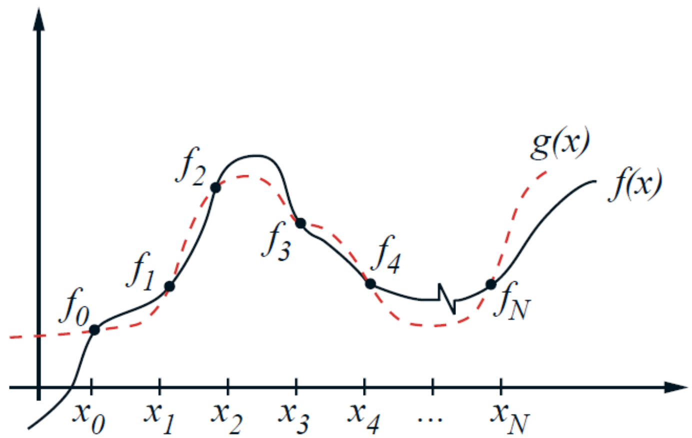
General 1st derivative approximation (obtained by Lagrange interpolation)



The interpolation nodes are given as:

$$(x_0\,,\quad f(x_0))$$
$$(x_1\,,\quad f(x_1))$$
$$(x_2\,,\quad f(x_2))$$
$$\dots$$
$$(x_N\,,\quad f(x_N))$$

By Lagrange Interpolation Theorem (Thm 3.3):

$$f(x) = \sum_{k=0}^{n} f(x_k) L_{N,k}(x) + \frac{(x-x_0)\cdots(x-x_N)}{(N+1)!} f^{(N+1)}(\xi(x)) \qquad (1)$$

Take 1st derivative for Eq. (1):

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

Set $x = x_j$, with x_j being x-coordinate of one of interpolation nodes. $j = 0, \dots, N$.

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

The error of (N+1)-point formula is $\frac{f^{(N+1)}(\xi(x))}{(N+1)!} \prod_{\substack{k=0;\\ k\neq j}}^{N} (x_j - x_k)$.

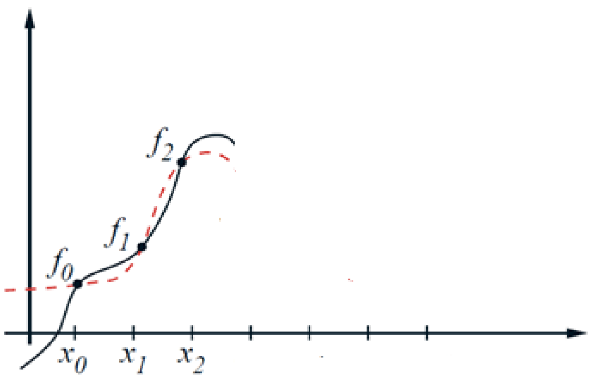
Example. The three-point formula with error to approximate $f'(x_j)$.

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

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

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.



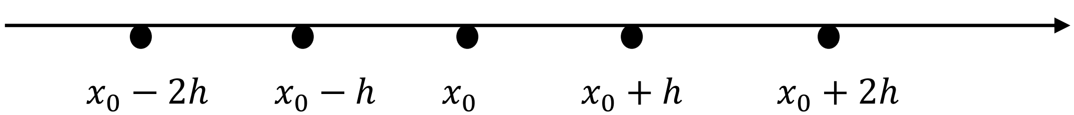
Thus $x_1 = x_0 + h$; and $x_2 = x_0 + 2h$.

1. $f'(x_0) = \frac{1}{2h}[-3f(x_0) + 4f(x_1) - f(x_2)] + \frac{h^2}{3}f^{(3)}(\xi(x_0))$ (three-point endpoint formula)
2. $f'(x_1) = \frac{1}{2h}[-f(x_0) + f(x_2)] + \frac{h^2}{6}f^{(3)}(\xi(x_1))$ (three-point midpoint formula)
3. $f'(x_2) = \frac{1}{2h}[f(x_0) - 4f(x_1) + 3f(x_2)] + \frac{h^2}{3}f^{(3)}(\xi(x_2))$ (three-point endpoint formula)

Figure 1. Schematic for three-point formula

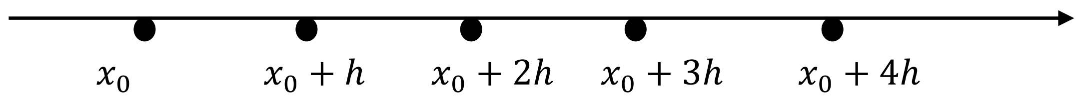
Mostly used five-point formula

1. Five-point midpoint formula



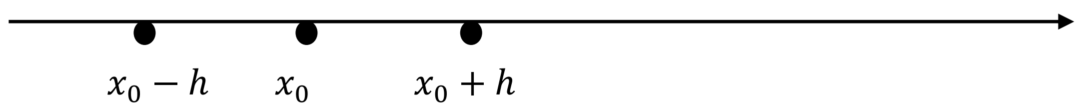
$$f'(x_0) = \frac{1}{12h}[f(x_0 - 2h) - 8f(x_0 - h) + 8f(x_0 + h) - f(x_0 + 2h)] + \frac{h^4}{30} f^{(5)}(\xi)$$

2. Five-point endpoint formula



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

2nd derivative approximation (obtained by Taylor polynomial)



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

$$f(x_0 + h) = f(x_0) + f'(x_0)h + \tfrac{1}{2} f''(x_0)h^2 + \tfrac{1}{6} f'''(x_0)h^3 + \tfrac{1}{24} f^{(4)}(\xi_1)h^4 \qquad (3)$$

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

$$f(x_0 - h) = f(x_0) - f'(x_0)h + \tfrac{1}{2} f''(x_0)h^2 - \tfrac{1}{6} f'''(x_0)h^3 + \tfrac{1}{24} f^{(4)}(\xi_2)h^4 \qquad (4)$$

Add Eqns. (3) and (4):

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

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 $f'(x_0) = \frac{1}{2h}[f(x_0+h) - f(x_0-h)] + \frac{h^2}{6} f^{(3)}\big(\xi(x_0)\big)$. 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., $f(x_0+h) = \tilde{f}(x_0+h) + e(x_0+h)$, and $f(x_0-h) = \tilde{f}(x_0-h) + e(x_0-h)$.

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

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

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

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