Numerieke methoden 2

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Exercise 5.1: (Least-squares method)

a) Let $A \in \mathbb{R}^{m \times n}$ with rank(A) = n. The condition number of A is defined by

$$\kappa_2(A) := \frac{\max_{x \neq 0} \frac{\|Ax\|_2}{\|x\|_2}}{\min_{x \neq 0} \frac{\|Ax\|_2}{\|x\|_2}}.$$
 (1)

1) Show that when A is invertible (so that m = n), $\kappa_2(A) = ||A||_2 ||A^{-1}||_2$, so the definitions of condition numbers coincide for quadratic matrices.

Answer. By definition we have

$$||A||_2 = \max_{x \neq 0} \frac{||Ax||_2}{||x||_2}$$

and

$$\kappa_2(A) = \frac{\max\limits_{x \neq 0} \frac{\|Ax\|_2}{\|x\|_2}}{\min\limits_{x \neq 0} \frac{\|Ax\|_2}{\|x\|_2}} = \|A\|_2 \cdot \frac{1}{\min\limits_{x \neq 0} \frac{\|Ax\|_2}{\|x\|_2}}$$

But

$$||A^{-1}||_{2} = \max_{x \neq 0} \frac{||A^{-1}x||_{2}}{||x||_{2}}$$

$$= \max_{x \neq 0} \frac{||A^{-1}x||_{2}}{||AA^{-1}x||_{2}}$$

$$= \max_{A^{-1}x \neq 0} \frac{||A^{-1}x||_{2}}{||AA^{-1}x||_{2}}$$

$$= \max_{y \neq 0} \frac{||y||_{2}}{||Ay||_{2}}$$

$$= \frac{1}{\min_{y \neq 0} \frac{||Ay||_{2}}{||y||_{2}}}$$

and we can conclude that $\kappa_2(A) = ||A||_2 ||A^{-1}||_2$.

2) Prove from (1) that for any $x, y \in \mathbb{R}^n$

$$\frac{\|y\|_2}{\|x\|_2} \le \kappa_2(A) \frac{\|Ay\|_2}{\|Ax\|_2}.$$
 (2)

Answer. We know that

$$\kappa_2(A) = \frac{\max_{x \neq 0} \frac{\|Ax\|_2}{\|x\|_2}}{\min_{x \neq 0} \frac{\|Ax\|_2}{\|x\|_2}} = \max_{x \neq 0} \frac{\|Ax\|_2}{\|x\|_2} \cdot \max_{y \neq 0} \frac{\|y\|_2}{\|Ay\|_2}$$
$$= \max_{x,y \neq 0} \frac{\|Ax\|_2}{\|x\|_2} \frac{\|y\|_2}{\|Ay\|_2}$$

Then we can conclude that

$$\kappa_2(A) \ge \frac{\|Ax\|_2}{\|x\|_2} \frac{\|y\|_2}{\|Ay\|_2} \quad \forall x, y \in \mathbb{R}^n - \{0\}$$

with this we have

$$\frac{\|y\|_2}{\|x\|_2} \le \kappa_2(A) \frac{\|Ay\|_2}{\|Ax\|_2}.$$

b) Let \bar{x} be the least-squares solution to $||Ax - b||_2 \to \min$. Show that the vector $A\bar{x} - b$ is perpendicular to the hyperplane spanned by the Ax's, i.e.

$$A\bar{x} - b \perp Ax, \quad \forall x \in \mathbb{R}^n$$

and therefore $||A\bar{x} - b||_2^2 + ||A\bar{x}||_2^2 = ||b||_2^2$ and $\cos(\theta) := \frac{||A\bar{x}||_2}{||b||_2} \le 1$ is well-defined.

Answer.

$$A\bar{x} - b \perp Ax$$

$$\langle Ax, A\bar{x} - b \rangle = 0 \iff$$

$$(Ax)^{t}(A\bar{x} - b) = 0 \iff$$

$$x^{t}A^{t}(A\bar{x} - b) = 0 \iff$$

$$x^{t}A^{t}A\bar{x} - x^{t}A^{t}b = 0 \iff$$

$$x^{t}(A^{t}A\bar{x} - A^{t}b) = 0 \text{ (Stelling 7)}$$

Take the particular \bar{x} , we just proved that $(A\bar{x}, A\bar{x} - b) = 0$. Then

$$||A\bar{x} - b||_{2}^{2} + ||A\bar{x}||_{2}^{2} = (A\bar{x} - b, A\bar{x} - b) + (A\bar{x}, A\bar{x})$$

$$= (A\bar{x}, A\bar{x}) - 2(A\bar{x}, b) + (b, b) + (A\bar{x}, A\bar{x})$$

$$= 2(A\bar{x}, A\bar{x}) - 2(A\bar{x}, b) + (b, b)$$

$$= 2(A\bar{x}, A\bar{x} - b) + (b, b)$$

$$= (b, b) = ||b||_{2}^{2}$$

Using Pitagoras' theorem we have $\cos(\theta) := \frac{\|A\bar{x}\|_2}{\|b\|_2} \le \frac{\|b\|_2}{\|b\|_2} = 1$.

c) Notice that Δx is the least-square solution to system $Ay = \Delta b$. Then applying a) and b) above, you can now prove

$$\frac{\|\Delta x\|_2}{\|\bar{x}\|_2} \le \frac{\kappa_2(A)}{\cos(\theta)} \frac{\|\Delta b\|_2}{\|b\|_2}.$$

Answer. Using the part (1) we have

$$\frac{\|\Delta x\|_2}{\|\bar{x}\|_2} \le \kappa_2(A) \frac{\|A\Delta x\|_2}{\|A\bar{x}\|_2}.$$

Moreover,

$$\begin{split} \frac{\|\Delta x\|_{2}}{\|\bar{x}\|_{2}} &\leq \kappa_{2}(A) \frac{\|A\Delta x\|_{2}}{\|A\bar{x}\|_{2}} \\ &= \kappa_{2}(A) \frac{\|A\Delta x\|_{2}}{\|A\bar{x}\|_{2}} \frac{\|A\bar{x}\|_{2}}{\|b\|_{2}} \frac{\|b\|_{2}}{\|A\bar{x}\|_{2}} \\ &= \kappa_{2}(A) \frac{\|A\Delta x\|_{2}}{\|b\|_{2}} \frac{\|b\|_{2}}{\|A\bar{x}\|_{2}} \\ &= \frac{\kappa_{2}(A)}{\cos(\theta)} \frac{\|A\Delta x\|_{2}}{\|b\|_{2}} \\ &\leq \frac{\kappa_{2}(A)}{\cos(\theta)} \frac{\|\Delta b\|_{2}}{\|b\|_{2}} \end{split}$$

Exercise 5.2: (Least-squares method)

a) Find a solution to $||Ax - b||_2 \to \min$ by solving the equation $A^T A \bar{x} = A^T b$ for

$$A = \begin{pmatrix} 1 & 3 \\ 1 & -1 \\ 1 & 1 \end{pmatrix}, \quad b = \begin{pmatrix} 5 \\ 1 \\ 0 \end{pmatrix}.$$

Compute the least-square error $||A\bar{x} - b||_2$ associated with the least-squares solution you found.

Answer. Define the new system

$$A^T A = \begin{pmatrix} 3 & 3 \\ 3 & 11 \end{pmatrix}$$

and

$$A^T b = \begin{pmatrix} 6\\14 \end{pmatrix}$$

Then

$$A^T A \bar{x} = A^T b \longrightarrow \bar{x} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

Now we can compute the error

$$A\bar{x} = \begin{pmatrix} 4 \\ 0 \\ 2 \end{pmatrix}$$

then

$$||A\bar{x} - b||_2 = ||\begin{pmatrix} -1\\-1\\2 \end{pmatrix}||_2 = \sqrt{6} = 2.4495$$

b) Use the factorization A = QU to find the least-squares solution $||Ax - b||_2 \to \min$ for

$$A = \begin{pmatrix} 2 & 3 \\ 2 & 4 \\ 1 & 1 \end{pmatrix}, \quad b = \begin{pmatrix} 7 \\ 3 \\ 1 \end{pmatrix}.$$

Answer. Using Given's rotations the factorization of A is A = QU with

$$Q = \begin{pmatrix} -0.5774 & 0.7071 & -0.4082 \\ -0.5774 & -0.7071 & -0.4082 \\ -0.5774 & 0 & -0.8165 \end{pmatrix}$$

and

$$U = \begin{pmatrix} -1.7321 & -1.7321 \\ 0 & 2.8284 \\ \mathbf{0} & \mathbf{0} \end{pmatrix}$$

then

$$\hat{b} = Q^T b = \begin{pmatrix} -3.4641 \\ 2.828 \\ \mathbf{2.4495} \end{pmatrix}$$

$$\begin{pmatrix} -1.7321 & -1.7321 \\ 0 & 2.8284 \end{pmatrix} \bar{x} = \begin{pmatrix} -3.4641 \\ 2.828 \end{pmatrix} \longrightarrow \bar{x} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$

Now we can compute the error

$$||A\bar{x} - b||_2 = ||-\sqrt{6}||_2 = 2.4495$$

Exercise 5.3: Non-uniqueness of minimalization problems

Consider the problem

$$\left\| \frac{x-1}{x} \right\|_1 \to \min.$$

Does it have a solution? Is it unique?

Answer.

Consider the problem

$$\begin{vmatrix} x-1 \\ x \end{vmatrix}_1 \to \min.$$

First we can compute the norm-1 of the vector

$$\begin{vmatrix} x - 1 \\ x \end{vmatrix} = |x - 1| + |x|$$

- Case 1. If $x \le 0$ then $|x 1| + |x| = -x + 1 x = 1 2x \ge 1$.
- Case 2. If 0 < x < 1 then |x 1| + |x| = x + 1 x = 1.
- Case 3. If $x \ge 1$ then $|x 1| + |x| = x 1 + x = 2x 1 \ge 1$.

And we can conclude

$$\begin{vmatrix} x - 1 \\ x \end{vmatrix}_1 = |x - 1| + |x| \ge 1 := \min, \quad \forall x$$

but the solution is not unique, because for every $x \in [0,1]$

$$\left\| \frac{x-1}{x} \right\|_1 = 1 = \min.$$

Exercise 5.4: Linear regression

Assume you are given a set of points (x_i, y_i) , $1 \le i \le N$, with $x_i \ne x_j, i \ne j$, and you want to find $m \in \mathbb{R}$ and $b \in \mathbb{R}$ such that, for f(x) := mx + b, these parameters minimize

$$\sum_{i=1}^{N} |f(x_i) - y_i|^2.$$

Show how to obtain m and b.

Answer.

Using ex.4.2 we know that $||Ax - c||_2 \to \min$ by solving $A^tAx = A^tc$ and now we want to minimize the following problem

$$\min_{m,b\in\mathbb{R}} \|mx - b - y\|_2^2$$

Define

$$A = \begin{pmatrix} x_1 & \cdots & 1 \\ \vdots & & \vdots \\ x_N & \cdots & 1 \end{pmatrix} \text{ and } c = \begin{pmatrix} y_1 \\ \vdots \\ y_N \end{pmatrix}$$

then

$$A^t A = \begin{pmatrix} \sum x_i^2 & \sum x_i \\ \sum x_i & N \end{pmatrix}$$
 and $A^t c = \begin{pmatrix} \sum x_i y_i \\ \sum y_i \end{pmatrix}$

We can solve $A^tAx = A^tc$ using Gaussian reduction:

$$\begin{pmatrix} \sum x_i^2 & \sum x_i & \sum x_i y_i \\ \sum x_i & N & \sum y_i \end{pmatrix} \xrightarrow{R_1:N:R_1 \text{ and } R_2:-\sum x_i:R_2} \begin{pmatrix} N \sum x_i^2 & N \sum x_i & N \sum x_i y_i \\ -(\sum x_i)^2 & -N \sum x_i & -\sum x_i \sum y_i \end{pmatrix}$$

$$\underbrace{\longrightarrow}_{R_2:R_1+R_2 \text{ and } R_1:1/N\cdot R_1} \begin{pmatrix} \sum x_i^2 & \sum x_i & \sum x_iy_i \\ N\sum x_i^2 - (\sum x_i)^2 & 0 & N\sum x_iy_i - \sum x_i\sum y_i \end{pmatrix}$$

Then
$$m = \frac{N \sum x_i y_i - \sum x_i \sum y_i}{N \sum x_i^2 - (\sum x_i)^2}$$
 and $b = \frac{\sum y_i - (m \sum x_i)}{N}$.