Gaussian elimination

Note Title

Let A be a square $m \times m$ matrix.

Idea - to transform A into an upper triangular matrix by introducing zeroes below the diagonal.

Suppose $A = \begin{array}{c} \begin{array}{cccc} a_1 & a_2 & \cdots & a_m \end{array} \\ \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1m} \\ a_{21} & & & \\ \vdots & & & \\ a_{m1} & a_{m2} & \cdots & a_{mm} \end{bmatrix} \end{array}$ such that A is invertible & $a_{ii} \neq 0 \; \forall i$.

Step 1: To annihilate $a_{21}, \ldots, a_{m1}$; assume $a_{11} \neq 0$.

- $R_2 - \frac{a_{21}}{a_{11}} R_1 \longleftrightarrow$ multiplying A on the left by

$$L_{21} = \begin{bmatrix} 1 & & & 0 \\ -\frac{a_{21}}{a_{11}} & 1 & & \\ \vdots & & \ddots & \\ 0 & & & 1 \end{bmatrix}$$

$\underbrace{L_{m1} \cdots L_{31} L_{21}}_{L_1} A$

- $R_3 - \frac{a_{31}}{a_{11}} R_1 \longleftrightarrow$ left multi. by $\begin{bmatrix} 1 & & & 0 \\ 0 & 1 & & \\ -\frac{a_{31}}{a_{11}} & & \ddots & \\ \vdots & & & 1 \end{bmatrix} = L_{31}$

$\vdots$

- $R_m - \frac{a_{m1}}{a_{11}} R_1 \longleftrightarrow$ L.M. by $\begin{bmatrix} 1 & & & 0 \\ 0 & 1 & & \\ \vdots & & \ddots & \\ 0 & & & \\ -\frac{a_{m1}}{a_{11}} & & & 1 \end{bmatrix} = L_{m1}$

Let $l_{21} = \frac{a_{21}}{a_{11}}$, $l_{31} = \frac{a_{31}}{a_{11}}$, $\ldots$, $l_{m1} = \frac{a_{m1}}{a_{11}}$.

$$L_1 = L_{m1} \cdots L_{31} L_{21} = \begin{bmatrix} 1 & & & & 0 \\ -l_{21} & \ddots & & & \\ -l_{31} & & \ddots & & \\ \vdots & & & \ddots & \\ -l_{m1} & & & & 1 \end{bmatrix}$$

$$L_1 A = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1m} \\ 0 & \boxed{a'_{22}} & \cdots & a'_{2m} \\ 0 & a'_{32} & \cdots & a'_{3m} \\ \vdots & \vdots & & \vdots \\ 0 & & & a'_{mm} \end{bmatrix}$$

$a'_{22} = a_{22}$ after row reduction

Assuming $a'_{22} \neq 0$, $L_{32} = \begin{bmatrix} 1 & & & \\ & 1 & & \\ & -l_{32} & \ddots & \\ & 0 & & \ddots \\ & \vdots & & & 1 \end{bmatrix}$ & so on.

$l_{32} = \frac{a'_{32}}{a'_{22}}$

Finally get L_2.

$$\text{Step } k: \quad A_{k-1} = \begin{array}{c c} & \begin{array}{cccccccc} L_1 & L_2 & L_3 & & L_{k-1} & k & & \end{array} \\ \begin{array}{c} \rightarrow \\ \rightarrow \\ \\ \\ k \\ \\ \end{array} & \begin{bmatrix} a_{11} & a_{12} & a_{13} & \cdots & a_{1k-1} & a_{1k} & \cdots & a_{1m} \\ 0 & a^1_{22} & a^1_{23} & & & \vdots & & a^1_{2m} \\ 0 & 0 & a^2_{33} & \ddots & & \vdots & & \\ \vdots & \vdots & & & a^{k-1}_{k-1,k-1} & \vdots & & \\ & & & & 0 & a^{k-1}_{kk} & & \\ & & & & \vdots & \vdots & & \\ & & & & 0 & \vdots & & \end{bmatrix} \end{array}$$

At each step we assume that $a^{k-1}_{kk} \neq 0$.

$$L_k = \begin{array}{c} \begin{array}{c} k \end{array} \\ \begin{bmatrix} 1 & & & & \\ & 1 & & & \\ & & \ddots & & \\ & & 1 & & \\ & & l_{k+1,k} & \ddots & \\ & & \vdots & & \ddots \\ & & l_{m,k} & & 1 \end{bmatrix} \end{array}, \quad \text{where } l_{k+1,k} = \frac{a^{k-1}_{k+1,k}}{a^{k-1}_{kk}}$$

$$l_{jk} = \frac{a^{k-1}_{jk}}{a^{k-1}_{kk}}$$

$$\& \quad A_k = L_k A_{k-1}$$

Continuing in this way, $\big(\underbrace{L_{m-1} L_{m-2} \cdots L_2 L_1}_{L^{-1}}\big) A = \mathcal{U}$ (say) (upper Δ^r)

Let $L = L_1^{-1} L_2^{-1} \cdots L_{m-1}^{-1}$, then $A = L\mathcal{U}$.
(the $L\mathcal{U}$-factorization of A).

Note that $L = \begin{bmatrix} 1 & & & 0 \\ l_{21} & 1 & & \\ l_{31} & l_{32} & \ddots & \\ \vdots & \vdots & \ddots & \\ l_{m1} & \cdots & l_{m,m-1} & 1 \end{bmatrix}$; $\det L = 1$.

If A is any square matrix with a_{ii} not necessarily $\neq 0$, then we have to introduce "pivoting".
This is done as follows -

Step 1: Let a_{j1} be the maximum among elements of the first column.

$$j \begin{bmatrix} 0 \\ 0 \\ 0 \\ 0 \\ a_{j1} \end{bmatrix} \qquad A \to \begin{bmatrix} a_{11} \\ \vdots \\ a_{j1} \\ \vdots \\ a_{m1} \end{bmatrix}$$

Then exchange rows j & 1.

i.e. left multiply by $E_{1j} = \begin{array}{c c} & \begin{array}{cccc} 1 & & j & \end{array} \\ \begin{array}{c} 1 \\ \\ j \\ \end{array} & \begin{bmatrix} 0 & \cdots & 1 & \\ \vdots & \ddots & \vdots & \\ 1 & \cdots & 0 & \\ & & & \ddots \; 1 \end{bmatrix} \end{array}$

So $\underset{P_1 =}{E_{1j}} A$ has a non-zero pivot a_{j1} at the (1, 1) spot.

Proceed as usual, form the matrix L_1 & $A_1 = L_1(P_1 A)$

$$A_1 = \begin{bmatrix} \alpha_{11} & \cdots & \alpha_{1m} \\ 0 & & \\ \vdots & & B \\ 0 & & \end{bmatrix}$$

· Next, choose max. from $\begin{pmatrix} a'_{22} \\ \vdots \\ a'_{m2} \end{pmatrix}$ to be the next pivot.

Step k: $\quad P_k = \begin{cases} I & \text{if } a_{kk}^{k-1} \text{ is the pivot.} \\ E_{kj} & \text{if pivot is } a_{jk}^{k-1}. \end{cases}$

$(\det P_k = \pm 1)$.

$$A_k = \left(L_k P_k \cdots \left(L_3 P_3 \left(L_2 P_2 (\underbrace{L_1 P_1 A}_{A_1})\right)\right)\right)$$

Continuing:

$$\underbrace{L_{m-1} P_{m-1} L_{m-2} P_{m-2} \cdots L_1 P_1}_{L^{-1}} A = U.$$

(check L^{-1} is actually lower Δ^r)

· Note that $\det U = \pm \det A$ depending on # of permutation matrices reqd.

· At each step $\det(A_k) = \pm \det A \neq 0$, atleast one of the elements $a_{jk}^{k-1} \neq 0$, so a pivot can be chosen.

· $\det A = \pm$ (product of pivots).

· U can be found irrespective of whether A is invertible or not.

If A is not invertible, $\exists A_k$ such that $a_{kj}^{k-1} = 0 \quad \forall k \leq j \leq n$
Then let $A_k = A_{k+1}$ & set $P_k = L_k = I$.

$$\begin{bmatrix} a_{11} & & * & \\ 0 & a_{22} & * & \\ \vdots & 0 & 0 & \cdots \\ & \vdots & 0 & \\ & & 0 & \end{bmatrix}$$

G.E.	LU factorization
without pivoting $\longrightarrow$	$A = LU$ ✓
with PP $\longrightarrow$	$PA = LU$ ✓
with CP $\longrightarrow$	$PAQ = LU$

Algorithms

I] G.E. without pivoting: $U = A$, $L = I$.

$m \times m$ matrix A.

(column) for $k = 1$ to $m-1$

  (row) for $j = k+1$ to m

$$l_{jk} = u_{jk} / u_{kk}$$

working on j^{th} row $\rightarrow$ $$u_{j,k:m} = u_{j,k:m} - l_{jk} \cdot u_{k,k:m}$$ (row reduction).

$$U = \begin{bmatrix} a_{11} & a_{12} & \cdots & a_{1m} \\ 0 & a_{22}^{1} & \cdots & a_{2m}^{1} \\ 0 & 0 & a_{33}^{2} \cdots & a_{3m}^{2} \\ & & & \end{bmatrix}$$

$$\begin{pmatrix} u_{j,k} \\ \vdots \\ u_{j,m} \end{pmatrix} \quad l_{jk} \quad \begin{pmatrix} u_{k,k} \\ u_{k,k+1} \\ u_{k,m} \end{pmatrix}$$

Operation count: each addition, subtraction, multi., division & sq. root counts as 1 flop.

$$\approx \frac{2}{3} m^3$$

II) G.E. with partial pivoting (GEPP).

At each step k, choose the largest among subdiagonal elements of the k^{th} column & use it as pivot (i.e. do corr. row exchanges)

Algorithm: $U = A$, $L = I$.

for $k = 1$ to $m-1$

if $u_{ii} = 0$ {
- select $i \geq k$ to maximize $|u_{ik}|$
- interchange rows u_i & u_k

  (for $j = 1$ to $k-1$
  $u_{kj} \leftrightarrow u_{ij}$)

} row exchanges do not contribute to flop count, but they make the algorithm slower.

  for $j = k+1$ to m

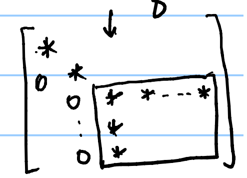
$$l_{jk} = u_{jk} / u_{kk}$$

$$u_{j,k:m} = u_{j,k:m} - l_{jk} u_{k,k:m}.$$

Operation count is same as before, but time reqd. is longer.

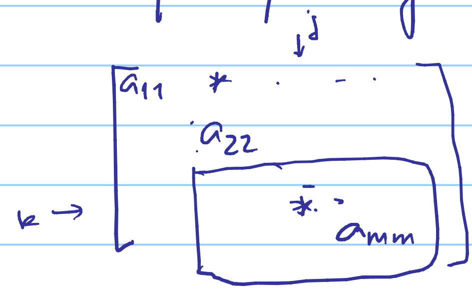
III) G.E. with complete pivoting (GECP).

At the k^{th} step, pivot is chosen from maximum of $(m-k)\times(m-k)$ elements.



This is rarely done in practice because selection of pivots takes a long time & improvement in stability is not considerable.

G.E. with complete pivoting -



$$L_{m-1}P_{m-1}\cdots\left(L_2P_2\left(\underbrace{L_1(P_1AQ_1)}_{A_1}\right)Q_2\cdots\right)Q_{m-1} = U.$$

$$L_{m-1}P_{m-1}\cdots L_1P_1 = \underbrace{(L'_{m-1}\cdots L'_1)}_{L^{-1}}\underbrace{(P_{m-1}\cdots P_1)}_{P}$$

$$L^{-1}PAQ = U.$$

$$PAQ = LU.$$

$$\overset{A}{\begin{bmatrix} [\;] & & \\ & & \\ & & \end{bmatrix}} = \overset{L}{\begin{bmatrix} [1\,1] & & 0 \\ & \ddots & \\ * & & 1 \end{bmatrix}} \overset{U}{\begin{bmatrix} [*] & * & * \\ & \ddots & \\ 0 & & * \end{bmatrix}}$$

Theorem: Let A be $n \times n$ nonsingular matrix.

A has an LU factorization $\iff \det \Delta_k \neq 0$ for each $1 \le k \le n$.

$A = LU$

Moreover, this factorization is unique.

$\Delta_k = k \times k$ top-left submatrix of A

$$= \begin{pmatrix} a_{11} & \cdots & a_{1k} \\ \vdots & \ddots & \\ a_{k1} & \cdots & a_{kk} \end{pmatrix}$$

$$\Delta_k^A = \Delta_k^L \Delta_k^U$$

Proof: If $A = LU$ is an LU factorization,

then $\det(\Delta_k^A) = \det(\Delta_k^L) \cdot \det(\Delta_k^U) \neq 0$.

Conversely, we proceed by induction on k.

$k=1$: $a_{11} \neq 0$, we can choose $P_1 = I$

(Enough to show that $P_k = I$)

Suppose $P_1, \dots, P_{k-1} = I$, so that $L_{k-1} L_{k-2} \cdots L_1 A = A_k$

$$\overset{k\times k}{\left(\begin{array}{ccc|c} 1 & & 0 & 0 \\ & 1 & & \\ & * & \ddots & \\ \hline & * & & \ddots\; 1 \end{array}\right)} \overset{k \times k \quad A}{\left(\begin{array}{ccc|c} a_{11} & \cdots & a_{1k} & \\ \vdots & \Delta_k & & * \\ a_{k1} & \cdots & a_{kk} & \\ \hline & * & & * \end{array}\right)} = \overset{U}{\left(\begin{array}{ccc|c} a_{11}^1 & \cdots & a_{1k}^1 & \\ & \ddots & a_{kk}^k & * \\ \hline 0 & & * & \\ & & * & \end{array}\right)}$$

$$0 \neq \det \Delta_k = \underbrace{a_{11}^1 \cdots}\, a_{kk}^k$$

so $a_{kk}^k \neq 0$, so it can be chosen as pivot.

$\therefore P_k = I$ $\square$

$$\overset{L_3}{\begin{pmatrix} 1 & & & \\ 0 & * & & \\ 0 & * & 0 & \\ \vdots & \vdots & & \ddots \\ 0 & * & & & 1 \end{pmatrix}} \overset{L_2}{\begin{pmatrix} 1 & & & \\ * & & & \\ * & 0 & & \\ * & & & 1 \end{pmatrix}} \overset{L_1}{\begin{pmatrix} a_{11} & & \cdots & a_{1k} \\ & a_{22} & & \\ \vdots & & & \\ a_{k1} & & \cdots & a_{kk} \end{pmatrix}} = \begin{pmatrix} a_{11}^1 & \cdots & \\ 0 & a_{22}^2 & \\ 0 & & \end{pmatrix}$$

$a_{11} \neq 0 \;\rightarrow\; a_{11}^1 \neq 0$

$a_{11} \cdot a_{22} - a_{12} a_{21} \neq 0 \qquad a_{22}^2 \neq 0$

$\vdots \qquad \vdots$

$$\overset{A}{\begin{bmatrix} [\,] & & \\ & & \\ & & \end{bmatrix}} = \overset{L}{\begin{bmatrix} [1\,1] & & 0 \\ & \ddots & \\ * & & 1 \end{bmatrix}} \overset{U}{\begin{bmatrix} [*] & & * \\ & * \ddots & \\ 0 & & * \end{bmatrix}}$$

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(Enough to show that $P_k = I$)

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$$\overset{k\times k}{\left(\begin{array}{ccc|c} 1 & & 0 & 0 \\ & 1 \ddots & & \\ & * & & \\ \hline & * & & \ddots\ 1 \end{array}\right)} \overset{A}{\left(\begin{array}{ccc|c} a_{11} & \cdots & a_{1k} & \\ \vdots & \Delta_k & & * \\ a_{k1} & \cdots & a_{kk} & \\ \hline & * & & * \end{array}\right)} = \overset{U}{\left(\begin{array}{ccc|c} a_{11}^1 & \cdots & a_{1k}^1 & \\ & \ddots & & * \\ 0 & & a_{kk}^k & \\ \hline & & * & \\ & & * & \end{array}\right)}$$

$$0 \neq \det \Delta_k = \underbrace{a_{11}^1 \cdots}\, a_{kk}^k$$

so $a_{kk}^k \neq 0$, so it can be chosen as pivot.

$\therefore P_k = I$ $\square$

$$\overset{L_3}{\begin{bmatrix} 1 & & & \\ 0 & \ddots & & \\ 0 & * & 0 & \\ \vdots & \vdots & & \ddots \\ 0 & * & & & 1 \end{bmatrix}} \overset{L_2}{\begin{bmatrix} 1 & & & \\ * & \ddots & & \\ * & 0 & \ddots & \\ * & & & 1 \end{bmatrix}} \overset{L_1}{\begin{bmatrix} a_{11} & & \cdots & a_{1k} \\ & a_{22} & & \\ \vdots & & & \\ a_{k1} & & \cdots & a_{kk} \end{bmatrix}} = \begin{bmatrix} a_{11}^1 & & \cdots \\ 0 & a_{22}^2 & \\ \vdots & & \\ 0 & & \end{bmatrix}$$

$a_{11} \neq 0 \implies a_{11}^1 \neq 0$

$a_{11}\cdot a_{22} - a_{12}a_{21} \neq 0 \qquad a_{22}^2 \neq 0$

$\vdots \qquad\qquad \vdots$