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Workbook for Numerical methods

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1 Root-finding for non-linear equations

Given a continuous function y = f(x), we find $\tilde{x} \in D_f$ such that

 $f(\tilde{x}) = 0.$

The value \tilde{x} is called **root** or **zero** of the function f.

1.1 Separation of roots

At first we have to determine number of roots and their positions, i.e. we need to find such intervals that each of these includes only one root. We can use the following theorem.

Theorem -

If the function f is continuous on the interval [a, b] and

$$f(a) \cdot f(b) < 0$$

then there is $\tilde{x} \in (a, b)$ such that $f(\tilde{x}) = 0$.

There are several ways how to find intervals such that each one of these includes only one root.

• We plot the graph of the function *f* and find points of intersection of this graph and the *x*-axis.



• We convert the equation f(x) = 0 into a form h(x) = g(x) and we find points of intersection of graphs of functions *h* and *g*.



• We tabulate values of the function *f* a find where their signs change.

- Example 1 ——

Separate all roots of the equation

 $x^3 - \ln(10 - x) = 0.$

We convert the given equation into such form to be able to plot graphs of functions on both sides of this equation.

$$x^{3} - \ln(10 - x) = 0$$

 $x^{3} = \ln(10 - x)$

We plot graphs of functions $g(x) = x^3$ and $h(x) = \ln(10 - x)$ and find points of intersection of these graphs.



It is obvious that the point of intersection is unique and lies within the interval [1,2]. To determine the root more precisely we tabulate function values of the function $f(x) = x^3 - \ln(10 - x)$ on this interval with the step 0.1. We round all values to two decimal places.

<i>x</i>	1	1.1	1.2	1.3	1.4	1.5	1.6	1.7	1.8	1.9	2
$f(x) \mid -1$.19	-0.85	-0.44	0.03	0.59	1.23	1.96	2.79	3.72	4.76	5.92

We can observe that sings of these function values change between 1.2 and 1.3. The function *f* is also evidently continuous on the mentioned interval. So the equation $x^3 - \ln(10 - x) = 0$ has unique root in the interval [1.2, 1.3].

- Example 2 —

Separate all roots of the equation

$$x - 4\cos^2(x) = 0.$$

Use the MATLAB to solve the problem.

We plot graph of the function $f(x) = x - 4\cos^2(x)$ and locate its point of intersection with the *x*-axis. We plot the graph on sufficiently long interval that naturally must be a subset of the function domain. We choose the interval [-10, 10].

>> fplot(@(x)x-4*cos(x).^2,[-10,10])
>> grid on



We can observe that all roots lie in the interval [0, 4]. So we plot the graph once more only on this shorter interval to determine the roots position more precisely.

```
>> fplot(@(x)x-4*cos(x).^2,[0,4])
>> grid on
```



There are three roots separated in intervals [1, 2], [2, 3] and [3, 4].

1.2 Bisection method

The aim of all methods is to find a sequence of numbers $x^{(1)}$, $x^{(2)}$, $x^{(3)}$, ..., $x^{(k)}$ that converges to the searched root \tilde{x} .

Assume that the root is separated in the interval [a, b]. We denote $a^{(1)} = a$, $b^{(1)} = b$, k = 1 in the beginning of calculations.

We determine the value $x^{(k)}$ as the mid-point of the interval $[a^{(k)}, b^{(k)}]$, i.e.

$$x^{(k)} = rac{a^{(k)} + b^{(k)}}{2}.$$

The next interval is chosen in accordace with signs of function values $f(a^{(k)})$, $f(x^{(k)})$, $f(b^{(k)})$.

If
$$f(a^{(k)})f(x^{(k)}) < 0$$
 then $a^{(k+1)} := a^{(k)}$, $b^{(k+1)} := x^{(k)}$.
If $f(x^{(k)})f(b^{(k)}) < 0$ then $a^{(k+1)} := x^{(k)}$, $b^{(k+1)} := b^{(k)}$.

Thus, we successively bisect intervals and their mid-points $\{x^{(k)}\}$ converge to the root \tilde{x} .





The calculation is terminated when the given accuracy is obtained, i.e. when the following holds

$$\frac{b^{(k)}-a^{(k)}}{2}\leq \varepsilon \ .$$

The last mid-point $x^{(k)}$ approximate the searched root \tilde{x} with the accuracy ε .

Find all roots of the equation $x^3 - \ln(10 - x) = 0$ using the bisection method with the accuracy $\varepsilon = 10^{-2}$.

We already know that the root lies in the interval [1.2, 1.3], i.e. $a^{(1)} = 1.2$, $b^{(1)} = 1.3$. The approximation error is $\frac{b^{(1)}-a^{(1)}}{2} = 0.05 > \varepsilon = 10^{-2}$ so we continue in calculations. We calculate the first approximation $x^{(1)}$ as the mid-point of this interval:

$$x^{(1)} = \frac{b^{(1)} + a^{(1)}}{2} = \frac{1.3 + 1.2}{2} = 1.25$$

Then we calculate values of the function $f(x) = x^3 - \ln(10 - x)$ at points $a^{(1)}, x^{(1)}, b^{(1)}$:

$$f(a^{(1)}) = -0.446, \quad f(x^{(1)}) = -0.2159, \quad f(b^{(1)}) = 0.0337$$

and determine interval $[a^{(2)}, b^{(2)}]$:

$$f(x^{(1)}) \cdot f(b^{(1)}) < 0 \Rightarrow a^{(2)} = x^{(1)} = 1.25, \quad b^{(2)} = b^{(1)} = 1.3.$$

The approximation error is $\frac{b^{(2)}-a^{(2)}}{2} = 0.025 > \varepsilon = 10^{-2}$ so we continue in calculations. We calculate the second approximation

$$x^{(2)} = \frac{a^{(2)} + b^{(2)}}{2} = \frac{1.25 + 1.3}{2} = 1.275$$

and determine interval $[a^{(3)}, b^{(3)}]$:

$$f(a^{(2)}) = -0.2159, \quad f(x^{(2)}) = -0.0935, \quad f(b^{(2)}) = 0.0337,$$

 $f(x^{(2)}) \cdot f(b^{(2)}) < 0 \Rightarrow a^{(3)} = x^{(2)} = 1.275 \quad b^{(3)} = b^{(2)} = 1.3.$

The approximation error is $\frac{b^{(3)}-a^{(3)}}{2} = 0.0125 > \varepsilon = 10^{-2}$ so we continue in calculations. We calculate the third approximation

$$x^{(3)} = \frac{a^{(3)} + b^{(3)}}{2} = \frac{1.275 + 1.3}{2} = 1.2875$$

and determine interval $[a^{(4)}, b^{(4)}]$:

$$f(a^{(3)}) = -0.0935, \quad f(x^{(3)}) = -0.0305, \quad f(b^{(3)}) = 0.0337,$$

 $f(x^{(3)}) \cdot f(b^{(3)}) < 0 \Rightarrow a^{(4)} = x^{(3)} = 1.2875, \quad b^{(4)} = b^{(3)} = 1.3.$

Because the approximation error fulfil $\frac{b^{(4)}-a^{(4)}}{2} = 0.0062 \le \varepsilon = 10^{-2}$, we can terminate our calculations.

We calculate the last approximation

		$x^{(4)} =$	$\frac{a^{(4)}+b^{(4)}}{2}$	$\frac{4)}{-} = \frac{1.28}{-}$	$\frac{75+1}{2}$	$\frac{1.3}{-} = 1.29$	938
k	$a^{(k)}$	$f(a^{(k)})$	$x^{(k)}$	$f(x^{(k)})$	$b^{(k)}$	$f(b^{(k)})$	$\frac{ b^{(k)}-a^{(k)} }{2}$
1	1.2	_	1.25	_	1.3	+	$0.05 > 10^{-2}$
2	1.25	_	1.275	_	1.3	+	$0.02 > 10^{-2}$
3	1.275	_	1.2875	_	1.3	+	$0.0125 > 10^{-2}$
4	1.2875	—	1.29 38	+	1.3	+	$0.0062 \leq 10^{-2}$

The resulting approximation of the given equation root is

$$\tilde{x} = 1.29 \pm 0.01$$

- Example 4 -

Find all roots of the equation

 $2x + 2 - e^x = 0$

using the bisection method with the accuracy $\varepsilon = 10^{-2}$. Use the MATLAB to solve the problem.

The first step is to separate roots. We define function f and plot its graph on a sufficient interval that we choose according to the domain of this function. Let us note that the domain of the function $f(x) = 2x + 2 - e^x$ is $D_f = \mathbb{R}$.

```
>> f=@(x) (2*x+2-exp(x))
f =
    @(x) (2*x+2-exp(x))
>> fplot(f,[-5,4])
>> grid on
```



It is obvious that there are two points of intersection of the function f graph and the *x*-axis included in intervals [-1,0] and [1,2].

Now we will calculate a root in the interval [1,2].

We input end-points of the interval as the variables a and b and set up the starting value of the approximation index k.

>> k=0; a=1; b=2;

In each step we increase the index k by one, calculate x(k) and the approximation error. We use the *if* statement to choose an interval for the next step.

```
>> k=k+1
k =
    1
>> x(k)=(a(k)+b(k))/2
x =
    1.5000
>> (b(k)-a(k))/2
ans =
    0.5000
>> if f(a(k))*f(x(k))<0, a(k+1)=a(k);b(k+1)=x(k);
else a(k+1)=x(k); b(k+1)=b(k);end</pre>
```

We repeat the following four statements until the approximation error is less than the given accuracy.

>> k=k+1
>> x(k) = (a(k)+b(k))/2
>> (b(k)-a(k))/2
>> if f(a(k))*f(x(k))<0, a(k+1)=a(k);b(k+1)=x(k);
else a(k+1)=x(k); b(k+1)=b(k);end</pre>

The given accuracy is achieved in the seventh step.

```
>> k=k+1
k =
    7
>> x(k)=(a(k)+b(k))/2
x =
    1.5000 1.7500 1.6250 1.6875 1.6563 1.6719 1.6797
>> (b(k)-a(k))/2
ans =
    0.0078
```

We write obtained data to a table.

k	$x^{(k)}$	$\frac{ b^{(k)}-a^{(k)} }{2}$
1	1.5000	$0.5 > 10^{-2}$
2	1.7500	$0.25 > 10^{-2}$
3	1.6250	$0.125 > 10^{-2}$
4	1.6875	$0.0625 > 10^{-2}$
5	1.6563	$0.0313 > 10^{-2}$
6	1.6719	$0.0156 > 10^{-2}$
7	1.6797	$0.0078 \leq 10^{-2}$

We round the last approximation to two decimal places according to the given accuracy. The resulting approximation of the searched root is:

 $\tilde{x} = 1.68 \pm 10^{-2}$.

The second root lying. in the interval [-1,0] can be found in analogous way. Approximations of all roots of the given equation are:

$$-0.77 \pm 10^{-2}$$
, 1.68 ± 10^{-2} .

1.3 Newton method

We find a sequence of numbers $x^{(0)}$, $x^{(1)}$, $x^{(2)}$, $x^{(3)}$, ..., $x^{(k)}$ that converges to the searched root \tilde{x} . The initial approximation $x^{(0)}$ is an arbitrary number from the interval [a, b] that we obtain by previous separation of roots. The principle of the Newton method is to construct a tangent line to the graph of the given function f at the point $[x^{(0)}, f(x^{(0)})]$. The point of intersection of this tangent line and the *x*-axis is the next approximation $x^{(1)}$. This process is repeated until the given accuracy is achieved.

Let the following assumptions be fulfilled:

- the first derivative f' does not change sign on the interval (a, b) (i.e. function f is either increasing or decreasing on (a, b));
- 2. the second derivative *f*["] does not change sign on the interval (*a*, *b*) (i.e. function *f* is either convex or concave on (*a*, *b*));
- 3. it holds $f(a) \cdot f(b) < 0$;
- 4. it holds $\left|\frac{f(a)}{f'(a)}\right| < b a$ and $\left|\frac{f(b)}{f'(b)}\right| < b a$.

Then the sequence $\{x^k\}$ calculated using the formula

$$x^{(k+1)} = x^{(k)} - \frac{f(x^{(k)})}{f'(x^{(k)})}$$

converges for an arbitrary initial approximation $x^{(0)} \in [a, b]$.

For k = 0



The calculation is terminated when the given accuracy ε is achieved, i.e. when

 $|x^{(k)}-x^{(k-1)}|\leq \varepsilon.$

Find all roots of the equation

Example 5

 $x^3 - \ln(10 - x) = 0$

using the Newton method with the accuracy $\varepsilon = 10^{-6}$.

We already know that the root lies in the interval [1.2, 1.3]. In the beginning we have to verify the Newton method assumptions, so we calculate the first and the second derivative of the function f,

$$f(x) = x^3 - \ln(10 - x), \quad f'(x) = 3 \cdot x^2 + \frac{1}{10 - x}, \quad f''(x) = 6 \cdot x + \frac{1}{(10 - x)^2}.$$

farther we check condition

$$\left|\frac{f(a)}{f'(a)}\right| = \left|\frac{-0.4468}{4.4336}\right| = 0.1008 > 0.1 = b - a$$
.

Thes condition is not fulfilled and that is why we have to shorten the interval in which the searched root is separated.



We can see that the searched root lies in the interval [1.25, 1.3]. Now we start to verify the assumptions on the new interval [1.25, 1.3]:

$$\left|\frac{f(a)}{f'(a)}\right| = \left|\frac{-0.2159}{4.8018}\right| = 0.0450 < 0.05 = b - a$$
$$\left|\frac{f(b)}{f'(b)}\right| = \left|\frac{0.0337}{5.1849}\right| = 0.0065 < 0.05 = b - a$$

We tabulate values of the first and the second derivative rounded to two decimal place.

x	$\int f'(x)$	f''(x)
1.25	4.80	7.51
1.26	4.88	7.57
1.27	4.95	7.63
1.28	5.03	7.69
1.29	5.11	7.75
1.3	5.19	7.81

From the table we can deduce that

$$f'(x) > 0$$
 on [1.25, 1.3]
 $f''(x) > 0$ on [1.25, 1.3]

Thus, all assumptions of the Newton method are verified. We choose the initial approximation $x^{(0)} = b = 1.3$.

We calculate the first approximation $x^{(1)}$

$$x^{(1)} = x^{(0)} - \frac{f(x^{(0)})}{f'(x^{(0)})} = 1.3 - \frac{0.03367697433946}{5.18494252873563} = 1.29350485098864$$

and the approximation error $|x^{(1)} - x^{(0)}| \doteq 0.007 > \varepsilon = 10^{-6}$. Calculations must continue. We calculate the second approximation $x^{(2)}$

$$x^{(2)} = x^{(1)} - \frac{f(x^{(1)})}{f'(x^{(1)})} = 1.29350485098864 - \frac{0.00016453367995}{5.13432117883453} = 1.29347280513989$$

and the approximation error $|x^2 - x^1| \doteq 0.00003 > \varepsilon = 10^{-6}$. Calculations must continue. We calculate the third approximation $x^{(3)}$

$$x^{(3)} = x^{(2)} - \frac{f(x^{(2)})}{f'(x^{(2)})} = 1.29347280513989 - \frac{0.0000000399178}{5.13407205040059} = 1.29347280436238$$

and the approximation error $|x^{(3)} - x^{(2)}| \doteq 0.000000008 = 8 \cdot 10^{-10} < \varepsilon = 10^{-6}$. The given accuracy is achieved and calculations can be terminated.

We write obtained data into the table:

k	$x^{(k)}$	$ x^{(k)} - x^{(k-1)} $
0	1.3	_
1	1.29350485098864	$0.007 > 10^{-6}$
2	1.29347280513989	$0.00003 > 10^{-6}$
3	1.29347280436238	$0.000000008 \le 10^{-6}$

The resulting approximation of the searched root is

$$\tilde{x} = 1.293473 \pm 10^{-6}.$$

- Example 6 —

Find all roots of the equation

 $x - 4\cos^2(x) = 0$

using the Newton method with the accuracy $\varepsilon = 10^{-8}$. Use the MATLAB to solve the problem.

Due to previous separation we know that there are three roots in intervals [1,2], [2,3] and [3, 4].

At first we attend to the root from the interval [3, 4]. We input end-points of this interval.

>> a=3; >> b=4;

Then we calculate the first and the second derivative of the given function.

$$f(x) = x - 4\cos^{2}(x)$$

$$f'(x) = 1 + 8\cos(x)\sin(x)$$

$$f''(x) = -8\sin^{2}(x) + 8\cos^{2}(x)$$

```
>> df=@(x)1+8*cos(x).*sin(x)
df =
    @(x)1+8*cos(x).*sin(x)
>> ddf=@(x)-8*sin(x).^2+8*cos(x).^2
ddf =
    @(x)-8*sin(x).^2+8*cos(x).^2
```

Now we can start verifying the assumptions.

We want to verify that values of derivatives do not change signs on the interval [3, 4]. Therefore we generate points from this interval with the step 0.1, input these as the vector x and calculate corresponding values of the first derivative.

```
>> x=a:0.1:b
x =
 Columns 1 through 6
 3.0000 3.1000 3.2000
                           3.3000
                                    3.4000
                                             3.5000
 Columns 7 through 11
 3.6000 3.7000 3.8000
                           3.9000
                                    4.0000
>> df(x)
ans =
 Columns 1 through 6
-0.1177 0.6676
                  1.4662
                           2.2462
                                    2.9765
                                             3.6279
 Columns 7 through 11
 4.1747 4.5948
                  4.8717
                           4.9942
                                    4.9574
```

However, the values of the first derivative change signs on [3, 4], so we have to shorten the interval of separation and to verify assumptions for this shorter one. We plot the graph of the given function on [3, 4].



It is obvious that the searched root lies in the interval [3.4, 3.6] where we again try to verify assumptions.

We input end-points of the new interval.

>> a=3.4; >> b=3.6;

We generate points from [3.4, 3.6] with the step 0.01 and calculate values of the first derivative at these points

```
>> x=a:0.01:b;
>> df(x)
ans =
 Columns 1 through 6
2.9765 3.0456 3.1139
                          3.1814 3.2480 3.3138
 Columns 7 through 12
3.3785 3.4424 3.5053
                          3.5671 3.6279
                                          3.6877
 Columns 13 through 18
 3.7464 3.8040 3.8605
                         3.9159 3.9701
                                          4.0230
 Columns 19 through 21
 4.0748 4.1254
               4.1747
```

as well as values of the second derivative

```
>> ddf(x)
ans =
 Columns 1 through 6
 6.9552 6.8747 6.7915
                         6.7056 6.6170 6.5258
 Columns 7 through 12
 6.4320 6.3355 6.2366
                         6.1351 6.0312
                                          5.9249
 Columns 13 through 18
 5.8162 5.7052 5.5919
                                 5.3587
                         5.4764
                                          5.2388
 Columns 19 through 21
 5.1168
       4.9928 4.8668
```

We can see that both derivatives do not change signs on the whole interval [3.4, 3.6]. The next step is to verify the condition $f(a) \cdot f(b) < 0$ that guarantees the root existence.

```
>> f(a)*f(b)
ans =
-0.1299
```

In the end we check validity of conditions $\left|\frac{f(a)}{f'(a)}\right| < b - a$ and $\left|\frac{f(b)}{f'(b)}\right| < b - a$.

```
>> abs(f(a)/df(a))
ans =
            0.1138
>> abs(f(b)/df(b))
ans =
            0.0918
```

Both values are less than b - a = 3.6 - 3.4 = 0.2.

Thus, all assumptions of the Newton method are verified for the interval [3.4, 3.6] and the sequence of approximations will converge to the given equation root for an arbitrary initial approximation $x^{(0)} \in [3.4.3.6]$.

Because the given accuracy is 10^{-8} , we need to know all output values with higher precision. Thas is why we set up longer form of outputs using the statement format long.

We input the initial approximation that can be arbitrary chosen from the interval [3.4, 3.6]. We choose the left end-point that is saved as *a*.

We calculate the first approximation and the approximation error. If this error is greater than given ε then the calculation continue.

We calculate next approximations and corresponding approximation errors. We test if the error is greater than given ε in each step.

```
>> x2=x1-f(x1)/df(x1)
x2 =
   3.50225628403900
>> abs(x2-x1)
ans =
   0.01156877372312
>> x3=x2-f(x2)/df(x2)
x3 =
   3.50214740099497
>> abs(x3-x2)
ans =
    1.088830440254540e-004
>> x4=x3-f(x3)/df(x3)
x4 =
   3.50214739121355
>> abs(x4-x3)
ans =
    9.781422338761558e-009
```

We write the obtained data into a table.

k	$x^{(k)}$	$ x^{(k)} - x^{(k-1)} $
0	3.4	
1	3.51382505776211	$0.11382505776211 > 10^{-8}$
2	3.50225628403900	$0.01156877372312 > 10^{-8}$
3	3.50214740099497	$1.088830440254540e - 004 > 10^{-8}$
4	3.50214739121355	$9.781422338761558e - 009 \le 10^{-8}$

The given accuracy $\varepsilon = 10^{-8}$ is achieved in the fourth step where the calculation is terminated. We round the value of $x^{(4)}$ to eight decimal places. The resulting approximation of the searched root is

$$\tilde{x} = 3.50214739 \pm 10^{-8}.$$

The other two roots can be found in analogous way. Approximations of all roots of the given equation are:

 1.03667388 ± 10^{-8} , 2.47646805 ± 10^{-8} , 3.50214739 ± 10^{-8} .

– Exercise 7 –

Find all roots of the equation

$$2x^3 - x^2 - x - 1 = 0$$

- a) using the bisection method with the accuracy $\varepsilon = 10^{-4}$,
- b) using the bisection method with the accuracy $\varepsilon = 10^{-4}$, use the MATLAB to solve the problem,
- c) using the Newton method with the accuracy $\varepsilon = 10^{-8}$,
- d) using the Newton method with the accuracy $\varepsilon = 10^{-8}$, use the MATLAB to solve the problem,
- e) using the bisection method and the Newton method, both with the accuracy $\varepsilon = 10^{-4}$. Compare obtained results, use the MATLAB to solve the problem.

2 Polynomial Interpolation

The interpolation problem

Given n + 1 pairs (x_i, y_i) of distinct nodes x_i and corresponding values y_i , the problem consists of finding a polynomial $p_n = p_n(x)$ that fulfils **the interpolation equalities**

$$p_n(x_i) = y_i, \quad i = 0, \ldots, n,$$

i.e. a polynomial whose graph passes the given points.

There exists unique interpolating polynomial of degree at most *n*. We introduce three different ways how to find this polynomial.



2.1 Interpolating polynomial in the standard form

The distinct nodes x_i and corresponding values y_i , i = 0, ..., n are given. Substituting the standard form of a polynomial

$$p_n(x) = a_0 + a_1 x + a_2 x^2 + \dots + a_n x^n$$

into the interpolation equalities $p_n(x_i) = y_i$ we obtain the system of linear equations

$$a_0 + a_1 x_i + a_2 x_i^2 + \dots + a_n x_i^n = y_i, \quad i = 0, \dots, n,$$

that can be written in the matrix form as

$$\begin{pmatrix} 1 & x_0 & x_0^2 & \dots & x_0^n \\ 1 & x_1 & x_1^2 & \dots & x_1^n \\ 1 & x_2 & x_2^2 & \dots & x_2^n \\ \vdots & \vdots & \vdots & \ddots & \vdots \\ 1 & x_n & x_n^2 & \dots & x_n^n \end{pmatrix} \cdot \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ \vdots \\ a_n \end{pmatrix} = \begin{pmatrix} y_0 \\ y_1 \\ y_2 \\ \vdots \\ y_n \end{pmatrix}.$$

The solution of this system of linear equations represents the coefficients $a_0, a_1, \ldots, a_n \in \mathbb{R}$ of the interpolating polynomial.

– Example 8 —

Find the interpolating polynomial in the standard form for the data

	i=0	i=1	i=2	i=3
x_i	$ 1 \\ 2$	45	6	9 1
<i>y</i> i		5	5	Ŧ

We seek for a cubic interpolating polynomial

$$p_3(x) = a_0 + a_1 x + a_2 x^2 + a_3 x^3$$

that we substitute into the interpolation equalities $p_n(x_i) = y_i$

$$p_{3}(1) = 2 \implies a_{0} + a_{1} \cdot 1 + a_{2} \cdot 1^{2} + a_{3} \cdot 1^{3} = 2$$

$$p_{3}(4) = 5 \implies a_{0} + a_{1} \cdot 4 + a_{2} \cdot 4^{2} + a_{3} \cdot 4^{3} = 5$$

$$p_{3}(6) = 3 \implies a_{0} + a_{1} \cdot 6 + a_{2} \cdot 6^{2} + a_{3} \cdot 6^{3} = 3$$

$$p_{3}(9) = 4 \implies a_{0} + a_{1} \cdot 9 + a_{2} \cdot 9^{2} + a_{3} \cdot 9^{3} = 4$$

The system of linear equations can be written in the matrix form:

$$\begin{pmatrix} 1 & 1 & 1 & 1 \\ 1 & 4 & 16 & 64 \\ 1 & 6 & 36 & 216 \\ 1 & 9 & 81 & 729 \end{pmatrix} \cdot \begin{pmatrix} a_0 \\ a_1 \\ a_2 \\ a_3 \end{pmatrix} = \begin{pmatrix} 2 \\ 5 \\ 3 \\ 4 \end{pmatrix}$$

We solve the system and we obtain the interpolating polynomial coefficients $a_0 = -2.6$, $a_1 = 5.8\overline{3}$, $a_2 = -1.31\overline{6}$, $a_3 = 0,08\overline{3}$.

The resulting interpolating polynomial is (coefficients are rounded to three decimal places)

$$p_3(x) = -2.6 + 5.833x - 1.317x^2 + 0.083x^3.$$



Find the interpolating polynomial in the standard form for the data $\underbrace{i=0 \quad i=1 \quad i=2}_{i=1}$

	1=0	1=1	1=2
x_i	0	3	4
y_i	2	1	5

```
Use the MATLAB to solve the problem.
```

```
>> x = [0; 3; 4]
>> y = [2; 1; 5]
>> M = [ones(3,1) x x.^2]
>> a = M\y
>> format rat
>> a
>> plot(x,y,'o')
>> grid on, hold on
>> p = @(x)a(1)+a(2)*x+a(3)*x.^2;
>> fplot(p, [0 4], 'r')
>> legend('nodes','interpolating polynomial')
```

2.2 Interpolating polynomial in the Lagrange form

The unique interpolating polynomial can be written in the Lagrange form

$$p_n(x) = y_0 l_0(x) + y_1 l_1(x) + \dots + y_n l_n(x)$$

where $l_0(x), l_1(x), \ldots, l_n(x)$ are the Lagrange basis of the interpolation problem, for $i = 1, \ldots, n$:

$$l_i(x) = \frac{(x - x_0) \cdots (x - x_{i-1})(x - x_{i+1}) \cdots (x - x_n)}{(x_i - x_0) \cdots (x_i - x_{i-1})(x_i - x_{i+1}) \cdots (x_i - x_n)}$$

The Lagrange basis have the following properties for i, j = 1, ..., n:

- $l_i(x)$ is the polynomial of degree n,
- $l_i(x_i) = 1$,
- $l_i(x_j) = 0$ for $i \neq j$.

- Example 10 ———

Find the interpolating polynomial in the Lagrange form for the data

	i=0	i=1	i=2	
x_i	0	3	4	
y_i	2	1	5	

Calculate the value of the polynom at the point x = 2.

We write the Lagrange basis corresponding to single nodes:

$$l_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} = \frac{(x-3)(x-4)}{(0-3)(0-4)} = \frac{1}{12}(x-3)(x-4),$$

$$l_1(x) = \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} = \frac{(x-0)(x-4)}{(3-0)(3-4)} = -\frac{1}{3}x(x-4),$$

$$l_2(x) = \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} = \frac{(x-0)(x-3)}{(4-0)(4-3)} = \frac{1}{4}x(x-3),$$

The interpolating polynomial is

$$p_{2}(x) = y_{0}l_{0}(x) + y_{1}l_{1}(x) + y_{2}l_{2}(x)$$

= $2 \cdot \frac{1}{12}(x-3)(x-4) + 1 \cdot \left(-\frac{1}{3}x(x-4)\right) + 5 \cdot \frac{1}{4}x(x-3)$
= $\frac{1}{6}(x-3)(x-4) - \frac{1}{3}x(x-4) + \frac{5}{4}x(x-3).$

The resulting form of the interpolating polynomial is

$$p_2(x) = \frac{1}{6}(x-3)(x-4) - \frac{1}{3}x(x-4) + \frac{5}{4}x(x-3) .$$

We calculate the value of the polynom p_2 at the point x = 2.

$$p_2(2) = \frac{1}{6}(2-3)(2-4) - \frac{1}{3}2(2-4) + \frac{5}{4}2(2-3)$$
$$= -\frac{5}{6}$$

- Example 11

Find the interpolating polynomial in the Lagrange form for the data

	i=0	i=1	i=2	i=3
x_i	1	4	6	9
y_i	2	5	3	4

The Lagrange basis corresponding to single nodes is:

$$l_0(x) = \frac{(x-x_1)(x-x_2)(x-x_3)}{(x_0-x_1)(x_0-x_2)(x_0-x_3)} = \frac{(x-4)(x-6)(x-9)}{(1-4)(1-6)(1-9)} = -\frac{1}{120}(x-4)(x-6)(x-9),$$

$$l_1(x) = \frac{(x-x_0)(x-x_2)(x-x_3)}{(x_1-x_0)(x_1-x_2)(x_1-x_3)} = \frac{(x-1)(x-6)(x-9)}{(4-1)(4-6)(4-9)} = \frac{1}{30}(x-1)(x-6)(x-9),$$

$$l_2(x) = \frac{(x-x_0)(x-x_1)(x-x_3)}{(x_2-x_0)(x_2-x_1)(x_2-x_3)} = \frac{(x-1)(x-4)(x-9)}{(6-1)(6-4)(6-9)} = -\frac{1}{30}(x-1)(x-4)(x-9),$$

$$l_3(x) = \frac{(x-x_0)(x-x_1)(x-x_2)}{(x_3-x_0)(x_3-x_1)(x_3-x_2)} = \frac{(x-1)(x-4)(x-6)}{(9-1)(9-4)(9-6)} = \frac{1}{120}(x-1)(x-4)(x-6),$$

The interpolating polynomial is:

$$p_{3}(x) = y_{0}l_{0}(x) + y_{1}l_{1}(x) + y_{2}l_{2}(x) + y_{3}l_{3}(x)$$

$$= 2 \cdot \left(-\frac{1}{120}(x-4)(x-6)(x-9) \right) + 5 \cdot \frac{1}{30}(x-1)(x-6)(x-9)$$

$$+ 3 \cdot \left(-\frac{1}{30}(x-1)(x-4)(x-9) \right) + 4 \cdot \frac{1}{120}(x-1)(x-4)(x-6)$$

$$= -\frac{1}{60}(x-4)(x-6)(x-9) + \frac{1}{6}(x-1)(x-6)(x-9) - \frac{1}{10}(x-1)(x-4)(x-9)$$

$$+ \frac{1}{30}(x-1)(x-4)(x-6)$$

The resulting form of the interpolating polynomial is

$$p_3(x) = -\frac{1}{60}(x-4)(x-6)(x-9) + \frac{1}{6}(x-1)(x-6)(x-9) \\ -\frac{1}{10}(x-1)(x-4)(x-9) + \frac{1}{30}(x-1)(x-4)(x-6)$$

2.3 Interpolating polynomial in the Newton form

The interpolating polynomial of degree *n* in the Newton form is defined by the formula

$$p_n(x) = y_0 + f[x_1, x_0](x - x_0) + f[x_2, x_1, x_0](x - x_0)(x - x_1) + f[x_3, x_2, x_1, x_0](x - x_0)(x - x_1)(x - x_2) + \cdots + f[x_n, \dots, x_0](x - x_0)(x - x_1) \cdots (x - x_{n-1}),$$

where $f[x_1, x_0]$ is the 1st divided difference, $f[x_2, x_1, x_0]$ is the 2nd divided difference, up to $f[x_n, \ldots, x_0]$ is the *n*-th divided difference.

Example for n = 4**.**

The interpolating polynomial in the Newton form for n = 4 is defined as

$$p_4(x) = y_0 + f[x_1, x_0](x - x_0) + f[x_2, x_1, x_0](x - x_0)(x - x_1) + f[x_3, x_2, x_1, x_0](x - x_0)(x - x_1)(x - x_2) + f[x_4, x_3, x_2, x_1, x_0](x - x_0)(x - x_1)(x - x_2)(x - x_3)$$

The calculation of the divided differences for n = 4 is realized in the following table:

i	x _i	y _i	$\begin{vmatrix} 1 \text{st} \\ f[x_{i+1}, x_i] \end{vmatrix}$	2nd $f[x_{i+2}, x_{i+1}, x_i]$	3rd $f[x_{i+3}, x_{i+2}, x_{i+1}, x_i]$	4th $f[x_{i+4}, x_{i+3}, x_{i+2}, x_{i+1}, x_i]$
0	x ₀	f_0	$ \begin{vmatrix} f[x_1, x_0] = \\ = \frac{y_1 - y_0}{x_1 - x_0} \end{aligned} $	$ f[x_2, x_1, x_0] = \\ = \frac{f[x_2, x_1] - f[x_1, x_0]}{x_2 - x_0} $	$f[x_3, x_2, x_1, x_0] = \frac{f[x_3, x_2, x_1] - f[x_2, x_1, x_0]}{x_3 - x_0}$	$ \begin{cases} f[x_4, x_3, x_2, x_1, x_0] = \\ = \frac{f[x_4, x_3, x_2, x_1] - f[x_3, x_2, x_1, x_0]}{x_4 - x_0} \end{cases} $
1	$ x_1 $	f_1	$ \int f[x_2, x_1] = \\ = \frac{y_2 - y_1}{x_2 - x_1} $	$f[x_3, x_2, x_1] = \frac{f[x_3, x_2] - f[x_2, x_1]}{x_3 - x_1}$	$f[x_4, x_3, x_2, x_1] = \frac{f[x_4, x_3, x_2] - f[x_3, x_2, x_1]}{x_4 - x_1}$	
2	x ₂	f_2	$ \int f[x_3, x_2] = \\ = \frac{y_3 - y_2}{x_3 - x_2} $	$f[x_4, x_3, x_2] = \frac{f[x_4, x_3] - f[x_3, x_2]}{x_4 - x_2}$		
3	<i>x</i> ₃	<i>f</i> ₃	$ \int f[x_4, x_3] = \\ = \frac{y_4 - y_3}{x_4 - x_3} $			
4	$ x_4 $	f_4				

– Example 12 –

Find the interpolating polynomial in the Newton form for the data

	i=0	i=1	i=2
x_i	0	3	4
f_i	2	1	5

The calculation of the divided differences is realized in the following table:

Using the values from the first row of the table we can write the interpolating polynomial.

$$p_{2}(x) = 2 - \frac{1}{3}(x - 0) + \frac{13}{12}(x - 0)(x - 3) = 2 - \frac{1}{3}x + \frac{13}{12}x(x - 3)$$

- Example 13 –

Find the interpolating polynomial in the Newton form for the data

	i=0	i=1	i=2	
x_i	0	3	4	
f_i	2	1	5	

Use the MATLAB to solve the problem.

```
>> x=[0,3,4];
>> y=[2,1,5];
>> format rat
>> n=length(x);
>> df0=y;
>> for i=1:n-1,df1(i)=(df0(i+1)-df0(i))/(x(i+1)-x(i));end
>> for i=1:n-2,df2(i)=(df1(i+1)-df1(i))/(x(i+2)-x(i));end
>> format short
>> xg=x(1):0.01:x(3);
>> yg=df0(1)+df1(1)*(xg-x(1))+df2(1)*(xg-x(1)).*(xg-x(2));
>> plot(x,y,'go')
>> hold on
>> plot(xg,yg)
>> legend('nodes','interpolating polynomial')
```

Exercise 14 –

Find the interpolating polynomial for the data

	i=0	i=1	i=2	i=3
x_i	0	1	3	5
y_i	2	-3	0	3

a) in the standard form,

- b) in the standard form, use the MATLAB to solve the problem,
- c) in the Lagrage form,
- d) in the Lagrange form, use the MATLAB to solve the problem,
- e) in the Newton form,
- f) in the Newton form, use the MATLAB to solve the problem.

3 Approximation by the least-squares method

The approximation problem

Given *n* pairs (x_i, y_i) of distinct nodes x_i and corresponding values y_i , the problem consists of finding a function $\varphi(x)$ that fulfils

$$\varphi(x_i) \approx y_i, \quad i=1,\ldots,n$$
.

3.1 Linear approximation

Assume we are given *n* pairs (x_i, y_i) , i = 1, ..., n of distinct nodes x_i and corresponding values y_i . We want to find such values $c_1, c_2 \in \mathbb{R}$, that the linear function $\varphi(x) = c_1 + c_2 x$ is the best approximation of the given data in the least-squares sense.



The following figure illustrates the given data and a straight line that represents the searched linear function $\varphi(x) = c_1 + c_2 x$.



We want to find the coefficients c_1, c_2 of the linear function $\varphi(x)$, for which the sum of areas of squares in the figure above is minimized. Because the area of the *i*-th square is $(c_1 + c_2x_i - y_i)^2$, we are looking for a minimum of the **price function**

$$\Phi(c_1, c_2) = \sum_{i=1}^n (c_1 + c_2 x_i - y_i)^2 \,.$$

The price function Φ is quadratic, therefore its minimum exists and is unique. We are to solve the problem to find a minimum of the function of two variables. The minimum [c_1 , c_2] of the price function Φ must fulfil the equations

$$\frac{\partial}{\partial c_1} \Phi(c_1, c_2) = 0,$$
$$\frac{\partial}{\partial c_2} \Phi(c_1, c_2) = 0.$$

Having calculated the partial derivatives we obtain

$$2\sum_{i=1}^{n} (c_1 + c_2 x_i - y_i) = 0,$$

$$2\sum_{i=1}^{n} (c_1 + c_2 x_i - y_i) x_i = 0,$$

that is the system of linear equations for the unknown coefficients c_1 , c_2 :

$$c_1 \sum_{i=1}^n 1 + c_2 \sum_{i=1}^n x_i = \sum_{i=1}^n y_i,$$

$$c_1 \sum_{i=1}^n x_i + c_2 \sum_{i=1}^n x_i^2 = \sum_{i=1}^n x_i y_i,$$

This system is called the **normal system of equations** and can be rewritten in a matrix form: (n + n) = (n + 1)

$$\begin{pmatrix} \sum_{i=1}^{n} 1 & \sum_{i=1}^{n} x_i \\ \sum_{i=1}^{n} x_i & \sum_{i=1}^{n} x_i^2 \end{pmatrix} \cdot \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^{n} y_i \\ \sum_{i=1}^{n} y_i x_i \end{pmatrix}$$

Example 15 —

Approximate the data from the table

x_i	-2	-1	1	2
y_i	10	4	6	3

in the sense of the least-squares method by the function

$$\varphi(x) = c_1 + c_2 x.$$

We write the normal system of equations in the matrix form

$$\begin{pmatrix} \sum_{i=1}^{4} 1 & \sum_{i=1}^{4} x_i \\ \sum_{i=1}^{4} x_i & \sum_{i=1}^{4} x_i^2 \end{pmatrix} \cdot \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^{4} y_i \\ \sum_{i=1}^{4} y_i x_i \end{pmatrix}$$

and calculate the sums:

$$\sum_{i=1}^{4} 1 = 1 + 1 + 1 + 1 = 4$$

$$\sum_{i=1}^{4} x_i = -2 + (-1) + 1 + 2 = 0$$

$$\sum_{i=1}^{4} x_i^2 = (-2)^2 + (-1)^2 + 1^2 + 2^2 = 10$$

$$\sum_{i=1}^{4} y_i = 10 + 4 + 6 + 3 = 23$$

$$\sum_{i=1}^{4} y_i x_i = 10 \cdot (-2) + 4 \cdot (-1) + 6 \cdot 1 + 3 \cdot 2 = -12$$

The normal system of equations is:

$$\begin{pmatrix} 4 & 0 \\ 0 & 10 \end{pmatrix} \cdot \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 23 \\ -12 \end{pmatrix}$$

The unique solution of this system is $c_1 = \frac{23}{4}$, $c_2 = -\frac{6}{5}$. Therefore the linear function that represents the best linear approximation of the given data in the least-squares method sense is



- Example 16 –

Approximate the data from the table

x_i	-2	-1	1	2
y_i	10	4	6	3

in the sense of the least-squares method by the function

$$\varphi(x) = c_1 + c_2 x.$$

```
>> x=[-2 -1 1 2];
>> y=[10 4 6 3];
>> n=length(x);
>> M=[n sum(x); sum(x) sum(x.^2)];
>> v=[sum(y); sum(y.*x)];
>> c=M\v;
>> hold on
>> plot(x,y,'ro')
>> xg=x(1):0.01:x(n);
>> yg=c(1)+c(2)*xg;
>> plot(xg,yg)
```

3.2 Approximation by two functions

Assume we are given *n* pairs (x_i, y_i) , i = 1, ..., n of distinct nodes x_i and corresponding values y_i as well as two functions $\varphi_1(x)$ a $\varphi_2(x)$. We want to find such values $c_1, c_2 \in \mathbb{R}$, that the function $\varphi(x) = c_1\varphi_1(x) + c_2\varphi_2(x)$ is the best approximation of the given data in the least-squares sense.

Analogously to the case of linear approximation, we obtain the unknown coefficients $c_1, c_2 \in \mathbb{R}$ as the minimum of the price function

$$\Phi(c_1, c_2) = \sum_{i=1}^n (c_1 \varphi_1(x_i) + c_2 \varphi_2(x_i) - y_i)^2,$$

i.e. as the solution of the normal system of equations

$$c_{1}\sum_{i=1}^{n} (\varphi_{1}(x_{i}))^{2} + c_{2}\sum_{i=1}^{n} \varphi_{1}(x_{i}) \cdot \varphi_{2}(x_{i}) = \sum_{i=1}^{n} y_{i} \cdot \varphi_{1}(x_{i}),$$

$$c_{1}\sum_{i=1}^{n} \varphi_{2}(x_{i}) \cdot \varphi_{1}(x_{i}) + c_{2}\sum_{i=1}^{n} (\varphi_{2}(x_{i}))^{2} = \sum_{i=1}^{n} y_{i} \cdot \varphi_{2}(x_{i})$$

or in the matrix form

$$\begin{pmatrix}\sum_{i=1}^{n} (\varphi_1(x_i))^2 & \sum_{i=1}^{n} \varphi_1(x_i) \cdot \varphi_2(x_i)\\ \sum_{i=1}^{n} \varphi_2(x_i) \cdot \varphi_1(x_i) & \sum_{i=1}^{n} (\varphi_2(x_i))^2 \end{pmatrix} \cdot \begin{pmatrix}c_1\\c_2\end{pmatrix} = \begin{pmatrix}\sum_{i=1}^{n} y_i \cdot \varphi_1(x_i)\\ \sum_{i=1}^{n} y_i \cdot \varphi_2(x_i)\end{pmatrix}$$

For example, if we want to approximate by the function

$$\varphi(x) = c_1 x^2 + c_1 \sin(x) ,$$

then the normal system of equations is:

$$c_1 \sum_{i=1}^n x_i^4 + c_2 \sum_{i=1}^n x_i^2 \sin(x_i) = \sum_{i=1}^n y_i x_i^2,$$

$$c_1 \sum_{i=1}^n x_i^2 \sin(x_i) + c_2 \sum_{i=1}^n \sin^2(x_i) = \sum_{i=1}^n y_i \sin(x_i)$$

or in the matrix form

$$\begin{pmatrix} \sum_{i=1}^n x_i^4 & \sum_{i=1}^n x_i^2 \sin(x_i) \\ \sum_{i=1}^n x_i^2 \sin(x_i) & \sum_{i=1}^n \sin^2(x_i) \end{pmatrix} \cdot \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^n y_i x_i^2 \\ \sum_{i=1}^n y_i \sin(x_i) \end{pmatrix}.$$

- Example 17 —

Approximate the data from the table

$x_i \mid$	1	2	3	5	7	10
y_i	0	3	5	8	8	7

in the sense of the least-squares method by the function

 $\varphi(x) = c_1 \ln(x) + c_2 x.$

We write the normal system of equations in the matrix form

$$\begin{pmatrix} \sum_{i=1}^{6} \ln^{2}(x_{i}) & \sum_{i=1}^{6} x_{i} \ln(x_{i}) \\ \sum_{i=1}^{6} x_{i} \ln(x_{i}) & \sum_{i=1}^{6} x_{i}^{2} \end{pmatrix} \cdot \begin{pmatrix} c_{1} \\ c_{2} \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^{6} y_{i} \ln(x_{i}) \\ \sum_{i=1}^{6} y_{i} x_{i} \end{pmatrix}$$

and calculate the sums:

$$\sum_{i=1}^{6} \ln^2(x_i) = \ln^2(1) + \ln^2(2) + \ln^2(3) + \ln^2(5) + \ln^2(7) + \ln^2(10) = 13.3662$$

$$\sum_{i=1}^{6} x_i \ln(x_1) = 1 \cdot \ln(1) + 2 \cdot \ln(2) + 3 \cdot \ln(3) + 5 \cdot \ln(5)$$

$$+7 \cdot \ln(7) + 10 \cdot \ln(10) = 49.3765$$

$$\sum_{i=1}^{6} x_i^2 = 1^2 + 2^2 + 3^2 + 5^2 + 7^2 + 10^2 = 188$$

$$\sum_{i=1}^{6} y_i \ln(x_i) = 0 \cdot \ln(1) + 3 \cdot \ln(2) + 5 \cdot \ln(3) + 8 \cdot \ln(5)$$

$$+8 \cdot \ln(7) + 7 \cdot \ln(10) = 52.1334$$

$$\sum_{i=1}^{6} y_i x_i = 0 \cdot 1 + 3 \cdot 2 + 5 \cdot 3 + 8 \cdot 5 + 8 \cdot 7 + 7 \cdot 10 = 187$$

The normal system of equations is:

$$\begin{pmatrix} 13.3662 & 49.3765 \\ 49.3765 & 188 \end{pmatrix} \cdot \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 52.1334 \\ 187 \end{pmatrix}$$

The unique solution of this system is $c_1 = 7.5896$, $c_2 = -0.9987$.

Therefore the best approximation of the given data in the least-squares method sense has the form

$$\varphi(x) = 7.58961 \ln(x) - 0.9987x$$



Example 18 ———

Approximate the data from the table

x_i	1	2	3	5	7	10
y_i	0	3	5	8	8	7

in the sense of the least-squares method by the function

$$\varphi(x) = c_1 \ln(x) + c_2 x.$$

Use the MATLAB to solve the problem.

```
>> x=[1,2,3,5,7,10]
>> y=[0,3,5,8,8,7];
>> n=length(x);
>> M=[sum(log(x).^2 sum(log(x)*x); sum(x.*log(x)) sum(x.^2)];
>> v=[sum(y.*log(x)); sum(y.*x)];
>> c=M\v
>> hold on
>> plot(x,y,'ro')
>> xg=x(1):0.01:x(n);
>> yg=c(1)*log(xg)+c(2)*xg;
>> plot(xg,yg)
```

3.3 Approximation by *k* functions

Assume we are given *n* pairs (x_i, y_i) , i = 1, ..., n of distinct nodes x_i and corresponding values y_i as well as *k* functions $\varphi_1(x)$, $\varphi_2(x)$, ..., $\varphi_k(x)$. We want to find such values $c_1, c_2, ..., c_k \in \mathbb{R}$, that the function $\varphi(x) = c_1\varphi_1(x) + c_2\varphi_2(x) + \cdots + c_k\varphi_k(x)$ is the best approximation of the given data in the least-squares sense.

These coefficients $c_1, c_2, ..., c_k \in \mathbb{R}$ we obtain as the solution of the normal system of equations

$$c_{1}\sum_{i=1}^{n} (\varphi_{1}(x_{i}))^{2} + c_{2}\sum_{i=1}^{n} \varphi_{1}(x_{i}) \cdot \varphi_{2}(x_{i}) + c_{3}\sum_{i=1}^{n} \varphi_{1}(x_{i}) \cdot \varphi_{3}(x_{i}) + \dots + c_{k}\sum_{i=1}^{n} \varphi_{1}(x_{i}) \cdot \varphi_{k}(x_{i})$$
$$= \sum_{i=1}^{n} y_{i} \cdot \varphi_{1}(x_{i}),$$

$$c_{1}\sum_{i=1}^{n}\varphi_{2}(x_{i})\cdot\varphi_{1}(x_{i})+c_{2}\sum_{i=1}^{n}(\varphi_{2}(x_{i}))^{2}+c_{3}\sum_{i=1}^{n}\varphi_{2}(x_{i})\cdot\varphi_{3}(x_{i})+\dots+c_{k}\sum_{i=1}^{n}\varphi_{2}(x_{i})\cdot\varphi_{k}(x_{i})$$

$$=\sum_{i=1}^{n}y_{i}\cdot\varphi_{2}(x_{i}),$$

$$\vdots$$

$$c_{1}\sum_{i=1}^{n}\varphi_{k}(x_{i})\cdot\varphi_{1}(x_{i})+c_{2}\sum_{i=1}^{n}\varphi_{k}(x_{i})\cdot\varphi_{2}(x_{i})+c_{3}\sum_{i=1}^{n}\varphi_{k}(x_{i})\cdot\varphi_{3}(x_{i})+\dots+c_{k}\sum_{i=1}^{n}(\varphi_{k}(x_{i}))^{2}$$

$$=\sum_{i=1}^{n}y_{i}\cdot\varphi_{k}(x_{i}).$$

For k = 3: We want to find the values $c_1, c_2, c_3 \in \mathbb{R}$ for the function $\varphi(x) = c_1\varphi_1(x) + c_2\varphi_2(x) + c_k\varphi_3(x)$. The normal system of equations is

$$c_{1}\sum_{i=1}^{n} (\varphi_{1}(x_{i}))^{2} + c_{2}\sum_{i=1}^{n} \varphi_{1}(x_{i}) \cdot \varphi_{2}(x_{i}) + c_{3}\sum_{i=1}^{n} \varphi_{1}(x_{i}) \cdot \varphi_{3}(x_{i}) = \sum_{i=1}^{n} y_{i} \cdot \varphi_{1}(x_{i}),$$

$$c_{1}\sum_{i=1}^{n} \varphi_{2}(x_{i}) \cdot \varphi_{1}(x_{i}) + c_{2}\sum_{i=1}^{n} (\varphi_{2}(x_{i}))^{2} + c_{3}\sum_{i=1}^{n} \varphi_{2}(x_{i}) \cdot \varphi_{3}(x_{i}) = \sum_{i=1}^{n} y_{i} \cdot \varphi_{2}(x_{i}),$$

$$c_{1}\sum_{i=1}^{n} \varphi_{3}(x_{i}) \cdot \varphi_{1}(x_{i}) + c_{2}\sum_{i=1}^{n} \varphi_{3}(x_{i}) \cdot \varphi_{2}(x_{i}) + c_{3}\sum_{i=1}^{n} (\varphi_{3}(x_{i}))^{2} = \sum_{i=1}^{n} y_{i} \cdot \varphi_{3}(x_{i})$$

or in the matrix form

$$\begin{pmatrix} \sum_{i=1}^{n} (\varphi_1(x_i))^2 & \sum_{i=1}^{n} \varphi_1(x_i) \cdot \varphi_2(x_i) & \sum_{i=1}^{n} \varphi_1(x_i) \cdot \varphi_3(x_i) \\ \sum_{i=1}^{n} \varphi_2(x_i) \cdot \varphi_1(x_i) & \sum_{i=1}^{n} (\varphi_2(x_i))^2 & \sum_{i=1}^{n} \varphi_2(x_i) \cdot \varphi_3(x_i) \\ \sum_{i=1}^{n} \varphi_3(x_i) \cdot \varphi_1(x_i) & \sum_{i=1}^{n} \varphi_3(x_i) \cdot \varphi_2(x_i) & \sum_{i=1}^{n} (\varphi_3(x_i))^2 \end{pmatrix} \cdot \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^{n} y_i \cdot \varphi_1(x_i) \\ \sum_{i=1}^{n} y_i \cdot \varphi_2(x_i) \\ \sum_{i=1}^{n} y_i \cdot \varphi_3(x_i) \end{pmatrix}.$$

- Example 19 -

Approximate the data from the table

$x_i \mid$	1	2	3	5	7	10
$y_i \mid$	0	3	5	8	8	7

in the sense of the least-squares method by the function

$$\varphi(x) = c_1 + c_2 x + c_3 x^2.$$

We write the normal system of equations in the matrix form

$$\begin{pmatrix} \sum_{i=1}^{6} 1 & \sum_{i=1}^{6} x_i & \sum_{i=1}^{6} x_i^2 \\ \sum_{i=1}^{6} x_i & \sum_{i=1}^{6} x_i^2 & \sum_{i=1}^{6} x_i^3 \\ \sum_{i=1}^{6} x_i^2 & \sum_{i=1}^{6} x_i^3 & \sum_{i=1}^{6} x_i^4 \end{pmatrix} \cdot \begin{pmatrix} c_1 \\ c_2 \\ c_3 \end{pmatrix} = \begin{pmatrix} \sum_{i=1}^{6} y_i \\ \sum_{i=1}^{6} y_i x_i \\ \sum_{i=1}^{6} y_i x_i^2 \end{pmatrix}$$

and calculate the sums:

$$\sum_{i=1}^{6} 1 = 1 + 1 + 1 + 1 + 1 + 1 = 6$$

$$\sum_{i=1}^{6} x_i = 1 + 2 + 3 + 5 + 7 + 10 = 28$$

$$\sum_{i=1}^{6} x_i^2 = 1^2 + 2^2 + 3^2 + 5^2 + 7^2 + 10^2 = 188$$

$$\sum_{i=1}^{6} x_i^3 = 1^3 + 2^3 + 3^3 + 5^3 + 7^3 + 10^3 = 1504$$

$$\sum_{i=1}^{6} x_i^4 = 1^4 + 2^4 + 3^4 + 5^4 + 7^4 + 10^4 = 13124$$

$$\sum_{i=1}^{6} y_i = 0 + 3 + 5 + 8 + 8 + 7 = 31$$

$$\sum_{i=1}^{6} y_i x_i = 0 \cdot 1 + 3 \cdot 2 + 5 \cdot 3 + 8 \cdot 5 + 8 \cdot 7 + 7 \cdot 10 = 187$$

$$\sum_{i=1}^{6} y_i x_i^2 = 0 \cdot 1^2 + 3 \cdot 2^2 + 5 \cdot 3^2 + 8 \cdot 5^2 + 8 \cdot 7^2 + 7 \cdot 10^2 = 1349$$

The normal system of equations is:

$$\begin{pmatrix} 6 & 28 & 188 \\ 28 & 188 & 1504 \\ 188 & 1504 & 13124 \end{pmatrix} \cdot \begin{pmatrix} c_1 \\ c_2 \end{pmatrix} = \begin{pmatrix} 31 \\ 187 \\ 1349 \end{pmatrix}$$

The unique solution of this system is $c_1 = -2.63963$, $c_2 = 3.16090$, $c_3 = -0.22163$.

The best quadratic approximation of the given data in the least-squares method sense) has the form

$$\varphi(x) = -2.63963 + 3.16090x - 0.22163x^2$$



- Example 20 —

Approximate the data from the table

x_i	1	2	3	5	7	10
y_i	0	3	5	8	8	7

in the sense of the least-squares method by the function

$$\varphi(x) = c_1 + c_2 x + c_3 x^2.$$

Use the MATLAB to solve the problem.

```
>> x=[1,2,3,5,7,10];
>> y=[0,3,5,8,8,7];
>> n=length(x);
>> M=[n sum(x) sum(x.^2); sum(x) sum(x.^2) sum(x.^3); sum(x.^2)
    sum(x.^3) sum(x.^4)];
>> v=[sum(y); sum(y.*x); sum(y.*x.^2)];
>> c=M\v
>> hold on
>> plot(x,y,'ro')
>> xg=x(1):0.01:x(n);
>> yg=c(1)+c(2)*xg+c(3)*x.^2;
>> plot(xg,yg)
```

– Exercise 21 —

Approximate the data from the table

x _i	1	2	3.5	4.5	6	7	7.5
y _i	4.2	5	5.5	7	7.8	8.5	8.1

in the sense of the least-squares method

a) by the linear function

$$\zeta(x) = a_1 + a_2 x,$$

b) by the function

$$\varphi(x)=b_1\mathrm{e}^x+b_2x,$$

c) by the quadratic function

$$\theta(x) = c_1 + c_2 x + c_3 x^2.$$

Compare the obtained results both graphically and numerically. Use the MATLAB to solve the problem.

4 Numerical differentiation

4.1 The first derivative

Given distinct nodes x_i and corresponding function values $f(x_i)$ of a function f, the problem is to approximate values of the first derivative $f'(x_i)$ at the given nodes. Because the value $f'(x_i)$ is the slope of the tangent line to the graph of the function f at the point $[x_i, f(x_i)]$, we can approximate it by a slope of a proper secant line.

Using a secant line corresponding to nodes x_i and x_{i+1} we obtain the **forward difference**



Using a secant line corresponding to nodes x_{i-1} and x_i we obtain the **backward difference**



Using a secant line corresponding to nodes x_{i-1} and x_{i+1} we obtain the **central difference**



In practice, the central difference is usually the most accurate approximation of the derivative value.

- Example 22 –

Approximate the derivative of the data

	i=1	i=2	i=3	i=4	i=5
x_i	0	1	2	3	4
y_i	40	50	20	25	30

using the forward difference.

We calculate the approximate value of the derivative $y'(x_1)$

$$y'(x_1) = rac{y_2 - y_1}{x_2 - x_1} = rac{50 - 40}{1 - 0} = 10$$
 ,

approximate value of the derivative $y'(x_3)$

$$y'(x_2) = \frac{y_3 - y_2}{x_3 - x_2} = \frac{20 - 50}{2 - 1} = -30$$
,

approximate value of the derivative $y'(x_3)$

$$y'(x_3) = \frac{y_4 - y_3}{x_4 - x_3} = \frac{25 - 20}{3 - 2} = 5$$

approximate value of the derivative $y'(x_4)$

$$y'(x_4) = \frac{y_5 - y_4}{x_5 - x_4} = \frac{30 - 25}{4 - 3} = 5.$$

Table of the obtained approximate values of the derivatives at the nodes:

x_i	0 1	2	3	4
$y'(x_i) \mid 1$	0 -30	5	5	

The approximate value of the derivative $y'(x_5)$ cannot be calculated by the forward difference because there is no following node there.

- Example 23 –

Approximate the derivative of the data

	i=1	i=2	i=3	i=4	i=5
x_i	0	1	2	3	4
y _i	40	50	20	25	30

using the backward difference.

We calculate the approximate value of the derivative $y'(x_2)$

$$y'(x_2) = \frac{y_2 - y_1}{x_2 - x_1} = \frac{50 - 40}{1 - 0} = 10$$

approximate value of the derivative $y'(x_3)$

$$y'(x_3) = \frac{y_3 - y_2}{x_3 - x_2} = \frac{20 - 50}{2 - 1} = -30$$
,

approximate value of the derivative $y'(x_4)$

$$y'(x_4) = \frac{y_4 - y_3}{x_4 - x_3} = \frac{25 - 20}{3 - 2} = 5$$

approximate value of the derivative $y'(x_5)$

$$y'(x_5) = \frac{y_5 - y_4}{x_5 - x_4} = \frac{30 - 25}{4 - 3} = 5.$$

Table of the obtained approximate values of the derivatives at the nodes:

x_i	0	1	2	3	4
$y'(x_i)$	—	10	-30	5	5

The approximate value of the derivative $y'(x_1)$ cannot be calculated by the backward difference because there is no previous node there.

- Example 24 —

Approximate the derivative of the data

	i=1	i=2	i=3	i=4	i=5
x_i	0	1	2	3	4
y_i	40	50	20	25	30

using the central difference.

We calculate the approximate value of the derivative $y'(x_2)$

$$y'(x_2) = \frac{y_3 - y_1}{x_3 - x_1} = \frac{20 - 40}{2 - 0} = -10$$
,

approximate value of the derivative $y'(x_3)$

$$y'(x_3) = \frac{y_4 - y_2}{x_4 - x_2} = \frac{25 - 50}{3 - 1} = -\frac{25}{2} = -12.5$$
,

approximate value of the derivative $y'(x_4)$

$$y'(x_4) = \frac{y_5 - y_3}{x_5 - x_3} = \frac{30 - 20}{4 - 2} = 5$$

Table of the obtained approximate values of the derivatives at the nodes:

x_i	0	1	2	3	4
$y'(x_i)$		-10	-12.5	5	

The approximate values of the derivatives $y'(x_1)$ and $y'(x_5)$ cannot be calculated by the central difference because there are no required near by nodes there.

- Example 25 –

Approximate the derivative of the data

	i=1	i=2	i=3	i=4	i=5
x_i	0	1	2	3	4
y_i	40	50	20	25	30

using the central difference at the interior nodes, the forward difference at the first node and the backward difference at the last node.

All needed approximate values of the derivative $y'(x_i)$ were calculated in previous examples.

Table of the obtained approximate values of the derivatives at the nodes:

$x_i \mid 0$	1	2	3	4
$y'(x_i) \mid 10$	-10	-12.5	5	5

– Example 26 –

Approximate the derivative of the data

	i=1	i=2	i=3	i=4	i=5
x_i	0	1	2	3	4
y_i	40	50	20	25	30

using the central difference at the interior nodes, the forward difference at the first node and the backward difference at the last node.

Use the MATLAB to solve the problem.

```
>> x=[0 1 2 3 4];
>> y=[40 50 20 25 30];
>> n=length(x);
>> yd(1)=(y(2)-y(1))/(x(2)-x(1));
>> for i=2:n-1, yd(i)=(y(i+1)-y(i-1))/(x(i+1)-x(i-1)); end
>> yd(n)=(y(n)-y(n-1))/(x(n)-x(n-1));
```

4.2 The second derivative

Given distinct nodes x_i and corresponding function values $f(x_i)$ of a function f, values of the second derivative $f''(x_i)$ at the given nodes can be approximated by the formula:

$$f''(x_i) \approx \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{(x_{i+1} - x_i)(x_i - x_{i-1})}.$$



If the nodes are equidistant with the step *h* then the formula above can be simplified to the form: f(x,y) = 2f(x,y) + f(x,y)

$$f''(x_i) \approx \frac{f(x_{i+1}) - 2f(x_i) + f(x_{i-1})}{h^2}.$$

- Example 27 ——

Approximate the second derivative of the data

	i=1	i=2	i=3	i=4	i=5
x_i	0	1	2	3	4
y_i	40	50	20	25	30

We calculate the approximate value of the second derivative $y''(x_2)$

$$y''(x_2) = \frac{y_3 - 2y_2 + y_1}{(x_3 - x_2)(x_2 - x_1)} = \frac{20 - 2 \cdot 50 + 40}{(2 - 1)(1 - 0)} = -40$$
,

approximate value of the second derivative $y''(x_3)$

$$y''(x_3) = \frac{y_4 - 2y_3 + y_2}{(x_4 - x_3)(x_3 - x_2)} = \frac{25 - 2 \cdot 20 + 50}{(3 - 2)(2 - 1)} = 35$$
,

approximate value of the second derivative $y''(x_4)$

$$y''(x_4) = \frac{y_5 - 2y_4 + y_3}{(x_5 - x_4)(x_4 - x_3)} = \frac{30 - 2 \cdot 25 + 20}{(4 - 3)(3 - 2)} = 0.$$

Table of the obtained approximate values of the second derivatives at the nodes:

x_i	0	1	2	3	4
$y''(x_i) \mid$		-40	35	0	

– Example 28 —

Approximate the second derivative of the data

```
>> x=[0 1 2 3 4];
>> y=[40 50 20 25 30];
>> h= 1;
>> n=length(x)
>> for i=2:n-1, ydd(i)=(f(x(i+1))-2*f(x(i))+f(x(i-1)))/(h^2); end
c Exercise 29
```

The data are given in table:

x_i	2	4	6	8	10	12	14
y_i	12.4	5.3	3.2	4.5	7.1	8.6	11.6

- a) Approximate the derivative of the data using the central difference at the interior nodes, the forward difference at the first node and the backward difference at the last node.
- b) Approximate the derivative of the data using the central difference at the interior nodes, the forward difference at the first node and the backward difference at the last node. Use the MATLAB to solve the problem.
- c) Approximate the second derivative of the data using the central difference at the interior nodes, the forward difference at the first node and the backward difference at the last node.
- d) Approximate the second derivative of the data using the central difference at the interior nodes, the forward difference at the first node and the backward difference at the last node. Use the MATLAB to solve the problem.

5 Numerical integration



5.1 The rectangle rule

We approximate the function *f* by the constant interpolating polynomial $p_0(x)$ with the node $x_0 = \frac{a+b}{2}$.



This approximation can be integrated analytically and we obtain **the rectangle rule**:

$$I_{rect} = (b-a)f\left(\frac{a+b}{2}\right)$$

– Example 30 –

Evaluate the definite integral

$$\int_0^6 \frac{x}{1+x^2} \,\mathrm{d}x$$

using the rectangle rule.

We have
$$a = 0$$
, $b = 6$ and $f(x) = \frac{x}{1 + x^2}$.

The rectangle rule.

$$I_{rect} = (b-a)f\left(\frac{a+b}{2}\right) = (6-0)f(3) = (6-0)\frac{3}{1+3^2}$$
$$= \frac{18}{10} = 1.8$$

– Example 31 –

Evaluate the definite integral

$$\int_0^6 \frac{x}{1+x^2} \,\mathrm{d}x$$

using the rectangle rule. Use the MATLAB to solve the problem.

>> f=@(x)x./(1+x.^2);
>> a=0; b=6;
>> I=(b-a)*f((a+b)/2)

5.2 The trapezoidal rule

We approximate the function *f* by the linear interpolating polynomial $p_1(x)$ with the nodes $x_0 = a$, $x_1 = b$.



The linear approximation can be also integrated analytically and we obtain **the trapezoidal rule**:

$$I_{trap} = \frac{b-a}{2} \left(f(a) + f(b) \right).$$

- Example 32 ——

Evaluate the definite integral

$$\int_0^6 \frac{x}{1+x^2} \,\mathrm{d}x$$

using the trapezoidal rule.

We have
$$a = 0$$
, $b = 6$ and $f(x) = \frac{x}{1 + x^2}$.

The trapezoidal rule.

$$I_{trap} = \frac{b-a}{2} \left(f(a) + f(b) \right) = \frac{6-0}{2} \left(f(0) + f(6) \right)$$
$$= 3 \left(\frac{0}{1+0^2} + \frac{6}{1+6^2} \right) = \frac{18}{37} = 0.4865$$

– Example 33 —

Evaluate the definite integral

$$\int_0^6 \frac{x}{1+x^2} \,\mathrm{d}x$$

using the trapezoidal rule.

Use the MATLAB to solve the problem.

>> f=@(x)x./(1+x.^2);
>> a=0; b=6;
>> I=(b-a)/2*(f(a)+f(b))

5.3 The Simpson's rule

We approximate the function *f* by the quadratic interpolating polynomial $p_2(x)$ with the nodes $x_0 = a$, $x_1 = \frac{a+b}{2}$, $x_2 = b$.



The quadratic approximation can be also integrated analytically and we obtain

$$I_{Simps} = \frac{b-a}{6} \left(f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right).$$

- Example 34 –

Evaluate the definite integral

$$\int_0^6 \frac{x}{1+x^2} \,\mathrm{d}x$$

using the Simpson's rule.

We have
$$a = 0$$
, $b = 6$ and $f(x) = \frac{x}{1 + x^2}$.

The Simpson's rule.

$$I_{Simps} = \frac{b-a}{6} \left(f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right) = \frac{6-0}{6} (f(0) + 4f(3) + f(6))$$
$$= 1 \left(\frac{0}{1+0^2} + 4\frac{3}{1+3^2} + \frac{6}{1+6^2} \right) = 0 + \frac{12}{10} + \frac{6}{37} = 1.3622$$

– Example 35 –

Evaluate the definite integral

$$\int_0^6 \frac{x}{1+x^2} \,\mathrm{d}x$$

using the Simpson's rule. Use the MATLAB to solve the problem.

>> f=@(x)x./(1+x.^2);
>> a=0; b=6;
>> I=(b-a)/6*(f(a)+4*f((a+b)/2)+f(b))

5.4 The composite rectangle rule

If we want to integrate the function f over the interval [a, b] using the composite rectangle rule, we have to divide the given interval into n equidistant subintervals of the length h = (b - a)/n with the nodes $x_i = a + ih, i = 0, 1, ..., n$.



The formula of the composite rectangle rule with the step h is then of the form

$$I_{CR} = h \sum_{i=1}^{n} f\left(\frac{x_{i-1}+x_i}{2}\right).$$

Example 36 —

Evaluate the definite integral

$$\int_{-1}^{1} \mathrm{e}^{x} \,\mathrm{d}x$$

using the composite rectangle rule for n = 4.

We equate n = 4, so that the step is $h = \frac{b-a}{n} = 0.5$ and we obtain the nodes $x_0 = -1$, $x_1 = -0.5$, $x_2 = 0$, $x_3 = 0.5$ a $x_4 = 1$.

$$I_{CR} = h \sum_{i=1}^{n} f\left(\frac{x_{i-1} + x_i}{2}\right)$$

= $h\left(f(\frac{x_0 + x_1}{2}) + f(\frac{x_1 + x_2}{2}) + f(\frac{x_2 + x_3}{2}) + f(\frac{x_3 + x_4}{2})\right)$
= $0.5(e^{-0.75} + e^{-0.25} + e^{0.25} + e^{0.75}) \doteq 2.3261.$

- Example 37 —

Evaluate the definite integral

$$\int_{-1}^{1} e^{x} dx$$

using the composite rectangle rule for n = 4.

```
>> f = @(x) exp(x)
>> a = -1; b = 1;
>> n = 4; h = (b-a)/n;
>> xmid = a+h/2:h:b-h/2;
>> y = f(xmid);
>> I=h*sum(y)
```

5.5 The composite trapezoidal rule

If we want to integrate the function f over the interval [a, b] using the composite trapezoidal rule, we have to divide the given interval into n equidistant subintervals of the length h = (b - a)/n with the nodes $x_i = a + ih$, i = 0, 1, ..., n.



The formula of the composite trapezoidal rule with the step h is then of the form

$$I_{CT} = \frac{h}{2} \left(f(x_0) + 2 \sum_{i=1}^{n-1} f(x_i) + f(x_n) \right).$$

- Example 38 -

Evaluate the definite integral

$$\int_{-1}^{1} \mathrm{e}^{x} \,\mathrm{d}x$$

using the composite trapezoidal rule for n = 4.

We equate n = 4, so that the step is $h = \frac{b-a}{n} = 0.5$ and we obtain the nodes $x_0 = -1$, $x_1 = -0.5$, $x_2 = 0$, $x_3 = 0.5$ a $x_4 = 1$.

$$I_{CT} = \frac{h}{2} \left(f(x_0) + 2 \sum_{i=1}^{n-1} f(x_i) + f(x_n) \right)$$

= $\frac{h}{2} \left(f(x_0) + 2 \left(f(x_1) + f(x_2) + f(x_3) \right) + f(x_n) \right)$
= $\frac{0.5}{2} (e^{-1} + 2(e^{-0.5} + e^0 + e^{0.5}) + e^1) \doteq 2.3992.$

- Example 39 -

Evaluate the definite integral

$$\int_{-1}^{1} e^{x} dx$$

using the composite trapezoidal rule for n = 4.

```
>> f = @(x) exp(x);
>> a = -1; b = 1;
>> n = 4; h = (b-a)/n;
>> x = a:h:b;
>> y = f(x);
>> I=h/2*(y(1)+2*sum(y(2:n))+y(n+1))
```

5.6 The composite Simpson's rule

If we want to integrate the function f over the interval [a, b] using the composite Simpson's rule, we have to divide the given interval into n equidistant subintervals where n has to be an even number. The length of each subinterval is h = (b - a)/n and we obtain an odd number of the nodes $x_i = a + ih$, i = 0, 1, ..., n.



The formula of the composite Simpson's rule with the step h is then of the form

$$I_{CS} = \frac{h}{3} \left(f(x_0) + 4 \sum_{\substack{i=1\\i \text{ even}}}^{n-1} f(x_i) + 2 \sum_{\substack{i=2\\i \text{ odd}}}^{n-2} f(x_i) + f(x_n) \right).$$

– Example 40 -

Evaluate the definite integral

$$\int_{-1}^{1} \mathrm{e}^{x} \,\mathrm{d}x$$

using the composite Simpson's rule for n = 4.

We exact n = 4, so that the step is $h = \frac{b-a}{n} = 0.5$ and we obtain the nodes $x_0 = -1$, $x_1 = -0.5$, $x_2 = 0$, $x_3 = 0.5$ a $x_4 = 1$.

$$I_{CS} = \frac{h}{3} \left(f(x_0) + 4 \sum_{i=1}^{n/2} f(x_{2i-1}) + 2 \sum_{i=1}^{n/2-1} f(x_{2i}) + f(x_{2m}) \right)$$

= $\frac{h}{3} \left(f(x_0) + 4 \left(f(x_1) + f(x_3) \right) + 2f(x_2) + f(x_4) \right)$
= $\frac{0.5}{3} (e^{-1} + 4(e^{-0.5} + e^{0.5}) + 2e^0 + e^1) \doteq 2.3512.$

- Example 41 -

Evaluate the definite integral

$$\int_{-1}^{1} \mathrm{e}^{x} \,\mathrm{d}x$$

using the composite Simpson's rule for n = 4.

```
>> f = @(x) exp(x);
>> a = -1; b = 1;
>> n = 4; h = (b-a)/n;
>> x = a:h:b;
>> y = f(x);
>> I=h/3*(y(1)+4*sum(y(2:2:n))+2*sum(y(3:2:n-1))+y(n+1))
```

5.7 The evaluation of the integral with the given accuracy

We calculate the approximate value I_h of the integral using the integration formula with the step *h*. Consequently, we calculate the approximate value $I_{h/2}$ with the half-length step h/2. We stop the calculation, if the following holds

$$|I_h - I_{h/2}| \leq \varepsilon.$$

The composite trapezoidal rules for n = 1, 2, 4



The composite Simpson's rules for n = 2, 4, 8



We define the function f and input the limits of integration as the variables a, b.

>> f = @(x)log(x)./sqrt(9-x.^2);
>> a = 1;
>> b = exp(1);

We set n = 2 in the first step. We input the vector of the nodes as the variable x.

>> n = 2; >> h = (b-a)/n; >> x = a:h:b; >> y = f(x);

Because we aim at the accuracy 10^{-8} , we can not take up with the four decimal places that the MATLAB display in the standard short format. We have to switch the output format to long.

>> format long

We calculate the approximate value of the given integral and input it as the variable Inew.

We save the obtained value as the variable I. Then we double the value of *n* and repeat all calculations. Finally we evaluate the error approximation $|I_h - I_{2h}|$

We repeat the previous seven statements till the error is greater than 10^{-8} . We round the result to eight decimal places and write it as

	$\int_{1}^{e} \frac{\ln \pi}{\sqrt{9}}$	$\frac{x}{-x^2} \mathrm{d}x = 0.5$	$0661191 \pm 10^{-8}.$
n	$ $ I_h	$ I_h - I_{2h} $	$\varepsilon = 10^{-8} = 0.000000001$
2	0.52733592		0
4	0.51036199	0.01697393	$> 10^{-8}$
8	0.50708297	0.00327902	$> 10^{-8}$
16	0.50665442	0.00042855	$> 10^{-8}$
32	0.50661499	0.00003943	$> 10^{-8}$
64	0.50661211	0.00000288	$> 10^{-8}$
128	0.50661192	0.00000019	$> 10^{-8}$
256	0.50661191	0.00000001	$> 10^{-8}$
512	0.50661191	0.00000000	$\leq 10^{-8}$

- Exercise 43 –

Evaluate the definite integral

$$\int_{1}^{3} \frac{2^{x}}{x^{2} + x + 3} \, \mathrm{d}x$$

- a) using the composite trapezoidal rule for n = 4 and for n = 8, compare the results,
- b) using the composite trapezoidal rule for n = 4 and for n = 8. compare the results, use the MATLAB to solve the problem,
- c) using the composite Simpson's rule for n = 4 and for n = 8, compare the results,

use the MATLAB to solve the problem,

- d) using the composite trapezoidal formula with the given accuracy $\varepsilon = 10^{-4}$, use the MATLAB to solve the problem,
- e) using the composite Simpson's formula with the given accuracy $\varepsilon = 10^{-8}$, use the MATLAB to solve the problem.

6 Numerical solution of ordinary differential equations

The initial-value problem for the ordinary differential equation We find the continuous function y = y(x) that on the interval [a, b] fulfil the differential equation

$$y'(x) = f(x, y(x))$$

and the initial condition

$$y(a)=c.$$

To solve the problem numerically we divide the interval [a, b] into n equidistant subintervals of the length h = (b - a)/n with the nodes $x_0 = a, x_1, x_2, ..., x_n = b$, i.e.

$$x_{i} = a + ih, \quad i = 0, 1, \dots, n.$$

$$h \quad h \quad h \quad h$$

$$x_{0} \quad x_{1} \quad x_{2} \quad x_{3} \quad b = x_{4}$$

To these nodes we assign values $y_0 = c, y_1, y_2, ..., y_n$ that approximate values of the analytical solution $y(x_0), y(x_1), y(x_2), ..., y(x_n)$.

Thus the **numerical solution** of the initial-value problem is a set of n + 1 discrete points $[x_i; y_i]$, i = 0, 1, ..., n.



6.1 Euler method

At first we calculate the nodes

$$x_i = a + ih, \quad i = 0, 1, \dots, n.$$

We consider the differential equation

$$y'(x) = f(x, y(x)),$$

in a node x_i and we replace the accurate value of the solution $y(x_i)$ by its approximation y_i .

Next we approximate the derivative on the left side using the numerical formula

$$y'(x_i) = f(x_i, y(x_i)) \approx \frac{y_{i+1} - y_i}{h} = f(x_i, y_i).$$

If the values x_i , y_i are known, we can calculate an unknown value y_{i+1}

$$\frac{y_{i+1} - y_i}{h} = f(x_i, y_i)$$

$$y_{i+1} - y_i = h \cdot f(x_i, y_i)$$

$$y_{i+1} = y_i + h \cdot f(x_i, y_i)$$

The initial value y_0 is given by the initial condition and the other values y_{i+1} we can calculate by the derived formula.

$$y_0 = c$$

for $i = 0, \dots, n-1$
$$y_{i+1} = y_i + hf(x_i, y_i),$$

Example 44 ———

Solve the initial-value problem

 $y' = x^2 - 0.2y, \quad y(-2) = -1$

on the interval [-2, 3] using the Euler method with the step h = 1.

At first we specify the number *n* of subintervals into which we divide the given interval [a,b]

$$n = \frac{b-a}{h} = \frac{3-(-2)}{1} = 5$$

Then we calculate the nodes:

$$x_{0} = a = -2$$

$$x_{1} = a + h = -2 + 1 = -1$$

$$x_{2} = a + 2h = -2 + 2 = 0$$

$$x_{3} = a + 3h = 1$$

$$x_{4} = a + 4h = 2$$

$$x_{5} = a + 5h = 3$$

The value $y_0 = -1$ is given by the initial condition, other values y_i for i = 1, ..., 5 can be calculated by the formula $y_{i+1} = y_i + hf(x_i, y_i)$. There it holds $f(x, y) = x^2 - 0.2y$ and h = 1, so the computational formula is of the form:

$$y_{i+1} = y_i + x_i^2 - 0.2y_i$$

$y_0 = -1$	(given initial value)
$y_1 = y_0 +$	$hf(x_0, y_0) = y_0 + x_0^2 - 0.2y_0 = -1 + (-2)^2 - 0.2 \cdot (-1) = 3.2$
$y_2 = y_1 +$	$hf(x_1, y_1) = y_1 + x_1^2 - 0.2y_1 = 3.2 + (-1)^2 - 0.2 \cdot 3.2 = 3.56$
$y_3 = y_1 +$	$hf(x_2, y_2) = y_2 + x_2^2 - 0.2y_2 = 2.848$
$y_4 = y_1 +$	$hf(x_3, y_3) = y_3 + x_3^2 - 0.2y_3 = 3.2784$
$y_5 = y_1 +$	$hf(x_4, y_4) = y_4 + x_4^2 - 0.2y_4 = 6.6227$

In the end we write the calculated values of the obtained numerical solution of the initialvalue problem to a table

x_i	-2	-1	0	1	2	3
y_i	-1	3.2	3.56	2.848	3.2784	6.6227

and plot the graph of this numerical solution:



Example 45 –

Solve the initial-value problem

$$y' = x^2 - 0.2y, \quad y(-2) = -1$$

on the interval [-2, 3] using the Euler method with the step h = 1. Use the MATLAB to solve the problem.

```
>> a=-2; b=3; c=-1;
>> f=@(x,y)(x.^2-0.2*y);
>> h=1; n=(b-a)/h;
>> x=a:h:b;
>> y(1)=c;
>> for i=1:n, y(i+1)=y(i)+h*f(x(i),y(i)); end
>> [x;y]
>> plot(x,y,'b.-')
```

6.2 Heun method

The equidistant nodes are the same as for the Euler method, i.e.

$$x_i = a + ih, i = 0, 1, \dots, n.$$

The value y_0 is also given by the initial condition $y_0 = c$.

The method principle is that for every i = 0, ..., n - 1 the value y_i is already known and the value y_{i+1} is to be found. In contrast to the Euler method, in each step we first have to evaluate auxiliary constants k_1, k_2 and next we calculate the value y_{i+1} from these:

$$y_0 = c$$

for $i = 0, ..., n - 1$
 $k_1 = hf(x_i, y_i)$
 $k_2 = hf(x_i + h, y_i + k_1)$
 $y_{i+1} = y_i + \frac{1}{2}(k_1 + k_2)$

- Example 46 —

Solve the initial-value problem

$$y' = x^2 - 0.2y, \quad y(-2) = -1$$

on the interval [-2, 3] using the Heun method with the step h = 1.

At first we calculate the number of subintervals into which we divide the given interval [a, b]

$$n = \frac{b-a}{h} = \frac{3-(-2)}{1} = 5$$

and the nodes

$$x_{0} = a = -2$$

$$x_{1} = a + h = -2 + 1 = -1$$

$$x_{2} = a + 2h = -2 + 2 = 0$$

$$x_{3} = a + 3h = 1$$

$$x_{4} = a + 4h = 2$$

$$x_{5} = a + 5h = 3$$
.

The initial condition determine the value $y_0 = -1$. In following steps we first evaluate constants k_1 , k_2 and using these we calculate the required value y_{i+1} .

 $y_0 = -1$ (initial condition)

Since it holds $f(x, y) = x^2 - 0.2y$ and h = 1 in this example, the calculations look like as follows:

for
$$i = 0$$

 $k_1 = hf(x_0, y_0) = 1 \cdot ((-2)^2 - 0.2 \cdot (-1)) = 4.2$
 $k_2 = hf(x_0 + h, y_0 + k_1) = 1 \cdot ((-2 + 1)^2 - 0.2 \cdot (-1 + 4.2)) = 0.36$
 $y_1 = y_0 + \frac{1}{2}(k_1 + k_2) = -1 + \frac{1}{2}(4.2 + 0.36) = 1.28$

for
$$i = 1$$

$$k_{1} = hf(x_{1}, y_{1}) = 1 \cdot ((-1)^{2} - 0.2 \cdot 1.28) = 0.744$$

$$k_{2} = hf(x_{1} + h, y_{1} + k_{1}) = 1 \cdot ((-1 + 1)^{2} - 0.2 \cdot (1.28 + 0.744)) = -0.4048$$

$$y_{2} = y_{1} + \frac{1}{2}(k_{1} + k_{2}) = 1.28 + \frac{1}{2}(0.744 + (-0.4048)) = 1.4496$$
for $i = 2$

$$k_{1} = hf(x_{2}, y_{2}) = -0.2899$$

$$k_{2} = hf(x_{2} + h, y_{2} + k_{1}) = 0.7681$$

$$y_{3} = y_{2} + \frac{1}{2}(k_{1} + k_{2}) = 1.6887$$
for $i = 3$

$$k_{1} = hf(x_{3}, y_{3}) = 0.6623$$

$$k_{2} = hf(x_{3} + h, y_{3} + k_{1}) = 3.5298$$

$$y_{4} = y_{3} + \frac{1}{2}(k_{1} + k_{2}) = 3.7847$$
for $i = 4$

$$k_{1} = hf(x_{4}, y_{4}) = 3.2431$$

$$k_{2} = hf(x_{4} + h, y_{4} + k_{1}) = 7.5944$$

$$y_{5} = y_{4} + \frac{1}{2}(k_{1} + k_{2}) = 9.2035$$

We write the obtained numerical solution values to a table:

x_i	-2	-1	0	1	2	3
y_i	-1	1.2800	1.4496	1.6887	3.7847	9.2035

- Example 47 —

Solve the initial-value problem

$$y' = x^2 - 0.2y, \quad y(-2) = -1$$

on the interval [-2, 3] using the Heun method with the step h = 1. Use the MATLAB to solve the problem.

```
>> a=-2; b=3; c=-1;
>> f=@(x,y)(x.^2-0.2*y);
>> h=1; n=(b-a)/h;
>> x=a:h:b;
>> y(1)=c;
>> for i=1:n,
    k1=h*f(x(i),y(i));
    k2=h*f(x(i+1),y(i)+k1);
    y(i+1)=y(i)+1/2*(k1+k2);
end
```

6.3 Runge-Kutta method RK4

The equidistant nodes are the same as before, i.e.

$$x_i = a + ih, i = 0, 1, \dots, n$$

and the value y_0 is again determined by the initial condition $y_0 = c$.

The method principle is that for every i = 0, ..., n - 1 the value y_i is already known and the value y_{i+1} is to be found. Analogous to the Heun method, in each step we first have to evaluate auxiliary constants k_1, k_2, k_3, k_4 and next we calculate the value y_{i+1} from these:

for
$$i = 0, ..., n - 1$$

$$y_0 = c$$

$$k_1 = hf(x_i, y_i)$$

$$k_2 = hf(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_1)$$

$$k_3 = hf(x_i + \frac{1}{2}h, y_i + \frac{1}{2}k_2)$$

$$k_4 = hf(x_i + h, y_i + k_3)$$

$$y_{i+1} = y_i + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4)$$

Example 48 –

Solve the initial-value problem

$$y' = y - x^2 + 2$$
, $y(0) = -1$

on the interval [0, 2] using the Runge-Kutta method RK4 with the step h = 0.5.

We calculate the number of subintervals into which we divide the given interval [a, b]

$$n = \frac{b-a}{h} = \frac{2-0}{0.5} = 4$$

and the nodes

$$x_{0} = a = 0$$

$$x_{1} = a + h = 0 + 0.5 = 0.5$$

$$x_{2} = a + 2h = 0 + 1 = 1$$

$$x_{3} = a + 3h = 1 + 1.5 = 1.5$$

$$x_{4} = a + 4h = 0 + 2$$

The initial condition determine the value $y_0 = -1$. In consequent steps we first evaluate constants k_1, k_2, k_3, k_4 and using these we calculate the required value y_{i+1} .

 $y_0 = -1$ (initial condition)

Since it holds $f(x, y) = y - x^2 + 2$ and h = 0.5 in this example, the calculations look like as follows:

for
$$i = 0$$

 $k_1 = hf(x_0, y_0) = 0.5$
 $k_2 = hf(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}k_1) = 0.5938$
 $k_3 = hf(x_0 + \frac{1}{2}h, y_0 + \frac{1}{2}k_2) = 0.6172$
 $k_4 = hf(x_0 + h, y_0 + k_3) = 0.6836$
 $y_1 = y_0 + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) =$
 $= -1 + \frac{1}{6}(0.5 + 2 \cdot 0.5938 + 2 \cdot 0.6172 + 0.6836) = -0.3991$
for $i = 1$
 $k_1 = hf(x_1, y_1) = 0.6755$
 $k_2 = hf(x_1 + \frac{1}{2}h, y_1 + \frac{1}{2}k_2) = 0.6912$
 $k_4 = hf(x_1 + h, y_1 + k_3) = 0.6461$
 $y_2 = y_1 + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) = 0.2809$
for $i = 2$
 $k_1 = hf(x_2, y_2) = 0.6405$
 $k_2 = hf(x_2 + \frac{1}{2}h, y_2 + \frac{1}{2}k_2) = 0.4890$
 $k_4 = hf(x_2 + h, y_2 + k_3) = 0.2600$
 $y_3 = y_2 + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) = 0.7671$
for $i = 3$
 $k_1 = hf(x_2, y_2) = 0.2586$
 $k_2 = hf(x_3 + \frac{1}{2}h, y_3 + \frac{1}{2}k_2) = -0.1684$
 $k_4 = hf(x_3 + h, y_3 + k_3) = -0.7007$
 $y_4 = y_3 + \frac{1}{6}(k_1 + 2k_2 + 2k_3 + k_4) = 0.6096$

We write the obtained numerical solution to a table

x_i	0	0.5	1	1.5	2
y_i	-1	-0.3991	0.2809	0.7671	0.6096

and plot this solution graph:



– Example 49 –

Solve the initial-value problem

$$y' = y - x^2 + 2$$
, $y(0) = -1$

on the interval [0, 2] using the Runge-Kutta method RK4 with the step h = 0.5. Use the MATLAB to solve the problem.

```
>> a=0; b=2; c=-1;
>> f=@(x,y)(y-x.^2+2);
>> h=0.5; n=(b-a)/h;
>> x=a:h:b;
>> y(1)=c;
>> for i=1:n
k1=h*f(x(i),y(i))
k2=h*f(x(i)+h/2,y(i)+1/2*k1);
k3=h*f(x(i)+h/2,y(i)+1/2*k2);
k4=h*f(x(i)+h,y(i)+k3);
y(i+1)=y(i)+1/6*(k1+2*k2+2*k3+k4);
end
```

– Exercise 50 –

Solve the initial-value problem

$$y' = \frac{3y - 2x}{x + y}, \ y(3) = 2$$

on the interval [3,6]

- a) using the Euler method with the step h = 0.5,
- b) using the Euler method with the step h = 0.5, use the MATLAB to solve the problem,
- c) using the Heun method with the step h = 0.5, use the MATLAB to solve the problem,
- d) using the Runge-Kutta method RK4 with the step h = 0.5, use the MATLAB to solve the problem,
- e) using the Euler method and the Runge-Kutta method RK4 both with the same step h = 0.5, compare values of both numerical solutions in a table as well as graphically, use the MATLAB to solve the problem.

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