

Gauss elimination with partial pivoting

Note Title

11/27/2010

$$Ax = b$$

Assumption: A is invertible, $\det(A) \neq 0$.

$$\begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & & & \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} b_1 \\ b_2 \\ \vdots \\ b_n \end{bmatrix}$$

We consider the elements in the first column
and let $|a_{k1}| = \max_{1 \leq i \leq n} |a_{i1}|$.

Then since A is invertible, $a_{k1} \neq 0$

Interchange the first and the k th row.

Interchange the first and the k-th row :

$$\begin{matrix} \rightarrow \\ \rightarrow \end{matrix}
 \begin{bmatrix} a_{k1} & a_{k2} & \dots & a_{kn} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & & & \\ a_{11} & a_{12} & \dots & a_{1n} \\ \vdots & & & \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix}
 \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_k \\ \vdots \\ x_n \end{bmatrix}
 =
 \begin{bmatrix} b_k \\ b_2 \\ \vdots \\ b_1 \\ \vdots \\ b_n \end{bmatrix}$$

Define $m_{i1} = \frac{a_{i1}}{a_{k1}}$, $i \neq k$, $i=1, \dots, n$

$$\tilde{R}_i \longrightarrow \tilde{R}_i - m_{i1} \tilde{R}_k$$

Note that $|m_{i1}| \leq 1$

$$\begin{bmatrix} \tilde{a}_{11} & \tilde{a}_{21} & \dots & \tilde{a}_{n1} \\ 0 & \tilde{a}_{22}^{(1)} & \dots & \tilde{a}_{2n}^{(1)} \\ \vdots & \vdots & \ddots & \vdots \\ 0 & \tilde{a}_{n2}^{(1)} & \dots & \tilde{a}_{nn}^{(1)} \end{bmatrix} \begin{bmatrix} x_1 \\ x_2 \\ \vdots \\ x_n \end{bmatrix} = \begin{bmatrix} \tilde{b}_1 \\ \tilde{b}_2^{(1)} \\ \vdots \\ \tilde{b}_n^{(1)} \end{bmatrix}$$

Let $|\tilde{a}_{k2}^{(1)}| = \max_{2 \leq i \leq n} |\tilde{a}_{i2}^{(1)}| \neq 0$ (why?)

Interchange 2nd and kth equation, define

$$m_{i2} = \frac{\tilde{a}_{i2}^{(1)}}{\tilde{a}_{k2}^{(1)}}, \quad i \neq k, \quad i = 2, \dots, n \quad \text{and perform}$$

$$\bar{R}_i \rightarrow \bar{R}_i - m_{i2} \bar{R}_2, \quad i = 3, \dots, n \quad \text{Continue...}$$

$$A = [a_{ij}] : n \times n \text{ matrix}, e_j = \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} \leftarrow j^{\text{th}} \text{ place}$$

$$A e_j = \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1j} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2j} & \dots & a_{2n} \\ \vdots & & & & & \\ a_{n1} & a_{n2} & \dots & a_{nj} & \dots & a_{nn} \end{bmatrix} \begin{bmatrix} 0 \\ \vdots \\ 0 \\ 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix} = \begin{bmatrix} a_{1j} \\ a_{2j} \\ \vdots \\ a_{nj} \end{bmatrix} = C_j$$

$$e_i^T A = [a_{i1} \ a_{i2} \ \dots \ a_{in}] = R_i$$

$$A = [Ae_1 \quad Ae_2 \quad \dots \quad Ae_n]$$

$$B = [Be_1 \quad Be_2 \quad \dots \quad Be_n] = [C_1 \quad C_2 \quad \dots \quad C_n]$$

$$\begin{aligned} AB &= [ABe_1 \quad ABe_2 \quad \dots \quad ABe_n] \\ &= [AC_1 \quad AC_2 \quad \dots \quad AC_n] \end{aligned}$$

We have seen before that the operation

$$R_i \rightarrow R_i - m_{i1} R_1 \quad a_{ij}^{(1)} = a_{ij} - m_{i1} a_{1j}$$

can be performed by premultiplying A by an elementary matrix.

$$\begin{bmatrix} 1 & 0 & \dots & 0 \\ -m_{21} & 1 & \dots & 0 \\ \vdots & \vdots & \ddots & \vdots \\ -m_{n1} & 0 & & 1 \end{bmatrix} \begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix} = A^{(1)}$$

$E^{(1)}$

Note that

$$\begin{bmatrix} 1 & 0 & \dots & 0 \\ 0 & 1 & \dots & 0 \\ \vdots & & & \\ 0 & 0 & \dots & 1 \end{bmatrix} \xrightarrow{R_i - m_{i1} R_1} \begin{bmatrix} 1 & 0 & \dots & 0 \\ -m_{21} & 1 & \dots & 0 \\ \vdots & & & \\ -m_{n1} & 0 & \dots & 1 \end{bmatrix}$$

I $E^{(1)}$

We now show that the interchange of two rows of a matrix is equivalent to premultiplying by a permutation matrix obtained by interchanging the corresponding rows of the Identity matrix.

$$P_1 = [e_k \ e_2 \ \dots \ e_{k-1} \ e_1 \ e_{k+1} \ \dots \ e_n]$$

$$\begin{aligned} AP_1 &= [Ae_k \ Ae_2 \ \dots \ Ae_{k-1} \ Ae_1 \ Ae_{k+1} \ \dots \ Ae_n] \\ &= [C_k \ C_2 \ \dots \ C_{k-1} \ C_1 \ C_{k+1} \ \dots \ C_n] \end{aligned}$$

AP_1 : Interchange of the 1st and
the k th column of A

$e_i^T A = R_i$: i th row of A

$$P_1 A = \begin{bmatrix} e_k^T \\ e_2^T \\ \vdots \\ e_{k-1}^T \\ e_1^T \\ \vdots \\ e_n^T \end{bmatrix} A = \begin{bmatrix} e_k^T A \\ e_2^T A \\ \vdots \\ e_{k-1}^T A \\ e_1^T A \\ \vdots \\ e_n^T A \end{bmatrix} = \begin{bmatrix} R_k \\ R_2 \\ \vdots \\ R_{k-1} \\ R_1 \\ \vdots \\ R_n \end{bmatrix}$$

Interchange of
the 1st and the
 k th row.

$I : R_1 \leftrightarrow R_k \quad (C_1 \leftrightarrow C_k) : P_1$

$$P_1^T = P_1, \quad P_1^2 = I$$

$P_1 A$: Interchange of the 1st and the k th
row

$A P_1$: Interchange of the 1st and the
 k th column

Thus reduction of A to an upper triangular matrix U using partial pivoting can be represented as

$$E_{n-1} P_{n-1} E_{n-2} P_{n-2} \dots E_1 P_1 A = U,$$

where P_i 's are permutation matrices.

The above equation can be rewritten as

$$E'_{n-1} E'_{n-2} \dots E'_1 \underbrace{P_{n-1} P_{n-2} \dots P_1}_P A = U.$$

Consider $E_2 P_2 E_1 P_1 A = U$ ($n=3$).

Note that $P_2^2 = I$.

Hence $U = E_2 \underbrace{P_2 E_1 P_2}_{P_2 E_1 P_2} P_1 A$

Define

$$E_1' = P_2 E_1 P_2$$

Then

$$U = E_2 E_1' P_2 P_1 A$$

We now show that E_1' is also unit lower triangular

$$E_1 = \begin{bmatrix} 1 & 0 & 0 \\ -m_{21} & 1 & 0 \\ -m_{31} & 0 & 1 \end{bmatrix}$$

$$P_2 = \begin{bmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{bmatrix}$$

$P_2 E_1$: Interchange of 2nd & 3rd row of E_1

$$P_2 E_1 = \begin{bmatrix} 1 & 0 & 0 \\ -m_{31} & 0 & 1 \\ -m_{21} & 1 & 0 \end{bmatrix}$$

$(P_2 E_1) P_2$: Interchange of the
second and third columns of
 $P_2 E_1$

$$E_1' = P_2 E_1 P_2 = \begin{bmatrix} 1 & 0 & 0 \\ -m_{31} & 1 & 0 \\ -m_{21} & 0 & 1 \end{bmatrix}$$

: lower triangular unit

Gauss elimination with partial pivoting

$$PA = LU,$$

where P : permutation matrix

L : unit lower triangular matrix

U : upper triangular matrix.

$$\det(P) = \pm 1, \quad \det(L) = 1, \quad \det(U) = \pm \det(A)$$

$$|l_{ij}| \leq 1$$

Suppose that $A = [a_{ij}]$ is diagonally dominant by columns:

$$\sum_{\substack{i=1 \\ i \neq j}}^n |a_{ij}| \leq |a_{jj}|, \quad j = 1, \dots, n.$$

$$\Rightarrow \sum_{i=2}^n |a_{i1}| \leq |a_{11}|$$

No need of row interchanges

$$\begin{bmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \vdots & \vdots & & \vdots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{bmatrix}$$

Inverse of a matrix

Classical formula : $A^{-1} = \frac{1}{\det(A)} \text{adj}(A)$

Calculation of determinant in the classical way :
more than $n!$ flops .

$n!$ grows much faster than n^3 .

$$A X = I : A [x_1, x_2, \dots, x_n] = [e_1, e_2, \dots, e_n]$$

Solve $A X_i = e_i, i = 1, \dots, n$.

Cost : LU decomposition (once) : $\frac{n^3}{3}$ flops

forward & backward substitution (n times) : $n^2 \times n = n^3$

Calculation of the determinant

$$PA = LU \Rightarrow \det(A) = \pm \det(U)$$

Sign depends on the number of row interchanges

Cost: $\frac{n^3}{3}$ flops

Complete Pivoting

$$Ax = b, \quad A: \text{invertible.}$$

First step: Let $|a_{k\ell}| = \max_{1 \leq i, j \leq n} |a_{ij}|$. n^2 comparisons

Interchange the 1st and kth row and the 1st and lth column.

$\tilde{A} = P_1 A Q_1$: Perform Gauss elimination to obtain

$$\tilde{A}^{(1)} = \begin{bmatrix} a_{k\ell} & \tilde{A}_{12} \\ 0 & \tilde{A}_{22} \end{bmatrix}$$

$$E_1 \tilde{A} = \tilde{A}^{(1)}$$

$$E_1 P_1 A Q_1 = \tilde{A}^{(1)}$$

2nd Step: $\tilde{A}_{22} = [\tilde{a}_{ij}^{(1)}] : 2 \leq i, j \leq n$

$$\text{Let } |\tilde{a}_{ks}^{(1)}| = \max_{2 \leq i, j \leq n} |\tilde{a}_{ij}^{(1)}|$$

Interchange 2nd and kth row and
2nd and lth column of $\tilde{A}^{(1)}$ and introduce
zeros in the second column below diagonal

$$E_2 P_2 \tilde{A}^{(1)} Q_2 = \tilde{A}^{(2)}$$

$$E_2 P_2 \overset{\uparrow}{E_1} P_1 A Q_1 Q_2 = \tilde{A}^{(2)}$$

Complete Pivoting

$$PAQ = LU,$$

P, Q : permutation matrices,

L : unit lower triangular

U : upper triangular

n^3 comparisons : expensive