

# Chapter 17 C-implementation

$$PAP' = LDL'$$

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Reference: [1] H. M. Deitel, P. J. Deitel, C++ How to Program 5-th edition

# OutLine

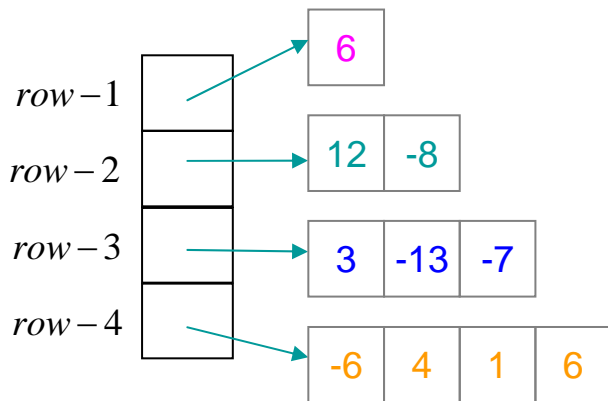
- Data structure of lower triangle matrix
- Function overloading in C++
- Implementation of  $PAP' = LDL'$

# row-major versus col-major

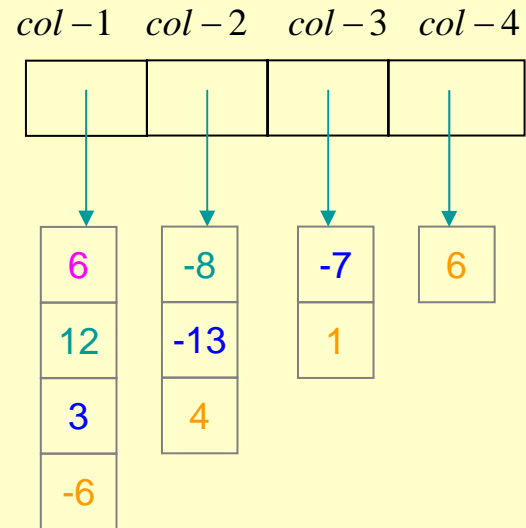
Logical index : 2D

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

row-major based



col-major based



We choose col-major representation

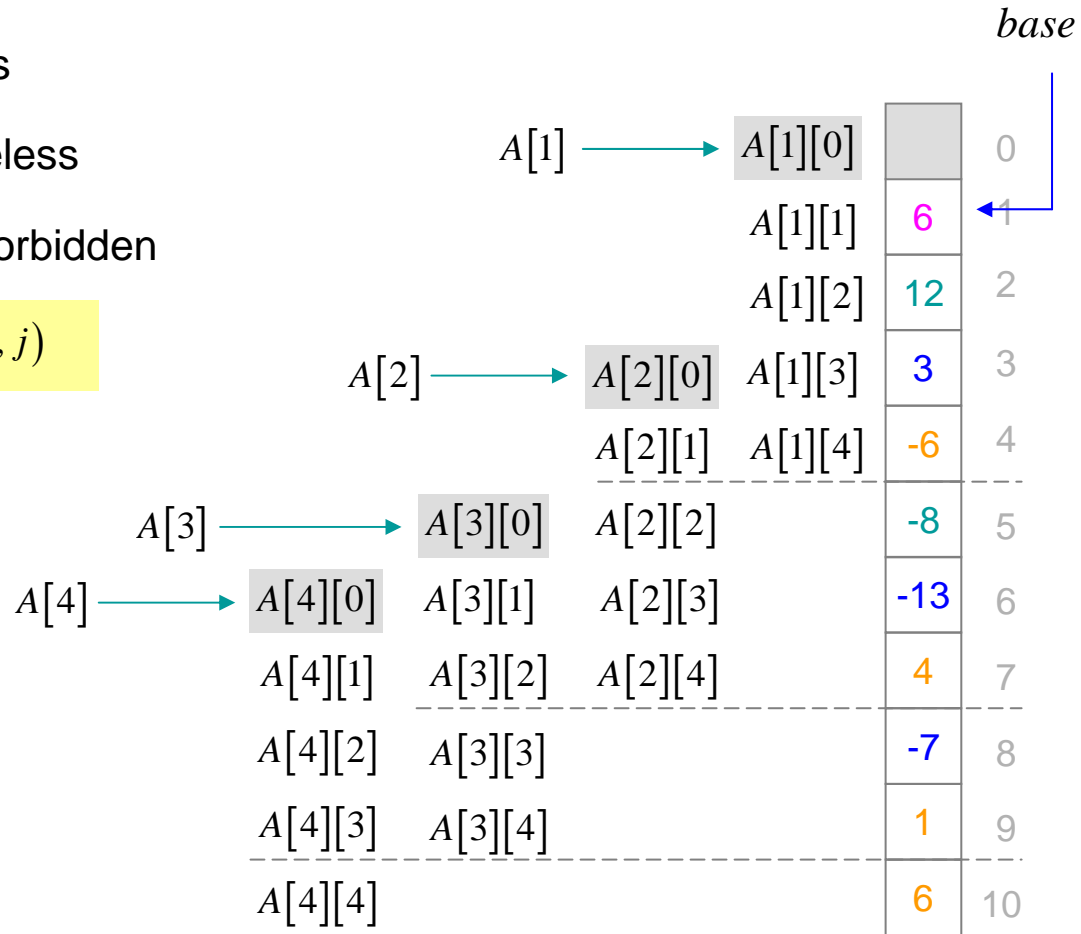
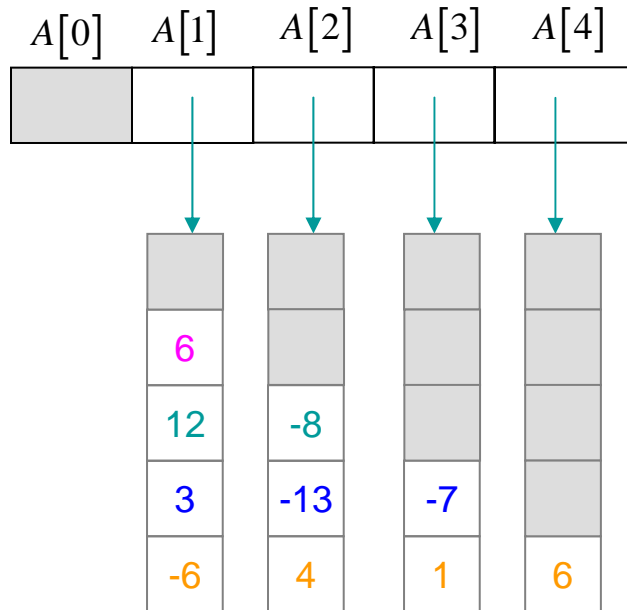
# column-major: method 1 (square-matrix based)

|    |     |     |    |
|----|-----|-----|----|
| 6  | 12  | 3   | -6 |
| 12 | -8  | -13 | 4  |
| 3  | -13 | -7  | 1  |
| -6 | 4   | 1   | 6  |

Keep properties

- 1  $A[0]$  is useless
- 2  $A[k][0]$  is forbidden
- 3  $A[j][i] \equiv A(i, j)$

column-major based



- 4  $A[j][i]$  is valid only for  $i \geq j$   $\left( A[2][1] = -6 = A(4,1) ? \right)$
- 5  $A[1] = base - 1$ ,  $A[2] = A[1] + 3$ ,  $A[3] = A[2] + 2$ ,  $A[4] = A[3] + 1$

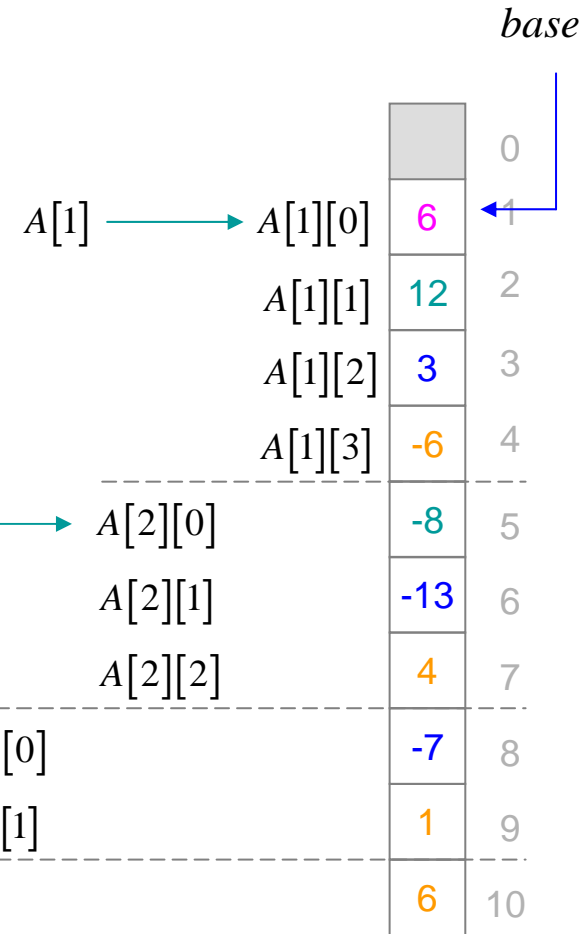
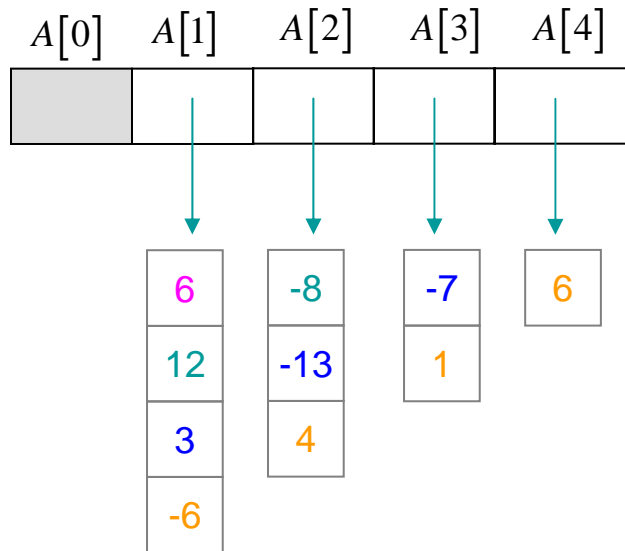
# column-major: method 2 (triangle-matrix based)

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

Keep properties

- 1  $A[0]$  is useless
- 2  $A[k][0]$  is forbidden
- 3  ~~$A[j][i] = A(i, j)$~~

column-major based



- 4  $A(i, j) = A[j][i - j]$  for  $i \geq j$

Index rule is more complicated

# Data structure of matrix and its method

## lowerTriangleMatrix.h

```
#ifndef LOWERTRIANGLEMATRIX_H
#define LOWERTRIANGLEMATRIX_H

#include "global.h" // declaration of doublereal
#include "matrix.h"

#include <stdio.h>
#include <iostream> // type of I/O
#include <iomanip> // manipulate I/O
using namespace std ;

typedef struct lowerTriangleMatrix
{
    integer m ;
    integer n ;
    orderVar sel ; // col-major or row-major
    int isSym ; // isSym > 0 : A is symmetry
    doublereal **A ;
} lowerTriangleMatrix ;

typedef lowerTriangleMatrix* lowerTriangleMatrixHandler ;

// lowerTriangleMatrix constructor
void zeros( lowerTriangleMatrixHandler* Ah_ptr, integer m, integer n, orderVar sel, int isSym ) ;

// destructor
void dealloc( lowerTriangleMatrixHandler Ah ) ;

// show content of matrix in standard form
void disp( lowerTriangleMatrixHandler Ah, ostream& out ) ;

doublereal norm( lowerTriangleMatrixHandler Ah, matrix_keyword p ) ;

// y = A*x
void matvec( lowerTriangleMatrixHandler Ah, matrixHandler xh, matrixHandler yh ) ;

// copy A to A_shadow
void duplicate( lowerTriangleMatrixHandler Ah, lowerTriangleMatrixHandler Ah_shadow ) ;

#endif // LOWERTRIANGLEMATRIX_H
```



method 1

A is symmetric, but we only store lower triangle part

The same name as those in matrix.h

# Constructor [1]

## lowerTriangleMatrix.cpp

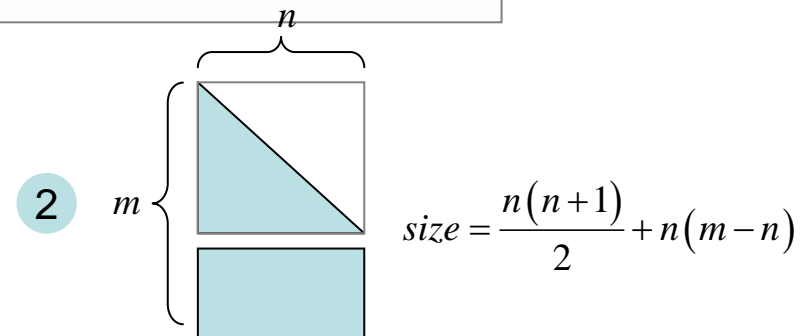
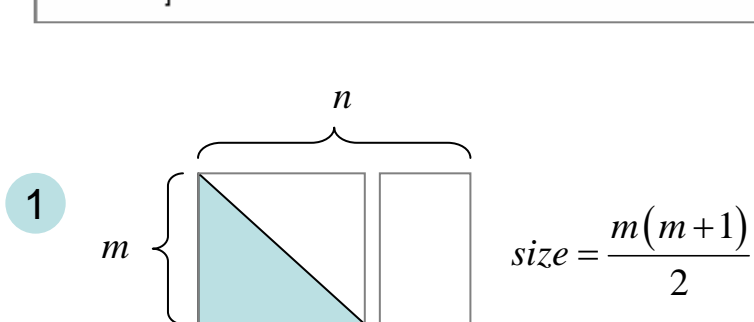
```
// lowerTriangleMatrix constructor
void zeros( lowerTriangleMatrixHandler* Ah_ptr, integer m, integer n, orderVar sel, int isSym )
{
    integer j ;
    doublereal **A ;
    doublereal *memA ; // contiguous memory block of A
    integer size ; // number of entries in matrix A

    assert( Ah_ptr ) ;
    assert( 0 < m ) ; assert( 0 < n ) ;

    // allocate an empty handler
    *Ah_ptr = (lowerTriangleMatrixHandler) malloc( sizeof(lowerTriangleMatrix) ) ;
    assert( *Ah_ptr ) ;

    if ( COL_MAJOR == sel ){
        // A[0] is useless, A[j] means pointer of column j
        A = (doublereal **) malloc( sizeof(doublereal *)*(n+1) ) ;
        assert( A ) ;

        if ( m < n ){
            1 size = m*(m+1) ;
            size = size >> 1 ; // size = m(m+1)/2
        }else{
            2 size = n*(n+1) ;
            size = size >> 1 ;
            size += n*(m-n) ; // size = n(n-1)/2 + n(m-n)
        }
    }
}
```



# Constructor [2]

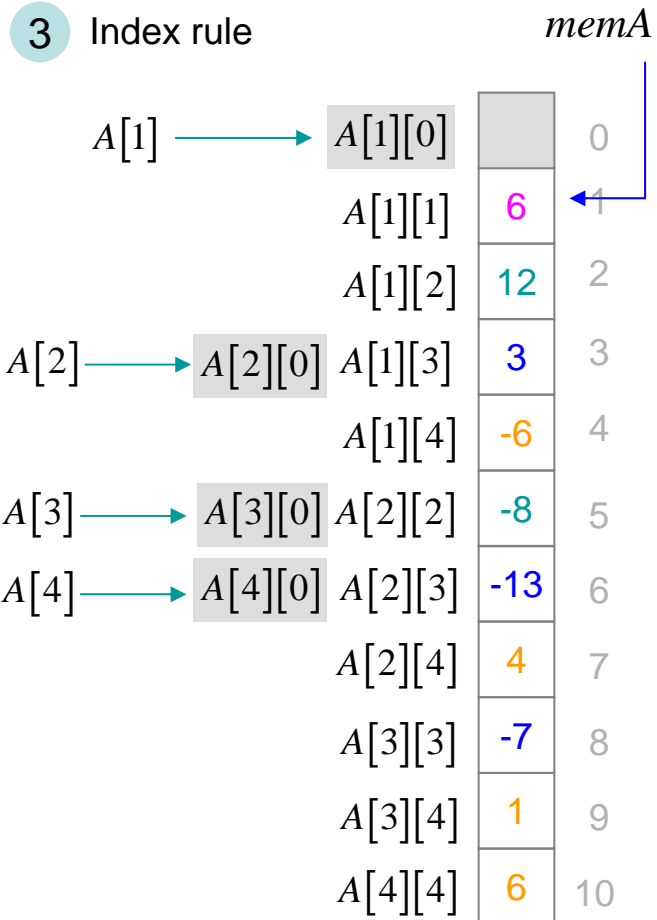
## lowerTriangleMatrix.cpp

```

#ifdef HIGH_PRECISION_PACKAGE
    memA = new doublereal [size] ;
#else
    memA = (doublereal*) malloc( sizeof(doublereal)*size );
#endif
assert( memA );
for ( j=0 ; j < size ; j++){
    memA[j] = 0.0 ; // reset matrix A as zero matrix
}
A[1] = memA - 1 ; // A[0] is useless
for ( j=1 ; j < n ; j++){
    3    A[j+1] = (doublereal*)A[j] + m-j ;
}
}else{
    printf("Error: we don't support row-major so far\n");
    exit(1) ;
}
// set parameter of a matrix
(*Ah_ptr)->m = m ; (*Ah_ptr)->n = n ; (*Ah_ptr)->sel = sel ; (*Ah_ptr)->A = A ;
(*Ah_ptr)->isSym = isSym ;
if ( 0 != isSym ){
    if ( m != n ){
        4    cerr << "A is symmetry, then A must be square matrix" << endl ;
        exit(1) ;
    }
}
}
}

```

|    |     |     |    |
|----|-----|-----|----|
| 6  | 12  | 3   | -6 |
| 12 | -8  | -13 | 4  |
| 3  | -13 | -7  | 1  |
| -6 | 4   | 1   | 6  |



4 When matrix A is symmetric, it must be square and we store lower triangle part of A,

Difference from full matrix is 3 4



# destructor

## lowerTriangleMatrix.cpp

```

void dealloc( lowerTriangleMatrixHandler Ah )
{
    // step 1: dealloc contiguous memory block
    #ifdef HIGH_PRECISION_PACKAGE
    delete [] ( (double*) (Ah->A[1]) + 1 );
    #else
    free( (double*) (Ah->A[1]) + 1 );
    #endif

    // step 2: dealloc column-index array
    free( Ah->A );

    // step 3: dealloc matrix handler
    free( Ah );
}
    
```

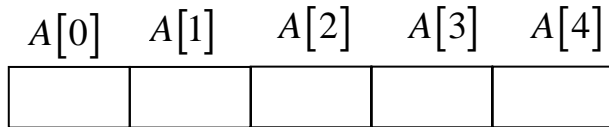
Pointer arithmetic, remember to do casting

1

2

3

2 free pointer array



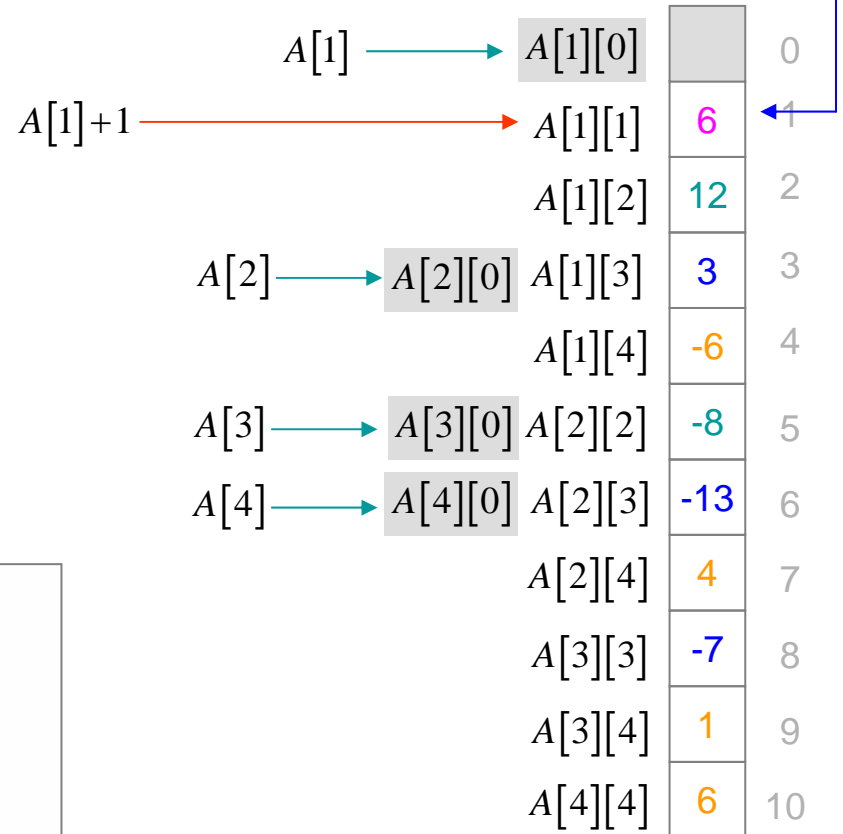
3 free lowerTriangleMatrix handler

```

typedef struct lowerTriangleMatrix
{
    integer m ;
    integer n ;
    orderVar sel ; // col-major or row-major
    int isSym ; // isSym > 0 : A is symmetry
    doublereal **A ;
} lowerTriangleMatrix ;

typedef lowerTriangleMatrix* lowerTriangleMatrixHandler ;
    
```

memA



# Input/Output

## lowerTriangleMatrix.cpp

```
// show content of matrix in standard form
void disp( lowerTriangleMatrixHandler Ah, ostream& out )
{
    int i, j ;
    doublereal **A ;
    integer m, n ;

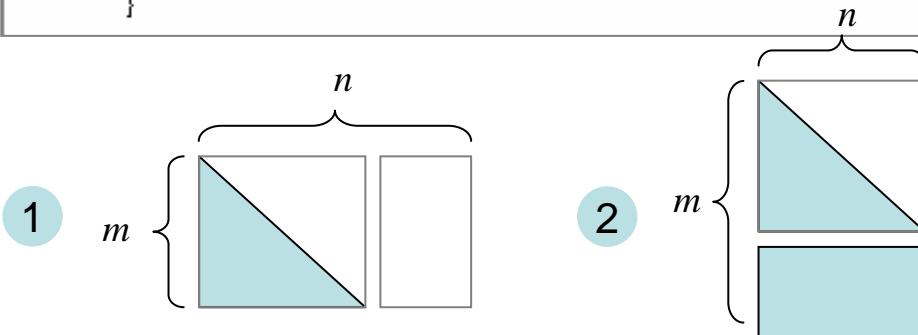
    assert( Ah ) ;
    assert( COL_MAJOR == Ah->sel ) ;

    out.precision(4) ;
    out << std::fixed ;

    if ( Ah->isSym ){
        out << "dimension of symmetric matrix is (" << Ah->m << ", "
            << Ah->n << ") with col-major" << endl ;
    }else{
        out << "dimension of lower triangle matrix is (" << Ah->m << ", "
            << Ah->n << ") with col-major" << endl ;
    }

    A = Ah->A ; m = Ah->m ; n = Ah->n ;
    if ( m < n ){
        1 for( i=1 ; i <= m ; i++ ){
            for( j=1 ; j <= i ; j++ ){
                out << setw(10) << A[j][i] ;
            }
            out << endl ;
        }
    }
}
```

```
}else{ // m >= n
    2 for( i=1 ; i <= n ; i++ ){
        for( j=1 ; j <= i ; j++ ){
            out << setw(10) << A[j][i] ;
        }
        out << endl ;
    }
    for ( i=n+1 ; i <= m ; i++){
        for( j=1 ; j <= n ; j++ ){
            out << setw(10) << A[j][i] ;
        }
        out << endl ;
    }
} // if ( m < n )
out.precision(16) ;
out << std::scientific ;
}
```



No matter what  $A$  is symmetric or not, we only report lower triangle part

# Simple driver

## main.cpp

```
#include "global.h"
#include <stdio.h>
#include "lowerTriangleMatrix.h"

void test_matrix( void );

int main( int argc, char* argv[] )
{
#ifdef HIGH_PRECISION_PACKAGE
    unsigned int old_cw;
    fpu_fix_start(&old_cw);
#endif

#ifdef DO_ARPREC
    mp::mp_init(ARPREC_NDIGITS);
#endif

    // ----- main code -----

    test_matrix();

    // ----- end main code -----

#ifdef DO_ARPREC
    mp::mp_finalize();
#endif

#ifdef HIGH_PRECISION_PACKAGE
    fpu_fix_end(&old_cw);
#endif

    return 0 ;
}
```

```
void test_matrix( void )
{
    integer m = 4 ;
    integer n = 4 ;
    lowerTriangleMatrixHandler Ah ;
    doublereal **A ;

    zeros( &Ah, m, n, COL_MAJOR, 1 ) ;
    A = Ah->A ;

    A[1][1] = 6. ; A[1][2] = 12. ; A[1][3] = 3. ; A[1][4] = -6. ;
    A[2][2] = -8. ; A[2][3] = -13. ; A[2][4] = 4. ;
    A[3][3] = -7. ; A[3][4] = 1. ;
    A[4][4] = 6. ;

    disp( Ah, cout ) ;

    dealloc( Ah ) ;
}
```

```
C:\WINDOWS\system32\cmd.exe
dimension of symmetric matrix is (4,4) with col-major
6.0000
12.0000  -8.0000
3.0000  -13.0000  -7.0000
-6.0000  4.0000  1.0000  6.0000
請按任意鍵繼續 . . .
```

Advantage of method 1: index rule is the same as that of full matrix, one only notices

$A[j][i]$  is valid only for  $i \geq j$

Question: how can we verify  $A[j][i]$  is valid only for  $i \geq j$  automatically?



```

double real norm_sym( lowerTriangleMatrixHandler Ah, matrix_keyword p )
{
    integer m, n ;
    double real sum ;
    double real sumMax ;
    double real **A ;
    int i, j ;

    m = Ah->m ; n = Ah->n ;
    A = Ah->A ;
    if ( INF_NORM == p ){
        sumMax = 0.0 ;
        for ( i = 1 ; i <= m ; i++ ){
            sum = 0.0 ;
            for ( j = 1 ; j <= i ; j++){
                sum += fabs( A[j][i] ) ;
            }
            for( j = i+1 ; j <= n ; j++ ){
                sum += fabs( A[i][j] ) ;
            }
            if ( sum > sumMax ){
                sumMax = sum ;
            }
        } // for each row
    } else if ( ONE_NORM == p ){
        sumMax = 0.0 ;
        for ( j = 1 ; j <= n ; j++ ){
            sum = 0.0 ;
            for ( i = 1 ; i < j ; i++){
                sum += fabs( A[i][j] ) ; // A[i][j] = A[j][i]
            }
            for ( i = j ; i <= m ; i++){
                sum += fabs( A[j][i] ) ;
            }
            if ( sum > sumMax ){
                sumMax = sum ;
            }
        } // for each col
    } else{
        printf("TWO_NORM is NOT implement\n");
        exit(1) ;
    }
    return sumMax ;
}

```

## lowerTriangleMatrix.cpp

```

#include <stdio.h>
#include <stdlib.h>
#include <assert.h>
#include <math.h>

#include "lowerTriangleMatrix.h"

// private supplement function
double real norm_sym( lowerTriangleMatrixHandler Ah, matrix_keyword p ) ;
double real norm_nonsym( lowerTriangleMatrixHandler Ah, matrix_keyword p ) ;

// implement p = 1, 2 and inf
double real norm( lowerTriangleMatrixHandler Ah, matrix_keyword p )
{
    assert( Ah ) ;
    assert( COL_MAJOR == Ah->sel ) ;

    double real val ;
    if ( Ah->isSym ){
        val = norm_sym( Ah, p ) ;
    } else{
        val = norm_nonsym( Ah, p ) ;
    }
    return val ;
}

```

“norm\_sym” and “norm\_nonsym” are private, means that user don't need to know them and we declare them in lowerTriangleMatrix.cpp, NOT in lowerTriangleMatrix.h which user looks at

## Matrix norm [2]

lowerTriangleMatrix.cpp

```
double norm_nonsym( lowerTriangleMatrixHandler Ah, matrix_keyword p )
{
    integer m, n ;
    doublereal sum ;
    doublereal sumMax ;
    doublereal **A ;
    int i, j ;

    m = Ah->m ; n = Ah->n ;
    A = Ah->A ;
    if ( INF_NORM == p ){
        sumMax = 0.0 ;
        for ( i = 1 ; i <= m ; i++ ){
            sum = 0.0 ;
            for ( j = 1 ; j <= i ; j++){
                sum += fabs( A[j][i] ) ;
            }
            if ( sum > sumMax ){
                sumMax = sum ;
            }
        }
        // for each row
    }else if ( ONE_NORM == p ){
        sumMax = 0.0 ;
        for ( j = 1 ; j <= n ; j++ ){
            sum = 0.0 ;
            for ( i = j ; i <= m ; i++){
                sum += fabs( A[j][i] ) ;
            }
            if ( sum > sumMax ){
                sumMax = sum ;
            }
        }
        // for each col
    }else{
        printf("TWO_NORM is NOT implement\n");
        exit(1) ;
    }
    return sumMax ;
}
```

symmetric : norm\_sym

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

nonsymmetric : norm\_nonsym

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

$$y = Ax$$

only A is lower triangle matrix (either symmetric or non-symmetric), x and y are full matrices.

```
// y = A*x
void matvec( lowerTriangleMatrixHandler Ah, matrixHandler xh,
            matrixHandler yh)
{
    integer m, n, s ;

    assert( Ah ) ; assert( xh ) ; assert( yh ) ;
    assert( COL_MAJOR == Ah->sel ) ;
    assert( COL_MAJOR == xh->sel ) ;
    assert( COL_MAJOR == yh->sel ) ;

    m = Ah->m ; n = Ah->n ; s = xh->n ;

    assert(n == xh->m) ;
    assert(m == yh->m) ; assert(s == yh->n) ;

    if ( Ah->isSym ){
        matvec_sym( Ah, xh, yh ) ;
    }else{
        matvec_nonsym( Ah, xh, yh ) ;
    }
}
```

```
void matvec_nonsym( lowerTriangleMatrixHandler Ah, matrixHandler xh,
                  matrixHandler yh)
{
    integer m, n, s ;
    integer i, j, k ;
    doublereal **A ;
    doublereal **x ;
    doublereal **y ;

    m = Ah->m ; n = Ah->n ; s = xh->n ;
    A = Ah->A ; x = xh->A ; y = yh->A ;
    // y = x(1)*A(:,1) + sum_{j}( x(j)*A(:,j) )
    for ( k=1 ; k <= s ; k++){
        for ( i=1 ; i <= m ; i++){
            y[k][i] = A[1][i] * x[k][1] ;
        }
        for ( j=2 ; j <= n ; j++){
            // A is lower triangle part of A
            for ( i=j ; i <= m ; i++){
                y[k][i] += A[j][i] * x[k][j] ;
            }
        } // for each col-j
    } // for each vector x(:,k)
}
```

```
void matvec_sym( lowerTriangleMatrixHandler Ah, matrixHandler xh,
                matrixHandler yh)
{
    integer m, n, s ;
    integer i, j, k ;
    doublereal **A ;
    doublereal **x ;
    doublereal **y ;

    m = Ah->m ; n = Ah->n ; s = xh->n ;
    A = Ah->A ; x = xh->A ; y = yh->A ;
    // y = x(1)*A(:,1) + sum_{j}( x(j)*A(:,j) )
    for ( k=1 ; k <= s ; k++){
        for ( i=1 ; i <= m ; i++){
            y[k][i] = A[1][i] * x[k][1] ;
        }
        for ( j=2 ; j <= n ; j++){
            for ( i=1 ; i < j ; i++){
                // i < j, A(i,j) = A(j,i)
                y[k][i] += A[i][j] * x[k][j] ;
            }
            for ( i=j ; i <= m ; i++){
                y[k][i] += A[j][i] * x[k][j] ;
            }
        } // for each col-j
    } // for each vector x(:,k)
}
```

# OutLine

- Data structure of lower triangle matrix
- Function overloading in C++
- Implementation of  $PAP' = LDL'$



## Function overloading in C++

- C++ enables several functions fo the **same name** to be defined, as long as these functions have different sets of parameter
  - (1) parameter type
  - (2) number of parameters
  - (3) order of parameter type
- when an overloaded function is called, the C++ compiler selects the proper function by examining (1) number (2) types (3) order of the arguments in the call.
- the only one function which cannot be overloaded is "main" since it is the entry point.
- Advantage: overloading functions that perform closely related tasks can make programs more readable

# Function overloading of matrix data type

## 1 constructor

```
void zeros( matrixHandler * , integer m, integer n, orderVar sel ) ;  
void zeros( int_matrixHandler * , integer m, integer n, orderVar sel ) ;  
void zeros( lowerTriangleMatrixHandler* , integer m, integer n, orderVar sel, int isSym ) ;
```

## 2 destructor

```
void dealloc( matrixHandler Ah ) ;  
void dealloc( int_matrixHandler Ah ) ;  
void dealloc( lowerTriangleMatrixHandler Ah ) ;
```

## 3 I/O

```
void disp( matrixHandler Ah , ostream& out ) ;  
void disp( int_matrixHandler Ah, ostream& out ) ;  
void disp( lowerTriangleMatrixHandler Ah, ostream& out ) ;
```

## 4 metric

```
doublereal norm( matrixHandler Ah, matrix_keyword p ) ;  
doublereal norm( lowerTriangleMatrixHandler Ah, matrix_keyword p ) ;
```

•  
•  
•

# OutLine

- Data structure of lower triangle matrix
- Function overloading in C++
- Implementation of  $PAP' = LDL'$

# Algorithm ( $PAP' = LDL'$ , partial pivot ) [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  $A^{(1)} := A$ ,  ~~$L^{(0)} = I$~~ ,  $P^{(0)} = (1, 2, 3, \dots, n)$  and  $pivot = zero(n)$ ,  $\alpha = \frac{1 + \sqrt{17}}{8} \approx 0.6404$

```

int bunch_kaufman( lowerTriangleMatrixHandler Ah, int_matrixHandler Ph,
                  int_matrixHandler pivoth, doublereal alpha )
{
    .
    .
    .

    assert( Ah ) ; assert( Ph ) ; assert( pivoth ) ;
    assert( COL_MAJOR == Ah->sel ) ;
    assert( COL_MAJOR == Ph->sel ) ;
    assert( COL_MAJOR == pivoth->sel ) ;

    m = Ah->m ; n = Ah->n ;
    assert( m == n ) ;
    assert( 0 != Ah->isSym ) ; // A must be symmetric matrix

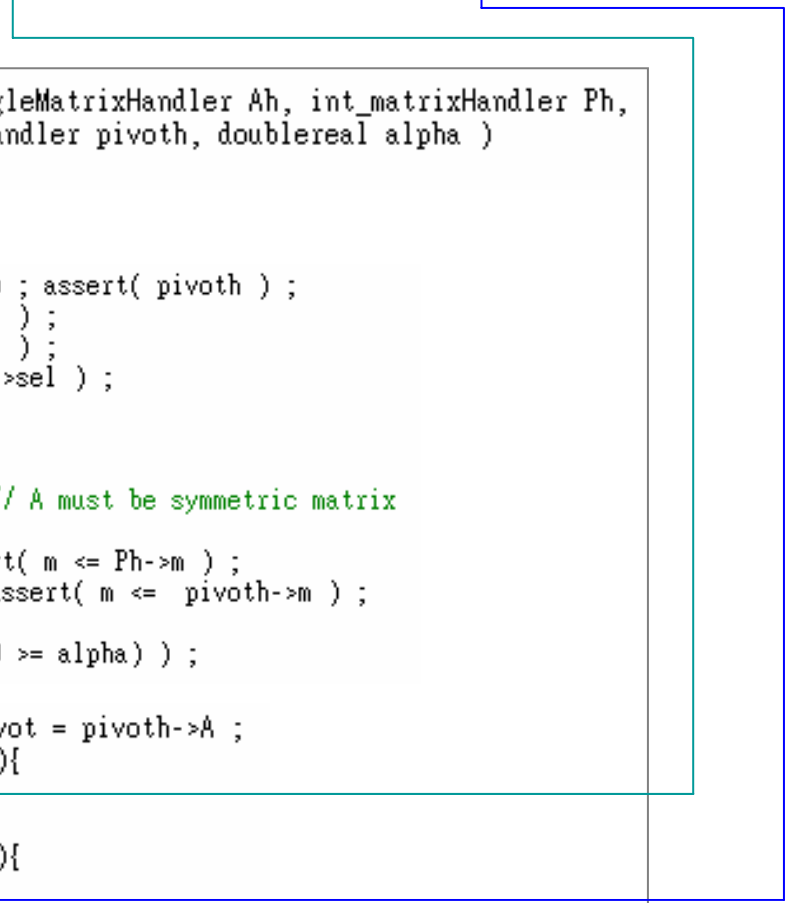
    assert( 1 == Ph->n ) ; assert( m <= Ph->m ) ;
    assert( 1 == pivoth->n ) ; assert( m <= pivoth->m ) ;

    assert( (0 <= alpha) && (1.0 >= alpha) ) ;

    A = Ah->A ; P = Ph->A ; pivot = pivoth->A ;
    for ( i = 1 ; i <= n ; i++){
        P[1][i] = i ;
    }
    for ( i = 1 ; i <= n ; i++){
        pivot[1][i] = 0 ;
    }
}

```

verification



## Algorithm ( $PAP' = LDL'$ , partial pivot ) [2]

(1) we store lower triangle matrix  $L$  and block diagonal matrix  $D$  into storage of matrix  $A$

(2) permutation matrix  $P$  and pivot sequence  $pivot$  are of type *int\_matrix*

$k = 1$

**while**  $k \leq (n-1)$

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

$$A^{(k)} = \left( \begin{array}{ccc|ccc} D_1 & 0 & \dots & 0 & \dots & 0 \\ 0 & \ddots & & & & \\ \vdots & & D_s & \dots & \dots & 0 \\ \hline \vdots & & 0 & a_{k,k}^{(k)} & \dots & a_{n,k}^{(k)} \\ \vdots & & \vdots & \vdots & & \vdots \\ 0 & \dots & 0 & a_{n,k}^{(k)} & \dots & a_{nn}^{(k)} \end{array} \right) \quad \text{update original matrix } A, \text{ where } D_i : 1 \times 1 \text{ or } 2 \times 2$$

$$L^{(k-1)} = \left( \begin{array}{c|c} \overbrace{\left( \begin{array}{c|c} W & O \\ \hline M & I \end{array} \right)}^{k-1} & \end{array} \right) \} k-1 \quad \text{combines all lower triangle matrix and store in } L$$

# Algorithm ( PAP' = LDL', partial pivot ) [3]

1 compute  $\lambda_1 = \max_{k+1 \leq j \leq n} |A_{j1}| = |A_{r1}|, \quad r \geq k$

```

// step 1: compute lambda_1 = max{|a(j,k)|: k+1<=j<=n}
lambda_1 = 0.0 ;
for( i = k ; i <= n ; i++ ){
    tmp = fabs( A[k][i] ) ;
    if ( tmp > lambda_1 ){
        lambda_1 = tmp ;
        r = i ;
    }
}
// for each row
    
```

```

53 % step 1: compute lambda_1 = max(|a(j,k)|: k+1<=j<=n)
54 %
55 [lambda_1, j] = max( abs(A(k:n,k)) ) ;
56 r = k + j - 1 ;
    
```

Case 1:  $|a_{kk}| \geq \alpha \lambda_1$  1x1 pivot no interchange

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

$$\left\{ \begin{array}{l} L(k+1:n, k) \leftarrow c/a_{kk}^{(k)} \\ A(k+1:n, k+1:n) - = cc^T/a_{kk}^{(k)} \end{array} \right. \quad \text{then } A = L^{(k-1)} L^{(k)} A^{(k+1)} L^{(k)} (L^{(k-1)})^T$$

**Technique problem:** if we store  $L$  into memory block of  $A$ , then  $L(k+1:n, k)$  will overwrite  $c = A(k+1:n, k)$  such that  $A(k+1:n, k+1:n) - = cc^T/a_{kk}^{(k)}$  fails. We use a temporary storage  $L(1:n, 2)$

# Algorithm ( $PAP' = LDL'$ , partial pivot ) [4]

do 1x1 pivot :

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

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

```

78 % step 2: do 1x1 pivot,
79 %   L(k+1:n, k ) <-- c/A(k,k)
80 %   A(k+1:n, k+1:n) -= c*c'/A(k,k)
81 %
82   L(k+1:n, k      ) = A(k+1:n,k)/A(k,k) ;
83   A(k+1:n, k+1:n) = A(k+1:n, k+1:n) - L(k+1:n,k)*A(k+1:n,k)' ;
84   A(k+1:n, k      ) = zero_vec(k+1:n) ;
85

```

```

matrixHandler Lh ;
double real **L ;

zeros( &Lh, n, 2, COL_MAJOR );
L = Lh->A ;

//   L(k+1:n, k      ) = A(k+1:n,k)/A(k,k) ;
//   a_kk = A[k][k] ;
//   for( i = k+1 ; i <= n ; i++){
//       L[1][i] = A[k][i] / a_kk ;
//   }
//   A(k+1:n, k+1:n) = A(k+1:n, k+1:n) - L(k+1:n,k)*A(k+1:n,k)'
// remember: only update lower triangle part
//   for (j = k+1 ; j <= n ; j++){
//       tmp = A[k][j] ; // A(k,j) = A(j,k)
//       for( i = j ; i <= n ; i++){
//           A[j][i] -= L[1][i] * tmp ;
//       } // for each row ;
//   } // for each column
// store L into A
//   for( i = k+1 ; i <= n ; i++){
//       A[k][i] = L[1][i] ;
//   }

```

We must update lower triangle part of matrix **A** only.

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

```
// step 3: update k <- k+1 and pivot(k) = 1
    pivot[1][k] = 1 ;
    k = k+1 ;
```

```
86 %
87 % step 3: update k <- k+1 and pivot(k) = 1
88 %
89     pivot(k) = 1 ;
90     k = k+1 ;
```

When case 1 is not satisfied, we compute

$$\lambda_r \equiv \max_{j \neq r} |a_{j,r}| = \text{maximum of off-diagonal elements in column } r$$

```
// step 4: find lambda_r = maximum of off-diagonal of col-r
// r < n : lambda_r = max( max(abs(A(r,k:r-1))), max(abs(A(r+1:n,r))) )
// r = n : lambda_r = max(abs(A(r,k:r-1)))
    lambda_r = 0.0 ;
    for( j = k ; j < r ; j++ ){
        tmp = fabs( A[j][r] ) ;
        if ( tmp > lambda_r ){
            lambda_r = tmp ;
        }
    }
    // for each column
    if ( r < n ){
        for( i = r+1 ; i <= n ; i++ ){
            tmp = fabs( A[r][i] ) ;
            if ( tmp > lambda_r ){
                lambda_r = tmp ;
            }
        }
    }
    // for each column
// if ( r < n )
```

```
%
% step 4: find lambda_r = maximum of off-diagonal of col-r
%
% if ( r < n )
%     lambda_r = max( max(abs(A(r,k:r-1))), max(abs(A(r+1:n,r))) ) ;
% else
%     lambda_r = max(abs(A(r,k:r-1))) ;
% end
```





# Algorithm ( $PAP' = LDL'$ , partial pivot ) [7]

Case 3:  $|a_{rr}| \geq \alpha \lambda_r$     1×1 pivot    do interchange

define permutation  $P = (1:k-1, r, k+1:r-1, k, r+1:n)$  to do symmetric permutation

7  $P(k) \leftrightarrow P(r)$

```

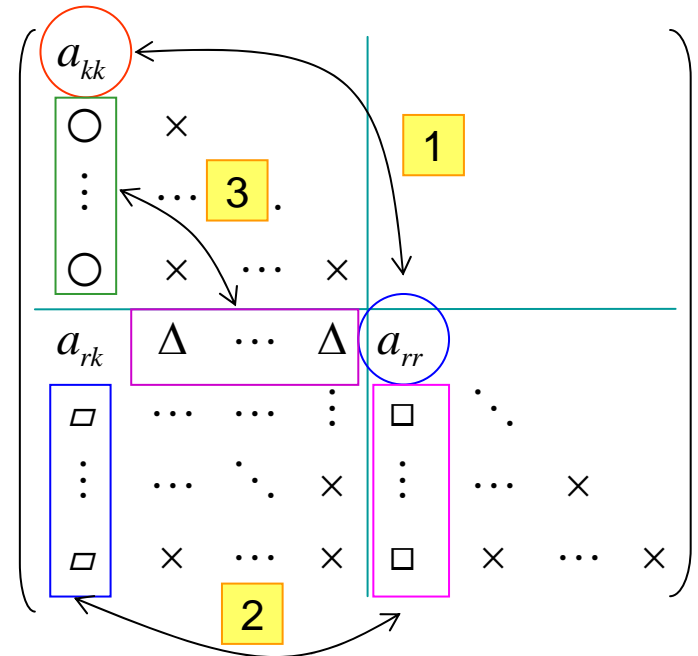
int_tmp = P[1][k] ;
P[1][k] = P[1][r] ;
P[1][r] = int_tmp ;
    
```

```

tmp = P(k) ;
P(k) = P(r) ;
P(r) = tmp ;
    
```

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

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



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

```
//
// step 8: compute A_tilda_{k} = P_{k} * A_{k} * (P_{k})'
// (1) A(k,k) <--> A(r, r)
    tmp      = A[k][k] ;
    A[k][k]  = A[r][r] ;
    A[r][r]  = tmp ;
// (2) A(r+1:n, k) <--> A(r+1:n, r)
    for ( i = r+1 ; i <= n ; i++ ){
        tmp      = A[r][i] ;
        A[r][i]  = A[k][i] ;
        A[k][i]  = tmp ;
    }
// (3) A(k+1:r-1, k) <--> A(r, k+1:r-1)
    for ( i = k+1 ; i < r ; i++){
        tmp      = A[k][i] ;
        A[k][i]  = A[i][r] ;
        A[i][r]  = tmp ;
    }
```

```
145 %
146 % step 8: compute A_tilda_{k} = P_{k} * A_{k} * (P_{k})'
147 % (1) A(k,k) <--> A(r, r)
148 % (2) A(r+1:n, k) <--> A(r+1:n, r)
149 % (3) A(k+1:r-1, k) <--> A(r, k+1:r-1)
150 %
151     tmp      = A(k,k) ;
152     A(k,k)  = A(r,r) ;
153     A(r,r)  = tmp ;
154
155     tmp(r+1:n) = A(r+1:n, r) ;
156     A(r+1:n, r) = A(r+1:n, k) ;
157     A(r+1:n, k) = tmp(r+1:n) ;
158
159     tmp_vec(k+1:r-1) = A(k+1:r-1, k) ;
160     A(k+1:r-1, k) = A(r, k+1:r-1)' ;
161     A(r, k+1:r-1) = tmp_vec(k+1:r-1)' ;
162
```

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

# Algorithm ( $PAP' = LDL'$ , partial pivot ) [9]

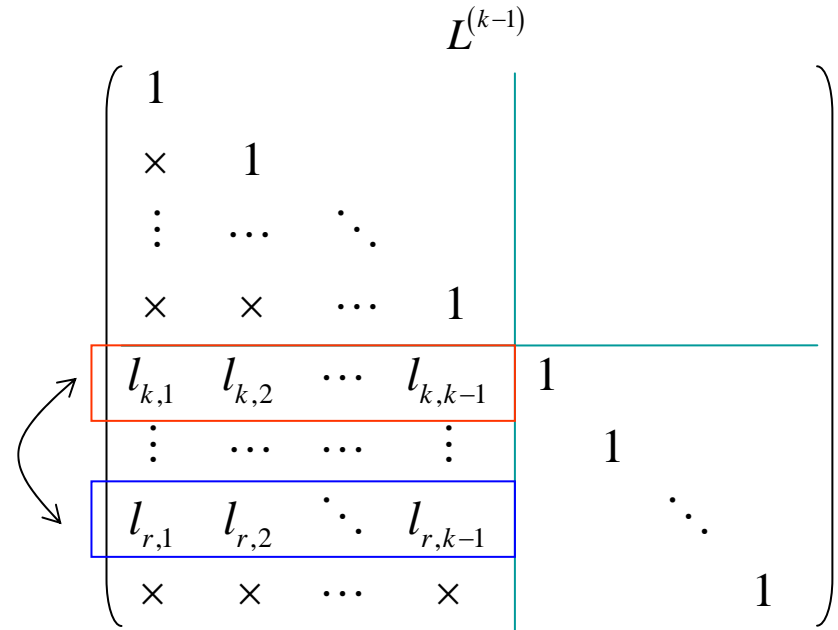
To compute  $\tilde{L}^{(k-1)} = P_k L^{(k-1)} P_k^T$

9 We only update lower triangle matrix  $L$

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

then

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



```

//
// step 9: compute L_tilda_{k} = P_{k} * L_{k} * (P_{k})'
-//   L(k, 1:k-1) <--> L(r, 1:k-1)
    if ( 1 < k ){
        for ( j = 1 ; j < k ; j++){
            tmp = A[j][k] ;
            A[j][k] = A[j][r] ;
            A[j][r] = tmp ;
        }
    }
-// if ( k > 1)
    
```

```

163 %
164 % step 9: compute L_tilda_{k} = P_{k} * L_{k} * (P_{k})'
165 %   L(k, 1:k-1) <--> L(r, 1:k-1)
166 %
167     if ( k > 1 )
168         tmp_vec(1:k-1) = L(k,1:k-1)' ;
169         L(k, 1:k-1)     = L(r, 1:k-1) ;
170         L(r, 1:k-1)     = tmp_vec(1:k-1)' ;
171     end
    
```

we store lower triangle matrix  $L$  into storage of matrix  $A$

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

$\left\{ \begin{array}{l} L(k+1:n, k) \leftarrow c/a_{kk}^{(k)} \\ A(k+1:n, k+1:n) \leftarrow B - cc^T/a_{kk}^{(k)} \end{array} \right.$  then  $P^{(k)} A (P^{(k)})^T = \tilde{L}^{(k-1)} L^{(k)} A^{(k+1)} (L^{(k)})^T (\tilde{L}^{(k-1)})^T$

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

The same as code in case 1

Case 4:  $|a_{rr}| < \alpha \lambda_r$  2x2 pivot do interchange

define permutation  $P = (1:k, r, k+2:r-1, k+1, r+1:n)$ , change  $a_{rk}$  to  $a_{k+1,k}$

12  $P(k+1) \leftrightarrow P(r)$

```
int_tmp = P[1][k+1] ;
P[1][k+1] = P[1][r] ;
P[1][r] = int_tmp ;
```

```
tmp = P(k+1) ;
P(k+1) = P(r) ;
P(r) = tmp ;
```

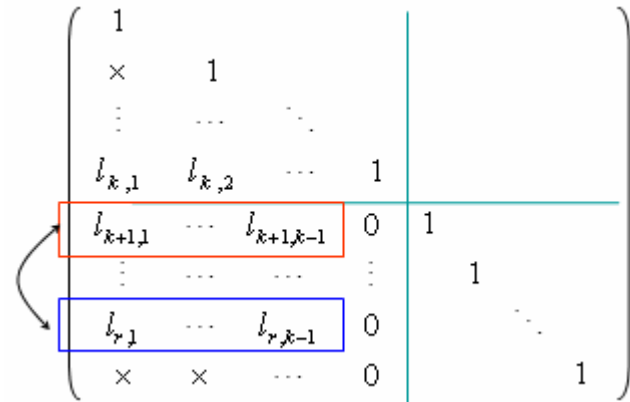


14 do interchange row  $k+1 \leftrightarrow r$

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

then

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



```

// to compute L_tilda_{k} = P_{k} * L_{k} * (P_{k})'
    if ( k > 1){
% // step 14: do interchange row k+1 <--> r
-//      L(k+1, 1:k-1) <--> L(r, 1:k-1)
        for ( j = 1 ; j < k ; j++ ){
            tmp = A[j][k+1] ;
            A[j][k+1] = A[j][r] ;
            A[j][r] = tmp ;
        }
    } // if ( k > 1)
    
```

```

    if ( k > 1 )
%
% step 14: do interchange row k+1 <--> r
%      L(k+1, 1:k-1) <--> L(r, 1:k-1)
%
        tmp_vec(1:k-1) = L(k+1,1:k-1)' ;
        L(k+1 , 1:k-1) = L(r , 1:k-1) ;
        L(r , 1:k-1) = tmp_vec(1:k-1)' ;
    end % if ( k > 1 )
    
```

15

do 2x2 pivot :

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

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

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

$$\text{do 2x2 pivot : } \begin{cases} L(k+2:n, k:k+1) \leftarrow cE^{-1} \\ A(k+2:n, k+2:n) \leftarrow cE^{-1}c^T \end{cases}$$

```
// compute inv(E)
detE = A[k][k] * A[k+1][k+1] - A[k][k+1]*A[k+1][k] ;
invE_11 = A[k+1][k+1] / detE ;
invE_22 = A[k][k] / detE ;
invE_12 = -A[k][k+1] / detE ;
invE_21 = invE_12 ;
// L(k+2:n, k:k+1) = A(k+2:n, k:k+1)*inv(E) ;
for ( i = k+2 ; i <= n ; i++ ){
    L[1][i] = A[k][i] * invE_11 + A[k+1][i]* invE_21 ;
    L[2][i] = A[k][i] * invE_12 + A[k+1][i]* invE_22 ;
}
// A(k+2:n, k+2:n) = A(k+2:n, k+2:n) - L(k+2:n, k:k+1)* (A(k+2:n, k:k+1)') ;
for ( j = k+2 ; j <= n ; j++){
    for ( i = j ; i <= n ; i++){
        A[j][i] -= L[1][i] * A[k][j] + L[2][i] * A[k+1][j] ;
    } // for each row
} // for each col
// store L into A
for ( i = k+2 ; i <= n ; i++ ){
    A[k ][i] = L[1][i] ;
    A[k+1][i] = L[2][i] ;
}
```

$$E = \begin{pmatrix} a_{k,k} & a_{k+1,k} \\ a_{k+1,k} & a_{k+1,k+1} \end{pmatrix}$$

$$E^{-1} = \frac{1}{\det E} \begin{pmatrix} a_{k+1,k+1} & -a_{k+1,k} \\ -a_{k+1,k} & a_{k,k} \end{pmatrix}$$

```
%
% step 15: do 2x2 pivoting
%
E(1,1) = A(k , k) ;
E(2,1) = A(k+1, k) ;
E(1,2) = E(2,1) ;
E(2,2) = A(k+1,k+1) ;

L(k+2:n, k:k+1) = A(k+2:n, k:k+1)*inv(E) ;
A(k+2:n, k+2:n) = A(k+2:n, k+2:n) - L(k+2:n, k:k+1) * (A(k+2:n, k:k+1)') ;
A(k+2:n, k ) = zero_vec(k+2:n) ;
A(k+2:n, k+1) = zero_vec(k+2:n) ;
```



16  $k \leftarrow k+2$  and  $\text{pivot}(k) = 2$

```
// step 16: update pivot(k) = 2 and k <-- k+2
    pivot[1][k] = 2 ;
    k = k + 2 ;
```

```
%
% step 16: update pivot(k) = 2 and k <-- k+2
%
    pivot(k) = 2 ;
    k = k + 2 ;
```

*endwhile*

```
// terminatin condition for pivot array
// when k = n-1, do 1x1 pivoting, after leaving while loop, pivot(n) = 0,
-// we must correct pivot(n) = 1 (implicit 1x1 pivoting)
    if ( 0 == pivot[1][n] ){
        if ( 1 == pivot[1][n-1] ){
            pivot[1][n] = 1 ;
        }
    }
}
```

```
% terminatin condition for pivot array
% when k = n-1, do 1x1 pivoting, after leaving while loop, pivot(n) = 0,
% we must correct pivot(n) = 1 (implicit 1x1 pivoting)
%
if ( 0 == pivot(n) )
    if ( 1 == pivot(n-1) )
        pivot(n) = 1 ;
    end
end
```

## Example: partial pivot

$$A = \begin{pmatrix} 6 & 12 & 3 & -6 \\ 12 & -8 & -13 & 4 \\ 3 & -13 & -7 & 1 \\ -6 & 4 & 1 & 6 \end{pmatrix} \quad \alpha = \frac{1 + \sqrt{17}}{8}$$

Bunch-Kaufman (partial pivot)

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

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

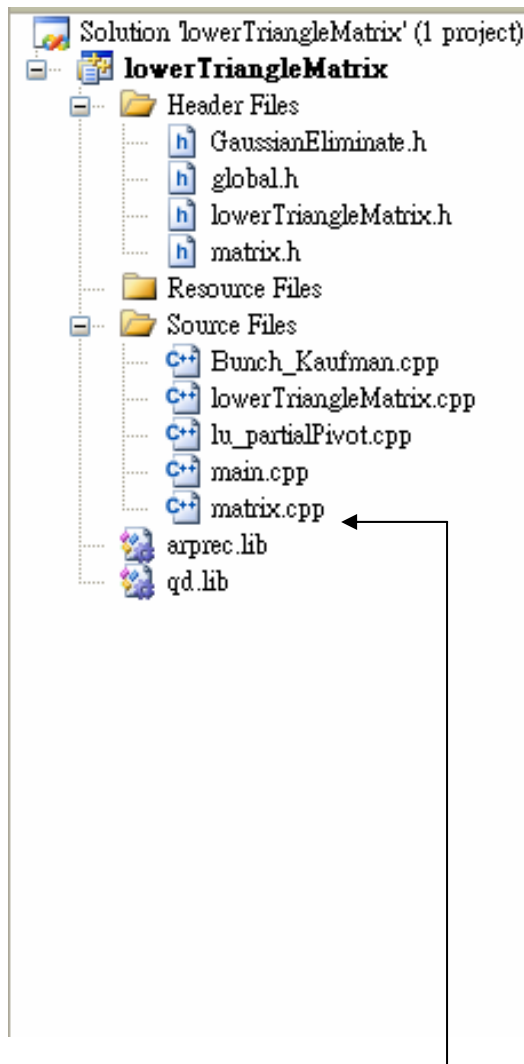
$$L = \begin{pmatrix} 1 & & & \\ & 1 & & \\ 0 & -0.5 & 1 & \\ -0.6875 & 0.5938 & -0.6875 & 1 \end{pmatrix}$$

$$D = \begin{pmatrix} 6 & & & \\ 12 & -8 & & \\ & & 8 & \\ & & & -1 \end{pmatrix}$$

$$L + D \rightarrow mem(A) = \begin{pmatrix} 6 & & & \\ 12 & -8 & & \\ 0 & -0.5 & 8 & \\ -0.6875 & 0.5938 & -0.6875 & -1 \end{pmatrix}$$

## driver for example [1]

main.cpp



```
#include "global.h"
#include <stdio.h>
#include "lowerTriangleMatrix.h"
#include "GaussianEliminate.h"

void test_BunchKaufman( void );

int main( int argc, char* argv[] )
{
#ifdef HIGH_PRECISION_PACKAGE
    unsigned int old_cw;
    fpu_fix_start(&old_cw);
#endif

#ifdef DO_ARPREC
    mp::mp_init(ARPREC_NDIGITS);
#endif

    // ----- main code -----

    test_BunchKaufman();

    // ----- end main code -----

#ifdef DO_ARPREC
    mp::mp_finalize();
#endif

#ifdef HIGH_PRECISION_PACKAGE
    fpu_fix_end(&old_cw);
#endif
    return 0 ;
}
```

Test example

We need full matrix representation of  $x, b$  of linear system  $Ax = b$  and permutation matrix  $P$ , pivot sequence *pivot*

## driver for example [2]

```
void test_BunchKaufman( void )
{
    integer m = 4 ;
    integer n = 4 ;
    lowerTriangleMatrixHandler Ah ;
    lowerTriangleMatrixHandler Ah_dup;
    int_matrixHandler Ph ;
    int_matrixHandler pivoth ;
    matrixHandler bh ;
    matrixHandler xh ; // x = inv(A)*b
    matrixHandler bh_hat ; // b_hat = A*x
    matrixHandler rh ; // residual r = b - Ax
    doublereal r_supnorm ;
    int isSingular ;
    doublereal **A ;
    doublereal **b ;
    doublereal alpha ;

    zeros( &Ah, m, n, COL_MAJOR, 1 ) ;
    A = Ah->A ;

    A[1][1] = 6. ; A[1][2] = 12. ; A[1][3] = 3. ; A[1][4] = -6. ;
                A[2][2] = -8. ; A[2][3] = -13. ; A[2][4] = 4. ;
                A[3][3] = -7. ; A[3][4] = 1. ;
                A[4][4] = 6. ;

    cout << "configuration of matrix A" << endl ;
    disp( Ah, cout ) ;

    zeros( &Ah_dup, m, n, COL_MAJOR, 1 ) ;
    duplicate( Ah, Ah_dup ) ;

    zeros( &Ph, m, 1, COL_MAJOR ) ;
    zeros( &pivoth, m, 1, COL_MAJOR ) ;
    alpha = (1.0 + sqrt(17.0))/8.0 ;
    // step 2: factorization, PAP' = LDL'
    cout.precision(4) ;
    cout << std::fixed ;
    isSingular = bunch_kaufman_v2( Ah, Ph, pivoth, alpha ) ;

    cout << "\nPAP' = LDL' : store L and D into A: with alpha = " << alpha << endl ;
    disp( Ah, cout ) ;

    cout << "\npermutation matrix P:\n" ;
    disp( Ph, cout ) ;

    cout << "\npivot matrix pivot:\n" ;
    disp( pivoth, cout ) ;
}
```

|         |        |         |    |
|---------|--------|---------|----|
| 6       |        |         |    |
| 12      | -8     |         |    |
| 0       | -0.5   | 8       |    |
| -0.6875 | 0.5938 | -0.6875 | -1 |

C:\WINDOWS\system32\cmd.exe

configuration of matrix A

dimension of symmetric matrix is (4,4) with col-major

```
6.0000
12.0000 -8.0000
3.0000 -13.0000 -7.0000
-6.0000 4.0000 1.0000 6.0000
```

PAP' = LDL' : store L and D into A: with alpha = 0.6404

dimension of symmetric matrix is (4,4) with col-major

```
6.0000
12.0000 -8.0000
-0.0000 -0.5000 8.0000
-0.6875 0.5938 -0.6875 -1.0000
```

permutation matrix P:

dimension of matrix is (4,1) with col-major

```
1
2
4
3
```

pivot matrix pivot:

dimension of matrix is (4,1) with col-major

```
2
0
1
1
```

# Report

- Implement PAP' = LDL' and linear solver in C/C++
- describe program structure
- How to verify your program
- Comparison with MATLAB implementation
- Memory usage (do you need extra storage?)
- Speedup strategy