Gaussian Elimination: with partial pivoting

$$\left[\begin{array}{cccc|c} 0.02 & 0.01 & 0 & 0 & 0.02 \\ 1 & 2 & 1 & 0 & 1 \\ 0 & 1 & 2 & 1 & 4 \\ 0 & 0 & 100 & 200 & 800 \end{array}\right]$$

1. Find entry in the first column with the largest absolute value – pivot.
2. Interchange row (if required) to take the pivot element to the first row – pivot row

$$\left[\begin{array}{cccc|c} 0.02 & 0.01 & 0 & 0 & 0.02 \\ 1 & 2 & 1 & 0 & 1 \\ 0 & 1 & 2 & 1 & 4 \\ 0 & 0 & 100 & 200 & 800 \end{array}\right] \xrightarrow{R_1 \leftrightarrow R_2} \left[\begin{array}{cccc|c} 1 & 2 & 1 & 0 & 1 \\ 0.02 & 0.01 & 0 & 0 & 0.02 \\ 0 & 1 & 2 & 1 & 4 \\ 0 & 0 & 100 & 200 & 800 \end{array}\right]$$

3. Gaussian elimination: $R_2 \to R_2 - 0.02\,R_1;\ R_3 \to R_3;\ R_4 \to R_4$

$$\left[\begin{array}{cccc|c} 1 & 2 & 1 & 0 & 1 \\ 0 & -0.03 & -0.02 & 0 & 0 \\ 0 & 1 & 100 & 200 & 800 \\ 0 & 0 & 0.04 & 200 & 800 \end{array}\right]$$

4. Find new pivot and switch rows (if necessary)

$$\left[\begin{array}{cccc|c} 1 & 2 & 1 & 0 & 1 \\ 0 & -0.03 & -0.02 & 0 & 0 \\ 0 & 1 & 2 & 1 & 4 \\ 0 & 0 & 100 & 200 & 800 \end{array}\right] \xrightarrow{R_3 \leftrightarrow R_2} \left[\begin{array}{cccc|c} 1 & 2 & 1 & 0 & 1 \\ 0 & 1 & 2 & 1 & 4 \\ 0 & -0.03 & -0.02 & 0 & 0 \\ 0 & 0 & 100 & 200 & 800 \end{array}\right]$$

5. Apply Gaussian elimination: $R_3 \to R_3 + 0.03\, R_2$

$$\left[\begin{array}{cccc|c} 1 & 2 & 1 & 0 & 1 \\ 0 & 1 & 2 & 1 & 4 \\ 0 & 0 & 0.04 & 0.03 & 0.12 \\ 0 & 0 & 100 & 200 & 800 \end{array}\right]$$

6. Find new pivot and switch rows (if required)

$$\left[\begin{array}{cccc|c} 1 & 2 & 1 & 0 & 1 \\ 0 & 1 & 2 & 1 & 4 \\ 0 & 0 & 0.04 & 0.03 & 0.12 \\ 0 & 0 & 100 & 200 & 800 \end{array}\right] \to \left[\begin{array}{cccc|c} 1 & 2 & 1 & 0 & 1 \\ 0 & 1 & 2 & 1 & 4 \\ 0 & 0 & 100 & 200 & 800 \\ 0 & 0 & 0.04 & 0.03 & 0.12 \end{array}\right]$$

7. Gaussian Elimination: $R_4 \to R_4 - 0.0004\, R_3$

$$\left[\begin{array}{cccc|c} 1 & 2 & 1 & 0 & 1 \\ 0 & 1 & 2 & 1 & 4 \\ 0 & 0 & 100 & 200 & 800 \\ 0 & 0 & 0 & -0.05 & -0.2 \end{array}\right]$$

Back Substitution

$-0.05\, x_4 = -0.2;\, x_4 = 4$

$100x_3 + 200x_4 = 800;\; x_3 = 0$

$x_2 + 2\, x_3 + x_4 = 4;\; x_2 = 0$

$x_1 + 2x_2 + x_3 = 1;\, x_1 = 1$

Reduction in rounding error. Avoid addition/ subtraction with very small/large numbers.

Example

$$\begin{bmatrix} 3 & -13 & 9 & 3 \\ -6 & 4 & 1 & -18 \\ 6 & -2 & 2 & 4 \\ 12 & -8 & 6 & 10 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \\ x_3 \end{bmatrix} = \begin{bmatrix} -19 \\ -34 \\ 16 \\ 26 \end{bmatrix}$$

Index vector: $l = [1, 2, 3, 4]$

Scale vector: $s = [13, 18, 6, 12]$ (does not change throughout the procedure)

Determine the first pivot row:

$$\left\{ \frac{|a_{l_i,1}|}{s_{l_i}} : i = 1, 2, 3, 4 \right\} = \left\{ \frac{3}{13}, \frac{6}{18}, \frac{6}{6}, \frac{12}{12} \right\} = \{0.23, 0.33, 1.0, 1.0\}$$

Choose index j as the first occurence of the largest value of $\frac{a_{l_i,j}}{s_{l_i}}$.

Row 3 is the pivot equation in step 1 of elimination $(k = 1)$.

Example

Interchange entries l_k and l_j in the index vector l. New index vector $l = [3, 2, 1, 4]$

$R_1 \to R_1 - (1/2)\, R_3;\ R_2 \to R_2 - (-1) R_3;\ R_4 \to R_4 - 2\, R_3$

$$\begin{bmatrix} 3 & -13 & 9 & 3 & -19 \\ -6 & 4 & 1 & -18 & -34 \\ 6 & -2 & 2 & 4 & 16 \\ 12 & -8 & 6 & 10 & 26 \end{bmatrix} \to \begin{bmatrix} 0 & -12 & 8 & 1 & -27 \\ 0 & 2 & 3 & -14 & -18 \\ 6 & -2 & 2 & 4 & 16 \\ 0 & 4 & 2 & 2 & -6 \end{bmatrix}$$

Next step ($k = 2$) index vector $l = [3, 2, 1, 4]$, scan ratios corresponding to rows $2, 1, 4$.

$\left\{ \frac{|a_{l_i,2}|}{s_{l_i}} : i = 2, 3, 4 \right\} = \left\{ \frac{2}{18}, \frac{12}{13}, \frac{4}{12} \right\} \approx \{0.11, 0.92, 0.33\}$

Interchange $l_2 \leftrightarrow l_3$ in the index vector: $l = [3, 1, 2, 4]$. Pivot equation is row 1.

Example

$R_2 \to R_2 - (-1/6)\, R_1; R_4 \to R_4 - (1/3) R_1$

$$\begin{bmatrix} 0 & -12 & 8 & 1 & -27 \\ 0 & 2 & 3 & -14 & -18 \\ 6 & -2 & 2 & 4 & 16 \\ 0 & 4 & 2 & 2 & -6 \end{bmatrix} \to \begin{bmatrix} 0 & -12 & 8 & 1 & -27 \\ 0 & 0 & 13/3 & -83/6 & -45/2 \\ 6 & -2 & 2 & 4 & 16 \\ 0 & 0 & -2/3 & 5/3 & 3 \end{bmatrix}$$

For $k = 3$, compare ratios corresponding to rows 2 and 4

$\left\{\frac{a_{l_i,3}}{s_{l_i}}\,(i = 3, 4)\right\} = \left\{\frac{13/3}{18}, \frac{2/3}{12}\right\} \approx \{0.24, 0.06\}$ $\quad l = [3, 1, 2, 4]$, index vector unchanged, pivot row is R_2, $\ l_3 = 2$, $R_4 \to R_4 - (-2/13)\, R_2$

$$\begin{bmatrix} 0 & -12 & 8 & 1 & -27 \\ 0 & 0 & 13/3 & -83/6 & -45/2 \\ 6 & -2 & 2 & 4 & 16 \\ 0 & 0 & -2/3 & 5/3 & 3 \end{bmatrix} \to \begin{bmatrix} 0 & -12 & 8 & 1 & -27 \\ 0 & 0 & 13/3 & -83/6 & -45/2 \\ 6 & -2 & 2 & 4 & 16 \\ 0 & 0 & 0 & -6/13 & -6/13 \end{bmatrix}$$

Example: back substitution

$l = [3, 1, 2, 4]$ Sequence for back substitution: 4, 2, 1, 3

$x_4 = \frac{1}{-6/13}[-6/13] = 1$

$x_3 = \frac{1}{13/3}[(-45/2) + (83/6)(1)] = -2$

$x_2 = \frac{1}{-12}[-27 - 8(-2) - 1(1)] = 1$

$x_1 = \frac{1}{6}[16 + 2(1) - 2(-2) - 4(1)] = 3$

Algorithm: Gaussian Elimination with scaled partial pivoting

Initialize row index vector $l = [1, \ldots, n]$ and scale vector $s_i = \max_{(1 \leqslant j \leqslant n)} (|a_{\mathrm{ij}}|)$

function GEspp$(n, a_{\mathrm{ij}}, l_i, b_i)$

integer i, j, k, n;   real $r, \mathrm{rmax}, \mathrm{smax}, \mathrm{xmult}$

real array $(a_{\mathrm{ij}})_{1:n \times 1:n}$, $(l_i)_{1:n}$, $(s_i)_{1:n}$,$(b_i)_{1:n}$

for $i = 1{:}\, n$ do

    $l_i \leftarrow i$

    $\mathrm{smax} \leftarrow 0$

    for $j = 1{:}\, n$ do

        $\mathrm{smax} \leftarrow \max(\mathrm{smax}, |a_{\mathrm{ij}}|)$

    end for

    $s_i \leftarrow \mathrm{smax}$

end for

Algorithm: Gaussian Elimination with scaled partial pivoting

for $k = 1 : n-1$ do (index k is the column index in which new $0s$ are created)

    rmax ← 0
    for i = k : n do
        r ← |a_{l_i,k} / s_{l_i}| (choose correct pivot row based on greatest ratio)
        if (r > rmax) then
            rmax ← r
            j ← i
        end if
    end for
 (Interchange the indices in the index vector)
    l_j ↔ l_k
    for i = k+1 : n do
        xmult ← a_{l_i,k} / a_{l_k,k}
        a_{l_i,k} ← xmult
        for j = k+1 : n do
            a_{l_i,j} ← a_{l_i,j} − (xmult) a_{l_k,j}
        end for
    end for

end for b

for $k = 1 : n-1$ do

  for $i = k+1 : n$ do

$b_{l_i} = b_{l_i} - a_{l_i,k} b_{l_k}$

end for

end for

end function GEspp

```
function x_i = backsub(n, a_ij, l_i, b_i)
integer i, k, n; real sum; array (real) (a_ij)_{1:n×1:n}, (l_i)_{1:n}, (b_i)_{1:n}(x_i)_{1:n}
for k = 1:n−1 do
    for i = k+1:n do
        b_{l_i} ← b_{l_i} − a_{l_i,k} b_{l_k}
    end for
end for
x_n ← b_{l_n} / a_{l_n,n}
for i = n−1:−1:1 do
    sum ← b_{l_i}
    for j = i+1:n do
    sum ← sum − a_{l_i,j} x_j
    end for
    x_i = sum / a_{l_i,i}
end for
end function backsub
```

Why do we require scaled partial pivoting?

Can I solve using Gaussian Elimination $(A \to U)$ without row interchange?

$$\begin{pmatrix} 0 & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$$

Let us consider a small number $\epsilon \ll 1$

Consider

$$\begin{pmatrix} \epsilon & 1 \\ 1 & 1 \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 \end{pmatrix}$$

Gaussian elimination - first stage

$$\begin{pmatrix} \epsilon & 1 \\ 0 & 1 - \epsilon^{-1} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \end{pmatrix} = \begin{pmatrix} 1 \\ 2 - \epsilon^{-1} \end{pmatrix}$$

$x_2 = \frac{2 - \epsilon^{-1}}{1 - \epsilon^{-1}}$; $x_1 = (1 - x_2)\epsilon^{-1}$

Exact solution is $x_1 = 1, x_2 = 1$

Pivoting strategy (Interchange row)

$$\begin{pmatrix} 1 & 1 \\ \epsilon & 1 \end{pmatrix}\begin{pmatrix} x_2 \\ x_1 \end{pmatrix}=\begin{pmatrix} 2 \\ 1 \end{pmatrix}$$

$$\begin{pmatrix} 1 & 1 \\ 0 & 1-\epsilon \end{pmatrix}\begin{pmatrix} x_2 \\ x_1 \end{pmatrix}=\begin{pmatrix} 2 \\ 1-2\epsilon \end{pmatrix}$$

$$\begin{aligned} x_1 &= \frac{1-2\epsilon}{1-\epsilon} \approx 1 \\ x_2 &= 2 - x_1 \approx 1 \end{aligned}$$

LU decomposition/ factorization

$$A = \begin{pmatrix} 1 & -2 & 3 \\ 2 & -5 & 12 \\ 0 & 2 & -10 \end{pmatrix}$$

Perform Gaussian elimination (forward elimination) and store multipliers

$$A' = \begin{pmatrix} 1 & -2 & 3 \\ (2) & -1 & 6 \\ (0) & (-2) & 2 \end{pmatrix}$$

$$L = \begin{pmatrix} 1 & 0 & 0 \\ 2 & 1 & 0 \\ 0 & -2 & 1 \end{pmatrix}, U = \begin{pmatrix} 1 & -2 & 3 \\ 0 & -1 & 6 \\ 0 & 0 & 2 \end{pmatrix}; \text{ LU} = A$$

LU

Let the pivot matrix be denoted by P

Pivot matrix P is the identity matrix with the rows interchanged when the rows of A are interchanged. e.g. $P = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$

In MATLAB type

$>[L \quad U \quad P] = \mathrm{lu}(A)$.

Solve $A\boldsymbol{x} = \boldsymbol{b}$, $PA\boldsymbol{x} = P\boldsymbol{b} = \boldsymbol{d}$, $\qquad LU\boldsymbol{x} = \boldsymbol{d}$, $\quad$ Define $\boldsymbol{y} = U\boldsymbol{x}$

$\therefore L\boldsymbol{y} = d$ $\quad$ Solve $\boldsymbol{y}$ by forward substitution.

Solve $U\boldsymbol{x} = \boldsymbol{y}$ by back substitution for $\boldsymbol{x}$.

LU Decomposition

Matlab example

```
A=rand(5,5)

[L U P] = lu(A)

b = rand(5,1)

d = P*b

y = L\d

x = U\y

rnorm=norm(A*x - b)
```

Algorithm for LU factorization

```
function [L, U] = myLU(A)
[n,n] = size(A);
for k = 1:n
    if abs(A(k,k)) < sqrt(eps)
        disp(['Small pivot element in column' int2str(k)])
    end
    L(k,k)=1;
    for i=k+1:n
        L(i,k)=A(i,k)/A(k,k);
        for j = k+1:n
            A(i,j) =A(i,j) - L(i,k)*A(k,j);
        end
    end
    for j=k:n
      U(k,j)=A(k,j)
    end
end
```