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:

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

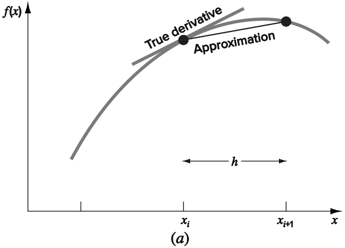
- solving for the derivative:

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

- truncating higher-order terms gives:

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

error $\quad \mathcal{O}(h)$

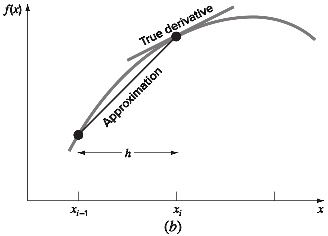


Backward difference differentiation formula

derivative backward approximation

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

error $\quad \mathcal{O}(h)$



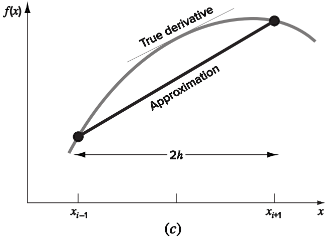
follows from backward Taylor series expansion at $x_{i-1} = x_i - h$ about x_i

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

Centered difference differentiation formula

derivative centered difference approximation

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



follows by subtracting

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

from

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

Improved forward difference formula

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

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

- subtracting from 2 times

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

gives

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

this is a second derivative approximation

Improved forward difference formula

- substitute into (9.1) gives

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

- collecting terms:

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

  accuracy improved to $\mathcal{O}(h^2)$

- 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

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

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

Second derivative

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

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

Third derivative

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

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

Fourth derivative

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

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

Backward finite-divided difference formulas

First derivative

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

Second derivative

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

Third derivative

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

Fourth derivative

$$f^{(4)}(x_i) = \frac{f(x_i)-4f(x_{i-1})+6f(x_{i-2})-4f(x_{i-3})+f(x_{i-4})}{h^4}, \quad \mathcal{O}(h)$$
$$f^{(4)}(x_i) = \frac{3f(x_i)-14f(x_{i-1})+26f(x_{i-2})-24f(x_{i-3})+11f(x_{i-4})-2f(x_{i-5})}{h^4}, \quad \mathcal{O}(h^2)$$

Centered finite-divided-difference formulas

First derivative

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

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

Second derivative

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

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

Third derivative

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

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

Fourth derivative

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

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

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 $\mathcal{O}(h^2)$

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

$\varepsilon_t = 5.82\%$

Backward difference $\mathcal{O}(h^2)$

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

$\varepsilon_t = 3.77\%$

Centered difference $\mathcal{O}(h^4)$

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

$\varepsilon_t = 0\%$

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 $h_2 = h_1/2$:

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

same idea holds for derivatives:

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

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

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:

$$D(h_1) = \frac{0.2 - 1.2}{2 \times 0.5} = -1.0, \quad \varepsilon_t = -9.6\%$$

$$D(h_2) = \frac{0.6363281 - 1.1035156}{2 \times 0.25} = -0.934375, \quad \varepsilon_t = -2.4\%$$

- Richardson extrapolation:

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

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 $(x_0, y_0), (x_1, y_1), (x_2, y_2)$:

$$
\begin{aligned}
f(x) = {} & f(x_0)\,\frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} + f(x_1)\,\frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} \\
& + f(x_2)\,\frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)}
\end{aligned}
$$

differentiating the interpolating polynomial yields

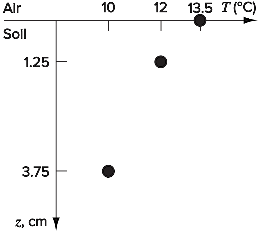
$$
\begin{aligned}
f'(x) = {} & f(x_0)\,\frac{2x-x_1-x_2}{(x_0-x_1)(x_0-x_2)} + f(x_1)\,\frac{2x-x_0-x_2}{(x_1-x_0)(x_1-x_2)} \\
& + f(x_2)\,\frac{2x-x_0-x_1}{(x_2-x_0)(x_2-x_1)}
\end{aligned}
$$

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

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

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

we have

$$\frac{dT}{dz}\bigg|_{z=0} = 13.5\frac{2(0)-1.25-3.75}{(0-1.25)(0-3.75)} + 12\frac{2(0)-0-3.75}{(1.25-0)(1.25-3.75)} + 10\frac{2(0)-0-1.25}{(3.75-0)(3.75-1.25)}$$

$$= -14.4 + 14.4 - 1.333 = -1.333\ °C/\text{cm}$$

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

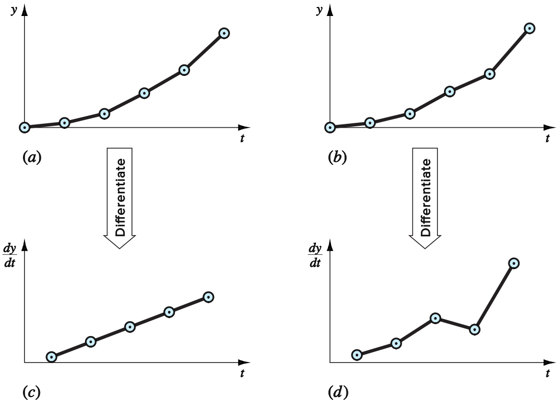
$$(x_1, f(x_1)),\ (x_2, f(x_2)),\ (x_3, f(x_3)),\ (x_4, f(x_4))$$

resulting derivative is

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

Differentiation noisy data

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



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)