pivoting

Consider the linear system $Ax = b$ using arithmetic with 4 digits:

$$A = \begin{pmatrix} 3.1 \cdot 10^{-4} & 1 \\ 1 & 1 \end{pmatrix}, \qquad b = \begin{pmatrix} -3 \\ -7 \end{pmatrix}, \qquad x_{exact} = \begin{pmatrix} -4.001246... \\ -2.99875... \end{pmatrix}$$

Then $l_{21} = 1/(3.1 \cdot 10^{-4}) \approx 3.226 \cdot 10^3$ and thus

$$L = \begin{pmatrix} 1 & 0 \\ 3.226 \cdot 10^3 & 1 \end{pmatrix}, \qquad U = \begin{pmatrix} 3.1 \cdot 10^{-4} & 1 \\ 0 & -3.225 \cdot 10^4 \end{pmatrix},$$

$$y = L^{-1}b = \begin{pmatrix} -3 \\ 9.671 \cdot 10^3 \end{pmatrix},$$

$$x = U^{-1}y = \begin{pmatrix} \frac{1}{3.1 \cdot 10^{-4}}(-3 - (-2.999)) \\ -2.999 \end{pmatrix} = \begin{pmatrix} -3.226 \\ -2.999 \end{pmatrix}$$

Observation:

during the back substition step all digits of x_1 were lost due to cancellation

intuitive explanation:

the small pivot a_{11} leads to large intermediate results. The final result is of moderate size, which is obtained by the subtraction of two numbers of similar size.

row pivoting

$$A = \begin{pmatrix} 3.1 \cdot 10^{-4} & 1 \\ 1 & 1 \end{pmatrix}, \qquad b = \begin{pmatrix} -3 \\ -7 \end{pmatrix}, \qquad x_{exakt} = \begin{pmatrix} -4.001246... \\ -2.99875... \end{pmatrix}$$

interchanging first and second row of A yields:

$$A_{per} = \begin{pmatrix} 1 & 1 \\ 3.1 \cdot 10^{-4} & 1 \end{pmatrix}, \qquad b_{per} = \begin{pmatrix} -7 \\ -3 \end{pmatrix},$$

and thus

$$L_{per} = \begin{pmatrix} 1 & 0 \\ 3.1 \cdot 10^{-4} & 1 \end{pmatrix}, \qquad U_{per} = \begin{pmatrix} 1 & 1 \\ 0 & 1 - l_{21} = 0.9997 \end{pmatrix},$$

$$y = L_{per}^{-1} b_{per} = \begin{pmatrix} -7 \\ -2.998 \end{pmatrix}, \qquad x = U_{per}^{-1} y = \begin{pmatrix} -4.001 \\ -2.999 \end{pmatrix}$$

$\Longrightarrow$ correct result up to rounding errors

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note: $L_{per} U_{per} = PA$ for the permutation matrix $P = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix}$.

example of an LU-factorization with row pivoting

$$A = A^{(1)} = \begin{pmatrix} 0.5 & 2 & 8.75 \\ 1 & 2 & 3 \\ 0.5 & 5 & 6.5 \end{pmatrix}, \qquad b^{(1)} = \begin{pmatrix} 11.25 \\ 6 \\ 12 \end{pmatrix} \quad \text{sol.: } (1,1,1)^\top$$

seek pivot in the first column: $\Longrightarrow$ interchange 1st and 2nd row:

$$\widetilde{A}^{(1)} = \begin{pmatrix} 1 & 2 & 3 \\ 0.5 & 2 & 8.75 \\ 0.5 & 5 & 6.5 \end{pmatrix}, \qquad \widetilde{b}^{(1)} = \begin{pmatrix} 6 \\ 11.25 \\ 12 \end{pmatrix}$$

elimination step: $l_{21} = 0.5$, $l_{31} = 0.5$ and thus

$$A^{(2)} = \begin{pmatrix} 1 & 2 & 3 \\ 0 & 1 & 7.25 \\ 0 & 4 & 5 \end{pmatrix}, \qquad b^{(2)} = \begin{pmatrix} 6 \\ 8.25 \\ 9 \end{pmatrix}, \qquad L^{(1)} = \begin{pmatrix} 1 & & \\ -0.5 & 1 & \\ -0.5 & & 1 \end{pmatrix},$$

example of an LU-factorization with row pivoting

$$A^{(2)} = \begin{pmatrix} 1 & 2 & 3 \\ 0 & 1 & 7.25 \\ 0 & 4 & 5 \end{pmatrix}, \qquad b^{(2)} = \begin{pmatrix} 6 \\ 8.25 \\ 9 \end{pmatrix}, \qquad L^{(1)} = \begin{pmatrix} 1 & & \\ -0.5 & 1 & \\ -0.5 & & 1 \end{pmatrix},$$

seek pivot in 2nd column: compare merely $a_{22}^{(2)}$ und $a_{32}^{(2)}$.
Since $|a_{32}^{(2)}| > |a_{22}^{(2)}|$ interchange the 2nd and 3rd row:

$$\widetilde{A}^{(2)} = \begin{pmatrix} 1 & 2 & 3 \\ 0 & 4 & 5 \\ 0 & 1 & 7.25 \end{pmatrix}, \qquad \widetilde{b}^{(2)} = \begin{pmatrix} 6 \\ 9 \\ 8.25 \end{pmatrix},$$

elimination step: $l_{32} = \frac{1}{4}$. We obtain the final matrix U and L as:

$$U = A^{(3)} = \begin{pmatrix} 1 & 2 & 3 \\ 0 & 4 & 5 \\ 0 & 0 & 6 \end{pmatrix}, \qquad b^{(3)} = \begin{pmatrix} 6 \\ 9 \\ 6 \end{pmatrix} \qquad L = \begin{pmatrix} 1 & 0 & 0 \\ 0.5 & 1 & 0 \\ 0.5 & 0.25 & 1 \end{pmatrix}$$

computation of the permutation matrix P, such that $PA = LU$

track the row permutations:

1. step: $\pi = (1, 2, 3)$
2. step: $\pi = (2, 1, 3)$
3. step: $\pi = (2, 3, 1)$

We expect that we have computed an LU-factorization of the following matrix:

$$\widetilde{A} := \begin{pmatrix} A_{2,:} \\ A_{3,:} \\ A_{1,:} \end{pmatrix}$$

$$P_\pi = \begin{pmatrix} 0 & 0 & 1 \\ 1 & 0 & 0 \\ 0 & 1 & 0 \end{pmatrix} \qquad \Longrightarrow P := P_\pi^{-1} = P_\pi^\top = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix}$$

one checks that $PA = \widetilde{A}$ and

$$LU = \begin{pmatrix} 1 & 0 & 0 \\ 0.5 & 1 & 0 \\ 0.5 & 0.25 & 1 \end{pmatrix} \cdot \begin{pmatrix} 1 & 2 & 3 \\ 0 & 4 & 5 \\ 0 & 0 & 6 \end{pmatrix} = \begin{pmatrix} 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{pmatrix} \cdot \begin{pmatrix} 0.5 & 2 & 8.75 \\ 1 & 2 & 3 \\ 0.5 & 5 & 6.5 \end{pmatrix} = PA$$

Gaussina eliminiation with (partial) pivoting

Input: invertible $\mathbf{A} \in \mathbb{R}^{n \times n}$

Output: factorization $\mathbf{PA} = \mathbf{LU}$, where $\mathbf{A}$ is overwritten by $\mathbf{U}$:

$u_{ij} = a_{\pi(i),j}$ and $\mathbf{P} = \mathbf{P}_\pi^{-1} = \mathbf{P}_\pi^\top$ is implicitly given by the vector π

$\pi := (1, 2, \ldots, n)$
for $k = 1 : (n-1)$ do
  seek $p \in \{k, \ldots, n\}$ s.t. $|a_{pk}| \geq |a_{ik}| \qquad \forall i \geq k$
  interchange k-th and p-th entry of vector π
  for $i = (k+1) : n$ do
    $l_{\pi(i),k} := \frac{a_{\pi(i),k}}{a_{\pi(k),k}}$
    for $j = (k+1) : n$ do
      $a_{\pi(i),j} := a_{\pi(i),j} - l_{\pi(i),k}\, a_{\pi(k),j}$
    end for
  end for
end for