Exercise 5. (Conjugate gradient method)

Solve the linear system

$$\begin{pmatrix} 1 & 0 & 0 \\ 0 & 2 & 0 \\ 0 & 0 & 3 \end{pmatrix} \begin{pmatrix} x \\ y \\ z \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} \quad \Leftrightarrow \quad A\boldsymbol{x} = \boldsymbol{b}$$

using the conjugate-gradient method.

Solution

Define

$$f(\boldsymbol{x}) = \frac{1}{2}\boldsymbol{x}^T A\boldsymbol{x} - \boldsymbol{b}^T\boldsymbol{x} \quad \Rightarrow \quad \nabla f(\boldsymbol{x}) = A\boldsymbol{x} - \boldsymbol{b}.$$

If $\boldsymbol{x}^*$ minimizes $f(\boldsymbol{x})$, then $\nabla f(\boldsymbol{x}^*) = 0$, and $\boldsymbol{x}^*$ will be the solution of the linear system.

We use the conjugate-gradient method for the minimization of $f(\boldsymbol{x})$.

- First step.

$$\boldsymbol{x}^0 = \begin{pmatrix} 0 \\ 0 \\ 0 \end{pmatrix}, \nabla f(\boldsymbol{x}^0) = \begin{pmatrix} -1 \\ -1 \\ -1 \end{pmatrix}, \boldsymbol{z}^1 = -\nabla f(\boldsymbol{x}^0) = \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix}.$$

Minimizing $f(x^0 + \alpha_1 \boldsymbol{z}^1)$ with respect to α_1 we get

$$\alpha_1^* = -\frac{(\boldsymbol{z}^1)^T \nabla f(\boldsymbol{x}^0)}{(\boldsymbol{z}^1)^T A(\boldsymbol{z}^1)} = \frac{1}{2}.$$

- $$\boldsymbol{x}^1 = x^0 + \alpha_1^* \boldsymbol{z}^1 = \begin{pmatrix} 1/2 \\ 1/2 \\ 1/2 \end{pmatrix}, \quad \Rightarrow \quad \nabla f(\boldsymbol{x}^1) = \begin{pmatrix} -1/2 \\ 0 \\ 1/2 \end{pmatrix}.$$

So

$$\boldsymbol{z}^2 = -\nabla f(\boldsymbol{x}^1) + \frac{(\nabla f(\boldsymbol{x}^1))^T \nabla f(\boldsymbol{x}^1)}{(\nabla f(\boldsymbol{x}^0))^T \nabla f(\boldsymbol{x}^0)} \boldsymbol{z}^1 = \begin{pmatrix} 1/2 \\ 0 \\ -1/2 \end{pmatrix} + \frac{1/2}{3} \begin{pmatrix} 1 \\ 1 \\ 1 \end{pmatrix} = \begin{pmatrix} 2/3 \\ 1/6 \\ -1/3 \end{pmatrix}.$$

Minimizing $f(x^1 + \alpha_2 \boldsymbol{z}^2)$ with respect to α_2 we get

$$\alpha_2^* = -\frac{(\boldsymbol{z}^2)^T \nabla f(\boldsymbol{x}^1)}{(\boldsymbol{z}^2)^T A(\boldsymbol{z}^2)} = \frac{1/2}{5/6} = \frac{3}{5}.$$

- $$\boldsymbol{x}^2 = x^1 + \alpha_2^* \boldsymbol{z}^2 = \begin{pmatrix} 9/10 \\ 3/5 \\ 3/10 \end{pmatrix}, \quad \Rightarrow \quad \nabla f(\boldsymbol{x}^2) = \begin{pmatrix} -1/10 \\ 1/5 \\ -1/10 \end{pmatrix}.$$

So

$$\boldsymbol{z}^3 = -\nabla f(\boldsymbol{x}^2) + \frac{(\nabla f(\boldsymbol{x}^2))^T \nabla f(\boldsymbol{x}^2)}{(\nabla f(\boldsymbol{x}^1))^T \nabla f(\boldsymbol{x}^1)} \boldsymbol{z}^2 = \begin{pmatrix} 1/10 \\ -1/5 \\ 1/10 \end{pmatrix} + \frac{6/100}{1/2} \begin{pmatrix} 2/3 \\ 1/6 \\ -1/3 \end{pmatrix} = \begin{pmatrix} 9/50 \\ -9/50 \\ 3/50 \end{pmatrix}.$$

Minimizing $f(x^2 + \alpha_3 \boldsymbol{z}^3)$ with respect to α_3 we get

$$\alpha_3^* = -\frac{(\boldsymbol{z}^3)^T \nabla f(\boldsymbol{x}^2)}{(\boldsymbol{z}^3)^T A(\boldsymbol{z}^3)} = \frac{3/50}{27/250} = \frac{5}{9}.$$

- $$\boldsymbol{x}^3 = x^2 + \alpha_3^* \boldsymbol{z}^3 = \begin{pmatrix} 1 \\ 1/2 \\ 1/3 \end{pmatrix},$$

which is the minimum searched.