Section 4.1 Numerical Differentiation

Motivation.

- Consider to solve Black-Scholes equation $\frac{\partial f}{\partial t}+\frac{1}{2}\sigma^2S^2\frac{\partial^2 f}{\partial S^2}+rS\frac{\partial f}{\partial S}-rf=0$. Here f is the price of a derivative security, t is time, S is the varying price of the underlying asset, r is the risk-free interest rate, and σ is the market volatility.
- The heat equation of a plate: $\frac{\partial u}{\partial t}=k\left(\frac{\partial^2 u}{\partial x^2}+\frac{\partial^2 u}{\partial y^2}\right)$. Here k is the heat-diffusivity coefficient.

Goal: Compute accurate approximation to the derivative(s) of a function.

The derivative of f at x_0 is: $f'(x_0)=\lim_{h\to 0}\frac{f(x_0+h)-f(x_0)}{h}$.

Obviously, when h is small, $\frac{f(x_0+h)-f(x_0)}{h}$ is a "good" approximation to $f'(x_0)$.

What is the error of approximation?

Big idea:

Build an interpolating polynomial to approximate $f(x)$, then use the derivative of the interpolating polynomial as the approximation of the $f'(x_0)$.

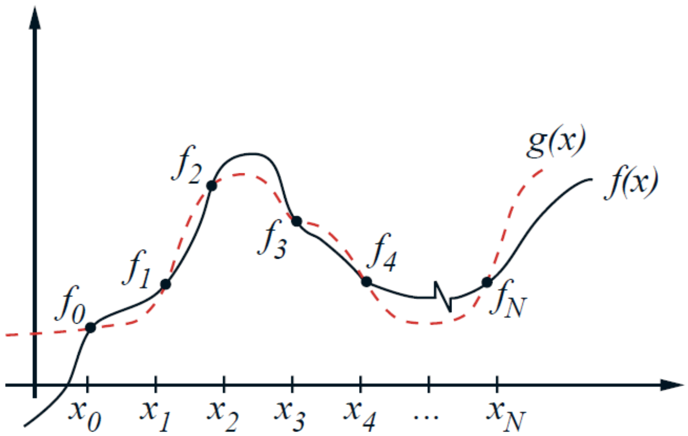
Example: Consider to approximate $f'(x_0)$ using two points x_0 and $x_0 + h$.

Example 4.4.1 Use forward difference formula with $h = 0.1$ to approximate the derivative of $f(x) = \ln(x)$ at $x_0 = 1.8$. Determine the bound of the approximation error.

Forward-difference: $f'(x_0) \approx \frac{f(x_0+h)-f(x_0)}{h}$ when $h > 0$.

Backward-difference: $f'(x_0) \approx \frac{f(x_0+h)-f(x_0)}{h}$ when $h < 0$.

1st derivative approximation (obtained by Lagrange interpolation)



The interpolation points are given as:

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

By Lagrange Interpolation Theorem (**Thm 3.3**):

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

Take 1st derivative for Eq. (1):

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

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

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

---- (N+1)-point formula with error to approximate $f'(x_j)$ **(4.2)**

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

Remark: $f'(x_j) \approx \sum_{k=0}^{n} f(x_k) L'_{N,k}(x_j)$

Example. Derive 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 $(x_2, f(x_2))$.

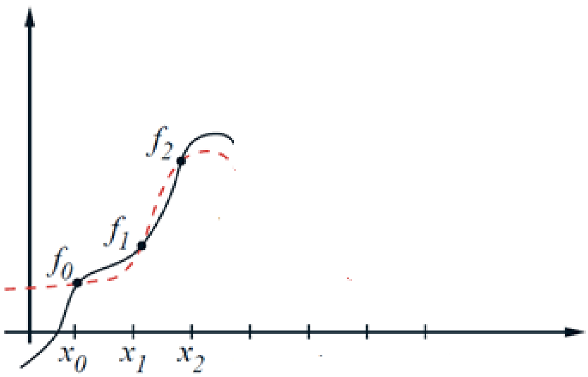
$$f'(x_j) = f(x_0)\left[\frac{2x_j - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)}\right] + f(x_1)\left[\frac{2x_j - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)}\right]$$

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

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 with error) **(4.4)**

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 with error) **(4.5)**

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 with error) **(4.4.1)**

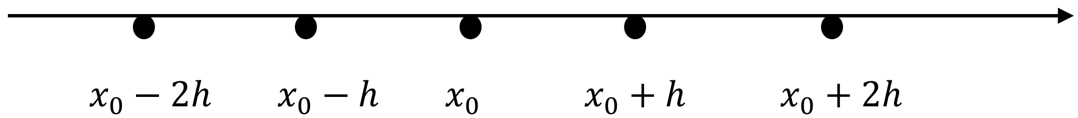
Remark: Eq. **(4.4)** in textbook is:

$$f'(x_0) = \frac{1}{2h}[-3f(x_0) + 4f(x_0 + h) - f(x_0 + 2h)] + \frac{h^2}{3}f^{(3)}\big(\xi(x_0)\big)$$

h can be both positive and negative

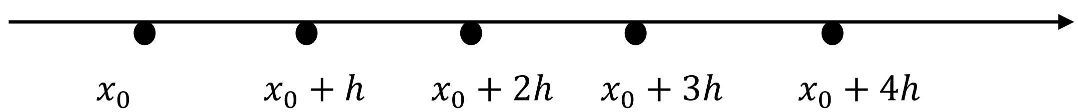
Mostly used five-point formula

1.Five-point midpoint formula



$$f'(x_0) = \frac{1}{12h}[f(x_0 - 2h) - 8f(x_0 - h) + 8f(x_0 + h) - f(x_0 + 2h)] + \frac{h^4}{30} f^{(5)}(\xi) \qquad \mathbf{(4.6)}$$

2.Five-point endpoint formula

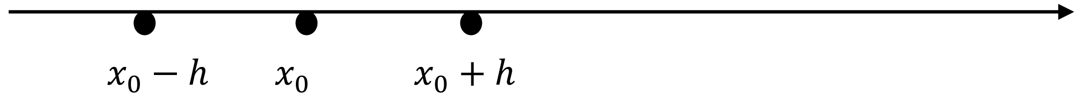


$$f'(x_0) = \frac{1}{12h}[-25f(x_0) + 48f(x_0 + h) - 36f(x_0 + 2h) + 16f(x_0 + 3h) - 3f(x_0 + 4h)] + \frac{h^4}{5} f^{(5)}(\xi) \qquad \mathbf{(4.7)}$$

Example 4.1.2 Values for $f(x) = xe^x$ are given in the following table. Use all applicable 3-point and 5-point formulas to approximate $f'(2.0)$.

x	1.8	1.9	2.0	2.1	2.2
$f(x)$	10.889365	12.703199	14.778112	17.148957	19.855030

2nd derivative approximation (obtained by Taylor polynomial)



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

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

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

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

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

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

Example 3. Values for $f(x) = xe^x$ are given in the following table. Use second derivative approximation formula to approximate $f''(2.0)$.

x	1.8	1.9	2.0	2.1	2.2
$f(x)$	10.889365	12.703199	14.778112	17.148957	19.855030

Solution: $f''(2.0) \approx \frac{1}{(0.1)^2}[f(1.9) - 2f(2.0) + f(2.1)] =$

Or

$$f''(2.0) \approx \frac{1}{(0.2)^2}[f(1.8) - 2f(2.0) + f(2.2)] =$$

Round-Off Error Instability

Let the round-off errors associated with $f(x_0 + h)$ and $f(x_0 - h)$ be $e(x_0 + h)$ and $e(x_0 - h)$, respectively.

Then $f(x_0 + h) = \tilde{f}(x_0 + h) + e(x_0 + h)$;

$f(x_0 - h) = \tilde{f}(x_0 - h) + e(x_0 - h)$.

Here $\tilde{f}(x_0 + h)$ and $\tilde{f}(x_0 - h)$ are actual values used by computer.

The total error of approximation using three-point midpoint formula:

$$f'(x_0) - \frac{\tilde{f}(x_0 + h) - \tilde{f}(x_0 - h)}{2h} = \frac{e(x_0 + h) - e(x_0 - h)}{2h} - \frac{h^2}{6} f^{(3)}(\xi_1)$$

Assume round-off errors are bounded by $\varepsilon \geq 0$, $\left|f^{(3)}(\xi_1)\right| \leq M$.

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. As h reduces, $\frac{\varepsilon}{h}$ grows;
2. In practice, it's rare to let h be too small;
3. Let the total error be $\frac{\varepsilon}{h} + \frac{h^2}{6} M$, a minimum of the total error occurs at

$$h = \left(\frac{3\varepsilon}{M}\right)^{\frac{1}{3}}.$$