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Numerik 1 – Homework 3

Deadline: 22.03.2024, 10:00 PM

Upload any relevant code and a PDF with everything other than the code (comments, proofs, etc...). The content of the PDF file must be clearly readable and, for the codes, it must be clear which file (or part of file) solves which exercise.

Hint. *If you use Python you may find useful the packages* `numpy` *and* `matplotlib.pyplot`.

Note: You can not use preimplemented functions that automatically let you interpolate and evaluate polynomials (such as `polyfit`, `polyval`) or differentiate functions (such as `gradient`, `diff`) to solve the exercises.

Exercise 1 (theoretical task, points: 5)
Consider a sufficiently smooth function $f(x) : [a, b] \to \mathbb{R}$ and a set of equidistant nodal points $X = \left\{x_{-k}, x_{-k+1}, \dots, x_{-1}, x_0, x_1, \dots, x_{m-1}, x_m | x_i = x_0 + i\dot{h}\right\}$ such that $X \subset [a, b]$. By constructing the polynomial interpolation $P_{k+n}(x)$ of $f(x)$ on the nodal points X and differentiating $P_{k+n}(x)$, complete the following tasks:

(a) Prove that differential operator $D_a(h)[x_0] = \frac{f_{-2}-4f_{-1}+3f_0}{2h}$ approximates $f'(x_0)$ for $X = \{x_{-2}, x_{-1}, x_0\}$, where $x_{-2} = x_0 - 2h$, $x_{-1} = x_0 - h$, $h > 0$ is a positive parameter.

(b) Prove that differential operator $D_b(h)[x_0] = \frac{-2f_{-1}-3f_0+6f_1-f_2}{6h}$ approximates $f'(x_0)$ for $X = \{x_{-1}, x_0, x_1, x_2\}$, where $x_{-1} = x_0 - h$, $x_1 = x_0 + h$, $x_2 = x_0 + 2h$.

(c) Prove that differential operator $D_c(h)[x_0] = \frac{f_{-1}-2f_0+f_1}{h^2}$ approximates $f''(x_0)$ for $X = \{x_{-1}, x_0, x_1\}$, where $x_{-1} = x_0 - h$, $x_1 = x_0 + h$.

Note: We denote $f(x_k)$ as f_k to save space.

Exercise 2 (theoretical task, points: 5)
Let an expression $D(h)[x_0]$ (a difference operator, h is a distance between chosen equidistant nodal points) approximate the p-th derivative of $f(x)$ in the point x_0: $D(h)[x_0] \approx f^{(p)}(x_0)$. We say that $D(h)[x_0]$ approximates $f^{(p)}(x_0)$ with a d-th order if the following expression is satisfied:

$$E(h)[x_0] = |f^{(p)}(x_0) - D(h)[x_0]| \leq Ch^d, \tag{1}$$

where C is some constant.

One can obtain the estimation in Eq. (1) using the Taylor series for $f(x)$ at the point x_0. For example, for the simplest "forward difference" operator $D(h)[x_0] = \frac{f_1-f_0}{h}$, which approximates $f'(x_0)$, we get:

$$\begin{aligned}
E(h)[x_0] &= \left|f'(x_0) - \frac{f_1 - f_0}{h}\right| = \left|f'(x_0) - \frac{f(x_0+h) - f(x_0)}{h}\right| = \\
&= \{\text{use the Taylor series for } f(x_0+h) \text{ at } x = x_0\} = \\
&= \left|f'(x_0) - \frac{f(x_0) + hf'(x_0) + 0.5h^2 f''(\xi) - f(x_0)}{h}\right| = \\
&= \left|f'(x_0) - f'(x_0) - 0.5hf''(\xi)\right| = 0.5h|f''(\xi)|,
\end{aligned}$$

where $\xi \in (x_0, x_0+h)$. We now assume that $f(x) \in C^2[a,b]$, which gives us $|f''(x)| \leq M$, $\forall x \in [a,b]$. Now we can deduce that

$$E(h)[x_0] \leq Ch, \;\; C = 0.5M,$$

which means that the "forward difference" operator approximates the first derivative with the first order.

Using the Taylor series for $f(x)$ at the point x_0 for the difference operators $D_a(h)[x_0]$, $D_b(h)[x_0]$ and $D_c(h)[x_0]$ from the previous exercise, complete the following tasks:

(a) Prove that $D_a(h)[x_0]$ approximates $f'(x_0)$ with the second order (assuming $f(x) \in C^3[a,b]$).

(b) Prove that $D_b(h)[x_0]$ approximates $f'(x_0)$ with the third order (assuming $f(x) \in C^4[a,b]$).

(c) Prove that $D_c(h)[x_0]$ approximates $f''(x_0)$ with the second order (assuming $f(x) \in C^3[a,b]$).

Exercise 3 (programming task, points: 6)

(a) For each of the difference operators $D_a(h)[x_0]$, $D_b(h)[x_0]$ and $D_c(h)[x_0]$ from Ex. 1, code a function with Python/Matlab.
INPUTS:

- fi: an array of values $\{f(x_{-k}), \ldots, f(x_0), \ldots, f(x_m)\}$ needed for the formula,
- h: the distance between mesh nodes (real number),

OUTPUT: The value of $D_*(f)[x_0]$ in point $x = x_0$.

(b) Consider a function $f(x) = \frac{1}{0.4x}$ and a point $x_0 = 10$. Using the functions from (a), compute the values of $D_a(h)[x_0]$, $D_b(h)[x_0]$ and $D_c(h)[x_0]$ for different values of h: $h = \{2^n \,|\, n = 0, -1, -2, \cdots - 10\}$. Compute the errors:

$$E_a(h) = |D_a(h)[x_0] - f'(x_0)|,$$
$$E_b(h) = |D_b(h)[x_0] - f'(x_0)|,$$
$$E_c(h) = |D_c(h)[x_0] - f''(x_0)|,$$

For each of the errors plot a graph in logarithmic scale: $(\log_2 h, \log_2 E_*(h))$. What order of convergence do you observe?

Hint. *In order to determine the order of convergence, remember that the error in Eq. (1) behaves like a polynomial function of h:*

$$E(h) \approx Ch^d,$$
$$\log_2 E(h) \approx \tilde{C} + d \log_2 h,$$

so in case of the d-th order the error (in logarithmic scale) should be a linear function with a slope coefficient d. Therefore you need to plot "helper functions" h^d and compare the slopes.

(c) Code a similar to (a) function to compute a simple "forward difference" operator: $D_+(h)[x_0] = \frac{f_1 - f_0}{h}$. For the same function $f(x) = \frac{1}{0.4x}$ and point $x_0 = 10$, compute the values of $D_+(f)[x_0]$ for different values of h: $h = \{2^n \,|\, n = 0, -1, -2, \cdots - 60\}$ and compute the errors:

$$E_+(h) = |D_+(h)[x_0] - f'(x_0)|$$

Plot a graph in logarithmic scale: $(\log_2 h, \log_2 E_+(h))$. How can you explain the behaviour of $E_+(h)$ for small h?

Hint. *Note that $f(x_0) = f(10) = 1/4 = 2^{-2}$ can be computed without any rounding errors. So the "real" error is $E_+(h) = |\frac{\tilde{f}_1 - f_0}{h} - f'(x_0)|$, where $\tilde{f}_1 = f_1 + \varepsilon$, ε - is the rounding error of f_1. One can investigate $E_+(h)$ as a function of h and determine an optimal value h_{opt}, for which the error is minimal.*