Gaussian Elim with (row) pivoting 16 Oct '23

What if, at some stage of the elim, the pivot element (i.e., the diagonal element used as the denominator of the multiplier) is zero?

e.g.,

$$A = \begin{bmatrix} 1 & 2 & 1 \\ 1 & 2 & 4 \\ 1 & 3 & 3 \end{bmatrix}, \quad L_1 = \begin{bmatrix} 1 & 0 & 0 \\ -1 & 1 & 0 \\ -1 & 0 & 1 \end{bmatrix}$$

$$L_1 A = \begin{bmatrix} 1 & 2 & 1 \\ 0 & 0 & 3 \\ 0 & 1 & 2 \end{bmatrix}.$$

Cannot use row $\hat{②}$ to elim $\hat{a}_{32}$ from row $\hat{③}$.

Solution: Swap rows $\hat{②}$ and $\hat{③}$.

$$P_2 (L_1 A) = \begin{bmatrix} 1 & 2 & 1 \\ 0 & 1 & 2 \\ 0 & 0 & 3 \end{bmatrix}. \quad (\text{Now } \Delta^r)$$

permutation matrix

A similar problem occurs if $\hat{a}_{22}$ is very small in magnitude (which is more common).

e.g., (not same as above)

$$L_1 A = \begin{bmatrix} 1 & 2 & 1 \\ 0 & 10^{-16} & 3 \\ 0 & 1 & 2 \end{bmatrix} \qquad L_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -10^{+16} & 1 \end{bmatrix}$$

$$L_2(L_1 A) = \begin{bmatrix} 1 & 2 & 1 \\ 0 & 10^{-16} & 3 \\ 0 & 0 & * \end{bmatrix}, \quad * = 2 - 10^{+16} \cdot 3,$$

very large relative to the other elements in the matrix.

This could even be an entire submatrix that gets amplified.

Problem: This amplifies roundoff of $*$ obscenely.

Roundoff error can be shown to be directly proportional to the largest element that occurs during the factorization.

Solution: row (partial) pivoting

When eliminating the k^{th} column, first look for row j, $j > k$, with the largest-magnitude element in column k, then swap rows j and k.

e.g., (continuing from previous)

$$P_2(L_1 A) = \begin{bmatrix} 1 & 2 & 1 \\ 0 & 1 & 2 \\ 0 & 10^{-16} & 3 \end{bmatrix} \qquad L_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & -10^{-16} & 1 \end{bmatrix}$$

$$L_2(P_2 L_1 A) = \begin{bmatrix} 1 & 2 & 1 \\ 0 & 1 & 2 \\ 0 & 0 & * \end{bmatrix}, \quad \text{where } * = 3 - 10^{-16} \cdot 2 \approx 3. \ ☺$$

e.g.,

$$\begin{bmatrix} 2 & 6 & 6 \\ 3 & 5 & 12 \\ 6 & 6 & 12 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 10 \\ 25 \\ 30 \end{bmatrix}.$$

Step 1 pivot (i.e., swap rows)

exchange rows ① & ③ (6 is largest in 1^{st} col)

$$P_1 A x = P_1 b, \qquad P_1 = \begin{bmatrix} 0 & 0 & 1 \\ 0 & 1 & 0 \\ 1 & 0 & 0 \end{bmatrix}$$

$$\begin{bmatrix} 6 & 6 & 12 \\ 3 & 5 & 12 \\ 2 & 6 & 6 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} 30 \\ 25 \\ 10 \end{bmatrix}$$

Now subtract $1/2$ R1 from R2, and $1/3$ R1 from R3.

Note that all multipliers are at most 1 in magnitude. (Good for roundoff error propagation)

$$L_1(P_1 A x) = L_1(P_1 b)$$

$$\begin{bmatrix} 6 & 6 & 12 \\ 0 & 2 & 6 \\ 0 & 4 & 2 \end{bmatrix} x = \begin{bmatrix} 30 \\ 10 \\ 10 \end{bmatrix}$$

$$P_2(L_1 P_1 A x) = P_2(L_1 P_1 b)$$

$$\begin{bmatrix} 6 & 6 & 12 \\ 0 & 4 & 2 \\ 0 & 2 & 6 \end{bmatrix} x = \begin{bmatrix} 30 \\ 10 \\ 10 \end{bmatrix}, \qquad P_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

$$L_2(P_2 L_1 P_1 A x) = L_2(P_2 L_1 P_1 b)$$

$$\begin{bmatrix} 6 & 6 & 12 \\ 0 & 4 & 2 \\ 0 & 0 & 5 \end{bmatrix} x = \begin{bmatrix} 30 \\ 10 \\ 5 \end{bmatrix}$$

$$\underbrace{L_2 P_2 L_1 P_1 A}_{U} x = \underbrace{L_2 P_2 L_1 P_1 b}_{\tilde{b}}.$$

How to extract a factorization when row pivoting is used to control roundoff error propagation?

From the above example,

$$L_2 P_2 L_1 P_1 A = U$$

$$\Leftrightarrow L_2 P_2 L_1 \underbrace{P_2 P_2}_{I} P_1 A = U$$

$$\Leftrightarrow L_2 \underbrace{(P_2 L_1 P_2)}_{\tilde{L}_1} P_2 P_1 A = U$$

Claim: $\tilde{L}_1$ is a modified Gauss transform.

e.g.,

$$P_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix} \qquad L_1 = \begin{bmatrix} 1 & 0 & 0 \\ \ell_{21} & 1 & 0 \\ \ell_{31} & 0 & 1 \end{bmatrix}$$

$$((P_2 L_1) P_2) = \begin{bmatrix} 1 & 0 & 0 \\ \ell_{31} & 0 & 1 \\ \ell_{21} & 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

$$= \underbrace{\begin{bmatrix} 1 & 0 & 0 \\ \ell_{31} & 1 & 0 \\ \ell_{21} & 0 & 1 \end{bmatrix}}_{\tilde{L}_1}$$

← interchanges 2^{nd} & 3^{rd} cols, fixing the structure back to being a Gauss transform

Note: $\tilde{L}_1$ is L_1 with the selected multipliers swapped.

Can prove this in general — see A2! Similar proof technique as for Lemma 1 and Lemma 2.

(In the book)

Continuing,

$$L_2 P_2 L_1 P_1 A = U$$

$$\Leftrightarrow L_2 P_2 L_1 \underbrace{P_2 P_2}_{I} P_1 A = U$$

$$\Leftrightarrow L_2 \underbrace{(P_2 L_1 P_2)}_{\tilde{L}_1} P_2 P_1 A = U$$

$$\Leftrightarrow L_2 \tilde{L}_1 P_2 P_1 A = U$$

$$\Leftrightarrow \underbrace{P_2 P_1}_{P} A = \underbrace{\tilde{L}_1^{-1} L_2^{-1}}_{L} U$$

$$\Leftrightarrow PA = LU.$$

How to solve $Ax = b$ given $PA = LU$?

$$Ax = b \Leftrightarrow PAx = Pb$$

$$\Leftrightarrow L \underbrace{Ux}_{d} = \tilde{b}$$

Then:

(i) solve $Ld = \tilde{b}$ for d, forwards (recall L is unit lower Δ^r and U is upper Δ^r)

(ii) solve $Ux = d$ for x, backwards.

What if, at some stage k of the elim, the diagonal and everything below it is exactly zero?

$$L_{k-1} L_{k-2} \cdots L_1 A = \begin{bmatrix} 0 & \ddots & & \\ \vdots & & 0 & \\ \vdots & & 0 & \\ \vdots & & \vdots & \\ 0 & \cdots & 0 & \end{bmatrix}$$

k^{th} column

Don't have to touch this column! It's already zeroed.

However, $u_{kk} = 0 \Rightarrow U$ is singular (not invertible). (This means A is singular.)

We still have a factorization, but when using it to solve $Ax = b$,

$\cdots$ $Ux = d$ but U is singular.

Either no sol^n, or infinite family of sol^{n}s, depending on what d is.

e.g., $Ux = d$

$$\begin{bmatrix} 2 & 5 & 4 \\ 0 & 0 & 1 \\ 0 & 0 & 2 \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ x_3 \end{bmatrix} = \begin{bmatrix} d_1 \\ d_2 \\ d_3 \end{bmatrix}$$

$$\Rightarrow 2x_3 = d_3 \ \wedge \ x_3 = d_2.$$

If $d_3 = 2d_2$, then x_2 is a free parameter. (For any x_2, there is a sol^n.)

O/w, system is inconsistent.