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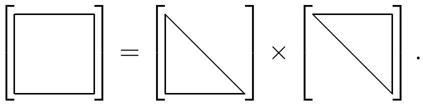
Easter 1997

# Numerical Analysis – Lecture 1

## 1 LU factorization of matrices

### 1.1 Definition and applications

Let $A$ be a real $n \times n$ matrix. We say that the $n \times n$ matrices $L$ and $U$ are an *LU factorization* of $A$ if *(1)* $L$ is lower-triangular (i.e., $L_{i,j} = 0$, $i < j$), *(2)* $U$ is upper-triangular, $U_{i,j} = 0$, $i > j$, and *(3)* $A = LU$. Therefore the factorization takes the form



**Application 1** Calculation of a determinant: $\det A = \det L \det U = \prod_{k=1}^{n} L_{k,k} \prod_{k=1}^{n} U_{k,k}$.

**Application 2** Testing nonsingularity: $A = LU$ is nonsingular iff all the diagonal elements of $L$ and $U$ are nonzero.

**Application 3** Solution of linear systems: Let $A = LU$ and suppose we wish to solve $A\boldsymbol{x} = \boldsymbol{b}$. This is the same as $L(U\boldsymbol{x}) = \boldsymbol{b}$, which we decompose into $L\boldsymbol{y} = \boldsymbol{b}$, $U\boldsymbol{x} = \boldsymbol{y}$. Both latter systems are triangular and can be calculated easily. Thus, $L_{1,1}y_1 = b_1$ gives $y_1$, next $L_{2,1}y_1 + L_{2,2}y_2 = b_2$ yields $y_2$ etc. Having found $\boldsymbol{y}$, we solve for $\boldsymbol{x}$ by reversing the order: $U_{n,n}x_n = y_n$ gives $x_n$, $U_{n-1,n-1}x_{n-1} + U_{n-1,n}x_n = y_{n-1}$ produces $x_{n-1}$ and so on.

**Application 4** The inverse of $A$: It is straightforward to devise a direct way of calculating the inverse of triangular matrices, subsequently forming $A^{-1} = U^{-1}L^{-1}$.

### 1.2 The calculation of LU factorization

We denote the *columns* of $L$ by $\boldsymbol{l}_1, \boldsymbol{l}_2, \ldots, \boldsymbol{l}_n$ and the *rows* of $U$ by $\boldsymbol{u}_1^{\mathrm{T}}, \boldsymbol{u}_2^{\mathrm{T}}, \ldots, \boldsymbol{u}_n^{\mathrm{T}}$. Hence

$$A = LU = [\ \boldsymbol{l}_1 \quad \boldsymbol{l}_2 \quad \cdots \quad \boldsymbol{l}_n\ ] \begin{bmatrix} \boldsymbol{u}_1^{\mathrm{T}} \\ \boldsymbol{u}_2^{\mathrm{T}} \\ \vdots \\ \boldsymbol{u}_n^{\mathrm{T}} \end{bmatrix} = \sum_{k=1}^{n} \boldsymbol{l}_k \boldsymbol{u}_k^{\mathrm{T}}. \tag{1.1}$$

Since the first $k-1$ components of $\boldsymbol{l}_k$ and $\boldsymbol{u}_k$ are all zero, each rank-one matrix $\boldsymbol{l}_k\boldsymbol{u}_k^{\mathrm{T}}$ has zeros in its first $k$ rows and columns.

Assume that the factorization exists and that $A$ is nonsingular. Since $\boldsymbol{l}_k\boldsymbol{u}_k^{\mathrm{T}}$ stays the same if we replace $\boldsymbol{l}_k \to \alpha\boldsymbol{l}_k$, $\boldsymbol{u}_k \to \alpha^{-1}\boldsymbol{u}_k$, where $\alpha \neq 0$, we may assume w.l.o.g. that all diagonal elements of $L$ equal one. In other words, the $k$th row of $\boldsymbol{l}_k\boldsymbol{u}_k^{\mathrm{T}}$ is $\boldsymbol{u}_k^{\mathrm{T}}$ and its $k$th column is $U_{k,k}$ times $\boldsymbol{l}_k$.

We commence from $k = 1$. Since the first elements of $\boldsymbol{l}_k$ and $\boldsymbol{u}_k$ are zero for $k \geq 2$, it follows from (1.1) that $\boldsymbol{u}_1^{\mathrm{T}}$ is the first row of $A$ and $\boldsymbol{l}_1$ is the first column of $A$, divided by $A_{1,1}$ (so that $L_{1,1} = 1$!).

Having found $\boldsymbol{l}_1$ and $\boldsymbol{u}_1$, we form the matrix $A - \boldsymbol{l}_1\boldsymbol{u}_1^{\mathrm{T}} = \sum_{k=2}^{n} \boldsymbol{l}_k\boldsymbol{u}_k^{\mathrm{T}}$. The first row & column of $A$ are zero and it follows that $\boldsymbol{u}_2^{\mathrm{T}}$ is the second row of $A - \boldsymbol{l}_1\boldsymbol{u}_1^{\mathrm{T}}$, while $\boldsymbol{l}_2$ is its second column, scaled so that $L_{2,2} = 1$.

**The LU algorithm:** Set $A_0 := A$. For all $k = 1, 2, \ldots, n$ set $\boldsymbol{u}_k^{\mathrm{T}}$ to the $k$th row of $A_{k-1}$ and $\boldsymbol{l}_k$ to the $k$th column of $A_{k-1}$, scaled so that $L_{k,k} = 1$. Further, calculate $A_k := A_{k-1} - \boldsymbol{l}_k\boldsymbol{u}_k^{\mathrm{T}}$ before incrementing $k$.

Note that all elements in the first $k$ rows & columns of $A_k$ are zero. Hence, we can use the storage of the original $A$ to accumulate $L$ and $U$.

## 1.3 Relation to Gaussian elimination

The equation $A_k = A_{k-1} - \boldsymbol{l}_k\boldsymbol{u}_k^{\mathrm{T}}$ has the property that the $j$th row of $A_k$ is the $j$th row of $A_{k-1}$ minus $L_{j,k}$ times $\boldsymbol{u}_k^{\mathrm{T}}$ (the $k$th row of $A_{k-1}$). Moreover, the multipliers $L_{k,k}, L_{k+1,k}, \ldots, L_{n,k}$ are chosen so that the outcome of this *elementary row operation* is that the $k$th column of $A_k$ is zero. This construction is analogous to Gaussian elimination for solving $A\boldsymbol{x} = \boldsymbol{b}$. An important difference is that in LU we do not consider the right hand side $\boldsymbol{b}$ until the factorization is complete. This is useful e.g. when there are many right hand sides, in particular if not all the $\boldsymbol{b}$'s are known at the outset.

## 1.4 Pivoting

Naive LU factorization fails when, for example, $A_{1,1} = 0$. The remedy is to exchange rows of $A$, a technique called *column pivoting.* This is equivalent to picking a suitable equation for eliminating the first unknown in Gaussian elimination. Specifically, column pivoting means that, having obtained $A_{k-1}$, we exchange two rows of $A_{k-1}$ so that the element of largest magnitude in the $k$th column is in the 'pivotal position' $(k, k)$. In other words,

$$|(A_{k-1})_{k,k}| = \max\{|(A_{k-1})_{j,k}| \,:\, j = 1, 2, \ldots, n\}.$$

Of course, the same exchange is required in the part of $L$ that has been formed already (i.e., the first $k-1$ columns). Also, we need to record the permutation of rows to solve for the right hand side and/or to compute the determinant.

This procedure copes with zeros at the pivot position, except when the whole $k$th column of $A_k$ is zero – in that case it is usual to let $\boldsymbol{l}_k$ be the $k$th unit vector (and, as before, choose $\boldsymbol{u}_k^{\mathrm{T}}$ as the $k$th row of $A_k$).

An important advantage of this procedure is that every element of $L$ has magnitude at most one. This avoids not just division by zero but also tends to reduce the chance of very large numbers occuring during the factorization, a phenomenon that might lead to accumulation of *roundoff error* and to *ill conditioning.*

In *row pivoting* one exchanges columns of $A_{k-1}$, rather than rows (sic!), whereas *total pivoting* corresponds to exchange of both rows and columns, so that the modulus of the pivotal element $(A_{k-1})_{k,k}$ is maximized.

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