General 1st derivative approximation (obtained by Lagrange interpolation)

The interpolation nodes are given as:

\[(x_0, \ f(x_0))\]
\[(x_1, \ f(x_1))\]
\[(x_2, \ f(x_2))\]
\[\ldots\]
\[(x_N, \ f(x_N))\]

By Lagrange Interpolation Theorem (Thm 3.3):

\[f(x) = \sum_{k=0}^{N} f(x_k)L_{N,k}(x) + \frac{(x-x_0)\ldots(x-x_N)}{(N+1)!} f^{(N+1)}(\xi(x)) \quad (1)\]

Take 1st derivative for Eq. (1):

\[f'(x) = \sum_{k=0}^{n} f(x_k)L'_{N,k}(x) + \frac{(x-x_0)\ldots(x-x_N)}{(N+1)!}\left(\frac{d}{dx}f^{(N+1)}(\xi(x))\right) + \frac{1}{(N+1)!}\left(\frac{d((x-x_0)\ldots(x-x_N))}{dx}\right)f^{(N+1)}(\xi(x))\]

Set \(x = x_j\), with \(x_j\) being \(x\)-coordinate of one of interpolation nodes. \(j = 0, \ldots, N\).

\[f'(x_j) = \sum_{k=0}^{n} f(x_k)L'_{N,k}(x_j) + \frac{f^{(N+1)}(\xi(x))}{(N+1)!} \prod_{k=0; k \neq j}^{N} (x_j - x_k) \quad \text{(N+1)-point formula to approximate } f'(x_j).\]

The error of \((N+1)\)-point formula is \[\frac{f^{(N+1)}(\xi(x))}{(N+1)!} \prod_{k=0; k \neq j}^{N} (x_j - x_k).\]
Example. The three-point formula with error to approximate $f'(x_j)$.

Let interpolation nodes be $(x_0, f(x_0)), (x_1, f(x_1))$ and $(x_2, f(x_2))$.

$$f'(x_j) = f(x_0) \left[ \frac{2x_j - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)} \right] + f(x_1) \left[ \frac{2x_j - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} \right] + f(x_2) \left[ \frac{2x_j - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)} \right] + \frac{f^{(3)}(\xi(x))}{6} \prod_{k=0; k \neq j}^{2} (x_j - x_k)$$

Mostly used three-point formula (see Figure 1)

Let $x_0, x_1$, and $x_2$ be equally spaced and the grid spacing be $h$.

Thus $x_1 = x_0 + h$; and $x_2 = x_0 + 2h$.

1. $f'(x_0) = \frac{1}{2h} \left[ -3f(x_0) + 4f(x_1) - f(x_2) \right] + \frac{h^2}{3} f^{(3)}(\xi(x_0))$ (three-point endpoint formula)

2. $f'(x_1) = \frac{1}{2h} \left[ -f(x_0) + f(x_2) \right] + \frac{h^2}{6} f^{(3)}(\xi(x_1))$ (three-point midpoint formula)

3. $f'(x_2) = \frac{1}{2h} \left[ f(x_0) - 4f(x_1) + 3f(x_2) \right] + \frac{h^2}{3} f^{(3)}(\xi(x_2))$ (three-point endpoint formula)

Figure 1. Schematic for three-point formula

Mostly used five-point formula

1. Five-point midpoint formula
2. Five-point endpoint formula

\[ f'(x_0) = \frac{1}{12h} [f(x_0 - 2h) - 8f(x_0 - h) + 8f(x_0 + h) - f(x_0 + 2h)] + \frac{h^4}{30} f^{(5)}(\xi) \]

\[ f''(x_0) = \frac{1}{12h} [-25f(x_0) + 48f(x_0 + h) - 36f(x_0 + 2h) + 16f(x_0 + 3h) - 3f(x_0 + 4h)] + \frac{h^4}{5} f^{(5)}(\xi) \]

**2\textsuperscript{nd} derivative approximation (obtained by Taylor polynomial)**

Approximate \( f(x_0 + h) \) by expansion about \( x_0 \):

\[ f(x_0 + h) = f(x_0) + f'(x_0)h + \frac{1}{2} f''(x_0)h^2 + \frac{1}{6} f'''(x_0)h^3 + \frac{1}{24} f^{(4)}(\xi_1)h^4 \]  

(3)

Approximate \( f(x_0 - h) \) by expansion about \( x_0 \):

\[ f(x_0 - h) = f(x_0) - f'(x_0)h + \frac{1}{2} f''(x_0)h^2 - \frac{1}{6} f'''(x_0)h^3 + \frac{1}{24} f^{(4)}(\xi_2)h^4 \]  

(4)

Add Eqns. (3) and (4):

\[ f(x_0 - h) + f(x_0 + h) = 2f(x_0) + f''(x_0)h^2 + \left[ \frac{1}{24} f^{(4)}(\xi_1)h^4 + \frac{1}{24} f^{(4)}(\xi_2)h^4 \right] \]

Thus

**Second derivative midpoint formula**

\[ f''(x_0) = \frac{1}{h^2} [f(x_0 - h) - 2f(x_0) + f(x_0 + h)] - \frac{h^2}{12} f^{(4)}(\xi) \]
**Round-Off Error Instability**

**Question:** what happens if \( h \) is too small?

Consider \( f'(x_0) = \frac{1}{2h} [f(x_0 + h) - f(x_0 - h)] + \frac{h^2}{6} f^{(3)}(\xi(x_0)) \). Suppose \( f(x_0 + h) \) and \( f(x_0 - h) \) are evaluated with round-off error \( e(x_0 + h) \) and \( e(x_0 - h) \) respectively, i.e., \( f(x_0 + h) = \hat{f}(x_0 + h) + e(x_0 + h) \), and \( f(x_0 - h) = \hat{f}(x_0 - h) + e(x_0 - h) \).

The total error of approximation is: \( f'(x_0) - \frac{\hat{f}(x_0 + h) - \hat{f}(x_0 - h)}{2h} = \frac{e(x_0 + h) - e(x_0 - h)}{2h} - \frac{h^2}{6} f^{(3)}(\xi(x_0)) \).

Suppose the round-off errors \( e(x_0 + h) \) and \( e(x_0 - h) \) are bounded by some number \( \varepsilon > 0 \), and \( |f^{(3)}(x)| < M \).

Then \( \left| f'(x_0) - \frac{\hat{f}(x_0 + h) - \hat{f}(x_0 - h)}{2h} \right| \leq \frac{\varepsilon}{h} + \frac{h^2}{6} M. \)

**Remark:** 1. To reduce the truncation error, \( \frac{h^2}{6} M \), \( h \) has to be reduced.

2. When \( h \) is reduced, \( \frac{\varepsilon}{h} \) grows.

**Optimal choice of \( h \):** minimum of \( e(h) = \frac{\varepsilon}{h} + \frac{h^2}{6} M \) occurs at \( h = \sqrt[3]{\frac{3\varepsilon}{M}}. \)