DDA 3005 — Numerical Methods

Solutions 3

Problem 1 (Computing the LU Factorization): (approx. *20* points)
Calculate the LU factorization (with pivoting) of the matrix

$$\boldsymbol{A} = \begin{bmatrix} 1 & \frac{5}{3} & 1 & 1 \\ 2 & -1 & -1 & 0 \\ 3 & -1 & 0 & 1 \\ -2 & 1 & -4 & 0 \end{bmatrix}.$$

For each step of the algorithm, clearly mark the current $\boldsymbol{L}$ and $\boldsymbol{U}$ factor and the pivot element. State the final LU factorization and permutation matrix $\boldsymbol{P}$.

Solution : The largest element (magnitude-wise) in the first column of $\boldsymbol{A}$ is 3. Hence, we first swap the first and third row of $\boldsymbol{A}$:

$$\boldsymbol{A} \ \to \ \boldsymbol{A}_1 = \boldsymbol{P}_1 \boldsymbol{A} = \begin{bmatrix} 3 & -1 & 0 & 1 \\ 2 & -1 & -1 & 0 \\ 1 & \frac{5}{3} & 1 & 1 \\ -2 & 1 & -4 & 0 \end{bmatrix}$$

and the first $\boldsymbol{L}_1$ and $\boldsymbol{U}_1$ factor are given by

$$\boldsymbol{L}_1 = \boldsymbol{M}_1^{-1} = \begin{bmatrix} 1 & & & \\ \frac{2}{3} & 1 & & \\ \frac{1}{3} & 0 & 1 & \\ -\frac{2}{3} & 0 & 0 & 1 \end{bmatrix}, \ \boldsymbol{U}_1 = \boldsymbol{M}_1 \boldsymbol{A}_1 = \begin{bmatrix} 3 & -1 & 0 & 1 \\ 0 & \frac{2}{3} - 1 & -1 & -\frac{2}{3} \\ 0 & \frac{1}{3} + \frac{5}{3} & 1 & 1 - \frac{1}{3} \\ 0 & 1 - \frac{2}{3} & -4 & \frac{2}{3} \end{bmatrix} = \begin{bmatrix} 3 & -1 & 0 & 1 \\ 0 & -\frac{1}{3} & -1 & -\frac{2}{3} \\ 0 & 2 & 1 & \frac{2}{3} \\ 0 & \frac{1}{3} & -4 & \frac{2}{3} \end{bmatrix}$$

The largest element in the column $[-\frac{1}{3}, 2, \frac{1}{3}]^\top$ is 2; we change row 2 and 3:

$$\boldsymbol{A}_2 = \boldsymbol{P}_2 \boldsymbol{P}_1 \boldsymbol{A} = \begin{bmatrix} 1 & & & \\ \frac{1}{3} & 1 & & \\ \frac{2}{3} & 0 & 1 & \\ -\frac{2}{3} & 0 & 0 & 1 \end{bmatrix} \begin{bmatrix} 3 & -1 & 0 & 1 \\ 0 & 2 & 1 & \frac{2}{3} \\ 0 & -\frac{1}{3} & -1 & -\frac{2}{3} \\ 0 & \frac{1}{3} & -4 & \frac{2}{3} \end{bmatrix}$$

To form $\boldsymbol{L}_2$ we add the multiplier $[-\frac{1}{6}, \frac{1}{6}]^\top$ in the second column of $\boldsymbol{L}_1$; we obtain:

$$\boldsymbol{L}_2 = \begin{bmatrix} 1 & & & \\ \frac{1}{3} & 1 & & \\ \frac{2}{3} & -\frac{1}{6} & 1 & \\ -\frac{2}{3} & \frac{1}{6} & 0 & 1 \end{bmatrix}, \ \boldsymbol{U}_2 = \boldsymbol{M}_2 \boldsymbol{A}_2 = \begin{bmatrix} 3 & -1 & 0 & 1 \\ 0 & 2 & 1 & \frac{2}{3} \\ 0 & 0 & \frac{1}{6} - 1 & \frac{2}{3}(\frac{1}{6} - 1) \\ 0 & 0 & -\frac{1}{6} - 4 & \frac{2}{3}(1 - \frac{1}{6}) \end{bmatrix} = \begin{bmatrix} 3 & -1 & 0 & 1 \\ 0 & 2 & 1 & \frac{2}{3} \\ 0 & 0 & -\frac{5}{6} & -\frac{5}{9} \\ 0 & 0 & -\frac{25}{6} & \frac{5}{9} \end{bmatrix}$$

The largest element in the column $[-\frac{5}{6}, -\frac{25}{6}]^\top$ is $-\frac{25}{6}$; we exchange row 3 and 4:

$$\boldsymbol{A}_3 = \boldsymbol{P}_3 \boldsymbol{P}_2 \boldsymbol{P}_1 \boldsymbol{A} = \begin{bmatrix} 1 & & & \\ \frac{1}{3} & 1 & & \\ -\frac{2}{3} & \frac{1}{6} & 1 & \\ \frac{2}{3} & -\frac{1}{6} & 0 & 1 \end{bmatrix} \begin{bmatrix} 3 & -1 & 0 & 1 \\ 0 & 2 & 1 & \frac{2}{3} \\ 0 & 0 & -\frac{25}{6} & \frac{5}{9} \\ 0 & 0 & -\frac{5}{6} & -\frac{5}{9} \end{bmatrix}.$$

To form $\boldsymbol{L}_3$, we add the multiplier $-\frac{5}{6}/(-\frac{25}{6}) = \frac{1}{5}$ to the third column in $\boldsymbol{L}_2$; this yields:

$$\boldsymbol{L}_3 = \begin{bmatrix} 1 & & & \\ \frac{1}{3} & 1 & & \\ -\frac{2}{3} & \frac{1}{6} & 1 & \\ \frac{2}{3} & -\frac{1}{6} & \frac{1}{5} & 1 \end{bmatrix}, \quad \text{and} \quad \boldsymbol{U}_3 = \boldsymbol{M}_3\boldsymbol{A}_3 = \begin{bmatrix} 3 & -1 & 0 & 1 \\ 0 & 2 & 1 & \frac{2}{3} \\ 0 & 0 & -\frac{25}{6} & \frac{5}{9} \\ 0 & 0 & 0 & -\frac{2}{3} \end{bmatrix}$$

The permutations swapped the rows: $1 \leftrightarrow 3$, $2 \leftrightarrow 3$, and $3 \leftrightarrow 4$. In total, we have:

$$\begin{bmatrix} & & 1 & \\ 1 & & & \\ & & & 1 \\ & 1 & & \end{bmatrix} \begin{bmatrix} 1 & \frac{5}{3} & 1 & 1 \\ 2 & -1 & -1 & 0 \\ 3 & -1 & 0 & 1 \\ -2 & 1 & -4 & 0 \end{bmatrix} = \boldsymbol{PA} = \boldsymbol{LU} = \begin{bmatrix} 1 & & & \\ \frac{1}{3} & 1 & & \\ -\frac{2}{3} & \frac{1}{6} & 1 & \\ \frac{2}{3} & -\frac{1}{6} & \frac{1}{5} & 1 \end{bmatrix} \begin{bmatrix} 3 & -1 & 0 & 1 \\ 0 & 2 & 1 & \frac{2}{3} \\ 0 & 0 & -\frac{25}{6} & \frac{5}{9} \\ 0 & 0 & 0 & -\frac{2}{3} \end{bmatrix}.$$

Problem 2 (Properties of Triangular Matrices): (approx. *20* points)
In this exercise, we investigate additional theoretical properties of triangular matrices.

a) Let $\boldsymbol{A} \in \mathbb{R}^{n\times n}$ be a nonsingular upper triangular matrix. Show that $\boldsymbol{A}^{-1}$ is an upper triangular matrix.

   Hint: This result can be shown via induction over the dimension n using suitable decompositions of the involved matrices.

b) Suppose that $\boldsymbol{A} \in \mathbb{R}^{n\times n}$ is a unit lower triangular matrix. Prove that the matrix $\boldsymbol{A}^{-1}$ is unit lower triangular as well.

Solution :

a) We can show this result via induction over the dimension n. For the base case $n = 1$, this property is obviously true. Now, let $\tilde{\boldsymbol{A}} \in \mathbb{R}^{(n+1)\times(n+1)}$ be a nonsingular upper triangular matrices. We can decompose $\tilde{\boldsymbol{A}}$ and $\tilde{\boldsymbol{A}}^{-1}$ as follows

$$\tilde{\boldsymbol{A}} = \begin{pmatrix} \boldsymbol{A} & \boldsymbol{a} \\ \boldsymbol{0} & \alpha \end{pmatrix} \quad \text{and} \quad \tilde{\boldsymbol{A}}^{-1} = \begin{pmatrix} \boldsymbol{B} & \boldsymbol{b} \\ \boldsymbol{c}^\top & \beta \end{pmatrix},$$

   where $\boldsymbol{A} \in \mathbb{R}^{n\times n}$ is an upper triangular matrix and we have $\boldsymbol{B} \in \mathbb{R}^{n\times n}$, $\boldsymbol{a}, \boldsymbol{b}, \boldsymbol{c} \in \mathbb{R}^n$, and $\alpha, \beta \in \mathbb{R}$. Next, let us consider the matrix products

$$\begin{pmatrix} \boldsymbol{I} & \boldsymbol{0} \\ \boldsymbol{0} & 1 \end{pmatrix} = \tilde{\boldsymbol{A}}\tilde{\boldsymbol{A}}^{-1} = \begin{pmatrix} \boldsymbol{A} & \boldsymbol{a} \\ \boldsymbol{0} & \alpha \end{pmatrix} \begin{pmatrix} \boldsymbol{B} & \boldsymbol{b} \\ \boldsymbol{c}^\top & \beta \end{pmatrix} = \begin{pmatrix} \boldsymbol{AB} + \boldsymbol{ac}^\top & \boldsymbol{Ab} + \beta\boldsymbol{a} \\ \alpha\boldsymbol{c}^\top & \alpha\beta \end{pmatrix}.$$

   and

$$\begin{pmatrix} \boldsymbol{I} & \boldsymbol{0} \\ \boldsymbol{0} & 1 \end{pmatrix} = \tilde{\boldsymbol{A}}^{-1}\tilde{\boldsymbol{A}} = \begin{pmatrix} \boldsymbol{B} & \boldsymbol{b} \\ \boldsymbol{c}^\top & \beta \end{pmatrix} \begin{pmatrix} \boldsymbol{A} & \boldsymbol{a} \\ \boldsymbol{0} & \alpha \end{pmatrix} = \begin{pmatrix} \boldsymbol{BA} & \boldsymbol{Ba} + \alpha\boldsymbol{b} \\ \boldsymbol{c}^\top\boldsymbol{A} & \boldsymbol{c}^\top\boldsymbol{a} + \alpha\beta \end{pmatrix}.$$

   From these expressions, we can infer $\alpha \neq 0$ (otherwise $\tilde{\boldsymbol{A}}$ is not invertible) and $\boldsymbol{c} = \boldsymbol{0}$. It then follows $\boldsymbol{AB} = \boldsymbol{BA} = \boldsymbol{I}$, i.e., $\boldsymbol{B} = \boldsymbol{A}^{-1}$. Thus, by the induction hypothesis, $\boldsymbol{B}$ is an upper triangular matrix which verifies that $\tilde{\boldsymbol{A}}^{-1}$ is upper triangular.

b) We can follow the previous proof by additionally assuming that $\boldsymbol{A}$ and $\tilde{\boldsymbol{A}}$ are unit upper triangular matrices, i.e., $\alpha = 1$. Then, we can directly infer $\beta = 1$, i.e., $\tilde{\boldsymbol{A}}^{-1}$ must be unit upper triangular as well (by induction). To cover the case where $\boldsymbol{A}$ is unit lower triangular, we note that $\boldsymbol{A}^\top$ is unit upper triangular and we have $(\boldsymbol{A}^\top)^{-1} = (\boldsymbol{A}^{-1})^\top$.

Problem 3 (Solving Linear Least Squares): (approx. *15* points)
Let $\boldsymbol{A} \in \mathbb{R}^{m \times n}$, $m \geq n$, and $\boldsymbol{b} \in \mathbb{R}^m$ be given and suppose that $\boldsymbol{A}$ has full column rank.

Let $\tilde{\boldsymbol{Q}}_r \tilde{\boldsymbol{R}} = [\boldsymbol{A}\ \boldsymbol{b}] \in \mathbb{R}^{m \times (n+1)}$ be the reduced QR factorization of the extended matrix $\tilde{\boldsymbol{A}} = [\boldsymbol{A}\ \boldsymbol{b}]$. Let us further consider the decomposition

$$\tilde{\boldsymbol{R}} = \begin{bmatrix} \boldsymbol{R} & \boldsymbol{p} \\ & \rho \end{bmatrix}$$

where $\boldsymbol{R} \in \mathbb{R}^{n \times n}$ is upper triangular, $\boldsymbol{p} \in \mathbb{R}^n$, and $\rho \in \mathbb{R}$, and let $\boldsymbol{x} \in \mathbb{R}^n$ be the solution of the linear least squares problem

$$\min_{\boldsymbol{x} \in \mathbb{R}^n} \|\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}\|_2.$$

Show that $\boldsymbol{R}\boldsymbol{x} = \boldsymbol{p}$ and $|\rho| = \|\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}\|_2$.

Hint: Decompose $\tilde{\boldsymbol{Q}}_r$ via $\tilde{\boldsymbol{Q}}_r = [\boldsymbol{Q}_r\ \boldsymbol{q}]$.

Solution : As mentioned, we use the partitioning $\tilde{\boldsymbol{Q}}_r$ via $\tilde{\boldsymbol{Q}}_r = [\boldsymbol{Q}_r\ \boldsymbol{q}]$ with $\boldsymbol{Q}_r \in \mathbb{R}^{m \times n}$ and $\boldsymbol{q} \in \mathbb{R}^m$. Then, we obtain

$$\begin{bmatrix} \boldsymbol{A} & \boldsymbol{b} \end{bmatrix} = \tilde{\boldsymbol{Q}}_r \tilde{\boldsymbol{R}} = \begin{bmatrix} \boldsymbol{Q}_r & \boldsymbol{q} \end{bmatrix} \begin{bmatrix} \boldsymbol{R} & \boldsymbol{p} \\ & \rho \end{bmatrix} = \begin{bmatrix} \boldsymbol{Q}_r \boldsymbol{R} & \boldsymbol{Q}_r \boldsymbol{p} + \rho \boldsymbol{q} \end{bmatrix}.$$

Hence, $\boldsymbol{Q}_r$ and $\boldsymbol{R}$ form a reduced QR factorization of $\boldsymbol{A}$ — $\boldsymbol{A} = \boldsymbol{Q}_r \boldsymbol{R}$ — and we have $\boldsymbol{Q}_r \boldsymbol{p} + \rho \boldsymbol{q} = \boldsymbol{b}$. Multiplying this equation with $\boldsymbol{Q}_r^\top$ and using $\boldsymbol{Q}_r^\top \boldsymbol{Q}_r = \boldsymbol{I}$ and $\boldsymbol{Q}_r^\top \boldsymbol{q} = 0$ (the matrix $\tilde{\boldsymbol{Q}}_r$ is orthogonal), this yields

$$\boldsymbol{p} = \boldsymbol{Q}_r^\top \boldsymbol{b}.$$

As shown in the lecture, the solution $\boldsymbol{x}$ of the linear least squares problem $\min_{\boldsymbol{x} \in \mathbb{R}^n} \|\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}\|_2$ is characterized via

$$\boldsymbol{R}\boldsymbol{x} = \boldsymbol{Q}_r^\top \boldsymbol{b} = \boldsymbol{p}$$

($\boldsymbol{A} = \boldsymbol{Q}_r \boldsymbol{R}$ is a reduced QR factorization of $\boldsymbol{A}$). Thus, it holds that $\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b} = \boldsymbol{Q}_r \boldsymbol{R}\boldsymbol{x} - \boldsymbol{b} = \boldsymbol{Q}_r \boldsymbol{p} - \boldsymbol{b} = -\rho \boldsymbol{q}$ and using $\|\boldsymbol{q}\| = 1$, we can infer $\|\boldsymbol{A}\boldsymbol{x} - \boldsymbol{b}\|_2 = |\rho|$.

Problem 4 (LU vs. QR Factorizations): (approx. *45* points)
For $n \in \mathbb{N}$, the so-called *Wilkinson*-matrix $\boldsymbol{W} \in \mathbb{R}^{n \times n}$ and its inverse $\boldsymbol{W}^{-1}$ are given by

$$\boldsymbol{W} = \begin{bmatrix} 1 & & & & 1 \\ -1 & 1 & & & 1 \\ -1 & -1 & \ddots & & 1 \\ \vdots & \vdots & \ddots & \ddots & \vdots \\ -1 & -1 & \dots & -1 & 1 \end{bmatrix} \quad \text{and} \quad \boldsymbol{W}^{-1} = \begin{bmatrix} \frac{1}{2} & -\frac{1}{4} & -\frac{1}{8} & & \cdots & -\frac{1}{2^{n-1}} & -\frac{1}{2^{n-1}} \\ & \frac{1}{2} & -\frac{1}{4} & -\frac{1}{8} & \cdots & -\frac{1}{2^{n-2}} & -\frac{1}{2^{n-2}} \\ & & \frac{1}{2} & -\frac{1}{4} & \cdots & -\frac{1}{2^{n-3}} & -\frac{1}{2^{n-3}} \\ & & & \ddots & \ddots & & \vdots \\ & & & & \ddots & & \vdots \\ & & & & & \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & \frac{1}{4} & \frac{1}{8} & \cdots & & \frac{1}{2^{n-1}} & \frac{1}{2^{n-1}} \end{bmatrix}.$$

a) Verify that the matrices

$$\boldsymbol{L} = \begin{bmatrix} 1 & & & & \\ -1 & 1 & & & \\ -1 & -1 & \ddots & & \\ \vdots & \vdots & \ddots & \ddots & \\ -1 & -1 & \dots & -1 & 1 \end{bmatrix} \quad \text{and} \quad \boldsymbol{U} = \begin{bmatrix} 1 & & & & 1 \\ & 1 & & & 2 \\ & & \ddots & & \vdots \\ & & & 1 & 2^{n-2} \\ & & & & 2^{n-1} \end{bmatrix}$$

define an LU factorization of the Wilkinson-matrix $\boldsymbol{W}$.

b) Calculate the condition number of $\boldsymbol{W}$ with respect to the norm $\|\cdot\|_\infty$. (Here, $\|\cdot\|_\infty$ denotes the maximum absolute row sum). Is the matrix $\boldsymbol{W}$ generally well- or ill-conditioned?

c) Compute the inverse matrix $\boldsymbol{L}^{-1}$ and show that $\|\boldsymbol{L}\|_\infty = n$ and $\|\boldsymbol{L}^{-1}\|_\infty = 2^{n-1}$.

d) Use Householder transformations to compute a QR factorization of $\boldsymbol{W}$ in the case $n = 4$.

Clearly mark and perform the corresponding updates step-by-step. You only need to state the final upper triangular $\boldsymbol{R}$ factor, i.e., computation of $\boldsymbol{Q}$ is not required.

e) Let us consider the linear system of equations $\boldsymbol{W}\boldsymbol{x} = \boldsymbol{b}$ and the associated LU algorithm

$$\boldsymbol{W}\boldsymbol{x} = \boldsymbol{b} \quad \Longleftrightarrow \quad \boldsymbol{L}\boldsymbol{U}\boldsymbol{x} = \boldsymbol{b} \quad \Longleftrightarrow \quad \boldsymbol{x} = \boldsymbol{U}^{-1}(\boldsymbol{L}^{-1}\boldsymbol{b}) \tag{1}$$

(using forward- and back-substitution to compute $\boldsymbol{y} = \boldsymbol{L}^{-1}\boldsymbol{b}$ and $\boldsymbol{x} = \boldsymbol{U}^{-1}\boldsymbol{y}$, respectively). Is the LU algorithm (1) generally an accurate method to solve the linear system $\boldsymbol{W}\boldsymbol{x} = \boldsymbol{b}$? Explain your answer!

Provide a suitable experiment that confirms your answer numerically. For instance, write a test program (in `MATLAB` or `Python`) and generate $\boldsymbol{W}$ and random vectors $\boldsymbol{b} \sim \mathcal{N}(0,1)^n$ for different n. Using the true inverse $\boldsymbol{W}^{-1}$ and $\boldsymbol{x}^* = \boldsymbol{W}^{-1}\boldsymbol{b}$, you can then report and compare the forward errors $\|\boldsymbol{x}^* - \boldsymbol{x}\|/\|\boldsymbol{x}^*\|$ where $\boldsymbol{x}$ is computed via (1).

Repeat your experiments for the QR-based algorithm

$$\boldsymbol{W}\boldsymbol{x} = \boldsymbol{b} \quad \Longleftrightarrow \quad \boldsymbol{Q}\boldsymbol{R}\boldsymbol{x} = \boldsymbol{b} \quad \Longleftrightarrow \quad \boldsymbol{x} = \boldsymbol{R}^{-1}(\boldsymbol{Q}^\top\boldsymbol{b})$$

(with back-substitution to compute $\boldsymbol{x} = \boldsymbol{R}^{-1}(\boldsymbol{Q}^\top\boldsymbol{b})$). You can use `MATLAB` or `Python` in-built code to obtain the QR factorizations of $\boldsymbol{W}$. Does this method perform differently from the LU-based approach? Can you explain your numerical observations?

Solution :

a) We can decompose $\boldsymbol{L}$ and $\boldsymbol{U}$ as follows:

$$\boldsymbol{L} = \begin{pmatrix} \tilde{\boldsymbol{L}} & \boldsymbol{0} \\ -\mathbb{1}^\top & 1 \end{pmatrix} \quad \text{and} \quad \boldsymbol{U} = \begin{pmatrix} \boldsymbol{I} & \boldsymbol{u} \\ \boldsymbol{0} & 2^{n-1} \end{pmatrix}.$$

where $\tilde{\boldsymbol{L}} \in \mathbb{R}^{(n-1)\times(n-1)}$ is a smaller $(n-1)\times(n-1)$-dimensional version of $\boldsymbol{L}$ and $\boldsymbol{u} = (1, 2, \ldots, 2^{n-2})^\top \in \mathbb{R}^{n-1}$. We then have

$$\boldsymbol{L}\boldsymbol{U} = \begin{pmatrix} \tilde{\boldsymbol{L}} & \boldsymbol{0} \\ -\mathbb{1}^\top & 1 \end{pmatrix} \begin{pmatrix} \boldsymbol{I} & \boldsymbol{u} \\ \boldsymbol{0} & 2^{n-1} \end{pmatrix} = \begin{pmatrix} \tilde{\boldsymbol{L}} & \tilde{\boldsymbol{L}}\boldsymbol{u} \\ -\mathbb{1}^\top & 2^{n-1} - \mathbb{1}^\top\boldsymbol{u} \end{pmatrix}.$$

Furthermore, using the geometric series $\sum_{k=0}^{n-1} x^k = \frac{1-x^n}{1-x}$, $(x \neq 1)$, it holds that $(\tilde{\boldsymbol{L}}\boldsymbol{u})_i = 2^{i-1} - \sum_{k=0}^{i-2} 2^k = 2^{i-1} - \frac{1-2^{i-1}}{1-2} = 1$ for all i. This proves $\boldsymbol{L}\boldsymbol{U} = \boldsymbol{W}$, i.e., $\boldsymbol{L}\boldsymbol{U}$ is an LU factorization of $\boldsymbol{W}$.

b) It holds that $\|\boldsymbol{W}\|_\infty = n$. Using the explicit representation of $\boldsymbol{W}^{-1}$, we further have

$$\|\boldsymbol{W}^{-1}\|_\infty = \sum_{i=1}^{n-1} \frac{1}{2^i} + \frac{1}{2^{n-1}} = \frac{1-\frac{1}{2^n}}{1-\frac{1}{2}} - 1 + \frac{1}{2^{n-1}} = 1$$

and $\operatorname{cond}(\boldsymbol{W}) = \|\boldsymbol{W}\|_\infty \|\boldsymbol{W}^{-1}\|_\infty = n$. Consequently, the matrix $\boldsymbol{W}$ is generally well-conditioned (unless $n \to \infty$).

c) We can compute $\boldsymbol{L}^{-1}$ directly via $\boldsymbol{L}^{-1} = \boldsymbol{U}\boldsymbol{W}^{-1}$:

$$
\begin{aligned}
\boldsymbol{U}\boldsymbol{W}^{-1} &= \begin{bmatrix} 1 & & & & & & 1 \\ & 1 & & & & & 2 \\ & & 1 & & & & 4 \\ & & & \ddots & & & \vdots \\ & & & & 1 & & 2^{n-3} \\ & & & & & 1 & 2^{n-2} \\ & & & & & & 2^{n-1} \end{bmatrix} \begin{bmatrix} \frac{1}{2} & -\frac{1}{4} & -\frac{1}{8} & & \cdots & -\frac{1}{2^{n-1}} & -\frac{1}{2^{n-1}} \\ & \frac{1}{2} & -\frac{1}{4} & -\frac{1}{8} & \cdots & -\frac{1}{2^{n-2}} & -\frac{1}{2^{n-2}} \\ & & \frac{1}{2} & -\frac{1}{4} & \cdots & -\frac{1}{2^{n-3}} & -\frac{1}{2^{n-3}} \\ & & & \ddots & \ddots & & \vdots \\ & & & & \ddots & & \vdots \\ & & & & & \frac{1}{2} & -\frac{1}{2} \\ \frac{1}{2} & \frac{1}{4} & \frac{1}{8} & \cdots & & \frac{1}{2^{n-1}} & \frac{1}{2^{n-1}} \end{bmatrix} \\
&= \begin{bmatrix} 1 & & & & & \\ 1 & 1 & & & & \\ 2 & 1 & 1 & & & \\ 4 & 2 & 1 & 1 & & \\ \vdots & \vdots & & \ddots & \ddots & \\ 2^{n-2} & 2^{n-3} & \cdots & 2 & 1 & 1 \end{bmatrix}.
\end{aligned}
$$

(We can use our knowledge about $\boldsymbol{L}^{-1}$ being a lower unit triangular matrix to significantly simplify this calculation. In particular, we only need to compute the subdiagonal entries of $\boldsymbol{L}^{-1}$ which are easy to obtain).

Alternatively, we can consider the linear system of equations

$$
\boldsymbol{L}\boldsymbol{x} = \begin{pmatrix} 1 & & & & \\ -1 & 1 & & & \\ -1 & -1 & \ddots & & \\ \vdots & \vdots & \ddots & \ddots & \\ -1 & -1 & \cdots & -1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ \vdots \\ x_n \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ \vdots \\ b_n \end{pmatrix} = \boldsymbol{b}.
$$

We then have $x_1 = b_1$, $x_2 = b_2 + x_1 = b_1 + b_2$, $x_3 = b_3 + x_1 + x_2 = 2b_1 + b_2 + b_3$, $x_4 = b_4 + x_1 + x_2 + x_3 = 4b_1 + 2b_2 + b_3 + b_4$ and x_n is given by

$$
x_n = b_n + \sum_{i=1}^{n-1} x_i = \sum_{i=1}^{n-1} 2^{n-1-i} b_i + b_n. \tag{2}
$$

This expression can be verified inductively. The base case $n = 1$ is obvious. Let us assume that the formula (2) is correct for x_n and let us consider x_{n+1}:

$$
\begin{aligned}
x_{n+1} = b_{n+1} + \sum_{i=1}^{n} x_i &= b_{n+1} + \sum_{i=1}^{n} \sum_{j=1}^{i-1} 2^{i-1-j} b_j + b_i = b_{n+1} + \sum_{j=1}^{n} \left[1 + \textstyle\sum_{i=1}^{n-j} 2^{i-1} \right] b_j \\
&= b_{n+1} + \sum_{j=1}^{n} \left[1 + \frac{1 - 2^{n-j}}{(1-2)} \right] b_j = \sum_{j=1}^{n} 2^{n-j} b_j + b_{n+1},
\end{aligned}
$$

where the used the induction hypothesis for $x_1, \ldots, x_n$. This shows that

$$
\boldsymbol{L}^{-1} = \begin{bmatrix} 1 & & & & & \\ 1 & 1 & & & & \\ 2 & 1 & 1 & & & \\ 4 & 2 & 1 & 1 & & \\ \vdots & \vdots & & \ddots & \ddots & \\ 2^{n-2} & 2^{n-3} & \cdots & 2 & 1 & 1 \end{bmatrix}.
$$

Finally, we obtain $\|\boldsymbol{L}\|_\infty = n$ and $\|\boldsymbol{L}^{-1}\|_\infty = 1 + \sum_{i=0}^{n-2} 2^i = 2^{n-1}$.

d) Setting $\boldsymbol{w}_1 = (1,-1,-1,-1)^\top$, we can compute the first Householder vector

$$\|\boldsymbol{w}_1\| = 2, \quad \alpha_1 = -\|\boldsymbol{w}_1\| = -2, \quad \boldsymbol{v}_1 = \boldsymbol{w}_1 - \alpha_1 \boldsymbol{e}_1 = \begin{bmatrix} 1 \\ -1 \\ -1 \\ -1 \end{bmatrix} + \begin{bmatrix} 2 \\ 0 \\ 0 \\ 0 \end{bmatrix} = \begin{bmatrix} 3 \\ -1 \\ -1 \\ -1 \end{bmatrix}.$$

We further have $\|\boldsymbol{v}_1\| = \sqrt{9+1+1+1} = \sqrt{12}$. Setting $\boldsymbol{H}_1 = \boldsymbol{I} - 2\frac{\boldsymbol{v}_1\boldsymbol{v}_1^\top}{\|\boldsymbol{v}_1\|^2}$, this yields

$$\boldsymbol{H}_1\boldsymbol{W} = \begin{bmatrix} \alpha_1 & \tilde{\boldsymbol{w}}_1^\top \\ \boldsymbol{0} & \boldsymbol{W}_1 \end{bmatrix},$$

where

$$\begin{bmatrix} \tilde{\boldsymbol{w}}_1^\top \\ \boldsymbol{W}_1 \end{bmatrix} = \boldsymbol{H}_1 \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 1 \\ -1 & 1 & 1 \\ -1 & -1 & 1 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 1 \\ -1 & 1 & 1 \\ -1 & -1 & 1 \end{bmatrix} - \frac{1}{6}\boldsymbol{v}_1 \begin{bmatrix} 1 & 0 & 0 \end{bmatrix} = \begin{bmatrix} -\frac{1}{2} & 0 & 1 \\ \frac{7}{6} & 0 & 1 \\ -\frac{5}{6} & 1 & 1 \\ -\frac{5}{6} & -1 & 1 \end{bmatrix}.$$

We can continue with the reduction of $\boldsymbol{W}_1$. Setting $\boldsymbol{w}_2 = (\frac{7}{6}, -\frac{5}{6}, -\frac{5}{6})^\top$, it follows

$$\|\boldsymbol{w}_2\| = \frac{1}{6}\sqrt{99} = \frac{\sqrt{11}}{2}, \quad \alpha_2 = -\|\boldsymbol{w}_2\| = -\frac{\sqrt{11}}{2}, \quad \boldsymbol{v}_2 = \boldsymbol{w}_2 - \alpha_2\boldsymbol{e}_1 = \begin{bmatrix} \frac{7}{6} + \frac{\sqrt{11}}{2} \\ -\frac{5}{6} \\ -\frac{5}{6} \end{bmatrix}.$$

Using $\|\boldsymbol{v}_2\|^2 = (\frac{7}{6} + \frac{\sqrt{11}}{2})^2 + \frac{50}{36} = \frac{99}{36} + \frac{7}{6}\sqrt{11} + \frac{11}{4} = \sqrt{11}(\frac{7}{6} + \frac{\sqrt{11}}{2})$ and setting $\boldsymbol{H}_2 = \boldsymbol{I} - 2\frac{\boldsymbol{v}_2\boldsymbol{v}_2^\top}{\|\boldsymbol{v}_2\|^2}$, we obtain

$$\boldsymbol{H}_2\boldsymbol{W}_1 = \begin{bmatrix} \alpha_2 & \tilde{\boldsymbol{w}}_2^\top \\ \boldsymbol{0} & \boldsymbol{W}_2 \end{bmatrix},$$

where

$$\begin{bmatrix} \tilde{\boldsymbol{w}}_2^\top \\ \boldsymbol{W}_2 \end{bmatrix} = \boldsymbol{H}_2 \begin{bmatrix} 0 & 1 \\ 1 & 1 \\ -1 & 1 \end{bmatrix} = \begin{bmatrix} 0 & 1 \\ 1 & 1 \\ -1 & 1 \end{bmatrix} - \frac{2}{\sqrt{11}(\frac{7}{6} + \frac{\sqrt{11}}{2})}\boldsymbol{v}_2 \begin{bmatrix} 0 & \frac{\sqrt{11}}{2} - \frac{1}{2} \end{bmatrix} = \begin{bmatrix} 0 & \frac{1}{\sqrt{11}} \\ 1 & \star \\ -1 & \star \end{bmatrix}$$

and $\star = 1 + \frac{\sqrt{11}-1}{\sqrt{11}(\frac{7}{6}+\frac{\sqrt{11}}{2})}\frac{5}{6} = 1 + \frac{5\sqrt{11}-5}{\sqrt{11}(7+3\sqrt{11})} = \frac{12\sqrt{11}+28}{\sqrt{11}(7+3\sqrt{11})} = \frac{4}{\sqrt{11}}$. We continue with the reduction of $\boldsymbol{W}_2$. Setting $\boldsymbol{w}_3 = (1,-1)^\top$, we have

$$\|\boldsymbol{w}_3\| = \sqrt{2}, \quad \alpha_3 = -\|\boldsymbol{w}_3\| = -\sqrt{2}, \quad \boldsymbol{v}_3 = \boldsymbol{w}_3 - \alpha_3\boldsymbol{e}_1 = \begin{bmatrix} 1 + \sqrt{2} \\ -1 \end{bmatrix},$$

and $\|\boldsymbol{v}_3\|^2 = (1+\sqrt{2})^2 + 1 = 4 + 2\sqrt{2}$. Setting $\boldsymbol{H}_3 = \boldsymbol{I} - 2\frac{\boldsymbol{v}_3\boldsymbol{v}_3^\top}{\|\boldsymbol{v}_3\|^2}$, we obtain

$$\boldsymbol{H}_3\boldsymbol{W}_2 = \begin{bmatrix} \alpha_3 & \tilde{w}_3 \\ 0 & W_3 \end{bmatrix},$$

where

$$\begin{bmatrix} \tilde{w}_3 \\ W_3 \end{bmatrix} = \boldsymbol{H}_3 \begin{bmatrix} \frac{4}{\sqrt{11}} \\ \frac{4}{\sqrt{11}} \end{bmatrix} = \begin{bmatrix} \frac{4}{\sqrt{11}} \\ \frac{4}{\sqrt{11}} \end{bmatrix} - \frac{2}{4+2\sqrt{2}}\boldsymbol{v}_3 \cdot \frac{4\sqrt{2}}{\sqrt{11}} = \begin{bmatrix} \frac{4}{\sqrt{11}} \\ \frac{4}{\sqrt{11}} \end{bmatrix} - \frac{4}{\sqrt{11}(1+\sqrt{2})} \begin{bmatrix} 1+\sqrt{2} \\ -1 \end{bmatrix} = \begin{bmatrix} 0 \\ \square \end{bmatrix}.$$

and $\square = \frac{4}{\sqrt{11}}(1 + \frac{1}{1+\sqrt{2}}) = \frac{4\sqrt{2}}{\sqrt{11}}$. Consequently, the final $\boldsymbol{R}$ factor is given by

$$\boldsymbol{R} = \begin{bmatrix} -2 & -\frac{1}{2} & 0 & 1 \\ 0 & -\frac{\sqrt{11}}{2} & 0 & \frac{1}{\sqrt{11}} \\ 0 & 0 & -\sqrt{2} & 0 \\ 0 & 0 & 0 & \frac{4\sqrt{2}}{\sqrt{11}} \end{bmatrix}.$$

e) The condition number of $\boldsymbol{L}$ is given by $\mathrm{cond}(\boldsymbol{L}) = \|\boldsymbol{L}\|_\infty \|\boldsymbol{L}^{-1}\|_\infty = 2^{n-1}n$. This number grows exponentially with n. In particular, we have $\mathrm{cond}(\boldsymbol{L}) > 10^{16}$ for $n \geq 50$. Hence, $\boldsymbol{L}$ is generally ill-conditioned which affects the accuracy of the forward-substitution $\boldsymbol{y} = \boldsymbol{L}^{-1}\boldsymbol{b}$. Hence, although the condition number of $\boldsymbol{W}$ is moderate, we expect the LU algorithm to be inaccurate for this special example.

Next, let us consider the QR factorization-based approach. Due to $\|\boldsymbol{q}\|_\infty \leq \|\boldsymbol{q}\|_2$ for all $\boldsymbol{q} \in \mathbb{R}^m$, the orthonormality of the matrix $\boldsymbol{Q}$ implies $\|\boldsymbol{Q}\|_\infty, \|\boldsymbol{Q}^{-1}\|_\infty \leq 1$. Hence, it follows $\|\boldsymbol{R}\|_\infty = \|\boldsymbol{Q}^\top \boldsymbol{W}\|_\infty \leq n$ and $\|\boldsymbol{R}^{-1}\|_\infty = \|\boldsymbol{W}^{-1}\boldsymbol{Q}\|_\infty \leq 1$. This shows that $\boldsymbol{R}$ is generally well-conditioned. Thus, in contrast to the LU-based method, we expect this QR method to produce accurate results.

The `MATLAB` code below can be used to demonstrate these observations. (The associated `Python` code is similar and will be shared online). The results are shown in Figure 1 and illustrate that the LU algorithm is generally not accurate in this case. By contrast, the results returned by the QR method are accurate. Notice that $\boldsymbol{x}^*$ is computed using the true inverse $\boldsymbol{W}^{-1}$.

Notice that this behavior is *not typical* for the LU factorization (especially if pivoting is used). In general, the LU algorithm performs more favorably and in a more stable way. Numerical instabilities can only be observed for highly constructed ("academic") examples.

```
dim     = [10,50,75,100,250,500,1000];

err_lu  = zeros(length(dim),1);
err_qr  = zeros(length(dim),1);

rng(20241023)

for i = 1:length(dim)
    m           = dim(i);

    % Wilkinson-Matrix
    A           = 2*eye(m)-tril(ones(m)); A(:,m) = 1;

    % Build Inverse of Wilkinson-Matrix
    d1          = [1/2,-1./2.^(2:1:m-1)];
    d2          = 1./2.^(m-1:-1:1);
    d3          = d2(end:-1:1);
    T           = triu(toeplitz(d1));
    Ainv        = [T,-d2';d3,1/2^(m-1)];

    b           = randn(m,1);

    % Solve via LU factorization
    [L,U,p]     = lu(A,'vector');
```

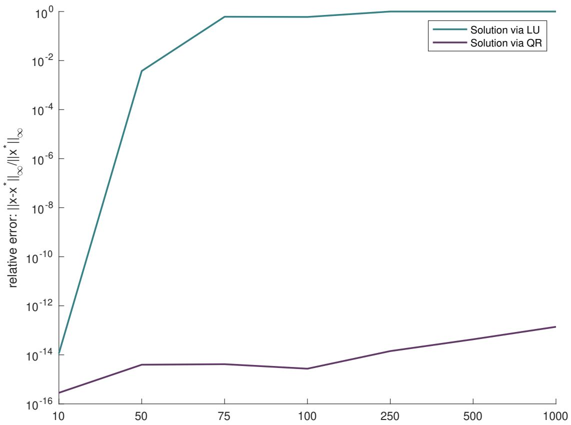

Figure 1: Logarithmic plot of the forward error $\|\boldsymbol{x}^* - \boldsymbol{x}\|/\|\boldsymbol{x}^*\|$ where $\boldsymbol{x}^* = \boldsymbol{W}^{-1}\boldsymbol{b}$ and $\boldsymbol{x} = \boldsymbol{U}^{-1}(\boldsymbol{L}^{-1}\boldsymbol{b})$ or $\boldsymbol{x} = \boldsymbol{R}^{-1}(\boldsymbol{Q}^\top\boldsymbol{b})$ for $n \in \{10, 50, 75, 100, 250, 500, 1000\}$ and $\boldsymbol{b} \sim \mathcal{N}(0,1)^n$.

```
    x           = U\(L\b(p));

    % Solve via QR factorization
    [Q,R]       = qr(A);
    y           = R\(Q'*b);

    % True solution
    sol         = Ainv*b;

    err_lu(i)   = norm(sol-x,'inf')/norm(sol,'inf');
    err_qr(i)   = norm(sol-y,'inf')/norm(sol,'inf');
end

figure;
hold on
plot(1:length(dim),log10(err_lu),'Color',[53,130,134]/255,'MarkerSize',12,'LineWidth
    ',1.5);
plot(1:length(dim),log10(err_qr),'Color',[98,56,105]/255,'MarkerSize',12,'LineWidth'
    ,1.5);
hold off

xticklabels(dim);
ytickformat('10^{%g}');

ylabel('dimension');
ylabel('relative error: ||x-x^*||_\infty/||x^*||_\infty');

legend('Solution via LU','Solution via QR');

saveas(gcf,'acc_lu_qr.eps','epsc');
```