)$ for non-uniform grid and $O(h^2)$ uniform grid

Numerical Differentiation: Finite Difference

Consistency: A numerical expression for the derivative is consistent if the leading order term in the Truncation Error (*TE*) satisfies the following:

$$\lim_{h \to 0} TE = 0$$

If the leading order term in the truncation error is:

$$TE = Kh^p \text{ or } O(h^p) \text{ where, } p \in I$$

the numerical differentiation scheme is consistent if ,

$$p \geq 1$$

Numerical Differentiation: Finite Difference

Modified Wave Number analysis for periodic functions:

Consider the periodic basis function:

$$f(x) = e^{-ikx} \qquad f'(x) = -ike^{-ikx} = -ikf(x)$$

If we evaluate the true derivative at a node $x = x_j$:

$$f'(x_j) = -ikf(x_j) \quad \text{or} \quad f_j' = -ikf_j$$

Numerical derivative using the 2nd order accurate central difference scheme at the same node is:

$$f_j' = \frac{f_{j+1} - f_{j-1}}{2h} = \frac{e^{-ik(x_j+h)} - e^{-ik(x_j-h)}}{2h} = -i\frac{\sin kh}{h} f_j$$

$$f_j' = -ik' f_j \qquad \text{where,} \quad k' = \frac{\sin kh}{h}$$

Numerical Differentiation: Finite Difference

Modified Wave Number analysis for periodic functions:

True derivative at a node $x = x_j$: $f_j' = -ikf_j$

Numerical derivative using the 2nd order central difference scheme at the same node: $f_j' = -ik'f_j$

$$k' = \frac{\sin kh}{h}$$

or

$$k'h = \sin kh$$