Numerieke technieken en optimalisatie

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All computation may be done with Matlab.

Exercise 1.1: Warm-up

a) Suppose that in a biological system there are n species of animals and m sources of food. Let x_j represent the population of the jth species, for each $j = 1, \cdots, n$; b_i represent the available daily supply of the ith food; and a_{ij} represent the amount of the ith food consumed on the average by a member of the jth species. The linear system

$$\begin{aligned} a_{11}x_1 + a_{12}x_2 + \cdots + a_{1n}x_n &= b_1 \\ a_{21}x_1 + a_{22}x_2 + \cdots + a_{2n}x_n &= b_2 \\ \vdots &= \vdots \\ a_{m1}x_1 + a_{m2}x_2 + \cdots + a_{mn}x_n &= b_m \end{aligned}$$

represents an equilibrium where there is a daily supply of food to precisely meet the average daily consumption of each species. Let

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

1. If $x = (100, 50, 35, 40)^t$ and $b = (350, 270, 90)^t$ is there sufficient food to satisfy the average daily consumption?.

Answer. For each ith food ($i = 1, 2, 3$) we need to show that $[Ax]_i := [\hat{b}]_i \leq [b]_i$.

$$Ax = \hat{b} = \begin{pmatrix} 320 \\ 250 \\ 75 \end{pmatrix}$$

clearly, $\hat{b} \leq b$ component-wise and there is an extra supply of food $b^\star = b - \hat{b} = (302015)^t$.

2. What is the maximum number of animals of each species that could be individually added to the system with the supply of food still meeting the consumption?

Answer. For each jth specie ($j = 1, 2, 3, 4$) we need to find Δx_j such that

$$\max_{\Delta x_j} \{[A(x + \Delta x_j \vec{e}_j)]_i \leq [b]_i,\ i = 1, 2, 3\}$$

$$\max_{\Delta x_j} \left\{[A \Delta x_j \vec{e}_j]_i \leq [b]_i - [\hat{b}]_i,\ i = 1, 2, 3\right\}$$

$$\max_{\Delta x_j} \left\{[A \Delta x_j \vec{e}_j]_i \leq [b]_i - [\hat{b}]_i,\ i = 1, 2, 3\right\}$$

After some algebraic operations we find that $\Delta x_1 \leq 20$, $\Delta x_2 \leq 15$, $\Delta x_3 \leq 10$ and $\Delta x_4 \leq 10$.

b) Suppose that our computer can only store 2 significant digits (the first two nonzero digits of a number, e.g. 0.967 stored as 0.97, 1.23 stored as 1.2). Consider the linear systems given by augmented matrices

$$\begin{pmatrix} .001 & 1 & 3 \\ 1 & 2 & 5 \end{pmatrix} \quad \text{and} \quad \begin{pmatrix} 1 & 2 & 5 \\ .001 & 1 & 3 \end{pmatrix}$$

Do the elimination exactly, round the numbers in the results to 2 significant digits. Then use backward substitution to find the solutions. What do you observe? Which solution is accurate?

Answer. For the first matrix we have:

$$\begin{pmatrix} .001 & 1 & 3 \\ 1 & 2 & 5 \end{pmatrix} \overrightarrow{1000 \cdot R1} \begin{pmatrix} 1 & 1000 & 3000 \\ 1 & 2 & 5 \end{pmatrix} \overrightarrow{R2 - R1} \begin{pmatrix} 1 & 1000 & 3000 \\ 0 & -998 & -2995 \end{pmatrix}$$
$$\overrightarrow{-R2/998} \begin{pmatrix} 1 & 1000 & 3000 \\ 0 & 1 & 3 \end{pmatrix} \overrightarrow{R1 - 1000 \cdot R2} \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 3 \end{pmatrix}$$

For the second matrix we have:

$$\begin{pmatrix} 1 & 2 & 5 \\ .001 & 1 & 3 \end{pmatrix} \overrightarrow{R2 - 0.01 \cdot R1} \begin{pmatrix} 1 & 2 & 5 \\ 0 & 0.998 \approx 1 & 2.995 \approx 3 \end{pmatrix} \overrightarrow{R1 - 2 \cdot R2} \begin{pmatrix} 1 & 0 & -1 \\ 0 & 1 & 3 \end{pmatrix}$$

Then $x_1 = (0, 3)^t$ and $x_2 = (-1, 3)^t$.

When we compute the result of Ax_1 and Ax_2 we obtain:

$$Ax_1 = \begin{pmatrix} 3 \\ 6 \end{pmatrix} \text{ and } Ax_2 = \begin{pmatrix} 5 \\ 3 \end{pmatrix}$$

This means that the solution x_2 is more accurate.

Exercise 1.2: (Norm of a matrix)

The norm of a square matrix A, w.r.t. to a vector norm $\|\cdot\|$, is defined by $||A|| := \sup_{x \neq 0} \frac{||Ax||}{||x||}$.

a) Prove that for any $A, B \in \mathbb{R}^{n \times n}$:

1) $||A|| = \sup_{||x||=1} ||Ax||$

Answer. If $x \neq 0$ then we can define $u = \frac{x}{||x||}$ and $||u|| = 1$,

$$\begin{aligned} ||A|| :&= \sup_{x \neq 0} \frac{||Ax||}{||x||} \\ &= \sup_{x \neq 0} ||A\frac{x}{||x||}|| = \sup_{||u||=1} ||Au|| \end{aligned}$$

2) $||A + B|| \leq ||A|| + ||B||$

Answer.

$$\begin{aligned} ||A+B|| :&= \sup_{x\neq 0} \frac{||(A+B)x||}{||x||} = \sup_{x\neq 0} \frac{||Ax+Bx||}{||x||} \\ &\leq \sup_{x\neq 0} \frac{||Ax||+||Bx||}{||x||} = \sup_{x\neq 0} \frac{||Ax||}{||x||} + \sup_{x\neq 0} \frac{||Ax||}{||x||} \\ &= ||A|| + ||B|| \end{aligned}$$

3) $||AB|| \leq ||A||||B||$

Answer. Case $x = 0$ is trivial. For all $x \neq 0$, first we show that $\|Ax\| \leq \|A\|\|x\|$:

$$\begin{aligned} \frac{||Ax||}{||x||} &\leq \sup_{y\neq 0} \frac{||Ay||}{||y||} \\ &= \sup_{y\neq 0} ||A\frac{y}{||y||}|| = ||A|| \longrightarrow ||Ax|| \leq ||A||||x|| \end{aligned}$$

Therefore we have that:

$$\begin{aligned} ||AB|| &= \sup_{||u||=1} ||ABu|| \leq \sup_{||u||=1} ||A||||Bu|| \\ &= ||A|| \sup_{||u||=1} ||Bu|| = ||A||||B|| \end{aligned}$$

Exercise 1.3: (Condition Number)

The condition number of an invertible matrix is defined as $\kappa(A) = \|A\|\|A^{-1}\|$.

a) Prove that the following are true for invertible A and B.

1) $\kappa(A) = \kappa(A^{-1})$ and $\kappa(A) \geq 1$;

Answer. For the first part we have:

$$\kappa(A^{-1}) = \|A^{-1}\|\|(A^{-1})^{-1}\| = \|A^{-1}\|\|A\| = \|A\|\|A^{-1}\| = \kappa(A)$$

Moreover,

$$1 = \|A\,A^{-1}\| \leq \|A\|\|A^{-1}\| = \kappa(A)$$

2) $\kappa(AB) \leq \kappa(A)\kappa(B)$;

Answer. Using the definition of the condition number we have:

$$\begin{aligned} \kappa(AB) &= \|AB\|\|(AB)^{-1}\| = \|AB\|\|B^{-1}A^{-1}\| \\ &\leq \|A\|\|B\|\|B^{-1}\|\|A^{-1}\| \\ &= \|A\|\|A^{-1}\|\,\|B\|\|B^{-1}\| = \kappa(A)\kappa(B) \end{aligned}$$

3) $\kappa(aA) = \kappa(A)$ for any $a \in \mathbb{R}^{\neq 0}$.

Answer. Assume $a \in \mathbb{R}^{\neq 0}$, using the definition of condition number we have:

$$\begin{aligned} \kappa(aA) &= \|aA\|\|(aA)^{-1}\| = \|aA\|\|\frac{1}{a}A^{-1}\| \\ &= a\,\frac{1}{a}\,\|A\|\|A^{-1}\| = \kappa(A) \end{aligned}$$

b) Solve the following two linear systems $Ax = b$ given by augmented matrices

$$\begin{pmatrix} 1 & 1/2 & 3/2 \\ 1/2 & 1/3 & 1 \end{pmatrix}, \quad \text{and} \quad \begin{pmatrix} 1 & 1/2 & 3/2 \\ 1/2 & 1/3 & 5/6 \end{pmatrix}.$$

What do you observe? Compute the condition number $\kappa_2(A)$ here.

Answer.

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A = [ 1  1/2;  1/2  1/3]

% normA   = sqrt(max(eig(A'*A)))
% normA1  = norm(A,2)
condA    = cond(A)

b1 = [3/2  1]'
b2 = [3/2  5/6]'

sol1  = A\b1
sol2  = A\b2

err1  = A*sol1-b2
err2  = A*sol2-b1


cota1  = condA*norm(inv(A)*b1)*norm(b1-b2)/norm(b1)
cota2  = condA*norm(inv(A)*b2)*norm(b1-b2)/norm(b2)

delta_X  = norm(sol1-sol2)
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The condition number is $\kappa_2(A) = 19.28$, *it is an indicator of how much a change Δb can affect the solution x of $Ax = b$.*

$$\|\Delta x\| \leq \kappa(A)\|Ab_1\|\frac{\|\Delta b\|}{\|b_1\|} = 5.34$$

$$\|\Delta x\| \leq \kappa(A)\|Ab_2\|\frac{\|\Delta b\|}{\|b_2\|} = 2.64$$

$$\|\Delta x\|_{real} = 2.23$$

Exercise 1.4: (Perturbations and eigenvalues)

a) Let A be a symmetric and positive definite matrix. Show that $x = \sum_{i=1}^{n}(c_i/\lambda_i)v_i$ is the solution of the linear system $Ax = b$ if and only if $b = \sum_{i=1}^{n} c_i v_i$, where λ_i are the eigenvalues of A and v_i are the corresponding eigenvalues.

Answer. - Suppose that $x = \sum_{i=1}^{n}(c_i/\lambda_i)v_i$ is the solution of $Ax = b$, then

$$Ax = \sum_{i=1}^{n}(c_i/\lambda_i)\, A\, v_i = \sum_{i=1}^{n}(c_i/\lambda_i)\, \lambda_i\, v_i = \sum_{i=1}^{n} c_i v_i$$

- Suppose that $b = \sum_{i=1}^n c_i v_i$, then

$$b = \sum_{i=1}^n c_i v_i = \sum_{i=1}^n c_i \frac{\lambda_i v_i}{\lambda_i} = \sum_{i=1}^n c_i \frac{A v_i}{\lambda_i} = A \sum_{i=1}^n c_i \frac{v_i}{\lambda_i} = Ax$$

b) Consider the following linear system

$$\begin{pmatrix} 1001 & 1000 \\ 1000 & 1001 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \end{pmatrix}.$$

Using (a) explain why, when $b = (2001, 2001)^T$, a small change $\Delta b = (1, 0)^T$ produces large variations in the solution, while, conversely, when $b = (1, -1)^T$, a small variation $\Delta x = (0.001, 0)^T$ in the solution induces a large change in b.

Answer. The eigenvalues of A are $\lambda = 1, 2001$ and the eigenvector are $v = (1, 1)^t, (1, -1)^t$.
First we assume small changes in b:

$$b = \begin{pmatrix} 2001 \\ 2001 \end{pmatrix} = 2001 \begin{pmatrix} 1 \\ 1 \end{pmatrix} + 0 \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$
$$b + \Delta b = \begin{pmatrix} 2002 \\ 2001 \end{pmatrix} = \underbrace{2001.5}_{c1} \begin{pmatrix} 1 \\ 1 \end{pmatrix} + \underbrace{0.5}_{c2} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

and the solution affected as follows

$$x = \frac{2001}{2001} \begin{pmatrix} 1 \\ 1 \end{pmatrix} + 0 \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \begin{pmatrix} 1 \\ 1 \end{pmatrix}$$
$$\hat{x} = \frac{2001.5}{2001} \begin{pmatrix} 1 \\ 1 \end{pmatrix} + \frac{1}{2} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \begin{pmatrix} 1.5 \\ 0.5 \end{pmatrix}$$

Small changes in b $\rightarrow$ other eigenvalue gains importance.

On the other hand, assume small changes in x:

$$b = \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \underbrace{0}_{c1} \begin{pmatrix} 1 \\ 1 \end{pmatrix} + \underbrace{1}_{c2} \begin{pmatrix} 1 \\ -1 \end{pmatrix} \longrightarrow x = 0 + \frac{1}{1} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

and $\hat{x} = x + \Delta x$ is such that:

$$\hat{x} = \begin{pmatrix} 1.001 \\ -1 \end{pmatrix} = \frac{c1}{2001} \begin{pmatrix} 1 \\ 1 \end{pmatrix} + \frac{c2}{1} \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$
$$\hat{b} = \frac{2001}{2001} \begin{pmatrix} 1 \\ 1 \end{pmatrix} + \frac{2001}{2000} \begin{pmatrix} 1 \\ -1 \end{pmatrix} = \begin{pmatrix} 2.001 \\ 0 \end{pmatrix} \neq \begin{pmatrix} 1 \\ -1 \end{pmatrix}$$

Small changes in x $\rightarrow$ other eigenvalue gains importance.

This is a typical behaviour when one has large difference in eigenvalues and big condition number $\kappa(A) = 2000$.

Exercise 1.5: (QU decomposition)

a) (Prove Theorem 2) Let $Q, \bar{Q} \in \mathbb{R}^{n\times n}$ be orthogonal matrices. Show that

1) $\|Qx\|_2 = \|x\|_2$ for any $x \in \mathbb{R}$. Thus, $\|QA\|_2 = \|A\|_2$ for any $A \in \mathbb{R}^{n\times n}$.

Answer.

$$\|Qx\|_2 = \sqrt{(Qx)^t(Qx)^t} = \sqrt{x^tQ^tQx} = \sqrt{x^tx} = \|x\|_2$$
$$\|QA\|_2 = \sup_{||u||_2=1} ||QAu||_2 = \sup_{||u||_2=1} ||Au||_2 = ||A||_2$$

2) $\kappa_2(Q) = 1$.

Answer.

$$\kappa_2(Q) = \|Q\|_2\|Q^{-1}\|_2 = \sqrt{\lambda_{max}(Q^tQ)}\sqrt{\lambda_{max}((Q^{-1})^t(Q^{-1}))} = \sqrt{\lambda_{max}(I)}\sqrt{\lambda_{max}(I)} = 1$$

3) $Q\bar{Q}$ is orthogonal.

Answer.

$$(Q\bar{Q})^{-1} = \bar{Q}^{-1}Q^{-1} = \bar{Q}^tQ^t = (Q\bar{Q})^t$$

b) If $A = QU$ is the QU decomposition of A, show that $Ax = b$ is equivalent to a upper-triangular system.

Answer.

$$A = QU \rightarrow Ax = b \rightarrow QUx = b$$
$$Ux = Q^{-1}b = Q^tb = \bar{b} \rightarrow Ux = \bar{b}$$