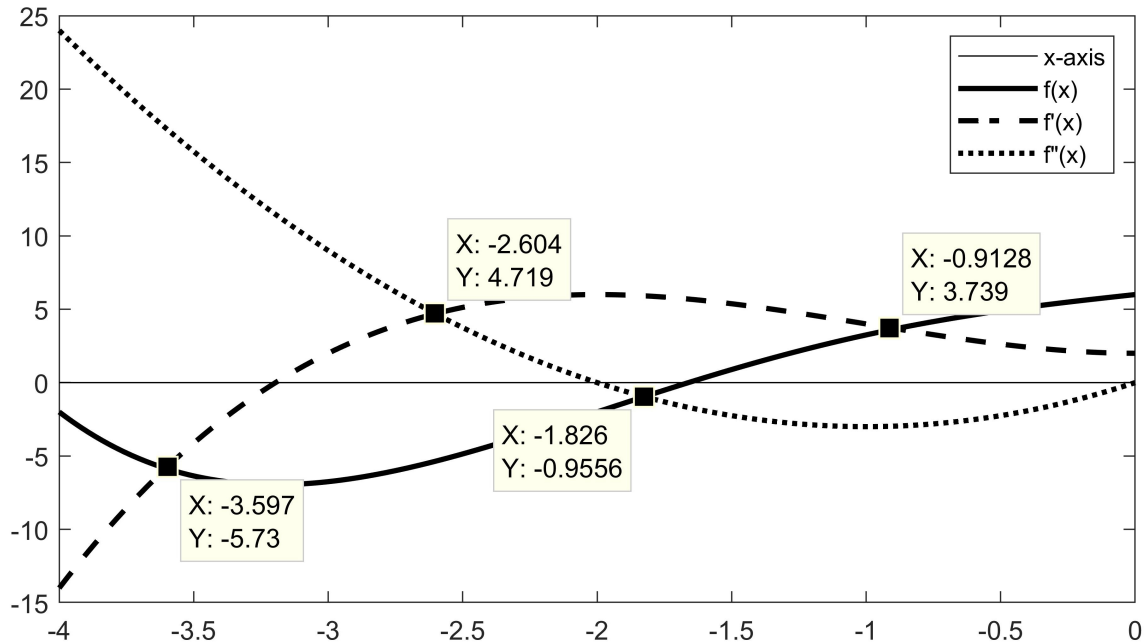
Numerical methods, midterm test II (2018/19 autumn, A), Solution

PROBLEM 1. (6p) We would like to approximate the zero nearest to -1.5 of the function $f(x) = x^4/4 + x^3 + 2x + 6$ using Newton's method. Let us consider the possible initial points $x_0 = -3.5$, $x_0 = -2.5$, $x_0 = -1.8$, $x_0 = -1.5$ or $x_0 = 0$. One of these points ensures monotone convergence. Choose this initial point to start the method and give an estimate to the zero of the function after two iteration steps. (The graph of the function and the derivatives can be seen in the figure.)



Solution: We see from the figure that we have to start the iteration at the point $x_0 = -1.8$. (Here we have $f(x_0)f''(x_0) > 0$ and the derivatives do not change sign between this point and the zero of the function.) We get

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} = -1.6628$$

and

$$x_2 = x_1 - \frac{f(x_1)}{f'(x_1)} = -1.6607.$$

Thus $x^\star \approx -1.6607$.

PROBLEM 2. (2+5p) Let $\mathbf{A} = \begin{bmatrix} 3 & 2 & 0 & 0 \\ 2 & 3 & 2 & 0 \\ 0 & 2 & 3 & 2 \\ 0 & 0 & 2 & 3 \end{bmatrix}$. Show that all eigenvalues of the matrix are real and located in the interval $[-1, 7]$.

We are searching for the nearest eigenvalue to 1. Use an appropriate iterative method to find this eigenvalue (perform only one step with the method starting at the vector $[-2, 1, 1, -2]^T$ and then give an estimation to the corresponding eigenvalue).

Solution: The matrix is symmetric, thus all its eigenvalues are real. All the Gershgorin circles are located at $3+0\mathtt{i}$ in the complex plane, and their radius is 2 and 4. This means that the eigenvalues are located between $3-4=-1$ and $3+4=7$.

The eigenvalue nearest to 1 can be approximated by the inverse iteration. Thus we have to compute the product

$$\overline{\mathbf{x}}_1 = \begin{bmatrix} 2 & 2 & 0 & 0 \\ 2 & 2 & 2 & 0 \\ 0 & 2 & 2 & 2 \\ 0 & 0 & 2 & 2 \end{bmatrix}^{-1} \cdot \begin{bmatrix} -2 \\ 1 \\ 1 \\ -2 \end{bmatrix}$$

(we have subtracted 1s from the diagonal elements of $\mathbf{A}$). In order to avoid matrix inversion we solve the system

$$\begin{bmatrix} 2 & 2 & 0 & 0 \\ 2 & 2 & 2 & 0 \\ 0 & 2 & 2 & 2 \\ 0 & 0 & 2 & 2 \end{bmatrix} \cdot \overline{\mathbf{x}}_1 = \begin{bmatrix} -2 \\ 1 \\ 1 \\ -2 \end{bmatrix}$$

with Gaussian elimination. We obtain $\overline{\mathbf{x}}_1 = [-5/2, 3/2, 3/2, -5/2]^T$. Then the corresponding eigenvalue can be approximated by the Rayleigh coefficient

$$\lambda \approx \frac{\overline{\mathbf{x}}_1^T \mathbf{A} \overline{\mathbf{x}}_1}{\overline{\mathbf{x}}_1^T \overline{\mathbf{x}}_1} = 1.7647.$$

Problem 3. (3+4p) We have determined the natural cubic spline interpolation $s(x)$ of the points $(0,1)$, $(1,2)$, $(2,1)$ and $(3,2)$. We obtained

$$s(x) = \begin{cases} -2x^3/3 + 5x/3 + 1, & x \in [0,1] \\ s_2(x), & x \in [1,2] \\ -2x^3/3 + 6x^2 - 49x/3 + 15, & x \in [2,3]. \end{cases}$$

Give the polynomial $s_2(x)$ on the interval $[1,2]$ using Hermite–Fejér interpolation.
We interpolate $s(x)$ on the nodes: $x_0 = 0$, $x_1 = 3$. Give an upper bound for the interpolation error on the interval $[0,3]$.

Solution: $s_2'(1) = s_1'(1) = -1/3$ and $s_2'(2) = s_3'(2) = -1/3$. The polynomial s_2 can be obtained from the divided difference table

$$\begin{array}{cccccc} 1 & 2 & & & & \\ & & -1/3 & & & \\ 1 & 2 & & -2/3 & & \\ & & -1 & & 4/3 & . \\ 2 & 1 & & 2/3 & & \\ & & -1/3 & & & \\ 2 & 1 & & & & \end{array}$$

Thus

$$s_2(x) = 2 - \frac{1}{3}(x-1) - \frac{2}{3}(x-1)^2 + \frac{4}{3}(x-1)^2(x-2).$$

To compute the interpolation error we apply the error formula

$$E \le \frac{M_2}{2!}\frac{h^2}{4}1! = \frac{4 \cdot 3^2}{2 \cdot 4} = 4.5.$$

M_2 can be obtained as follows. M_2 is an upper bound for the absolute value of $s''(x)$ on $[0,3]$. Because $s''(0) = 0$, $s''(1) = -4$, $s''(2) = 4$, and $s''(3) = 0$ and $s''(x)$ is piecewise linear and continuous, we obtain that 4 is a good choice for M_2.

PROBLEM 4. (7p) We are going to solve the equation $2x = \tan x$. Show that the sequence produced by the iteration $x_{k+1} = \arctan(2x_k)$ converges to the solution of the equation for any initial point from the interval $[1, 1.5]$. Give an estimate for the number of steps that are needed to approximate the solution within the error tolerance 10^{-6}. Let the starting point be $x_0 = 1$.

Solution: Let $F(x) = \arctan 2x$. Finding the fixed point of F is equivalent to finding the root of the equation.

We use Banach's fixed point theorem. Because $\arctan 2x$ is a monotonically increasing function and $F(1) = 1.107$ and $F(1.5) = 1.249$, we have that $F([1, 1.5]) \subset [1, 1.5]$. Moreover,

$$|F'(x)| = \frac{2}{1 + (2x)^2} \leq \frac{2}{5} =: q < 1,$$

that is F is a contraction with contraction coefficient $q = 2/5$. Thus the function F has a unique fixed point $x^\star$ in $[1, 1.5]$ (which is the root of the equation $2x = \tan x$) and $x^\star$ is the limit of the sequence generated by the iteration $x_{k+1} = F(x_k)$ with any starting element $x_0 \in [1, 1.5]$.

If $x_0 = 1$, then $x_1 = \arctan 2 \approx 0.107$, and we have the error estimate

$$|x_k - x^\star| \leq \frac{q^k}{1-q}|x_1 - x_0| \leq \frac{(2/5)^k}{1-(2/5)} 0.108 \leq 10^{-6}.$$

Thus $k \geq 13.2$ steps are enough to guarantee the required error level.

PROBLEM 5. (3+1+3p) Apply the composite midpoint rule to give an estimation to the definite integral $\int_1^4 x \log x \, \mathrm{d}x$ (exact value is 7.3404) using three equidistant subintervals.

Estimate the error we may expect when we would use 6 subintervals.

How many subintervals should we use to estimate the exact integral value within the error tolerance 10^{-4}?

Solution:

$$\int_1^4 x \log x \, \mathrm{d}x \approx 1 \cdot (1.5 \log 1.5 + 2.5 \log 2.5 + 3.5 \log 3.5) = 7.2832$$

We see from the exact value that the error of this approximation is about 0.0568.

When we halve the step size then the error must be quartered (the convergence order of the midpoint rule is 2), that is we can expect an error of 0.0142.

The error estimate

$$|I(f) - I_{mid}(f)| \leq \frac{h^2 M_2 (b-a)}{24} \leq \frac{h^2 \cdot 1 \cdot 3}{24} \leq 10^{-4}$$

(M_2 is an upper bound for the absolute value of the second derivative $(x \log x)'' = 1/x$ on the interval $[1, 4]$). This shows that $h \leq 0.0283$, that is dividing the interval into more than 106.06 subintervals is enough to produce an approximation to the exact integral value within the error tolerance 10^{-4}.

PROBLEM 6. (4+2p) Give a suitable trigonometric interpolation polynomial to the points $(0, 3)$, $(2\pi/3, 1)$, $(4\pi/3, 2)$.

Assume that the above points were taken from the graph of a three times continuously differentiable function f. Using the centered difference formula on the given points, give an approximation to the value $f'(4\pi/3)$.

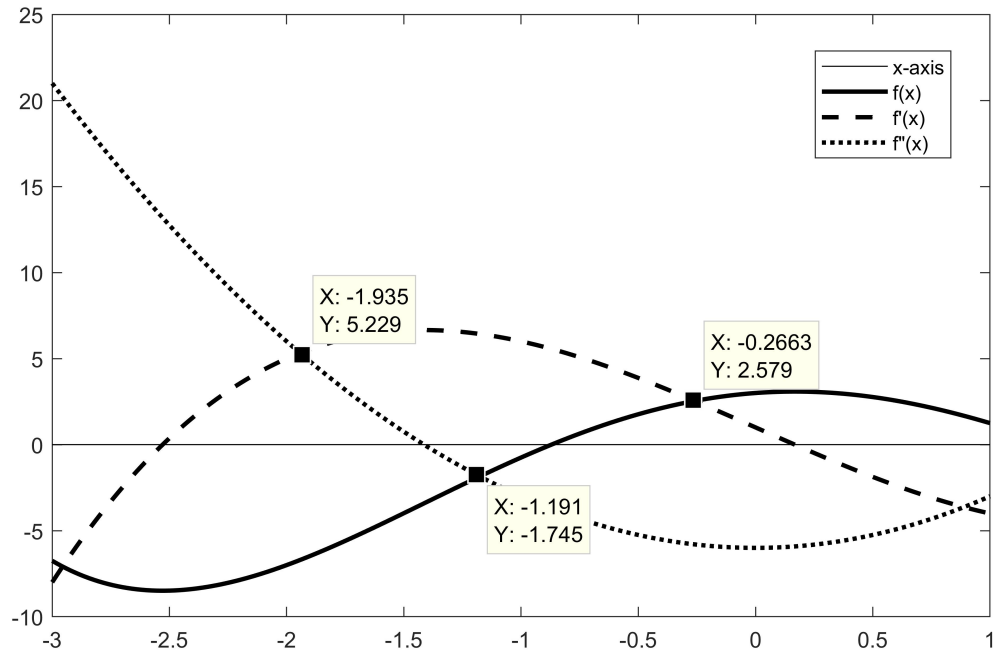
Solution: A first degree trigonometric polynomial is enough to interpolate. The coefficients of the polynomial can be computed using the usual expressions. Thus we obtain $t(x) = 2 + \cos x + (-1/\sqrt{3}) \sin x$.

Using the periodicity of the function we obtain

$$f'\left(\frac{4\pi}{3}\right) \approx \frac{3-1}{2 \cdot (2\pi/3)} = \frac{3}{2\pi} \approx 0.4775.$$

Numerical methods, midterm test II (2018/19 autumn, B), solution

PROBLEM 1. (6p) We would like to approximate the zero nearest to -1 of the function $f(x) = x^4/4 - 3x^2 + x + 3$ using Newton's method. Let us consider the possible initial points $x_0 = -2.5$, $x_0 = -1.8$, $x_0 = -1.2$, $x_0 = -0.5$ or $x_0 = 0.5$. One of these points ensures monotone convergence. Choose this initial point to start the method and give an estimate to the zero of the function after two iteration steps. (The graph of the function and the derivatives can be seen in the figure.)



Solution: We see from the figure that we have to start the iteration at the point $x_0 = -1.2$. (Here we have $f(x_0)f''(x_0) > 0$ and the derivatives do not change sign between this point and the zero of the function.) We get

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} = -0.8907$$

and

$$x_2 = x_1 - \frac{f(x_1)}{f'(x_1)} = -0.8706.$$

Thus $x^\star \approx -0.8706$.

PROBLEM 2. (2+5p) Let $\mathbf{A} = \begin{bmatrix} 1 & 2 & 0 & 0 \\ 2 & 1 & 2 & 0 \\ 0 & 2 & 1 & 2 \\ 0 & 0 & 2 & 1 \end{bmatrix}$. Show that all eigenvalues of the matrix are real and located in the interval $[-3, 5]$.

We are searching for the nearest eigenvalue to -1. Use an appropriate iterative method to find this eigenvalue (perform only one step with the method starting at the vector $[2, -1, -1, 2]^T$ and then give an estimation to the corresponding eigenvalue).

Solution: The matrix is symmetric, thus all its eigenvalues are real. All the Gershgorin circles are located at $1 + 0\mathtt{i}$ in the complex plane, and their radius is 2 and 4. This means that the eigenvalues are located between $1 - 4 = -3$ and $1 + 4 = 5$.

The eigenvalue nearest to -1 can be approximated by the inverse iteration. Thus we have to compute the product

$$\overline{\mathbf{x}}_1 = \begin{bmatrix} 2 & 2 & 0 & 0 \\ 2 & 2 & 2 & 0 \\ 0 & 2 & 2 & 2 \\ 0 & 0 & 2 & 2 \end{bmatrix}^{-1} \cdot \begin{bmatrix} 2 \\ -1 \\ -1 \\ 2 \end{bmatrix}$$

(we have subtracted -1s from the diagonal elements of $\mathbf{A}$). In order to avoid matrix inversion we solve the system

$$\begin{bmatrix} 2 & 2 & 0 & 0 \\ 2 & 2 & 2 & 0 \\ 0 & 2 & 2 & 2 \\ 0 & 0 & 2 & 2 \end{bmatrix} \cdot \overline{\mathbf{x}}_1 = \begin{bmatrix} 2 \\ -1 \\ -1 \\ 2 \end{bmatrix}$$

with Gaussian elimination. We obtain $\overline{\mathbf{x}}_1 = [5/2, -3/2, -3/2, 5/2]^T$. Then the corresponding eigenvalue can be approximated by the Rayleigh coefficient

$$\lambda \approx \frac{\overline{\mathbf{x}}_1^T \mathbf{A} \overline{\mathbf{x}}_1}{\overline{\mathbf{x}}_1^T \overline{\mathbf{x}}_1} = -0.2353.$$

Problem 3. (3+4p) We have determined the natural cubic spline interpolation $s(x)$ of the points $(0, 2)$, $(1, 1)$, $(2, 2)$ and $(3, 1)$. We obtained

$$s(x) = \begin{cases} 2x^3/3 - 5x/3 + 2, & x \in [0, 1] \\ s_2(x), & x \in [1, 2] \\ 2x^3/3 - 6x^2 + 49x/3 - 12, & x \in [2, 3]. \end{cases}$$

Give the polynomial $s_2(x)$ on the interval $[1, 2]$ using Hermite–Fejér interpolation.
We interpolate $s(x)$ on the nodes: $x_0 = 0$, $x_1 = 3$. Give an upper bound for the interpolation error on the interval $[0, 3]$.

Solution: $s_2'(1) = s_1'(1) = 1/3$ and $s_2'(2) = s_3'(2) = 1/3$. The polynomial s_2 can be obtained from the divided difference table

$$\begin{array}{cccccc} 1 & 1 & & & & \\ & & 1/3 & & & \\ 1 & 1 & & 2/3 & & \\ & & 1 & & -4/3 & . \\ 2 & 2 & & -2/3 & & \\ & & 1/3 & & & \\ 2 & 2 & & & & \end{array}$$

Thus

$$s_2(x) = 1 + \frac{1}{3}(x-1) + \frac{2}{3}(x-1)^2 - \frac{4}{3}(x-1)^2(x-2).$$

To compute the interpolation error we apply the error formula

$$E \le \frac{M_2}{2!}\frac{h^2}{4}1! = \frac{4 \cdot 3^2}{2 \cdot 4} = 4.5.$$

M_2 can be obtained as follows. M_2 is an upper bound for the absolute value of $s''(x)$ on $[0,3]$. Because $s''(0) = 0$, $s''(1) = 4$, $s''(2) = -4$, and $s''(3) = 0$ and $s''(x)$ is piecewise linear and continuous, we obtain that 4 is a good choice for M_2.

Problem 4. (7p) We are going to solve the equation $3x = \tan x$. Show that the sequence produced by the iteration $x_{k+1} = \arctan(3x_k)$ converges to the solution of the equation for any initial point from the interval $[1,2]$. Give an estimate for the number of steps that are needed to approximate the solution within the error tolerance 10^{-5}. Let the starting point be $x_0 = 2$.

Solution: Let $F(x) = \arctan 3x$. Finding the fixed point of F is equivalent to finding the root of the equation.

We use Banach's fixed point theorem. Because $\arctan 3x$ is a monotonically increasing function and $F(1) = 1.2490$ and $F(2) = 1.4056$, we have that $F([1,2]) \subset [1,2]$. Moreover,

$$|F'(x)| = \frac{3}{1+(3x)^2} \le \frac{3}{10} =: q < 1,$$

that is F is a contraction with contraction coefficient $q = 3/10$. Thus the function F has a unique fixed point $x^\star$ in $[1,2]$ (which is the root of the equation $3x = \tan x$) and $x^\star$ is the limit of the sequence generated by the iteration $x_{k+1} = F(x_k)$ with any starting element $x_0 \in [1,2]$.

If $x_0 = 2$, then $x_1 = \arctan 6 \approx 1.4056$, and we have the error estimate

$$|x_k - x^\star| \le \frac{q^k}{1-q}|x_1 - x_0| \le \frac{(3/10)^k}{1-(3/10)}0.6 \le 10^{-5}.$$

Thus $k \ge 10.138$ steps are enough to guarantee the required error level.

Problem 5. (3+1+3p) Apply the composite midpoint rule to give an estimation to the definite integral $\int_2^5 x \log x \, \mathrm{d}x$ (exact value is 13.4817) using three equidistant subintervals.

Estimate the error we may expect when we would use 6 subintervals.

How many subintervals should we use to estimate the exact integral value within the error tolerance 10^{-5}?

Solution:

$$\int_2^5 x \log x \, \mathrm{d}x \approx 1 \cdot (2.5 \log 2.5 + 3.5 \log 3.5 + 4.5 \log 4.5) = 13.4437$$

We see from the exact value that the error of this approximation is about 0.0380.

When we halve the step size then the error must be quartered (the convergence order of the midpoint rule is 2), that is we can expect an error of 0.0095.

The error estimate

$$|I(f) - I_{mid}(f)| \le \frac{h^2 M_2 (b-a)}{24} \le \frac{h^2 \cdot (1/2) \cdot 3}{24} \le 10^{-5}$$

(M_2 is an upper bound for the absolute value of the second derivative $(x \log x)'' = 1/x$ on the interval $[2,5]$). This shows that $h \le 0.0125$, that is dividing the interval into more than 237.17 subintervals is enough to produce an approximation to the exact integral value within the error tolerance 10^{-5}.

Problem 6. (4+2p) Give a suitable trigonometric interpolation polynomial to the points $(0, 2)$, $(2\pi/3, 1)$, $(4\pi/3, 3)$.

Assume that the above points were taken from the graph of a three times continuously differentiable function f. Using the centered difference formula on the given points, give an approximation to the value $f'(4\pi/3)$.

<u>Solution:</u> A first degree trigonometric polynomial is enough to interpolate. The coefficients of the polynomial can be computed using the usual expressions. Thus we obtain $t(x) = 2 + (-2/\sqrt{3}) \sin x$.

Using the periodicity of the function we obtain

$$f'\left(\frac{4\pi}{3}\right) \approx \frac{2-1}{2 \cdot (2\pi/3)} = \frac{3}{4\pi} \approx 0.2387.$$