Numerical Differentiation and Integration

Differentiation:

Calculus def.:

$$f'(x) \; \lim_{h\to 0} \frac{f(x+h)-f(x)}{h}$$

Idea: approximate numerically using small h

Finite Difference Approximation

Consider Taylor series centered at x:

Ⓐ $f(x+h) = f(x) + f'(x)\cdot h + \frac{f''(x)}{2!}h^2 + \frac{f'''(x)}{3!}h^3 \ldots$

Ⓑ $f(x-h) = f(x) - f'(x)\cdot h + \frac{f''(x)}{2!}h^2 - \frac{f'''(x)}{3!}h^3 \ldots$

Forward Difference Approximation

Use Ⓐ:

$$f(x+h) = f(x) + f'(x)\cdot h + \frac{f''(x)}{2!}h^2 + \frac{f'''(x)}{3!}h^3 \ldots$$

$$\frac{f(x+h)-f(x)}{h} = f'(x) + \underbrace{\frac{f''(x)}{2!}h + \frac{f'''(x)}{3!}h^2}_{\text{if } h \text{ small, truncate}} \ldots$$

$\Rightarrow$ $f'(x) \approx \frac{f(x+h)-f(x)}{h}$ w/ approximation error $O(h)$

Backward Difference Approximation

Use Ⓑ:

$$f(x-h) = f(x) - f'(x)h + \frac{f''(x)}{2!}h^2 - \frac{f'''(x)}{3!}h^3 + \ldots$$

$$\frac{f(x)-f(x-h)}{h} = f'(x) - \underbrace{\frac{f''(x)}{2!}h + \frac{f'''(x)}{3!}h^2}_{h \text{ small} \rightarrow \text{ truncate}} + \ldots$$

$\Rightarrow$ $f'(x) \approx \frac{f(x)-f(x-h)}{h}$ with approx. error $O(h)$

Centered Difference (1st Deriv.)

Use Ⓐ−Ⓑ:

$$f(x+h) = f(x) + f'(x)h + \frac{f''(x)}{2!}h^2 + \frac{f'''(x)}{3!}h^3 + \dots$$

$$f(x-h) = f(x) - f'(x)h + \frac{f''(x)}{2!}h^2 - \frac{f'''(x)}{3!}h^3 + \dots$$

subtract:

$$f(x+h) - f(x-h) = 2f'(x)h + \frac{2f'''(x)}{3!}h^3 + \dots$$

$$\Rightarrow \frac{f(x+h)-f(x-h)}{2h} = f'(x) + \underbrace{\frac{f'''(x)}{3!}h^2 + \dots}_{h \text{ small} \to \text{truncate}}$$

$\Rightarrow$ $f'(x) \approx \frac{f(x+h)-f(x-h)}{2h}$ with approx. error $O(h^2)$

Rmk.

1. Typically used for tabulated data $\{(x_i, f_i)\}_{i=1}^{n}$ or solving differential equations. Else, can use symbolic $f'(x)$.
2. Want h sufficiently small, but not so small as to lead to cancellation of significant digits. $(f(x+h)-f(x))$
   - one remedy: centered diff.s
3. In practice, if h is much smaller than $\sqrt{\varepsilon}$, round-off errors will dominate

   Double precision : $\sqrt{\varepsilon_d} \approx 10^{-8}$

   Single precision : $\sqrt{\varepsilon_s} \approx 10^{-4}$

Centered Difference (2nd Deriv.)

Use Ⓐ+Ⓑ:

$$f(x+h) = f(x) + f'(x)h + \frac{f''(x)}{2!}h^2 + \frac{f'''(x)}{3!}h^3 + \dots$$

$$f(x-h) = f(x) - f'(x)h + \frac{f''(x)}{2!}h^2 - \frac{f'''(x)}{3!}h^3 + \dots$$

$$f(x+h) + f(x-h) = 2f(x) + f''(x)h^2 + \frac{2f^{(4)}(x)}{4!}h^4 + \dots$$

$$\Rightarrow \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} = f''(x) + \underbrace{\frac{2f^{(4)}(x)}{4!}h^2 + \dots}_{h \text{ small} \to \text{truncate}}$$

$$\Rightarrow f''(x) \approx \frac{f(x+h) - 2f(x) + f(x-h)}{h^2} \text{ with approx. error } O(h^2)$$

Ex. Poisson's Eqn in 1-D

$$\frac{-d^2u}{dx^2} = f(x) \qquad 0 < f(x) < 1 \qquad \text{(DE)}$$

where $f(x)$ is given, $u(x)$ is unknown.

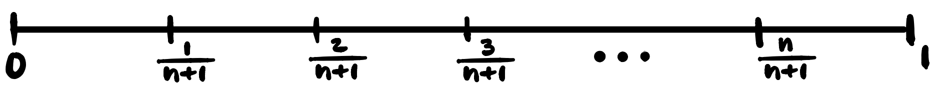
Assume Dirichlet's boundary conditions:

$u(0) = 0 = u(1)$

One approach to solve (DE):

Discretize & use linear algebra. That is:

- try to compute an approx. solution at $n+2$ equally-spaced points, x_i :



- denote $u_i = u(x_i)$ and $f_i = f(x_i)$
- try to turn (DE) into a linear system using finite diff. approx.

$$\frac{d^2u(x)}{dx^2} \approx \frac{u(x+h) - 2u(x) + u(x-h)}{h^2}$$

$$= \frac{u(x_{i+1}) - 2u(x_i) + u(x_{i-1})}{h^2}$$

$$= \frac{u_{i+1} - 2u_i + u_{i-1}}{h^2}$$

$\therefore$ Poisson eqn. $\to$ approximation:

$$\frac{-u_{i+1} + 2u_i - u_{i-1}}{h^2} = f_i \qquad i = 1, 2, \dots n$$

or $-u_{i+1} + 2u_i - u_{i-1} = h^2 f_i \qquad i = 1, 2, \dots n$

- since boundary conditions imply $u_0 = u_{n+1} = 0$, we can obtain the system of eqns:

$$
\begin{array}{ll}
i=1 & 2u_1 - u_2 = h^2 f_1 \\
i=2 & -u_1 + 2u_2 - u_3 = h^2 f_2 \\
i=3 & -u_2 + 2u_3 - u_4 = h^2 f_3 \\
\vdots & \\
i=n-1 & -u_{n-2} + 2u_{n-1} - u_n = h^2 f_{n-1} \\
i=n & -u_{n-1} + 2u_n = h^2 f_n
\end{array}
$$

$$
\Rightarrow \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & \cdots & \\ & -1 & 2 & -1 & \\ \vdots & & \ddots & & \\ & & & 2 & -1 \\ & & & -1 & 2 \end{bmatrix} \begin{bmatrix} u_1 \\ u_2 \\ \vdots \\ \\ u_n \end{bmatrix} = h^2 \begin{bmatrix} f_1 \\ f_2 \\ \vdots \\ \\ f_n \end{bmatrix}
$$

$$\Rightarrow A\underline{u} = \underline{b}$$

MATLAB: `u = A\b`