PMS – Exercise Sheet 8

Exercise 1

Initialization

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

$$b = \begin{pmatrix} 6 \\ 6 \\ 6 \end{pmatrix}$$

$$x_0 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

First iteration

$$d_0 = b - A * x_0 = \begin{pmatrix} 6 \\ 6 \\ 6 \end{pmatrix} - \begin{pmatrix} 1 & 1 & 4 \\ 1 & 1 & 1 \\ 4 & 1 & 1 \end{pmatrix} * \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} = \begin{pmatrix} 6 \\ 6 \\ 6 \end{pmatrix}$$

$$r_0 = d_0 = \begin{pmatrix} 6 \\ 6 \\ 6 \end{pmatrix}$$

$$\alpha_0 = \frac{r_0{}^T * r_0}{d_0{}^T * A * d_0} = \frac{\begin{pmatrix} 6 \\ 6 \\ 6 \end{pmatrix}^T * \begin{pmatrix} 6 \\ 6 \\ 6 \end{pmatrix}}{\begin{pmatrix} 6 \\ 6 \\ 6 \end{pmatrix}^T * \begin{pmatrix} 1 & 1 & 4 \\ 1 & 1 & 1 \\ 4 & 1 & 1 \end{pmatrix} * \begin{pmatrix} 6 \\ 6 \\ 6 \end{pmatrix}} = \frac{1}{5}$$

$$x_1 = x_0 + \alpha_0 d_0 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix} + \frac{1}{5} \begin{pmatrix} 6 \\ 6 \\ 6 \end{pmatrix} = \begin{pmatrix} \frac{6}{5} \\ \frac{6}{5} \\ \frac{6}{5} \end{pmatrix}$$

Second iteration

$$r_1 = r_0 - \alpha_0 A * d_0 = \begin{pmatrix} 6 \\ 6 \\ 6 \end{pmatrix} - \frac{1}{5} \begin{pmatrix} 1 & 1 & 4 \\ 1 & 1 & 1 \\ 4 & 1 & 1 \end{pmatrix} * \begin{pmatrix} 6 \\ 6 \\ 6 \end{pmatrix} = \begin{pmatrix} -\frac{6}{5} \\ \frac{12}{5} \\ -\frac{6}{5} \end{pmatrix}$$

$$\beta_1 = \frac{{r_1}^T r_1}{{r_0}^T r_0} = \frac{\begin{pmatrix} -\frac{6}{5} \\ \frac{12}{5} \\ -\frac{6}{5} \end{pmatrix}^T * \begin{pmatrix} -\frac{6}{5} \\ \frac{12}{5} \\ -\frac{6}{5} \end{pmatrix}}{\begin{pmatrix} 6 \\ 6 \\ 6 \end{pmatrix}^T * \begin{pmatrix} 6 \\ 6 \\ 6 \end{pmatrix}} = \frac{2}{25}$$

$$d_1 = r_1 + \beta_1 d_0 = \begin{pmatrix} -\frac{6}{5} \\ \frac{12}{5} \\ -\frac{6}{5} \end{pmatrix} + \frac{2}{25} \begin{pmatrix} 6 \\ 6 \\ 6 \end{pmatrix} = \begin{pmatrix} -\frac{18}{25} \\ \frac{72}{25} \\ -\frac{18}{25} \end{pmatrix}$$

$$\alpha_1 = \frac{{r_1}^T * r_1}{{d_1}^T * A * d_1} = \frac{\begin{pmatrix} -\frac{6}{5} \\ \frac{12}{5} \\ -\frac{6}{5} \end{pmatrix}^T * \begin{pmatrix} -\frac{6}{5} \\ \frac{12}{5} \\ -\frac{6}{5} \end{pmatrix}}{\begin{pmatrix} -\frac{18}{25} \\ \frac{72}{25} \\ -\frac{18}{25} \end{pmatrix}^T * \begin{pmatrix} 1 & 1 & 4 \\ 1 & 1 & 1 \\ 4 & 1 & 1 \end{pmatrix} * \begin{pmatrix} -\frac{18}{25} \\ \frac{72}{25} \\ -\frac{18}{25} \end{pmatrix}} = \frac{5}{3}$$

$$x_2 = x_1 + \alpha_1 d_1 = \begin{pmatrix} \frac{6}{5} \\ \frac{6}{5} \\ \frac{6}{5} \end{pmatrix} + \frac{5}{3} \begin{pmatrix} -\frac{18}{25} \\ \frac{72}{25} \\ -\frac{18}{25} \end{pmatrix} = \begin{pmatrix} 0 \\ 6 \\ 0 \end{pmatrix}$$

$$r_2 = r_1 - \alpha_1 A * d_1 = \begin{pmatrix} -\frac{6}{5} \\ \frac{12}{5} \\ -\frac{6}{5} \end{pmatrix} - \frac{5}{3} \begin{pmatrix} 1 & 1 & 4 \\ 1 & 1 & 1 \\ 4 & 1 & 1 \end{pmatrix} * \begin{pmatrix} -\frac{18}{25} \\ \frac{72}{25} \\ -\frac{18}{25} \end{pmatrix} = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}$$

Stop, residuum $r_2 = 0 \Rightarrow$ the calculated optimum $x_2 = \begin{pmatrix} 0 \\ 6 \\ 0 \end{pmatrix}$ will not change anymore.

Exercise 2

a) As each step of the algorithm finds the local minimum of one dimension, for a 3-dimensional systems it will at most take three iterations.

b) In large systems, the conjugate gradient algorithm allows for fast approximation, doing only a few iterations until the solution is "good enough". Gauss elimination does not allow this.

   Additionally, it is sufficient to know the product Ax (in physical calculations, this equals calculating forces). This is an advantage over other approaches, where A has to be known explicitly, especially when A is very sparse.

c) A has to be a symmetric, positive-definite matrix. All symmetric matrices are also square.

d)
   - A negative-definite $\Rightarrow$ global maximum can be found with CG. In our opinion, the algorithm will work nevertheless, as $d_i^T A d_i$ will be negative, which leads to ascending steps.
   - According to the lecture: A singular positive indefinite $\Rightarrow$ No unique minimum. CG calculates just one possible Minimum. (Note: We are not sure whether positive *in*definite matrices even exist...)
   - A indefinite $\Rightarrow$ saddlepoint problem. CG won't work (or one step-size should be ∞, because one can find a point at which one can walk indefinitely and still get smaller objective function values).

- A not square $\Rightarrow$ if $A \in \mathbb{R}^{m \times n}$ with $m > n$ (A has more rows than colums) this is a *linear curve fitting problem*. This can be solved by decomposing A in a specific way and solving another system of linear equations (which can again be done using CG).