STAT 309: MATHEMATICAL COMPUTATIONS I
FALL 2021
PROBLEM SET 2

For the coding problems, use any program you like but present your codes and results in a way that is comprehensible to someone who is unfamiliar with that program (e.g. comment your codes appropriately).

1. The files required for this problem can be found in the subfolder `hw2` under 'Files' in Canvas or at `http://www.stat.uchicago.edu/~lekheng/courses/309/stat309-hw2/`. The matrix in `processed.mat` (Matlab format) or `processed.txt` (comma separated, plain text) is a 49×7 matrix where each row is indexed by a country in `row.txt` and each column is indexed by a demographic variable in `column.txt`, ordered as in the respective files. So for example, if we denote the matrix by

$$A = \begin{bmatrix} \mathbf{a}_1^{\mathsf{T}} \\ \mathbf{a}_2^{\mathsf{T}} \\ \vdots \\ \mathbf{a}_{49}^{\mathsf{T}} \end{bmatrix} = [\boldsymbol{\alpha}_1, \dots, \boldsymbol{\alpha}_7] = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{17} \\ a_{21} & a_{22} & \cdots & a_{27} \\ \vdots & \vdots & \ddots & \vdots \\ a_{49,1} & a_{49,2} & \cdots & a_{49,7} \end{bmatrix} \in \mathbb{R}^{49 \times 7},$$

then $a_{23} = -0.2743$ is Austria's population per square kilometers (row index 2 = Austria, column index 3 = population per square kilometers). As you probably notice, this matrix has been slightly preprocessed. If you want to see the raw data, you can find them in `raw.txt` (e.g. the actual value for Austria's population per square kilometers is 84) but you don't need the raw data for this problem.

(a) Show that to plot the projections of the row vectors (i.e., samples) $\mathbf{a}_1, \dots, \mathbf{a}_{49} \in \mathbb{R}^7$ onto the two-dimensional subspace $\operatorname{span}\{\mathbf{v}_j, \mathbf{v}_k\} \cong \mathbb{R}^2$, we may simply plot the n points

$$\{(\sigma_j u_{ij}, \sigma_k u_{ik}) \in \mathbb{R}^2 : i = 1, \dots, 49\}$$

where $U = [u_{ij}] \in \mathbb{R}^{49 \times 49}$ and $\Sigma = \operatorname{diag}(\sigma_1, \dots, \sigma_p) \in \mathbb{R}^{49 \times 7}$ are the matrix of left singular vectors and matrix of singular values respectively.

(b) Find the first two right singular vectors of A, $\mathbf{v}_1, \mathbf{v}_2 \in \mathbb{R}^7$. Project the data onto the two-dimensional space $\operatorname{span}\{\mathbf{v}_1, \mathbf{v}_2\} \cong \mathbb{R}^2$. Plot this in a graph where the x- and y-axes correspond to $\mathbf{v}_1$ and $\mathbf{v}_2$ respectively and where the points correspond to the countries — label each point by the country it corresponds to. Identify the two obvious outliers.

(c) Now do the same with the two left singular vectors of A, $\mathbf{u}_1, \mathbf{u}_2 \in \mathbb{R}^{49}$. Project the column vectors (i.e., variables) $\boldsymbol{\alpha}_1, \dots, \boldsymbol{\alpha}_7 \in \mathbb{R}^{49}$ onto the two-dimensional space $\operatorname{span}\{\mathbf{u}_1, \mathbf{u}_2\} \cong \mathbb{R}^2$ and plot this in a graph as before. Note that in this case, the points correspond to the demographic variables — label them accordingly.

(d) Overlay the two graphs in (b) and (c). Identify the two demographic variables near the two outlier countries — these explain why the two countries are outliers.

(e) Remove the two outlier countries and redo (b) with this 47×7 matrix. This allows you to see features that were earlier obscured by the outliers. Which two European countries are most alike Japan?

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The graphs[1] in (b) and (c) are called *scatter plots* and the overlayed one in (d) is called a *biplot*. See `http://en.wikipedia.org/wiki/Biplot` for more information. The reason we didn't need to adjust the scale of the axes using the singular values of A like in the Wikipedia description is because the preprocessing has taken care of the scaling; if we had started from the raw data, then we would need to deal with this complication.

2. Let $A, B \in \mathbb{R}^{m\times n}$.

(a) Suppose $n \le m$. Show that

$$\min_{X^{\mathsf{T}}X=I} \|AX - B\|_F$$

is given by $X = UV^{\mathsf{T}}$ where $A^{\mathsf{T}}B = U\Sigma V^{\mathsf{T}}$ is a singular value decomposition.

(b) Suppose A has full column rank. Show that the following method produces a symmetric matrix $X \in \mathbb{R}^{n\times n}$ that solves

$$\min_{X^{\mathsf{T}}=X} \|AX - B\|_F. \tag{2.1}$$

(i) Show that the SVD of A takes the form

$$A = U \begin{bmatrix} \Sigma \\ O \end{bmatrix} V^{\mathsf{T}}$$

where $U \in \mathbb{R}^{m\times m}$, $V \in \mathbb{R}^{n\times n}$ are unitary matrices and $\Sigma = \operatorname{diag}(\sigma_1, \dots, \sigma_n) \in \mathbb{R}^{n\times n}$ is a diagonal matrix.

(ii) Show that

$$\|AX - B\|_F^2 = \|\Sigma Y - C_1\|_F^2 + \|C_2\|_F^2$$

where $Y = V^{\mathsf{T}}XV$ and $C = \begin{bmatrix} C_1 \\ C_2 \end{bmatrix} = U^{\mathsf{T}}BV$.

(iii) Note that Y must be symmetric if X is. Show that

$$\|\Sigma Y - C_1\|_F^2 = \sum_{i=1}^{n} |\sigma_i y_{ii} - c_{ii}|^2 + \sum_{j>i} \left(|\sigma_i y_{ij} - c_{ij}|^2 + |\sigma_j y_{ij} - c_{ji}|^2 \right)$$

and deduce that the minimum value of (2.1) is attained when

$$y_{ij} = \frac{\sigma_i c_{ij} + \sigma_j c_{ji}}{\sigma_i^2 + \sigma_j^2}$$

for all $i, j = 1, \dots, n$.

(c) Show that

$$\min_{X\in\mathbb{R}^{n\times m}} \|AX - I_m\|_F$$

has a unique solution when A has full column rank. What is the minimum length solution, i.e., where $\|X\|_F$ is minimum?

3. Let $A \in \mathbb{C}^{m\times n}$ and $\mathbf{b} \in \mathbb{C}^m$. We will discuss a variant of $A\mathbf{x} \approx \mathbf{b}$ where the error occurs only in A. Note that in ordinary least squares we assume that the error occurs only in $\mathbf{b}$ while in total least squares we assume that it occurs in both A and $\mathbf{b}$.

(a) Show that if $0 \ne \mathbf{x} \in \mathbb{C}^n$, then

$$\left\| A \left(I - \frac{\mathbf{x}\mathbf{x}^*}{\mathbf{x}^*\mathbf{x}} \right) \right\|_F^2 = \|A\|_F^2 - \frac{\|A\mathbf{x}\|_2^2}{\mathbf{x}^*\mathbf{x}}.$$

[1] One point to observe is that all the information needed for all three plots are already contained in the SVD of A, i.e., in U, Σ, and V; it is just a matter of deciding which numbers to plot against which numbers.

(b) Show that the matrix

$$E = \frac{(\mathbf{b} - A\mathbf{x})\mathbf{x}^*}{\mathbf{x}^*\mathbf{x}} \in \mathbb{C}^{m\times n}$$

has the smallest 2-norm among all $E \in \mathbb{C}^{m\times n}$ that satisfy

$$(A+E)\mathbf{x} = \mathbf{b}.$$

(c) Let A, $\mathbf{b}$, and $\mathbf{x}$ be given and fixed. What are the solutions of

$$\min_{(A+E)\mathbf{x}=\mathbf{b}} \|E\|_2 \qquad \text{and} \qquad \min_{(A+E)\mathbf{x}=\mathbf{b}} \|E\|_F$$

where the minimum is taken over all $E \in \mathbb{C}^{m\times n}$ such that $(A+E)\mathbf{x} = \mathbf{b}$?

(d) Given $\mathbf{a} \in \mathbb{C}^n$, $\mathbf{b} \in \mathbb{C}^m$, and $\delta > 0$. Show how to solve the problems

$$\min_{\|E\|_F \le \delta} \|E\mathbf{a} - \mathbf{b}\|_2 \qquad \text{and} \qquad \max_{\|E\|_F \le \delta} \|E\mathbf{a} - \mathbf{b}\|_2$$

over all $E \in \mathbb{C}^{m\times n}$.

4. In the following, $\kappa(A) := \|A\|\|A^\dagger\|$ for $A \in \mathbb{C}^{m\times n}$ where $\|\cdot\|$ denotes a submultiplicative matrix norm. We will write $\kappa_p(A)$ if the norm involved is a matrix p-norm.

(a) Show that for any nonzero $A \in \mathbb{C}^{m\times n}$,

$$\kappa(A) \ge 1.$$

(b) Show that for any $A \in \mathbb{C}^{m\times n}$,

$$\kappa_2(A^*A) = \kappa_2(A)^2$$

but that in general

$$\kappa(A^*A) \ne \kappa(A)^2.$$

(c) Show that for nonsingular $A, B \in \mathbb{C}^{n\times n}$,

$$\kappa(AB) \le \kappa(A)\kappa(B).$$

Is this true in general without the nonsingular condition?

(d) Let $Q \in \mathbb{C}^{m\times n}$ be a matrix with orthonormal columns. Show that

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

Is this true if Q has orthonormal rows instead? Is this true with κ_1 or κ_∞ in place of κ_2?

(e) Let $R \in \mathbb{C}^{n\times n}$ be a nonsingular upper-triangular matrix. Show that

$$\kappa_\infty(R) \ge \frac{\max_{i=1,\dots,n}|r_{ii}|}{\min_{i=1,\dots,n}|r_{ii}|}.$$

(f) Show that for any nonsingular $A \in \mathbb{C}^{n\times n}$,

$$\kappa(A) \ge \max\left\{\frac{\|AX - I\|}{\|XA - I\|}, \frac{\|XA - I\|}{\|AX - I\|}\right\}.$$

(*Hint:* $AX - I = A(XA - I)A^{-1}$.)

5. We will examine the effect of various parameters on the accuracy of a computed solution to a nonsingular linear system. Relevant commands in Matlab syntax are given in brackets.

(a) Generate $A = [a_{ij}] \in \mathbb{R}^{n\times n}$ as follows:

(i) a_{ij} randomly generated from a standard normal distribution [`randn(n)`];

(ii) a Hilbert matrix, i.e., $a_{ij} = 1/(i+j-1)$ [`hilb(n)`];

(iii) a Pascal matrix, i.e., the entries $a_{ij} = \binom{i+j}{i}$ [`pascal(n)`];

(iv) a magic square, i.e., the entries a_{ij}'s are the integers $1, 2, \dots, n^2$ arranged in a way that A has equal row, column, and diagonal sums [`magic(n)`].

$$\texttt{hilb(4)} = \begin{bmatrix} 1 & 1/2 & 1/3 & 1/4 \\ 1/2 & 1/3 & 1/4 & 1/5 \\ 1/3 & 1/4 & 1/5 & 1/6 \\ 1/4 & 1/5 & 1/6 & 1/7 \end{bmatrix}, \quad \texttt{pascal(4)} = \begin{bmatrix} 1 & 1 & 1 & 1 \\ 1 & 2 & 3 & 4 \\ 1 & 3 & 6 & 10 \\ 1 & 4 & 10 & 20 \end{bmatrix}, \quad \texttt{magic(4)} = \begin{bmatrix} 16 & 2 & 3 & 13 \\ 5 & 11 & 10 & 8 \\ 9 & 7 & 6 & 12 \\ 4 & 14 & 15 & 1 \end{bmatrix}$$

For simplicity, we will assume that A is stored exactly with no errors even though this is only true for those matrices with integer-valued entries.

(b) Generate $\mathbf{x}$ and $\mathbf{b} \in \mathbb{R}^n$ as follows:
  (i) $\mathbf{x} = [1, \dots, 1]^{\mathsf{T}}$ [`ones(n,1)`];
  (ii) $\mathbf{b} = A\mathbf{x}$ [`b = A*x`].

(c) For each A generated as above, perform the following for $n = 5, 10, 15, \dots, 500$.
  (i) Solve $A\mathbf{x} = \mathbf{b}$ using your program to get $\widehat{\mathbf{x}}$ [`xhat = A\\b`]. Note that in general the result computed by your program will not be exactly the true solution $\mathbf{x} = A^{-1}\mathbf{b}$ because of roundoff errors that occurred during computations.
  (ii) Compute $\Delta\mathbf{b} = A\widehat{\mathbf{x}} - \mathbf{b}$ and record the values of $\|\mathbf{x} - \widehat{\mathbf{x}}\|/\|\mathbf{x}\|$, $\kappa(A) = \|A\|\|A^{-1}\|$ and $\kappa(A)\|\Delta\mathbf{b}\|/\|\mathbf{b}\|$for $\|\cdot\| = \|\cdot\|_1$, $\|\cdot\|_2$, and $\|\cdot\|_\infty$.
  (iii) Present everything for the $n = 5$ case but only tabulate the relevant trend for general $n > 5$ in a graph.

(d) Discuss and explain the effects of different choices of A, $\mathbf{b}$, $\|\cdot\|$, and n have on the accuracy of the computed solution $\widehat{\mathbf{x}}$.

(e) Instead of solving the linear system directly, compute A^{-1} and then $\widehat{\mathbf{x}} := A^{-1}\mathbf{b}$ [`xhat = inv(A)*b`]. Comment on the accuracy of this approach. Provide numerical evidence to support your conclusion.

(f) Write a program that computes the $(1,1)$-entry of the matrix A^{-1} that does not involve computing A^{-1}, i.e., if $A^{-1} = [b_{ij}]$, you want the value b_{11} but you are not allowed to compute A^{-1}.

6. Let $A \in \mathbb{R}^{n\times n}$ be nonsingular and let $\mathbf{0} \neq \mathbf{b} \in \mathbb{R}^n$. Let $\mathbf{x} = A^{-1}\mathbf{b} \in \mathbb{R}^n$. In the following, $\Delta A \in \mathbb{R}^{n\times n}$ and $\Delta\mathbf{b} \in \mathbb{R}^n$ are some arbitrary matrix and vector. We assume that the norm on A satisfies $\|A\mathbf{x}\| \leq \|A\|\|\mathbf{x}\|$ for all $A \in \mathbb{R}^{n\times n}$ and all $\mathbf{x} \in \mathbb{R}^n$.

(a) Show that if $\Delta A \in \mathbb{R}^{n\times n}$ is any matrix satisfying

$$\frac{\|\Delta A\|}{\|A\|} < \frac{1}{\kappa(A)}, \tag{6.2}$$

then $A + \Delta A$ must be nonsingular. (*Hint*: If $A + \Delta A$ is singular, then there exists nonzero $\mathbf{v}$ such that $(A + \Delta A)\mathbf{v} = \mathbf{0}$).

(b) Suppose $(A + \Delta A)(\mathbf{x} + \Delta\mathbf{x}) = \mathbf{b}$ and $\hat{\mathbf{x}} = \mathbf{x} + \Delta\mathbf{x}$. Show that

$$\frac{\|\Delta\mathbf{x}\|}{\|\hat{\mathbf{x}}\|} \leq \kappa(A)\frac{\|\Delta A\|}{\|A\|}. \tag{6.3}$$

(c) Suppose $(A + \Delta A)(\mathbf{x} + \Delta\mathbf{x}) = \mathbf{b}$ and $\hat{\mathbf{x}} = \mathbf{x} + \Delta\mathbf{x}$ and (6.2) is satisfied. Show that

$$\frac{\|\Delta\mathbf{x}\|}{\|\mathbf{x}\|} \leq \frac{\kappa(A)\dfrac{\|\Delta A\|}{\|A\|}}{1 - \kappa(A)\dfrac{\|\Delta A\|}{\|A\|}}.$$

You may like to use the following outline:
  (i) Show that

$$\Delta\mathbf{x} = -A^{-1}\Delta A\hat{\mathbf{x}}$$

and so

$$\|\Delta\mathbf{x}\| \leq \kappa(A)\frac{\|\Delta A\|}{\|A\|}(\|\mathbf{x}\| + \|\Delta\mathbf{x}\|).$$

(ii) Rewrite this inequality as

$$\left(1-\kappa(A)\frac{\|\Delta A\|}{\|A\|}\right)\|\Delta\mathbf{x}\| \le \kappa(A)\frac{\|\Delta A\|}{\|A\|}\|\mathbf{x}\|$$

and use (6.2).

(d) Suppose $(A+\Delta A)\hat{\mathbf{x}} = \mathbf{b}+\Delta\mathbf{b}$ where $\hat{\mathbf{b}} = \mathbf{b}+\Delta\mathbf{b} \neq \mathbf{0}$ and $\hat{\mathbf{x}} = \mathbf{x}+\Delta\mathbf{x} \neq \mathbf{0}$. Show that

$$\frac{\|\Delta\mathbf{x}\|}{\|\hat{\mathbf{x}}\|} \le \kappa(A)\left(\frac{\|\Delta A\|}{\|A\|} + \frac{\|\Delta\mathbf{b}\|}{\|\hat{\mathbf{b}}\|} + \frac{\|\Delta A\|}{\|A\|}\frac{\|\Delta\mathbf{b}\|}{\|\hat{\mathbf{b}}\|}\right). \tag{6.4}$$

You may like to use the following outline:

(i) Show that

$$\Delta\mathbf{x} = A^{-1}(\Delta\mathbf{b} - \Delta A\hat{\mathbf{x}})$$

and so

$$\frac{\|\Delta\mathbf{x}\|}{\|\hat{\mathbf{x}}\|} \le \kappa(A)\left(\frac{\|\Delta A\|}{\|A\|} + \frac{\|\Delta\mathbf{b}\|}{\|A\|\|\hat{\mathbf{x}}\|}\right). \tag{6.5}$$

(ii) Show that

$$\frac{1}{\|\hat{\mathbf{x}}\|} \le \frac{\|A\| + \|\Delta A\|}{\|\hat{\mathbf{b}}\|}. \tag{6.6}$$

(iii) Combine (6.5) and (6.6) to get (6.4).

(e) Suppose $(A+\Delta A)\hat{\mathbf{x}} = \mathbf{b}+\Delta\mathbf{b}$ where $\hat{\mathbf{b}} = \mathbf{b}+\Delta\mathbf{b} \neq \mathbf{0}$ and $\hat{\mathbf{x}} = \mathbf{x}+\Delta\mathbf{x} \neq \mathbf{0}$ and (6.2) is satisfied. Use the same ideas in (b) to deduce that

$$\frac{\|\Delta\mathbf{x}\|}{\|\mathbf{x}\|} \le \frac{\kappa(A)\left(\dfrac{\|\Delta A\|}{\|A\|} + \dfrac{\|\Delta\mathbf{b}\|}{\|\mathbf{b}\|}\right)}{1-\kappa(A)\dfrac{\|\Delta A\|}{\|A\|}}.$$