Chapter 13 Gaussian Elimination (III)

Bunch-Parlett diagonal pivoting

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Reference: James R. *Bunch* and Linda *Kaufman*, Some Stable Methods for Calculating Inertia and Solving Symmetric Linear Systems, Mathematics of Computation, volume 31, number 137, January 1977, page 163-179

OutLine

- Preliminary
  - 1x1, 2x2 pivoting in Gaussian Elimination
  - real symmetric indefinite matrix
- Symmetric permutation
- LDL’ decomposition (diagonal pivoting)
- Example of complete diagonal pivoting
- Algorithm of complete diagonal pivoting

Pivoting in Traditional Gaussian Elimination

consider $A = A^{(1)} = \left(\begin{array}{c|ccc} 6 & -2 & 2 & 4 \\ \hline 12 & -8 & 6 & 10 \\ 3 & -13 & 9 & 3 \\ -6 & 4 & 1 & -18 \end{array}\right) \equiv \left(\begin{array}{c|c} E & d^T \\ \hline c & B \end{array}\right)$ $E = a_{11},\ c = \begin{pmatrix} 12 \\ 3 \\ -6 \end{pmatrix},\ d = \begin{pmatrix} -2 \\ 2 \\ 4 \end{pmatrix}$

then one step *LU*-factorization leads to $\left(\begin{array}{c|c} a_{11} & d^T \\ \hline c & B \end{array}\right) = \left(\begin{array}{c|c} 1 & \\ \hline c/a_{11} & I \end{array}\right)\left(\begin{array}{c|c} a_{11} & d^T \\ \hline & A^{(2)} \end{array}\right) = L^{(1)}U^{(1)}$

where $L^{(1)} \equiv \left(\begin{array}{c|ccc} 1 & & & \\ \hline 2 & 1 & & \\ 0.5 & & 1 & \\ -1 & & & 1 \end{array}\right) = \left(\begin{array}{c|c} 1 & 0 \\ \hline c/a_{11} & I_{3\times 3} \end{array}\right)$ and $U^{(1)} = \begin{pmatrix} a_{11} & d^T \\ & B \end{pmatrix} = \left(\begin{array}{c|ccc} 6 & -2 & 2 & 4 \\ \hline 0 & -4 & 2 & 2 \\ 0 & -12 & 8 & 1 \\ 0 & 2 & 3 & -14 \end{array}\right)$

It is easy to show $A^{(2)} \equiv B - \dfrac{cd^T}{a_{11}} = \begin{pmatrix} -4 & 2 & 2 \\ -12 & 8 & 1 \\ 2 & 3 & -14 \end{pmatrix}$ from Gaussian Elimination

We use principal submatrix $E = a_{11}$ as pivoting, called 1×1 pivoting since $E \in R^{1\times 1}$

Question: can we use 2×2 or higher $s\times s$ pivoting, i.e. $E \in R^{s\times s}$

2x2 pivoting in block Gaussian Elimination

$$A=\begin{array}{cc} \begin{array}{cc} \overbrace{\qquad}^{s} & \overbrace{\qquad}^{n-s} \end{array} & \\ \left(\begin{array}{c|c} E & d^T \\ \hline c & B \end{array}\right) & \begin{array}{l} \}\; s \\ \}\; m-s \end{array} \end{array}$$

If principal sub-matrix E is non-singular,

then one-step *GE* leads to
$$\left(\begin{array}{c|c} E & d^T \\ \hline c & B \end{array}\right)=\left(\begin{array}{c|c} I & \\ \hline cE^{-1} & I \end{array}\right)\left(\begin{array}{c|c} E & d^T \\ \hline & A^{(s+1)} \end{array}\right) \qquad A^{(s+1)}=B-cE^{-1}d^T$$

Example 1: 2×2 pivoting

$$A=A^{(1)}=\left(\begin{array}{cc|cc} 6 & -2 & 2 & 4 \\ 12 & -8 & 6 & 10 \\ \hline 3 & -13 & 9 & 3 \\ -6 & 4 & 1 & -18 \end{array}\right)\equiv\left(\begin{array}{c|c} E & d^T \\ \hline c & B \end{array}\right)=\left(\begin{array}{c|c} I & \\ \hline cE^{-1} & I \end{array}\right)\left(\begin{array}{c|c} E & d^T \\ \hline & A^{(3)} \end{array}\right) \qquad |A|_\infty=18$$

where
$$\left(\begin{array}{c|c} I & \\ \hline cE^{-1} & I \end{array}\right)=\left(\begin{array}{cc|cc} 1 & & & \\ & 1 & & \\ \hline -5.5 & 3 & 1 & \\ 0 & -0.5 & & 1 \end{array}\right)$$

$$|L|_\infty=5.5$$

and
$$\left(\begin{array}{c|c} E & d^T \\ \hline & A^{(3)} \end{array}\right)=\left(\begin{array}{cc|cc} 6 & -2 & 2 & 4 \\ 12 & -8 & 6 & 10 \\ \hline & & 2 & -5 \\ & & 4 & -13 \end{array}\right)$$

$$|U|_\infty=13$$

3x3 pivoting in block Gaussian Elimination

Example 2: 3×3 pivoting

$$A = A^{(1)} = \left(\begin{array}{ccc|c} 6 & -2 & 2 & 4 \\ 12 & -8 & 6 & 10 \\ 3 & -13 & 9 & 3 \\ \hline -6 & 4 & 1 & -18 \end{array}\right) \equiv \left(\begin{array}{c|c} E & d^T \\ \hline c & B \end{array}\right) = \left(\begin{array}{c|c} I & \\ \hline cE^{-1} & I \end{array}\right)\left(\begin{array}{c|c} E & d^T \\ \hline & A^{(4)} \end{array}\right) \qquad |A|_\infty = 18$$

where

$$\left(\begin{array}{c|c} I & \\ \hline cE^{-1} & I \end{array}\right) = \left(\begin{array}{ccc|c} 1 & & & \\ & 1 & & \\ & & 1 & \\ \hline 11 & -6.5 & 2 & 1 \end{array}\right)$$

$$|L|_\infty = 11$$

and

$$\left(\begin{array}{c|c} E & d^T \\ \hline & A^{(3)} \end{array}\right) = \left(\begin{array}{ccc|c} 6 & -2 & 2 & 4 \\ 12 & -8 & 6 & 10 \\ 3 & -13 & 9 & 3 \\ \hline & & & -3 \end{array}\right)$$

$$|U|_\infty = 13$$

Question: what is criterion to choose *1x1*, *2x2* or *3x3* pivoting?

stability

performance

Question: what is the ***cost*** to estimate the criterion ?

Real symmetry indefinite matrix A

$A=\begin{pmatrix} E & c^T \\ c & B \end{pmatrix}$ is symmetric implies $E=E^T$ and $B=B^T$

From linear algebra, if *A* is real symmetric, then *A* has real spectrum decomposition (譜分解)

$$AV_j=\lambda_j V_j \qquad \lambda_j \in R \text{ and } V_i^T V_j=\delta_i^j=\begin{cases} 1 & \text{if } i=j \\ 0 & \text{if } i\neq j \end{cases} \qquad \forall\ j=1,2,\cdots,n$$

or write in matrix form $AV=V\Lambda$ $\quad V=\left(V_1|V_2|\cdots|V_n\right)$ and $\Lambda=diag\left(\lambda_1,\lambda_2,\cdots,\lambda_n\right)=\begin{pmatrix} \lambda_1 & & \\ & \ddots & \\ & & \lambda_n \end{pmatrix}$

without loss of generality, we can rearrange eigen-values to be increasing

$$\lambda_1\leq\lambda_2\leq\cdots\leq\lambda_n$$

Definition: suppose matrix *A* is real symmetric, then we say "*A* is indefinite" if there exists an eigen-value of A less than zero. If *A* is nonsingular, then

$$\lambda_1\leq\lambda_2\leq\cdots\leq\lambda_k<0<\lambda_{k+1}\leq\cdots\leq\lambda_n$$

Thereafter we focus on *LU*-decomposition of symmetry indefinite matrix *A*

LU-factorization for real symmetry indefinite matrix A

$LU-$ factorization $$A=\left(\begin{array}{c|c} E & c^T \\ \hline c & B \end{array}\right)=\left(\begin{array}{c|c} I & \\ \hline cE^{-1} & I \end{array}\right)\left(\begin{array}{c|c} E & c^T \\ \hline & B-cE^{-1}c^T \end{array}\right)$$

LDL^T- factorization $$A=\left(\begin{array}{c|c} E & c^T \\ \hline c & B \end{array}\right)=\left(\begin{array}{c|c} I & \\ \hline cE^{-1} & I \end{array}\right)\left(\begin{array}{c|c} E & \\ \hline & B-cE^{-1}c^T \end{array}\right)\left(\begin{array}{c|c} I & E^{-1}c^T \\ \hline & I \end{array}\right)$$

where $L=\left(\begin{array}{c|c} I & \\ \hline cE^{-1} & I \end{array}\right)$ and $L^T=\left(\begin{array}{c|c} I & E^{-T}c^T \\ \hline & I \end{array}\right)=\left(\begin{array}{c|c} I & E^{-1}c^T \\ \hline & I \end{array}\right)$

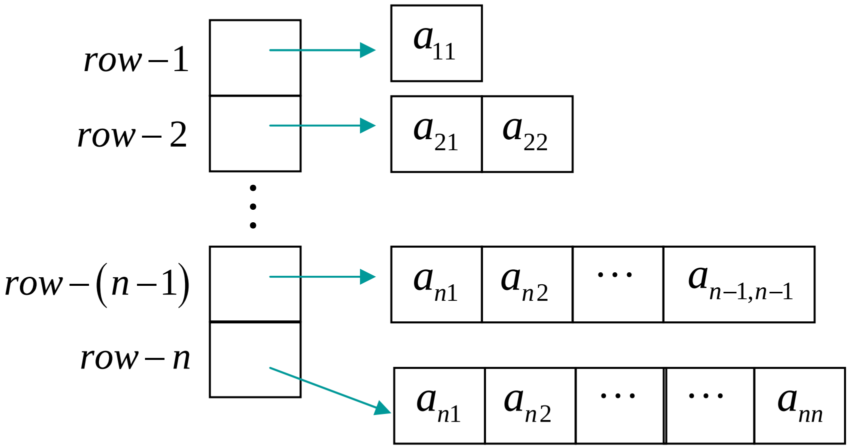
Question: why not *LU*-decomposition?

A is real symmetric, we only store lower triangle part of **A**, say

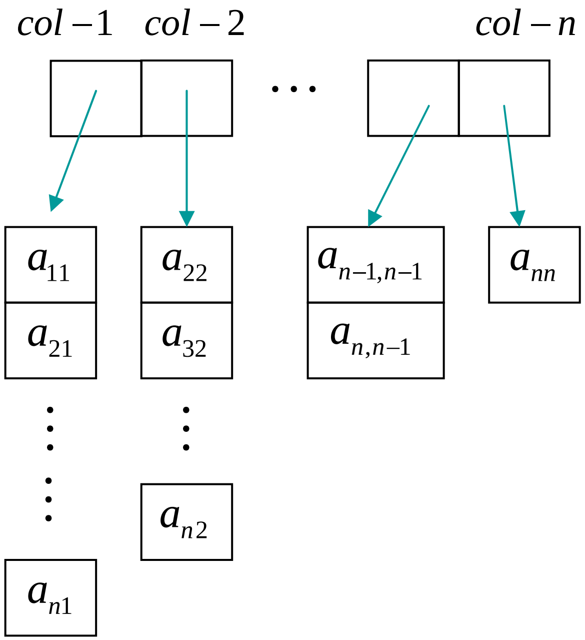
$$mem(A)=\begin{pmatrix} a_{11} & & & \\ a_{21} & a_{22} & & \\ \vdots & \vdots & \ddots & \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix}$$

Pointer array to store lower triangular part of A

row-major based



col-major based



Question: what is the cost to fetch one element of *A* ? That is, operation count for $A(i,j)$

Question: can you find another representation for lower part of matrix *A* ?

Question: if one uses row-major to store lower part of matrix *A,* then how to fetch a column of A efficiently?

OutLine

- Preliminary
- Symmetric permutation
  - change diagonal element to (1,1) position
  - change off-diagonal element to (2,1) position
  - implementation of symmetric permutation
- LDL’ decomposition (diagonal pivoting)
- Example of complete diagonal pivoting
- Algorithm of complete diagonal pivoting

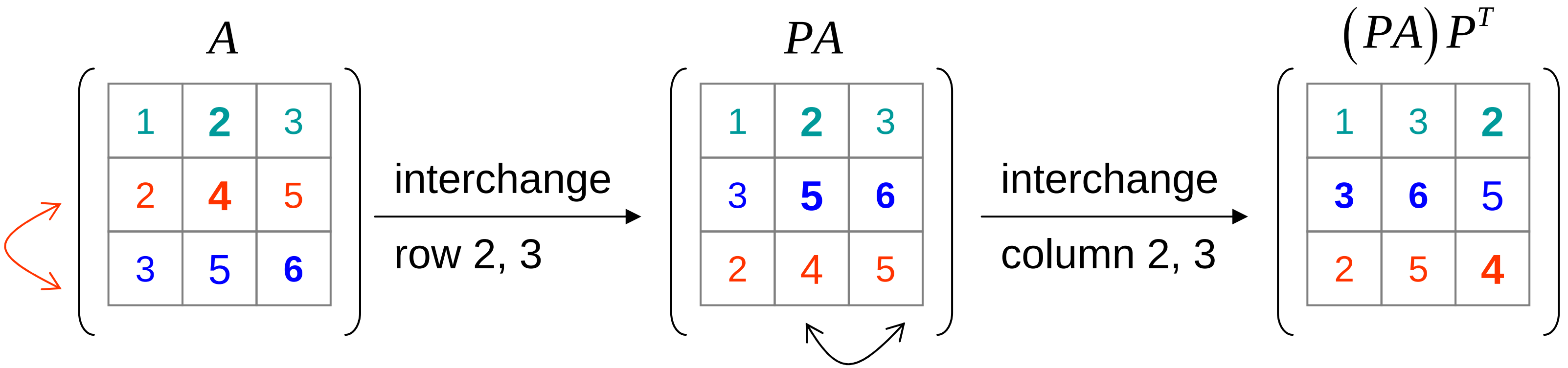
How to do permutation on real symmetry indefinite matrix A

Let $A = \begin{pmatrix} 1 & 2 & 3 \\ 2 & 4 & 5 \\ 3 & 5 & 6 \end{pmatrix}$ Define permutation matrix $P = (1,3,2) \equiv \begin{pmatrix} e_1^T \\ e_3^T \\ e_2^T \end{pmatrix} = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 0 & 1 \\ 0 & 1 & 0 \end{pmatrix}$

$$Px = \begin{pmatrix} e_1^T \\ e_3^T \\ e_2^T \end{pmatrix} x = \begin{pmatrix} e_1^T x \\ e_3^T x \\ e_2^T x \end{pmatrix} = \begin{pmatrix} x_1 \\ x_3 \\ x_2 \end{pmatrix} \xrightarrow{\text{interchange row 2, 3}} PA = \begin{pmatrix} 1 & 2 & 3 \\ 3 & 5 & 6 \\ 2 & 4 & 5 \end{pmatrix}$$

$$x^T P^T = (Px)^T = \begin{pmatrix} x_1 \\ x_3 \\ x_2 \end{pmatrix}^T = \begin{pmatrix} x_1 & x_3 & x_2 \end{pmatrix} \xrightarrow{\text{interchange column 2, 3}} AP^T = \begin{pmatrix} 1 & 3 & 2 \\ 2 & 5 & 4 \\ 3 & 6 & 5 \end{pmatrix}$$

Symmetric permutation: $A \to PAP^T$



$$\underset{A}{\begin{pmatrix} 1 & \mathbf{2} & 3 \\ 2 & \mathbf{4} & 5 \\ 3 & \mathbf{5} & \mathbf{6} \end{pmatrix}} \xrightarrow[\text{row 2, 3}]{\text{interchange}} \underset{PA}{\begin{pmatrix} 1 & \mathbf{2} & 3 \\ 3 & \mathbf{5} & \mathbf{6} \\ 2 & 4 & 5 \end{pmatrix}} \xrightarrow[\text{column 2, 3}]{\text{interchange}} \underset{(PA)P^T}{\begin{pmatrix} 1 & 3 & \mathbf{2} \\ \mathbf{3} & \mathbf{6} & 5 \\ 2 & 5 & \mathbf{4} \end{pmatrix}}$$

Change diagonal element to (1,1) position [1]

suppose we want to change $a_{33} = 8$ to position (*1,1*) , then consider permutation $P = (3,2,1,4)$ and do symmetric permutation on *A*, say PAP^T

$$\underset{A}{\begin{pmatrix} 1 & 2 & 3 & 4 \\ 2 & 5 & 6 & 7 \\ 3 & 6 & 8 & 9 \\ 4 & 7 & 9 & 10 \end{pmatrix}} \xrightarrow[\text{col 1, 3}]{\text{interchange}} \underset{AP^T}{\begin{pmatrix} 3 & 2 & 1 & 4 \\ 6 & 5 & 2 & 7 \\ 8 & 6 & 3 & 9 \\ 9 & 7 & 4 & 10 \end{pmatrix}} \xrightarrow[\text{row 1, 3}]{\text{interchange}} \underset{PAP^T}{\begin{pmatrix} 8 & 6 & 3 & 9 \\ 6 & 5 & 2 & 7 \\ 3 & 2 & 1 & 4 \\ 9 & 7 & 4 & 10 \end{pmatrix}}$$

Question: we only store lower triangle part of matrix *A*, above permutation does not work, how to modify it?

Observation 1:

$$\underset{A}{\begin{pmatrix} 1 & 2 & 3 & 4 \\ 2 & 5 & 6 & 7 \\ 3 & 6 & 8 & 9 \\ 4 & 7 & 9 & 10 \end{pmatrix}} \longrightarrow \underset{PAP^T}{\begin{pmatrix} 8 & 2 & 3 & 4 \\ 2 & 5 & 6 & 7 \\ 3 & 6 & 1 & 9 \\ 4 & 7 & 9 & 10 \end{pmatrix}}$$

Change diagonal element to (1,1) position [2]

$$\begin{tikzcd} a_{11} \arrow[r, "col-1\to col-3"] \arrow[rr, bend left] & a_{13} \arrow[r, "row-1\to row-3"] & a_{33} \end{tikzcd} \qquad \begin{tikzcd} a_{33} \arrow[r, "col-3\to col-1"] \arrow[rr, bend left] & a_{31} \arrow[r, "row-3\to row-1"] & a_{11} \end{tikzcd}$$

$$\begin{tikzcd} a_{13} \arrow[r, "col-3\to col-1"] \arrow[rr, bend left] & a_{11} \arrow[r, "row-1\to row-3"] & a_{31} \end{tikzcd} \qquad \begin{tikzcd} a_{31} \arrow[r, "col-1\to col-3"] \arrow[rr, bend left] & a_{33} \arrow[r, "row-3\to row-1"] & a_{13} \end{tikzcd}$$

Observation 2: we only need to update lower triangle part of *A* (diagonal term is excluded).

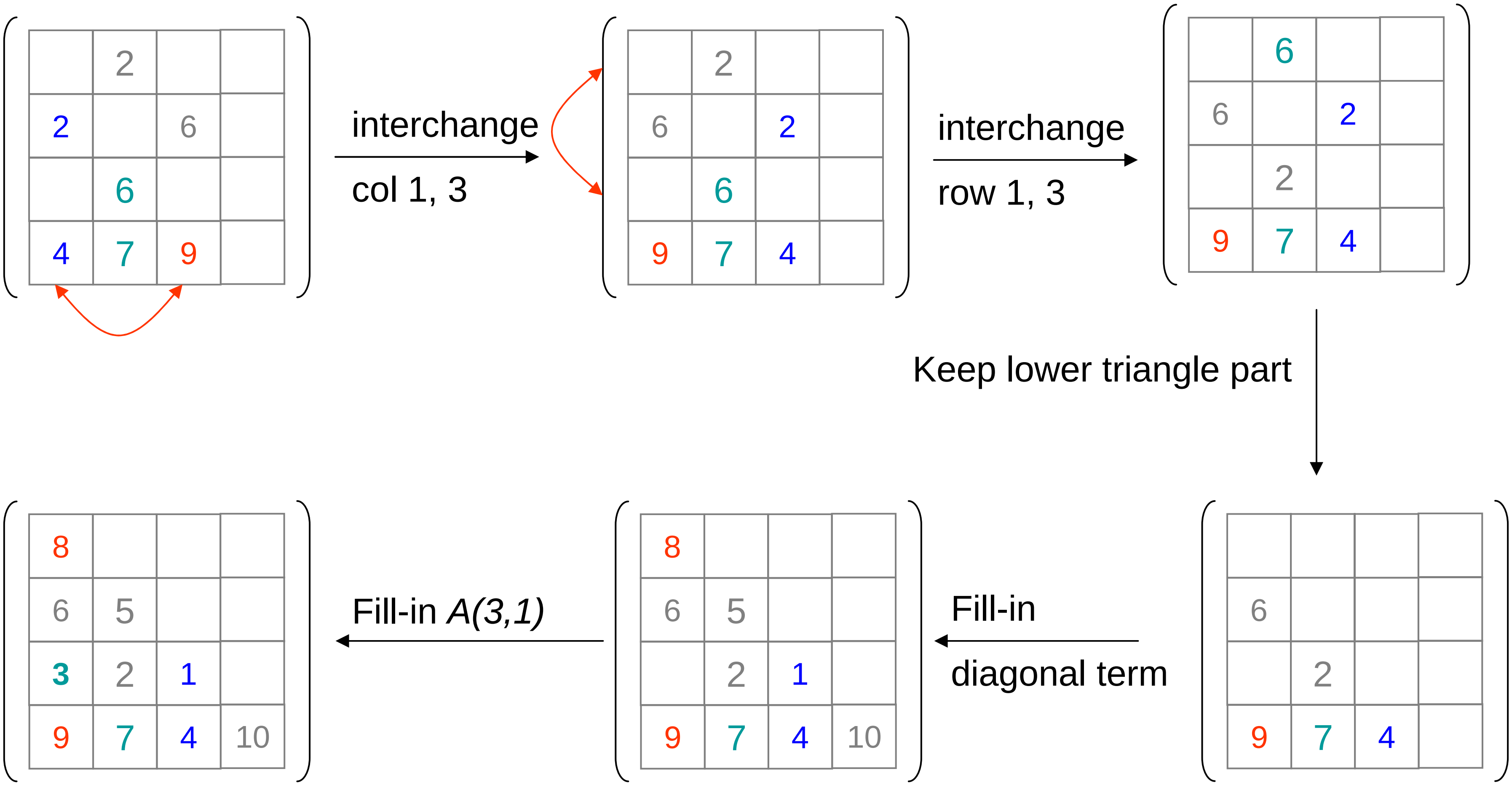
$$\begin{pmatrix} 8 & 2 & 3 & 4 \\ 2 & 5 & 6 & 7 \\ 3 & 6 & 1 & 9 \\ 4 & 7 & 9 & 10 \end{pmatrix} \longrightarrow \begin{pmatrix} & & & \\ 2 & & & \\ & 6 & & \\ 4 & 7 & 9 & \end{pmatrix}$$

diagonal term $a_{kk}\left(k\neq 1,3\right)\xrightarrow{col-1\leftrightarrow col-3} a_{kk} \xrightarrow{row-1\leftrightarrow row-3} a_{kk}$ does not changed

$$\left.\begin{array}{l} a_{11}\xrightarrow{col-1\leftrightarrow col-3,row-1\leftrightarrow row-3} a_{33} \\ a_{33}\xrightarrow{col-1\leftrightarrow col-3,row-1\leftrightarrow row-3} a_{11} \end{array}\right\} \text{we have changed}$$

$a_{13}=a_{31}$ does not changed

Change diagonal element to (1,1) position [3]



	2		
2		6	
	6		
4	7	9	

interchange

col 1, 3

	2		
6		2	
	6		
9	7	4	

interchange

row 1, 3

	6		
6		2	
	2		
9	7	4	

Keep lower triangle part

6			
	2		
9	7	4	

Fill-in

diagonal term

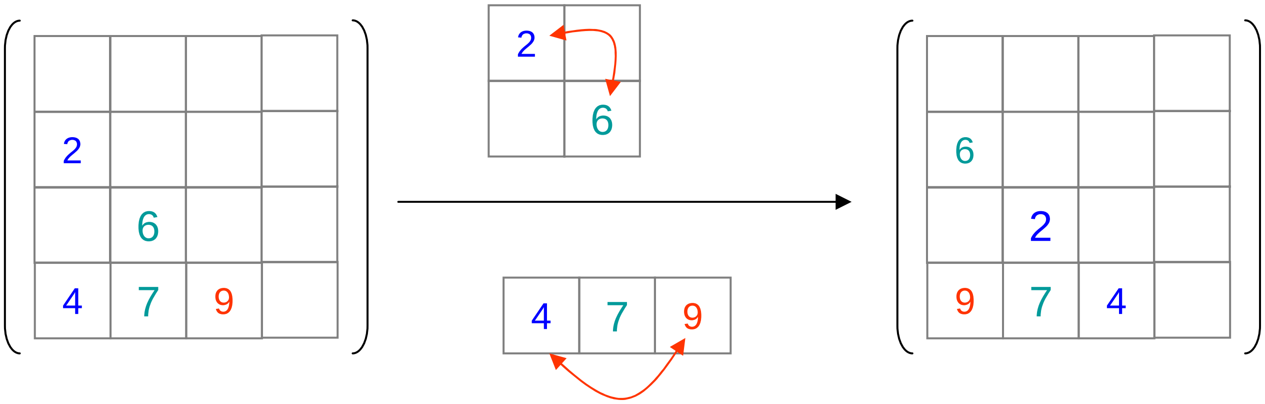
8			
6	5		
	2	1	
9	7	4	10

Fill-in *A(3,1)*

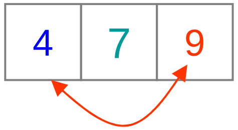
8			
6	5		
3	2	1	
9	7	4	10

Question: any compact form to represent above interchange?

Change diagonal element to (1,1) position [4]



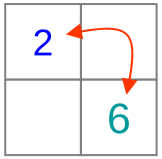
case 1:



$$a_{41}\left(i\neq 1,3\right)\xrightarrow{col-1\leftrightarrow col-3} a_{43}\xrightarrow{row-1\leftrightarrow row-3} a_{43}$$

$$a_{43}\left(i\neq 1,3\right)\xrightarrow{col-1\leftrightarrow col-3} a_{41}\xrightarrow{row-1\leftrightarrow row-3} a_{41}$$

case 2:



$$a_{21}\left(i\neq 1,3\right)\xrightarrow{col-1\leftrightarrow col-3} a_{23}\xrightarrow{row-1\leftrightarrow row-3} a_{23}\left(upper\ \ triangle\right)=a_{32}$$

$$a_{32}\left(j\neq 1,3\right)\xrightarrow{col-1\leftrightarrow col-3} a_{32}\xrightarrow{row-1\leftrightarrow row-3} a_{12}\left(upper\ \ triangle\right)=a_{21}$$

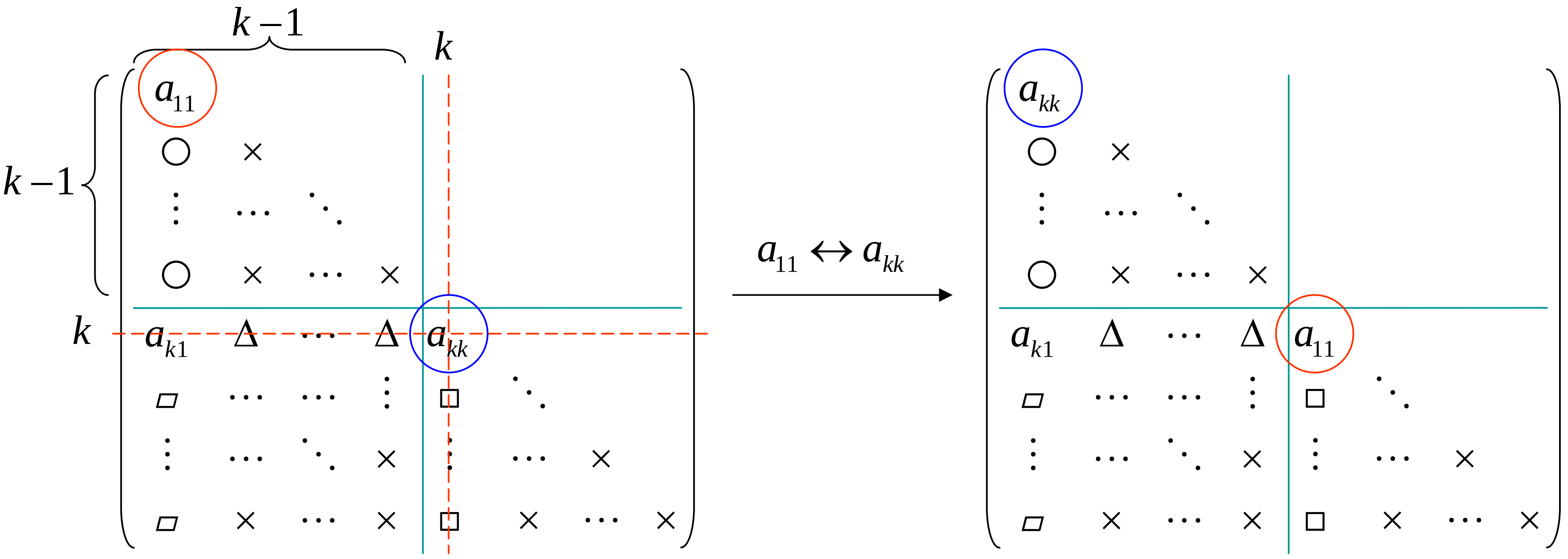
Change diagonal element to (1,1) position *[5]*

For general real symmetric matrix *A* with dimension *n*, suppose we want to change $a_{kk} \to a_{11}$

$$P=\left(\underset{1-th}{\underset{\uparrow}{k}},\ 2,3,\cdots k-1,\ \underset{k-th}{\underset{\uparrow}{1}},\ k+1,n\right)$$ interchanges rows $1,k$ or columns $1,k$

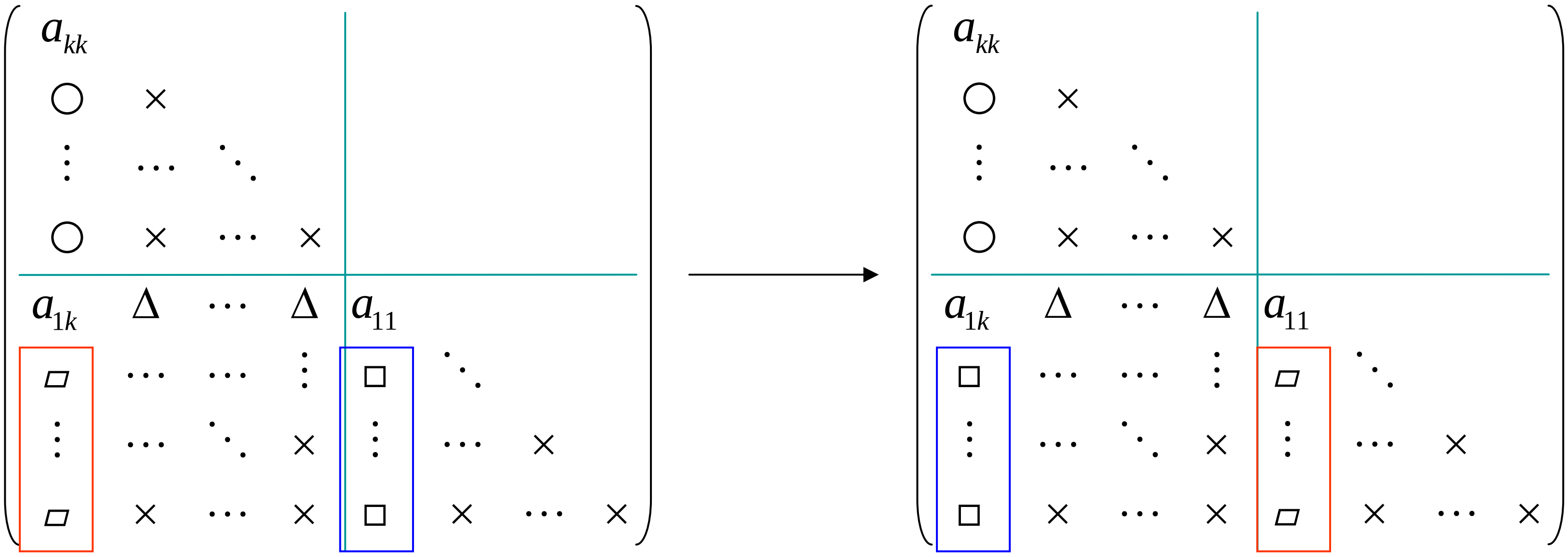
Step 1: interchange position *(1,1)* and *(k,k), i.e.* $a_{11} \leftrightarrow a_{kk}$

keep position *(k,1)* and *(1,k), i.e.* $a_{1k} = a_{k1}$ does not changed



Change diagonal element to (1,1) position [6]

Step 2: interchange column 1 and *k* below row *k+1*, i.e $A(k+1:n,1)\leftrightarrow A(k+1:n,k)$



$$A(i,1)(i>k)\xrightarrow{col-1\leftrightarrow col-k}A(i,k)\xrightarrow{row-1\leftrightarrow row-k}A(i,k)$$

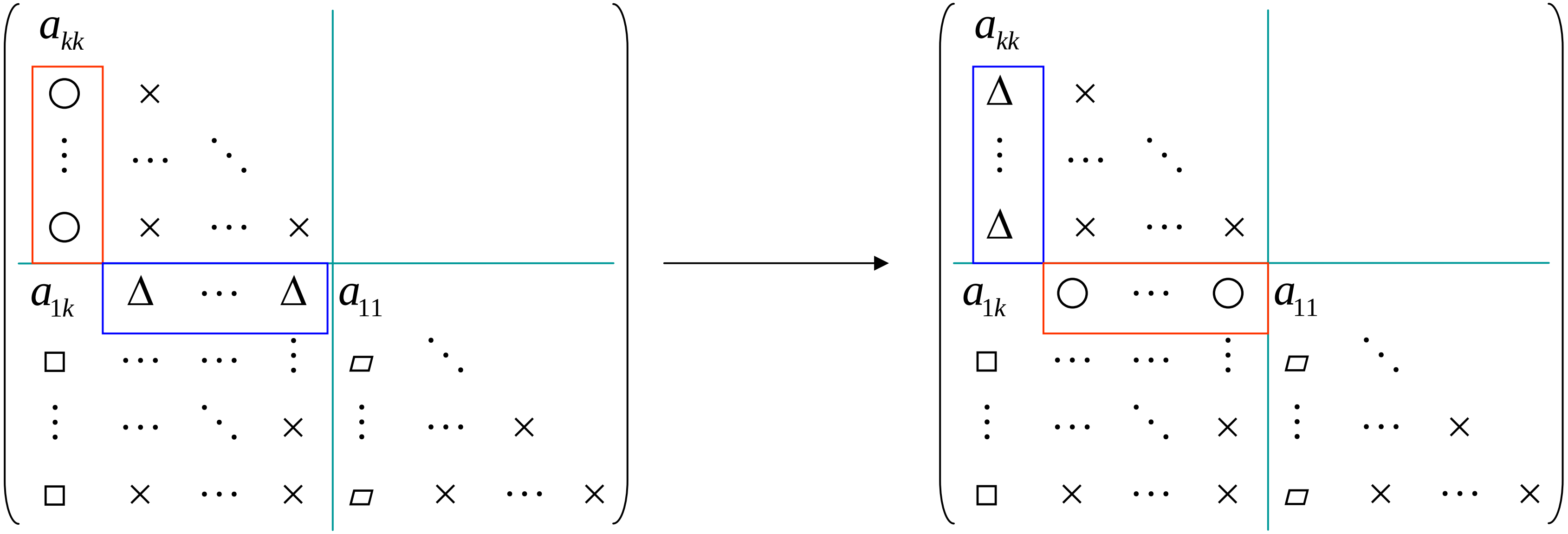
$$A(i,k)(i>k)\xrightarrow{col-1\leftrightarrow col-k}A(i,1)\xrightarrow{row-1\leftrightarrow row-k}A(i,1)$$

Therefore $A(i,1)\leftrightarrow A(i,k)\quad\forall\ k+1\le i\le n$

Change diagonal element to (1,1) position [7]

Step 3: interchange column 1 (from row-*2* to row-*(k-1)*) and row *k (from col-2 to col-(k-1))*

$$A(2:k-1,1) \leftrightarrow A(k,2:k-1)$$



$$A(i,1)(2 \le i < k) \xrightarrow{col-1 \leftrightarrow col-k} A(i,k) \xrightarrow{row-1 \leftrightarrow row-k} A(i,k)(upper\ triangle) = A(k,i)$$

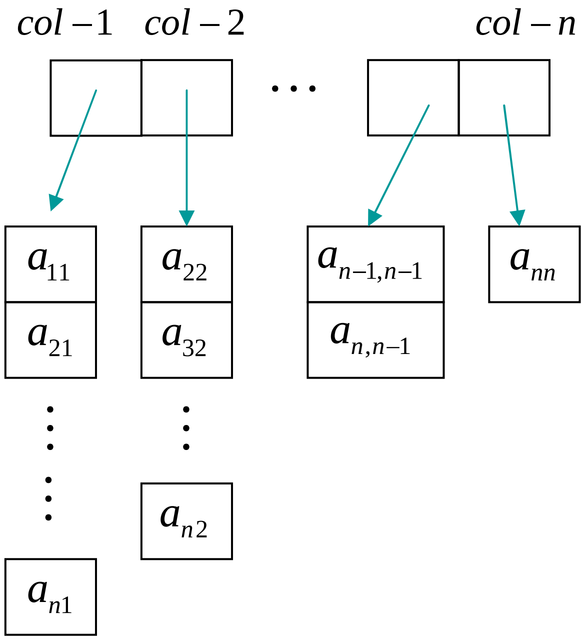
$$A(k,i)(2 \le i < k) \xrightarrow{col-1 \leftrightarrow col-k} A(k,i) \xrightarrow{row-1 \leftrightarrow row-k} A(1,i)(upper\ triangle) = A(i,1)$$

Therefore $A(i,1) \leftrightarrow A(k,i) \quad \forall\ 2 \le i \le k-1$

Implementation of symmetric permutation: swapping overhead [1]

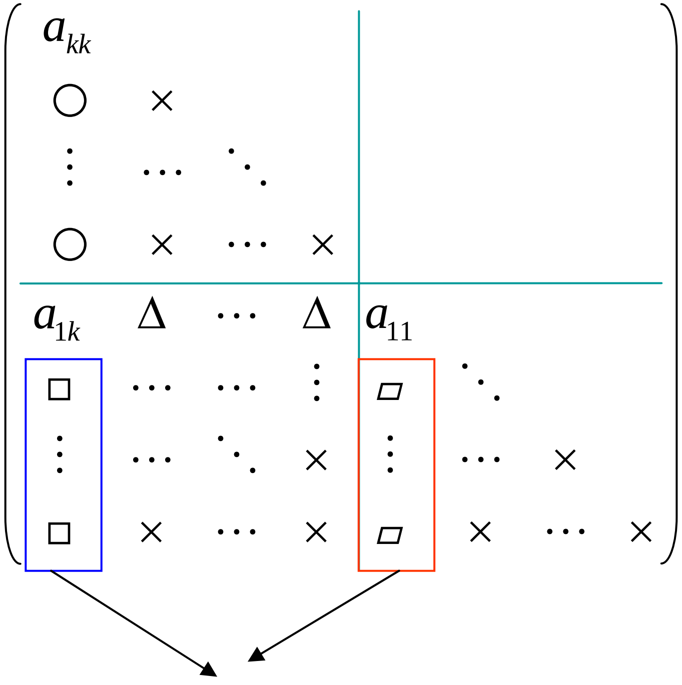
Suppose we use col-major based pointer array to store real symmetric matrix *A*

$$mem(A) = \begin{pmatrix} a_{11} & & & \\ a_{21} & a_{22} & & \\ \vdots & \vdots & \ddots & \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix}$$



Step 2: interchanging column 1 and *k* is O.K

since memory block is contiguous.

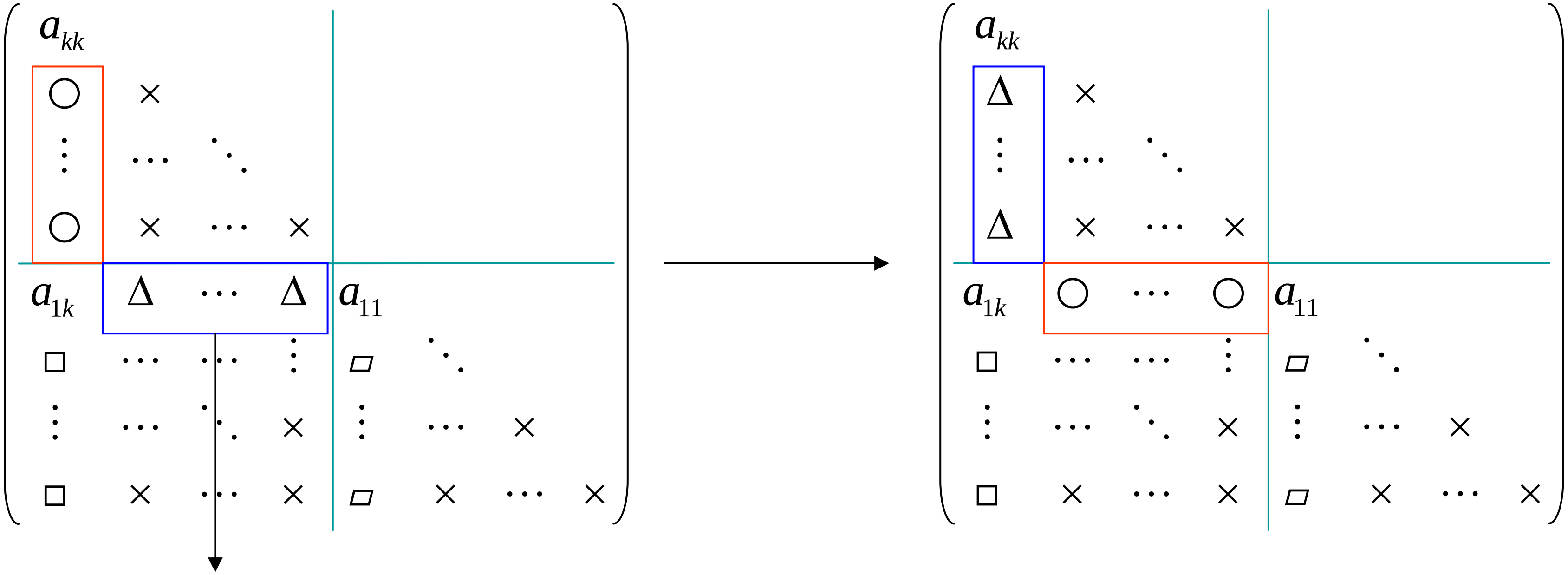


Contiguous memory block

Implementation of symmetric permutation: swapping overhead [2]

Step 3: interchanging column 1 and row *k, i.e.* $A(2:k-1,1) \leftrightarrow A(k,2:k-1)$

is **NOT** efficient since $A(k,2:k-1)$ is **NOT** contiguous.



NOT contiguous, swapping is very slow.

Observation: the situation is the same even we choose row-major based pointer array as storage strategy.

Solution: in order to avoid high swapping overhead, we should avoid permutation.

Change off-diagonal element to (2,1) position [1]

suppose we want to change $a_{43} = 9$ to position *(2,1),* then consider first permutation $P_1 = (1, 4, 3, 2)$ which change first index from 4 to 2

$$\overset{A}{\begin{pmatrix} 1 & \mathbf{2} & 3 & 4 \\ 2 & \mathbf{5} & 6 & 7 \\ 3 & 6 & \mathbf{8} & \mathbf{9} \\ 4 & 7 & \mathbf{9} & \mathbf{10} \end{pmatrix}} \xrightarrow[\text{col 2, 4}]{\text{interchange}} \overset{AP_1^T}{\begin{pmatrix} 1 & \mathbf{4} & 3 & 2 \\ 2 & \mathbf{7} & 6 & 5 \\ 3 & 9 & \mathbf{8} & \mathbf{6} \\ 4 & 10 & \mathbf{9} & \mathbf{7} \end{pmatrix}} \xrightarrow[\text{row 2, 4}]{\text{interchange}} \overset{P_1AP_1^T}{\begin{pmatrix} 1 & \mathbf{4} & 3 & 2 \\ 4 & \mathbf{10} & 9 & 7 \\ 3 & 9 & \mathbf{8} & \mathbf{6} \\ 2 & 7 & \mathbf{6} & \mathbf{5} \end{pmatrix}}$$

and second permutation $P_2 = (3, 2, 1, 4)$ which change second index from 3 to 1

$$\overset{P_1AP_1^T}{\begin{pmatrix} 1 & \mathbf{4} & 3 & 2 \\ 4 & \mathbf{10} & 9 & 7 \\ 3 & 9 & \mathbf{8} & \mathbf{6} \\ 2 & 7 & \mathbf{6} & \mathbf{5} \end{pmatrix}} \xrightarrow[\text{col 1, 3}]{\text{interchange}} \overset{\left(P_1AP_1^T\right)P_2^T}{\begin{pmatrix} 3 & \mathbf{4} & 1 & 2 \\ 9 & \mathbf{10} & 4 & 7 \\ 8 & 9 & \mathbf{3} & \mathbf{6} \\ 6 & 7 & \mathbf{2} & \mathbf{5} \end{pmatrix}} \xrightarrow[\text{row 1, 3}]{\text{interchange}} \overset{P_2\left(P_1AP_1^T\right)P_2^T}{\begin{pmatrix} 8 & \mathbf{9} & 3 & 6 \\ 9 & \mathbf{10} & 4 & 7 \\ 3 & 4 & \mathbf{1} & \mathbf{2} \\ 6 & 7 & \mathbf{2} & \mathbf{5} \end{pmatrix}}$$

Change off-diagonal element to (2,1) position [2]

$$A = \begin{pmatrix} 1 & 2 & 3 & 4 \\ 2 & 5 & 6 & 7 \\ 3 & 6 & 8 & 9 \\ 4 & 7 & 9 & 10 \end{pmatrix} \xrightarrow[\text{row and col 2, 4}]{\text{interchange}} P_1AP_1^T = \begin{pmatrix} 1 & 4 & 3 & 2 \\ 4 & 10 & 9 & 7 \\ 3 & 9 & 8 & 6 \\ 2 & 7 & 6 & 5 \end{pmatrix} \xrightarrow[\text{row and col 1, 3}]{\text{interchange}} P_2\left(P_1AP_1^T\right)P_2^T = \begin{pmatrix} 8 & 9 & 3 & 6 \\ 9 & 10 & 4 & 7 \\ 3 & 4 & 1 & 2 \\ 6 & 7 & 2 & 5 \end{pmatrix}$$

$$\left.\begin{array}{l} a_{43} \xrightarrow{row/col\ \ 2\leftrightarrow 4} a_{23} \xrightarrow{row/col\ \ 1\leftrightarrow 3} a_{21} \\ a_{44} \xrightarrow{row/col\ \ 2\leftrightarrow 4} a_{22} \xrightarrow{row/col\ \ 1\leftrightarrow 3} a_{22} \\ a_{33} \xrightarrow{row/col\ \ 2\leftrightarrow 4} a_{33} \xrightarrow{row/col\ \ 1\leftrightarrow 3} a_{11} \end{array}\right\} \longrightarrow \begin{pmatrix} a_{33} & \\ a_{43} & a_{44} \end{pmatrix} \to \begin{pmatrix} a_{11} & \\ a_{21} & a_{22} \end{pmatrix}$$

Observation: two permutation matrices can be computed easily since 2 ←→ 4 and 1 ←→ 3 are independent.

$$P_1 = (1,4,3,2) \xrightarrow{P_2 = (3,2,1,4)} P \equiv P_2P_1 = (3,4,1,2)$$

Change off-diagonal element to (2,1) position [3]

HOW to transform $a_{43} = 9$ to position *(2,1)*, under only lower triangle part of *A* is stored?

Observation 1: $a_{22} \leftrightarrow a_{44}$ and $a_{42} = a_{24}$ does not changed

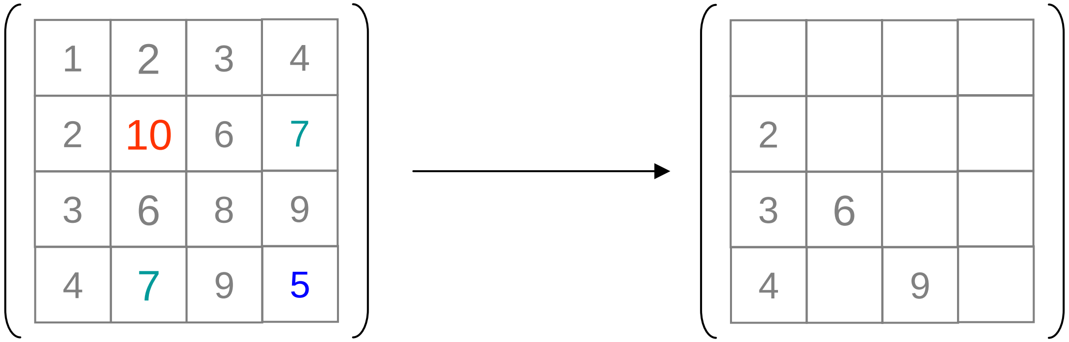
$$\overset{A}{\begin{pmatrix} 1 & 2 & 3 & 4 \\ 2 & 5 & 6 & 7 \\ 3 & 6 & 8 & 9 \\ 4 & 7 & 9 & 10 \end{pmatrix}} \xrightarrow[\text{row/col 2, 4}]{\text{interchange}} \overset{P_1 A P_1^T}{\begin{pmatrix} 1 & 4 & 3 & 2 \\ 4 & 10 & 9 & 7 \\ 3 & 9 & 8 & 6 \\ 2 & 7 & 6 & 5 \end{pmatrix}}$$

Step 1: interchange position (*4,4*) and (*2,2*), $a_{22} \leftrightarrow a_{44}$

$$\overset{A}{\begin{pmatrix} 1 & 2 & 3 & 4 \\ 2 & 5 & 6 & 7 \\ 3 & 6 & 8 & 9 \\ 4 & 7 & 9 & 10 \end{pmatrix}} \longrightarrow \begin{pmatrix} 1 & 2 & 3 & 4 \\ 2 & 10 & 6 & 7 \\ 3 & 6 & 8 & 9 \\ 4 & 7 & 9 & 5 \end{pmatrix}$$

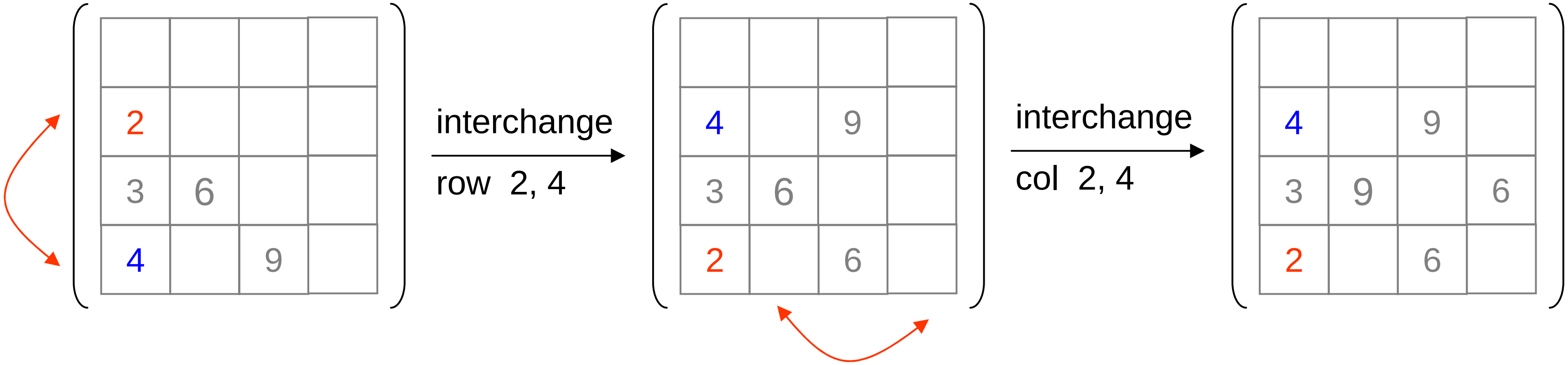
Change off-diagonal element to (2,1) position [4]

Observation 2: we only need to update lower triangle part of *A* (diagonal term is excluded).



$$\begin{pmatrix} 1 & 2 & 3 & 4 \\ 2 & 10 & 6 & 7 \\ 3 & 6 & 8 & 9 \\ 4 & 7 & 9 & 5 \end{pmatrix} \longrightarrow \begin{pmatrix} & & & \\ 2 & & & \\ 3 & 6 & & \\ 4 & & 9 & \end{pmatrix}$$

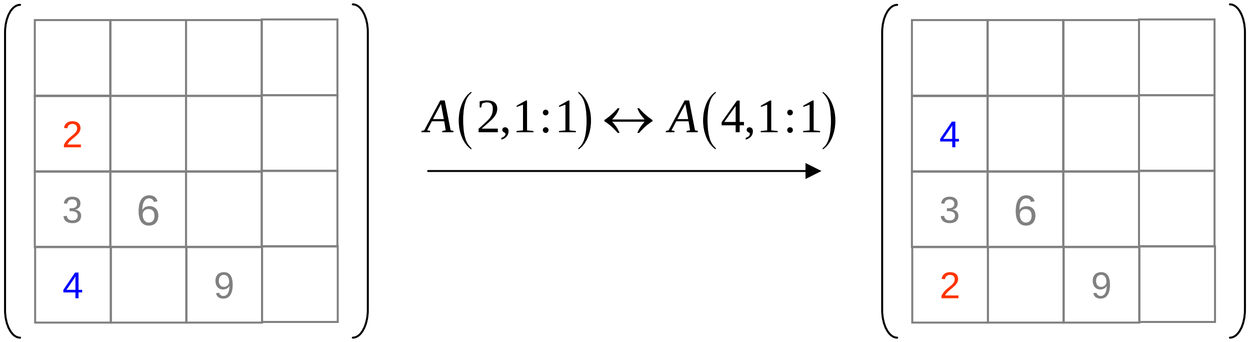
Step 2: interchange row 2 and *4* below col *2*, i.e $A(2,1:1) \leftrightarrow A(4,1:1)$



$$\begin{pmatrix} & & & \\ 2 & & & \\ 3 & 6 & & \\ 4 & & 9 & \end{pmatrix} \xrightarrow[\text{row 2, 4}]{\text{interchange}} \begin{pmatrix} & & & \\ 4 & & 9 & \\ 3 & 6 & & \\ 2 & & 6 & \end{pmatrix} \xrightarrow[\text{col 2, 4}]{\text{interchange}} \begin{pmatrix} & & & \\ 4 & & 9 & \\ 3 & 9 & & 6 \\ 2 & & 6 & \end{pmatrix}$$

NOTE: Interchanging column 2, 4 does not change position (*2,1*) and (*4,1*), it suffices to interchange position (2,1) and (4,1) first.

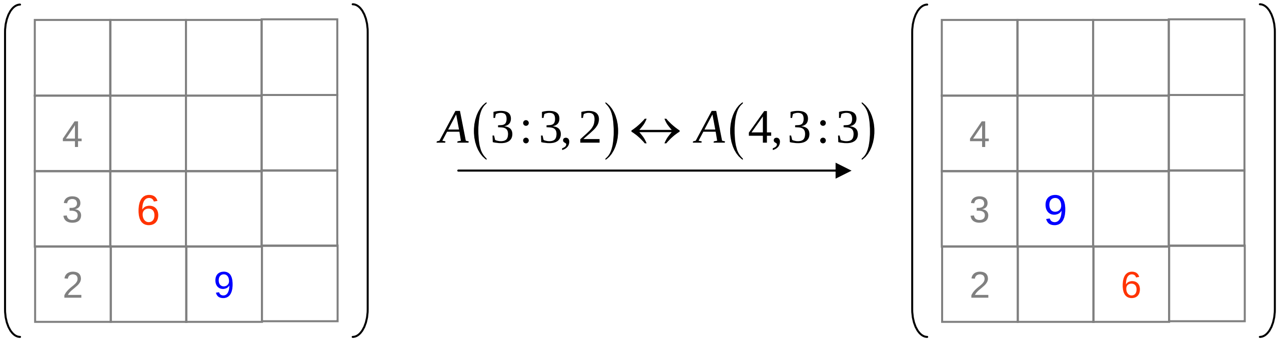
Change off-diagonal element to (2,1) position [5]



$$\begin{pmatrix} & & & \\ 2 & & & \\ 3 & 6 & & \\ 4 & & 9 & \end{pmatrix} \xrightarrow{A(2,1:1) \leftrightarrow A(4,1:1)} \begin{pmatrix} & & & \\ 4 & & & \\ 3 & 6 & & \\ 2 & & 9 & \end{pmatrix}$$

Step 3: interchange column 2 (from row-*3* to row-*3*) and row *4 (from col-3 to col-3)*

$$A(3:3,2) \leftrightarrow A(4,3:3)$$



$$\begin{pmatrix} & & & \\ 4 & & & \\ 3 & 6 & & \\ 2 & & 9 & \end{pmatrix} \xrightarrow{A(3:3,2) \leftrightarrow A(4,3:3)} \begin{pmatrix} & & & \\ 4 & & & \\ 3 & 9 & & \\ 2 & & 6 & \end{pmatrix}$$

$$a_{32} \xrightarrow{col-2 \leftrightarrow col-4} a_{34} \xrightarrow{row-2 \leftrightarrow row-4} a_{34}\,(upper\ \ triangle) = a_{43}$$

$$a_{43} \xrightarrow{col-2 \leftrightarrow col-4} a_{43} \xrightarrow{row-2 \leftrightarrow row-4} a_{23}\,(upper\ \ triangle) = a_{32}$$

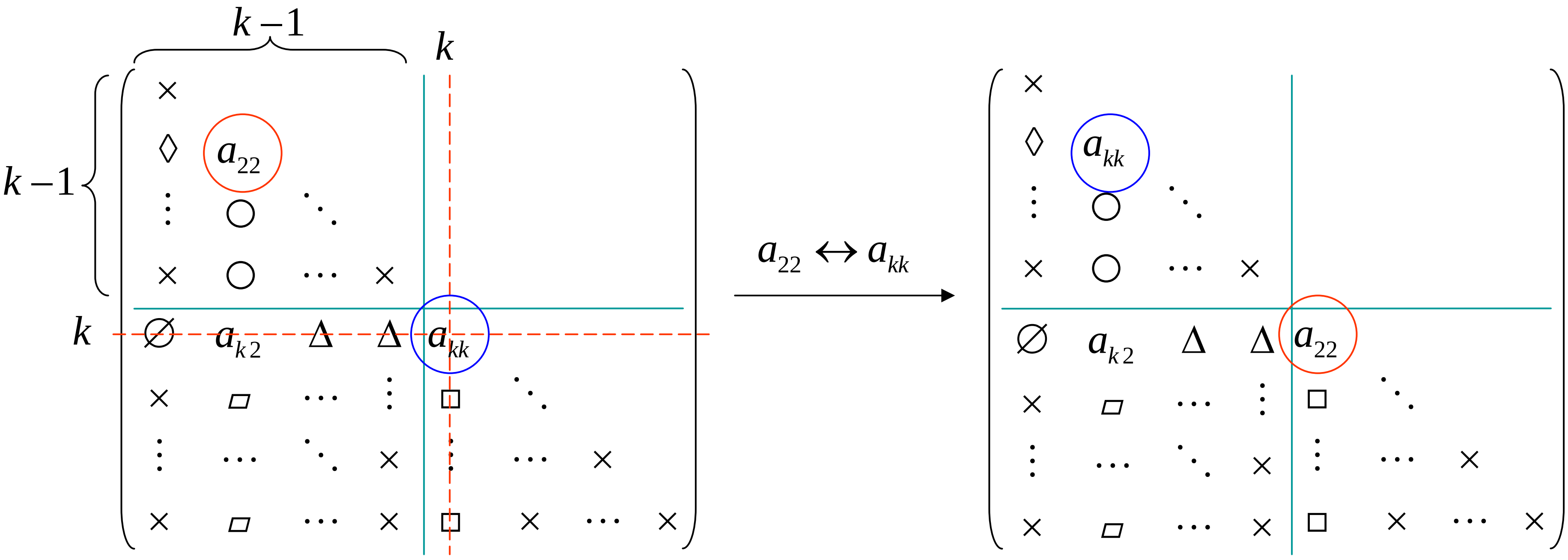
Change off-diagonal element to (2,1) position [6]

For general real symmetric matrix *A* with dimension *n*, suppose we want to change $a_{kk} \to a_{22}$

$P = \left(1,\ \underset{\substack{\uparrow \\ 2-th}}{k},\ 3,\cdots k-1,\ \underset{\substack{\uparrow \\ k-th}}{2},\ k+1, n\right)$ interchanges rows $2,k$ or columns $2,k$

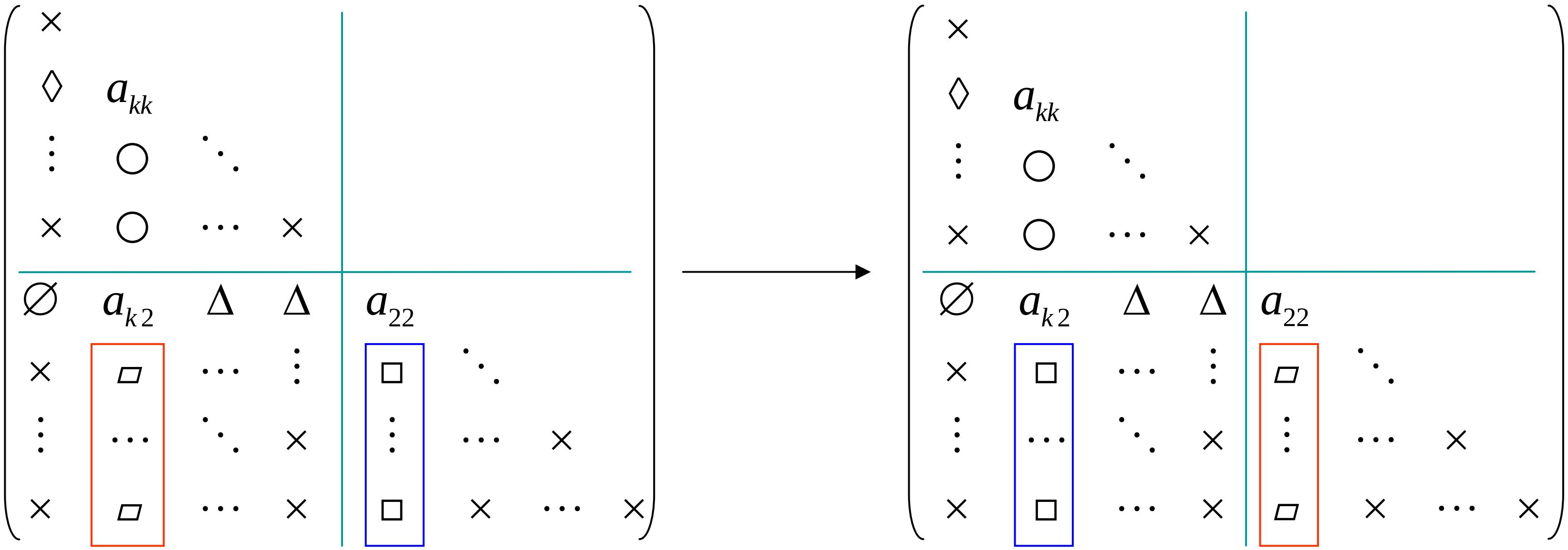
Step 1: interchange position *(2,2)* and *(k,k), i.e.* $a_{22} \leftrightarrow a_{kk}$

keep position *(k,2)* and *(2,k), i.e.* $a_{2k} = a_{k2}$ does not changed



Change off-diagonal element to (2,1) position [7]

Step 2: interchange column 2 and *k* below row *k+1*, i.e $A(k+1:n,2)\leftrightarrow A(k+1:n,k)$



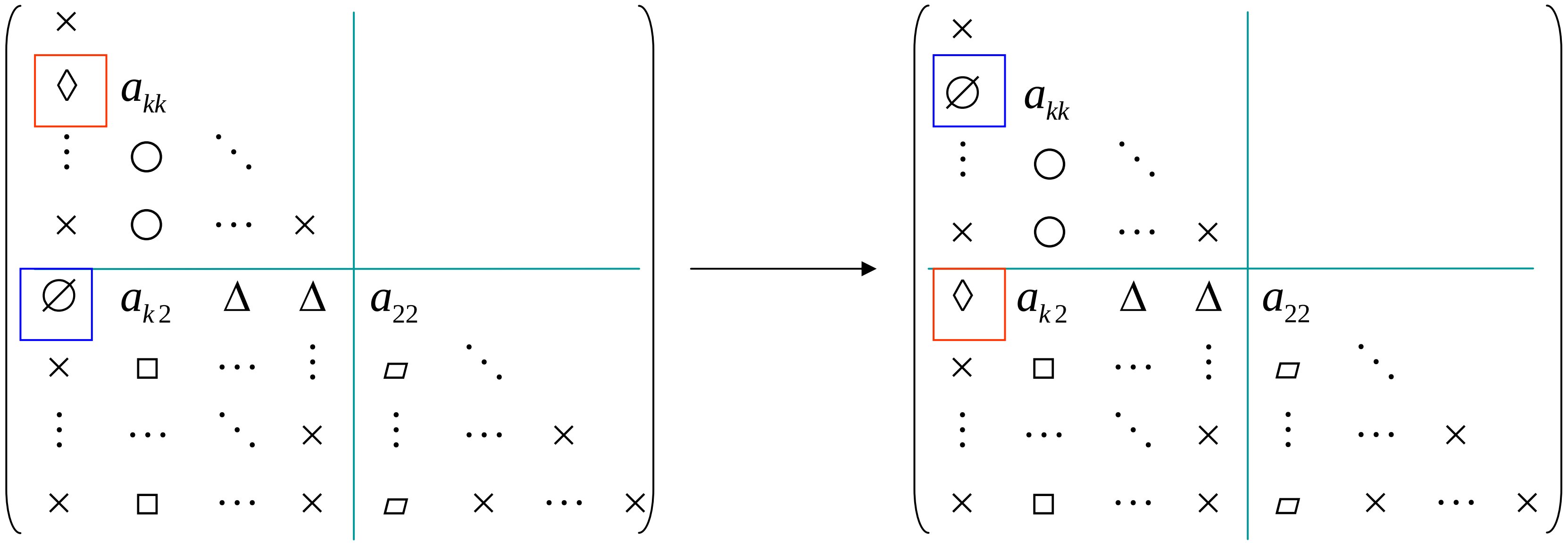
$$A(i,2)(i>k)\xrightarrow{col-2\leftrightarrow col-k}A(i,k)\xrightarrow{row-2\leftrightarrow row-k}A(i,k)$$

$$A(i,k)(i>k)\xrightarrow{col-2\leftrightarrow col-k}A(i,2)\xrightarrow{row-2\leftrightarrow row-k}A(i,2)$$

Therefore $A(i,2)\leftrightarrow A(i,k)\quad \forall\ k+1\le i\le n$

Change off-diagonal element to (2,1) position

Step 3: interchange row 2 (column 1) and *row k* (column1), i.e $A(2,1) \leftrightarrow A(k,1)$



$$A(2,1) \xrightarrow{col-2 \leftrightarrow col-k} A(2,1) \xrightarrow{row-2 \leftrightarrow row-k} A(k,1)$$

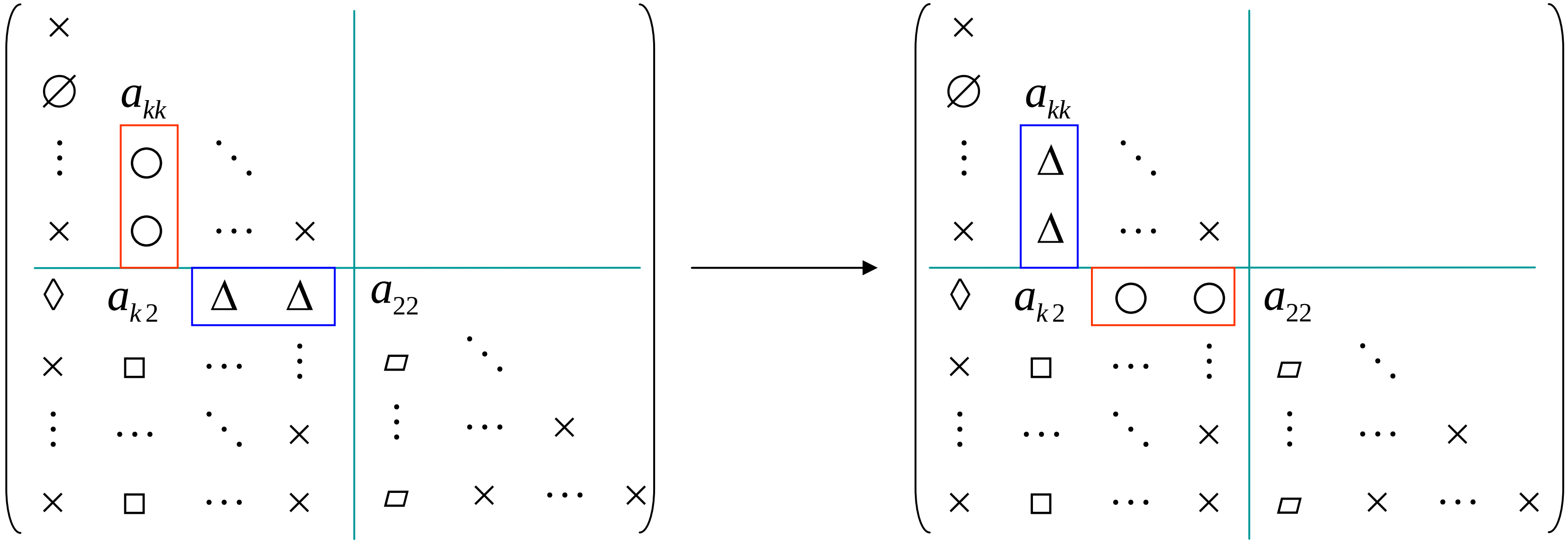
$$A(k,1) \xrightarrow{col-2 \leftrightarrow col-k} A(k,1) \xrightarrow{row-2 \leftrightarrow row-k} A(2,1)$$

Therefore $A(2,1) \leftrightarrow A(k,1)$

Change off-diagonal element to (2,1) position *[9]*

Step 4: interchange column 2 (from row-*3* to row-*(k-1)*) and row *k (from col-3 to col-(k-1))*

$$A(3:k-1,2) \leftrightarrow A(k,3:k-1)$$



$$A(i,2)(3\le i<k)\xrightarrow{col-2\leftrightarrow col-k}A(i,k)\xrightarrow{row-2\leftrightarrow row-k}A(i,k)(upper\ triangle)=A(k,i)$$

$$A(k,i)(3\le i<k)\xrightarrow{col-2\leftrightarrow col-k}A(k,i)\xrightarrow{row-2\leftrightarrow row-k}A(2,i)(upper\ triangle)=A(i,2)$$

Therefore $A(i,2)\leftrightarrow A(k,i) \quad \forall\ 3\le i\le k-1$

OutLine

- Preliminary
- Symmetric permutation
- LDL’ decomposition (diagonal pivoting)
  - growth rate of 1x1, 2x2 pivoting
  - criterion for pivot strategy
  - comparison to complete pivoting in *GE*
- Example of complete diagonal pivoting
- Algorithm of complete diagonal pivoting

LDL’ decomposition: 1x1, 2x2 pivoting

- diagonal pivoting method with complete pivoting: Bunch-Parlett, “Direct methods fro solving symmetric indefinite systems of linear equations,” SIAM J. Numer. Anal., v. 8, 1971, pp. 639-655

- diagonal pivoting method with partial pivoting: *Bunch-Kaufman*, “Some Stable Methods for Calculating Inertia and Solving Symmetric Linear Systems,” Mathematics of Computation, volume 31, number 137, January 1977, page 163-179

Growth rate in LDL' decomposition *[1]*

$$A \equiv \begin{pmatrix} E & c^T \\ c & B \end{pmatrix} = \begin{pmatrix} I & \\ cE^{-1} & I \end{pmatrix} \begin{pmatrix} E & \\ & A^{(n-s)} \end{pmatrix} \begin{pmatrix} I & E^{-1}c^T \\ & I \end{pmatrix}$$

E is of order s

Define $L = \begin{pmatrix} I & \\ cE^{-1} & I \end{pmatrix}$ and constant $\begin{cases} \mu_0 = \max\limits_{1\le i,j\le n} |A_{ij}| = \text{maximal element of matrix } A \\ \mu_1 = \max\limits_{1\le i\le n} |A_{ii}| = \text{maximal diagonal element of matrix } A \\ \nu = |\det E| \end{cases}$

Case 1: *s = 1*

$$A = \left(\begin{array}{c|ccc} a_{11} & a_{21} & \cdots & a_{n1} \\ \hline a_{21} & a_{22} & \cdots & \vdots \\ \vdots & \cdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{array}\right) = L\tilde{A}^{(n-1)}L^T$$

where $\tilde{A}^{(n-1)} = \begin{pmatrix} a_{11} & \\ & A^{(n-1)} \end{pmatrix}$ $E = a_{11}$ with $\nu = |\det E| = |a_{11}| > 0$

$c = \begin{pmatrix} a_{21} \\ a_{31} \\ \vdots \\ a_{n1} \end{pmatrix}$ with $c_j = a_{j+1,1}$ and $B = \begin{pmatrix} a_{22} & & & \\ a_{23} & a_{33} & & \\ \vdots & \cdots & \ddots & \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{pmatrix} = B^T$ with $B_{ij} = a_{i+1,j+1}$

Growth rate in LDL' decomposition *[2]*

$$cE^{-1} = \frac{1}{a_{11}} \begin{pmatrix} a_{21} \\ a_{31} \\ \vdots \\ a_{n1} \end{pmatrix} \rightarrow \left|cE^{-1}\right|_\infty \le \max_{2\le j\le n} \left|\frac{a_{j1}}{a_{11}}\right| \le \frac{1}{\nu} \max_{2\le j\le n} \left|a_{j1}\right| \le \frac{\mu_0}{\nu}$$

Therefore $\boxed{\left|L\right|_\infty = \max\left(1, \left|cE^{-1}\right|_\infty\right) \le \max\left(1, \frac{\mu_0}{\nu}\right)}$

Observation: in *PA=LU*, we choose $\left|a_{11}\right| = \max\left|A(:,1)\right|$ such that $\left|L\right|_\infty \le 1$

$$A^{(n-1)} = B - cE^{-1}c^T = B - \frac{cc^T}{a_{11}} \qquad A^{(n-1)}_{ij} = B_{ij} - \frac{c_i c_j}{a_{11}} = a_{i+1,j+1} - \frac{a_{i+1,1}a_{j+1,1}}{a_{11}}$$

$\left|A^{(n-1)}_{ij}\right| \le \left|a_{i+1,j+1}\right| + \frac{\left|a_{i+1,1}\right| \cdot \left|a_{j+1,1}\right|}{\left|a_{11}\right|} \le \mu_0 + \frac{\mu_0^2}{\nu}$ implies $\left|A^{(n-1)}\right|_\infty \le \mu_0 + \frac{\mu_0^2}{\nu}$

Therefore $\boxed{\left|\tilde{A}^{(n-1)}\right|_\infty \le \max\left(\left|a_{11}\right|, \left|A^{(n-1)}\right|_\infty\right) \le \max\left(\nu, \mu_0 + \frac{\mu_0^2}{\nu}\right) \le \mu_0 + \frac{\mu_0^2}{\nu}}$

Observation: large element growth will not occur for a 1×1 pivot if ν is large relative to μ_0

Growth rate in LDL' decomposition *[3]*

Case 2: *s = 2*

$$A = \left(\begin{array}{cc|cc} a_{11} & a_{21} & \cdots & a_{n1} \\ a_{21} & a_{22} & \cdots & \vdots \\ \hline \vdots & \cdots & \ddots & \vdots \\ a_{n1} & a_{n2} & \cdots & a_{nn} \end{array}\right) = L\tilde{A}^{(n-2)}L^T \quad \text{where} \quad \tilde{A}^{(n-2)} = \begin{pmatrix} E & \\ & A^{(n-2)} \end{pmatrix}, \quad L = \begin{pmatrix} I & \\ cE^{-1} & I \end{pmatrix} \quad \text{and} \quad A^{(n-2)} = B - cE^{-1}c^T$$

$$E = \begin{pmatrix} a_{11} & a_{21} \\ a_{21} & a_{22} \end{pmatrix} \quad \text{with} \quad \nu = \left|\det E\right| = \left|a_{11}a_{22} - a_{21}^2\right| > 0 \quad \text{and} \quad E^{-1} = \frac{1}{\det E}\begin{pmatrix} a_{22} & -a_{21} \\ -a_{21} & a_{11} \end{pmatrix}$$

$$c = \begin{pmatrix} a_{31} & a_{32} \\ a_{41} & a_{42} \\ \vdots & \vdots \\ a_{n1} & a_{n2} \end{pmatrix} \quad \text{with} \quad c_{ij} = a_{i+2,j} \quad \text{and} \quad B = \begin{pmatrix} a_{33} & & & \\ a_{43} & a_{44} & & \\ \vdots & \cdots & \ddots & \\ a_{n3} & a_{n4} & \cdots & a_{nn} \end{pmatrix} = B^T \quad \text{with} \quad B_{ij} = a_{i+2,j+2}$$

$$\left(cE^{-1}\right)_{ij} = c(i,:)E^{-1}(:,j) \quad \text{implies} \quad \begin{cases} \left(cE^{-1}\right)_{i1} = \begin{pmatrix} c_{i1} & c_{i2} \end{pmatrix} \dfrac{1}{\det E} \begin{pmatrix} a_{22} \\ -a_{21} \end{pmatrix} \\ \left(cE^{-1}\right)_{i2} = \begin{pmatrix} c_{i1} & c_{i2} \end{pmatrix} \dfrac{1}{\det E} \begin{pmatrix} -a_{21} \\ a_{11} \end{pmatrix} \end{cases}$$

Growth rate in LDL' decomposition *[4]*

for $2 < i$

$$\begin{cases} L_{i1} = \left(cE^{-1}\right)_{i-1,1} = \left(a_{i1} \quad a_{i2}\right)\dfrac{1}{\det E}\begin{pmatrix} a_{22} \\ -a_{21} \end{pmatrix} = \dfrac{a_{i1}a_{22} - a_{i2}a_{21}}{\det E} \\ L_{i2} = \left(cE^{-1}\right)_{i-1,2} = \left(a_{i1} \quad a_{i2}\right)\dfrac{1}{\det E}\begin{pmatrix} -a_{21} \\ a_{11} \end{pmatrix} = \dfrac{-a_{i1}a_{21} + a_{i2}a_{11}}{\det E} \end{cases}$$

$$\begin{cases} \left|L_{i1}\right| \le \dfrac{\left|a_{i1}\right|\left|a_{22}\right| + \left|a_{i2}\right|\left|a_{21}\right|}{\left|\det E\right|} \le \dfrac{\mu_0\mu_1 + \mu_0^2}{\nu} = \dfrac{\mu_0}{\nu}\left(\mu_0 + \mu_1\right) \\ \left|L_{i2}\right| \le \dfrac{\left|a_{i1}\right|\left|a_{21}\right| + \left|a_{i2}\right|\left|a_{11}\right|}{\left|\det E\right|} \le \dfrac{\mu_0\mu_0 + \mu_0\mu_1}{\nu} = \dfrac{\mu_0}{\nu}\left(\mu_0 + \mu_1\right) \end{cases}$$

Therefore $\boxed{\left|L\right|_\infty = \max\left(1, \left|cE^{-1}\right|_\infty\right) \le \max\left(1, \dfrac{\mu_0}{\nu}\left(\mu_0 + \mu_1\right)\right)}$

Growth rate in LDL’ decomposition [5]

$$A_{ij}^{(n-2)} = B_{ij} - \left(cE^{-1}\right)(i,:)\,c^T(:,j) = B_{ij} - c(i,:)\,E^{-1}c(j,:)$$

$$= a_{i+2,j+2} - \begin{pmatrix} a_{i+2,1} & a_{i+2,2} \end{pmatrix} \frac{1}{\det E} \begin{pmatrix} a_{22} & -a_{21} \\ -a_{21} & a_{11} \end{pmatrix} \begin{pmatrix} a_{j+2,1} \\ a_{j+2,2} \end{pmatrix}$$

$$= a_{i+2,j+2} - \frac{1}{\det E} \begin{pmatrix} a_{i+2,1}a_{22} - a_{i+2,2}a_{21} & -a_{i+2,1}a_{21} + a_{i+2,2}a_{11} \end{pmatrix} \begin{pmatrix} a_{j+2,1} \\ a_{j+2,2} \end{pmatrix}$$

$$= a_{i+2,j+2} - \frac{\left(a_{i+2,1}a_{22} - a_{i+2,2}a_{21}\right)a_{j+2,1} + \left(-a_{i+2,1}a_{21} + a_{i+2,2}a_{11}\right)a_{j+2,2}}{\det E}$$

$$\left|A_{ij}^{(n-2)}\right| \le \left|a_{i+2,j+2}\right| + \frac{\left(\left|a_{i+2,1}\right|\left|a_{22}\right| + \left|a_{i+2,2}\right|\left|a_{21}\right|\right)\left|a_{j+2,1}\right| + \left(\left|a_{i+2,1}\right|\left|a_{21}\right| + \left|a_{i+2,2}\right|\left|a_{11}\right|\right)\left|a_{j+2,2}\right|}{\left|\det E\right|}$$

$$\le \mu_0 + \frac{\left(\mu_0\mu_1 + \mu_0\mu_0\right)\mu_0 + \left(\mu_0\mu_0 + \mu_0\mu_1\right)\mu_0}{\nu} = \mu_0\left[1 + \frac{2\mu_0\left(\mu_0 + \mu_1\right)}{\nu}\right]$$

Therefore $$\boxed{\left|\tilde{A}^{(n-2)}\right|_\infty \le \max\left(\left|E\right|_\infty, \left|A^{(n-2)}\right|_\infty\right) \le \max\left(\mu_0, \mu_0\left[1 + \frac{2\mu_0\left(\mu_0 + \mu_1\right)}{\nu}\right]\right) = \mu_0\left[1 + \frac{2\mu_0\left(\mu_0 + \mu_1\right)}{\nu}\right]}$$

Criterion for pivot strategy [1]

Fix a number $0 < \alpha < 1$ (later on, we will determine optimal value of α)

$$A = A^{(n)} = \begin{pmatrix} E & c^T \\ c & B \end{pmatrix} = \begin{pmatrix} I & \\ cE^{-1} & I \end{pmatrix} \begin{pmatrix} E & \\ & A^{(n-s)} \end{pmatrix} L^T$$

$\mu_0 = \max_{1 \le i, j \le n} |A_{ij}| =$ maximal element of matrix *A*

$\mu_1 = \max_{1 \le i \le n} |A_{ii}| =$ maximal diagonal element of matrix *A*

$\nu = |\det E|$

Case 1: $\mu_1 \ge \alpha \mu_0$

suppose $\mu_1 = |A_{kk}| = \max_{1 \le i \le n} |A_{ii}|$ we interchange *1st* and *k-th* rows and columns by introducing permutation matrix $P_1 = (k, 2, 3, \cdots, k-1, 1, k+1, \cdots, n)$ and do symmetric permutation

$$\hat{A}^{(n)} = P_1 A^{(n)} P_1^T$$

$$A^{(n)} = \begin{pmatrix} a_{11} & \cdots & a_{k1} & \times \\ \vdots & \ddots & \vdots & \times \\ a_{k1} & \cdots & a_{kk} & \times \\ \times & \times & \times & \times \end{pmatrix} \longrightarrow \tilde{A}^{(n)} = \begin{pmatrix} a_{kk} & \cdots & a_{k1} & \times \\ \vdots & \ddots & \vdots & \times \\ a_{k1} & \cdots & a_{11} & \times \\ \times & \times & \times & \times \end{pmatrix}$$

Then do LDL^T on $\hat{A}^{(n)}$ with 1×1 pivot, written as $\hat{A}^{(n)} = \begin{pmatrix} \hat{a}_{11} & c^T \\ c & B \end{pmatrix} = \begin{pmatrix} 1 & \\ c / \tilde{a}_{11} & I \end{pmatrix} \begin{pmatrix} \hat{a}_{11} & \\ & A^{(n-1)} \end{pmatrix} L_1^T$

Criterion for pivot strategy [2]

Recall for 1×1 pivot, $A = L\tilde{A}^{(n-1)}L^T$, we have growth rate

$$\boxed{\left|L\right|_\infty \le \max\left(1, \frac{\mu_0}{\nu}\right)} \quad \text{and} \quad \boxed{\left|\tilde{A}^{(n-1)}\right|_\infty \le \mu_0 + \frac{\mu_0^2}{\nu}}$$

Now for $\hat{A}^{(n)} = \begin{pmatrix} \hat{a}_{11} & c^T \\ c & B \end{pmatrix} = \begin{pmatrix} 1 & \\ c/\tilde{a}_{11} & I \end{pmatrix} \begin{pmatrix} \hat{a}_{11} & \\ & A^{(n-1)} \end{pmatrix} L_1^T,$ $\quad \nu = \left|\hat{a}_{11}\right| = \left|a_{kk}\right| = \mu_1 \ge \alpha\mu_0$

$$\boxed{\left|L_1\right|_\infty \le \max\left(1, \frac{\mu_0}{\nu}\right) \le \max\left(1, \frac{1}{\alpha}\right) = \frac{1}{\alpha}} \quad \text{and} \quad \boxed{\left|\tilde{A}^{(n-1)}\right|_\infty \le \mu_0 + \frac{\mu_0^2}{\nu} \le \left(1 + \frac{1}{\alpha}\right)\mu_0}$$

Case 2: $\mu_1 < \alpha\mu_0$

suppose $\mu_0 = \left|A_{rq}\right| = \max_{1\le i,\, j\le n} \left|A_{ij}\right|, \quad r > q$, we interchange *q-th* and *1st* rows and columns,

and then *r-th* and *2nd* rows and columns by introducing permutation matrix

$$P_1 = \left(1, r, 3, \cdots, r-1, 2, r+1, \cdots, n\right)\cdot\left(q, 2, 3, \cdots, q-1, 1, q+1, \cdots, n\right)$$

and do symmetric permutation $\hat{A}^{(n)} = P_1 A^{(n)} P_1^T$

Question: we must change *q*←→1 first, then change *r* ←→2, why?

Criterion for pivot strategy [3]

$P_1 = (1, r, 3, \cdots, r-1, 2, r+1, \cdots, n) \cdot (q, 2, 3, \cdots, q-1, 1, q+1, \cdots, n)$ transforms $A_{rq} \to A_{21}$

① $r > q > 3$

$$P_1 = (\ q\ ,\ r,\ 3, \cdots, q-1,\ \underset{\substack{\uparrow \\ q-th}}{1},\ q+1, \cdots, r-1,\ \underset{\substack{\uparrow \\ r-th}}{2}\ , r+1, \cdots, n)$$

② $r > q = 3$

$$P_1 = (\ 3\ ,\ r,\ 1,\ 4, \cdots, r-1,\ \underset{\substack{\uparrow \\ r-th}}{2}\ , r+1, \cdots, n)$$

③ $3 = r > q = 2$ (boundary case)

$$P_1 = (1, 3, 2, 4, \cdots, n) \cdot (2, 1, 3, 4, \cdots, n) = (\ 2\ ,\ 3,\ 1,\ 4, \cdots, n)$$

$$\nparallel$$

but $(2, 1, 3, 4, \cdots, n) \cdot (1, 3, 2, 4, \cdots, n) = (\ 3\ ,\ 1,\ 2,\ 4, \cdots, n)$

Criterion for pivot strategy [4]

2×2 pivot

$$A^{(n)}=\begin{pmatrix} a_{11} & a_{21} & \cdots & a_{q1} & \times & \times & \times \\ \enclose{circle}{a_{21}} & a_{22} & \cdots & \vdots & \times & a_{r2} & \times \\ \vdots & \cdots & \ddots & \vdots & \times & \times & \times \\ a_{q1} & \cdots & \cdots & a_{qq} & \cdots & a_{rq} & \times \\ \times & \times & \times & \vdots & \ddots & \vdots & \times \\ \times & a_{r2} & \times & \enclose{circle}{a_{rq}} & \cdots & a_{rr} & \times \\ \times & \times & \times & \times & \times & \times & \times \end{pmatrix} \xrightarrow[q\leftrightarrow 1]{r\leftrightarrow 2} \hat{A}^{(n)}=\begin{pmatrix} a_{qq} & a_{rq} & \cdots & a_{q1} & \times & \times & \times \\ \enclose{circle}{a_{rq}} & a_{rr} & \cdots & \vdots & \times & a_{r2} & \times \\ \vdots & \cdots & \ddots & \vdots & \times & \times & \times \\ a_{q1} & \cdots & \cdots & a_{11} & \cdots & a_{21} & \times \\ \times & \times & \times & \vdots & \ddots & \vdots & \times \\ \times & a_{r2} & \times & \enclose{circle}{a_{21}} & \cdots & a_{22} & \times \\ \times & \times & \times & \times & \times & \times & \times \end{pmatrix}$$

Then do LDL^T on $\hat{A}^{(n)}$ with 2×2 pivot, written as $\hat{A}^{(n)}=\begin{pmatrix} E & c^T \\ c & B \end{pmatrix}=\begin{pmatrix} 1 & \\ cE^{-1} & I \end{pmatrix}\begin{pmatrix} E & \\ & A^{(n-2)} \end{pmatrix}L_1^T$

Recall for 2×2 pivot, $A=L\tilde{A}^{(n-2)}L^T$, we have growth rate

$$\boxed{\left|L\right|_\infty \le \max\left(1,\frac{\mu_0}{\nu}\left(\mu_0+\mu_1\right)\right)}$$

and

$$\boxed{\left|\tilde{A}^{(n-2)}\right|_\infty \le \mu_0\left[1+\frac{2\mu_0\left(\mu_0+\mu_1\right)}{\nu}\right]}$$

Criterion for pivot strategy [5]

Now for $\hat{A}^{(n)} = \begin{pmatrix} E & c^T \\ c & B \end{pmatrix} = \begin{pmatrix} 1 & \\ cE^{-1} & I \end{pmatrix} \begin{pmatrix} E & \\ & A^{(n-2)} \end{pmatrix} L_1^T$

$$\nu = \left|\det E\right| = \left|a_{qq}a_{rr} - a_{rq}^2\right| = a_{rq}^2 - a_{qq}a_{rr} \geq \mu_0^2 - \mu_1^2 > \left(1-\alpha^2\right)\mu_0^2$$

$$\boxed{\left|L_1\right|_\infty \leq \max\left(1, \frac{\mu_0}{\nu}\left(\mu_0 + \mu_1\right)\right) \leq \max\left(1, \frac{1}{1-\alpha}\right) = \frac{1}{1-\alpha}}$$

$$\boxed{\left|\tilde{A}^{(n-2)}\right|_\infty \leq \mu_0 \left[1 + \frac{2\mu_0\left(\mu_0+\mu_1\right)}{\nu}\right] \leq \left(1 + \frac{2}{1-\alpha}\right)\mu_0}$$

To sum up

Case 1: $\mu_1 \geq \alpha\mu_0$

$$\hat{A}^{(n)} = \begin{pmatrix} \hat{a}_{11} & c^T \\ c & B \end{pmatrix} = \begin{pmatrix} 1 & \\ c/\hat{a}_{11} & I \end{pmatrix} \begin{pmatrix} \hat{a}_{11} & \\ & A^{(n-1)} \end{pmatrix} L_1^T,$$

$$\boxed{\left|L_1\right|_\infty \leq \frac{1}{\alpha}} \quad \text{and} \quad \boxed{\left|\tilde{A}^{(n-1)}\right|_\infty \leq \left(1 + \frac{1}{\alpha}\right)\mu_0}$$

Case 2: $\mu_1 < \alpha\mu_0$

$$\hat{A}^{(n)} = \begin{pmatrix} E & c^T \\ c & B \end{pmatrix} = \begin{pmatrix} 1 & \\ cE^{-1} & I \end{pmatrix} \begin{pmatrix} E & \\ & A^{(n-2)} \end{pmatrix} L_1^T$$

$$\boxed{\left|L_1\right|_\infty \leq \frac{1}{1-\alpha}} \quad \text{and} \quad \boxed{\left|\tilde{A}^{(n-2)}\right|_\infty \leq \left(1 + \frac{2}{1-\alpha}\right)\mu_0}$$

Question: How to choose value of $0 < \alpha < 1$

Criterion for pivot strategy [6]

worst case analysis : choose $0<\alpha<1$ such that

$$\left[\text{growth rate of } 1\times 1 \text{ pivot } + \ 1\times 1 \text{ pivot}\right] \approx \left[\text{growth rate of } 2\times 2 \text{ pivot}\right]$$

or equivalently $\left[\text{growth rate of } 1\times 1 \text{ pivot}\right] \approx \sqrt{\left[\text{growth rate of } 2\times 2 \text{ pivot}\right]}$

Define $B(\alpha)=\max\left(1+\frac{1}{\alpha},\sqrt{1+\frac{2}{1-\alpha}}\right)$

$$\min_{0<\alpha<1} B(\alpha)=B(\alpha_0)=\frac{1+\sqrt{17}}{2}\approx 2.5616<2.57$$

where $\alpha_0=\frac{1+\sqrt{17}}{8}\approx 0.6404$ satisfies $1+\frac{1}{\alpha_0}=\sqrt{1+\frac{2}{1-\alpha_0}}$

Exercise: verify $\min_{0<\alpha<1} B(\alpha)=B(\alpha_0)=\frac{1+\sqrt{17}}{2}$ and $\alpha_0=\frac{1+\sqrt{17}}{8}$

Diagonal pivoting versus complete pivoting of Gaussian Elimination [1]

1 We must search for the largest element in each reduced matrix, this is a complete pivoting strategy analogous to Gaussian Elimination with complete pivoting

$$\boxed{\mu_0 = \max_{1\le i,j\le n} \left|A_{ij}\right| = \text{maximal element of matrix } A}$$

$$\mu_1 = \max_{1\le i\le n} \left|A_{ii}\right| = \text{ maximal diagonal element of matrix } A$$

complete pivoting of *GE (Gaussian Elimination)*

(1) find a $p,q \in \{k, k+1, \cdots, n\}$ such that $\boxed{\left|A_{pq}^{(k)}\right| = \max\left|A^{(k)}(k:n, k:n)\right|}$

(2) swap row $A^{(k)}(k,1:n)$ and row $A^{(k)}(p,1:n)$

(2) swap column $A^{(k)}(1:n,k)$ and column $A^{(k)}(1:n,q)$

then $PA\Pi = LU$ with $|L|_\infty \le 1$

Diagonal pivoting versus complete pivoting of Gaussian Elimination [2]

2 growth rate

diagonal pivoting $PAP^T = LDL^T$

$$\left|L\right|_\infty \le \max\left(\frac{1}{\alpha_0}, \frac{1}{1-\alpha_0}\right) = \max\left(1.56, 2.78\right) = 2.78$$

$$\left|D\right|_\infty \le B\left(\alpha_0\right)^{n-1} \mu_0 \le 2.57^{n-1} \mu_0$$

complete pivoting in *GE* $PA\Pi = LU$

$$\left|L\right|_\infty \le 1$$

$$\left|U\right|_\infty \le ?$$

Remark: Bunch [1] proves that the element growth in the diagonal pivoting method with complete pivoting is bounded by $3n \cdot f\left(n\right)$ in comparison with $\sqrt{n} \cdot f\left(n\right)$ for Gaussian Elimination with complete pivoting, where

$$f\left(n\right) = \sqrt{\prod_{k=2}^{n} k^{1/(k-1)}} < 1.8 \cdot n^{\frac{1}{4}\log n}$$

[1] J.R. Bunch, "Analysis of the diagonal pivoting method", SIAM J. Numer. Anal., v. 8, 1971, pp. 656-680

OutLine

- Preliminary
- Symmetric permutation
- LDL’ decomposition (diagonal pivoting)
- Example of complete diagonal pivoting
- Algorithm of complete diagonal pivoting

Example (complete pivoting) [1]

$$A^{(1)} = A$$

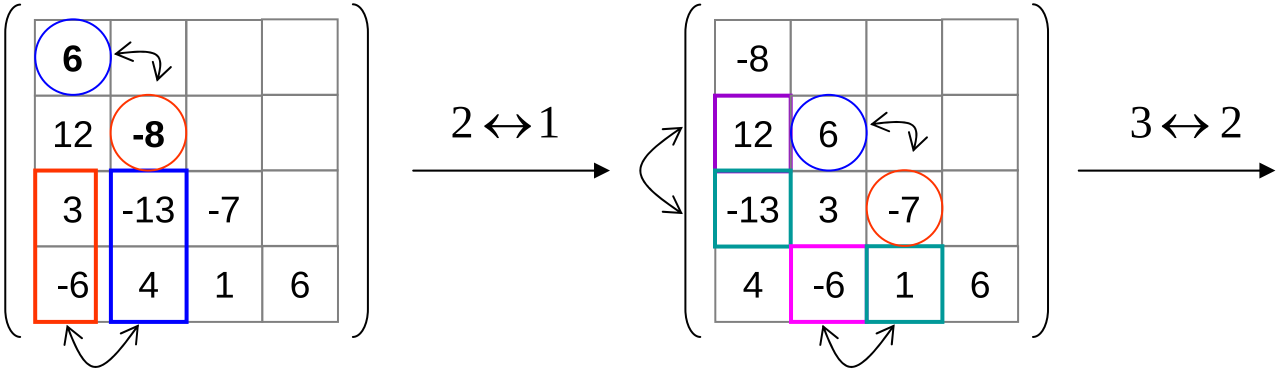
$$\begin{pmatrix} 6 & 12 & 3 & -6 \\ 12 & -8 & -13 & 4 \\ 3 & -13 & -7 & 1 \\ -6 & 4 & 1 & 6 \end{pmatrix}$$

$$\boxed{\mu_0 = \max_{1\le i,j\le n} \left|A_{ij}\right| = \left|A_{32}\right| = 13} \qquad \boxed{\mu_1 = \max_{1\le i\le n} \left|A_{ii}\right| = \left|A_{22}\right| = 8} \qquad \alpha_0 \approx 0.6404$$

$\mu_1 < \alpha_0 \mu_0 = 8.33$ we choose 2×2 pivot

swap row/column $2 \leftrightarrow 1$ and $3 \leftrightarrow 2$ by permutation matrix

$$P_1 = (2,3,1,4)$$



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

$$\left(\begin{array}{cc|cc} -8 & -13 & 12 & 4 \\ -13 & -7 & 3 & 1 \\ \hline 12 & 3 & 6 & -6 \\ 4 & 1 & -6 & 6 \end{array}\right)$$

$$\| $$

$$\begin{pmatrix} E & c^T \\ c & B \end{pmatrix}$$

Example (complete pivoting) [2]

$$P_1 A^{(1)} P_1^T = \tilde{A}^{(1)} = \begin{pmatrix} E & c^T \\ c & B \end{pmatrix} = \begin{pmatrix} I & \\ cE^{-1} & I \end{pmatrix} \begin{pmatrix} E & \\ & B - cE^{-1}c^T \end{pmatrix} \begin{pmatrix} I & \\ cE^{-1} & I \end{pmatrix}^T = L^{(1)} A^{(3)} \left(L^{(1)}\right)^T$$

$$\tilde{A}^{(1)} = P_1 A^{(1)} P_1^T \qquad\qquad L^{(1)} \qquad\qquad A^{(3)}$$

$$\left(\begin{array}{cc|cc} -8 & -13 & 12 & 4 \\ -13 & -7 & 3 & 1 \\ \hline 12 & 3 & 6 & -6 \\ 4 & 1 & -6 & 6 \end{array}\right) = \left(\begin{array}{cc|cc} 1 & & & \\ & 1 & & \\ \hline 0.3982 & -1.1681 & 1 & \\ 0.1327 & -0.3894 & & 1 \end{array}\right) \left(\begin{array}{cc|cc} -8 & -13 & & \\ -13 & -7 & & \\ \hline & & 4.7257 & -6.4248 \\ & & -6.4248 & 5.8584 \end{array}\right) \left(L^{(1)}\right)^T$$

Recursively do the same procedure for $A^{(3)}(3:4, 3:4)$

$$\boxed{\mu_0 = \max_{3 \le i, j \le 4} \left|A_{ij}^{(3)}\right| = \left|A_{43}^{(3)}\right| = 6.4248} \qquad \boxed{\mu_1 = \max_{3 \le i \le 4} \left|A_{ii}^{(3)}\right| = \left|A_{44}^{(3)}\right| = 5.8584} \qquad \alpha_0 \approx 0.6404$$

$\mu_1 > \alpha_0 \mu_0 = 4.1144$ we choose 1×1 pivot

swap row/column $3 \leftrightarrow 4$ by permutation matrix $P_3 = (1, 2, 4, 3)$ such that $A_{44}^{(3)} \rightarrow A_{33}^{(3)}$

$$P_3 \tilde{A}^{(1)} P_3^T = \left[P_3 L^{(1)} P_3^T\right]\left(P_3 A^{(3)} P_3^T\right)\left[P_3 \left(L^{(1)}\right)^T P_3^T\right] = \tilde{L}^{(1)} \tilde{A}^{(3)} \left(\tilde{L}^{(1)}\right)^T$$

Example (complete pivoting) [3]

Do symmetry permutation for $A^{(3)}$ and $L^{(1)}$

$$A^{(3)} = \left(\begin{array}{cc|cc} -8 & -13 & & \\ -13 & -7 & & \\ \hline & & 4.7257 & -6.4248 \\ & & -6.4248 & 5.8584 \end{array}\right) \xrightarrow{P_3 = (1,2,4,3)} \tilde{A}^{(3)} = P_3 A^{(3)} P_3^T = \left(\begin{array}{cc|cc} -8 & -13 & & \\ -13 & -7 & & \\ \hline & & 5.8584 & -6.4248 \\ & & -6.4248 & 4.7257 \end{array}\right)$$

$$L^{(1)} = \left(\begin{array}{cc|cc} 1 & & & \\ & 1 & & \\ \hline 0.3982 & -1.1681 & 1 & \\ 0.1327 & -0.3894 & & 1 \end{array}\right) \xrightarrow{P_3 = (1,2,4,3)} \tilde{L}^{(1)} = P_3 L^{(1)} P_3^T = \left(\begin{array}{cc|cc} 1 & & & \\ & 1 & & \\ \hline 0.1327 & -0.3894 & 1 & \\ 0.3982 & -1.1681 & & 1 \end{array}\right)$$

we do 1×1 pivot on $\tilde{A}^{(3)}(3:4,3:4) = \begin{pmatrix} 5.8584 & -6.4248 \\ -6.4248 & 4.7257 \end{pmatrix}$

Example (complete pivoting) [4]

$$\tilde{A}^{(3)}(3:4,3:4) = \begin{pmatrix} a_{33}^{(3)} & c^T \\ c & B \end{pmatrix} = \begin{pmatrix} 1 & \\ c/a_{33}^{(3)} & I \end{pmatrix} \begin{pmatrix} a_{33}^{(3)} & \\ & B - cc^T/a_{33}^{(3)} \end{pmatrix} \begin{pmatrix} I & \\ c/a_{33}^{(3)} & I \end{pmatrix}^T$$

$$\left(\begin{array}{c|c} 5.8584 & -6.4248 \\ \hline -6.4248 & 4.7257 \end{array}\right) = \left(\begin{array}{c|c} 1 & \\ \hline -1.0967 & 1 \end{array}\right) \left(\begin{array}{c|c} 5.8584 & \\ \hline & -2.3202 \end{array}\right) \left(\begin{array}{c|c} 1 & -1.0967 \\ \hline & 1 \end{array}\right)$$

Or write in original matrix form

$$\begin{array}{cccc} \tilde{A}^{(3)} = P_3 A^{(3)} P_3^T & & L^{(3)} & A^{(4)} \\ \left(\begin{array}{cc|cc} -8 & -13 & & \\ -13 & -7 & & \\ \hline & & 5.8584 & -6.4248 \\ & & -6.4248 & 4.7257 \end{array}\right) & = & \left(\begin{array}{cc|cc} 1 & & & \\ & 1 & & \\ \hline & & 1 & \\ & & -1.0967 & 1 \end{array}\right) & \left(\begin{array}{cc|cc} -8 & -13 & & \\ -13 & -7 & & \\ \hline & & 5.8584 & \\ & & & -2.3202 \end{array}\right) \left(L^{(3)}\right)^T \end{array}$$

$$P_3 P_1 A^{(1)} P_1^T P_3^T = P_3 \tilde{A}^{(1)} P_3^T = \tilde{L}^{(1)} \tilde{A}^{(3)} \left(\tilde{L}^{(1)}\right)^T = \tilde{L}^{(1)} L^{(3)} A^{(4)} \left(L^{(3)}\right)^T \left(\tilde{L}^{(1)}\right)^T$$

Example (complete pivoting) [5]

$$P_3P_1 = (1,2,4,3)\cdot(2,3,1,4) = (2,3,4,1)$$

$$\tilde{L}^{(1)}L^{(3)} = \begin{pmatrix} 1 & & & \\ & 1 & & \\ 0.1327 & -0.3984 & 1 & \\ 0.3982 & -1.1681 & -1.0967 & 1 \end{pmatrix}$$

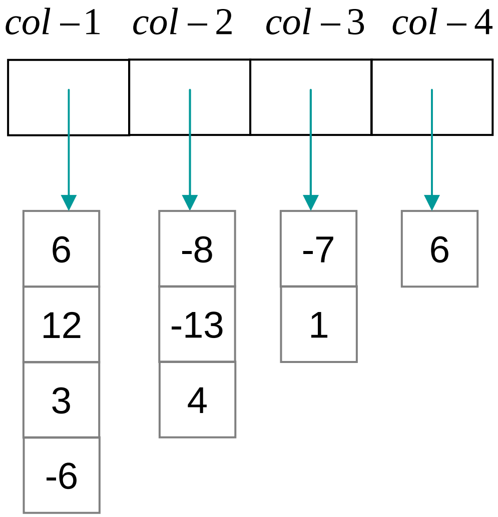
$$A^{(4)} = \begin{pmatrix} -8 & -13 & & \\ -13 & -7 & & \\ & & 5.8584 & \\ & & & -2.3202 \end{pmatrix}$$

In practice, we have two key issues

① we only store lower part of matrix A

$$A = \begin{pmatrix} 6 & & & \\ 12 & -8 & & \\ 3 & -13 & -7 & \\ -6 & 4 & 1 & 6 \end{pmatrix}$$

col-major based



Example (complete pivoting) [6]

② we store decomposition $\tilde{L}^{(1)}L^{(3)}$ and $A^{(4)}$ into original A

$$\tilde{L}^{(1)}L^{(3)} = \begin{pmatrix} 1 & & & \\ & 1 & & \\ 0.1327 & -0.3984 & 1 & \\ 0.3982 & -1.1681 & -1.0967 & 1 \end{pmatrix} \quad + \quad A^{(4)} = \begin{pmatrix} -8 & & & \\ -13 & -7 & & \\ & & 5.8584 & \\ & & & -2.3202 \end{pmatrix}$$

$$mem\left(\tilde{L}^{(1)}L^{(3)}\right) + mem\left(A^{(4)}\right) = \begin{pmatrix} -8 & & & \\ -13 & -7 & & \\ 0.1327 & -0.3984 & 5.8584 & \\ 0.3982 & -1.1681 & -1.0967 & -2.3202 \end{pmatrix}$$

Question: How can you judge correct decomposition $PAP^T = LDL^T$

from $mem\left(\tilde{L}^{(1)}L^{(3)}\right) + mem\left(A^{(4)}\right)$

Example (complete pivoting) [7]

Case 1: four 1x1 pivot

$$L = \begin{pmatrix} 1 & & & \\ 13 & 1 & & \\ 0.1327 & -0.3984 & 1 & \\ 0.3982 & -1.1681 & -1.0967 & 1 \end{pmatrix} \qquad D = \begin{pmatrix} -8 & & & \\ & -7 & & \\ & & 5.8584 & \\ & & & -2.3202 \end{pmatrix}$$

Case 2: two 2x2 pivot

$$L = \begin{pmatrix} 1 & & & \\ & 1 & & \\ 0.1327 & -0.3984 & 1 & \\ 0.3982 & -1.1681 & & 1 \end{pmatrix} \qquad D = \begin{pmatrix} -8 & & & \\ -13 & -7 & & \\ & & 5.8584 & \\ & & -1.0967 & -2.3202 \end{pmatrix}$$

Example (complete pivoting) [8]

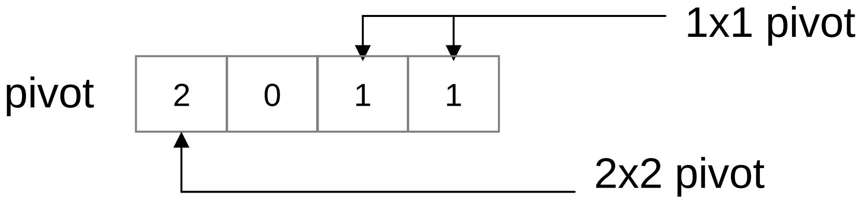
Case 3: 1x1 pivot + 2x2 pivot + 1x1 pivot

$$L = \begin{pmatrix} 1 & & & \\ -13 & 1 & & \\ 0.1327 & & 1 & \\ 0.3982 & -1.1681 & -1.0967 & 1 \end{pmatrix} \qquad D = \begin{pmatrix} -8 & & & \\ & -7 & & \\ & -0.3984 & 5.8584 & \\ & & & -2.3202 \end{pmatrix}$$

Case 4: 2x2 pivot + 1x1 pivot + 1x1 pivot

$$L = \begin{pmatrix} 1 & & & \\ & 1 & & \\ 0.1327 & -0.3984 & 1 & \\ 0.3982 & -1.1681 & -1.0967 & 1 \end{pmatrix} \qquad D = \begin{pmatrix} -8 & & & \\ -13 & -7 & & \\ & & 5.8584 & \\ & & & -2.3202 \end{pmatrix}$$

Solution: we need an array to record pivot sequence



pivot	2	0	1	1

OutLine

- Preliminary
- Symmetric permutation
- LDL’ decomposition (diagonal pivoting)
- Example of complete diagonal pivoting
- Algorithm of complete diagonal pivoting

Algorithm (PAP' = LDL')   [1]

Given symmetric indefinite matrix $A \in R^{n \times n}$, construct initial lower triangle matrix $L = I$

use permutation vector P to record permutation matrix $P^{(k)}$

let $A^{(1)} := A$, $L^{(0)} = I$, $P^{(0)} = (1,2,3,\cdots,n)$ and $pivot = zero(n)$, $\alpha = \frac{1+\sqrt{17}}{8} \approx 0.6404$

$k = 1$

while $k \le (n-1)$

we have compute $P^{(k-1)} A \left(P^{(k-1)}\right)^T = L^{(k-1)} A^{(k)} \left(L^{(k-1)}\right)^T$

$$A^{(k)} = \left(\begin{array}{ccc|ccc} D_1 & 0 & \cdots & 0 & \cdots & 0 \\ 0 & \ddots & & & & \\ \vdots & & D_s & \cdots & \cdots & 0 \\ \hline \vdots & & 0 & a^{(k)}_{k,k} & \cdots & a^{(k)}_{n,k} \\ \vdots & & \vdots & \vdots & & \vdots \\ 0 & \cdots & 0 & a^{(k)}_{n,k} & \cdots & a^{(k)}_{nn} \end{array}\right)$$

update original matrix A , where $D_i : 1 \times 1$ or 2×2

$$L^{(k-1)} = \left(\begin{array}{c|c} \overbrace{W}^{k-1} & O \\ \hline M & I \end{array}\right) \begin{array}{l} \}k-1 \\ \\ \end{array}$$

combines all lower triangle matrix and store in L

Algorithm (PAP' = LDL') *[2]*

1 compute $\mu_0 = \max_{k\le i,j\le n} \left|A_{ij}\right| = \left|A_{rq}\right|$ and $\mu_1 = \max_{k\le i\le n} \left|A_{ii}\right| = A_{\eta\eta}$

Case 1: $\mu_1 \ge \alpha\mu_0$

define permutation $P_k = \left(1,2,3,\cdots,k-1,\eta,k+1,\cdots,\eta-1,k,\eta+1,\cdots n\right)$ to do symmetric permutation

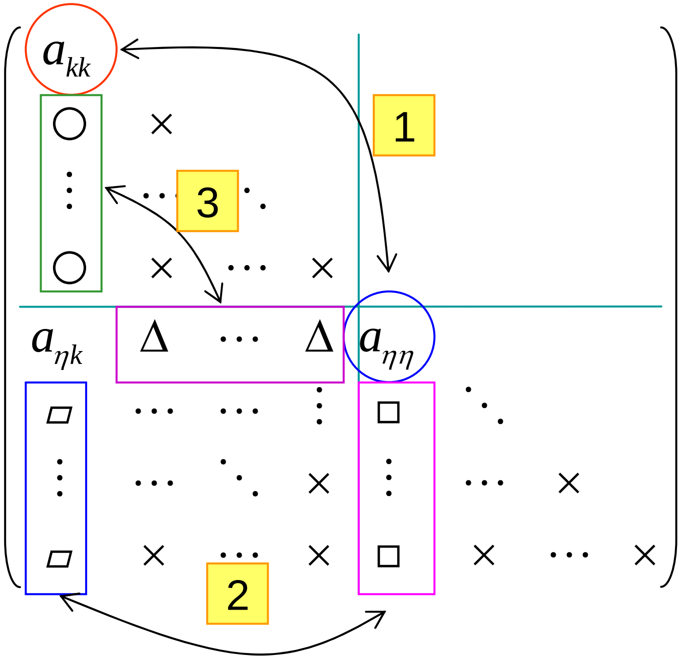
2 $P(k) \leftrightarrow P(\eta)$

To compute $\tilde{A}^{(k)} = P_k A^{(k)} P_k^T$, we only update lower triangle of $A^{(k)}$

3

$$\begin{cases} \boxed{1} \; A(k,k) \leftrightarrow A(\eta,\eta) \\ \boxed{2} \; A(\eta+1:n,k) \leftrightarrow A(\eta+1:n,\eta) \\ \boxed{3} \; A(k+1:\eta-1,k) \leftrightarrow A(\eta,k+1:\eta-1) \end{cases}$$

then $\tilde{A}^{(k)} = \left(\begin{array}{c|cc} D_{k-1} & & \\ \hline & a_{kk}^{(k)} & c^T \\ & c & B \end{array}\right)$, $a_{kk}^{(k)} := a_{\eta\eta}$



Algorithm (PAP' = LDL') *[3]*

To compute $\tilde{L}^{(k-1)} = P_k L^{(k-1)} P_k^T$

4 We only update lower triangle matrix L

$$L(k,1:k-1) \leftrightarrow L(\eta,1:k-1)$$

$$L^{(k-1)}$$

$$\begin{pmatrix}\begin{array}{cccc|cccc}
1 & & & & & & & \\
\times & 1 & & & & & & \\
\vdots & \cdots & \ddots & & & & & \\
\times & \times & \cdots & 1 & & & & \\
\hline
l_{k,1} & l_{k,2} & \cdots & l_{k,k-1} & 1 & & & \\
\vdots & \cdots & \cdots & \vdots & & 1 & & \\
l_{\eta,1} & l_{\eta,2} & \ddots & l_{\eta,k-1} & & & \ddots & \\
\times & \times & \cdots & \times & & & & 1
\end{array}\end{pmatrix}$$

then

$$P^{(k)} A \left(P^{(k)}\right)^T = \tilde{L}^{(k-1)} \tilde{A}^{(k)} \left(\tilde{L}^{(k-1)}\right)^T$$

5 do 1x1 pivot : $\tilde{A}^{(k)} = \begin{pmatrix}\begin{array}{c|c|c} D_{k-1} & & \\ \hline & a_{kk}^{(k)} & c^T \\ \hline & c & B \end{array}\end{pmatrix} = \begin{pmatrix}\begin{array}{c|c|c} I & & \\ \hline & 1 & \\ \hline & c/a_{kk}^{(k)} & I \end{array}\end{pmatrix} \begin{pmatrix}\begin{array}{c|c|c} D_{k-1} & & \\ \hline & a_{kk}^{(k)} & \\ \hline & & B - cc^T/a_{kk}^{(k)} \end{array}\end{pmatrix} \left(L^{(k)}\right)^T$

$$\begin{cases} L(k+1:n,k) \leftarrow c/a_{kk}^{(k)} \\ A(k+1:n,k+1:n) -= cc^T/a_{kk}^{(k)} \end{cases}$$

then $P^{(k)} A \left(P^{(k)}\right)^T = \tilde{L}^{(k-1)} L^{(k)} A^{(k+1)} L^{(k)} \left(\tilde{L}^{(k-1)}\right)^T$

6 $k \leftarrow k+1$ and $pivot(k) = 1$

Algorithm (PAP' = LDL') [4]

Case 2: $\mu_1 < \alpha\mu_0$

define permutation $P_k = (1:k, r, k+2, \cdots, r-1, k+1, r+1, \cdots, n)\cdot(1:k-1, q, k+1, 3, \cdots, q-1, k, q+1, \cdots, n)$

to interchange *q-th* and *k-th* rows and columns, and then *r-th* and *(k+1)-th* rows and columns

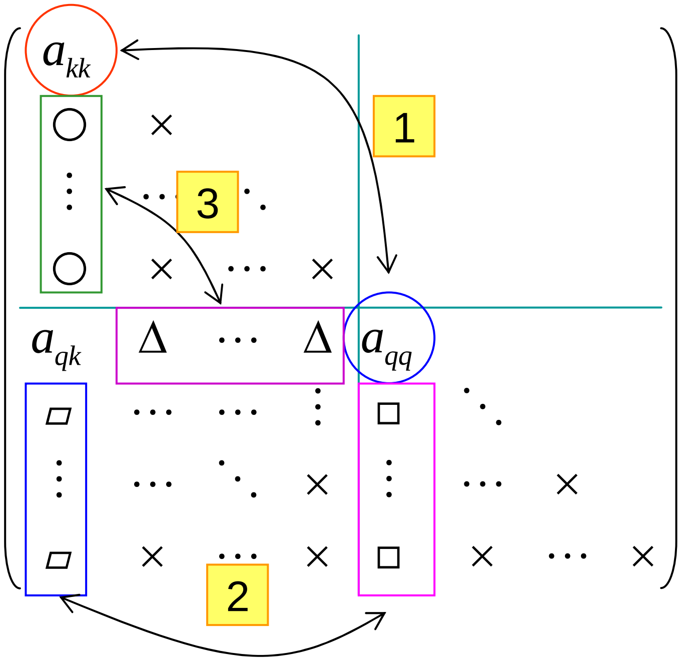
7 $P(k) \leftrightarrow P(q)$ and then $P(k+1) \leftrightarrow P(r)$

To compute $\tilde{A}^{(k)} = P_k A^{(k)} P_k^T$, we only update lower triangle of $A^{(k)}$

(1) do interchange row/col $k \leftrightarrow q$

8
- 1 $A(k,k) \leftrightarrow A(q,q)$
- 2 $A(q+1:n,k) \leftrightarrow A(q+1:n,q)$
- 3 $A(k+1:q-1,k) \leftrightarrow A(q,k+1:q-1)$

then $A^{(k)} \rightarrow \left(\begin{array}{c|cc} D_k & & \\ \hline & a_{qq}^{(k)} & c^T \\ & c & B \end{array}\right)$



Algorithm (PAP' = LDL') [5]

9 (2) do interchange row/col $k+1 \leftrightarrow r$

1 $A(k+1,k+1) \leftrightarrow A(r,r)$

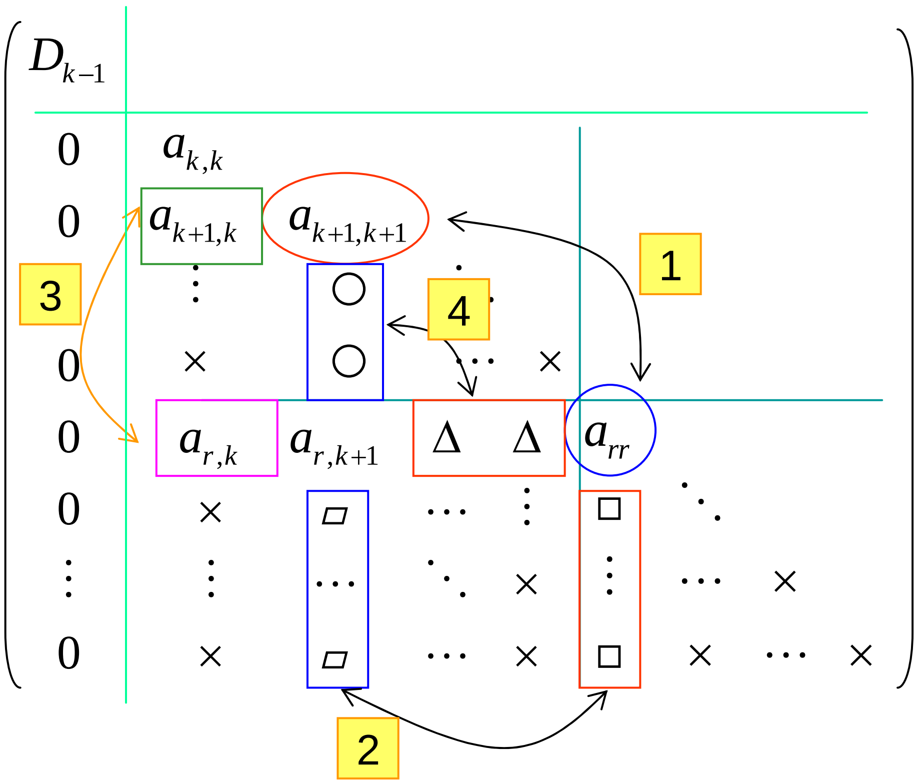
2 $A(r+1:n,k+1) \leftrightarrow A(r+1:n,r)$

3 $A(k+1,k) \leftrightarrow A(r,k)$

4 $A(k+2:r-1:k+1) \leftrightarrow A(r,k+2:r-1)$

then $\tilde{A}^{(k)} = \left(\begin{array}{c|cc} D_{k-1} & & \\ \hline & E & c^T \\ & c & B \end{array}\right)$

where $E = \begin{pmatrix} a_{qq}^{(k)} & a_{rq}^{(k)} \\ a_{rq}^{(k)} & a_{rr}^{(k)} \end{pmatrix}$



Algorithm (PAP’ = LDL’) [6]

To compute $\tilde{L}^{(k-1)} = P_k L^{(k-1)} P_k^T$

⑩ (1) do interchange row $k \leftrightarrow q$

$$L(k,1:k-1) \leftrightarrow L(q,1:k-1)$$

⑪ (2) do interchange row $k+1 \leftrightarrow r$

$$L(k+1,1:k-1) \leftrightarrow L(r,1:k-1)$$

$$L^{(k-1)}$$

$$\left(\begin{array}{cccc|cccc}
1 & & & & & & & \\
\times & 1 & & & & & & \\
\vdots & \cdots & \ddots & & & & & \\
\times & \times & \cdots & 1 & & & & \\
\hline
l_{k,1} & l_{k,2} & \cdots & l_{k,k-1} & 1 & & & \\
\vdots & \cdots & \cdots & \vdots & & 1 & & \\
l_{q,1} & l_{q,2} & \ddots & l_{q,k-1} & & & \ddots & \\
\times & \times & \cdots & \times & & & & 1
\end{array}\right)$$

then

$$P^{(k)} A \left(P^{(k)}\right)^T = \tilde{L}^{(k-1)} \tilde{A}^{(k)} \left(\tilde{L}^{(k-1)}\right)^T$$

$$\left(\begin{array}{cccc|cccc}
1 & & & & & & & \\
\times & 1 & & & & & & \\
\vdots & \cdots & \ddots & & & & & \\
l_{k,1} & l_{k,2} & \cdots & 1 & & & & \\
\hline
l_{k+1,1} & \cdots & l_{k+1,k-1} & 0 & 1 & & & \\
\vdots & \cdots & \cdots & \vdots & & 1 & & \\
l_{r,1} & \cdots & l_{r,k-1} & 0 & & & \ddots & \\
\times & \times & \cdots & 0 & & & & 1
\end{array}\right)$$

Algorithm (PAP' = LDL') [7]

12 do 2x2 pivot : $\tilde{A}^{(k)} = \begin{pmatrix} D_{k-1} & & \\ & E & c^T \\ & c & B \end{pmatrix} = \begin{pmatrix} I & & \\ & I & \\ & cE^{-1} & I \end{pmatrix} \begin{pmatrix} D_{k-1} & & \\ & E & \\ & & B - cE^{-1}c^T \end{pmatrix} \left(L^{(k)}\right)^T$

$$\begin{cases} L(k+2:n, k:k+1) \leftarrow cE^{-1} \\ A(k+2:n, k+2:n) -= cE^{-1}c^T \end{cases}$$

then $P^{(k)} A \left(P^{(k)}\right)^T = \tilde{L}^{(k-1)} L^{(k)} \boxed{A^{(k+2)}} L^{(k)} \left(\tilde{L}^{(k-1)}\right)^T$

$$A^{(k+2)} = \begin{pmatrix} D_{k-1} & & & \\ & D_k & & \\ & & a_{k+2,k+2}^{(k+2)} & \times \\ & & \times & \times \end{pmatrix}$$

13 $k \leftarrow k+2$ and $pivot(k) = 2$

$pivot(k:k+1) = [2,0]$ means $A(k:k+1, k:k+1) = D_k = \begin{pmatrix} d_{k,k} & d_{k+1,k} \\ d_{k+1,k} & d_{k+1,k+1} \end{pmatrix}$ is 2x2 pivot

endwhile

Question: recursion implementation

normal

- Initialization
  - check algorithm holds for *k=1*
- Recursion formula
  - check algorithm holds for *k or k+1*, if *k-1* is true
- Termination condition
  - check algorithm holds for *k=n-1*

abnormal

- Breakdown of algorithm
  - check which condition *PAP'=LDL'* fails

Extension
of algorithm

- No extension: algorithm works only for square, symmetric indefinite matrix.

MATLAB implementation [1]

Given a (full) symmetric indefinite matrix A , compute factorization $PAP^T = LDL^T$

return four quantities $P,\ D,\ L,\ pivot$

Remark: try to neglect upper triangle part of A in MATLAB implementation

Example :

$$A = \begin{pmatrix} 6 & 12 & 3 & -6 \\ 12 & -8 & -13 & 4 \\ 3 & -13 & -7 & 1 \\ -6 & 4 & 1 & 6 \end{pmatrix}$$

$$\alpha = \frac{1+\sqrt{17}}{8}$$

return :

$$P = \begin{pmatrix} 2 & 3 & 4 & 1 \end{pmatrix}$$

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

$$L = \begin{pmatrix} 1 & & & \\ & 1 & & \\ 0.1327 & -0.3984 & 1 & \\ 0.3982 & -1.1681 & -1.0967 & 1 \end{pmatrix}$$

$$D = \begin{pmatrix} -8 & & & \\ -13 & -7 & & \\ & & 5.8584 & \\ & & & -2.3202 \end{pmatrix}$$

MATLAB implementation [2]

When factorization is complete, $PAP^T = LDL^T$, you need to provide linear solver

$$Ax = b \longrightarrow \left(PAP^T\right)\left(Px\right) = Pb \longrightarrow LDL^T\left(Px\right) = Pb$$

① define $z = DL^T\left(Px\right)$, then $Lz = Pb \longrightarrow z = L^{-1}\left(Pb\right)$ by forward substitution

② define $y = L^T\left(Px\right)$, then $Dy = z \longrightarrow y = D^{-1}z$ by diagonal block inversion

Example: $D = \begin{pmatrix} a_1 & & & \\ & a_2 & a_3 & \\ & a_3 & a_4 & \\ & & & a_5 \end{pmatrix}$, then $D^{-1} = \begin{pmatrix} 1/a_1 & & \\ & \dfrac{1}{a_2a_4 - a_3^2}\begin{pmatrix} a_4 & -a_3 \\ -a_3 & a_2 \end{pmatrix} & \\ & & 1/a_5 \end{pmatrix}$

③ define $w = Px$, then $L^T w = y \longrightarrow w = \left(L^T\right)^{-1} y$ by backward substitution

However you cannot transpose L explicitly in MATLAB

④ $x = P^T w$, you must scan w once to determine x