

9. Numerical differentiation

- finite difference formulas
- Richardson extrapolation
- derivatives of unequally spaced data

Forward difference differentiation formula

- forward Taylor series expansion at $x_{i+1} = x_i + h$ about x_i :

$$f(x_{i+1}) = f(x_i) + f'(x_i)h + \frac{f''(x_i)}{2}h^2 + \dots$$

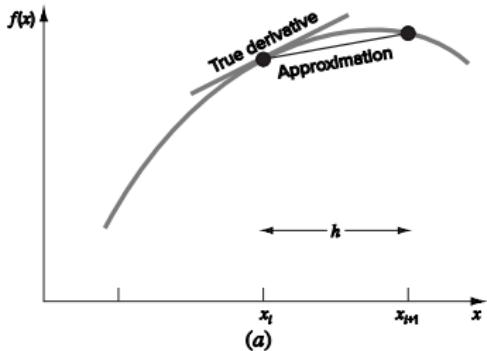
- solving for the derivative:

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h} - \frac{f''(x_i)}{2}h + O(h^2) \quad (9.1)$$

- truncating higher-order terms gives:

$$f'(x_i) \approx \frac{f(x_{i+1}) - f(x_i)}{h}$$

error $O(h)$



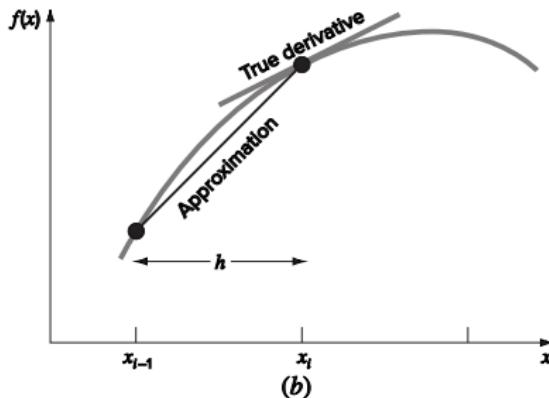
Backward difference differentiation formula

derivative backward approximation

$$f'(x_i) \approx \frac{f(x_i) - f(x_{i-1})}{h}, \quad \text{error } O(h)$$

follows from backward Taylor series expansion at $x_{i-1} = x_i - h$ about x_i

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



Centered difference differentiation formula

derivative centered difference approximation

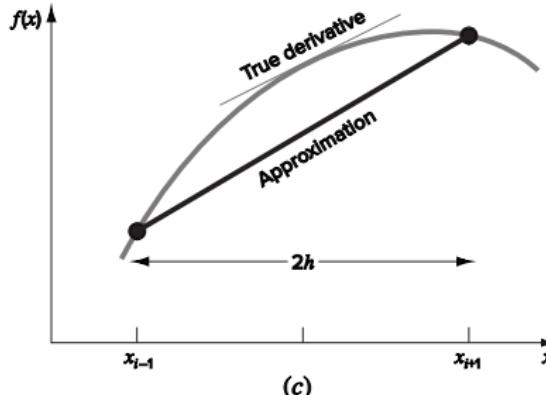
$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h}, \quad \text{error } O(h^2)$$

follows by subtracting

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

from

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



Improved forward difference formula

- high-accuracy divided-difference formulas can be generated by including additional terms from the Taylor series
- Taylor series at x_{i+2} about x_i with $x_{i+2} - x_i = 2h$:

$$f(x_{i+2}) = f(x_i) + f'(x_i)(2h) + \frac{f''(x_i)}{2!}(2h)^2 + \dots$$

- subtracting from 2 times

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

gives

$$f''(x_i) \approx \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2}, \quad \text{error } O(h)$$

this is a second derivative approximation

Improved forward difference formula

- substitute into (9.1) gives

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

- collecting terms:

$$f'(x_i) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} + O(h^2)$$

accuracy improved to $O(h^2)$

- similar formulas can be developed for backward and centered differences
- useful for estimating derivatives with greater accuracy from discrete data

Forward finite-divided-difference formulas

First derivative

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_i)}{h}, \quad O(h)$$

$$f'(x_i) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h}, \quad O(h^2)$$

Second derivative

$$f''(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + f(x_i)}{h^2}, \quad O(h)$$

$$f''(x_i) = \frac{-f(x_{i+3}) + 4f(x_{i+2}) - 5f(x_{i+1}) + 2f(x_i)}{h^2}, \quad O(h^2)$$

Third derivative

$$f^{(3)}(x_i) = \frac{f(x_{i+3}) - 3f(x_{i+2}) + 3f(x_{i+1}) - f(x_i)}{h^3}, \quad O(h)$$

$$f^{(3)}(x_i) = \frac{-3f(x_{i+4}) + 14f(x_{i+3}) - 24f(x_{i+2}) + 18f(x_{i+1}) - 5f(x_i)}{2h^3}, \quad O(h^2)$$

Fourth derivative

$$f^{(4)}(x_i) = \frac{f(x_{i+4}) - 4f(x_{i+3}) + 6f(x_{i+2}) - 4f(x_{i+1}) + f(x_i)}{h^4}, \quad O(h)$$

$$f^{(4)}(x_i) = \frac{-2f(x_{i+5}) + 11f(x_{i+4}) - 24f(x_{i+3}) + 26f(x_{i+2}) - 14f(x_{i+1}) + 3f(x_i)}{h^4}, \quad O(h^2)$$

Backward finite-divided difference formulas

First derivative

$$f'(x_i) = \frac{f(x_i) - f(x_{i-1})}{h}, \quad O(h)$$

$$f'(x_i) = \frac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{2h}, \quad O(h^2)$$

Second derivative

$$f''(x_i) = \frac{f(x_i) - 2f(x_{i-1}) + f(x_{i-2})}{h^2}, \quad O(h)$$

$$f''(x_i) = \frac{2f(x_i) - 5f(x_{i-1}) + 4f(x_{i-2}) - f(x_{i-3})}{h^2}, \quad O(h^2)$$

Third derivative

$$f^{(3)}(x_i) = \frac{f(x_i) - 3f(x_{i-1}) + 3f(x_{i-2}) - f(x_{i-3})}{h^3}, \quad O(h)$$

$$f^{(3)}(x_i) = \frac{5f(x_i) - 18f(x_{i-1}) + 24f(x_{i-2}) - 14f(x_{i-3}) + 3f(x_{i-4})}{2h^3}, \quad O(h^2)$$

Fourth derivative

$$f^{(4)}(x_i) = \frac{f(x_i) - 4f(x_{i-1}) + 6f(x_{i-2}) - 4f(x_{i-3}) + f(x_{i-4})}{h^4}, \quad O(h)$$

$$f^{(4)}(x_i) = \frac{3f(x_i) - 14f(x_{i-1}) + 26f(x_{i-2}) - 24f(x_{i-3}) + 11f(x_{i-4}) - 2f(x_{i-5})}{h^4}, \quad O(h^2)$$

Centered finite-divided-difference formulas

First derivative

$$f'(x_i) = \frac{f(x_{i+1}) - f(x_{i-1})}{2h}, \quad O(h^2)$$

$$f'(x_i) = \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h}, \quad O(h^4)$$

Second derivative

$$f''(x_i) = \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2}, \quad O(h^2)$$

$$f''(x_i) = \frac{-f(x_{i+2}) + 16f(x_{i+1}) - 30f(x_i) + 16f(x_{i-1}) - f(x_{i-2})}{12h^2}, \quad O(h^4)$$

Third derivative

$$f^{(3)}(x_i) = \frac{f(x_{i+2}) - 2f(x_{i+1}) + 2f(x_{i-1}) - f(x_{i-2})}{2h^3}, \quad O(h^2)$$

$$f^{(3)}(x_i) = \frac{-f(x_{i+3}) + 8f(x_{i+2}) - 13f(x_{i+1}) + 13f(x_{i-1}) - 8f(x_{i-2}) + f(x_{i-3})}{8h^3}, \quad O(h^4)$$

Fourth derivative

$$f^{(4)}(x_i) = \frac{f(x_{i+2}) - 4f(x_{i+1}) + 6f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{h^4}, \quad O(h^2)$$

$$f^{(4)}(x_i) = \frac{-f(x_{i+3}) + 12f(x_{i+2}) - 39f(x_{i+1}) + 56f(x_i) - 39f(x_{i-1}) + 12f(x_{i-2}) - f(x_{i-3})}{6h^4}, \quad O(h^4)$$

Example

before, we estimated the derivative of

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

at $x = 0.5$ using finite divided differences and a step size of $h = 0.25$:

	forward	backward	centered
order	$O(h)$	$O(h)$	$O(h^2)$
estimate	-1.155	-0.714	-0.934
$\varepsilon_t (\%)$	-26.5	21.7	-2.4

errors were computed on the basis of the true value $f'(0.5) = -0.9125$

repeat this computation, but employ the high-accuracy formulas

Example

data needed is

$$x_{i-2} = 0, f(x_{i-2}) = 1.2, \quad x_{i-1} = 0.25, f(x_{i-1}) = 1.1035156$$

$$x_i = 0.5, f(x_i) = 0.925$$

$$x_{i+1} = 0.75, f(x_{i+1}) = 0.6363281, \quad x_{i+2} = 1, f(x_{i+2}) = 0.2$$

Forward difference $O(h^2)$

$$f'(0.5) = \frac{-f(x_{i+2}) + 4f(x_{i+1}) - 3f(x_i)}{2h} = \frac{-0.2 + 4(0.6363281) - 3(0.925)}{2(0.25)} = -0.859375$$

$$\varepsilon_t = 5.82\%$$

Backward difference $O(h^2)$

$$f'(0.5) = \frac{3f(x_i) - 4f(x_{i-1}) + f(x_{i-2})}{2h} = \frac{3(0.925) - 4(1.1035156) + 1.2}{2(0.25)} = -0.878125$$

$$\varepsilon_t = 3.77\%$$

Centered difference $O(h^4)$

$$f'(0.5) = \frac{-f(x_{i+2}) + 8f(x_{i+1}) - 8f(x_{i-1}) + f(x_{i-2})}{12h} = -0.9125$$

$$\varepsilon_t = 0\%$$

Outline

- finite difference formulas
- **Richardson extrapolation**
- derivatives of unequally spaced data

Richardson extrapolation

to this point, we have seen that there are two ways to improve derivative:

1. decrease the step size
2. use a higher-order formula that employs more points

recall Richardson extrapolation for integrals

$$I \approx I(h_2) + \frac{1}{\left(\frac{h_1}{h_2}\right)^2 - 1} [I(h_2) - I(h_1)]$$

for $h_2 = h_1/2$:

$$I \approx \frac{4}{3}I(h_2) - \frac{1}{3}I(h_1)$$

same idea holds for derivatives:

$$D \approx \frac{4}{3}D(h_2) - \frac{1}{3}D(h_1)$$

for centered difference accuracy improves $O(h^2) \rightarrow O(h^4)$

Example

estimate the first derivative of

$$f(x) = -0.1x^4 - 0.15x^3 - 0.5x^2 - 0.25x + 1.2$$

at $x = 0.5$ with step sizes $h_1 = 0.5$, $h_2 = 0.25$; true value: $f'(0.5) = -0.9125$

- centered differences:

$$D(h_1) = \frac{0.2 - 1.2}{1} = -1.0, \quad \varepsilon_t = -9.6\%$$

$$D(h_2) = \frac{0.6363281 - 1.1035156}{0.5} = -0.934375, \quad \varepsilon_t = -2.4\%$$

- Richardson extrapolation:

$$D = \frac{4}{3}(-0.934375) - \frac{1}{3}(-1.0) = -0.9125$$

perfect result since $f(x)$ is a fourth-order polynomial

Outline

- finite difference formulas
- Richardson extrapolation
- **derivatives of unequally spaced data**

Derivatives via Lagrange second-order polynomial

fit a quadratic Lagrange polynomial to 3 adjacent points $(x_0, y_0), (x_1, y_1), (x_2, y_2)$

$$f'(x) = f(x_0) \frac{(x - x_1)(x - x_2)}{(x_0 - x_1)(x_0 - x_2)} + f(x_1) \frac{(x - x_0)(x - x_2)}{(x_1 - x_0)(x_1 - x_2)} \\ + f(x_2) \frac{(x - x_0)(x - x_1)}{(x_2 - x_0)(x_2 - x_1)}$$

differentiating the interpolating polynomial yields

$$f'(x) = f(x_0) \frac{2x - x_1 - x_2}{(x_0 - x_1)(x_0 - x_2)} + f(x_1) \frac{2x - x_0 - x_2}{(x_1 - x_0)(x_1 - x_2)} \\ + f(x_2) \frac{2x - x_0 - x_1}{(x_2 - x_0)(x_2 - x_1)}$$

- works for unequally spaced points
- valid derivative approximation anywhere within the interval
- $O(h^2)$ accuracy for spacing $x_{i+1} - x_i = O(h)$ (same as centered differences)

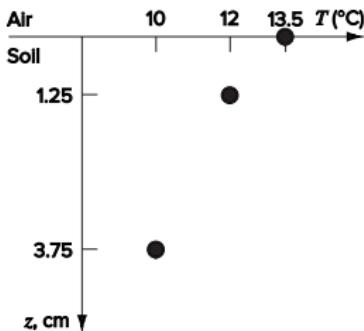
Example: differentiating unequally spaced data

soil temperature measurements at depths:

(0, 13.5°C), (1.25, 12°C), (3.75, 10°C)

compute heat flux heat flux

$$q(0) = -k\rho C \left. \frac{dT}{dz} \right|_{z=0}$$



with $k = 3.5 \times 10^{-7} \text{ m}^2/\text{s}$, $\rho = 1800 \text{ kg/m}^3$, $C = 840 \text{ J/(kg}^\circ\text{C)}$

we have

$$\begin{aligned} \left. \frac{dT}{dz} \right|_{z=0} &= 13.5 \frac{2(0)-1.25-3.75}{(0-1.25)(0-3.75)} + 12 \frac{2(0)-0-3.75}{(1.25-0)(1.25-3.75)} + 10 \frac{2(0)-0-1.25}{(3.75-0)(3.75-1.25)} \\ &= -14.4 + 14.4 - 1.333 = -1.333 \text{ } ^\circ\text{C/cm} \end{aligned}$$

heat flux:

$$q(0) = -3.5 \times 10^{-7} (1800)(840)(-133.333) = 70.56 \text{ W/m}^2$$

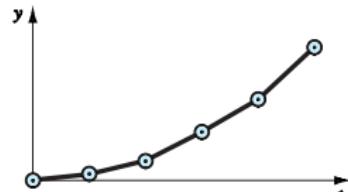
Derivatives via Lagrange third-order polynomial

differentiate the 3rd-order Lagrange polynomial fitted to four adjacent points resulting derivative is

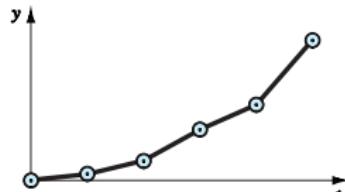
$$\begin{aligned}f'(x) &= \frac{3x^2 - 2(x_2 + x_3 + x_4)x + (x_2x_3 + x_2x_4 + x_3x_4)}{(x_1 - x_2)(x_1 - x_3)(x_1 - x_4)} f(x_1) \\&\quad + \frac{3x^2 - 2(x_1 + x_3 + x_4)x + (x_1x_3 + x_1x_4 + x_3x_4)}{(x_2 - x_1)(x_2 - x_3)(x_2 - x_4)} f(x_2) \\&\quad + \frac{3x^2 - 2(x_1 + x_2 + x_4)x + (x_1x_2 + x_1x_4 + x_2x_4)}{(x_3 - x_1)(x_3 - x_2)(x_3 - x_4)} f(x_3) \\&\quad + \frac{3x^2 - 2(x_1 + x_2 + x_3)x + (x_1x_2 + x_1x_3 + x_2x_3)}{(x_4 - x_1)(x_4 - x_2)(x_4 - x_3)} f(x_4)\end{aligned}$$

Differentiation noisy data

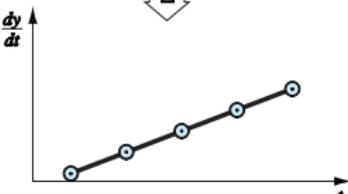
shortcoming of numerical differentiation is that it tends to amplify errors in the data



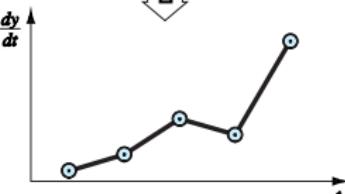
(a)



(b)



(c)



(d)

References and further readings

- S. C. Chapra and R. P. Canale. *Numerical Methods for Engineers* (8th edition). McGraw Hill, 2021. (Ch. 23)
- S. C. Chapra. *Applied Numerical Methods with MATLAB for Engineers and Scientists* (5th edition). McGraw Hill, 2023. (Ch. 21)