Theorem Let A be an $n \times n$ nonsingular matrix. Then A has a unique LU decomposition if and only if all the leading principal submatrices of A are nonsingular.

Proof: Suppose A has an LU decomposition. Consider the partitioning $A = \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix}$ where A_{11} is the $k \times k$ leading principal submatrix of A with $1 \leq k \leq n-1$. Partitioning, L and U conformally gives,

$$A = LU \Rightarrow \begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} = \begin{bmatrix} L_{11} & \\ L_{21} & L_{22} \end{bmatrix} \begin{bmatrix} U_{11} & U_{12} \\ & U_{22} \end{bmatrix}.$$

Then

$$A_{11} = L_{11}U_{11} \Rightarrow \det A_{11} = \det(L_{11}U_{11}) = \det L_{11} \det U_{11} = \det U_{11} = \prod_{i=1}^{k} u_{ii},$$

where u_{ii} are the diagonal entries of U. As A is nonsingular and $A = LU$, so is U. Therefore $u_{ii} \neq 0$ for all $i = 1, \dots, n$. Hence A_{11} is nonsingular as $\det A_{11} = \prod_{i=1}^{k} u_{ii} \neq 0$. Since A_{11} is an arbitrary leading principal submatrix of A, all leading principal submatrices of A must be nonsingular.

Conversely, suppose that all the leading principal submatrices of A are nonsingular. To prove that A has a *unique* LU decomposition, we proceed by induction on the order n of A. If $n = 1$, then trivially, $A = [a_{11}] = [1][a_{11}]$ is a unique LU decomposition. Suppose that all nonsingular matrices of size at most $n-1$ whose leading principal submatrices are all nonsingular, have a unique LU decomposition. Consider the partition $A = \begin{bmatrix} \widehat{A} & a \\ b^T & a_{nn} \end{bmatrix}$ where $\widehat{A}$ is the leading principal submatrix of A of size $n-1$, a is the column vector of first $n-1$ entries of the last column of A and b^T is the row vector of first $n-1$ entries of the last row of A. As all leading principal submatrices of A are nonsingular, $\widehat{A}$ is nonsingular and all its leading principal submatrices are also nonsingular. Therefore by assumption, it has a unique LU decomposition, say, $\widehat{A} = \widehat{L}\widehat{U}$. Since $\widehat{A}$ is nonsingular, $\widehat{U}$ is also nonsingular. Thus the system $\widehat{U}^T x = b$ has a unique solution. Let this be l. Also let u be the unique solution of $\widehat{L}x = a$ and $u_{nn} = a_{nn} - l^T u$. Then as $\widehat{L}u = a$, $\widehat{U}^T l = b$ and $a_{nn} = u_{nn} + l^T u$,

$$A = \begin{bmatrix} \widehat{L}\widehat{U} & a \\ b^T & a_{nn} \end{bmatrix} = \underbrace{\begin{bmatrix} \widehat{L} & \\ l^T & 1 \end{bmatrix}}_{=:L} \underbrace{\begin{bmatrix} \widehat{U} & u \\ & u_{nn} \end{bmatrix}}_{=:U},$$

which gives an LU decomposition of A. Note that this is a unique LU decomposition as $\widehat{L}$, $\widehat{U}$ l, u

and u_{nn} are all unique. Hence the proof follows by induction for all nonsingular matrices whose leading principal submatrices are all nonsingular. $\square$

Theorem Given any square matrix A, there exists a permutation matrix P such that PA has an LU decomposition.

Proof: The proof is by induction on the size of A. Suppose A is a $n \times n$ matrix. If $n = 1$, then the statement holds trivially as $A = [a_{11}] = [1][a_{11}]$. Suppose the statement holds for all matrices of order $n-1$ or less. The proof is divided into two cases.

Case I. Suppose the $(1,1)$ entry of A is nonzero. Partitioning A as

$$A = \left[\begin{array}{c|c} a_{11} & a^T \\ \hline b & \widehat{A} \end{array}\right],$$

where a^T is the row vector of the last $n-1$ entries of the first row of A, b is the column vector of the last $n-1$ entries of the first column of A and $\widehat{A}$ is the trailing principal submatrix of A of order $n-1$, we have

$$A = \left[\begin{array}{c|c} 1 & \\ \hline \frac{b}{a_{11}} & I_{n-1} \end{array}\right] \left[\begin{array}{c|c} a_{11} & a^T \\ \hline & \widehat{A} - \frac{b}{a_{11}} a^T \end{array}\right] \tag{1}$$

Since $\widehat{A} - \frac{b}{a_{11}} a^T$ is of size $n-1$, by induction hypothesis, there exists a permutation $\widehat{P}$ such that $\widehat{P}(\widehat{A} - \frac{b}{a_{11}} a^T) = \widehat{L}\widehat{U}$ is an LU decomposition. Thus $\widehat{A} - \frac{b}{a_{11}} a^T = \widehat{P}^T \widehat{L}\widehat{U}$. Using this in (1),

$$A = \left[\begin{array}{c|c} 1 & \\ \hline \frac{b}{a_{11}} & I_{n-1} \end{array}\right] \left[\begin{array}{c|c} a_{11} & a^T \\ \hline & \widehat{P}^T \widehat{L}\widehat{U} \end{array}\right] = \left[\begin{array}{c|c} 1 & \\ \hline \frac{b}{a_{11}} & \widehat{P}^T \end{array}\right] \left[\begin{array}{c|c} 1 & \\ \hline & \widehat{L} \end{array}\right] \left[\begin{array}{c|c} a_{11} & a^T \\ \hline & \widehat{U} \end{array}\right]. \tag{2}$$

Now $\left[\begin{array}{c|c} 1 & \\ \hline \frac{b}{a_{11}} & \widehat{P}^T \end{array}\right] \left[\begin{array}{c|c} 1 & \\ \hline & \widehat{L} \end{array}\right] = \left[\begin{array}{c|c} 1 & \\ \hline & \widehat{P}^T \end{array}\right] \left[\begin{array}{c|c} 1 & \\ \hline \widehat{P}\frac{b}{a_{11}} & I_{n-1} \end{array}\right] \left[\begin{array}{c|c} 1 & \\ \hline & \widehat{L} \end{array}\right] = \left[\begin{array}{c|c} 1 & \\ \hline & \widehat{P}^T \end{array}\right] \left[\begin{array}{c|c} 1 & \\ \hline \widehat{P}\frac{b}{a_{11}} & \widehat{L} \end{array}\right].$

Using this in (2),

$$A = \left[\begin{array}{c|c} 1 & \\ \hline & \widehat{P}^T \end{array}\right] \left[\begin{array}{c|c} 1 & \\ \hline \widehat{P}\frac{b}{a_{11}} & \widehat{L} \end{array}\right] \left[\begin{array}{c|c} a_{11} & a^T \\ \hline & \widehat{U} \end{array}\right] \Rightarrow \left[\begin{array}{c|c} 1 & \\ \hline & \widehat{P} \end{array}\right] A = \left[\begin{array}{c|c} 1 & \\ \hline \widehat{P}\frac{b}{a_{11}} & \widehat{L} \end{array}\right] \left[\begin{array}{c|c} a_{11} & a^T \\ \hline & \widehat{U} \end{array}\right].$$

Setting $P = \left[\begin{array}{c|c} 1 & \\ \hline & \widehat{P} \end{array}\right]$, $L = \left[\begin{array}{c|c} 1 & \\ \hline \widehat{P}\frac{b}{a_{11}} & \widehat{L} \end{array}\right]$ and $U = \left[\begin{array}{c|c} a_{11} & a^T \\ \hline & \widehat{U} \end{array}\right]$, gives $PA = LU$ and the proof follows by induction in this case.

Case II. Suppose the $(1,1)$ entry of A is zero. If the whole first column of A is 0, then

$$A = \left[\begin{array}{c|c} 0 & a^T \\ \hline 0 & \widehat{A} \end{array}\right],$$

where again a^T is the row vector of the last $n-1$ entries of the first row of A and $\widehat{A}$ is the trailing principal submatrix of A of order $n-1$. By induction hypothesis, there is a permutation matrix $\widehat{P}$ such that $\widehat{P}\widehat{A} = \widehat{L}\widehat{U}$ is an LU decomposition. Therefore,

$$A = \left[\begin{array}{c|c} 0 & a^T \\ \hline 0 & \widehat{P}^T\widehat{L}\widehat{U} \end{array}\right] = \left[\begin{array}{c|c} 1 & \\ \hline & \widehat{P}^T \end{array}\right] \left[\begin{array}{c|c} 1 & \\ \hline & \widehat{L} \end{array}\right] \left[\begin{array}{c|c} 0 & a^T \\ \hline 0 & \widehat{U} \end{array}\right] \Rightarrow \left[\begin{array}{c|c} 1 & \\ \hline & \widehat{P} \end{array}\right] A = \left[\begin{array}{c|c} 1 & \\ \hline & \widehat{L} \end{array}\right] \left[\begin{array}{c|c} 0 & a^T \\ \hline 0 & \widehat{U} \end{array}\right].$$

Setting $P = \left[\begin{array}{c|c} 1 & \\ \hline & \widehat{P} \end{array}\right]$, $L = \left[\begin{array}{c|c} 1 & \\ \hline & \widehat{L} \end{array}\right]$ and $U = \left[\begin{array}{c|c} 0 & a^T \\ \hline 0 & \widehat{U} \end{array}\right]$, gives $PA = LU$.

Suppose the whole first column of A is not equal to 0. Then there is a transposition P_1 that interchanges the first row of A with some other row such that the $(1,1)$ entry of P_1A is not zero. Then arguing as in Case I, there exists a permutation $\widehat{P}$, such that $\widehat{P}(P_1A) = LU$ is an LU dcomposition of P_1A. Setting $P = \widehat{P}P_1$ gives $PA = LU$.

Therefore in either case, the proof follows by induction. $\square$