MTMM.00.005 Numerical Methods
Practical lesson 12: Numerical differentiation

April 30, 2019

To get a positive result, student has to solve all of the exercises given in practical lessons, explain the programming code and answer the questions.

The deadline for the 12th set of exercises is May 7th.

NB! In order to use the nonstandard packages as *numpy* and *matplotlib* one could use Command Prompt and type

```
H:\nm> "C:\Program Files\Anaconda3\python" <filename>.py
```

Here `H:\nm` is the folder for `<filename>.py`.

Numerical differentiation

For given equally spaced knots $x_i = x_0 + ih$, $i = 0, \ldots, n$, and function values $f(x_i) = f_i$, $i = 0, \ldots, n$, consider the problem of finding derivatives (or higher derivatives) of function f at these knots. Observe two-point formulas

$$f'(x_i) = \frac{f_{i+1} - f_i}{h} - \frac{h}{2} f''(\xi), \quad \xi \in [x_i, x_{i+1}], \tag{1}$$

$$f'(x_i) = \frac{f_i - f_{i-1}}{h} + \frac{h}{2} f''(\xi), \quad \xi \in [x_{i-1}, x_i] \tag{2}$$

and three-point formulas

$$f'(x_i) = \frac{f_{i+1} - f_{i-1}}{2h} - \frac{h^2}{6} f'''(\xi), \quad \xi \in [x_{i-1}, x_{i+1}], \tag{3}$$

$$f'(x_i) = \frac{-3f_i + 4f_{i+1} - f_{i+2}}{2h} + \frac{h^2}{3} f'''(\xi), \quad \xi \in [x_i, x_{i+2}], \tag{4}$$

$$f'(x_i) = \frac{3f_i - 4f_{i-1} + f_{i-2}}{2h} + \frac{h^2}{3} f'''(\xi), \quad \xi \in [x_{i-2}, x_i]. \tag{5}$$

If instead of the exact values f_i we use approximate values $\tilde{f}_i$ with the error $\varepsilon_i = |f_i - \tilde{f}_i|$ and decrease the step size h, the influence of unconditional error increases.

Example. Observe formula (3) and estimate the error

$$\left| f'(x_i) - \frac{\tilde{f}_{i+1} - \tilde{f}_{i-1}}{2h} \right| = \left| \frac{(f_{i+1} - \tilde{f}_{i+1}) - (f_{i-1} - \tilde{f}_{i-1})}{2h} - \frac{h^2}{6} f'''(\xi) \right| \leq \frac{\varepsilon}{h} + \frac{h^2}{6} M,$$

where $\varepsilon = \max\{\varepsilon_{i+1}, \varepsilon_{i-1}\}$ and $|f'''(\xi)| \leq M$, $\xi \in [x_{i-1}, x_{i+1}]$. If ε and M are accurate estimates, we can find an optimal h for which the error is minimal. For that we find stationary points of $e(h) = \frac{\varepsilon}{h} + \frac{h^2}{6} M$. Equation $e'(h) = -\frac{\varepsilon}{h^2} + \frac{h}{3} M = 0$ gives $h_{opt} = \sqrt[3]{\frac{3\varepsilon}{M}}$, since $e''(h_{opt}) = \frac{2\varepsilon}{h_{opt}^3} + \frac{M}{3} > 0$, we have a minima.

In practice it is impossible to find an optimal h since there is no information about $f'''(\xi)$ or any other (higher order) derivative included in remainder term. An important fact is that decreasing h does not always make the formula more accurate.

Exercise 1. The approximate values of $f(x)$ are given in the table. Use the most accurate formula from (3)–(5) to find the approximations to $f'(x)$. Find analytically $f'(x)$ and compute the actual errors $|f'(x) - \tilde{f}'(x)|$.

Choose data according to the value of α:

- If $\alpha \,⋮\, 4$, then

x	$\tilde{f}(x)$	$\tilde{f}'(x)$	$\lvert f'(x) - \tilde{f}'(x)\rvert$
1.1	9.025013		
1.2	11.023176		
1.3	13.463738		
1.4	16.444647		

$f(x) = e^{2x}$

- If $(\alpha - 1) \,⋮\, 4$, then

x	$\tilde{f}(x)$	$\tilde{f}'(x)$	$\lvert f'(x) - \tilde{f}'(x)\rvert$
8.1	16.944099		
8.3	17.564921		
8.5	18.190562		
8.7	18.820910		

$f(x) = x \ln x$

- If $(\alpha - 2) \,⋮\, 4$, then

x	$\tilde{f}(x)$	$\tilde{f}'(x)$	$\lvert f'(x) - \tilde{f}'(x)\rvert$
2.9	−2.8157787		
3.0	−2.9699775		
3.1	−3.0973190		
3.2	−3.1945433		

$f(x) = x \cos x$

- If $(\alpha - 3) \,⋮\, 4$, then

x	$\tilde{f}(x)$	$\tilde{f}'(x)$	$\lvert f'(x) - \tilde{f}'(x)\rvert$
2.0	0.9609060		
2.2	1.2433300		
2.4	1.5328910		
2.6	1.8260042		

$f(x) = 2(\ln x)^2$

Exercise 2. Find an approximation to $f'(x_\alpha)$ using formula (1) or (2), use $h = \dfrac{h_\alpha}{10^j}$, $j = 0, \ldots, 8$, as the step size. For the initial data $\tilde{f}_i$ use the function values with precision $|f_i - \tilde{f}_i| \le 0.5 \cdot 10^{-k}$, i.e., rounded to k digits after the decimal point. Print out the next table

i	h	$\tilde{f}'(x_\alpha)$	$\lvert f'(x_\alpha) - \tilde{f}'(x_\alpha)\rvert$
0			
$\vdots$			
8			

Find analytically the optimal step size h_{opt} for for the same formula (1) or (2) and given precision $\varepsilon = 0.5 \cdot 10^{-k}$ (the initial data $\tilde{f}_i$ is again rounded to k digits after the decimal point). For that you need to estimate the values of $f''(\xi)$ on specific interval. Is the theoretical h_{opt} consistent with the practical results?

Choose data according to the value of α:

- If $\alpha \,\vdots\, 4$, then
  $f(x) = e^{2x}$, $x_\alpha = 1.5$, $h_\alpha = 0.1$, $k = 6$
- If $(\alpha - 1) \,\vdots\, 4$, then
  $f(x) = x \ln x$, $x_\alpha = 3.3$, $h_\alpha = 0.2$, $k = 6$
- If $(\alpha - 2) \,\vdots\, 4$, then
  $f(x) = x \cos x$, $x_\alpha = 8.2$, $h_\alpha = 0.1$, $k = 7$
- If $(\alpha - 3) \,\vdots\, 4$, then
  $f(x) = 2(\ln x)^2$, $x_\alpha = 2.0$, $h_\alpha = 0.2$, $k = 7$