Numerieke technieken en optimalisatie

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Any questions? Do not hesitate to contact us!

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Exercise 4.1: (Conjugate gradient (CG) method)

Let $A \in \mathbb{R}^{n \times n}$ be a symmetric positive definite matrix, and let $\overline{x}$ be the solution to

$$A\overline{x} = b.$$

We say that u and v are conjugate if

$$(u, v)_A := (u, Av) = 0.$$

A corresponding norm is defined as $\| \cdot \|_A := (u, u)_A$.

a) Let $u, v \in \mathbb{R}^n \setminus \{0\}$. Prove that if $(u, v)_A = 0$, then u and v are linearly independent.

Answer. Supose $\alpha_1 u + \alpha_2 v = 0$ for some $\alpha_1, \alpha_2 \in \mathbb{R}$. Then

$$\begin{aligned}
(\alpha_1 u + \alpha_2 v, u)_A &= (0, u)_A \\
\alpha_1 (u, u)_A + \alpha_2 (v, u)_A &= (0, u)_A \\
\alpha_1 (u, Au) + \alpha_2 \cancel{(v, u)_A} &= 0 \\
\alpha_1 (u, Au) &= 0
\end{aligned}$$

Then α_1 should be 0. And

$$\begin{aligned}
(\alpha_1 u + \alpha_2 v, v)_A &= (0, v)_A \\
\alpha_1 (u, v)_A + \alpha_2 (v, v)_A &= (0, v)_A \\
\alpha_1 \cancel{(u, v)_A} + \alpha_2 (v, Av) &= 0 \\
\alpha_2 (v, Av) &= 0
\end{aligned}$$

Then α_2 should be 0. So we can conclude that u, v are L.I.

b) Let $U_k = \text{span}\{p_0, \dots, p_k\}$ with pairwise conjugate vectors p_k. Show that

$$x_{k+1} = \underset{x \in U_k}{\text{argmin}} \|x - \overline{x}\|_A$$

is equivalent to

$$x_{k+1} = \sum_{j=0}^{k} \frac{(p_j, b)}{(p_j, p_j)_A} p_j.$$

Answer. First we will show that $\operatorname{argmin}_{x\in U_k} \|x-\overline{x}\|_A = \operatorname{argmin}_{x\in U_k} F(x)$

$$\begin{aligned}
\|x-\overline{x}\|_A &= (x-\overline{x}, Ax-A\overline{x}) \\
&= (x-\overline{x}, Ax-b) \\
&= (x,Ax)-(x,b)-(\overline{x},Ax)+(\overline{x},b) \\
&= (x,Ax)-(x,b)-(A\overline{x},x)+(\overline{x},b) \longrightarrow \text{ Symmetry of } A \\
&= (x,Ax)-2(x,b)+(\overline{x},b)
\end{aligned}$$

Then we can reformulate our problem as

$$\begin{aligned}
\operatorname*{argmin}_{x\in U_k} \|x-\overline{x}\|_A &= \operatorname*{argmin}_{x\in U_k} \left[(x,Ax)-2(x,b)+(\overline{x},b)\right] \\
&= \operatorname*{argmin}_{x\in U_k} \left[\frac{1}{2}(x,Ax)-(x,b)\right] = \operatorname*{argmin}_{x\in U_k} F(x)
\end{aligned}$$

Now is enough to proof that $\operatorname{argmin}_{x\in U_k} F(x) = \sum_{j=0}^{k} \frac{(p_j,b)}{(p_j,p_j)_A} p_j$.

Notice that for all $x \in U_k$: $x = (\alpha_0 p_0 + \cdots + \alpha_k p_k)$ with $\alpha_i \in \mathbb{R}$ for $i = 1, \ldots, k$ and

$$\begin{aligned}
F(x) &= \frac{1}{2} x^T A x - x^T b \\
&= \frac{1}{2}(\alpha_0 p_0 + \cdots + \alpha_k p_k)^T A (\alpha_0 p_0 + \cdots + \alpha_k p_k) - (\alpha_0 p_0 + \cdots + \alpha_k p_k)^T b \\
&= \sum_{j=0}^{k} \frac{1}{2} (\alpha_j p_j)^T A (\alpha_j p_j) - \sum_{j=0}^{k} (\alpha_j p_j)^T b = \sum_{j=0}^{k} F(\alpha_j p_j)
\end{aligned}$$

Then $\operatorname{argmin}_{x\in U_k} F(x) = \operatorname{argmin}_{\alpha_j p_j \in U_k} \sum_{j=0}^{k} F(\alpha_j p_j) = \sum_{j=0}^{k} \operatorname{argmin}_{\alpha_j\in\mathbb{R}} F(\alpha_j p_j)$

For all $j = 1, \ldots, k$ we can compute $F(\alpha_j p_j) = \alpha_j \left[\frac{1}{2}\alpha_j p_j A p_j - p_j b\right]$ and

$$\frac{\partial F(\alpha_j p_j)}{\partial \alpha_j} = \alpha_j p_j^T A p_j - p_j^T b$$

then

$$\frac{\partial F(\alpha_j p_j)}{\partial \alpha_j} = 0 \iff \alpha_j = \frac{(p_j,b)}{(p_j,p_j)_A} := \bar{\alpha_j}$$

In conclusion

$$\begin{aligned}
\operatorname*{argmin}_{x\in U_k} \|x-\overline{x}\|_A &= \sum_{j=0}^{k} \operatorname*{argmin}_{\alpha_j\in U_k} F(\alpha_j p_j) \\
&= \bar{\alpha_j} p_j = \frac{(p_j,b)}{(p_j,p_j)_A} p_j
\end{aligned}$$

c) Prove that the CG method yields the exact solution after at most n steps.

Answer. The step number n of CG is

$$x_n = \sum_{j=0}^{n-1} \frac{(p_j,b)}{(p_j,p_j)_A} p_j$$

then for all $\ell = 0, \dots n-1$ we have

$$\begin{aligned} p_\ell^T A x_n &= \sum_{j=0}^{n-1} \frac{(p_j, b)}{(p_j, p_j)_A} p_\ell^T A p_j \\ &= \frac{(p_\ell, b)}{(p_\ell, p_\ell)_A} p_\ell^T A p_\ell \longrightarrow \text{ def. Conjugate } (\textbf{??}) \\ &= (p_\ell, b) \end{aligned}$$

In conclusion $[P]\, A x_n = [P]\, b$ where $[P]$ is the matrix with all the vectors p_ℓ and this implies that $A x_n = b$.

Exercise 4.2

a) Consider the following linear system:

$$\begin{pmatrix} 1 & 2 \\ 2 & 5 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 3 \\ 7 \end{pmatrix}$$

and the starting point $x^{(0)} = (2, 2)^T$.

1) Is it possible to apply the CG method to solve this linear system?

Answer. Yes, because $A = A^t$ and $\det(A - \lambda I) = (1-\lambda)(5-\lambda) - 4 = 0 \to \lambda_1 = 5.83$ and $\lambda_2 = 0.17$, i.e A is positive definite.

2) Find the quadratic functional (to minimize) associated to this system.

Answer.

$$\begin{aligned} F(x) &= \frac{1}{2} \begin{pmatrix} x \\ y \end{pmatrix}^t \begin{pmatrix} 1 & 2 \\ 2 & 5 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} - \begin{pmatrix} x \\ y \end{pmatrix}^t \begin{pmatrix} 3 \\ 7 \end{pmatrix} \\ &= \frac{1}{2} x^2 + 2xy + \frac{5}{2} y^2 - 3x - 7y \end{aligned}$$

3) Find the solution of this problem using the CG method.

Answer.

$$
\begin{aligned}
r_0 &= b - Ax = \begin{pmatrix} -3 \\ -7 \end{pmatrix} \\
p_0 &= r_0 \\
\alpha_0 &= \frac{r_0^t r_0}{p_0 t A p_0} = 0.1716 \\
x_1 &= \begin{pmatrix} 1.48 \\ 0.79 \end{pmatrix} \\
r_1 &= \begin{pmatrix} -0.0828 \\ 0.0355 \end{pmatrix} \\
\beta_1 &= 1.4005 \times 10^{-4} \\
p_1 &= \begin{pmatrix} -0.0833 \\ 0.0345 \end{pmatrix} \\
\alpha_1 &= 5.8272 \\
x_2 &= \begin{pmatrix} 1 \\ 1 \end{pmatrix} \\
r_2 &= \begin{pmatrix} -0.26 \\ 0.71 \end{pmatrix} \times 10^{-14} \\
\beta_2 &= 7.08 \times 10^{-27} \\
p_2 &= \begin{pmatrix} 0.2665 \\ 0.7105 \end{pmatrix} \times 10^{-14}
\end{aligned}
$$

The solution is $x_2 = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$.

b) Figure 1 is a contour plot of $F(X)$ for

$$
\begin{pmatrix} 2 & 1 \\ 1 & 3 \end{pmatrix} \begin{pmatrix} x \\ y \end{pmatrix} = \begin{pmatrix} 3 \\ 4 \end{pmatrix}
$$

Start at $x^{(0)} = (-2, 4)^T$ and sketch a few steps of the steepest descent method.

MATLAB CODE!!!

Exercise 4.3 (Matlab)

a) Suppose that an object can be at any one of $n+1$ equally spaced points $x_0, x_1, ..., x_n$. When an object is at location x_i , it is equally likely to move to either x_{i-1} or x_{i+1} and cannot directly move to any other location. Consider the probabilities $\{P_i\}_{i=0}^n$ that an object starting at location x_i will reach the left endpoint x_0 before reaching the right endpoint x_n. Clearly, $P_0 = 1$ and $P_n = 0$. Since the object can move to x_i only from x_{i-1} or x_{i+1} and does so with probability $\frac{1}{2}$ for each of these locations.

$$
P_i = \frac{1}{2} P_{i-1} + \frac{1}{2} P_{i+1} \quad \text{for each } i = 1, 2, ..., n-1.
$$

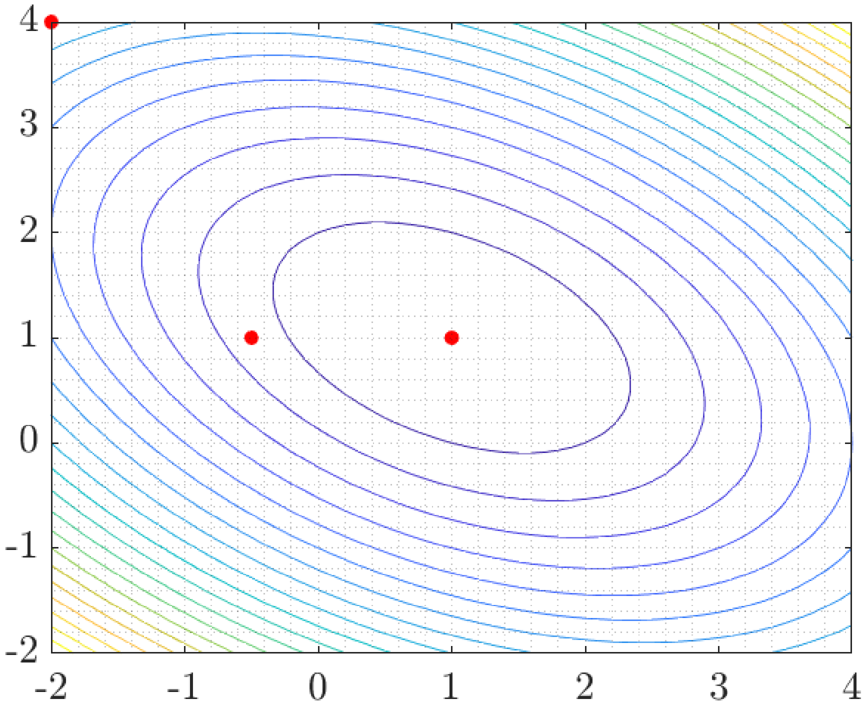

Figure 1: **Answer.** Exercise 4.2

(i) Show that

$$\begin{pmatrix} 1 & -\frac{1}{2} & & & & & \\ -\frac{1}{2} & 1 & -\frac{1}{2} & & & & \\ & -\frac{1}{2} & 1 & -\frac{1}{2} & & & \\ & & & \cdots & & & \\ & & & & -\frac{1}{2} & 1 & -\frac{1}{2} \\ & & & & & -\frac{1}{2} & 1 \end{pmatrix} \begin{pmatrix} P_1 \\ P_2 \\ \vdots \\ P_{n-1} \end{pmatrix} = \begin{pmatrix} \frac{1}{2} \\ 0 \\ \vdots \\ 0 \end{pmatrix}$$

b) Write a Matlab code to solve this system using conjugate gradient method. Test your code with $n = 10, 50, 100$.

c) Compare your results against a Monte Carlo simulation for this case.

Monte Carlo method is a class of numerical methods that relies on random sampling.
`- First, the input random variables are sampled.`
`- Second, for each sample, a calculation is performed to obtain the outputs. Due to the randomness in the inputs, the outputs are also random variables.`
`- Finally, the statistics of the output random variables are computed, which estimates the output.`

MATLAB CODE!!!