Gaussian Elimination with Partial Pivoting

While it is true that almost all nonsingular matrices can be triangularized using only Gauss Transforms (add multiple of one row to another), it does not make a good general purpose numerical method. The problem is caused, as you might suspect, by small pivot elements. Consider the $k^{th}$ step, zeroing the $(i, k)$ entries with multipliers $m_{ik} = -a_{ik}^{(k-1)}/a_{kk}^{(k-1)}$, $k+1, k+2, \ldots, n$:

$$a_i^{(k)} = a_i^{(k-1)} + m_{ik}a_k^{(k-1)},$$

giving

$$A^{(k)} = \begin{bmatrix} \hat{U}^{(k)} & X \\ 0 & \hat{A}^{(k)} \end{bmatrix}.$$  

If $a_{kk}^{(k-1)}$ is small, then $|m_{ik}|$ will be large, and two bad things will happen: (i) information in the entries of $A^{(k-1)}$ gets swamped when the large vector $m_{ik}a_k^{(k-1)}$ gets added to $a_i^{(k-1)}$, and (ii) that information is replaced by basically the same value for each row: $a_i^{(k)}$ will be mostly in the direction $a_k^{(k-1)}$ for all of the rows $i = k+1, k+2, \ldots, n$ of $A^{(k)}$, moving $\hat{A}^{(k)}$ closer to the set of singular matrices.

So it’s time to bring back row operation R2: Before zeroing the elements in column $k$, we find $\max_{k \leq j \leq n} |a_{jk}^{(k-1)}|$ (the $|\text{biggest}|$ element of the first column of $\hat{A}^{(k-1)}$). If that max occurs in row $p$, then we interchange rows $k$ and $p$ of $A^{(k-1)}$. This is called partial pivoting. Now the $|\text{biggest}|$ entry in the first row of the permuted $\hat{A}^{(k-1)}$ is in its $(1, 1)$ position, and thus all of the multipliers for this step satisfy $|m_{ik}| \leq 1$.

In the language of matrix operations: Before applying the Gauss transform $M_k$, we apply the permutation $P_{kp}$. The $k^{th}$ step of GE with partial pivoting (GEPP) is

$$A^{(k)} = M_kP_kA^{(k-1)},$$

and after $n - 1$ steps

$$A^{(n-1)} = M_{n-1}P_{n-1} \cdots M_2P_2M_1P_1A \equiv U.$$  

If $A$ is nonsingular, this can always be done. It does not give the $A = LU$ factorization as before, because the permutations (row interchanges) mess up the lower triangularity of $L$. In order to see what factorization we do get, we need to interpret the matrix $M_{n-1}P_{n-1} \cdots M_2P_2M_1P_1$. To that end, take $j < k \leq p$ and notice that an $e_j$ Gauss transform followed by a $(k, p)$ permutation is that permutation followed by a different (permutted $m_j$) $e_j$ Gauss transform:

$$P_kM_j = P_k(I + m_je_j^t) = P_k + P_km_je_j^tP_k^tP_k \equiv (I + \tilde{m}_je_j^t)P_k \equiv \tilde{M}_jP_k.$$  

Now define $N_i = I + n_ie_i^t$, where $n_i = P_{n-1} \cdots P_{i+1}m_i$.

$$M_{n-1}P_{n-1} \cdots M_2P_2M_1P_1 = (N_{n-1} \cdots N_2N_1)(P_{n-1} \cdots P_2P_1) \equiv L^{-1}P,$$

giving $PA = LU$. This simple change makes GE general purpose; in fact GEPP (and then forward and backward substitution) is the most often used method for solving $Ax = b$.  