Homework 3

Due Date: September 16 Grace Etzel

Complete the assignment in Google Colab and typeset your wite-up in LaTeX. Show all work and code, and provide clear justifications for your answers. Submissions that are messy or poorly organized may be returned with a grade of zero.

Link to Google Colab: link

Problem 1. Understanding operations counts and computational costs. Remember to show all steps; no coding required.

(a) The approximate operation count for the Gaussian elimination is $\frac{2n^3}{3}$. Estimate how much longer it would take to solve a system if the size n is quadrupled. Express your answer as a multiple of the original time.

Solution. We denote the quadrupled form as 4n. We plug this into the elimination to get

$$\frac{2(4n)^3}{3} = 64\left(\frac{2n^3}{3}\right).$$

That is, the cost increases by 64 units.

(b) Suppose your computer performs a back substitution for a 5000×5000 upper-triangular system in 0.005 seconds. Use the estimates

Back substitution:
$$n^2$$
, Elimination: $\frac{2n^3}{3}$.

to estimate how long it would take to perform a full Gaussian elimination for a 5000×5000 system. Round your answer to the nearest second.

Solution. Denote C_1 as the numerical cost for backward substitution. We are given

$$C_1 = n^2$$

= 5000^2
= $25,000,000$.

Next, we want to compute for a constant that allows to interchange between time units and cost units. So, let α denote this constant so that $C_1 = \alpha t$, where t is in seconds. Then, to solve for α we have

$$\alpha = \frac{C_1}{t}$$

$$= \frac{25,000,000}{0.005}$$

$$= 5,000,000,000.$$

Then, we denote C_2 as the Gaussian Elimination cost. To find the cost in time, we consider

$$t = \frac{C_2}{\alpha}$$

$$= \frac{\frac{2n^3}{3}}{\alpha}$$

$$= \frac{\frac{2(5000)^3}{3}}{50000000000}$$

$$= \frac{250}{15}$$

$$= \frac{50}{3}$$

This gives us a elimination time cost of 17 seconds.

- (c) On the same computer, assume back substitution for a 4000×4000 upper-triangular system takes 0.002 seconds. Now estimate:
 - The time required for forward elimination, and
 - The time for back substitution

when solving a general system of size 9000×9000 . Use the same operation count assumptions and round your answer to the nearest second.

Solution. We use the same notation as before. First, we find α , which gives us

$$\alpha = \frac{C_1}{t}$$

$$= \frac{4000^2}{0.002}$$

$$= 8,000,000,000.$$

Next, we are interested in solving for the forward elimination t time in seconds for a 9000×9000 matrix. That is,

$$t = \frac{C_2}{\alpha}$$

$$= \frac{\frac{2n^3}{3}}{\alpha}$$

$$= \frac{\frac{2(9000)^3}{3}}{\alpha}$$

$$= \frac{\frac{2(9000)^3}{3}}{8,000,000,000}$$

$$= 60.75.$$

That is, the cost for the forward elimination is 61 seconds. Next, we want to consider the cost for back substitution. Then,

$$t = \frac{n^2}{\alpha}$$

$$= \frac{9000^2}{8,000,000,000}$$

$$= 0.01.$$

That is, the backward substitution is 0.01 seconds.

- (d) Suppose you want to solve 1000 different systems, all with the same coefficient matrix A (of size 9000×9000) but different right-hand sides \vec{b} . Compare the total time required using
 - Full Gaussian elimination on each system, versus
 - LU decomposition once, followed by back substitution for each right-hand side.

Clearly justify which method is more efficient and by how much.

Solution. Note that the LU factorization costs about n^2 whereas the Gaussian elimination costs about $\frac{2n^3}{3}$. If we are solving 1000 different systems using a 9000 \times 9000 matrix, we can use the estimates above to compare the costs. For the LU factorization, we have

$$LU = 1000(0.01) = 10$$
 seconds

For the Gaussian Elimination, we have

Elimination =
$$1000(61) = 61,000$$
 seconds.

Then, the LU method takes 61+10=71. Notice that the LU method is more efficient, since it lowers costs by 60,929 seconds.

Problem 2. Solving Hilbert systems and analyzing conditioning. Let $H \in \mathbb{R}^{n \times n}$ be the Hilbert matrix with $H_{ij} = \frac{1}{i+j-1}$ and let $\vec{b} = 1$.

- (a) Hand Calculation for n = 3.
 - (1) Gaussian elimination: Solve $H\vec{x} = \vec{b}$ by elimination. Show the row operations (or the equivalent elimination steps) and the back-substitution, and report the final \vec{x}_{GE} .

Solution. When we compute H, we get

$$H = \begin{pmatrix} 1 & \frac{1}{2} & \frac{1}{4} \\ \frac{1}{2} & \frac{1}{3} & \frac{1}{4} \\ \frac{1}{3} & \frac{1}{4} & \frac{1}{5} \end{pmatrix}.$$

We will use Gaussian Elimination to find x_1 , x_2 , and x_3 :

$$\begin{pmatrix}
1 & \frac{1}{2} & \frac{1}{4} & 1 \\
\frac{1}{2} & \frac{1}{3} & \frac{1}{4} & 1 \\
\frac{1}{3} & \frac{1}{4} & \frac{1}{5} & 1
\end{pmatrix} (-\frac{1}{2}R_1 + R_2 \mapsto R_2) \qquad \begin{pmatrix}
1 & \frac{1}{2} & \frac{1}{4} & 1 \\
0 & \frac{1}{12} & \frac{1}{12} & \frac{1}{2} \\
\frac{1}{3} & \frac{1}{4} & \frac{1}{5} & 1
\end{pmatrix}$$

$$(-\frac{1}{3}R_1 + R_3 \mapsto R_3) \qquad \begin{pmatrix}
1 & \frac{1}{2} & \frac{1}{4} & 1 \\
0 & \frac{1}{12} & \frac{1}{12} & \frac{1}{2} \\
0 & \frac{1}{12} & \frac{4}{45} & \frac{2}{3}
\end{pmatrix}$$

$$(12R_2 \mapsto R_2) \qquad \begin{pmatrix}
1 & \frac{1}{2} & \frac{1}{4} & 1 \\
0 & 1 & 1 & 6 \\
0 & \frac{1}{12} & \frac{4}{45} & \frac{2}{3}
\end{pmatrix}$$

$$(-\frac{1}{12}R_2 + R_3 \mapsto R_3) \qquad \begin{pmatrix}
1 & \frac{1}{2} & \frac{1}{4} & 1 \\
0 & 1 & 1 & 6 \\
0 & 0 & \frac{1}{180} & \frac{1}{6}
\end{pmatrix}$$

$$(180R_3 \mapsto R_3) \qquad \begin{pmatrix}
1 & \frac{1}{2} & \frac{1}{4} & 1 \\
0 & 1 & 1 & 6 \\
0 & 0 & \frac{1}{180} & \frac{1}{6}
\end{pmatrix}$$

Next, we use backward substitution to obtain the solution. First, note that $x_3 = 30$. Then,

$$x_2 = 6 - x_3$$

= 6 - 30
= -24.

So, $x_2 = -24$. Then, we want to compute x_3 , which gives us

$$x_1 = 1 - \frac{x_2}{2} - \frac{x_3}{3}$$
$$= 1 - \frac{-24}{2} - \frac{30}{10}$$
$$= 3.$$

So,
$$\vec{x} = \begin{pmatrix} 3 \\ -24 \\ 30 \end{pmatrix}$$
.

(2) LU factorization (no pivoting): Compare H = LU; write L and U explicitly. Solve $L\vec{c} = \vec{b}$ and $U\vec{x} = \vec{c}$, and verify that \vec{x} matches \vec{x}_{GE} in part (1).

Solution. First, we would like to obtain U. Take the matrix from the previous problem:

$$\begin{pmatrix} 1 & \frac{1}{2} & \frac{1}{4} \\ 0 & \frac{1}{12} & \frac{1}{12} \\ 0 & \frac{1}{12} & \frac{4}{45} \end{pmatrix} \quad (-R_2 + R_3 \mapsto R_3) \qquad \begin{pmatrix} 1 & \frac{1}{2} & \frac{1}{4} \\ 0 & \frac{1}{12} & \frac{1}{12} \\ 0 & 0 & \frac{1}{180} \end{pmatrix} = U$$

Next, we form L by identifying the transformations to make U and placing them in their respective position:

$$L = \begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{2} & 1 & 0 \\ \frac{1}{3} & 1 & 1 \end{pmatrix}.$$

First, we perform forward substitution on $L\vec{c} = \vec{b}$, which gives the following transformation below:

$$L|\vec{b} = \begin{pmatrix} 1 & 0 & 0 & 1\\ \frac{1}{2} & 1 & 0 & 1\\ \frac{1}{3} & 1 & 1 & 1 \end{pmatrix}.$$

Then, using forward substition, where $c_1 = 1$, we can find c_2 and c_3 :

$$c_2 = 1 - \frac{c_1}{2}$$
$$= 1 - \frac{1}{2}$$
$$= \frac{1}{2}$$

and

$$c_3 = 1 - \frac{c_1}{3} - c_2$$

$$= 1 - \frac{1}{3} - \frac{1}{2}$$

$$= 1 - \frac{5}{6}$$

$$= \frac{1}{6}.$$

Next, we solve for $U\vec{x} = \vec{c}$, which is represented by the following transformation:

$$U|\vec{c} = \begin{pmatrix} 1 & \frac{1}{2} & \frac{1}{3} & 1\\ 0 & \frac{1}{12} & \frac{1}{12} & \frac{1}{2}\\ 0 & 0 & \frac{1}{180} & \frac{1}{6} \end{pmatrix}.$$

Then, we can use backward substitution to solve for \vec{x} . Notice that $x_3 = 30$. Notice that the steps for the backward substitution follow similarly to the backward

substitution in (1). Then,
$$\vec{x} = \begin{pmatrix} 3 \\ -24 \\ 30 \end{pmatrix}$$
.

(3) Conditional numbers: Compute

$$\kappa_{\infty}(H) = \|H\|_{\infty} \|H^{-1}\|_{\infty}, \quad \kappa_{2}(H) = \frac{\sigma_{\max}(H)}{\sigma_{\min}(H)}.$$

Give a 1-2 sentence interpretation of what each condition number says about the sensitivity of the solution to perturbations in b (and in H).

Solution. Define

$$\kappa_{\infty}(H) = \|H\|_{\infty} \|H^{-1}\|_{\infty}$$

To find max(H), we know that the largest sum of the rows is the first. So, we can say

$$||H||_{\infty} = 1 + \frac{1}{2} + \frac{1}{3} = \frac{11}{6}.$$

To find $||H^{-1}||_{\infty}$, we compute the inverse of H, which gives us

$$H^{-1} = \begin{pmatrix} 9 & -36 & 30 \\ -36 & 192 & -180 \\ 30 & -180 & 180 \end{pmatrix}.$$

The absolute value of the second row has the largest sum, so

$$||H^{-1}|| = |-36| + |192| + |-180|$$

= 408

Then, $\kappa_{\infty} = 408 \cdot \frac{11}{6}$. This tells us that small errors in \vec{b} may lead to large errors in \vec{x} . Next, we want to compute $\kappa_2(H)$. To do this, we first must find the singular values of H^TH . That is, we need to find the eigenvalues and square them. First, we find that

$$H^T H = \begin{pmatrix} \frac{49}{36} & \frac{3}{4} & \frac{21}{40} \\ \frac{3}{4} & \frac{61}{144} & \frac{3}{10} \\ \frac{21}{40} & \frac{3}{10} & \frac{769}{3600} \end{pmatrix}.$$

To set up computing the eigenvalues, we get

$$\det(H^T H - \lambda I) = \begin{vmatrix} \frac{49}{36} - \lambda & \frac{3}{4} & \frac{21}{40} \\ \frac{3}{4} & \frac{61}{144} - \lambda & \frac{3}{10} \\ \frac{21}{40} & \frac{3}{10} & \frac{769}{3600} - \lambda \end{vmatrix}$$

When we solve, we get $\lambda \approx 7.22, 0.015, 1.98$. Then, we can find $\sigma_{\text{max}} = \sqrt{7.22} \approx 2.687$ and $\sigma_{\text{min}} = \sqrt{0.015} = 0.122$. Then,

$$\kappa_2(H) = \frac{\sigma_{\text{max}}(H)}{\sigma_{\text{min}}(H)}$$

$$\approx \frac{2.687}{0.122}$$

$$\approx 22.$$

Accordingly, this tells that that a 1% error could lead to a 22%, which means that this systems is not very stable.

- (b) Timing the solvers: Solve $H\vec{x} = \vec{b}$ for $n \in \{2, 3, 5, 10\}$ using:
 - the lecture-note implementation of partial-pivoting LU (PA = LU), and
 - np.linalg.solve.

Compare their solutions. For each n when using the partial-pivoting LU, report in a table: n, time, and the residual norm $\|\vec{b} - H\vec{x}\|_2$. You can measure wall-clock time with time.perf_counter().

(c) Conditioning vs. Size: For each n, compute the conditional number with np.linalg.cond:

$$\kappa_2(H) = \text{np.linalg.cond}(H, 2).$$

Also report $\kappa_{\infty}(H)$. Discuss how condition numbers grow with n. Based on your results, comment on whether the Hilbert matrix is well-conditioned or ill-conditioned as n increases.

Solution. Consider the table in the Google colab on part (c). Notice that the condition numbers grow with n. This tells us that the Hilbert matrix is ill-conditioned as n increases.

Problem 3. LU decomposition with and without pivoting: Let

$$A(\varepsilon) = \begin{pmatrix} \varepsilon & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 2 \end{pmatrix}, \quad \vec{b} = \begin{pmatrix} 2 \\ 3 \\ 4 \end{pmatrix}, \quad \text{with} \quad \varepsilon = 10^{-12}.$$

(Keep ε symbolic in your hand work; substitute $\varepsilon=10^{-12}$ for the numeric comparison.)

- (a) Hand Calculation
 - (1) LU without pivoting: Perform A = LU. Write L and U explicitly and solve $L\vec{c} = \vec{b}, U\vec{x} = \vec{c}$. Show all steps, including the elimination process to obtain L and U, and the substitution steps to find x.

Solution. We begin by attempting the LU factorization.

$$\begin{pmatrix} \varepsilon & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 2 \end{pmatrix} \begin{pmatrix} -\frac{1}{\varepsilon}R_1 + R_2 \mapsto R_2 \end{pmatrix} \begin{pmatrix} \varepsilon & 1 & 1 \\ 0 & 1 - \frac{1}{\varepsilon} & 1 - \frac{1}{\varepsilon} \\ 1 & 1 & 2 \end{pmatrix}$$

$$\begin{pmatrix} -\frac{1}{\varepsilon}R_1 + R_3 \mapsto R_3 \end{pmatrix} \begin{pmatrix} \varepsilon & 1 & 1 \\ 0 & 1 - \frac{1}{\varepsilon} & 1 - \frac{1}{\varepsilon} \\ 0 & 1 - \frac{1}{\varepsilon} & 2 - \frac{1}{\varepsilon} \end{pmatrix}$$

$$\begin{pmatrix} -R_2 + R_3 \mapsto R_3 \end{pmatrix} \begin{pmatrix} \varepsilon & 1 & 1 \\ 0 & 1 - \frac{1}{\varepsilon} & 1 - \frac{1}{\varepsilon} \\ 0 & 0 & 1 \end{pmatrix} = U$$

That is, we have

$$L = \begin{pmatrix} 1 & 0 & 0 \\ \frac{1}{\varepsilon} & 1 & 0 \\ \frac{1}{\varepsilon} & 1 & 1 \end{pmatrix}.$$

So when we solve $L\vec{c} = \vec{b}$, with $c_1 = 2$, we get

$$c_2 = 3 - \frac{c_1}{\varepsilon}$$
$$= 3 - \frac{2}{\varepsilon}.$$

Then,

$$c_3 = 4 + \frac{c_1}{\varepsilon} - c_2$$
$$= 4 - \frac{2}{\varepsilon} - \left(2 - \frac{2}{\varepsilon}\right)$$
$$= 1.$$

Next, we solve for $U\vec{x} = \vec{c}$, with $x_3 = 1$, we get

$$x_2 = \frac{3 - \frac{2}{\varepsilon}}{1 - \frac{1}{\varepsilon}} - 1$$
$$= \frac{\frac{3\varepsilon - 2}{\varepsilon}}{\frac{\varepsilon - 1}{\varepsilon}} - 1$$
$$= \frac{3\varepsilon - 2}{\varepsilon - 1} - 1.$$

Finally,

$$x_1 = 4 - \left(\frac{3\varepsilon - 2}{\varepsilon - 1} - 1\right) - \frac{1}{\varepsilon}$$
$$= 4 - \frac{3\varepsilon - 2}{\varepsilon - 1} + \frac{\varepsilon - 1}{\varepsilon}$$
$$= -\frac{1}{\varepsilon - 1}.$$

That is, our final solution is $\vec{x} = \begin{pmatrix} -\frac{1}{\varepsilon-1} \\ \frac{3\varepsilon-2}{\varepsilon-1} - 1 \\ 1 \end{pmatrix}$.

(2) LU with partial pivoting: Compute PA = LU using partial pivoting. Write P, L and U explicitly and solve $L\vec{c} = P\vec{b}, U\vec{x} = \vec{c}$. Show all steps, including pivot selection, row swaps, elimination, and substitution processes.

Solution. We attempt a similar elimination as in the part above, except that we set

$$P = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}.$$

So, PA = LU gives us

$$\begin{pmatrix} 1 & 1 & 1 \\ \varepsilon & 1 & 1 \\ 1 & 1 & 2 \end{pmatrix} \quad (-\varepsilon R_1 + R_2 \mapsto R_2) \qquad \begin{pmatrix} 1 & 1 & 1 \\ 0 & 1 - \varepsilon & 1 - \varepsilon \\ 1 & 1 & 2 \end{pmatrix}$$

$$(-R_1 + R_3 \mapsto R_3) \qquad \begin{pmatrix} 1 & 1 & 1 \\ 0 & 1 - \varepsilon & 1 - \varepsilon \\ 0 & 0 & 1 \end{pmatrix} = U.$$

That is, we find that

$$L = \begin{pmatrix} 1 & 0 & 0 \\ \varepsilon & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix}$$

Next, we solve $L\vec{c} = P\vec{b}$, where $c_1 = 3$, we get

$$c_2 = 2 - \varepsilon c_2$$
$$= 2 - 3\varepsilon.$$

Then,

$$c_3 = 4 - 3$$
$$= 1.$$

Next, we would like to solve $U\vec{x} = \vec{c}$, where $x_3 = 1$. Then,

$$x_2 = \frac{2 - 3\varepsilon}{1 - \varepsilon} - 1$$
$$= \frac{3\varepsilon - 2}{\varepsilon - 1} - 1.$$

Finally, we get

$$x_1 = 3 - x_3 - x_2$$

$$= 3 - 1 - \left(\frac{2 - 3\varepsilon}{1 - \varepsilon} - 1\right)$$

$$= 3 - \frac{2 - 3\varepsilon}{1 - \varepsilon}$$

$$= \frac{1}{1 - \varepsilon}$$

$$= -\frac{1}{\varepsilon - 1}.$$

That is, our final solution is $\vec{x} = \begin{pmatrix} -\frac{1}{\varepsilon-1} \\ \frac{3\varepsilon-2}{\varepsilon-1} - 1 \\ 1 \end{pmatrix}$.

- (b) Numerical Comparison Using the code provided in the lecture notes, implement the following for $\varepsilon = 10^{-12}$:
 - -LU decomposition without pivoting (as in part (a)).
 - -LU decomposition with partial pivoting (as in part (b)).

Compute the numerical solutions to \vec{x} for both methods. Additionally, compute a reference solution using NumPy's np.linalg.solve(A, b). Present the results in a table comparing:

- The solutions \vec{x} from both methods and the reference solution.
- The absolute error $\|\vec{x}_{\text{method}} \vec{x}_{\text{ref}}\|_2$ for each method, where \vec{x}_{ref} is the NumPy solution.

Discuss the differences between the solutions and explain why partial pivoting matters for this system. In your discussion, consider:

- The effect of the small value $\varepsilon = 10^{-12}$ on the matrix's conditioning (you may compute the condition number $\kappa(A)$ using np.linalg.cond(A)).
- The role of partial pivoting in improving numerical stability, especially in the presence of small pivots.
- Any numerical issues (e.g., roundoff errors, small pivots) observed in the computations.

Solution. For the solution, please look at the Google colab.