# 1 Examples for Lectures 1-5

- These are some additional exercises to what we have done and explained at the laboratory.
- I did not include all the theory, in many parts I just wrote where you can find it in the lectures please read it before solving these examples.
- These exercises focus on the algorithms you should use. I did not include many examples regarding the approximation errors, remainder, etc. You can find these in your lectures.
- You also have other similar exercises solved in the lectures I indicated where you can find them.

**Example 1.1** Write the **Taylor polynomial of order** n around  $x_0 = 0$ , for the function  $f: (-1, \infty) \to \mathbb{R}$ ,  $f(x) = \ln(1+x)$ . What is the **error of the Taylor approximation**?

• For theory, see Lecture 1, pp. 1–3. For Taylor's formula in two dimensions, see pp. 4–5.

The Taylor polynomial of order n is defined as

$$T_n f(x) = \sum_{k=0}^n \frac{(x-x_0)^k}{k!} f^{(k)}(x_0) = f(x_0) + \frac{(x-x_0)}{1!} f'(x_0) + \frac{(x-x_0)^2}{2!} f''(x_0) + \dots + \frac{(x-x_0)^n}{n!} f^{(n)}(x_0).$$
 (1.1)

The error of approximation is

$$R_{n+1}(x) = \frac{(x-x_0)^{n+1}}{(n+1)!} f^{(n+1)}(\xi), \text{ with } \xi \text{ between } x \text{ and } x_0.$$
 (1.2)

We first need to find the kth order derivative of  $f(x) = \ln(1+x)$ .

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

$$f''(x) = (-1) \cdot (1+x)^{-2}$$

$$f'''(x) = (-1)(-2) \cdot (1+x)^{-3}$$

$$f^{(4)}(x) = (-1)(-2)(-3) \cdot (1+x)^{-4}$$
...
$$f^{(n)}(x) = (-1)^{n-1}(n-1)! \cdot (1+x)^{-n}, \ n \ge 1.$$

In our formula, we need the values of the derivatives at  $x_0 = 0$ , so it becomes

$$f^{(n)}(0) = (-1)^{n-1}(n-1)!, n \ge 1 \text{ and } f(0) = \ln(1) = 0.$$

We have the polynomial:

$$T_n f(x) = 0 + \frac{x}{1!} \cdot 0! - \frac{x^2}{2!} \cdot 1! + \frac{x^3}{3!} \cdot 2! - \frac{x^4}{4!} \cdot 3! + \dots + (-1)^{n-1} \frac{x^n}{n!} \cdot (n-1)!$$
$$= x - \frac{x^2}{2} + \frac{x^3}{3} - \frac{x^4}{4} + \dots + (-1)^{n-1} \frac{x^n}{n}$$

and the error of approximation:

$$R_{n+1}(x) = (-1)^n \frac{x^{n+1}}{(n+1)!} \cdot n! (1+\xi)^{-(n+1)} = (-1)^n \frac{x^{n+1}}{n+1} \cdot (1+\xi)^{-(n+1)} \text{ with } \xi \text{ between } x \text{ and } 0.$$

Example 1.2 Compute the finite difference table for the following given data

• For theory, see Lecture 2, pp. 8–9.

Since nothing is specified, we consider 'forward differences' (Lect. 2, Remark 4.11, pp. 9).

The "maximum order" for the finite difference table is nr. points -1, so, in our case it is 4. (we have 5 data). On the *first column*, we should put *the function's values*, in our case y.

у	$\Delta^1 y$	$\Delta^2 y$	$\Delta^3 y$	$\Delta^4 y$
$y_0 = 4$	$y_1 - y_0 = 13 - 4 = 9$	$\Delta^1 y_1 - \Delta^1 y_0 = 21 - 9 = 12$		
$y_1$ =13	$y_2 - y_1 = 34 - 13 = 21$	$\Delta^1 y_2 - \Delta^1 y_1 = 39 - 21 = 18$	$\Delta^2 y_2 - \Delta^2 y_1 = 24 - 18 = 6$	
$y_2 = 34$	$y_3 - y_2 = 73 - 34 = 39$	$\Delta^1 y_3 - \Delta^1 y_2 = 63 - 39 = 24$		
$y_3$ =73	$y_4 - y_3 = 136 - 73 = 63$			
$y_4 = 136$				

Example 1.3 Compute the backward difference table for the following given data

• For theory, see Lecture 2, pp. 8–9.

The "maximum order" for the finite difference table is nr. points -1, so, in our case it is 4. (we have 5 data). On the first column, we should put the function's values, in our case y.

У	$\nabla^1 y$	$\nabla^2 y$	$\nabla^3 y$	$\nabla^4 y$
4				
13	13-4=9			
34	34 - 13 = 21	21-9 = 12		
73	73 - 34 = 39	39-21 = 18	18-12=6	
136	136-73=63	63-39 = 24	24-18=6	6-6=0

Remark 1.4 For finite differences, the nodes should be equidistant.

Example 1.5 Compute the divided difference table for the following given data

• For theory, see Lecture 2, pp. 1–2.

The "maximum order" for the divided difference table is nr. points -1, so, in our case it is 3. (we have 4 data). On the *first column*, we should put the nodes (x), on the second column, we should put the values of the function on the nodes (f).

$x_i$	$f_i$	$\mathcal{D}_1 f_i$	$\mathcal{D}_2 f_i$	$\mathcal{D}_3 f_i$
$x_0 = 0$	1	$\frac{f_1 - f_0}{x_1 - x_0} = \frac{3 - 1}{1 - 0} = 2$	$\frac{\mathcal{D}_1 f_1 - \mathcal{D}_1 f_0}{x_2 - x_0} = \frac{23 - 2}{3 - 0} = 7$	$\frac{\mathcal{D}_2 f_1 - \mathcal{D}_2 f_0}{x_3 - x_0} = \frac{19 - 7}{4 - 0} = 3$
$x_1 = 1$	3	$\frac{f_2 - f_1}{x_2 - x_1} = \frac{49 - 3}{3 - 1} = 23$	$\frac{\mathcal{D}_1 f_2 - \mathcal{D}_1 f_1}{x_3 - x_1} = \frac{80 - 23}{4 - 1} = 19$	
$x_2 = 3$	49	$\frac{f_3 - f_2}{x_3 - x_2} = \frac{129 - 49}{4 - 3} = 80$	<b>V</b> 1	
$x_3 = 4$	129	_		

**Remark 1.6** For the 1st order  $(\mathcal{D}_1)$ , you divide by the difference of consecutive nodes  $(x_1 - x_0, x_2 - x_1)$  and so on...). For the 2nd order, you "skip" a node  $(x_2 - x_0, x_3 - x_1,...)$ . Then you "skip" 2 nodes  $(x_3 - x_0)$ , and so on...

**Example 1.7** Compute the divided difference table for the triple nodes  $x_0 = x_1 = x_2 = 0$ , the double nodes  $x_3 = x_4 = 1$  and the function  $f(x) = \arctan(x)$ .

From Lecture 2, pp. 2, Divided difference with multiple nodes, you have the following property:

The divided difference of order n at the node  $x_0$ , of multiplicity (n+1), is defined as

$$f[x_0,...,x_0] = \frac{f^{(n)}(x_0)}{n!}$$
, where  $x_0$  appears (n+1) times in [...].

In our case, since the first three nodes are equal, we will use for them f' and f'' (they have order of multiplicity 3). For the other two nodes, we will use f' (their order of multiplicity is 2). The derivatives of f are:

$$f'(x) = \frac{1}{x^2 + 1}, \quad f''(x) = \frac{-2x}{(x^2 + 1)^2}.$$

Our table becomes:

$$\begin{array}{|c|c|c|c|c|c|c|}\hline x_i & f_i & D_1 & D_2 & D_3 & D_4\\\hline x_0 = 0 & f(0) = 0 & f'(0) = 1 & \frac{f''(0)}{2!} = 0 & \frac{\frac{\pi}{4} - 1 - 0}{1 - 0} = \frac{\pi}{4} - 1 & \frac{\frac{3 - \pi}{2} - \frac{\pi}{4} + 1}{1 - 0} = \frac{10 - 3\pi}{4}\\\hline x_1 = 0 & f(0) = 0 & f'(0) = 1 & \frac{\frac{\pi}{4} - 1}{1 - 0} = \frac{\pi}{4} - 1 & \frac{\frac{1}{2} - \frac{\pi}{4} - \frac{\pi}{4} + 1}{1 - 0} = \frac{3 - \pi}{2}\\\hline x_2 = 0 & f(0) = 0 & \frac{\frac{\pi}{4} - 0}{1 - 0} = \frac{\pi}{4} & \frac{1}{2} - \frac{\pi}{4} & \frac{1}{1 - 0} = \frac{1}{2} - \frac{\pi}{4}\\\hline x_3 = 1 & f(1) = \frac{\pi}{4} & f'(1) = \frac{1}{2}\\\hline x_4 = 1 & f(1) = \frac{\pi}{4} & \end{array}$$

Remark 1.8 The denominator is computed here as usual in a divided difference table (with the rule of skipping nodes). Even if here we have always 1-0, these are not the same nodes - this happens only because the nodes are multiple.

Example 1.9 Compute the Lagrange polynomial for the following data using

#### 1. the fundamental formula

• For theory, see Lecture 2, pp. 11–15.

The fundamental formula for the Lagrange polynomial is:

$$L_n f(x) = \sum_{i=0}^n l_i(x) f(x_i)$$
 (1.3)

considering n+1 interpolation nodes given  $x_i$ , i=0,...,n, and the values of an unknown function f on these nodes,  $f(x_i)$ , i=0,...,n.

Remark 1.10 The values of the polynomial  $L_n f$  on the nodes should be the same as the values of the function!! (this is what interpolation means). So,  $L_n f(x_i) = f(x_i)$ , i = 0, ..., n. (this is how you could check if your computations were correct.)

The fundamental interpolation polynomials  $l_i$  are defined as

$$l_i(x) = \prod_{j=0, j\neq i}^n \frac{x - x_j}{x_i - x_j} = \frac{(x - x_0)(x - x_1) \cdot \dots \cdot (x - x_{i-1})(x - x_{i+1}) \cdot \dots \cdot (x - x_n)}{(x_i - x_0)(x_i - x_1) \cdot \dots \cdot (x_i - x_{i-1})(x_i - x_{i+1}) \cdot \dots \cdot (x_i - x_n)}$$

**Remark 1.11** On the numerator, the term  $(x-x_i)$  is missing, on the denominator the term  $(x_i-x_i)$  is missing!

So, in our case  $x_0 = 3$ ,  $x_1 = 4$ ,  $x_2 = 5$  and  $f(x_0) = 1$ ,  $f(x_1) = 2$ ,  $f(x_2) = 4$ . For  $l_0(x)$ , the terms that contain  $x_0$  will be missing from the numer. and denom.

$$l_0(x) = \frac{(x-x_1)(x-x_2)}{(x_0-x_1)(x_0-x_2)} = \frac{(x-4)(x-5)}{(3-4)(3-5)} = \frac{x^2-9x+20}{2}$$

For  $l_1(x)$ , the terms that contain  $x_1$  will be missing from the numer. and denom.

$$l_1(x) = \frac{(x-x_0)(x-x_2)}{(x_1-x_0)(x_1-x_2)} = \frac{(x-3)(x-5)}{(4-3)(4-5)} = \frac{x^2-8x+15}{-1} = -x^2+8x-15$$

For  $l_2(x)$ , the terms that contain  $x_2$  will be missing from the numer. and denom.

$$l_2(x) = \frac{(x-x_0)(x-x_1)}{(x_2-x_0)(x_2-x_1)} = \frac{(x-3)(x-4)}{(5-3)(5-4)} = \frac{x^2-7x+12}{2}$$

Now we substitute them in the eq. (1.3), for n = 2 and get

$$L_2f(x) = l_0(x) \cdot f(x_0) + l_1(x) \cdot f(x_1) + l_2(x) \cdot f(x_2) =$$

$$= \frac{x^2 - 9x + 20}{2} \cdot 1 + (-x^2 + 8x - 15) \cdot 2 + \frac{x^2 - 7x + 12}{2} \cdot 4 =$$

$$= \frac{x^2 - 9x + 20 - 4x^2 + 32x - 60 + 4x^2 - 28x + 48}{2} =$$

$$= \frac{x^2 - 5x + 8}{2}.$$

**Remark 1.12** To approximate f(3.5) using this polynomial, you simply have to compute

$$L_2f(3.5) = \frac{(3.5)^2 - 5 \cdot (3.5) + 8}{2} = \dots$$

## 2. the barycentric formula

• For theory, see Lecture 3, pp. 1–2.

The first barycentric formula for the Lagrange polynomial is

$$L_n f(x) = u(x) \sum_{i=0}^n \frac{w_i}{x - x_i} f(x_i),$$
 (1.4)

with

$$u(x) = \prod_{j=0}^{n} (x - x_j)$$
 and  $w_i = \frac{1}{u_i(x_i)} = \frac{1}{\prod_{j=0, j \neq i}^{n} (x_i - x_j)}$ .

First, let us compute u(x):

$$u(x) = (x - x_0)(x - x_1)(x - x_2) = (x - 3)(x - 4)(x - 5)$$
:

Now, let us compute the weights  $w_0, w_1, w_2$ :

$$w_0 = \frac{1}{(x_0 - x_1)(x_0 - x_2)} \text{ (the term } (x_0 - x_0) \text{ is missing), so } w_0 = \frac{1}{(3 - 4)(3 - 5)} = \frac{1}{2}.$$

$$w_1 = \frac{1}{(x_1 - x_0)(x_1 - x_2)} \text{ (the term } (x_1 - x_1) \text{ is missing), so } w_1 = \frac{1}{(4 - 3)(4 - 5)} = -1.$$

$$w_2 = \frac{1}{(x_2 - x_0)(x_2 - x_1)} \text{ (the term } (x_2 - x_2) \text{ is missing), so } w_2 = \frac{1}{(5 - 3)(5 - 4)} = \frac{1}{2}.$$

We also need  $\frac{w_i}{x-x_i}$ , so

$$\frac{w_0}{x-x_0} = \frac{\frac{1}{2}}{x-3} = \frac{1}{2(x-3)}, \quad \frac{w_1}{x-x_1} = -\frac{1}{x-4}, \quad \frac{w_2}{x-x_2} = \frac{1}{2(x-5)}.$$

We obtain:

$$L_2f(x) = (x-3)(x-4)(x-5) \left[ \frac{1}{2(x-3)} \cdot 1 - \frac{1}{x-4} \cdot 2 + \frac{1}{2(x-5)} \cdot 4 \right]$$

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

$$= \frac{x^2 - 9x + 20 - 4x^2 + 32x - 60 + 4x^2 - 28x + 48}{2} = \frac{x^2 - 5x + 8}{2}$$

as we obtained with the fundamental formula.

The second barycentric formula for the Lagrange polynomial is

$$L_n f(x) = \frac{\sum_{i=0}^{n} \frac{w_i}{x - x_i} f(x_i)}{\sum_{i=0}^{n} \frac{w_i}{x - x_i}},$$
(1.5)

with

$$w_i = \frac{1}{u_i(x_i)} = \frac{1}{\prod\limits_{j=0, j\neq i}^{n} (x_i - x_j)}.$$

First, let us compute  $w_0$ ,  $w_1$ ,  $w_2$ :

$$w_0 = \frac{1}{(x_0 - x_1)(x_0 - x_2)} \text{ (the term } (x_0 - x_0) \text{ is missing), so } w_0 = \frac{1}{(3 - 4)(3 - 5)} = \frac{1}{2}.$$

$$w_1 = \frac{1}{(x_1 - x_0)(x_1 - x_2)} \text{ (the term } (x_1 - x_1) \text{ is missing), so } w_1 = \frac{1}{(4 - 3)(4 - 5)} = -1.$$

$$w_2 = \frac{1}{(x_2 - x_0)(x_2 - x_1)} \text{ (the term } (x_2 - x_2) \text{ is missing), so } w_2 = \frac{1}{(5 - 3)(5 - 4)} = \frac{1}{2}.$$

We also need  $\frac{w_i}{x-x_i}$ , so

$$\frac{w_0}{x-x_0} = \frac{\frac{1}{2}}{x-3} = \frac{1}{2(x-3)}, \quad \frac{w_1}{x-x_1} = -\frac{1}{x-4}, \quad \frac{w_2}{x-x_2} = \frac{1}{2(x-5)}.$$

The numerator is

$$N = \frac{w_0}{x - x_0} \cdot f(x_0) + \frac{w_1}{x - x_1} \cdot f(x_1) + \frac{w_2}{x - x_2} \cdot f(x_2) =$$

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

$$= \frac{x^2 - 5x + 8}{2(x - 3)(x - 4)(x - 5)}.$$

The denominator is

$$M = \frac{w_0}{x - x_0} + \frac{w_1}{x - x_1} + \frac{w_2}{x - x_2} = \frac{1}{2(x - 3)} - \frac{1}{x - 4} + \frac{1}{2(x - 5)} =$$

$$= \frac{(x - 4)(x - 5) - 2(x - 3)(x - 5) + (x - 3)(x - 4)}{2(x - 3)(x - 4)(x - 5)} =$$

$$= \frac{2}{2(x - 3)(x - 4)(x - 5)}.$$

So, with the second barycentric formula  $L_2f(x)$  is

$$L_2f(x) = \frac{N}{M} = \frac{\frac{x^2 - 5x + 8}{2(x - 3)(x - 4)(x - 5)}}{\frac{2}{2(x - 3)(x - 4)(x - 5)}} = \frac{x^2 - 5x + 8}{2},$$

as we previously obtained using the fundamental formula and the first barycentric formula. ©

- For the limit of error of the Lagrange polynomial, see Lecture 2, pp. 15–16.
- For optimal choice of nodes (= roots of Chebyshev polynomial of first kind), see Lecture 2, pp. 16–18.
- For an example in which the Lagrange polynomial does not converge, see Lecture 2, pp. 18–19 (Runge's example).

**Example 1.13** Use the Neville's method to approximate f(3) using the data

• For theory, see Lecture 3, pp. 11–14 and for another example, see Lecture 3, pp. 15–16.

We have to construct the table

$$\begin{array}{c|ccccc} x_0 & P_{00} & & & & \\ x_1 & P_{10} & P_{11} & & & \\ x_2 & P_{20} & P_{21} & P_{22} & & \\ x_3 & P_{30} & P_{31} & P_{32} & \mathbf{P_{33}} \end{array}$$

where 
$$P_{i,0} = f(x_i)$$
,  $i = 0, ..., n$  and  $P_{i,j} = \frac{1}{x_i - x_{i-j}} \begin{vmatrix} x - x_{i-j} & P_{i-1,j-1} \\ x - x_i & P_{i,j-1} \end{vmatrix}$   $i \ge j > 0$ . We have  $x_0 = 0, x_1 = 1, x_2 = 2, x_3 = 4$ .

In our case, since we want to approx. f(3), x=3. The table becomes:

The computations are

$$P_{00} = f(x_0) = 1$$
,  $P_{10} = f(x_1) = 1$ ,  $P_{20} = f(x_2) = 2$ ,  $P_{30} = f(x_3) = 5$ ,

$$P_{11} = \frac{1}{x_1 - x_0} \begin{vmatrix} x - x_0 & P_{00} \\ x - x_1 & P_{10} \end{vmatrix} = 1 \cdot \begin{vmatrix} 3 & 1 \\ 2 & 1 \end{vmatrix} = 1$$

$$P_{21} = \frac{1}{x_2 - x_1} \begin{vmatrix} x - x_1 & P_{10} \\ x - x_2 & P_{20} \end{vmatrix} = 1 \cdot \begin{vmatrix} 2 & 1 \\ 1 & 2 \end{vmatrix} = 3$$

$$P_{31} = \frac{1}{x_3 - x_2} \begin{vmatrix} x - x_2 & P_{20} \\ x - x_3 & P_{30} \end{vmatrix} = \frac{1}{2} \cdot \begin{vmatrix} 1 & 2 \\ -1 & 5 \end{vmatrix} = \frac{7}{2}$$

$$P_{22} = \frac{1}{x_2 - x_0} \begin{vmatrix} x - x_0 & P_{11} \\ x - x_2 & P_{21} \end{vmatrix} = \frac{1}{2} \cdot \begin{vmatrix} 3 & 1 \\ 1 & 3 \end{vmatrix} = 4$$

$$P_{32} = \frac{1}{x_3 - x_1} \begin{vmatrix} x - x_1 & P_{21} \\ x - x_3 & P_{31} \end{vmatrix} = \frac{1}{3} \cdot \begin{vmatrix} 2 & 3 \\ -1 & \frac{7}{2} \end{vmatrix} = \frac{10}{3}$$

$$P_{33} = \frac{1}{x_3 - x_0} \begin{vmatrix} x - x_0 & P_{22} \\ x - x_3 & P_{32} \end{vmatrix} = \frac{1}{4} \cdot \begin{vmatrix} 3 & 4 \\ -1 & \frac{10}{2} \end{vmatrix} = \frac{7}{2}.$$

The approximation for f(3) will be  $P_{33}$ , so,  $\frac{7}{2}$ .

- The Lagrange polynomial of degree n, at the given point  $x = L_n f(x)$  will be the element  $P_{nn}$ .
- You can add a new node, case in which you have to add another row (the previous computations remain the same).

**Example 1.14** Use the **Aitken's method** to approximate f(3) using the data

• For theory, see Lecture 3, pp. 14 and for another example, see see Lecture 3, pp. 16

We have to construct the table

$$\begin{array}{c|ccccc} x_0 & P_{00} & & & & \\ x_1 & P_{10} & P_{11} & & & \\ x_2 & P_{20} & P_{21} & P_{22} & & \\ x_3 & P_{30} & P_{31} & P_{32} & \mathbf{P_{33}} \end{array}$$

where 
$$P_{i0} = f(x_i)$$
,  $i = 0, ..., n$  and  $P_{i,j+1} = \frac{1}{x_i - x_j} \begin{vmatrix} x - x_j & P_{jj} \\ x - x_i & P_{ij} \end{vmatrix}$   $i > j \ge 0$ .

We have  $x_0 = 0$ ,  $x_1 = 1$ ,  $x_2 = 2$ ,  $x_3 = 4$ .

In our case, since we want to approx. f(3), x=3. The table becomes: The computations are:

$$P_{00} = f(x_0) = 1$$
,  $P_{10} = f(x_1) = 1$ ,  $P_{20} = f(x_2) = 2$ ,  $P_{30} = f(x_3) = 5$ .

$$P_{11} = P_{1,0+1} = \frac{1}{x_1 - x_0} \begin{vmatrix} x - x_0 & P_{00} \\ x - x_1 & P_{10} \end{vmatrix} = 1 \cdot \begin{vmatrix} 3 & 1 \\ 2 & 1 \end{vmatrix} = 1$$

$$P_{21} = P_{2,0+1} = \frac{1}{x_2 - x_0} \begin{vmatrix} x - x_0 & P_{00} \\ x - x_2 & P_{20} \end{vmatrix} = \frac{1}{2} \cdot \begin{vmatrix} 3 & 1 \\ 1 & 2 \end{vmatrix} = \frac{5}{2}$$

$$P_{31} = P_{3,0+1} = \frac{1}{x_3 - x_0} \begin{vmatrix} x - x_0 & P_{00} \\ x - x_3 & P_{30} \end{vmatrix} = \frac{1}{4} \cdot \begin{vmatrix} 3 & 1 \\ -1 & 5 \end{vmatrix} = 4$$

$$P_{22} = P_{2,1+1} = \frac{1}{x_2 - x_1} \begin{vmatrix} x - x_1 & P_{11} \\ x - x_2 & P_{21} \end{vmatrix} = 1 \cdot \begin{vmatrix} 2 & 1 \\ 1 & \frac{5}{2} \end{vmatrix} = 4$$

$$P_{32} = P_{3,1+1} = \frac{1}{x_3 - x_1} \begin{vmatrix} x - x_1 & P_{11} \\ x - x_3 & P_{31} \end{vmatrix} = \frac{1}{3} \cdot \begin{vmatrix} 2 & 1 \\ -1 & 4 \end{vmatrix} = 3$$

$$P_{33} = P_{3,2+1} = \frac{1}{x_3 - x_2} \begin{vmatrix} x - x_2 & P_{22} \\ x - x_3 & P_{32} \end{vmatrix} = \frac{1}{2} \cdot \begin{vmatrix} 1 & 4 \\ -1 & 3 \end{vmatrix} = \frac{7}{2}.$$

The approximation for f(3) will be  $P_{33}$ , so,  $\frac{7}{2}$ .

- The Lagrange polynomial of degree n, at the given point  $x = L_n f(x)$  will be the element  $P_{nn}$ .
- You can add a new node, case in which you have to add another row (the previous computations remain the same).
- You can see that  $P_{ii}$  have the same values in both Aitken's and Neville's methods, only the other elements are different. This happens because  $P_{ii}$  is the Lagrange polynomial of degree i and the Lagrange polynomial is unique. All the above methods are just different ways to compute the polynomial, but the result should always be the same!

Example 1.15 Construct the Lagrange polynomial in the Newton form, using divided difference formula for the data  $\frac{x \mid 3 \mid 4 \mid 5}{f \mid 1 \mid 2 \mid 4}$ .

• For theory, see Lecture 3, pp. 3–5. For the remainder's formula and another example, see see Lecture 3, pp. 6–7.

The Newton form of the Lagrange pol. is

$$L_n f(x) = f(x_0) + (x - x_0) \mathcal{D}_1 + (x - x_0)(x - x_1) \mathcal{D}_2 + \dots + (x - x_0)(x - x_1) \dots (x - x_{n-1}) \mathcal{D}_n, \tag{1.6}$$

where  $\mathcal{D}_i = f[x_0, ..., x_i]$  is the divided difference of order i at the nodes  $x_0, ..., x_i$  (in our table  $\mathcal{D}_i = \mathcal{D}_i f_0$ ). You will use only the first row of the divided diff. table to get the required values. First, we have to construct the div. diff. table. So, we have

$$L_2(f) = f(x_0) + (x - x_0) \cdot \mathcal{D}_1 + (x - x_0)(x - x_1) \cdot \mathcal{D}_2$$

$$= 1 + (x - 3) \cdot 1 + (x - 3)(x - 4) \cdot \frac{1}{2} = 1 + x - 3 + \frac{1}{2}x^2 - \frac{7}{2}x + 6 =$$

$$= \frac{1}{2}x^2 - \frac{5}{2}x + 4.$$

Example 1.16 Construct the Lagrange polynomial in the Newton form, using finite differences in both cases - forward and backward, for the data  $\frac{x \mid 3 \mid 4 \mid 5}{f \mid 1 \mid 2 \mid 4}$ .

• For theory and another example, see Lecture 3, pp. 8–11.

#### a) forward differences

Newton's forward difference formula is:

$$L_n f(x) = f_0 + \binom{s}{1} \Delta f_0 + \binom{s}{2} \Delta^2 f_0 + \dots + \binom{s}{n} \Delta^n f_0 \tag{1.7}$$

with

$$f_0 = f(x_0), \quad \Delta^k f_0 = \Delta^{k-1} f_1 - \Delta^{k-1} f_0, \quad x_i = x_0 + ih, \quad i = 0, ..., n, \quad s = \frac{x - x_0}{h}, \quad \binom{s}{k} = \frac{s(s-1)...(s-k+1)}{k!}.$$

Note that the **nodes** should be **equidistant** since we have finite differences!

We construct the finite difference table (forward):

$$\begin{array}{c|cccc} f & \Delta^1 f & \Delta^2 f \\ \hline 1 & 2-1 = 1 & 2-1 = 1 \\ 2 & 4-2 = 2 & 4 \end{array}$$

$$x_0 = 3, \ h = 1 \implies s = \frac{x-3}{1} = x-3, \ n = 2$$

and obtain

$$L_2f(x) = \frac{1}{1} + {s \choose 1} \cdot 1 + {s \choose 2} \cdot 1 = 1 + \frac{s}{1!} + \frac{s(s-1)}{2!}$$
$$= 1 + x - 3 + \frac{(x-3)(x-4)}{2} = \frac{x^2 - 5x + 8}{2}.$$

#### b) backward differences

Newton's backward difference formula is:

$$L_n f(x) = f_n + \binom{s}{1} \nabla f_n + \binom{s+1}{2} \nabla^2 f_n + \dots + \binom{s+n-1}{n} \nabla^n f_n$$
 (1.8)

with

$$f_n = f(x_n), \quad \nabla^k f_n = \nabla^{k-1} f_n - \nabla^{k-1} f_{n-1}, \quad x_i = x_0 + ih, \quad i = 0, ..., n, \quad s = \frac{x - x_n}{h}, \quad \binom{s}{k} = \frac{s(s-1)...(s-k+1)}{k!}$$

Note that the **nodes** again should be **equidistant** to apply this method.

We construct the finite difference table (backward):

$$n = 2$$
,  $x_2 = 5$ ,  $h = 1 \implies s = \frac{x - 5}{1} = x - 5$ 

and obtain

$$L_2f(x) = 4 + {s \choose 1} \cdot 2 + {s+1 \choose 2} \cdot 1 = 1 + \frac{s}{1!} + \frac{s(s+1)}{2!}$$
$$= 4 + 2x - 10 + \frac{(x-5)(x-4)}{2} = \frac{x^2 - 5x + 8}{2}.$$

Example 1.17 Consider the double nodes  $x_0 = -1$  and  $x_1 = 1$ . Consider also f(-1) = -3, f'(-1) = 10, f(1) = 1, f'(1) = 2. Find the Hermite interpolation polynomial using the divided difference table for double nodes.

• For theory, other examples and estimation of the error, see Lecture 4, pp. 1–9. We will use the Newton's divided difference formula here (pp. 4–5).

**Remark 1.18** Hermite interpolation for double nodes can be used only when you know the values of f and f' for all the nodes!

First, we should compute the divided difference table with double nodes.

 $z_0 = x_0$ ,  $z_1 = x_0$ ,  $z_2 = x_1$ ,  $z_3 = x_1$ . You should also double the values of f. The difference appears when you compute the divided difference of first order. At the odd positions you have to put the derivative of f at the corresponding node. The other entries are computed in the usual manner.

Next, we will use the Newton form:

$$H_{2m+1}f(x) = f(z_0) + \sum_{i=1}^{2m+1} (x - z_0) \cdot \dots \cdot (x - z_{i-1}) \mathcal{D}_i, \tag{1.9}$$

with  $\mathcal{D}_i = \mathcal{D}_i f_0 = f[x_0, ..., x_i]$ , that is in our case

$$H_3f(x) = -3 + (x - z_0) \cdot \mathcal{D}_1 + (x - z_0)(x - z_1) \cdot \mathcal{D}_2 + (x - z_0)(x - z_1)(x - z_2) \cdot \mathcal{D}_3 =$$

$$= -3 + (x + 1) \cdot 10 + (x + 1)^2 \cdot (-4) + (x + 1)^2(x - 1) \cdot 2$$

$$= -3 + 10x + 10 - 4x^2 - 8x - 4 + 2x^3 - 2x^2 + 4x^2 - 4x + 2x - 2 =$$

$$= 2x^3 - 2x^2 + 1.$$

**Remark 1.19** A good way to check if your computations were right is by checking the interpolation conditions. Here, the polynomial  $H_3f$  should satisfy the following conditions:

$$H_3f(-1) = f(-1) = -3$$
,  $H_3f(1) = f(1) = 1$ ,  $H_3'f(-1) = f'(-1) = 10$ ,  $H_3'f(1) = f(1) = 2$ .

Indeed, they are all satisfied.

Example 1.20 Construct the interpolation polynomial that approximates the data

We first should decide what interpolation problem we have (Lagrange, Hermite, Birkhoff).

We have  $x_0 = -1$ ,  $x_1 = 1$ ,  $f(x_0) = 2$ ,  $f(x_1) = 2$ ,  $f'(x_0) = -4$ . We have some information about the derivative of f, we cannot use Lagrange interpolation, so we are left with either Hermite or Birkhoff. Since no derivative's order is skipped for the 2 nodes (we have f(-1),  $f'(-1) \rightarrow max$ . order for derivative is 1 and we have  $f(1) \rightarrow max$ . order is 0), we have to use **Hermite interpolation**. (The derivative's

maximum order doesn't have to be the same for each node. It is important not to skip any order from 0 to the max.).

We can still use the method of Newton's divided difference, but in this case only the first node is doubled (for the first node we know the values of f and f').

$$\begin{array}{|c|c|c|c|c|c|}\hline z_i & f_i & \mathcal{D}_1 f_i & \mathcal{D}_2 f_i \\ \hline z_0 = -1 & f(-1) = 2 & f'(-1) = -4 & \frac{\mathcal{D}_1 f_1 - \mathcal{D}_1 f_0}{z_2 - z_0} = \frac{0 - (-4)}{1 - (-1)} = 2 \\ \hline z_1 = -1 & f(-1) = 2 & \frac{f(1) - f(-1)}{z_2 - z_1} = \frac{2 - 2}{1 - (-1)} = 0 \\ \hline z_2 = 1 & f(1) = 2 & \hline \end{array}$$

Using Newton's form we get:

$$H_2f(x) = 2 + (x - z_0) \cdot (-4) + (x - z_0)(x - z_1) \cdot 2 = 2 - 4(x + 1) + 2(x + 1)^2 = 2x^2$$

Indeed, this polynomial satisfies the interpolation properties:

$$H_2f(-1) = 2 = f(-1), \quad H'_2f(-1) = -4 = f'(-1), \quad H_2f(1) = 2 = f(1).$$

**Remark 1.21** To approximate f(0) and f'(0), you compute  $H_2f(0) = 2 \cdot 0^2 = 0$  and  $H'_2f(0) = 4 \cdot 0 = 0$ .

**Remark 1.22** Newton form can also be used for other multiplicities of the nodes - pay attention at how you compute the divided difference table in that case (see Example 1.7).

#### Remark 1.23 Hermite polynomial is unique!

For other examples and estimations of the errors, see Lecture 4. There are other ways to compute Hermite polynomials:

- general case see Lecture 4, Theorem 1.6, Remark 1.7, pp. 10–11 with Hermite fundamental polynomials, given by relations (1.11), (1.12), (1.13);
- double nodes see Lecture 4, Theorem 1.1, pp. 2 with Hermite fundamental polynomials, given by relations (1.3), (1.4);
- cubic Hermite polynomial see Lecture 4, Example 1.2, pp. 3-4 for 2 double nodes.

**Example 1.24** Approximate  $f(\frac{1}{2})$  knowing the following information:  $x_0 = 0$ ,  $x_1 = 1$ ,  $f(x_0) = 1$ ,  $f'(x_0) = 2$  and  $f'(x_1) = -1$ .

Again, let's decide the interpolation problem we have. Since for  $x_1$  the value of f is missing, we cannot use Hermite interpolation, so we have to use **Birkhoff interpolation**.

In general, for m+1 given nodes,  $x_k$ , k=0,...,m, the max. degree of the polynomial is  $n=|I_0|+|I_1|+...+|I_m|-1$ , where  $|I_k|$  is the number of elements of  $I_k$  and  $I_k$  is the set that contains all the derivative's orders that are known for the node  $x_k$ .

In our case,  $I_0 = \{0,1\}$  (for  $x_0$  we know the val. for f and f')  $I_1 = \{1\}$  (for  $x_1$  we know only f'). So, the **max. degree of the Birkhoff pol.** is

$$n = |I_0| + |I_1| - 1 = 2 + 1 - 1 = 2.$$

This means that we will have a polynomial P of max. degree n = 2. First, in the Birkhoff case, we should check that the problem has a unique solution (Lagrange and Hermite polynomials have a unique solution, but Birkhoff does not have a solution all the time).

For this, let us denote  $P(x) = ax^2 + bx + c$  our polynomial. We will also need its derivative, P'(x) = 2ax + b. The polynomial P should satisfy the interpolation conditions

$$P(x_0) = f(x_0), P'(x_0) = f'(x_0), P'(x_1) = f'(x_1)$$
 (1.10)

which gives us

$$\begin{cases} a \cdot 0^2 + b \cdot 0 + c &= 1 \\ 2a \cdot 0 + b &= 2 \\ 2a \cdot 1 + b &= -1 \end{cases}$$
 (1.11)

The determinant below tells us if we have a unique solution  $(\neq 0)$ . It is constructed using the coefficients of the unknowns a, b, c, of the system (1.11) (as usual in a problem for linear systems)

$$\begin{vmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 2 & 1 & 0 \end{vmatrix} = -2 \neq 0$$

so we have a unique solution.

Now, the first method to obtain the Birkhoff polynomial is by solving the above system to find the coefficients a, b, c. From the second eq. we get b = 2, from the third eq. we get  $a = -\frac{3}{2}$  and from the first eq. we get c = 1, so our polynomial is

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

Indeed, all the interpolation conditions (1.10) are satisfied. To approximate  $f(\frac{1}{2})$ , we have to compute  $P(\frac{1}{2}) = -\frac{3}{8} + 1 + 1 = \frac{13}{8}$ .

Another method to solve the problem is by computing the Birkhoff polynomial in a more general way. For this, consider the following expression

$$B_n f(x) = \sum_{k=0}^{m} \sum_{j \in I_k} b_{kj}(x) \cdot f^{(j)}(x_k)$$

for m+1 nodes  $x_k$ , k=0,...,m, with  $f^{(j)}(x_k)$  denoting the derivative of order j of function f at the node  $x_k$  and the Birkhoff fundamental polynomials  $b_{kj}$  to be determined from the following properties:

$$\begin{split} b_{kj}^{(p)}(x_{\nu}) &= 0, \text{ when } k \neq \nu, \ p \in I_{\nu} \\ b_{kj}^{(p)}(x_{k}) &= \delta_{jp}, \text{ when } p \in I_{k}, \ j \in I_{k}, \text{ and } \nu, k = 0, ..., m \\ \delta_{jp} &= 0 \ (j \neq p) \text{ and } 1 \ (j = p). \end{split}$$

For example (not for our problem, but in general):

 $b_{01}(x_1) = 0$  (because  $0 \neq 1$ ).

 $b_{11}(x_1) = 0$  (we have 1 = 1, but  $b_{11}(x_1) = b_{11}^{(0)}(x_1)$  and  $0 \neq 1$ ).

 $b'_{11}(x_1) = 1$  (because 1=1 and 1=1).

In our case, we have

$$B_2f(x) = \sum_{k=0}^{1} \sum_{j \in I_k} b_{kj}(x) \cdot f^{(j)}(x_k) = b_{00}(x) \cdot f(x_0) + b_{01}(x) \cdot f'(x_0) + b_{11}(x) \cdot f'(x_1)$$
(1.12)

The unknowns here are the polynomials  $b_{00}$ ,  $b_{01}$  and  $b_{11}$ . Since the Birkhoff pol. should have the max. degree 2, we will write each of these 3 polynomials as a second degree pol.  $(ax^2 + bx + c)$  and determine the coeffs. a, b, c in each case, by using the fundamental properties:

•  $b_{00}(x) = ax^2 + bx + c$  and  $b'_{00}(x) = 2ax + b$ 

$$\begin{cases} b_{00}(x_0) = 1 \\ b'_{00}(x_0) = 0 \\ b'_{00}(x_1) = 0 \end{cases} \implies \begin{cases} b_{00}(0) = c = 1 \\ b'_{00}(0) = b = 0 \\ b'_{00}(1) = 2a + b = 0 \implies a = 0 \end{cases}$$
$$\implies b_{00}(x) = 1.$$

•  $b_{01}(x) = ax^2 + bx + c$  and  $b'_{01}(x) = 2ax + b$ 

$$\begin{cases} b_{01}(x_0) = 0 \\ b'_{01}(x_0) = 1 \\ b'_{01}(x_1) = 0 \end{cases} \implies \begin{cases} b_{01}(0) = c = 0 \\ b'_{01}(0) = b = 1 \\ b'_{01}(1) = 2a + b = 0 \implies a = -\frac{1}{2} \end{cases}$$
$$\implies b_{01}(x) = -\frac{1}{2}x^2 + x.$$

•  $b_{11}(x) = ax^2 + bx + c$  and  $b'_{11}(x) = 2ax + b$ 

$$\begin{cases} b_{11}(x_0) = c = 0 \\ b'_{11}(x_0) = b = 0 \\ b'_{11}(x_1) = 2a + b = 1 \implies a = \frac{1}{2} \end{cases}$$

$$\implies b_{11}(x) = \frac{1}{2}x^2.$$

Going back at eq. (1.12), we obtain

$$B_2(f) = 1 \cdot 1 + 2 \cdot \left(-\frac{1}{2}x^2 + x\right) - 1 \cdot \frac{1}{2}x^2 = 1 - x^2 + 2x - \frac{1}{2}x^2 = 1 - \frac{3}{2}x^2 + 2x + 1$$

Indeed, this polynomial is the same as what we obtain with the first method.

For other examples and estimations of the errors, see Lecture 5.

# 1 Examples for Lecture 6

**Example 1.1** For the points (1,1), (2,1), (3,0) construct a natural cubic spline that passes through them

• For theory, see Lecture 6, pp. 5–9. For another example, see pp. 10–11.

We have  $x_1 = 1$ ,  $x_2 = 2$ ,  $x_3 = 3$  and  $f_1 = f(x_1) = 1$ ,  $f_2 = f(x_2) = 1$ ,  $f_3 = f(x_3) = 0$ . So,  $f_3 = 1$ ,  $f_4 = 1$ ,  $f_5 = 1$ . Our spline will have the form

$$s(x) = \begin{cases} s_1(x), & x \in [1, 2] \\ s_2(x), & x \in [2, 3] \end{cases}$$

A property is that the spline, its first derivative and its second derivative are continuous at the nodes. Another one is that it interpolates the function at the nodes. Since we work with cubic splines,  $s_1$  and  $s_2$  need to be polynomials of degree 3, so they will have the form

$$s_i(x) = c_{i,0} + c_{i,1}(x - x_i) + c_{i,2}(x - x_i)^2 + c_{i,3}(x - x_i)^3, x \in [x_i, x_{i+1}], i = 1, 2.$$

The coefficients  $c_{i,0}$ ,  $c_{i,1}$ ,  $c_{i,2}$ ,  $c_{i,3}$  are given from (see Lect. 6, eq. (2.9))

$$\begin{split} c_{i,0} &= f_i \\ c_{i,1} &= m_i \\ c_{i,2} &= \frac{3f[x_i, x_{i+1}] - 2m_i - m_{i+1}}{h_i} \\ c_{i,3} &= \frac{m_{i+1} - 2f[x_i, x_{i+1}] + m_i}{h_i^2} \end{split}$$

where

$$f[x_i, x_{i+1}] = \frac{f_{i+1} - f_i}{x_{i+1} - x_i}$$

The unknowns here are  $m_i$ , which can be found from the following system (see Lect. 6, eq. (2.13), (2.14))

$$h_i m_{i-1} + 2(h_{i-1} + h_i) m_i + h_{i-1} m_{i+1} = 3(h_i f[x_{i-1}, x_i] + h_{i-1} f[x_i, x_{i+1}]), \ i = 2, ..., n-1.$$
 (1.1)

Some information about them is known from the type of the spline (natural, clamped, de Boor, etc.) (see Lect. 6, pp. 7–8).

In our case, since we have to construct a natural spline, we have

$$2m_1 + m_2 = 3f[x_1, x_2]$$

$$m_{n-1} + 2m_n = 3f[x_{n-1}, x_n]$$
(1.2)

**Remark 1.2**  $m_i$  are computed only once and then used to compute the coefficients of the spline on each subinterval.

The conditions (1.2) become in our case

$$2m_1 + m_2 = 3\frac{f_2 - f_1}{x_2 - x_1} = 3 \cdot 0 = 0$$

$$m_2 + 2m_3 = 3\frac{f_3 - f_2}{x_3 - x_2} = 3 \cdot (-1) = -3$$

From equation (1.1), since n = 3, we only have to write the eq. for i = 2, so:

$$h_2 m_1 + 2(h_1 + h_2)m_2 + h_1 m_3 = 3(h_2 \frac{f_2 - f_1}{x_2 - x_1} + h_1 \frac{f_3 - f_2}{x_3 - x_2}) \iff$$

$$m_1 + 4m_2 + m_3 = -3$$

We obtain the system

$$\begin{cases} 2m_1 + m_2 &= 0\\ m_1 + 4m_2 + m_3 &= -3\\ m_2 + 2m_3 &= -3 \end{cases}$$

with solutions

$$m_1 = \frac{1}{4}$$
,  $m_2 = -\frac{1}{2}$ ,  $m_3 = -\frac{5}{4}$ .

We now construct the coefficients  $c_{i,j}$  for  $s_1$  and  $s_2$ .

•  $s_1(x)$ :

$$c_{1,0} = f_1 = 1$$

$$c_{1,1} = m_1 = \frac{1}{4}$$

$$c_{1,2} = \frac{3f[x_1, x_2] - 2m_1 - m_2}{h_1} = 0$$

$$c_{1,3} = \frac{m_2 - 2f[x_1, x_2] + m_1}{h_1^2} = -\frac{1}{4}$$

$$\implies s_1(x) = 1 + \frac{1}{4}(x - x_1) + 0(x - x_1)^2 - \frac{1}{4}(x - x_1)^3 = 1 + \frac{1}{4}(x - 1) - \frac{1}{4}(x - 1)^3, \ x \in [1, 2]$$

•  $s_2(x)$ :

$$\begin{split} c_{2,0} &= f_2 = 1 \\ c_{2,1} &= m_2 = -\frac{1}{2} \\ c_{2,2} &= \frac{3f[x_2, x_3] - 2m_2 - m_3}{h_2} = -\frac{3}{4} \\ c_{2,3} &= \frac{m_3 - 2f[x_2, x_3] + m_2}{h_2^2} = \frac{1}{4} \end{split}$$

$$\implies s_2(x) = 1 - \frac{1}{2}(x - x_2) - \frac{3}{4}(x - x_2)^2 + \frac{1}{4}(x - x_2)^3 = 1 - \frac{1}{2}(x - 2) - \frac{3}{4}(x - 2)^2 + \frac{1}{4}(x - 2)^3, \ x \in [2, 3]$$

In conclusion, 
$$s(x) = \begin{cases} 1 + \frac{1}{4}(x-1) - \frac{1}{4}(x-1)^3, & x \in [1,2] \\ 1 - \frac{1}{2}(x-2) - \frac{3}{4}(x-2)^2 + \frac{1}{4}(x-2)^3, & x \in [2,3] \end{cases}$$

Another method to construct the splines is by imposing the continuity of the spline, of the first derivative and of the second derivative on the nodes, together with the condition of a natural spline  $(s''(x_1) = 0)$  and  $s''(x_n) = 0$  and the condition of interpolating the function on the nodes. We obtain

$$s_1(x_2) = s_2(x_2)$$
 (continuity at the nodes)  
 $s_1'(x_2) = s_2'(x_2)$  (continuity of first der. at the nodes)  
 $s_1''(x_2) = s_2''(x_2)$  (continuity of second der. at the nodes)  
 $s_1(x_1) = f_1$   
 $s_1(x_2) = f_2$   
 $s_2(x_2) = f_2$   
 $s_2(x_3) = f_3$  (interpolation conditions)  
 $s_1''(x_1) = 0$   
 $s_2''(x_3) = 0$  (natural spline conditions)

If we write again  $s_1$  and  $s_2$  as cubic polynomials:

$$s_1(x) = a_1 + b_1(x - x_1) + c_1(x - x_1)^2 + d_1(x - x_1)^3 = a_1 + b_1(x - 1) + c_1(x - 1)^2 + d_1(x - 1)^3$$

$$s_2(x) = a_2 + b_2(x - x_2) + c_2(x - x_2)^2 + d_2(x - x_2)^3 = a_2 + b_2(x - 2) + c_2(x - 2)^2 + d_2(x - 2)^3$$

and compute their first and second derivatives

$$s'_1(x) = b_1 + 2c_1(x-1) + 3d_1(x-1)^2$$

$$s'_2(x) = b_2 + 2c_2(x-2) + 3d_2(x-2)^2$$

$$s''_1(x) = 2c_1 + 6d_1(x-1)$$

$$s''_2(x) = 2c_2 + 6d_2(x-2)$$

we obtain the following system from the above conditions:

$$\begin{cases} a_1 + b_1 + c_1 + d_1 &= a_2 \\ b_1 + 2c_1 + 3d_1 &= b_2 \\ 2c_1 + 6d_1 &= 2c_2 \\ a_1 &= 1 \\ a_1 + b_1 + c_1 + d_1 &= 1 \\ a_2 &= 1 \\ a_2 + b_2 + c_2 + d_2 &= 0 \\ 2c_1 &= 0 \\ 2c_2 + 6d_2 &= 0 \end{cases} \iff \begin{cases} a_1 &= 1 \\ c_1 &= 0 \\ a_2 &= 1 \\ b_1 + d_1 &= 0 \\ b_1 + 3d_1 - b_2 &= 0 \\ 3d_1 - c_2 &= 0 \\ b_2 + c_2 + d_2 &= -1 \\ c_2 + 3d_2 &= 0 \end{cases}$$

which has the solution

$$a_1 = 1, b_1 = \frac{1}{4}, c_1 = 0, d_1 = -\frac{1}{4}$$
  
 $a_2 = 1, b_2 = -\frac{1}{2}, c_2 = -\frac{3}{4}, d_2 = \frac{1}{4}$ 

as we previously obtained.

**Example 1.3** Construct a complete cubic spline s that passes through the points (1,2), (2,3), (3,5) and has s'(1) = 2, s'(3) = 1.

$$x_1 = 1$$
,  $x_2 = 2$ ,  $x_3 = 3$ ,  $f_1 = 2$ ,  $f_2 = 3$ ,  $f_3 = 5$ ,  $n = 3$ ,  $h_1 = 1$ ,  $h_2 = 1$ .

The information we know in this case (complete/clamped spline) for  $m_i$  is  $m_1 = f'(x_1)$  and  $m_n = f'(x_n)$ . So we have

$$m_1 = 2$$
,  $m_3 = 1$ .

Writing again eq. (1.1), for i = 2, we get:

$$h_2 m_1 + 2(h_1 + h_2) m_2 + h_1 m_3 = 3(h_2 \frac{f_2 - f_1}{x_2 - x_1} + h_1 \frac{f_3 - f_2}{x_3 - x_2}) \iff 2 + 4m_2 + 1 = 3(1 + 2) \implies m_2 = \frac{3}{2}.$$

We now construct the coefficients  $c_{i,j}$  for  $s_1$  and  $s_2$ .

•  $s_1(x)$ :

$$c_{1,0} = f_1 = 2$$

$$c_{1,1} = m_1 = 2$$

$$c_{1,2} = \frac{3f[x_1, x_2] - 2m_1 - m_2}{h_1} = -\frac{5}{2}$$

$$c_{1,3} = \frac{m_2 - 2f[x_1, x_2] + m_1}{h_1^2} = \frac{3}{2}$$

$$\implies s_1(x) = 2 + 2(x - x_1) - \frac{5}{2}(x - x_1)^2 + \frac{3}{2}(x - x_1)^3 = 2 + 2(x - 1) - \frac{5}{2}(x - 1)^2 + \frac{3}{2}(x - 1)^3, \ x \in [1, 2]$$

•  $s_2(x)$ :

$$\begin{split} c_{2,0} &= f_2 = 3 \\ c_{2,1} &= m_2 = \frac{3}{2} \\ c_{2,2} &= \frac{3f[x_2, x_3] - 2m_2 - m_3}{h_2} = 2 \\ c_{2,3} &= \frac{m_3 - 2f[x_2, x_3] + m_2}{h_2^2} = -\frac{3}{2} \end{split}$$

$$\implies s_2(x) = 3 + \frac{3}{2}(x - x_2) + 2(x - x_2)^2 - \frac{3}{2}(x - x_2)^3 = 3 + \frac{3}{2}(x - 2) + 2(x - 2)^2 - \frac{3}{2}(x - 2)^3, \ x \in [2, 3]$$

In conclusion, 
$$s(x) = \begin{cases} 2 + 2(x-1) - \frac{5}{2}(x-1)^2 + \frac{3}{2}(x-1)^3, & x \in [1,2] \\ 3 + \frac{3}{2}(x-2) + 2(x-2)^2 - \frac{3}{2}(x-2)^3, & x \in [2,3] \end{cases}$$

**Remark 1.4** We can use here method 2 as in the previous example, but know we will not have the last two conditions (for the natural spline). Instead we will have the conditions for the clamped spline:  $s'(x_1) = s'_1(x_1) = 2$  and  $s'(x_3) = s'_2(x_3) = 1$ .

Remark 1.5 Another method is presented in Lect. 6, pp. 9-10 (Finding cubic splines using the second derivatives).

**Example 1.6** A clamped cubic spline s for a function f is defined as

$$s(x) = \begin{cases} s_1(x) & = 1 + ax + 2x^2 - 2x^3, \ x \in [0, 1] \\ s_2(x) & = 1 + b(x - 1) - 4(x - 1)^2 + 7(x - 1)^3, \ x \in [1, 2] \end{cases}$$

Compute f'(0) and f'(2).

We need to determine first a and b. We don't know the values of the function on the nodes 0, 1, 2 so the interpolation condition won't help us. We will use the conditions for continuity of the spline, its first der. and second der. at the nodes. Let us first compute s', s''.

$$s'(x) = \begin{cases} s'_1(x) &= a + 4x - 6x^2, \ x \in [0, 1] \\ s'_2(x) &= b - 8(x - 1) + 21(x - 1)^2, \ x \in [1, 2] \end{cases}$$

$$s''(x) = \begin{cases} s_1''(x) &= 4 - 12x, \ x \in [0, 1] \\ s_2''(x) &= -8 + 42(x - 1), \ x \in [1, 2] \end{cases}$$

We obtain

$$\begin{cases} s_1(1) = s_2(1) \\ s'_1(1) = s'_2(1) \\ s''_1(1) = s''_2(1) \end{cases}$$

which is equivalent to

$$\begin{cases} 1+a=1 \Longrightarrow a=0 \\ a-2=b \Longrightarrow b=-2 \\ -8=-8, "True" \end{cases}$$

We get:

$$f'(0) = s'(0) = s'_1(0) = 0$$
$$f'(2) = s'(2) = s'_2(2) = 11$$

**Example 1.7** • For theory, see Lecture 6, pp. 14–16. For another example, see pp. 17.

Fit the data from the table with

#### a) the best least squares line

The best least squares line is obtained by considering the linear polynomial (degree = 1) P(x) = ax + b, with the unknowns a and b. We have to minimize the error

$$E(a,b) = \sum_{i=1}^{n} (y_i - P(x_i))^2$$

where  $(y_i - P(x_i))$  is called residual. This minimization occurs when

$$\frac{\partial E}{\partial a} = 0$$
 and  $\frac{\partial E}{\partial b} = 0$ .

Remark 1.8 If  $P(x) = a_0 + a_1 x + ... + a_m x^m$ , then each  $\frac{\partial E}{\partial a_i} = 0$ , i = 0, ..., m.

In the general case, for n points and linear polynomial, we have

$$E(a,b) = \sum_{i=1}^{n} (y_i - ax_i - b)^2.$$

We obtain

$$\frac{\partial E}{\partial a} = 2\sum_{i=1}^{n} (y_i - ax_i - b) \cdot (-x_i) = -2\sum_{i=1}^{n} (x_i y_i - ax_i^2 - bx_i)$$

$$\frac{\partial E}{\partial b} = 2\sum_{i=1}^{n} (y_i - ax_i - b) \cdot (-1) = -2\sum_{i=1}^{n} (y_i - ax_i - b)$$

$$\frac{\partial E}{\partial a} = 0 \implies = -2\sum_{i=1}^{n} (x_i y_i - ax_i^2 - bx_i) = 0 \xrightarrow{\stackrel{:(-2)}{\longrightarrow}} \sum_{i=1}^{n} ax_i^2 + \sum_{i=1}^{n} bx_i = \sum_{i=1}^{n} x_i y_i$$

$$\frac{\partial E}{\partial b} = 0 \implies = -2\sum_{i=1}^{n} (y_i - ax_i - b) = 0 \xrightarrow{\stackrel{:(-2)}{\longrightarrow}} \sum_{i=1}^{n} ax_i + \sum_{i=1}^{n} b = \sum_{i=1}^{n} y_i$$

and finally

$$\begin{cases} a \sum_{i=1}^{n} x_{i}^{2} + b \sum_{i=1}^{n} x_{i} = \sum_{i=1}^{n} x_{i} y_{i} \\ a \sum_{i=1}^{n} x_{i} + b n = \sum_{i=1}^{n} y_{i} \end{cases}$$
(1.3)

In our case we have

so the system becomes

$$\begin{cases} 2 \cdot a + 0 \cdot b = 1 \\ 0 \cdot a + 3 \cdot b = 4 \end{cases} \Longrightarrow \begin{cases} a = \frac{1}{2} \\ b = \frac{4}{3} \end{cases}$$

so 
$$P(x) = \frac{1}{2}x + \frac{4}{3}$$
.

#### b) the best least squares polynomial of degree 2

Our polynomial will have the form  $P(x) = ax^2 + bx + c$ , with the unknowns a, b, c that will be obtain in a similar way as in the linear case. We have to minimize the error

$$E(a,b,c) = \sum_{i=1}^{n} (y_i - P(x_i))^2$$

which occurs when

$$\frac{\partial E}{\partial a} = 0, \frac{\partial E}{\partial b} = 0 \text{ and } \frac{\partial E}{\partial c} = 0.$$

In the general case, for n points and quadratic polynomial, we have

$$E(a,b,c) = \sum_{i=1}^{n} (y_i - ax_i^2 - bx_i - c)^2.$$

We obtain

$$\frac{\partial E}{\partial a} = 2\sum_{i=1}^{n} (y_i - ax_i^2 - bx_i - c) \cdot (-x_i^2) = -2\sum_{i=1}^{n} (x_i^2 y_i - ax_i^4 - bx_i^3 - cx_i^2)$$

$$\frac{\partial E}{\partial b} = 2\sum_{i=1}^{n} (y_i - ax_i^2 - bx_i - c) \cdot (-x_i) = -2\sum_{i=1}^{n} (x_i y_i - ax_i^3 - bx_i^2 - cx_i)$$

$$\frac{\partial E}{\partial c} = 2\sum_{i=1}^{n} (y_i - ax_i^2 - bx_i - c) \cdot (-1) = -2\sum_{i=1}^{n} (y_i - ax_i^2 - bx_i - c)$$

$$\frac{\partial E}{\partial a} = 0 \implies -2\sum_{i=1}^{n} (x_i^2 y_i - ax_i^4 - bx_i^3 - cx_i^2) = 0 \xrightarrow{:(-2)} \sum_{i=1}^{n} ax_i^4 + \sum_{i=1}^{n} bx_i^3 + \sum_{i=1}^{n} cx_i^2 = \sum_{i=1}^{n} x_i^2 y_i$$

$$\frac{\partial E}{\partial b} = 0 \implies = -2\sum_{i=1}^{n} (x_i y_i - ax_i^3 - bx_i^2 - cx_i) = 0 \xrightarrow{:(-2)} \sum_{i=1}^{n} ax_i^3 + \sum_{i=1}^{n} bx_i^2 + \sum_{i=1}^{n} cx_i = \sum_{i=1}^{n} x_i y_i$$

$$\frac{\partial E}{\partial c} = 0 \implies = -2\sum_{i=1}^{n} (y_i - ax_i^2 - bx_i - c) = 0 \xrightarrow{:(-2)} \sum_{i=1}^{n} ax_i^2 + \sum_{i=1}^{n} bx_i + \sum_{i=1}^{n} c = \sum_{i=1}^{n} y_i$$

and finally

$$\begin{cases} a \sum_{i=1}^{n} x_{i}^{4} + b \sum_{i=1}^{n} x_{i}^{3} + c \sum_{i=1}^{n} x_{i}^{2} = \sum_{i=1}^{n} x_{i}^{2} y_{i} \\ a \sum_{i=1}^{n} x_{i}^{3} + b \sum_{i=1}^{n} x_{i}^{2} + c \sum_{i=1}^{n} x_{i} = \sum_{i=1}^{n} x_{i} y_{i} \\ a \sum_{i=1}^{n} x_{i}^{2} + b \sum_{i=1}^{n} x_{i} + c n = \sum_{i=1}^{n} y_{i} \end{cases}$$

$$(1.4)$$

In our case, we have

so the system becomes

$$\begin{cases} 2 \cdot a + 0 \cdot b + 3 \cdot c = 3 \\ 0 \cdot a + 2 \cdot b + 0 \cdot c = 1 \\ 2 \cdot a + 0 \cdot b + 3 \cdot c = 4 \end{cases} \Longrightarrow \begin{cases} c = 1 \\ b = \frac{1}{2} \\ a = \frac{1}{2} \end{cases}$$

so 
$$P(x) = \frac{1}{2}x^2 + \frac{1}{2}x + 1$$
.

Example 1.9 Fit the data from the table with

a) a linear least squares polynomial

As in the previous example, we have P(x) = ax + b, with the unknowns a and b. They can be found from

$$\frac{\partial E}{\partial a} = 0, \quad \frac{\partial E}{\partial b} = 0$$

We will use the system (1.3), and for this we first compute

	$x_i$	$y_i$	$x_i^2$	$x_i y_i$
	-2	0	4	0
	-1	-3	1	3
	1	2	1	2
	2	2	4	4
	3	5	9	15
$\overline{\Sigma}$	3	6	19	24

so the system becomes

$$\begin{cases} 19 \cdot a + 3 \cdot b = 24 \\ 3 \cdot a + 5 \cdot b = 6 \end{cases} \implies \begin{cases} a = \frac{51}{43} \\ b = \frac{21}{43} \end{cases}$$

so 
$$P(x) = \frac{51}{43}x + \frac{21}{43}$$
.

b) the least squares polynomial of degree 2

 $P(x) = ax^2 + bx + c$ , with the unknowns a, b, c They can be found from

$$\frac{\partial E}{\partial a} = 0$$
,  $\frac{\partial E}{\partial b} = 0$ ,  $\frac{\partial E}{\partial c} = 0$ .

We will use the system (1.4), and for this we first compute

	$  x_i  $	$y_i$	$x_i^2$	$x_i y_i$	$x_i^3$	$x_i^4$	$x_i^2 y_i$
	-2	0	4	0	-8	16	0
	-1	-3	1	3	-1	1	-3
	1	2	1	2	1	1	2
	2	2	4	4	8	16	8
	3	5	9	15	27	81	45
$\sum$	3	6	19	24	27	115	52

so the system becomes

$$\begin{cases} 115 \cdot a + 27 \cdot b + 19 \cdot c = 52 \\ 27 \cdot a + 19 \cdot b + 3 \cdot c = 24 \\ 19 \cdot a + 3 \cdot b + 5 \cdot c = 6 \end{cases} \Longrightarrow \begin{cases} a = \frac{115}{308} \\ b = \frac{261}{308} \\ c = -\frac{8}{11} \end{cases}$$

so 
$$P(x) = \frac{115}{308}x^2 + \frac{261}{308}x - \frac{8}{11}$$
.

# 2 Examples for Lectures 7 – 8 (Numerical integration of functions)

**Example 2.1** • For theory, see Lecture 7, pp. 9–15.

Compute the integral  $I = \int_{0}^{\frac{\pi}{4}} \sin x \, dx$  using

• the trapezoidal rule

The trapezoidal rule is

$$\int_{a}^{b} f(x) dx = \frac{b-a}{2} [f(a) + f(b)] + R(f)$$

with

$$R(f) = -\frac{(b-a)^3}{12}f''(\xi), \ \xi \in (a,b).$$

So,

$$I = \frac{\frac{\pi}{4} - 0}{2} \left( \sin 0 + \sin \frac{\pi}{4} \right) = \frac{\pi}{8} \cdot \frac{\sqrt{2}}{2} = \frac{\pi\sqrt{2}}{16} \approx 0.277680183634898.$$

• Simpson's rule

The Simpson's rule is

$$\int_{a}^{b} f(x) dx = \frac{b-a}{6} \left[ f(a) + 4f\left(\frac{a+b}{2}\right) + f(b) \right] + R(f)$$

with

$$R(f) = -\frac{(b-a)^5}{2880} f^{(4)}(\xi), \ \xi \in (a,b).$$

So,

$$I = \frac{\frac{\pi}{4} - 0}{6} \left( \sin 0 + 4 \sin \frac{0 + \frac{\pi}{4}}{2} + \sin \frac{\pi}{4} \right) = \frac{\pi}{24} \cdot \left( 4 \sin \frac{\pi}{8} + \frac{\sqrt{2}}{2} \right) \approx 0.292932637839748$$

The exact value is 0.2928932188134525.

Example 2.2 Compute the integral  $\int_0^{\frac{\pi}{2}} \sin x \, dx$  using the rectangle (midpoint) formula. The rectangle (midpoint) formula is

$$\int_{a}^{b} f(x) dx = (b-a)f\left(\frac{a+b}{2}\right) + R(f)$$

with

$$R(f) = \frac{(b-a)^3}{24}f''(\xi), \ \xi \in (a,b).$$

So,

$$\int_0^{\frac{\pi}{2}} \sin x \, dx = \left(\frac{\pi}{2} - 0\right) \sin\left(\frac{0 + \frac{\pi}{2}}{2}\right) = \frac{\pi}{2} \sin\frac{\pi}{4} = \frac{\pi\sqrt{2}}{4} \approx 1.11072073454$$

The actual value is  $\cos 0 = 1$ .

**Example 2.3** Does the trapezoidal rule reproduce for the integral  $\int_{0}^{2} 3x \, dx$  the exact value?

Answer: Yes, because trapezoidal rule has the degree of precision 1, which means it gives the exact value for linear polynomials (=polynomials of degree 1).

Check:  $\int\limits_0^2 3x \; dx = \frac{2-0}{2} (3 \cdot 0 + 3 \cdot 2) = 6 \; \text{(with trapezoidal rule)}$ 

$$\int_{0}^{2} 3x \ dx = 3\frac{x^{2}}{2} \Big|_{0}^{2} = 3\frac{2^{2}}{2} - 3\frac{0^{2}}{2} = 6 \text{ (with usual computations)}.$$

Remark 2.4 The Simpson's rule has the degree of precision 3, which means that for polynomials of maximum degree 3, the formula returns the exact value.

#### Example 2.5

Simpson: 
$$\int_{1}^{2} (2x^{3} + 3x) dx = \frac{2 - 1}{6} \left[ \left( 2 \cdot 1^{3} + 3 \cdot 1 \right) + 4 \cdot \left( 2 \cdot \left( \frac{3}{2} \right)^{3} + 3 \cdot \frac{3}{2} \right) + \left( 2 \cdot 2^{3} + 3 \cdot 2 \right) \right] = \frac{1}{6} \cdot 72 = 12$$

$$\text{normal computation:} \quad \int_{1}^{2} \left(2x^3 + 3x\right) \, dx = \left(2\frac{x^4}{4} + 3\frac{x^2}{2}\right) \bigg|_{1}^{2} = \left(2\frac{2^4}{4} + 3\frac{2^2}{2}\right) - \left(2\frac{1^4}{4} + 3\frac{1^2}{2}\right) = 8 + 6 - \frac{1}{2} - \frac{3}{2} = 12.$$

**Remark 2.6** The remainder in each case also tells us about the degree of precision. Since in trapezoidal rule the remainder contains f'', it will be 0 for polynomials of maximum degree 1. The same happens in the rectangle rule. In the Simpson's rule, since we have  $f^{(4)}$ , the 4th derivative of polynomials of maximum degree 3 will be 0, so the degree of precision will be 3.

Remark 2.7 Other examples for trapezoidal, rectangle and Simpson formulas are found in Lecture 7, pp. 16–17.

Example 2.8 Compute  $I = \int_{1}^{2} \ln x \, dx$  using the composite (repeated) trapezoidal rule, for n = 3. The repeated trapezoidal rule is

$$\int_{a}^{b} f(x) dx = \frac{h}{2} [f(a) + 2(f_1 + \dots + f_{n-1}) + f(b)] + R_n(f)$$

with

$$R_n(f) = -\frac{h^2(b-a)}{12}f''(\xi), \ \xi \in (a,b)$$

and

$$f_i = f(x_i), \ x_i = a + ih, \ h = \frac{b-a}{n}, \ i = \overline{0, n}.$$

We have:  $i = \overline{0,3}$ ,  $h = \frac{1}{3}$ ,  $x_0 = 1$ ,  $x_1 = \frac{4}{3}$ ,  $x_2 = \frac{5}{3}$ ,  $x_3 = 2$ ,  $f(x) = \ln x$  and

$$I = \frac{1}{2 \cdot 3} \left[ \ln(1) + 2 \ln\left(\frac{4}{3}\right) + 2 \ln\left(\frac{5}{3}\right) + \ln(2) \right] = \frac{1}{6} \ln\left(\frac{16}{9} \cdot \frac{25}{9} \cdot 2\right) = \frac{1}{6} \ln\left(\frac{800}{81}\right) \approx 0.381693762165915.$$

The exact value is 0.3862943611198906.

Example 2.9 Compute  $I = \int_{0}^{1} \frac{1}{1+x} dx$  using the composite (repeated) Simpson's rule and n = 4. The repeated Simpson's formula is

$$\int_{a}^{b} f(x) dx = \frac{h}{3} \left[ f(a) + 4 \sum_{i=1}^{m} f_{2i-1} + 2 \sum_{i=1}^{m-1} f_{2i} + f(b) \right] + R_n(f)$$

with

$$R_n(f) = -\frac{h^4(b-a)}{180}f^{(4)}(\xi), \ \xi \in (a,b)$$

and

$$f_i = f(x_i), \ x_i = a + ih, \ h = \frac{b-a}{n}, \ i = \overline{0,n}, \ \mathbf{n} = 2\mathbf{m}.$$

We have: m = 2,  $h = \frac{1-0}{4} = \frac{1}{4}$ ,  $i = \overline{0,4}$ ,  $x_0 = 0$ ,  $x_1 = \frac{1}{4}$ ,  $x_2 = \frac{1}{2}$ ,  $x_3 = \frac{3}{4}$ ,  $x_4 = 1$ ,  $f(x) = \frac{1}{1+x}$  and

$$I = \frac{1}{4 \cdot 3} \left[ f(0) + 4 \sum_{i=1}^{2} f_{2i-1} + 2 \sum_{i=1}^{1} f_{2i} + f(1) \right] =$$

$$= \frac{1}{12} \left[ f(0) + 4 \cdot (f_1 + f_3) + 2f_2 + f(1) \right] = \frac{1}{12} \left[ 1 + 4 \left( \frac{1}{1 + \frac{1}{4}} + \frac{1}{1 + \frac{3}{4}} \right) + 2 \cdot \frac{1}{1 + \frac{1}{2}} + \frac{1}{2} \right]$$

$$= \frac{1}{12} \left( \frac{3}{2} + \frac{16}{5} + \frac{16}{7} + \frac{4}{3} \right) = \frac{1}{12} \cdot \frac{1747}{210} \approx 0.693253968253968.$$

The exact value is  $\ln 2 = 0.69314718056$ .

**Example 2.10** Compute the integral  $I = \int_1^2 \ln x \, dx$  using the composite (repeated) rectangle (midpoint) formula for n = 3.

The repeated rectangle (midpoint) formula is

$$\int_{a}^{b} f(x) dx = h \sum_{i=0}^{n-1} f\left(a + \left(i + \frac{1}{2}\right)h\right) + R_{n}(f)$$

with

$$R_n(f) = \frac{h^2(b-a)}{24}f''(\xi), \ \xi \in (a,b)$$

and

$$h = \frac{b-a}{n}.$$

We have  $h = \frac{1}{3}$  and

$$I = \frac{1}{3} \left[ f \left( 1 + \frac{1}{2} \cdot \frac{1}{3} \right) + f \left( 1 + \frac{3}{2} \cdot \frac{1}{3} \right) + f \left( 1 + \frac{5}{2} \cdot \frac{1}{3} \right) \right] =$$

$$= \frac{1}{3} \left[ f \left( \frac{7}{6} \right) f \left( \frac{9}{6} \right) + f \left( \frac{11}{6} \right) \right] = \frac{1}{3} \left( \ln \frac{7}{6} + \ln \frac{9}{6} + \ln \frac{11}{6} \right) = \frac{1}{3} \ln \left( \frac{693}{216} \right) \approx 0.38858386383.$$

The exact value is 0.3862943611198906.

Remark 2.11 Other examples for repeated trapezium, repeated Simpson, repeated rectangle formulas are found in Lecture 7, pp. 17.

The degree of exactness of a quadrature formula

$$\int_{a}^{b} f(x) \, dx = \sum_{k=0}^{m} A_{k} f(x_{k}) + R(f)$$

is n if:

- each  $R(e_j) = 0$ , for all j = 0, 1, ..., n and  $R(e_{n+1}) \neq 0$ , where:
  - \*  $e_m(x) = x^m;$

\* 
$$R(e_j) = \int_{a}^{b} x^j dx - \sum_{k=0}^{m} A_k e_j(x_k)$$

Practically, it reproduces exact the polynomials of maximum degree n.

**Example 2.12** Determine n such that the approximation error for the integral  $\int_0^{\pi} \sin(x) dx$  is less than  $2 \cdot 10^{-5}$  using

## a) composite trapezoidal rule

 $a=0, b=\pi, h=\frac{\pi}{n}$ . The remainder should be less than  $2\cdot 10^{-5}$ , so

$$|R(f)| < 2 \cdot 10^{-5}$$

For the remainder we need f''.  $f'(x) = \cos(x)$  and  $f''(x) = -\sin(x)$ , so

$$|R(f)| = \left| -\frac{h^2(b-a)}{12} f''(\xi) \right| = \left| \frac{\pi^3}{12n^2} (-\sin(\xi)) \right| = \frac{\pi^3}{12n^2} |\sin(\xi)|$$

Since  $\xi \in [0, \pi]$ , to ensure that the inequality holds for every point of the interval, we can find n from

$$|R(f)| \le \frac{\pi^3}{12n^2} \max_{x \in [0,\pi]} |\sin(x)| < 2 \cdot 10^{-5}$$

Now we work with the second inequality.  $\max_{x \in [0,\pi]} |\sin(x)| = 1$  which gives us

$$\frac{\pi^3}{12n^2} < \frac{2}{10^5} \implies \frac{12n^2}{\pi^3} > \frac{10^5}{2} \implies n^2 > \pi^3 \frac{10^5}{24} \approx 129192.8 \implies n = 360.$$

## b) composite Simpson's rule

For the remainder in this case we need  $f^{(4)}$ .  $f'(x) = \cos(x)$  and  $f''(x) = -\sin(x)$ ,  $f'''(x) = -\cos(x)$ ,  $f^{(4)}(x) = \sin(x)$ , so

$$|R(f)| = \left| -\frac{h^4(b-a)}{180} f^{(4)}(\xi) \right| = \frac{\pi^5}{180n^4} |\sin(\xi)|$$

Since  $\xi \in [0, \pi]$ , to ensure that the inequality holds for every point of the interval, we can find n from

$$|R(f)| \le \frac{\pi^5}{180n^4} \max_{x \in [0, \pi]} |\sin(x)| < 2 \cdot 10^{-5}$$

Now we work with the second inequality.  $\max_{x \in [0,\pi]} |\sin(x)| = 1$  which gives us

$$\frac{\pi^5}{180n^4} < \frac{2}{10^5} \implies \frac{180n^4}{\pi^5} > \frac{10^5}{2} \implies n^4 > \pi^5 \frac{10^5}{360} \approx 85005.4 \implies n = 18.$$

#### Example 2.13 Approximate ln 2 with two correct decimals, using the repeated rectangle formula.

Again we need to work with the remainder, and to obtain 2 correct decimals (see Lecture 1, pp. 12–13), we impose

$$|R(f)| < \frac{1}{2} \cdot 10^{-2}.$$

Furthermore, we need to determine the integral whose result is ln 2, to obtain the function we will work with. For example, we can consider

$$\ln 2 = \int_{1}^{2} \frac{1}{x} dx$$

so,  $f(x) = \frac{1}{x}$ , a = 1, b = 2,  $h = \frac{1}{n}$ . This implies

$$\left| \frac{h^2(b-a)}{24} f''(\xi) \right| < \frac{1}{2} \cdot 10^{-2} \implies \frac{1}{24n^2} |f''(\xi)| < \frac{1}{2} \cdot 10^{-2}.$$

But for  $\xi \in (1,2)$ :

$$\frac{1}{24n^2} |f''(\xi)| \le \frac{1}{24n^2} \max_{x \in [1,2]} |f''(x)|$$

so we impose the condition

$$\frac{1}{24n^2} \max_{x \in [1,2]} |f''(x)| < \frac{1}{200}.$$

$$f'(x) = -\frac{1}{x^2}$$
 and  $f''(x) = \frac{2}{x^3} \Longrightarrow \max_{x \in [1,2]} |f''(x)| = 2$ . We have:

$$\frac{2}{24n^2} < \frac{1}{200} \implies 12n^2 > 200 \implies n^2 > \frac{200}{12} = 16.(6) \implies n = 5.$$

$$\implies \ln 2 \approx \frac{1}{5} \left[ f\left(\frac{11}{10}\right) + f\left(\frac{13}{10}\right) + f\left(\frac{15}{10}\right) + f\left(\frac{17}{10}\right) + f\left(\frac{19}{10}\right) \right] =$$

$$= \frac{1}{5} \left(\frac{10}{11} + \frac{10}{13} + \frac{10}{15} + \frac{10}{17} + \frac{10}{19}\right) = 0.69190788571.$$

 $\ln 2 \approx 0.69314718056$ .

Example 2.14 Determine a quadrature formula of the form

$$\int_{-1}^{1} f(x) dx = A_1 f(-1) + A_2 f(x_2) + A_3 f(1)$$

that has the degree of precision d = 3.

Since d = 3, the formula should be exact for polynomials of maximum degree 3. This means

$$R(e_{0}) = R(e_{1}) = R(e_{2}) = R(e_{3}) = 0, \quad e_{j} = x^{j}.$$

$$\begin{cases}
R(e_{0}) = \int_{-1}^{1} e_{0}(x) dx - [A_{1}e_{0}(-1) + A_{2}e_{0}(x_{2}) + A_{3}e_{0}(1)] \\
R(e_{1}) = \int_{-1}^{1} e_{1}(x) dx - [A_{1}e_{1}(-1) + A_{2}e_{1}(x_{2}) + A_{3}e_{1}(1)] \\
R(e_{2}) = \int_{-1}^{1} e_{2}(x) dx - [A_{1}e_{2}(-1) + A_{2}e_{2}(x_{2}) + A_{3}e_{2}(1)] \\
R(e_{3}) = \int_{-1}^{1} e_{3}(x) dx - [A_{1}e_{3}(-1) + A_{2}e_{3}(x_{2}) + A_{3}e_{3}(1)]
\end{cases}$$

$$\begin{cases}
R(e_{0}) = \int_{-1}^{1} 1 dx - [A_{1} \cdot 1 + A_{2} \cdot 1 + A_{3} \cdot 1] \\
R(e_{1}) = \int_{-1}^{1} x dx - [A_{1} \cdot (-1) + A_{2}x_{2} + A_{3} \cdot 1] \\
R(e_{2}) = \int_{-1}^{1} x^{2} dx - [A_{1} \cdot 1 + A_{2}x_{2}^{2} + A_{3} \cdot 1] \\
R(e_{3}) = \int_{-1}^{1} x^{3} dx - [A_{1} \cdot (-1) + A_{2}x_{3}^{2} + A_{3} \cdot 1]
\end{cases}$$

$$\begin{cases}
A_{1} + A_{2} + A_{3} = 2 \\
-A_{1} + A_{2}x_{2} + A_{3} = 0 \\
A_{1} + A_{2}x_{2}^{2} + A_{3} = \frac{2}{3} \\
-A_{1} + A_{2}x_{2}^{2} + A_{3} = 0
\end{cases}$$

**Remark 2.15**  $e_0(1) = 1$ ,  $e_0(x) = 1$ , etc.  $e_1(x_1) = x_1$ ,  $e_1(2) = 2$ , etc.  $e_2(x_1) = x_1^2$ ,  $e_2(2) = 2^2 = 4$ , etc.

From the 2nd and 4th eq. (substraction) we get

$$A_2x_2(1-x_2^2)=0.$$

 $1-x_2^2$  cannot be 0, because in this case  $x_2$  would be 1 or -1 and the nodes should be distinct. So, we have either  $A_2 = 0$  or  $x_2 = 0$ .

If we substract eq. (1) and (3), we have

$$A_2(1-x_2^2) = \frac{4}{3}$$

so  $A_2$  cannot be 0, which means that  $x_2 = 0$ . Then we get  $A_2 = \frac{4}{3}$ . From eq. (4) we have  $A_1 = A_3$  (since  $x_2 = 0$ ) and from eq. (1),  $A_1 = A_3 = \frac{1}{3}$ .

$$\implies \int_{-1}^{1} f(x) dx = \frac{1}{3} f(-1) + \frac{4}{3} f(0) + \frac{1}{3} f(1).$$

**Example 2.16** Evaluate  $\int_{1}^{3} \frac{1}{t} dt$  using Gauss-Legendre quadrature with m = 3.

For the Legendre orthogonal polynomials, we have the weight function w(x) = 1 and the interval [-1,1]. We need first to transform the interval [1,3] in [-1,1].

We consider  $x = t - 2 \implies t = x + 2$ , dt = dx, so our integral becomes

$$I = \int_{-1}^{1} \frac{1}{x+2} \, dx.$$

The nodes of the quadrature are the zeros of the Legendre polynomial  $l_3$  (m = 3) (see Lecture 8, pp. 14–15, Remark 3.10 and the table). We have

$$l_3(x) = \left[ (x^2 - 1)^3 \right]^{""}$$

$$[(x^{2}-1)^{3}]' = 3(x^{2}-1)^{2} \cdot 2x = 6x(x^{2}-1)^{2}$$

$$[(x^{2}-1)^{3}]'' = [6x(x^{2}-1)^{2}]' = 6(x^{2}-1)^{2} + 6x \cdot 2(x^{2}-1) \cdot 2x = 6(x^{2}-1)(5x^{2}-1)$$

$$[(x^{2}-1)^{3}]''' = [6(x^{2}-1)(5x^{2}-1)]' = 6 \cdot 2x(5x^{2}-1) + 6(x^{2}-1) \cdot 10x = 24x(5x^{2}-3)$$

$$\implies l_{3}(x) = 24x(5x^{2}-3) = 0 \implies x_{1} = -\sqrt{\frac{3}{5}}, \quad x_{2} = 0, \quad x_{3} = \sqrt{\frac{3}{5}}.$$

For the coefficients  $A_1, A_2, A_3$  we use the system (see Lecture 8, pp. 13, eq. (3.23)):

$$\left\{ \begin{array}{l} A_1 + A_2 + A_3 = \mu_0 = \int_{-1}^1 1 \; dx = 2 \\ A_1 x_1 + A_2 x_2 + A_3 x_3 = \mu_1 = \int_{-1}^1 x \; dx = 0 \\ A_1 x_1^2 + A_2 x_2^2 + A_3 x_3^2 = \mu_2 = \int_{-1}^1 x^2 \; dx = \frac{2}{3} \end{array} \right. \iff \left\{ \begin{array}{l} A_1 + A_2 + A_3 = 2 \\ -\sqrt{\frac{3}{5}} A_1 + \sqrt{\frac{3}{5}} A_3 = 0 \\ \frac{3}{5} A_1 + \frac{3}{5} A_3 = \frac{2}{3} \end{array} \right.$$

From eq. (2) we have  $A_1 = A_3$  and from eq. (3) we have  $A_1 = A_3 = \frac{5}{9}$ . Finally, from eq. (1) we have  $A_2 = \frac{8}{9}$ .

$$\implies I = \int_{-1}^{1} \frac{1}{x+2} dx \approx \frac{5}{9} \cdot f\left(-\sqrt{\frac{3}{5}}\right) + \frac{8}{9} \cdot f\left(0\right) + \frac{5}{9} \cdot f\left(\sqrt{\frac{3}{5}}\right) \approx \frac{5}{9} \cdot \frac{1}{-\sqrt{\frac{3}{5}} + 2} + \frac{8}{9} \cdot \frac{1}{0+2} + \frac{5}{9} \cdot \frac{1}{\sqrt{\frac{3}{5}} + 2}$$

 $\Rightarrow I \approx 1.098039215686274.$ 

The exact value is  $\ln 3 = 1.098612288668110$ .

• Other examples for Gauss quadratures are found in Lecture 8, pp. 11–12, 15.

Remark 2.17 For examples of adaptive quadratures and Romberg's method, see Lecture 8, pp. 1–9 and what we have done at the lab.

# 3 Examples for Lectures 9-10

# (Numerical methods for solving linear systems)

#### 3.1 Direct methods

Example 3.1 Solve the system

$$\begin{cases} 2x_1 + 4x_3 + x_4 = 7 \\ 2x_2 + 4x_3 + x_4 = 7 \\ 2x_1 + 4x_2 + 3x_3 = 9 \\ x_1 + 2x_2 + 2x_4 = 5 \end{cases}$$

using the Gauss method with partial pivoting.

We start by writing the matrix A that contains the coefficients of the unknowns  $(x_1, x_2, x_3, x_4)$ . We also write  $\overline{A}$  which contains also the column vector b (the result of each equation), since the modifications should be performed on this column too.

$$A = \begin{pmatrix} 2 & 0 & 4 & 1 \\ 0 & 2 & 4 & 1 \\ 2 & 4 & 3 & 0 \\ 1 & 2 & 0 & 2 \end{pmatrix} \quad \text{and} \quad \overline{A} = \begin{pmatrix} 2 & 0 & 4 & 1 & | & 7 \\ 0 & 2 & 4 & 1 & | & 7 \\ 2 & 4 & 3 & 0 & | & 9 \\ 1 & 2 & 0 & 2 & | & 5 \end{pmatrix}.$$

On the first column of  $\overline{A}$ , the pivot (maximum element in absolute value) is  $a_{11} = 2$ , so we do not interchange any rows.  $a_{21} = 0$  so we let it the same, and to obtain  $a_{31} = 0$  and  $a_{41} = 0$ , we have to perform  $R_3 - R_1$  and  $R_4 - \frac{1}{2}R_1$ . (Don't forget to change also the column of free term b!)

$$\overline{A} \sim \begin{pmatrix} 2 & 0 & 4 & 1 & | & 7 \\ 0 & 2 & 4 & 1 & | & 7 \\ 0 & 4 & -1 & -1 & | & 2 \\ 0 & 2 & -2 & \frac{3}{2} & | & \frac{3}{2} \end{pmatrix}$$

On the second column (below the main diagonal - and including it), the maximum element in absolute value is  $a_{32} = 4$ , so we interchange  $R_2$  and  $R_3$ .

$$\overline{A} \sim \begin{pmatrix} 2 & 0 & 4 & 1 & | & 7 \\ 0 & 4 & -1 & -1 & | & 2 \\ 0 & 2 & 4 & 1 & | & 7 \\ 0 & 2 & -2 & \frac{3}{2} & | & \frac{3}{2} \end{pmatrix}$$

The pivot is now  $a_{22} = 4$ . Now, to obtain 0 below the main diagonal on the second column, we need  $a_{32} = 0$  and  $a_{42} = 0$ , so we perform  $R_3 - \frac{1}{2}R_2$  and  $R_4 - \frac{1}{2}R_2$ , obtaining

$$\overline{A} \sim \begin{pmatrix} 2 & 0 & 4 & 1 & | & 7 \\ 0 & 4 & -1 & -1 & | & 2 \\ 0 & 0 & \frac{9}{2} & \frac{3}{2} & | & 6 \\ 0 & 0 & -\frac{3}{2} & 2 & | & \frac{1}{2} \end{pmatrix}$$

On the third column, the maximum element in absolute value below the main diagonal (including it) is  $a_{33} = \frac{9}{2}$ , so we don't interchange anything. To obtain 0 below the main diagonal, we need  $a_{43} = 0$ , so we have to compute  $R_4 + \frac{1}{3}R_3$ , obtaining

$$\overline{A} \sim \begin{pmatrix} 2 & 0 & 4 & 1 & | & 7 \\ 0 & 4 & -1 & -1 & | & 2 \\ 0 & 0 & \frac{9}{2} & \frac{3}{2} & | & 6 \\ 0 & 0 & 0 & \frac{5}{2} & | & \frac{5}{2} \end{pmatrix}$$

Now, using backward substitution, we obtain

$$\frac{5}{2}x_4 = \frac{5}{2} \implies x_4 = 1$$

$$\frac{9}{2}x_3 + \frac{3}{2} \cdot 1 = 6 \implies x_3 = 1$$

$$4x_2 - 1 \cdot 1 - 1 \cdot 1 = 2 \implies x_2 = 1$$

$$2x_1 + 0 \cdot 1 + 4 \cdot 1 + 1 \cdot 1 = 7 \implies x_1 = 1$$

Remark 3.2 The theory can be found in Lecture 9, pp. 1–9. Other examples using the Gauss elimination with partial pivoting are in Lecture 9, pp. 7–8. Examples using the Gauss elimination with scaled partial pivoting and total pivoting are in Lecture 9, pp. 8–9.

Example 3.3 Solve the previous system using an LUP decomposition.

Starting with the matrix

$$A = \begin{pmatrix} 2 & 0 & 4 & 1 \\ 0 & 2 & 4 & 1 \\ 2 & 4 & 3 & 0 \\ 1 & 2 & 0 & 2 \end{pmatrix}$$

we see that the pivot on the first column is 2, so we do not interchange any rows. In this case, P has the

form  $P = \begin{pmatrix} 1\\2\\3\\4 \end{pmatrix}$  (the order of the rows in the matrix - we change it when we interchange rows.)

1.

$$A \sim \begin{pmatrix} 2 & 0 & 4 & 1 \\ \hline 0 & 2 & 4 & 1 \\ 2 & 4 & 3 & 0 \\ 1 & 2 & 0 & 2 \end{pmatrix}$$

2. A will look like this at the next step

$$A \sim \begin{pmatrix} 2 & 0 & 4 & 1 \\ \frac{0}{2} & & & \\ \frac{2}{2} & & & \\ \frac{1}{2} & & & \end{pmatrix} \sim \begin{pmatrix} 2 & 0 & 4 & 1 \\ 0 & & & \\ 1 & & & \\ \frac{1}{2} & & & \end{pmatrix}$$

3. To fill the empty space we compute the Schur complement from the coloured part:

$$\begin{pmatrix} 2 & 4 & 1 \\ 4 & 3 & 0 \\ 2 & 0 & 2 \end{pmatrix} - \frac{1}{2} \cdot \begin{pmatrix} 0 \\ 2 \\ 1 \end{pmatrix} \cdot \begin{pmatrix} 0 & 4 & 1 \end{pmatrix} = \begin{pmatrix} 2 & 4 & 1 \\ 4 & -1 & -1 \\ 2 & -2 & \frac{3}{2} \end{pmatrix}$$

and add it to our matrix

$$A \sim \begin{pmatrix} 2 & 0 & 4 & 1 \\ \hline 0 & 2 & 4 & 1 \\ 1 & 4 & -1 & -1 \\ \frac{1}{2} & 2 & -2 & \frac{3}{2} \end{pmatrix}$$

4. On the remaining part, second column, the pivot is 4, so we interchange  $R_2$  and  $R_3$ . Now P is

changed to 
$$P = \begin{pmatrix} 1 \\ 3 \\ 2 \\ 4 \end{pmatrix}$$
.

$$A \sim \begin{pmatrix} 2 & 0 & 4 & 1 \\ \hline 1 & 4 & -1 & -1 \\ 0 & 2 & 4 & 1 \\ \hline \frac{1}{2} & 2 & -2 & \frac{3}{2} \end{pmatrix}$$

A will have the form

$$A \sim \begin{pmatrix} 2 & 0 & 4 & 1 \\ 1 & 4 & -1 & -1 \\ 0 & \frac{2}{4} & & & \\ \frac{1}{2} & \frac{2}{4} & & & \end{pmatrix} \sim \begin{pmatrix} 2 & 0 & 4 & 1 \\ 1 & 4 & -1 & -1 \\ 0 & \frac{1}{2} & & & \\ \frac{1}{2} & \frac{1}{2} & & & \end{pmatrix}$$

5. Next Schur complement:

$$\begin{pmatrix} 4 & 1 \\ -2 & \frac{3}{2} \end{pmatrix} - \frac{1}{4} \cdot \begin{pmatrix} 2 \\ 2 \end{pmatrix} \cdot \begin{pmatrix} -1 & -1 \end{pmatrix} = \begin{pmatrix} \frac{9}{2} & \frac{3}{2} \\ -\frac{3}{2} & 2 \end{pmatrix}$$

We add it to our matrix

$$A \sim \begin{pmatrix} 2 & 0 & 4 & 1 \\ \hline 1 & 4 & -1 & -1 \\ 0 & \frac{1}{2} & \frac{9}{2} & \frac{3}{2} \\ \frac{1}{2} & \frac{1}{2} & -\frac{3}{2} & 2 \end{pmatrix}$$

6. On the remaining part the pivot is  $\frac{9}{2}$ , so we do not make any interchanges, P remains the same.

$$A \sim \begin{pmatrix} 2 & 0 & 4 & 1 \\ \hline 1 & 4 & -1 & -1 \\ 0 & \frac{1}{2} & \frac{9}{2} & \frac{3}{2} \\ \frac{1}{2} & \frac{1}{2} & -\frac{3}{2} & 2 \end{pmatrix}$$

Finally, A will have the form:

$$A \sim \begin{pmatrix} 2 & 0 & 4 & 1 \\ \hline 1 & 4 & -1 & -1 \\ 0 & \frac{1}{2} & \frac{9}{2} & \frac{3}{2} \\ \frac{1}{2} & \frac{1}{2} & -\frac{3}{2} \cdot \frac{2}{9} \end{pmatrix}$$

the missing part being computed from the last Schur complement

$$2 - \frac{2}{9} \cdot \left(-\frac{3}{2}\right) \cdot \frac{3}{2} = \frac{5}{2}$$

7. Finally,

$$A \sim \begin{pmatrix} 2 & 0 & 4 & 1 \\ 1 & 4 & -1 & -1 \\ 0 & \frac{1}{2} & \frac{9}{2} & \frac{3}{2} \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{3} & \frac{5}{2} \end{pmatrix}$$

8. L will be the lower triangular part of A, with 1 on the main diagonal, U will be the upper triangular

part of A and P will be the permutation matrix of the rows. Since  $P = \begin{pmatrix} 1 \\ 3 \\ 2 \\ 4 \end{pmatrix}$ , we have

$$L = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & \frac{1}{2} & 1 & 0 \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{3} & 1 \end{pmatrix}, \quad U = \begin{pmatrix} 2 & 0 & 4 & 1 \\ 0 & 4 & -1 & -1 \\ 0 & 0 & \frac{9}{2} & \frac{3}{2} \\ 0 & 0 & 0 & \frac{5}{2} \end{pmatrix}, \quad P = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}.$$

9. We have

$$PA = LU$$

Multiplying at right with x, we have

$$PAx = LUx$$

Knowing that Ax = b and denoting Ux = y, we have first to solve the system

$$Pb = Ly$$

which will be solve using forward substitution:

$$\begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & \frac{1}{2} & 1 & 0 \\ \frac{1}{2} & \frac{1}{2} & -\frac{1}{2} & 1 \end{pmatrix} \cdot \begin{pmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{pmatrix} = \begin{pmatrix} 7 \\ 9 \\ 7 \\ 5 \end{pmatrix}$$

$$\implies y_1 = 7, \ y_2 = 2, \ y_3 = 6, \ y_4 = \frac{5}{2}.$$

To find x, we have to solve Ux = y, by backward substitution:

$$\begin{pmatrix} 2 & 0 & 4 & 1 \\ 0 & 4 & -1 & -1 \\ 0 & 0 & \frac{9}{2} & \frac{3}{2} \\ 0 & 0 & 0 & \frac{5}{2} \end{pmatrix} \cdot \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} 7 \\ 2 \\ 6 \\ \frac{5}{2} \end{pmatrix}$$

that implies

$$x_4 = 1$$
,  $x_3 = 1$ ,  $x_2 = 1$ ,  $x_1 = 1$ 

The solution is  $x = \begin{pmatrix} 1 \\ 1 \\ 1 \\ 1 \end{pmatrix}$  as we obtained at the previous exercise.

Remark 3.4 For theory about LU and LUP decompositions, see Lecture 9, pp. 10–15. Other examples are found in Lecture 9, pp. 12–13 (LU), 14–15 (LUP).

Remark 3.5 There are two other factorization methods discussed in class (QR decomposition and Cholesky factorization). You can find the theory and examples in Lecture 10, pp. 1–3.

Example 3.6 Find the Cholesky decomposition of the matrix

$$A = \begin{pmatrix} 10 & 5 & 2 \\ 5 & 3 & 2 \\ 2 & 2 & 3 \end{pmatrix}$$

First, we can see that  $A = A^t$ , so the matrix is symmetric. Its eigenvalues (=solutions  $\lambda$  of the equation  $det(A - \lambda I_3) = 0$ ) are  $\approx 0.09$ , 2.6, 13.31 so real and positive, hence the matrix is positive definite. The algorithm is similar to the LU decomposition.

1.

$$A \sim \left(\begin{array}{c|cc} 10 & 5 & 2 \\ \hline 5 & 3 & 2 \\ 2 & 2 & 3 \end{array}\right)$$

2. A will look at the next step as

$$A \sim \begin{pmatrix} \frac{\sqrt{10}}{\frac{5}{\sqrt{10}}} & \frac{2}{\sqrt{10}} \\ \frac{5}{\sqrt{10}} & \\ \frac{2}{\sqrt{10}} & \\ \end{pmatrix} \sim \begin{pmatrix} \frac{\sqrt{10}}{\frac{\sqrt{10}}{2}} & \frac{\sqrt{10}}{5} \\ \frac{\sqrt{10}}{2} & \\ \frac{\sqrt{10}}{5} & \\ \end{pmatrix}$$

with the empty part computed by

$$\begin{pmatrix} 3 & 2 \\ 2 & 3 \end{pmatrix} - \begin{pmatrix} \frac{\sqrt{10}}{2} \\ \frac{\sqrt{10}}{5} \end{pmatrix} \cdot \begin{pmatrix} \frac{\sqrt{10}}{2} & \frac{\sqrt{10}}{5} \end{pmatrix} = \begin{pmatrix} 3 & 2 \\ 2 & 3 \end{pmatrix} - \begin{pmatrix} \frac{5}{2} & 1 \\ 1 & \frac{2}{5} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} & 1 \\ 1 & \frac{13}{5} \end{pmatrix}$$

We add it to our matrix

$$A \sim \begin{pmatrix} \frac{\sqrt{10}}{\sqrt{10}} & \frac{\sqrt{10}}{2} & \frac{\sqrt{10}}{5} \\ \frac{\sqrt{10}}{2} & \frac{1}{2} & 1 \\ \frac{\sqrt{10}}{5} & 1 & \frac{13}{5} \end{pmatrix}$$

3.

$$A \sim \begin{pmatrix} \frac{\sqrt{10}}{\sqrt{10}} & \frac{\sqrt{10}}{5} \\ \frac{\sqrt{10}}{2} & \frac{1}{2} & 1 \\ \frac{\sqrt{10}}{5} & 1 & \frac{13}{5} \end{pmatrix}$$

At the next step, A will have the form

$$A \sim \begin{pmatrix} \frac{\sqrt{10}}{2} & \frac{\sqrt{10}}{5} \\ \frac{\sqrt{10}}{2} & \sqrt{\frac{1}{2}} & \frac{1}{\sqrt{\frac{1}{2}}} \\ \frac{\sqrt{10}}{5} & \frac{1}{\sqrt{\frac{1}{2}}} & - \end{pmatrix} \sim \begin{pmatrix} \frac{\sqrt{10}}{2} & \frac{\sqrt{10}}{2} & \frac{\sqrt{10}}{5} \\ \frac{\sqrt{10}}{2} & \frac{\sqrt{2}}{2} & \sqrt{\frac{10}{2}} \\ \frac{\sqrt{10}}{5} & \frac{\sqrt{2}}{2} & - \end{pmatrix}$$

with the empty part computed by

$$\frac{13}{5} - \sqrt{2} \cdot \sqrt{2} = \frac{3}{5}$$

We put in the empty part:  $\sqrt{\frac{3}{5}}$  (!)

4. So, finally

$$A \sim \begin{pmatrix} \sqrt{10} & \frac{\sqrt{10}}{2} & \frac{\sqrt{10}}{5} \\ \frac{\sqrt{10}}{2} & \frac{\sqrt{2}}{2} & \sqrt{2} \\ \frac{\sqrt{10}}{5} & \sqrt{2} & \sqrt{\frac{3}{5}} \end{pmatrix}$$

5. Since Cholesky decomposition consists in writing  $A = R^t R$ , with R upper triangular, we have that (in A we put zeros below the main diagonal)

$$R = \begin{pmatrix} \sqrt{10} & \frac{\sqrt{10}}{2} & \frac{\sqrt{10}}{5} \\ 0 & \frac{\sqrt{2}}{2} & \sqrt{2} \\ 0 & 0 & \sqrt{\frac{3}{5}} \end{pmatrix}.$$

Remark 3.7 At the lab we have solved a system using its Cholesky decomposition.

#### 3.2 Iterative methods

Example 3.8 Determine the approximate solution for the system

$$\begin{cases} 5x_1 + x_2 - x_3 = 7 \\ x_1 + 5x_2 + x_3 = 7 \\ x_1 + x_2 + 5x_3 = 7 \end{cases}$$

with the initial approximation  $x^{(0)} = (0,0,0)^T$  using

a) Jacobi method in 3 steps;

We can see that the matrix

$$A = \begin{pmatrix} 5 & 1 & -1 \\ 1 & 5 & 1 \\ 1 & 1 & 5 \end{pmatrix}$$

is diagonally dominant since

$$|a_{11}| = |5| > |a_{12}| + |a_{13}| = |1| + |-1| = 2$$
  
 $|a_{22}| = |5| > |a_{21}| + |a_{23}| = |1| + |1| = 2$   
 $|a_3| = |5| > |a_{31}| + |a_{32}| = |1| + |1| = 2$ 

hence the method will converge (no matter what the initial approximation  $x^{(0)}$  is).

To apply the method, we have to express the unknown  $x_k$  from the equation k with respect to the other unknowns. So, we have

$$\begin{cases} x_1 = \frac{7 - x_2 + x_3}{5} \\ x_2 = \frac{7 - x_1 - x_3}{5} \\ x_3 = \frac{7 - x_1 - x_2}{5} \end{cases}$$
(3.1)

Now, the Jacobi method consists in expressing  $x^{(k)}$  (the unknown x at step k) using the previous approximations  $x^{(k-1)}$ . We have:

$$\begin{cases} x_1^{(1)} = \frac{7 - x_2^{(0)} + x_3^{(0)}}{5} = \frac{7 - 0 + 0}{5} = \frac{7}{5} = 1.4\\ x_2^{(1)} = \frac{7 - x_1^{(0)} - x_3^{(0)}}{5} = \frac{7 - 0 - 0}{5} = \frac{7}{5} = 1.4\\ x_3^{(1)} = \frac{7 - x_1^{(0)} - x_2^{(0)}}{5} = \frac{7 - 0 - 0}{5} = \frac{7}{5} = 1.4 \end{cases}$$

Next, on the second iteration we have:

$$\begin{cases} x_1^{(2)} = \frac{7 - x_2^{(1)} + x_3^{(1)}}{5} = \frac{7 - \frac{7}{5} + \frac{7}{5}}{5} = \frac{7}{5} = 1.4\\ x_2^{(2)} = \frac{7 - x_1^{(1)} - x_3^{(1)}}{5} = \frac{7 - \frac{7}{5} - \frac{7}{5}}{5} = \frac{21}{25} = 0.84\\ x_3^{(2)} = \frac{7 - x_1^{(1)} - x_2^{(1)}}{5} = \frac{7 - \frac{7}{5} - \frac{7}{5}}{5} = \frac{21}{25} = 0.84 \end{cases}$$

and the last one:

$$\begin{cases} x_1^{(3)} = \frac{7 - x_2^{(2)} + x_3^{(2)}}{5} = \frac{7 - \frac{21}{25} + \frac{21}{25}}{5} = \frac{7}{5} = 1.4 \\ x_2^{(3)} = \frac{7 - x_1^{(2)} - x_3^{(2)}}{5} = \frac{7 - \frac{7}{5} - \frac{21}{25}}{5} = \frac{119}{125} = 0.952 \\ x_3^{(3)} = \frac{7 - x_1^{(2)} - x_2^{(2)}}{5} = \frac{7 - \frac{7}{5} - \frac{21}{25}}{5} = \frac{119}{125} = 0.952 \end{cases}$$

**Remark 3.9** Another way to compute is if we consider A = D - L - U, with

$$D = \begin{pmatrix} 5 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 5 \end{pmatrix}, \quad -L = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 1 & 0 \end{pmatrix}, \quad -U = \begin{pmatrix} 0 & 1 & -1 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}$$

then we have

$$x^{(k+1)} = D^{-1}(L+U)x^{(k)} + D^{-1}b.$$

b) Gauss-Seidel method in 2 steps;

The method converges because A is diagonally dominant. The difference between Jacobi and Gauss-Seidel is that in this case, we have to replace the unknowns with their most recent approximations. So, if we are at the step k, when we compute  $x_3^{(k)}$ , we won't use  $x_1$  and  $x_2$  from the previous step  $(x_1^{(k-1)}, x_2^{(k-1)})$ , but instead we will use their values from the current step, since we have already determined them. Using again (3.1), we obtain

$$\begin{cases} x_1^{(1)} = \frac{7 - x_2^{(0)} + x_3^{(0)}}{5} = \frac{7 - 0 + 0}{5} = \frac{7}{5} = 1.4 \\ x_2^{(1)} = \frac{7 - x_1^{(1)} - x_3^{(0)}}{5} = \frac{7 - \frac{7}{5} - 0}{5} = \frac{28}{25} = 1.12 \\ x_3^{(1)} = \frac{7 - x_1^{(1)} - x_2^{(1)}}{5} = \frac{7 - \frac{7}{5} - \frac{28}{25}}{5} = \frac{112}{125} = 0.896 \end{cases}$$

Next, we have:

$$\begin{cases} x_1^{(2)} = \frac{7 - x_2^{(1)} + x_3^{(1)}}{5} = \frac{7 - \frac{28}{25} + \frac{112}{125}}{5} = \frac{847}{625} = 1.3552 \\ x_2^{(2)} = \frac{7 - x_1^{(2)} - x_3^{(1)}}{5} = \frac{7 - \frac{847}{625} - \frac{112}{125}}{5} = \frac{2968}{3125} = 0.94976 \\ x_3^{(2)} = \frac{7 - x_1^{(2)} - x_2^{(2)}}{5} = \frac{7 - \frac{847}{625} - \frac{2968}{3125}}{5} = \frac{14672}{15625} = 0.939008 \end{cases}$$

**Remark 3.10** Again if we consider A = D - L - U, with

$$D = \begin{pmatrix} 5 & 0 & 0 \\ 0 & 5 & 0 \\ 0 & 0 & 5 \end{pmatrix}, \quad -L = \begin{pmatrix} 0 & 0 & 0 \\ 1 & 0 & 0 \\ 1 & 1 & 0 \end{pmatrix}, \quad -U = \begin{pmatrix} 0 & 1 & -1 \\ 0 & 0 & 1 \\ 0 & 0 & 0 \end{pmatrix}$$

we have

$$x^{(k+1)} = (D-L)^{-1}Ux^{(k)} + (D-L)^{-1}b.$$

c) SOR method for  $\omega = \frac{1}{2}$  in 2 steps.

It is similar to Gauss-Seidel method. First, we compute an intermediary point  $\tilde{x}^{(k)}$  as in Gauss-

Seidel and then  $x^{(k)} = \omega \tilde{x}^{(k)} + (1 - \omega) x^{(k-1)}$ . So, for (3.1), we have:

$$\begin{cases} \tilde{x_1}^{(1)} = \frac{7 - x_2^{(0)} + x_3^{(0)}}{5} = \frac{7 - 0 + 0}{5} = \frac{7}{5} = 1.4 \\ x_1^{(1)} = \omega \tilde{x_1}^{(1)} + (1 - \omega) x_1^{(0)} = \frac{1}{2} \cdot 1.4 + \frac{1}{2} \cdot 0 = 0.7 \\ \tilde{x_2}^{(1)} = \frac{7 - x_1^{(1)} - x_3^{(0)}}{5} = \frac{7 - 0.7 - 0}{5} = 1.26 \\ x_2^{(1)} = \omega \tilde{x_2}^{(1)} + (1 - \omega) x_2^{(0)} = \frac{1}{2} \cdot 1.26 + \frac{1}{2} \cdot 0 = 0.63 \\ \tilde{x_3}^{(1)} = \frac{7 - x_1^{(1)} - x_2^{(1)}}{5} = \frac{7 - 0.7 - 0.63}{5} = 1.134 \\ x_3^{(1)} = \omega \tilde{x_3}^{(1)} + (1 - \omega) x_3^{(0)} = \frac{1}{2} \cdot 1.134 + \frac{1}{2} \cdot 0 = 0.567 \end{cases}$$

And the second iteration is

$$\begin{cases} \tilde{x_1}^{(2)} = \frac{7 - x_2^{(1)} + x_3^{(1)}}{5} = \frac{7 - 0.63 + 0.567}{5} = 1.3874 \\ x_1^{(2)} = \omega \tilde{x_1}^{(2)} + (1 - \omega) x_1^{(1)} = \frac{1}{2} \cdot 1.3874 + \frac{1}{2} \cdot 0.7 = 1.0437 \\ \tilde{x_2}^{(2)} = \frac{7 - x_1^{(2)} - x_3^{(1)}}{5} = \frac{7 - 1.0437 - 0.567}{5} = 1.07786 \\ x_2^{(2)} = \omega \tilde{x_2}^{(2)} + (1 - \omega) x_2^{(1)} = \frac{1}{2} \cdot 1.07786 + \frac{1}{2} \cdot 0.63 = 0.85393 \\ \tilde{x_3}^{(2)} = \frac{7 - x_1^{(2)} - x_2^{(2)}}{5} = \frac{7 - 1.0437 - 0.85393}{5} = 1.020474 \\ x_3^{(2)} = \omega \tilde{x_3}^{(2)} + (1 - \omega) x_3^{(1)} = \frac{1}{2} \cdot 1.020474 + \frac{1}{2} \cdot 0.567 = 0.793737 \end{cases}$$

**Remark 3.11** The exact solution is (1.4; 0.9(3); 0.9(3)).

Remark 3.12 See the **theory** and other **examples** for the three Iterative methods in Lecture 10, pp. 4–12.

# 4 Examples for Lecture 11 (Nonlinear equations in $\mathbb{R}$ )

**Example 4.1** Consider the equation  $x^3 - 2x^2 = 5$ . Give the next two iterations for approximating the solution of this equation using:

1. Newton's method starting with  $x_0 = 2$ .

Considering the equation f(x) = 0 (in our case we will have  $f(x) = x^3 - 2x^2 - 5$ ), for Newton's method the next iteration is obtained from

$$x_{k+1} = x_k - \frac{f(x_k)}{f'(x_k)}$$

for a starting value  $x_0$ . This method is a *one-step method*, i.e., to obtain an approximation for  $x_k$  we need only the previous approximation  $x_{k-1}$ , in particular we only need one starting value.

$$f'(x) = (x^3 - 2x^2 - 5)' = 3x^2 - 4x$$

The next two iterations are:

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} = 2 - \frac{f(2)}{f'(2)} = 2 - \frac{-5}{4} = \frac{13}{4} = 3.25$$

and

$$x_2 = x_1 - \frac{f(x_1)}{f'(x_1)} = 3.25 - \frac{f(3.25)}{f'(3.25)} = 3.25 - \frac{8.2}{18.68} \approx 2.81.$$

Remark 4.2 See another example in Lecture 11, pp. 10–11 and the theory on pp. 10–13.

2. secant method starting with  $x_0 = 1$  and  $x_1 = 3$ .

The secant method is a two-step method (we need two previous approximations to get a new one) and it has the formula

$$x_{k+1} = x_k - \frac{x_k - x_{k-1}}{f(x_k) - f(x_{k-1})} f(x_k)$$

for two starting values  $x_0$  and  $x_1$ . In our case we have:

$$x_2 = x_1 - \frac{x_1 - x_0}{f(x_1) - f(x_0)} f(x_1) = 3 - \frac{3 - 1}{f(3) - f(1)} f(3) = 3 - \frac{2 \cdot 4}{4 - (-6)} = 3 - 0.8 = 2.2$$

and the second approximation

$$x_3 = x_2 - \frac{x_2 - x_1}{f(x_2) - f(x_1)} f(x_2) = 2.2 - \frac{2.2 - 3}{f(2.2) - f(3)} f(2.2) = 2.2 - \frac{-0.8 \cdot (-4.03)}{-4.03 - 4} = 2.2 + \frac{0.8 \cdot 4.03}{8.03} \approx 2.60.$$

Remark 4.3 See another example in Lecture 11, pp. 8 and the theory on pp. 7–9.

3. bisection method starting with  $a_0=1$  and  $b_0=3$ .

The bisection method is based on the following algorithm: If  $f(a) \cdot f(b) < 0$  with f continuous on [a,b], then there is at least one root of f in (a,b).

Let  $[a,b] = [a_0,b_0]$ . First we check if  $f(a_0) \cdot f(b_0) < 0$  and then we compute the middle of the interval [a,b], i.e.,  $c_0 = \frac{a_0 + b_0}{2}$  and we check:

- if  $f(c_0) \cdot f(b_0) < 0$ , then the root is in the interval  $[c_0, b_0]$  and we consider  $a_1 = c_0$  and  $b_1 = b_0$ ;
- otherwise (if  $f(a_0) \cdot f(c_0) < 0$ ), then the root is in  $[a_0, c_0]$  and we consider  $a_1 = a_0$  and  $b_1 = c_0$ .

We apply then the same steps on the new interval  $[a_1, b_1]$  and so on. In our case, we have :

$$f(a_0) \cdot f(b_0) = f(1) \cdot f(3) = (1^3 - 2 \cdot 1^2 - 5) \cdot (3^3 - 2 \cdot 3^2 - 5) = (-6) \cdot 4 = -24 < 0.$$

so

$$c_0 = \frac{a_0 + b_0}{2} = \frac{1+3}{2} = 2.$$

Next, we check:

$$f(c_0) \cdot f(b_0) = f(2) \cdot f(3) = (-5) \cdot 4 = -20 < 0$$

and the root must be in the interval  $[c_0, b_0] = [2, 3]$ . This is why we set  $a_1 = c_0$  and  $b_1 = b_0$  and we move in the interval  $[a_1, b_1] = [2, 3]$ . This time we have

$$c_1 = \frac{a_1 + b_1}{2} = \frac{2+3}{2} = 2.5$$

$$f(c_1) \cdot f(b_1) = f(2.5) \cdot f(3) = (-1.875) \cdot 4 < 0,$$

so the root must be in the interval  $[c_1, b_1] = [2.5, 3]$ . We set  $a_2 = c_1$  and  $b_2 = b_1$  and we move in the interval  $[a_2, b_2] = [2.5, 3]$ , with  $c_2 = \frac{2.5+3}{2} = 2.75$ .

Remark 4.4 See another example in Lecture 11, pp. 4–5 and the theory on pp. 3–6.

**Example 4.5** Show that  $g(x) = \pi + \frac{1}{2}\sin(\frac{x}{2})$  has a unique fixed point on  $[0, 2\pi]$ . Estimate the number of iterations required to achieve  $10^{-2}$  accuracy for the solution of g(x) = x. Compute the first two iterates.

**Remark 4.6** The Banach Theorem can be found on pp. 15. We will use a little modification for it (easier to apply) which can be found on pp. 16 (Th. 3.5.).

We have  $g'(x) = \frac{1}{4}\cos(\frac{x}{2})$ , so it is obvious that  $g \in C^1([0, 2\pi])$  (= derivable, which implies continuous, and with the first derivative also continuous on  $[0, 2\pi]$ ). Now we have to show that  $g([0, 2\pi]) \subseteq [0, 2\pi]$ . We compute the table of variation for g.

$$g'(x) = 0 \implies \frac{1}{4}\cos(\frac{x}{2}) = 0 \implies \cos(\frac{x}{2}) = 0 \xrightarrow{x \in [0, 2\pi]} x = \pi.$$

$$\begin{array}{c|ccccc}
x & 0 & \pi & 2\pi \\
\hline
g'(x) & + & 0 & - \\
g(x) & \nearrow & \searrow
\end{array}$$

$$g(0) = \pi, \ g(\pi) = \pi + \frac{1}{2}, \ g(2\pi) = \pi$$

and together with the continuity of g, we have that  $\text{Im} g = [\pi, \pi + \frac{1}{2}] \subseteq [0, 2\pi]$ .

Now we have to check that  $\lambda = \max_{x \in [0,2\pi]} |g'(x)| < 1$ .

$$|g'(x)| = \left|\frac{1}{4}\cos\left(\frac{x}{2}\right)\right| = \frac{1}{4}\left|\cos\left(\frac{x}{2}\right)\right| \le \frac{1}{4} \cdot 1 = \frac{1}{4} \implies \lambda = \frac{1}{4} < 1.$$

So all the conditions of Banach Theorem are fulfilled. So g has a unique fixed point  $\alpha \in [0, 2\pi]$  (i.e., the eq. g(x) = x has a unique solution). Another result is that **the sequence** 

$$x_{n+1} = g(x_n)$$

will converge to the solution  $\alpha$  of the equation g(x) = x as  $n \to \infty$ , for any choice of initial approximation  $x_0 \in [0, 2\pi]$ .

We can take for example  $x_0 = \pi$ . Then the first two iterates are

$$x_1 = g(x_0) = \pi + \frac{1}{2}\sin\frac{\pi}{2} = \pi + \frac{1}{2}$$

and

$$x_2 = g(x_1) = \pi + \frac{1}{2}\sin\frac{\pi + \frac{1}{2}}{2} = \dots$$

To obtain the accuracy of  $10^{-2}$ , we use the result:

$$|x_n - \alpha| \le \frac{\lambda^n}{1 - \lambda} |x_1 - x_0|, \ n \ge 1$$

and we impose that

$$\frac{\lambda^n}{1-\lambda}|x_1 - x_0| \le 10^{-2}$$

which obviously will impose that  $|x_n - \alpha| \le 10^{-2}$ .

$$\frac{\lambda^n}{1-\lambda}|x_1 - x_0| \le 10^{-2} \iff \frac{\frac{1}{4^n}}{1-\frac{1}{4}} \left| \pi + \frac{1}{2} - \pi \right| \le \frac{1}{100} \iff 100$$

$$\iff \frac{1}{3 \cdot 4^{n-1}} \cdot \frac{1}{2} \le \frac{1}{100} \iff 6 \cdot 4^{n-1} \ge 100 \iff 4^{n-1} \ge \frac{100}{6} = 16.(6) \implies n = 4.$$

Remark 4.7 The theory is in Lecture 11, pp. 14-16. Examples are in Lecture 11, pp. 17.

**Example 4.8** Approximate  $\sqrt{10}$  using two iterations of the Newton's method.

If we let  $x = \sqrt{10}$ , then  $x^2 = 10$  and  $x^2 - 10 = 0$  so we can consider the equation f(x) = 0 with  $f(x) = x^2 - 10$  and f'(x) = 2x. f(3) = -1 < 0, f(4) = 6 > 0 so we can take the interval [3, 4].

Let the first approximation be 4, so  $x_0 = 4$ . We have then

$$x_1 = x_0 - \frac{f(x_0)}{f'(x_0)} = 4 - \frac{6}{8} = \frac{26}{8} = 3.25$$

and

$$x_2 = x_1 - \frac{f(x_1)}{f'(x_1)} = 3.25 - \frac{0.5625}{6.5} \approx 3.16.$$

**Remark 4.9** If you have to solve the equation f(x) = 0, but you do not have the interval, you can use the following result:

If f is continuous on [a,b] and  $f(a) \cdot f(b) < 0$ , then there is at least one point  $c \in (a,b)$  such that f(c) = 0.

So, first try to find two values of the function f of opposite signs to determine the interval. Then you can use a suitable method to solve the nonlinear equation f(x) = 0. You can use other results from Calculus (Rolle's Theorem, monotony of function - table of variation, etc.) to find more about the roots.

Some notions are found in Lecture 11, pp. 1–2.

Remark 4.10 See Lecture 12 for Newton's method for nonlinear systems (pp. 8–10), Numerical approximation for multiple roots (pp. 4–8).