

Assignment 3

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1. Deriving a second derivative approximation formula

We are looking for an equation that approximates the second derivative and is of the form

$$f''(x) = \lambda_1 f(x) + \lambda_2 f(x+h) + \lambda_3 f(x-h) + \lambda_4 f(x+2h) + \lambda_5 f(x-2h) \quad (1)$$

We can start by finding the Taylor expansions of each function

$$f(x) = f(x)$$

$$f(x+h) = f(x) + hf'(x) + \frac{h^2}{2!}f''(x) + \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{(4)}(x) + \mathcal{O}(h^5)$$

$$f(x-h) = f(x) - hf'(x) + \frac{h^2}{2!}f''(x) - \frac{h^3}{3!}f'''(x) + \frac{h^4}{4!}f^{(4)}(x) - \mathcal{O}(h^5)$$

$$f(x+2h) = f(x) + 2hf'(x) + 2hf''(x) + \frac{8h^3}{3!}f'''(x) + \frac{16h^4}{4!}f^{(4)}(x) + \mathcal{O}(h^5)$$

$$f(x-2h) = f(x) - 2hf'(x) + 2hf''(x) - \frac{8h^3}{3!}f'''(x) + \frac{16h^4}{4!}f^{(4)}(x) - \mathcal{O}(h^5)$$

and then, after collecting coefficients of derivatives of f , Equation 1 looks like this, ignoring the error term

$$\begin{aligned} f''(x) = & (\lambda_1 + \lambda_2 + \lambda_3 + \lambda_4 + \lambda_5)f(x) + (\lambda_2 - \lambda_3 + 2\lambda_4 - 2\lambda_5)hf'(x) \\ & + (\lambda_2 + \lambda_3 + 4\lambda_4 + 4\lambda_5)h^2f''(x) + (\lambda_2 - \lambda_3 + 8\lambda_4 - 8\lambda_5)h^3f'''(x) \\ & + (\lambda_2 + \lambda_3 + 16\lambda_4 + 16\lambda_5)h^4f^{(4)}(x) \end{aligned} \quad (2)$$

Now we can equate coefficients of derivatives on either side of the equation, which we can turn into a matrix equation:

$$\begin{pmatrix} 1 & 1 & 1 & 1 & 1 \\ 0 & 1 & -1 & 2 & -2 \\ 0 & 1 & 1 & 4 & 4 \\ 0 & 1 & -1 & 8 & -8 \\ 0 & 1 & 1 & 16 & 16 \end{pmatrix} \begin{pmatrix} \lambda_1 \\ \lambda_2 \\ \lambda_3 \\ \lambda_4 \\ \lambda_5 \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ \frac{2}{h^2} \\ 0 \\ 0 \end{pmatrix}$$

Solving this equation (finding the inverse of the 5×5 matrix) gives us values for our λ 's, which are:

$$\lambda_1 = \frac{-30}{12h^2}; \quad \lambda_2 = \frac{16}{12h^2}; \quad \lambda_3 = \frac{16}{12h^2}; \quad \lambda_4 = \frac{-1}{12h^2}; \quad \lambda_5 = \frac{-1}{12h^2}$$

Finally, we have Equation 1 becoming

$$\begin{aligned} f''(x) &= \frac{-30f(x) + 16f(x+h) + 16f(x-h) - f(x+2h) - f(x-2h)}{12h^2} \\ &= \frac{-f(x-2h) + 16f(x-h) - 30f(x) + 16f(x+h) - f(x+2h)}{12h^2} \end{aligned} \quad (3)$$

2. Evaluating an integral with the Composite Trapezoid Method

We aim to evaluate the following integral using the composite trapezoid method, using n equal subintervals

$$\int_a^b \frac{4}{1+x^2} dx = \pi \quad (4)$$

Firstly, we can look at the general form of the trapezoid method for approximating an integral:

$$\int_a^b f(x) dx = \underbrace{\frac{h}{2} \sum_{i=0}^{n-1} [f(x_i) + f(x_{i+1})]}_{\text{approximation}} - \underbrace{\frac{h^2}{12}(b-a)f''(c)}_{\text{error}} \quad (5)$$

where n is the number of equal subintervals between a and b , $h = (b-a)/n$, and $c \in [a, b]$. c is arbitrary but we choose it to be the point which maximises the function on the given interval in order to look at the "worst case scenario", if you will. Applying