Section 4.1 Numerical Differentiation

Motivation Examples (differential equations)

1. Consider to solve Black-Scholes equation $\frac{\partial f}{\partial t}+\frac{1}{2}\sigma^2 S^2 \frac{\partial^2 f}{\partial S^2}+rS\frac{\partial f}{\partial S}-rf=0$. 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.
2. 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.
- Remark: The derivative of f at x_0 is: $f'(x_0)=\lim_{h\to 0}\frac{f(x_0+h)-f(x_0)}{h}$.

Developing Derivative Approximation Formula

- **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 0. Consider to approximate $f'(x_0)$ using two points x_0 and $x_0 + h$.

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

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

- **Example 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 (Later)

General 1st Derivative Approximation Formulas

- The interpolation points are given as: $\left(x_0, f(x_0)\right), \left(x_1, f(x_1)\right), \ldots (x_N, f(x_N))$

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

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

- Take 1st derivative for Eq. (1):

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

- Set $x = x_j$, with x_j being x-coordinate of one of interpolation nodes. $j = 0, \dots, N$.
- $f'(x_j) = \sum_{k=0}^{N} f(x_k) L'_{N,k}(x_j) + \frac{f^{(N+1)}\left(\xi(x_j)\right)}{(N+1)!} \prod_{\substack{k=0; \\ k \neq j}}^{N} (x_j - x_k)$
- $\sum_{k=0}^{N} f(x_k) L'_{N,k}(x_j)$ -- **(N+1)-point formula to approximate** $f'(x_j)$
- $\frac{f^{(N+1)}\left(\xi(x_j)\right)}{(N+1)!} \prod_{\substack{k=0; \\ k \neq j}}^{N} (x_j - x_k)$ **is the error of approximation.**
- **Remark:** $f'(x_j) \approx \sum_{k=0}^{n} f(x_k) L'_{N,k}(x_j)$ ← **Finite Difference Formula**

Three-Point Formulas

- Let interpolation points be $(x_0, f(x_0))$, $(x_1, f(x_1))$ and $(x_2, f(x_2))$. Let x_0, x_1, and x_2 be equally spaced and the grid spacing be h.

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

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

Three-Point Formulas

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

  (three-point endpoint formula with error) **(4.4)**

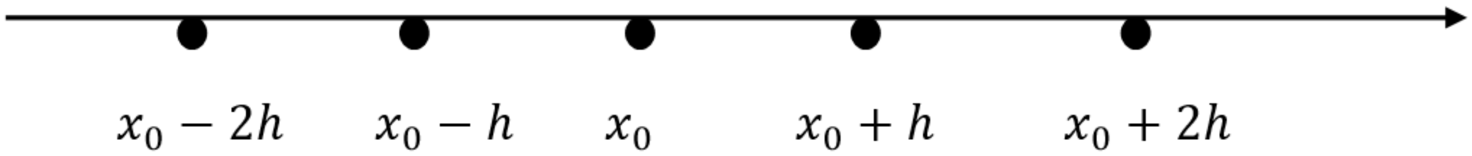
Remark: h can be both positive and negative.

- $f'(x_1) = \frac{1}{2h}[-f(x_0) + f(x_2)] + \frac{h^2}{6} f^{(3)}(\xi(x_1))$

  (three-point midpoint formula with error) **(4.5)**

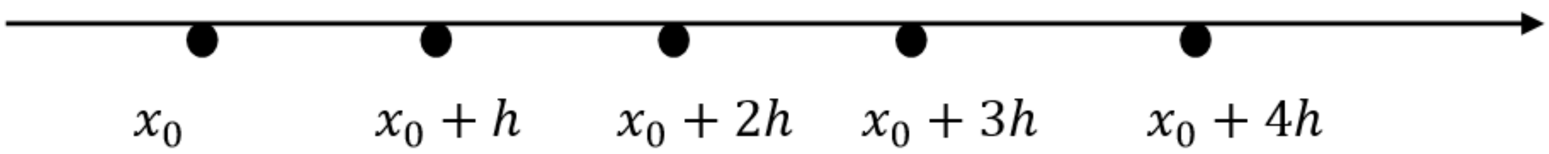
Mostly Used Five-Point Formulas

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

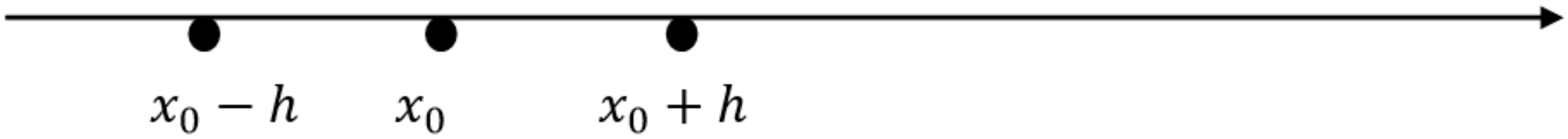


$$f'(x) = \frac{1}{12h}\left[-25f(x_0) + 48f(x_0 + h) - 36f(x_0 + 2h) + 16f(x_0 + 3h) - 3f(x_0 + 4h)\right] + \frac{h^4}{5} f^{(5)}(\xi) \qquad \textbf{(4.7)}$$

- **Example 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 Formulas



1. Expand $f(x_0 + h)$ about x_0:
   $$f(x_0 + h) = f(x_0) + f'(x_0)h + \frac{1}{2}f''(x_0)h^2 + \frac{1}{6}f'''(x_0)h^3 + \frac{1}{24}f^{(4)}(\xi_1)h^4$$
2. Expand $f(x_0 - h)$ about x_0:
   $$f(x_0 - h) = f(x_0) - f'(x_0)h + \frac{1}{2}f''(x_0)h^2 - \frac{1}{6}f'''(x_0)h^3 + \frac{1}{24}f^{(4)}(\xi_2)h^4$$
3. Add above Eqns.

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

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