02601 Introduction to numerical algorithms

Homework assignment 1

Hand in on DTU Learn before 26 September 10pm

1 Multiple choice (40%)

Each question has only ONE correct answer. In the pdf file with your answers, you just need type the number of the answer. You get 10% for a correct answer, 0% for no answer, and -5% for a wrong answer.

A – Data fitting. We need to compute a least-squares fit to the following data:

k	0	1	2	3	4
x_k	-1	1	3	5	7
y_k	-0.5	2	5	11	20

The fit function is of the form

$$F(x) = a\cos(x) + b\exp(x). \tag{1}$$

Please find the correct answers to the following three questions.

Question A1: Let $\boldsymbol{y} = [y_0, \cdots, y_4]^T$ and $\boldsymbol{c} = [a, b]^T$. Set up the normal equation

$$A^T A\boldsymbol{c} = A^T\boldsymbol{y}. \tag{2}$$

The sizes of the system matrix and the right-hand side of the normal equation (2) are

1. 5×2 and 5×1, respectively.
2. 5×2 and 1×5, respectively.
3. 2×5 and 2×1, respectively.
4. 2×2 and 2×1, respectively.
5. 2×2 and 1×2, respectively.

Question A2: The solution of (2) is:

1. $a \approx -1.3337$, $b \approx 0.0078$.
2. $a \approx -2.0244$, $b \approx 0.0169$.
3. $a \approx -1.4658$, $b \approx 0.0203$.
4. $a \approx 3.6603$, $b \approx -2.0244$.

B – Convergence of a numerical algorithm. A numerical algorithm depends on a parameter n, which, for example, tells us how many subintervals the interval is split into. Consider the errors with respect to the value of n shown in the table:

n	1	2	3	4	5
error	3.77	0.94	0.42	0.24	0.15

(3)

Which statement describes the convergence of the algorithm best?

1. The error is proportional to $1/n$
2. The error is proportional to $1/n^2$
3. The error is proportional to $1/n^3$
4. The error is proportional to $1/n^4$

C – Bisection. A function f is continuous on the interval $x \in [0, 1]$ and has a simple root at $x = x^* = 2/5$. Moreover, we know that $f(0) = -1$ and $f(1) = 1$. We search the root of the function by the bisection method with the starting interval $I_0 = [0, 1]$, and the corresponding estimate of the root x^* is denoted by x_0. After the first iteration, the new interval $I_1 = [0, 1/2]$ is as large as the half of the starting interval, and the bisection method gives a new estimate x_1 to the root x^*. Which statement in the following is correct?

1. We cannot use bisection method in this case.
2. $|x^* - x_0| > |x^* - x_1|$
3. $|x^* - x_0| < |x^* - x_1|$
4. $|x^* - x_0| = |x^* - x_1|$

2 Data fitting (20%)

k	x_k	y_k
1	0	1
2	1	2
3	2	5
4	3	10
5	4	17

Table 1: The table of data for fitting.

We want to fit the data (x_k, y_k), $k = 1, \ldots, 5$, in the Table 1 by a function in the form:

$$y = F(x) = a \sin(x) + b\, x^2 + c, \quad x \in \mathbb{R}. \tag{4}$$

2.1) Use Python to set up the normal equation for calculating the coefficients a, b and c, and state both the system matrix and the right-hand side in the normal equation with 4 significant digits.

2.2) Use Python to solve the normal equation, and state the solutions of a, b and c with 3 significant digits.

2.3) Calculate the sum of the absolute errors,

$$S = \sum_{k=1}^{5} |y_k - F(x_k)|,$$

and state S with 3 significant digits. Comment on the value for the parameter a that you found.

3 Convergence of Newton's method for double root

Objective: Newton's method (page 127) has quadratic convergence for computing a simple root (Theorem 1 page 129). In the exercise 3.2, we have checked it. Now we consider using Newton's method to calculate a double root *r, i.e. $f(r) = 0$, $f'(r) = 0$ and $f''(r) \neq 0$.*
In this exercise, we will study how Newton's method converges in the case of double root. Here, we consider the function

$$f(x) = (x-2)^2\,(x-8). \tag{5}$$

We will see that a modified version of Newton's method can still reach quadratic convergence, and we will use the above function to check it.

Question 1 – Python (10%)

Similar as in Exercise 3.2, run an experiment to study the convergence of Newton's method on (5) to a double root. Use the starting point $x_0 = 4.6$ and $nmax = 12$ iterations. Does it converge quadratically?

Question 2 – theory (10%)

In this question, we consider a general function f. In the book page 131 and Exercise 3.2.35, **modified Newton's method** is introduced, and the iteration step is defined as

$$x_{n+1} = x_n - m\,\frac{f(x_n)}{f'(x_n)}\ , \qquad n = 0, 1, 2, \ldots \tag{6}$$

where m is the multiplicity of the zero. In this exercise, we only consider the case $m = 2$.

Now we will derive (but not strictly prove) that the convergence of this method is quadratic for a double root. Specifically, we will obtain a formula *in similar form* as in (1) in page 130; but our concrete formula has a different factor.

First, according to (6) we can easily show that

$$e_{n+1} = x_{n+1} - r = e_n - 2\,\frac{f(x_n)}{f'(x_n)}\ . \tag{7}$$

The sign of the error e_{n+1} is opposite to the one in the bottom of page 129; but it will make the proof a bit easier.

Then, we use Taylor's Theorem on f and f':

$$f(x_n) = f(r+e_n) = f(r) + f'(r)\,e_n + \frac{1}{2}\,f''(r)\,e_n^2 + \frac{1}{6}f'''(\xi_n)\,e_n^3 \tag{8}$$

$$f'(x_n) = f'(r+e_n) = f'(r) + f''(r)\,e_n + \frac{1}{2}\,f'''(\zeta_n)\,e_n^2 \tag{9}$$

where ξ_n and ζ_n lie between r and x_n. These two Taylor series are a bit different as the one on top of page 130, but again it will make the proof easier. Substitute these two Taylor series into (7). You should obtain an expression in the form as

$$e_{n+1} = \left(\frac{\square}{\square}\right)\,e_n^2\ . \tag{10}$$

Note that you can simplify the expression (10) by recalling that r is a double root, i.e., $f(r)=0$, $f'(r)=0$ and $f''(r)\neq 0$.

If you are stuck on your way, just write down what you have got.

Question 3 – Python (10%)

Modify your Python function such that it implements the iteration (6) with $m=2$, and check if the modified method converges quadratically when finding the double root $r=2$ for the function (5). According to your results, which value does the ratio $|e_n/e_{n-1}^2|$ converge to approximately? Use the starting point $x_0 = 4.6$ and $nmax = 5$ iterations.

Question 4 – theory (10%)

For a specific function f which is given in (5), use the result from Question 2 to estimate the constant $\left(\frac{\square}{\square}\right)$ in the formula (10), which gives us the theoretical constant for quadratic convergence. Note that e_n tends to 0 as n goes to the infinite. You can use this fact to further simplify the constant formula in (10). Compare this constant with the one numerically estimated in Question 3. Are they the same?