Gauss elimination and LU factorization - breakdown

Recall a point in the Gauss elimination algorithm:
if $a_{kk} \neq 0$, $a_{ik} = a_{ik} / a_{kk}$, else quit   /* a_{kk} pivot */
Clearly, if $a_{kk} = 0$, this algorithm cannot be applied in the form it was given.

For example, the GE algorithm, as it was given, cannot be applied to the matrix

$$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$$

although it is easy to solve a system with such a matrix.

Gauss elimination and LU factorization - instability

Consider a computer system with three decimal digits floating-point arithmetic with rounding. In this system, the numbers can be represented as $\pm 0.d_1 d_2 d_3 \times 10^e$, where $0 \leq d_i \leq 9$, and e some exponent, positive, negative or zero, with finite but large number of digits. E.g.
1 is represented $.100 \times 10^1$,
0.0001 is represented $.100 \times 10^{-3}$,
1.234 is represented $.123 \times 10^1$, and
1.236 is represented $.124 \times 10^1$,
1.001 is represented $.100 \times 10^1$, etc.

Gauss elimination and LU factorization - instability

Using exact (fractional or with enough decimals) arithmetic, apply GE to the matrix

$$A = \begin{bmatrix} -0.001 & 1 \\ 1 & 1 \end{bmatrix}.$$

We have

$$L = \begin{bmatrix} 1 & 0 \\ -1000 & 1 \end{bmatrix}, U = \begin{bmatrix} -0.001 & 1 \\ 0 & 1001 \end{bmatrix}$$

Now solve $Ax = b$ with $b = [1, 2]^T$, using the L, U factors obtained above, that is, solve $Ly = b$, $Ux = y$. In exact (fractional or with enough decimals) arithmetic, we obtain $y = [1, 1002]^T$, $x = [1000/1001, 1002/1001]^T \approx [0.999, 1.001]^T$.

Gauss elimination and LU factorization - instability

If, though, we apply GE to

$$A = \begin{bmatrix} -0.001 & 1 \\ 1 & 1 \end{bmatrix}$$

doing *all* computations in three decimal digits floating-point arithmetic, we have

$$L^* = \begin{bmatrix} 1 & 0 \\ -1000 & 1 \end{bmatrix}, U^* = \begin{bmatrix} -0.001 & 1 \\ 0 & 1000 \end{bmatrix}$$

Now solve $Ax = b$ with $b = [1, 2]^T$, using the L^*, U^* factors obtained above, that is, solve $L^* y^* = b$, $U^* x = y^*$. Doing *all* computations in three decimal digits floating-point arithmetic, we obtain $y^* = [1, 1000]^T$, $x^* = [0, 1]^T$. This solution vector is completely incorrect: $x^*{}_1$ does not have any correct digit.

The problem stems from the large (in abs. value) numbers appearing in L and U, which numbers stem, themselves, from the small denominator in the multiplier $l_{21} = -\dfrac{1}{0.001}$.

Gauss elimination and LU factorization - instability

Let’s interchange the rows of the matrix and of the right-hand side, and let’s repeat the procedure. In exact arithmetic, we obtain

$$A = \begin{bmatrix} 1 & 1 \\ -0.001 & 1 \end{bmatrix}$$

$$L = \begin{bmatrix} 1 & 0 \\ -0.001 & 1 \end{bmatrix}, U = \begin{bmatrix} 1 & 1 \\ 0 & 1.001 \end{bmatrix}.$$

Now solve $Ax = b$ with $b = [1, 2]^T$, using the L, U factors obtained above, that is, solve $Ly = b$, $Ux = y$. We obtain $y = [2, 1.002]^T$, $x = [1.001, 0.999]^T$, which is the correct solution. Also, in three decimal digits floating-point arithmetic,

$$L^* = \begin{bmatrix} 1 & 0 \\ -0.001 & 1 \end{bmatrix}, U^* = \begin{bmatrix} 1 & 1 \\ 0 & 1 \end{bmatrix}.$$

Solving $L^* y^* = b$, $U^* x^* = y^*$, doing *all* computations in three decimal digits floating-point arithmetic, we obtain $y^* = [2, 1]^T$, $x^* = [1, 1]^T$, which is correct to the third digit. The error is at the level of 10^{-3}, something natural, since we used three decimal digits.

Gauss elimination and LU factorization - interchanges of rows - pivoting

Pivoting in GE is a technique according to which rows (or columns or both rows and columns) are interchanged, so that zero or very small in absolute value denominators in multipliers are avoided. Thus the applicability and/or stability of GE is enhanced. Through GE with pivoting, we are either able to solve systems not solvable due to zero denominators, or able to solve systems with better accuracy than without pivoting.

Row pivoting: reorder rows of the matrix. ($P_r A = LU$, P_r permutation matrix)
Column pivoting: reorder columns of the matrix. ($AP_c = LU$, P_c permutation matrix)
Partial pivoting: row or column pivoting (one of the two).
Complete pivoting: reorder both rows and columns of the matrix. ($P_r A P_c = LU$)
Symmetric pivoting: reorder both rows and columns of the matrix, but apply the same reordering to both rows and columns. ($PAP^T = LU$)

The most common form of pivoting is row pivoting, so we often omit the term ‘‘row’’ or ‘‘partial’’.

Notes:
Reordering rows (columns) of matrix A is equivalent to pre-multiplying (post-multiplying) A by a permutation matrix.

Gauss elimination and LU factorization -- pivoting

The strategy followed in (row) pivoting is summarized as follows:

At the kth GE step, before the multipliers at column k, rows $k+1, \cdots, n$, are computed, a search along the kth column from row k to row n is performed, to identify the largest in absolute value element. This element becomes the *pivot*. Assume the pivot belongs to row s, i.e. $|a_{sk}| = \max\{|a_{ik}|, i = k, \cdots, n\}$. If $s \neq k$, rows k and s are interchanged.
In most standard implementations, this interchange is done by indirect indexing. That is, an integer vector, say *ipiv*, of size n or $n-1$ is used to refer to the indices of rows. For example, we can define *ipiv* (size $n-1$) by using the following idea: *ipiv(k)* = s means that rows k and s were interchanged during the kth elimination step. If *ipiv(k)* = k, then no interchange took place at the kth elimination step. (We could also keep track of the permutation vector - size n - corresponding to the permutation matrix reflecting the interchanges.) The result of one or more interchanges of rows of A is a reordering of the rows of A.
After the possible interchange of rows, the multipliers are computed as usual, and the elimination step proceeds.

Gauss elimination and LU factorization -- pivoting -- algorithm

Gauss elimination with partial pivoting algorithm for general $n \times n$ matrices

for k = 1 to n-1 do
  find row s with $\max_{i=k}^{n} \{|a_{ik}|\}$ ($s = \arg\max_{i=k}^{n} \{|a_{ik}|\}$)   /* a_{sk} pivot */
  if $a_{sk} = 0$, matrix is singular, quit
  interchange rows k and s
  for i = k+1 to n do
    $a_{ik} = a_{ik} / a_{kk}$ /* a_{kk} pivot */
    for j = k+1 to n do
      $a_{ij} = a_{ij} - a_{ik} a_{kj}$ /* a_{ik} multiplier */
    endfor
  endfor
endfor

Cost: The algorithm requires $\sum_{k=1}^{n-1} (n-k) = \sum_{k=1}^{n-1} k = \frac{(n-1)n}{2} \approx \frac{n^2}{2}$ comparisons in addition to the flops of the algorithm without pivoting.

Asymptotically, it has the same cost as the no pivoting algorithm, i.e. $\frac{n^3}{3}$.

Gauss elimination (GE) and LU factorization with pivoting -- example

Consider the linear system $Ax = b$, where

$$A = \begin{bmatrix} 1 & -2 & -4 & -3 \\ 2 & 0 & -1 & 2 \\ -1 & 2 & 2 & -1 \\ 3 & 0 & -3 & 6 \end{bmatrix}, \; x = \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix}, \; b = \begin{bmatrix} 2 \\ -1 \\ 4 \\ 9 \end{bmatrix}.$$

The system can be also described with the so-called **augmented** matrix

$$[A \colon b] = \left[\begin{array}{rrrrcr} 1 & -2 & -4 & -3 & : & 2 \\ 2 & 0 & -1 & 2 & : & -1 \\ -1 & 2 & 2 & -1 & : & 4 \\ 3 & 0 & -3 & 6 & : & 9 \end{array}\right].$$

Gauss elimination (GE) and LU factorization with pivoting -- example step 1

$k = 1$

Find along column 1 (rows 1 to 4) the maximum in absolute value element, and interchange its row with row 1.

$$\left[\begin{array}{rrrrcr} 1 & -2 & -4 & -3 & : & 2 \\ 2 & 0 & -1 & 2 & : & -1 \\ -1 & 2 & 2 & -1 & : & 4 \\ \mathbf{3} & 0 & -3 & 6 & : & 9 \end{array}\right] \rightarrow \left[\begin{array}{rrrrcr} 3 & 0 & -3 & 6 & : & 9 \\ 2 & 0 & -1 & 2 & : & -1 \\ -1 & 2 & 2 & -1 & : & 4 \\ 1 & -2 & -4 & -3 & : & 2 \end{array}\right], \; P_1 = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}$$

$$ipiv = [4, \cdot, \cdot]$$

Eliminate x_1 from rows (equations) 2 to 4 through the row operations

$\rho_2^{(1)} \leftarrow \rho_2 - 2/3\rho_1$
$\rho_3^{(1)} \leftarrow \rho_3 + 1/3\rho_1$
$\rho_4^{(1)} \leftarrow \rho_4 - 1/3\rho_1$

$$\rightarrow \left[\begin{array}{rrrrcr} 3 & 0 & -3 & 6 & : & 9 \\ 2/3 & 0 & 1 & -2 & : & -7 \\ -1/3 & 2 & 1 & 1 & : & 7 \\ 1/3 & -2 & -3 & -5 & : & -1 \end{array}\right] = [A^{(1)} \colon b^{(1)}]$$

Notes: The part of A below the ‘‘stair-step’’ belongs to L, but we overlay the elements of L within $A^{(k)}$ for being concise and for indicating that we save memory when doing the related computation.

ipiv is a vector or one-dimensional array. Relation $ipiv(k) = s$ denotes that rows k and s were interchanged in the kth step of the algorithm.

Gauss elimination (GE) and LU factorization with pivoting -- example step 2

$k = 2$

Find along column 2 (rows 2 to 4) the maximum in absolute value element, and interchange its row with row 2.

$$\left[\begin{array}{rrrrcr} 3 & 0 & -3 & 6 & : & 9 \\ 2/3 & 0 & 1 & -2 & : & -7 \\ -1/3 & \mathbf{2} & 1 & 1 & : & 7 \\ 1/3 & -2 & -3 & -5 & : & -1 \end{array}\right] \rightarrow \left[\begin{array}{rrrrcr} 3 & 0 & -3 & 6 & : & 9 \\ -1/3 & 2 & 1 & 1 & : & 7 \\ 2/3 & 0 & 1 & -2 & : & -7 \\ 1/3 & -2 & -3 & -5 & : & -1 \end{array}\right], \; P_2 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}$$

$$ipiv = [4, 3, \cdot]$$

Eliminate x_2 from rows (equations) 3 to 4 through the row operations

$\rho_3^{(2)} \leftarrow \rho_3^{(1)} - 0\rho_2^{(1)}$
$\rho_4^{(2)} \leftarrow \rho_4^{(1)} + \frac{2}{2}\rho_2^{(1)}$

$$\rightarrow \left[\begin{array}{rrrrcr} 3 & 0 & -3 & 6 & : & 9 \\ -1/3 & 2 & 1 & 1 & : & 7 \\ 2/3 & 0 & 1 & -2 & : & -7 \\ 1/3 & -1 & -2 & -4 & : & 6 \end{array}\right] = [A^{(2)} \colon b^{(2)}]$$

Gauss elimination (GE) and LU factorization with pivoting -- example step 3

$k = 3$

Find along column 3 (rows 3 to 4) the maximum in absolute value element, and interchange its row with row 3.

$$\left[\begin{array}{rrrrcr} 3 & 0 & -3 & 6 & : & 9 \\ -1/3 & 2 & 1 & 1 & : & 7 \\ 2/3 & 0 & 1 & -2 & : & -7 \\ 1/3 & -1 & \mathbf{-2} & -4 & : & 6 \end{array}\right] \rightarrow \left[\begin{array}{rrrrcr} 3 & 0 & -3 & 6 & : & 9 \\ -1/3 & 2 & 1 & 1 & : & 7 \\ 1/3 & -1 & -2 & -4 & : & 6 \\ 2/3 & 0 & 1 & -2 & : & -7 \end{array}\right], \; P_3 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$$

$$ipiv = [4, 3, 4]$$

Eliminate x_3 from row (equation) 4 through the row operation

$\rho_4^{(3)} \leftarrow \rho_4^{(2)} + \frac{1}{2}\rho_3^{(2)}$

$$\rightarrow \left[\begin{array}{rrrrcr} 3 & 0 & -3 & 6 & : & 9 \\ -1/3 & 2 & 1 & 1 & : & 7 \\ 1/3 & -1 & -2 & -4 & : & 6 \\ 2/3 & 0 & -1/2 & -4 & : & -4 \end{array}\right] = [A^{(3)} \colon b^{(3)}]$$

Gauss elimination (GE) and LU factorization with pivoting -- attention

We obtained

$$\begin{bmatrix} 3 & 0 & -3 & 6 \\ -1/3 & 2 & 1 & 1 \\ 1/3 & -1 & -2 & -4 \\ 2/3 & 0 & -1/2 & -4 \end{bmatrix} \to L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -1/3 & 1 & 0 & 0 \\ 1/3 & -1 & 1 & 0 \\ 2/3 & 0 & -1/2 & 1 \end{bmatrix}, U = \begin{bmatrix} 3 & 0 & -3 & 6 \\ 0 & 2 & 1 & 1 \\ 0 & 0 & -2 & -4 \\ 0 & 0 & 0 & -4 \end{bmatrix}$$

Attention: Relation $A = LU$ no longer holds; but we have $PA = LU$, where $P = P_3 P_2 P_1$, i.e.,

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

More specifically:

Gauss elimination (GE) and LU factorization with pivoting -- properties

We know that each row interchange to a matrix A is equivalent to pre-multiplying A by a permutation matrix P.

The steps of GE with pivoting can be expressed as

Initially: $Ax = b$

Step 1: $M^{(1)} P_1 A x = M^{(1)} P_1 b$ or $A^{(1)} x = b^{(1)}$

Step 2: $M^{(2)} P_2 M^{(1)} P_1 A x = M^{(2)} P_2 M^{(1)} P_1 b$ or $A^{(2)} x = b^{(2)}$

Step 3: $M^{(3)} P_3 M^{(2)} P_2 M^{(1)} P_1 A x = M^{(3)} P_3 M^{(2)} P_2 M^{(1)} P_1 b$ or $A^{(3)} x = b^{(3)}$ or $Ux = c$

From above, we have $M^{(3)} P_3 M^{(2)} P_2 M^{(1)} P_1 A = U$. It can be shown that this relation is equivalent to $PA = LU$, where $P = P_3 P_2 P_1$.
Caution: While $M^{(k)}$ are lower triangular, the matrix $M^{(3)} P_3 M^{(2)} P_2 M^{(1)} P_1$ is not necessarily lower triangular.

Gauss elimination (GE) and LU factorization with pivoting -- properties

Repeat: The matrix $M^{(3)} P_3 M^{(2)} P_2 M^{(1)} P_1$ is not necessarily lower triangular. In the example, we have

$$M^{(3)} P_3 M^{(2)} P_2 M^{(1)} P_1 = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 1/3 \\ 1 & 0 & 1 & 0 \\ 1/2 & 1 & 1/2 & -2/3 \end{bmatrix},$$

$$L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -1/3 & 1 & 0 & 0 \\ 1/3 & -1 & 1 & 0 \\ 2/3 & 0 & -1/2 & 1 \end{bmatrix}, L^{-1} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 1/3 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ -2/3 & 1/2 & 1/2 & 1 \end{bmatrix}$$

We observe that L^{-1} is of the same type as $M^{(3)} P_3 M^{(2)} P_2 M^{(1)} P_1$ but with some or all columns in different order. We can actually show that $L^{-1} = M^{(3)} P_3 M^{(2)} P_2 M^{(1)} P_1 P^{-1}$, i.e. $L^{-1} = M^{(3)} P_3 M^{(2)} P_2 M^{(1)} P_1 P_1^{-1} P_2^{-1} P_3^{-1}$.

Gauss elimination (GE) and LU factorization with pivoting -- properties

In the general $n \times n$ case, at the kth step of GE with pivoting ($k = 1, \cdots, n-1$) we have

$$M^{(k)} P_k M^{(k-1)} P_{k-1} \cdots M^{(1)} P_1 A x = M^{(k)} P_k M^{(k-1)} P_{k-1} \cdots M^{(1)} P_1 b \quad \text{or } A^{(k)} x = b^{(k)}$$

From above, we have

$$M^{(n-1)} P_{n-1} M^{(n-2)} P_{n-2} \cdots M^{(1)} P_1 A = U. \tag{2.4}$$

It can be shown that (2.4) is equivalent to

$$PA = LU, \text{ where } P = P_{n-1} P_{n-2} \cdots P_1, \tag{2.5}$$

and L unit lower triangular.
It can also be shown that

$$L = P P_1 (M^{(1)})^{-1} P_2 (M^{(2)})^{-1} \cdots P_{n-1} (M^{(n-1)})^{-1} \tag{2.6}$$

$$L^{-1} = M^{(n-1)} P_{n-1} M^{(n-2)} P_{n-2} \cdots M^{(1)} P_1 P^{-1} \tag{2.7}$$

Gauss elimination (GE) and LU factorization with pivoting -- properties

Matrices P_k are derived from $\mathbf{I}$ by interchanging two rows and are called **elementary permutation matrices**.

As permutation matrices, they are also orthogonal: $P_k^{-1} = P_k^T$.
As elementary permutation matrices, they are also symmetric: $P_k = P_k^T$.

Thus we have: $P_k = P_k^{-1}$, $P_k P_k = \mathbf{I}$ (**idempotent** matrices).

Matrix $P = P_{n-1} P_{n-2} \cdots P_1$ is a permutation matrix (therefore also orthogonal), however, neither necessarily elementary permutation matrix, nor necessarily symmetric. In the example,

$$P_1 = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix}, P_2 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix}, P_3 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}, P = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

Solution of linear systems by GE/LU with pivoting

There are two ways of solving $Ax = b$ on GE with pivoting (GEpiv).

The first applies GEpiv to A and b simultaneously, and obtains an upper triangular matrix U and a transformed vector $c = b^{(n-1)}$, such that $Ax = b$ (or $[A\colon b]$) is equivalent to $Ux = c$ (or $[U\colon c]$), then applies back substitution to $Ux = c$ to compute x. In this case, the multipliers are computed, but do not need to be stored. Note that, when GEpiv is applied to A and b, both the row permutations and the elimination operations are applied to both A and b. The permutation matrix P (or the *ipiv* vector) does not need to be stored for the solution process.

The second, applies GEpiv to A, and obtains the L and U factors and the permutation matrix P, such that $PA = LU$, then applies f/s to $Lc = Pb$ to compute an intermediate vector c, and then applies b/s to $Ux = c$, to compute x. In this case, the multipliers are computed and stored in the strictly lower triangular part of A. The permutation matrix P is not explicitly stored, but the vector *ipiv* is, and from that the relevant information can be extracted.

Solution of linear systems by GE/LU with pivoting -- GEpiv to A and b

First way: In the example,

$$[A^{(3)}\colon b^{(3)}] = \begin{bmatrix} 3 & 0 & -3 & 6 & : & 9 \\ -1/3 & 2 & 1 & 1 & : & 7 \\ 1/3 & -1 & -2 & -4 & : & 6 \\ 2/3 & 0 & -1/2 & -4 & : & -4 \end{bmatrix}$$

and back substitution is applied to solve $Ux = c$, i.e.

$$\begin{bmatrix} 3 & 0 & -3 & 6 \\ 0 & 2 & 1 & 1 \\ 0 & 0 & -2 & -4 \\ 0 & 0 & 0 & -4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 9 \\ 7 \\ 6 \\ -4 \end{bmatrix}$$

Back substitution to $Ux = c$ of the example gives

$$\begin{bmatrix} 3 & 0 & -3 & 6 \\ 0 & 2 & 1 & 1 \\ 0 & 0 & -2 & -4 \\ 0 & 0 & 0 & -4 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{bmatrix} = \begin{bmatrix} 9 \\ 7 \\ 6 \\ -4 \end{bmatrix} \Rightarrow \begin{array}{l} x_4 = -4/(-4) = 1 \\ x_3 = (6 - (-4)x_4)/(-2) = (6+4)/(-2) = 10/(-2) = -5 \\ x_2 = (7 - x_4 - x_3)/2 = (7 - 1 - (-5))/2 = 11/2 \\ x_1 = (9 - 6x_4 - (-3)x_3 - 0x_2)/3 = \\ \quad = (9 - 6 + 3(-5))/3 = -4 \end{array}$$

Thus, $x = [-4, 11/2, -5, 1]^T$ is the solution vector for $Ax = b$.

Solution of linear systems by GE/LU with pivoting -- GEpiv to A

Second way: In the example, A is decomposed into

$$\begin{bmatrix} 3 & 0 & -3 & 6 \\ -1/3 & 2 & 1 & 1 \\ 1/3 & -1 & -2 & -4 \\ 2/3 & 0 & -1/2 & -4 \end{bmatrix} \to L = \begin{bmatrix} 1 & 0 & 0 & 0 \\ -1/3 & 1 & 0 & 0 \\ 1/3 & -1 & 1 & 0 \\ 2/3 & 0 & -1/2 & 1 \end{bmatrix}, U = \begin{bmatrix} 3 & 0 & -3 & 6 \\ 0 & 2 & 1 & 1 \\ 0 & 0 & -2 & -4 \\ 0 & 0 & 0 & -4 \end{bmatrix}$$

with

$$P = P_3 P_2 P_1 = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix} \cdot \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{bmatrix} \cdot \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix}$$

We have $PA = LU$. From relations $Ax = b$ and $PA = LU$, we get $LUx = Pb$, thus the solution of $Ax = b$ is computed by

- computing $\hat{b} = Pb$ (row interchanges to b)
- applying f/s to $Lc = \hat{b}$
- applying b/s to $Ux = c$.

Solution of linear systems by GE/LU with pivoting -- GEpiv to A

In the example,

$$\hat{b} = Pb = \begin{bmatrix} 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 2 \\ -1 \\ 4 \\ 9 \end{bmatrix} = \begin{bmatrix} 9 \\ 4 \\ 2 \\ -1 \end{bmatrix}$$

Solve $Lc = \hat{b}$ with f/s

$$\begin{bmatrix} 1 & 0 & 0 & 0 \\ -1/3 & 1 & 0 & 0 \\ 1/3 & -1 & 1 & 0 \\ 2/3 & 0 & -1/2 & 1 \end{bmatrix} \begin{bmatrix} c_1 \\ c_2 \\ c_3 \\ c_4 \end{bmatrix} \begin{bmatrix} 9 \\ 4 \\ 2 \\ -1 \end{bmatrix} \Rightarrow \begin{aligned} c_1 &= 9 \\ c_2 &= 4 - (-1/3)c_1 = 4 + 1/3 \cdot 9 = 7 \\ c_3 &= 2 - (1/3)c_1 - (-1)c_2 = 2 - 1/3 \cdot 9 + 7 = 6 \\ c_4 &= -1 - (2/3)c_1 - 0c_2 - (-1/2)c_3 = \\ &= -1 - 2/3 \cdot 9 + 1/2 \cdot 6 = -4 \end{aligned}$$

Note that c above is the same as $c = b^{(n-1)}$, we had computed using the first way.
Then, solve $Ux = c$ with b/s as in page 127, to obtain the same solution vector x as before.

Solution of linear systems by GE/LU with pivoting

The two ways are mathematically equivalent and involve the same computational cost. However, when we need to solve several linear systems with the same matrix and different right-hand side vectors, we should adopt the second way, apply GE/LU once, store the L and U factors and the *ipiv* vector, then apply row interchanges and a pair of f/s and b/s to each right-hand side vector.
Cost for solving m linear systems of size $n \times n$ with the same matrix: $\frac{n^3}{3} + m(\frac{n^2}{2} + \frac{n^2}{2}) = \frac{n^3}{3} + mn^2$ flops, $\frac{n^2}{2} + mn$ divisions, and $\frac{n^2}{2}$ comparisons.

Scaling and GE/LU with partial pivoting

Recall: In three decimal digits floating-point arithmetic, GE/LU without pivoting applied to $Ax = b$, with

$$A = \begin{bmatrix} -0.001 & 1 \\ 1 & 1 \end{bmatrix}, b = \begin{bmatrix} 1 \\ 2 \end{bmatrix}, \quad (2.8)$$

produced inaccurate results, while, GE/LU with pivoting applied to the same system produced reasonably accurate results.
Consider now solving $Ax = b$, with

$$A = \begin{bmatrix} -1 & 1000 \\ 1 & 1 \end{bmatrix}, b = \begin{bmatrix} 1000 \\ 2 \end{bmatrix}, \quad (2.9)$$

using GE/LU with pivoting. It is clear that GEpiv applied to $Ax = b$ with (2.9) will not interchange the rows, and GEpiv will produce the same results as the no pivoting GE applied to $Ax = b$ with (2.8). This discrepancy comes from bad scaling. If we scale each equation so that the largest element in each row is equal to 1, and then apply GEpiv in three decimal digits floating-point arithmetic, we will get the reasonably accurate results of GEpiv applied to $Ax = b$ with (2.8).

Aside: $Ax = b$ with A, b as in (2.8) is equivalent to $Ax = b$ with A, b as in (2.9).

GE/LU with scaled partial pivoting

Gauss elimination with scaled partial pivoting algorithm for general $n \times n$ matr.

for $i = 1$ to n do
    $t = \max_{j=1}^{n} \{|a_{ij}|\}$
    if $t = 0$, the system is singular, quit
    for $j = 1$ to n do
        $a_{ij} = a_{ij} / t$
    endfor
endfor
apply Gauss elimination with partial pivoting algorithm

Operation counts:
The algorithm requires $n(n-1) \approx n^2$ comparisons and equal number of divisions in addition to the flops and comparisons required by the partial pivoting (no scaling) algorithm. There are variations of this algorithm that save about half of the divisions (by scaling only the multipliers as they are generated during the elimination process). The bottom-line is that, it requires approximately the same amount of work as the no-pivoting algorithm ($n^3/3$). Thus, scaled partial pivoting (though it does not always improve the results as magically as in the example) is considered a useful technique for improving the accuracy of GE.

Complete pivoting

Complete pivoting strategy: At the kth GE step, before the multipliers at column k, rows $k+1, \cdots, n$, are computed, a search in the submatrix of size $(n-k+1) \times (n-k+1)$ is performed, to identify the largest in absolute value element. This element becomes the *pivot*. Assume the pivot belongs to row l, and column m, i.e. $|a_{lm}| = \max\{|a_{ij}|, i = k, \cdots, n, j = k, \cdots, n\}$. If $l \neq k$, rows k and l are interchanged, and if $m \neq k$, columns k and m are interchanged.

Gauss elimination with complete pivoting algorithm for general $n \times n$ matrices

for k = 1 to n-1 do
    $(l, m) = \arg \max_{i=k, j=k}^{n} \{|a_{ij}|\}$ /* a_{lm} pivot */
    if $a_{lm} = 0$, the system is singular, quit
    interchange rows k and l and columns k and m
    for i = k+1 to n do
        $a_{ik} = a_{ik} / a_{kk}$ /* a_{kk} pivot */
        for j = k+1 to n do
            $a_{ij} = a_{ij} - a_{ik} a_{kj}$ /* a_{ik} multiplier */
        endfor
    endfor
endfor

Complete pivoting

Operation counts:

The algorithm requires $\sum_{k=1}^{n-1} (n-k)^2 = \sum_{k=1}^{n-1} k^2 = \frac{n(n-1)(2n-1)}{6} \approx \frac{n^3}{3} = O(n^3)$ comparisons in addition to the flops required by the no-pivoting algorithm.

Asymptotically, it requires approximately twice the amount of work of the no-pivoting algorithm ($\frac{n^3}{3}$).

For this reason, although complete pivoting can improve the accuracy of GE on certain (pathological) cases further than scaled partial pivoting, it is rarely used.

Effect of pivoting to special matrices

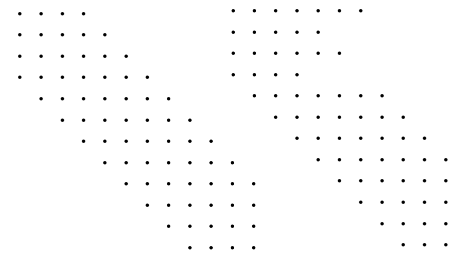
Symmetric matrices:

- Row (or column or complete) pivoting may destroy the symmetry of a matrix. Symmetric pivoting (same reordering to both rows and columns) preserves symmetry.

Banded matrices ((l, u)-banded):

- Partial (row or column) pivoting may alter the bandwidth, but preserves *some* bandedness. More specifically,
  - Row pivoting applied to an (l, u)-banded matrix generates (at most) l additional non-zero superdiagonals, i.e., U is $(0, u+l)$−banded, while L has at most $l+1$ non-zero elements per column.
  - Column piv. applied to an (l, u)-banded matrix generates (at most) u additional non-zero subdiagonals, i.e., L is $(u+l, 0)$−banded.
- Complete pivoting may destroy any bandedness.

Example: possible interchange of rows



MATLAB -- LU factorization of matrices and solution of linear systems

MATLAB has a function `lu` that returns the LU factorization of a matrix under various pivoting strategies.

The most common form of using `lu` is `[L, U, P] = lu(A)` This returns the LU factorization of A with partial (row) pivoting (no scaling), so that $PA = LU$, where L unit lower triangular, U upper triangular, and P permutation matrix representing the row interchanges.

Another form of using `lu` is `[L, U, p] = lu(A, 'vector')` This does the same as above, except that it returns the permutation vector in p instead of the permutation matrix.

To obtain scaled partial pivoting, we can use

```
D = diag(1./max(abs(A')));
[L, U, P] = lu(D*A);
```


MATLAB -- LU factorization of matrices and solution of linear systems

If `lu` is used in the simple form `[L_1, U] = lu(A)` it returns a permuted unit lower triangular matrix L_1 and an upper triangular matrix U so that $A = L_1 U$. The relations that hold between the matrices returned by `lu` in

```
[L_1, U_1] = lu(A)
[L, U, P] = lu(A)
```

are $L_1 = P^T L$, and $U_1 = U$.
(Recall that $P^T = P^{-1}$, since P is a permutation matrix, hence orthogonal.)

MATLAB -- LU factorization of matrices and solution of linear systems

To obtain the **solution** of a linear system $Ax = b$, MATLAB has a special operator: ‘‘\’’ (backslash). More specifically, `x = A\b` gives the solution of $Ax = b$. Internally, the backslash operator uses some version of GE, as well as forward and back substitutions.

Important note:
Whenever the solution of a linear system, $Ax = b$, is needed, use
`x = A\b`.

Although mathematically, `x = inv(A)*b` is equivalent to `x = A\b`, computationally, the two expressions are **very** different, with the former (using `inv`) being much heavier in computational load. Therefore, if the inverse of the matrix is not needed explicitly, the use of `inv` must be avoided, especially for large matrices.

Mathematical software

General information and free mathematical software

GAMS: Guide to Available Mathematical Software in `http://gams.nist.gov/` (by NIST, the National Institute of Standards and Technology of U.S.A.)

Netlib Repository in `http://www.netlib.org/`

For Linear Algebra

Jack Dongarra’s survey in
`http://www.netlib.org/utk/people/JackDongarra/la-sw.html`

BLAS: Basic Linear Algebra Subprograms in `http://www.netlib.org/blas/`

LINPACK: direct solution of linear systems in
`http://www.netlib.org/linpack/`

ITPACK and **NSPCG**: iterative solution of linear systems (including methods for non symmetric matrices) in `http://www.netlib.org/itpack/`

EISPACK: eigenvalue/eigenvector computation in
`http://www.netlib.org/eispack/`

Mathematical software

Free mathematical software (cont.)

LAPACK: direct solution of linear systems & eigenvalue/eigenvector computation optimized for shared-memory parallel and vector computers in
`http://www.netlib.org/lapack/`
`http://math.nist.gov/lapack++/`
`http://www.netlib.org/lapack90/`
(supersedes some of the previous packages)

Free alternatives to matlab:
`http://www.dspguru.com/dsp/links/matlab-clones/`
`http://page.math.tu-berlin.de/˜ehrhardt/matlab_alternatives.html`

Mathematical software

Commercial mathematical software

MATLAB: Matrix Laboratory
`http://www.mathworks.com/`
direct and iterative solution of linear systems, eigenvalue/eigenvector computation, solution of non-linear systems, interpolation, approximation, numerical integration, solution of differential equations, optimization, statistics, symbolic computation, etc.

IMSL: International Mathematical Software Library
complete set of mathematical software as above.

NAG: Numerical Algorithms Group
complete set of mathematical software as above.

Maple:
`http://www.maplesoft.com/`
symbolic computation as well as a fairly good set of numerical computation routines.

Aside: Effect of permutation matrix to another matrix -- examples

$$A = \begin{bmatrix} 1 & 0 & 3 \\ 4 & 5 & 0 \\ 0 & 8 & 9 \end{bmatrix}, P = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}, PA = \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \cdot \begin{bmatrix} 1 & 0 & 3 \\ 4 & 5 & 0 \\ 0 & 8 & 9 \end{bmatrix} = \begin{bmatrix} 4 & 5 & 0 \\ 0 & 8 & 9 \\ 1 & 0 & 3 \end{bmatrix}$$

$$AP = \begin{bmatrix} 1 & 0 & 3 \\ 4 & 5 & 0 \\ 0 & 8 & 9 \end{bmatrix} \cdot \begin{bmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} = \begin{bmatrix} 3 & 1 & 0 \\ 0 & 4 & 5 \\ 9 & 0 & 8 \end{bmatrix}, P^T = \begin{bmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{bmatrix}, PAP^T = \begin{bmatrix} 5 & 0 & 4 \\ 8 & 9 & 0 \\ 0 & 3 & 1 \end{bmatrix}$$

$$P = \begin{bmatrix} 0 & 0 & 1 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}, A = \begin{bmatrix} 11 & 12 & 0 & 14 & 0 \\ 21 & 22 & 23 & 0 & 0 \\ 0 & 32 & 33 & 34 & 0 \\ 0 & 0 & 43 & 44 & 45 \\ 0 & 0 & 0 & 54 & 55 \end{bmatrix}, P^T = \begin{bmatrix} 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix}$$

$$PAP^T = (PA)P^T = \begin{bmatrix} 0 & 32 & 33 & 34 & 0 \\ 21 & 22 & 23 & 0 & 0 \\ 0 & 0 & 43 & 44 & 45 \\ 11 & 12 & 0 & 14 & 0 \\ 0 & 0 & 0 & 54 & 55 \end{bmatrix} \cdot \begin{bmatrix} 0 & 0 & 0 & 1 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 1 & 0 & 0 & 0 & 0 \\ 0 & 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 33 & 32 & 34 & 0 & 0 \\ 23 & 22 & 0 & 21 & 0 \\ 43 & 0 & 44 & 0 & 45 \\ 0 & 12 & 14 & 11 & 0 \\ 0 & 0 & 54 & 0 & 55 \end{bmatrix}$$

Aside: Permutation vectors and matrices

Permutation vector p: a vector of n components whose values are the integers $1, \cdots, n$, but possibly not in that order.

Let $p = (k_1, k_2, \cdots, k_n)^T$ be a permutation vector. Define a permutation matrix P by

$$P_{ij} = \begin{cases} 1 & \text{if } j = k_i \\ 0 & \text{otherwise.} \end{cases}$$

Then PA permutes the rows of A according to the permutation p, i.e.

$$PA = \begin{bmatrix} a_{k_1,1} & a_{k_1,2} & \cdots & a_{k_1,n} \\ a_{k_2,1} & a_{k_2,2} & \cdots & a_{k_2,n} \\ . & . & & . \\ . & . & & . \\ . & . & & . \\ a_{k_n,1} & a_{k_n,2} & \cdots & a_{k_n,n} \end{bmatrix}$$

and AP permutes the columns of A according to the permutation p.

Permutation vector for previous 3×3 example: $p = [2, 3, 1]^T$.
Permutation vector for previous 5×5 example: $p = [3, 2, 4, 1, 5]^T$.
Attention: The pivotal vector in the GEpiv example, is *not* a permutation vector.