Gaussian Elimination.

We now analyze ~~that~~ the most basic algorithm for solving $Ax=b$.

Definition. A permutation matrix P is an identity matrix with permuted rows.

We Know:

Lemma. Let P, P_1, P_2 be permutation matrices and X be any $n \times n$ matrix.

1. PX is X with rows permuted.
   XP is X with columns permuted.
2. $P^{-1} = P^T$ (or P is an orthogonal matrix)
3. $\det(P) = \pm 1$
4. $P_1 P_2$ is also a permutation matrix.

The proof is homework.

Algorithm. (Gauss Elimination)

1. Factorize A into $A = PLU$ where

   P = permutation matrix

   L = a lower triangular matrix with 1's on the diagonal

   U = nonsingular upper triangular matrix

2. Solve $PLUx = b$ for LUx using $P^{-1} = P^T$ and writing

$$P^{-1}(PLUx) = P^{-1}b$$
$$LUx = P^T b$$

   This permutes the entries of b.

3. Solve $LUx = P^T b$ for Ux using back substitution:

$$\begin{bmatrix} 1 & & & \\ a_{21} & 1 & & \\ a_{31} & a_{32} & 1 & \\ \cdot & \cdots & \cdots & 1 \end{bmatrix} \begin{bmatrix} (Ux)_1 \\ \\ \\ (Ux)_n \end{bmatrix} = \begin{bmatrix} (P^T b)_1 \\ \\ \\ (P^T b)_n \end{bmatrix}$$

We know

$$(Ux)_1 = (P^T b)_1$$

$$(Ux)_2 = (P^T b)_2 - a_{21}(Ux)_1$$

$$\vdots$$

$$(Ux)_n = (P^T b)_n - \sum_{i=1}^{n-1} a_{ni}(Ux)_i$$

so it isn't hard to solve a lower triangular system. The resulting vector is $L^{-1}(P^T b)$.

4. Solve $Ux = L^{-1}(P^T b)$ for x by forward substitution.

$$\begin{bmatrix} a_{11} & a_{12} & \cdots & \cdots \\ & a_{22} & \cdots & \cdots \\ & & a_{33} & \cdots \\ & & & \ddots \\ & & & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} L^{-1}(P^T b)_1 \\ \vdots \\ L^{-1}(P^T b)_n \end{bmatrix}$$

This works just like back substitution except we start by solving for x_n

and work our way back to x_1 rather than vice versa.

A few points are worth making before we go on.

1) We compute P, L, and U rather than A^{-1}. In fact, we don't explicitly compute L^{-1} or U^{-1} either.

2) Once we have P, L, and U, solving for a new right hand side is very inexpensive.

Now why do we need the permutation matrix P?

Definition. The leading $j \times j$ principal submatrix of A is the upper left $j \times j$ block submatrix.

Theorem. The following are equivalent:

$\exists$ a unique unit lower triangular L and nonsingular upper triangular U so that $A = LU$

$$\Updownarrow$$

all leading principal submatrices of A are nonsingular.

Proof. Suppose $A = LU$. Then for any j, we can write A in block form

$$\begin{bmatrix} A_{11} & A_{12} \\ A_{21} & A_{22} \end{bmatrix} = \begin{bmatrix} L_{11} & 0 \\ L_{21} & L_{22} \end{bmatrix} \begin{bmatrix} U_{11} & U_{12} \\ 0 & U_{22} \end{bmatrix}$$

$$= \begin{bmatrix} L_{11}U_{11} & L_{11}U_{12} \\ L_{21}U_{11} & L_{21}U_{12} + L_{22}U_{22} \end{bmatrix}$$

where A_{11}, L_{11}, U_{11} are $j \times j$ matrices.

Now

$$\det A_{11} = \det(L_{11}U_{11})$$
$$= \det(L_{11}) \cdot \det(U_{11})$$

We now need a useful linear algebra fact:

Fact. If B is lower (or upper) triangular, then $\det B = \prod_{i=1}^{n} b_{ii}$.

Thus

$$\det L_{11} \cdot \det U_{11} = 1 \cdot \prod_{k=1}^{j} (U_{11})_{kk} \neq 0$$

since L is unit (1's on diagonal), and U is nonsingular (if $\prod_{k=1}^{j}(U_{11})_{kk} = 0$, $\det U = \prod_{k=1}^{n} U_{kk} = 0$).

This proves $\Downarrow$.

Now we prove $\Uparrow$ by induction on n.
For $n=1$, $[a] = [1] \cdot [a]$ where $[a]$ is nonsingular if $a \neq 0$ and there is only one leading principal submatrix.

So suppose we know:

1) $\tilde{A}$ is an $n \times n$ matrix with all leading principal submatrices nonsingular.

2) For $(n-1) \times (n-1)$ matrices, all leading principal submatrices nonsingular $\Rightarrow$ $\exists$ a unique LU decomposition.

So write

$$\tilde{A} = \begin{bmatrix} A & b \\ c^T & \delta \end{bmatrix}$$

where A is $(n-1) \times (n-1)$, b, c are vectors in $\mathbb{R}^{n-1}$, and δ is a scalar.

we know $A = LU$. If we can complete this to an LU decomposition of $\tilde{A}$, we have

$$\begin{bmatrix} A & b \\ c^T & \delta \end{bmatrix} = \begin{bmatrix} L & 0 \\ \ell^T & 1 \end{bmatrix} \begin{bmatrix} U & u \\ 0 & \eta \end{bmatrix}$$

$$= \begin{bmatrix} LU & Lu \\ \ell^T U & \ell^T u + \eta \end{bmatrix}$$

So we need to choose u, ℓ, η so that

$$Lu = b, \quad \ell^T U = c^T, \quad \eta + \ell^T u = \delta$$

The first equation can clearly be solved by back substitution, the second can be written

$U^T \ell = c$, and again solved by back substitution

The last equation can be solved as

$\eta = \delta - \ell^T u$ once we know ℓ, u.

Clearly, ℓ, u, η are determined uniquely.

We need only check η nonzero.
But

$$0 \neq \det \tilde{A} = \det \begin{bmatrix} L & 0 \\ \ell^T & 1 \end{bmatrix} \det \begin{bmatrix} \mathcal{U} & u \\ 0 & \eta \end{bmatrix}$$

$$= 1 \cdot (\det \mathcal{U}) \cdot \eta$$

and $\det \mathcal{U} \neq 0$ by induction. $\square$.

This explains why we need permutations: for example the matrix

$$A = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}$$ has singular leading principal 1×1 and 2×2 submatrices

and so has no LU decomposition.

Of course, we haven't proved that a suitable permutation will give any nonsingular matrix nonsingular leading principal submatrices.

In fact, this is true:

Theorem. If A is nonsingular, there exist permutations P_1 and P_2 so that

$$P_1 A = LU \quad \text{and} \quad A P_2 = LU$$

where L is unit lower triangular, U is nonsingular upper triangular. ~~Further, there are (different~~ ~~the statements holds with ei~~

Proof. See Demmel, p. 40 for a messy, but basically straightforward proof by induction on n.