

Today: Numerical Differentiation

- Examples deriving formulas
- Applications to differential equations

Announcement: No office hour on Monday, May 25 (Memorial Day)

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Example 1. Prove the following forward difference formula when f is a smooth function:

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

Taylor expansion about a :

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

Expand $f(x_0+h)$ about x_0

$$\begin{aligned} f(x_0+h) &= f(x_0) + f'(x_0)(\cancel{x_0}+h-\cancel{x_0}) + \frac{f''(x_0)}{2!}(\cancel{x_0}+h-\cancel{x_0})^2 \\ &\quad + \frac{f'''(x_0)}{3!}(\cancel{x_0}+h-\cancel{x_0})^3 + \dots \end{aligned}$$

$$f(x_0+h) = f(x_0) + h f'(x_0) + \frac{h^2}{2!} f''(x_0) + \frac{h^3}{3!} f'''(x_0) + O(h^4)$$

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Example 1. continued

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

$$f(x_0 + h) = f(x_0) + h f'(x_0) + \frac{h^2}{2!} f''(x_0) + \frac{h^3}{3!} f'''(x_0) + O(h^4)$$

$$h f'(x_0) = f(x_0 + h) - f(x_0) - \frac{h^2}{2!} f''(x_0) - \frac{h^3}{3!} f'''(x_0) + O(h^4)$$

$$f'(x_0) = \frac{f(x_0 + h) - f(x_0)}{h} - \frac{h}{2} f''(x_0) - \frac{h^2}{3!} f'''(x_0) + O(h^3) \checkmark$$

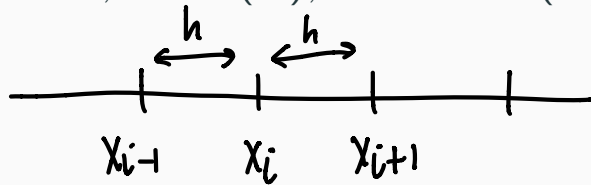
↑
order $O(h)$

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Example 2. Let $u(x)$ and $a(x)$ be smooth functions. Determine the order of accuracy of

$$\frac{(a_{i+1} + a_i)(u_{i+1} - u_i) - (a_i + a_{i-1})(u_i - u_{i-1}))}{2h^2}$$

as an approximation to $\left. \frac{d}{dx} \left(a(x) \frac{du}{dx} \right) \right|_{x_i}$ where h is the mesh width, $x_i = ih$, $a_i = a(x_i)$, and $u_i = u(x_i)$.



$$x_{i+1} = x_i + h$$

$$x_{i-1} = x_i - h$$

Taylor expansions:

$$a(x_{i+1}) = a(x_i) + a'(x_i)(x_{i+1} - x_i) + \frac{a''(x_i)}{2!}(x_{i+1} - x_i)^2 + \dots$$

$$a(x_{i+1}) = a(x_i) + ha'(x_i) + \frac{h^2}{2!}a''(x_i) + O(h^3)$$

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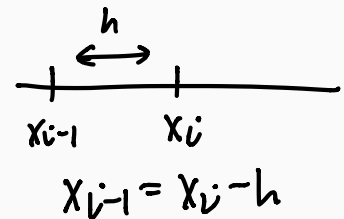
Example 2. continued

$$\frac{(a_{i+1} + a_i)(u_{i+1} - u_i) - (a_i + a_{i-1})(u_i - u_{i-1}))}{2h^2}$$

$$a(x_{i+1}) = a(x_i) + ha'(x_i) + \frac{h^2}{2!} a''(x_i) + O(h^3)$$

$$a_{i+1} = a_i + ha'_i + \frac{h^2}{2} a''_i + O(h^3)$$

$$u_{i+1} = u_i + hu'_i + \frac{h^2}{2} u''_i + O(h^3)$$



$$\begin{aligned} a(x_{i-1}) &= a(x_i) + a'(x_i)(x_{i-1} - x_i) + \frac{a''(x_i)}{2!} (x_{i-1} - x_i)^2 + \dots \\ &= a(x_i) - ha'(x_i) + \frac{h^2}{2} a''(x_i) + O(h^3) \end{aligned}$$

$$a_{i-1} = a_i - ha'_i + \frac{h^2}{2} a''_i + O(h^3)$$

$$u_{i-1} = u_i - hu'_i + \frac{h^2}{2} u''_i + O(h^3)$$

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Example 2. continued

$$\frac{(a_{i+1} + a_i)(u_{i+1} - u_i) - (a_i + a_{i-1})(u_i - u_{i-1})}{2h^2}$$

$$a_{i+1} = a_i + ha_i' + \frac{h^2}{2}a_i'' + o(h^3)$$

$$u_{i+1} = u_i + hu_i' + \frac{h^2}{2}u_i'' + o(h^3)$$

$$a_{i-1} = a_i - ha_i' + \frac{h^2}{2}a_i'' + o(h^3)$$

$$u_{i-1} = u_i - hu_i' + \frac{h^2}{2}u_i'' + o(h^3)$$

Plug in :

$$\frac{1}{2h^2} \left((2a_i + ha_i' + \frac{h^2}{2}a_i'' + o(h^3))(hu_i' + \frac{h^2}{2}u_i'' + o(h^3)) - (2a_i - ha_i' + \frac{h^2}{2}a_i'' + o(h^3))(hu_i' - \frac{h^2}{2}u_i'' + o(h^3)) \right)$$

$$= \frac{1}{2h^2} \left(2a_i hu_i' + h^2 a_i u_i'' + h^2 a_i' u_i' + o(h^3) - (2h a_i u_i' - h^2 a_i u_i'' - h^2 a_i' u_i' + o(h^3)) \right)$$

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Example 2. continued

$$\left. \frac{d}{dx} \left(a(x) \frac{du}{dx} \right) \right|_{x_i} = a'(x_i) u'(x_i) + a(x_i) u''(x_i)$$

$$= a'_i u'_i + a_i u''_i$$

$$\begin{aligned} & \frac{(a_{i+1} + a_i)(u_{i+1} - u_i) - (a_i + a_{i-1})(u_i - u_{i-1}))}{2h^2} \\ &= \frac{1}{2h^2} \left(\cancel{2a_i h u'_i} + h^2 a_i u''_i + h^2 a'_i u'_i + O(h^3) \right. \\ & \quad \left. - (\cancel{2h a_i u'_i} - h^2 a_i u''_i - h^2 a'_i u'_i + O(h^3)) \right) \\ &= \frac{1}{2h^2} \left(h^2 a_i u''_i + h^2 a'_i u'_i + h^2 a_i u''_i + h^2 a'_i u'_i + O(h^3) \right) \\ &= \frac{1}{2h^2} \left(2h^2 a_i u''_i + 2h^2 a'_i u'_i + O(h^3) \right) \\ &= \underline{a_i u''_i + a'_i u'_i} + \underline{O(h)} \end{aligned}$$

order $O(h)$

Example 2. continued

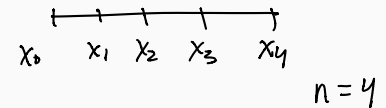
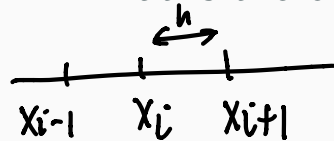
$$\frac{(a_{i+1} + a_i)(u_{i+1} - u_i) - (a_i + a_{i-1})(u_i - u_{i-1})}{2h^2}$$

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Example 3. Consider the boundary-value problem

$$y'' = q(x)y + r(x), \quad \text{for } a \leq x \leq b, \quad y(a) = \alpha, y(b) = \beta$$

Using standard centered-difference approximations for $y''(x_i)$, derive the system of equations whose solution can be used to approximate the solution to this problem. What is the order of accuracy of your approximation?



Taylor expansions:

$$\begin{aligned} y(x_{i+1}) &= y(x_i) + y'(x_i)(x_{i+1} - x_i) + \frac{y''(x_i)}{2}(x_{i+1} - x_i)^2 \\ &\quad + \frac{y'''(x_i)}{3!}(x_{i+1} - x_i)^3 + \dots \end{aligned}$$

$$y_{i+1} = y_i + h y_i' + \frac{h^2}{2} y_i'' + \frac{h^3}{3!} y_i''' + O(h^4)$$

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Example 3. continued

$$\underline{y''} = q(x)y + r(x), \quad \text{for } a \leq x \leq b, \quad y(a) = \alpha, y(b) = \beta$$

$$\begin{aligned} y_{i+1} &= y_i + h y_i' + \frac{h^2}{2} y_i'' + \frac{h^3}{3!} y_i''' + O(h^4) \\ + y_{i-1} &= y_i - h y_i' + \frac{h^2}{2} y_i'' - \frac{h^3}{3!} y_i''' + O(h^4) \end{aligned}$$

$$y_{i+1} + y_{i-1} = 2y_i + h^2 y_i'' + O(h^4)$$

$$\frac{h^2 y_i''}{h^2} = \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} + \frac{O(h^4)}{h^2}$$

$$y_i'' = \frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} + O(h^2) \quad \boxed{\text{order } O(h^2)}$$

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Example 3. continued

$$y'' = q(x)y + r(x), \quad \text{for } a \leq x \leq b, \quad \underline{y(a) = \alpha, y(b) = \beta}$$

$$\frac{y_{i+1} - 2y_i + y_{i-1}}{h^2} = q_i y_i + r_i$$

$$\begin{array}{ccccccc} x_0 & x_1 & x_2 & & \dots & & x_n \\ | & | & | & & & & | \\ a & & & & & & b \end{array}$$

$$\frac{y_{i+1} - (q_i h^2 + 2)y_i + y_{i-1}}{h^2} = r_i$$

$$\begin{aligned} y_0 &= y(x_0) = y(a) = \alpha \\ y_n &= y(x_n) = y(b) = \beta \end{aligned}$$

$$i=1: \quad \frac{y_2 - (q_1 h^2 + 2)y_1 + y_0}{h^2} = r_1 \Rightarrow \frac{y_2 - (q_1 h^2 + 2)y_1}{h^2} = r_1 - \frac{\alpha}{h^2}$$

$$i=2, 3, \dots, n-2$$

$$i=2: \quad \frac{y_3 - (q_2 h^2 + 2)y_2 + y_1}{h^2} = r_2$$

$$i=n-1: \quad \frac{y_n - (q_{n-1} h^2 + 2)y_{n-1} + y_{n-2}}{h^2} = r_{n-1}$$

$$\frac{-(q_{n-1} h^2 + 2)y_{n-1} + y_{n-2}}{h^2} \equiv r_{n-1} - \frac{\beta}{h^2}$$

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Example 3. continued

$$\frac{y_{i+1} - (q_i h^2 + 2)y_i + y_{i-1}}{h^2} = r_i$$

$$y'' = q(x)y + r(x), \quad \text{for } a \leq x \leq b, \quad y(a) = \alpha, y(b) = \beta$$

$$\underbrace{\begin{pmatrix} -q_1 - \frac{2}{h^2} & \frac{1}{h^2} & & \\ \frac{1}{h^2} & -q_2 - \frac{2}{h^2} & \frac{1}{h^2} & \\ & \ddots & \ddots & \ddots \\ & & \frac{1}{h^2} & -q_{n-2} - \frac{2}{h^2} & \frac{1}{h^2} \\ & & & \frac{1}{h^2} & -q_{n-1} - \frac{2}{h^2} \end{pmatrix}}_{\underline{A}} \underbrace{\begin{pmatrix} y_1 \\ y_2 \\ \vdots \\ y_{n-2} \\ y_{n-1} \end{pmatrix}}_{\underline{y}} = \underbrace{\begin{pmatrix} r_1 - \frac{\alpha}{h^2} \\ r_2 \\ \vdots \\ r_{n-2} \\ r_{n-1} - \frac{\beta}{h^2} \end{pmatrix}}_{\underline{b}}$$

$\underline{y} = \underline{A} \backslash \underline{b}$

$$\frac{y_2 - (q_1 h^2 + 2)y_1}{h^2} = r_1 - \frac{\alpha}{h^2}$$

$$\frac{y_3 - (q_2 h^2 + 2)y_2 + y_1}{h^2} = r_2$$

Example 3. continued

$$y'' = q(x)y + r(x), \quad \text{for } a \leq x \leq b, \quad y(a) = \alpha, y(b) = \beta$$

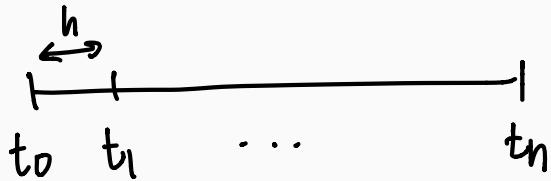
SIR Model: The SIR model is a simple compartmental model. The model consists of three compartments: **S**usceptible, **I**nfected, **R**ecovered. These variables represent the population in each compartment at a particular time. The SIR model can be expressed as the following system of differential equations:

$$\begin{aligned}\frac{dS}{dt} &= -\beta \frac{IS}{N} \\ \frac{dI}{dt} &= \beta \frac{IS}{N} - \gamma I \\ \frac{dR}{dt} &= \gamma I\end{aligned}$$

$R_0 = \frac{\beta}{\gamma}$ is called the “basic reproduction number”, i.e. the expected number of new infections from a single infection in a population where all subjects are susceptible.

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Example 4. Using the forward difference formula, program the SIR model in MATLAB. Try different parameters and initial values.



$$S(t_i) = S_i$$

$$I(t_i) = I_i$$

$$R(t_i) = R_i$$

$$\frac{dS}{dt} = -\beta \frac{IS}{N}$$

$$\frac{dI}{dt} = \beta \frac{IS}{N} - \gamma I$$

$$\frac{dR}{dt} = \gamma I$$

Forward difference

$$f'_i \approx \frac{f_{i+1} - f_i}{h}$$

"Forward Euler Method"

$$\frac{S_{i+1} - S_i}{h} = -\beta \frac{I_i S_i}{N} \longrightarrow S_{i+1} = S_i - h \beta \frac{I_i S_i}{N}$$

$$\frac{I_{i+1} - I_i}{h} = \beta \frac{I_i S_i}{N} - \gamma I_i \longrightarrow I_{i+1} = I_i + h \left(\beta \frac{I_i S_i}{N} - \gamma I_i \right)$$

$$\frac{R_{i+1} - R_i}{h} = \gamma I_i \longrightarrow R_{i+1} = R_i + h \gamma I_i$$