Numerical Analysis MATH50003 (2025–26) Problem Sheet 5

In this problem sheet we investigate the LU, PLU and Cholesky factorisations by-hand. These are all mathematically equivalent to Gaussian elimination, but by writing it as a matrix factorisation we make it more amenable to implementation on a computer and reveal an underlying, intuitive structure. The PLU factorisation is how general linear systems are solved in practice on a computer, whilst the Choleksy factorisation can be used in the special case of symmetric positive definite matrices for better performance. Mathematically, an important property of Cholesky factorisations is that they include an algorithm to proof that matrix is positive definite.

Our first problem investigates LU factorisation and PLU factorisation, corresponding to Gaussian elimination with or without pivoting:

Problem 1 Compute the LU factorisation (if possible) and the PLU factorisation, where the entry of largest magnitude is always permuted to the diagonal, of the following matrices:

$$
\begin{bmatrix} 1 & 2 & 0 \\ 3 & 1 & 2 \\ 0 & 5 & 1 \end{bmatrix}, \begin{bmatrix} 0 & 5 & 5 & 5 \\ 1 & 2 & 0 & 0 \\ 3 & 3 & 3 & 0 \\ 0 & 0 & 3 & 1 \end{bmatrix}
$$

SOLUTION

Matrix 1 For the LU factorisation we have:

$$
A = \begin{bmatrix} 1 & 2 & 0 \\ 3 & 1 & 2 \\ 0 & 5 & 1 \end{bmatrix} = \underbrace{\begin{bmatrix} 1 & & \\ 3 & 1 & \\ 0 & 0 & 1 \end{bmatrix}}_{L_1} \begin{bmatrix} 1 & 2 & 0 \\ & -5 & 2 \\ & 5 & 1 \end{bmatrix}
$$

We now have

$$
A_2 = \begin{bmatrix} -5 & 2 \\ 5 & 1 \end{bmatrix} = \underbrace{\begin{bmatrix} 1 & \\ -1 & 1 \end{bmatrix}}_{L_2} \begin{bmatrix} -5 & 2 \\ & 3 \end{bmatrix}
$$

We can put it together to find:

$$
A = \underbrace{\begin{bmatrix} 1 & & \\ 3 & 1 & \\ 0 & -1 & 1 \end{bmatrix}}_{L} \underbrace{\begin{bmatrix} 1 & 2 & 0 \\ & -5 & 2 \\ 0 & 0 & 3 \end{bmatrix}}_{U}
$$

For the PLU factorisation we need to permute the largest entry to the diagonal each stage:

$$
\underbrace{\begin{bmatrix} 0 & 1 & \\ 1 & 0 & \\ & & 1 \end{bmatrix}}_{P_1} A = \begin{bmatrix} 3 & 1 & 2 \\ 1 & 2 & 0 \\ 0 & 5 & 1 \end{bmatrix} = \underbrace{\begin{bmatrix} 1 & & \\ 1/3 & 1 & \\ 0 & 0 & 1 \end{bmatrix}}_{L_1} \begin{bmatrix} 3 & 1 & 2 \\ 1 & 5/3 & -2/3 \\ 0 & 5 & 1 \end{bmatrix}
$$

We now permute again since $5 > 5/3$:

$$
\underbrace{\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}}_{P_2} A_2 = \begin{bmatrix} 5 & 1 \\ 5/3 & -2/3 \end{bmatrix} = \underbrace{\begin{bmatrix} 1 & \\ 1/3 & 1 \end{bmatrix}}_{L_2} \begin{bmatrix} 5 & 1 \\ & -1 \end{bmatrix}
$$

1

We thus have:

$$P_1 A = L_1 \begin{bmatrix} 1 & \\ & P_2^\top L_2 \end{bmatrix} \underbrace{\begin{bmatrix} 3 & 1 & 2 \\ & 5 & 1 \\ & & -1 \end{bmatrix}}_{U} = \begin{bmatrix} 1 & \\ & P_2^\top \end{bmatrix} \underbrace{\begin{bmatrix} 1 & & \\ 0 & 1 & \\ 1/3 & 1/3 & 1 \end{bmatrix}}_{L} U,$$

that is,

$$P = \begin{bmatrix} 1 & \\ & P_2 \end{bmatrix} P_1 = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$$

Matrix 2

This has no LU factorisation since the first entry is 0 so we only deduce the PLU. First permute the largest entry to the diagonal by a simple swap and factor:

$$\underbrace{\begin{bmatrix} 0 & & 1 & \\ & 1 & & \\ 1 & & 0 & \\ & & & 1 \end{bmatrix}}_{P_1} A = \begin{bmatrix} 3 & 3 & 3 \\ 1 & 2 & \\ 5 & 5 & 5 \\ & 3 & 1 \end{bmatrix} = \underbrace{\begin{bmatrix} 1 & & \\ 1/3 & 1 & \\ & & 1 \\ & & & 1 \end{bmatrix}}_{L_1} \begin{bmatrix} 3 & 3 & 3 \\ & 1 & -1 \\ & 5 & 1 & 2 \\ & & 3 & 1 \end{bmatrix}$$

We repeat with the subslice:

$$\underbrace{\begin{bmatrix} 0 & 1 & \\ 1 & 0 & \\ & & 1 \end{bmatrix}}_{P_2} A_2 = \begin{bmatrix} 5 & 5 & 5 \\ 1 & -1 & \\ & 3 & 1 \end{bmatrix} = \underbrace{\begin{bmatrix} 1 & & \\ 1/5 & 1 & \\ 0 & & 1 \end{bmatrix}}_{L_2} \begin{bmatrix} 5 & 5 & 5 \\ & -2 & -1 \\ & 3 & 1 \end{bmatrix}$$

Finally, we have

$$\underbrace{\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}}_{P_3} A_3 = \begin{bmatrix} 3 & 1 \\ -2 & -1 \end{bmatrix} = \underbrace{\begin{bmatrix} 1 & \\ -2/3 & 1 \end{bmatrix}}_{L_3} \underbrace{\begin{bmatrix} 3 & 1 \\ & -1/3 \end{bmatrix}}_{U_3}$$

We now need to swap the lower matrices and permutations which we do one step at a time. We already know $A_3 = P_3^\top L_3 U_3$ which tells us that

$$A_2 = P_2^\top L_2 \begin{bmatrix} \alpha_2 & \boldsymbol{w}_2^\top \\ & A_3 \end{bmatrix} = P_2^\top \begin{bmatrix} 1 & \\ & P_3^\top \end{bmatrix} \begin{bmatrix} 1 & \\ P_3 \boldsymbol{v}_2/\alpha_2 & L_3 \end{bmatrix} \begin{bmatrix} \alpha_2 & \boldsymbol{w}_2^\top \\ & U_3 \end{bmatrix}$$

$$= \underbrace{\begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}}_{\tilde{P}_2^\top} \underbrace{\begin{bmatrix} 1 & & \\ 0 & 1 & \\ 1/5 & -2/3 & 1 \end{bmatrix}}_{\tilde{L}_2} \underbrace{\begin{bmatrix} 5 & 5 & 5 \\ & 3 & 1 \\ & & -1/3 \end{bmatrix}}_{\tilde{U}_2}$$

Finally,

$$A = P_1^\top L_1 \begin{bmatrix} \alpha_1 & \boldsymbol{w}_1^\top \\ & A_2 \end{bmatrix} = P_1^\top \begin{bmatrix} 1 & \\ & \tilde{P}_2^\top \end{bmatrix} \begin{bmatrix} 1 & \\ \tilde{P}_2 \boldsymbol{v}_1/\alpha_1 & \tilde{L}_2 \end{bmatrix} \begin{bmatrix} \alpha_1 & \boldsymbol{w}_1^\top \\ & \tilde{U}_2 \end{bmatrix}$$

$$= \underbrace{\begin{bmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \end{bmatrix}}_{P^\top} \underbrace{\begin{bmatrix} 1 & & & \\ 0 & 1 & & \\ 0 & 0 & 1 & \\ 1/3 & 1/5 & -2/3 & 1 \end{bmatrix}}_{L} \underbrace{\begin{bmatrix} 3 & 3 & 3 & 0 \\ & 5 & 5 & 5 \\ & & 3 & 1 \\ & & & -2/3 \end{bmatrix}}_{U}$$

We now turn to Cholesky factorisations, which are a special way of computing LU factorisations when the matrix is symmetric-positive definite. In fact, we can use the factorisation to prove a symmetric matrix is positive definite:

Problem 2 By computing the Cholesky factorisation, determine which of the following matrices are symmetric positive definite:

$$\begin{bmatrix} 1 & -1 \\ -1 & 3 \end{bmatrix}, \begin{bmatrix} 1 & 2 & 2 \\ 2 & 1 & 2 \\ 2 & 2 & 1 \end{bmatrix}, \begin{bmatrix} 4 & 2 & 2 & 1 \\ 2 & 4 & 2 & 2 \\ 2 & 2 & 4 & 2 \\ 1 & 2 & 2 & 4 \end{bmatrix}$$

SOLUTION

A matrix is symmetric positive definite (SPD) if and only if it has a Cholesky factorisation, so the task here is really just to compute Cholesky factorisations (by hand). Since our goal is to tell if the Cholesky factorisations exist, we do not have to compute L_k's. We only need to see if the factorisation process can continue to the end.

Matrix 1

$$A_0 = \begin{bmatrix} 1 & -1 \\ -1 & 3 \end{bmatrix}$$

and $A_1 = 3 - \frac{(-1) \times (-1)}{1} > 0$, so Matrix 1 is SPD.

Matrix 2

$$A_0 = \begin{bmatrix} 1 & 2 & 2 \\ 2 & 1 & 2 \\ 2 & 2 & 1 \end{bmatrix}$$

Then

$$A_1 = \begin{bmatrix} 1 & 2 \\ 2 & 1 \end{bmatrix} - \begin{bmatrix} 2 \\ 2 \end{bmatrix} \begin{bmatrix} 2 & 2 \end{bmatrix} = \begin{bmatrix} -3 & -2 \\ -2 & -3 \end{bmatrix}$$

and finally $A_1[1,1] \leq 0$, so Matrix 2 is not SPD.

Matrix 3

$$A_0 = \begin{bmatrix} 4 & 2 & 2 & 1 \\ 2 & 4 & 2 & 2 \\ 2 & 2 & 4 & 2 \\ 1 & 2 & 2 & 4 \end{bmatrix}$$

and then

$$A_1 = \begin{bmatrix} 4 & 2 & 2 \\ 2 & 4 & 2 \\ 2 & 2 & 4 \end{bmatrix} - \frac{1}{4} \begin{bmatrix} 2 \\ 2 \\ 1 \end{bmatrix} \begin{bmatrix} 2 & 2 & 1 \end{bmatrix} = \frac{1}{4} \begin{bmatrix} 12 & 4 & 6 \\ 4 & 12 & 6 \\ 6 & 6 & 15 \end{bmatrix}$$

Furthermore

$$4A_2 = \begin{bmatrix} 12 & 6 \\ 6 & 15 \end{bmatrix} - \frac{1}{12} \begin{bmatrix} 4 \\ 6 \end{bmatrix} \begin{bmatrix} 4 & 6 \end{bmatrix} = \frac{4}{3} \begin{bmatrix} 8 & 3 \\ 3 & 9 \end{bmatrix}$$

and finally $3A_3 = 9 - \frac{3 \times 3}{8} > 0$, so Matrix 4 is SPD.

END

We can take this idea further and use the Cholesky factorisation to prove certain families of matrices are symmetric positive definite, for example, the following tridiagonal matrix (which we will see later is related to solving ordinary differential equations numerically):

Problem 3(a) Use the Cholesky factorisation to prove that the following $n \times n$ matrix is symmetric positive definite for any n:

$$\Delta_n := \begin{bmatrix} 2 & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & \ddots & \\ & & \ddots & \ddots & -1 \\ & & & -1 & 2 \end{bmatrix}$$

Hint: consider a matrix $K_n^{(\alpha)}$ that equals Δ_n apart from the top left entry which is $\alpha > 1$ and use a proof by induction.

SOLUTION

Consider the first step of the Cholesky factorisation:

$$\Delta_n = \begin{bmatrix} 2 & -\boldsymbol{e}_1^\top \\ -\boldsymbol{e}_1 & \Delta_{n-1} \end{bmatrix} = \underbrace{\begin{bmatrix} \sqrt{2} & \\ \frac{-\boldsymbol{e}_1}{\sqrt{2}} & I \end{bmatrix}}_{L_1} \begin{bmatrix} 1 & \\ & \Delta_{n-1} - \frac{\boldsymbol{e}_1 \boldsymbol{e}_1^\top}{2} \end{bmatrix} \underbrace{\begin{bmatrix} \sqrt{2} & \frac{-\boldsymbol{e}_1^\top}{\sqrt{2}} \\ & I \end{bmatrix}}_{L_1^\top}$$

The bottom right is merely Δ_{n-1} but with a different $(1,1)$ entry! This hints at a strategy of proving by induction.

Assuming $\alpha > 1$ write

$$K_n^{(\alpha)} := \begin{bmatrix} \alpha & -1 & & & \\ -1 & 2 & -1 & & \\ & -1 & 2 & \ddots & \\ & & \ddots & \ddots & -1 \\ & & & -1 & 2 \end{bmatrix} = \begin{bmatrix} \sqrt{\alpha} & \\ \frac{-\boldsymbol{e}_1}{\sqrt{\alpha}} & I \end{bmatrix} \begin{bmatrix} 1 & \\ & K_{n-1}^{(2-1/\alpha)} \end{bmatrix} \begin{bmatrix} \sqrt{\alpha} & \frac{-\boldsymbol{e}_1^\top}{\sqrt{\alpha}} \\ & I \end{bmatrix}$$

Note if $n = 1$ this is trivially SPD. Hence assume $K_{n-1}^{(\alpha)}$ is SPD for all $\alpha > 1$. If $\alpha > 1$ then $2 - 1/\alpha > 1$. Hence by induction and the fact that $\Delta_n = K_n^{(2)}$ we conclude that Δ_n has a Cholesky factorisation and hence is symmetric positive definite.

END

Problem 3(b) Deduce its Cholesky factorisations: $\Delta_n = L_n L_n^\top$ where L_n is lower triangular.

SOLUTION

We can write down the factors explicitly: define $\alpha_1 := 2$ and

$$\alpha_{k+1} = 2 - 1/\alpha_k.$$

Let's try out the first few:

$$\alpha_1 = 2, \alpha_2 = 3/2, \alpha_3 = 4/3, \alpha_4 = 5/4, \ldots$$

The pattern is clear and one can show by induction that $\alpha_k = (k+1)/k$. Thus we have the Cholesky factorisation

$$\Delta_n = \begin{bmatrix} \sqrt{2} & & & & \\ -1/\sqrt{2} & \sqrt{3/2} & & & \\ & -\sqrt{2/3} & \sqrt{4/3} & & \\ & & \ddots & \ddots & \\ & & & -\sqrt{(n-1)/n} & \sqrt{(n+1)/n} \end{bmatrix}$$

$$\underbrace{\phantom{\begin{bmatrix} \sqrt{2} & & & & \\ -1/\sqrt{2} & \sqrt{3/2} & & & \\ & -\sqrt{2/3} & \sqrt{4/3} & & \\ & & \ddots & \ddots & \\ & & & -\sqrt{(n-1)/n} & \sqrt{(n+1)/n} \end{bmatrix}}}_{L_n}$$

$$\times \begin{bmatrix} \sqrt{2} & -1/\sqrt{2} & & & \\ & \sqrt{3/2} & -\sqrt{2/3} & & \\ & & \ddots & \ddots & \\ & & & \sqrt{n/(n-1)} & -\sqrt{(n-1)/n} \\ & & & & \sqrt{(n+1)/n} \end{bmatrix}$$

$$\underbrace{\phantom{\begin{bmatrix} \sqrt{2} & -1/\sqrt{2} & & & \\ & \sqrt{3/2} & -\sqrt{2/3} & & \\ & & \ddots & \ddots & \\ & & & \sqrt{n/(n-1)} & -\sqrt{(n-1)/n} \\ & & & & \sqrt{(n+1)/n} \end{bmatrix}}}_{L_n^\top}$$

END

An alternative to an LU factorisation is a UL factorisation, where one uses row-eliminations beginning with the bottom row. Here we investigate the Cholesky analogue, which we call a *reverse* Cholesky factorisation:

Problem 3 Show that a matrix $A \in \mathbb{R}^{n \times n}$ is symmetric positive definite if and only if it has a *reverse* Cholesky factorisation of the form

$$A = UU^\top$$

where U is upper triangular with positive entries on the diagonal.

SOLUTION

Note $\boldsymbol{x}^\top UU^\top \boldsymbol{x} = \|U^\top \boldsymbol{x}\| > 0$ since U is invertible.

For the other direction, we replicate the proof by induction for standard Cholesky, beginning in the bottom right instead of the top left. Again the basis case is trivial. Since all diagonal entries are positive we can write

$$A = \begin{bmatrix} K & \boldsymbol{v} \\ \boldsymbol{v}^\top & \alpha \end{bmatrix} = \underbrace{\begin{bmatrix} I & \frac{\boldsymbol{v}}{\sqrt{\alpha}} \\ & \sqrt{\alpha} \end{bmatrix}}_{U_1} \begin{bmatrix} K - \frac{\boldsymbol{v}\boldsymbol{v}^\top}{\alpha} & \\ & 1 \end{bmatrix} \underbrace{\begin{bmatrix} I & \\ \frac{\boldsymbol{v}^\top}{\sqrt{\alpha}} & \sqrt{\alpha} \end{bmatrix}}_{U_1^\top}$$

By assumption $K - \frac{\boldsymbol{v}\boldsymbol{v}^\top}{\alpha} = \tilde{U}\tilde{U}^\top$ hence we have

$$A = \underbrace{U_1 \begin{bmatrix} \tilde{U} & \\ & 1 \end{bmatrix}}_{U} \underbrace{\begin{bmatrix} \tilde{U}^\top & \\ & 1 \end{bmatrix} U_1^\top}_{U^\top}$$

END

5