# Unit 1.2 Special Matrices

Numerical Analysis

EE/NTHU

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Numerical Analysis (EE/NTHU)

Unit 1.2 Special Matrices

## Cholesky Decomposition

- A special case of the matrix factorization
- Matrix A needs to be symmetric and positive definite

$$\mathbf{A} = \mathbf{A}^T \tag{1.2.1}$$

$$\mathbf{x}^T \mathbf{A} \mathbf{x} > 0$$
, for any  $\mathbf{x} \neq \mathbf{0}$ . (1.2.2)

Then we can factorize A to

$$\mathbf{A} = \mathbf{L}\mathbf{L}^T. \tag{1.2.3}$$

where  ${f L}$  is a lower triangular matrix, i.e.,  $\ell_{ij}=0$ , if j>i.

For example

$$\begin{bmatrix} a_{11} & a_{21} & a_{31} \\ a_{21} & a_{22} & a_{32} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} \ell_{11} & 0 & 0 \\ \ell_{21} & \ell_{22} & 0 \\ \ell_{31} & \ell_{32} & \ell_{33} \end{bmatrix} \begin{bmatrix} \ell_{11} & \ell_{21} & \ell_{31} \\ 0 & \ell_{22} & \ell_{32} \\ 0 & 0 & \ell_{33} \end{bmatrix}$$

## Cholesky Decomposition – Example

$$\begin{bmatrix} a_{11} & a_{21} & a_{31} \\ a_{21} & a_{22} & a_{32} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} \ell_{11} & 0 & 0 \\ \ell_{21} & \ell_{22} & 0 \\ \ell_{31} & \ell_{32} & \ell_{33} \end{bmatrix} \begin{bmatrix} \ell_{11} & \ell_{21} & \ell_{31} \\ 0 & \ell_{22} & \ell_{32} \\ 0 & 0 & \ell_{33} \end{bmatrix}$$

$$a_{11} = \ell_{11}\ell_{11}$$

$$a_{21} = \ell_{11}\ell_{21}$$

$$a_{31} = \ell_{11}\ell_{31}$$

$$a_{22} = \ell_{22}\ell_{22} + \ell_{21}\ell_{21}$$

$$a_{32} = \ell_{31}\ell_{21} + \ell_{22}\ell_{32}$$

$$a_{33} = \ell_{31}\ell_{31} + \ell_{32}\ell_{32} + \ell_{33}\ell_{33}$$

$$\ell_{11} = \sqrt{a_{11}}$$

$$\ell_{21} = a_{21}/\ell_{11}$$

$$\ell_{21} = a_{31}/\ell_{11}$$

$$\ell_{22} = \sqrt{a_{22} - \ell_{21}\ell_{21}}$$

$$\ell_{22} = \sqrt{a_{22} - \ell_{21}\ell_{21}}$$

$$\ell_{32} = (a_{32} - \ell_{31}\ell_{21})/\ell_{22}$$

$$\ell_{33} = \sqrt{a_{33} - \ell_{31}\ell_{31} - \ell_{32}\ell_{32}}$$

- Note that the number of variables in Cholesky decomposition is smaller than LU decomposition
  - Cholesky is 2X faster than LU decomposition

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## Cholesky Decomposition - Properties

#### Theorem 1.2.1

For any positive definite (symmetric) matrix A the matrix  $A^{-1}$  exists and is also positive definite. All principal submatrices of a positive definite matrix is also positive definite, and all principal minors of a positive definite matrix are positive.

- If  $\mathbf{x} \neq \mathbf{0}$ ,  $\mathbf{x}^T \mathbf{A} \mathbf{x} > 0$ , thus  $\mathbf{A} \mathbf{x} \neq \mathbf{0}$ , and  $\mathbf{A}^{-1}$  exists.
- ullet Let  $\mathbf{y} = \mathbf{A}\mathbf{x}$  then

$$\mathbf{y}^T \mathbf{A}^{-1} \mathbf{y} = \mathbf{x}^T \mathbf{A} \mathbf{A}^{-1} \mathbf{A} \mathbf{x} = \mathbf{x}^T \mathbf{A} \mathbf{x} > 0.$$

• Partition  $\mathbf{x}$  to  $\begin{bmatrix} \mathbf{x}_1 & \mathbf{x}_2 \end{bmatrix}$ , where  $\mathbf{x}_2$  corresponds to the principal submatrix and  $\mathbf{x}_1$  is not. Then since  $\mathbf{x}^T \mathbf{A} \mathbf{x} > \mathbf{0}$ ,  $\mathbf{y} = \begin{bmatrix} \mathbf{0} & \mathbf{x}_2 \end{bmatrix}$  we also have  $\mathbf{y}^{-1} \mathbf{A} \mathbf{y} > \mathbf{0}$ .

#### Theorem 1.2.2

For any positive definite symmetric matrix  $\mathbf{A}$  there is a unique lower triangular matrix  $\mathbf{L}$ ,  $\ell_{ii}=0$  if i>i, with  $\ell_{ii}>0$ , such that  $\mathbf{A}=\mathbf{L}\mathbf{L}^T$ .

ullet Note that this theorem also holds if  ${f A}$  is Hermitian,  ${f A}={f A}^H$  then  ${f A}={f L}{f L}^H.$ 

## Cholesky Decomposition – Algorithm

- In-place Cholesky decomposition
  - ullet Only lower triangle of  ${f A}$  is affected
  - Forward and backward substitutions need to modified accordingly

#### gorithm 1.2.3. Cholesky Decomposition

```
void Cholesky(double A[n][n])
01
02
    {
03
       int i, j, k;
04
05
       for (i=0; i<n; i++) {
          A[i][i]=sqrt(A[i][i]);
06
          for (j=i+1; j<n; j++) {
07
              A[j][i] /= A[i][i];
80
09
          for (j=i+1; j<n; j++) {
10
              for (k=i+1; k<=j; k++)
11
12
                 A[j][k] -= A[j][i]*A[k][i];
          }
13
14
       }
15
   }
```

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## $\mathbf{LDL}^T$ Decomposition

• For symmetric positive definite matrices it is also possible to decompose matrix A into the following form:

$$\mathbf{A} = \mathbf{L}\mathbf{D}\mathbf{L}^{T}.\tag{1.2.4}$$

Where  ${f L}$  is a lower triangle matrix with  ${f 1}$ 's on the diagonal and  ${f D}$  is a diagonal matrix.

For example

$$\begin{bmatrix} a_{11} & a_{21} & a_{31} \\ a_{21} & a_{22} & a_{32} \\ a_{31} & a_{32} & a_{33} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 \\ \ell_{21} & 1 & 0 \\ \ell_{31} & \ell_{32} & 1 \end{bmatrix} \begin{bmatrix} d_{11} & 0 & 0 \\ 0 & d_{22} & 0 \\ 0 & 0 & d_{33} \end{bmatrix} \begin{bmatrix} 1 & \ell_{21} & \ell_{31} \\ 0 & 1 & \ell_{32} \\ 0 & 0 & 1 \end{bmatrix}$$

$$= \begin{bmatrix} d_{11} & 0 & 0 \\ d_{11}\ell_{21} & d_{22} & 0 \\ d_{11}\ell_{31} & d_{22}\ell_{32} & d_{33} \end{bmatrix} \begin{bmatrix} 1 & \ell_{21} & \ell_{31} \\ 0 & 1 & \ell_{32} \\ 0 & 0 & 1 \end{bmatrix}$$

$$= \begin{bmatrix} d_{11} & d_{11}\ell_{21} & d_{11}\ell_{31} \\ d_{11}\ell_{21} & d_{22} + d_{11}\ell_{21}^2 & \ell_{21}d_{11}\ell_{31} + d_{22}\ell_{32} \\ d_{11}\ell_{31} & \ell_{31}d_{11}\ell_{21} + d_{22}\ell_{32} & d_{11}\ell_{31}^2 + d_{22}\ell_{32}^2 + d_{33} \end{bmatrix}$$

# $\mathbf{LDL}^T$ Decomposition, $\mathsf{II}$

- Decomposition process is similar.
  - In-place decomposition feasible.

#### Requirements:

$$a_{11} = d_{11}$$

$$a_{21} = d_{11}\ell_{21}$$

$$a_{31} = d_{11}\ell_{31}$$

$$a_{22} = d_{22} + d_{11}\ell_{21}^{2}$$

$$a_{32} = \ell_{31}d_{11}\ell_{21} + d_{22}\ell_{32}$$

$$a_{33} = d_{33} + d_{11}\ell_{31}^{2} + d_{22}\ell_{32}^{2}$$

#### Solving unknowns:

$$d_{11} = a_{11}$$

$$\ell_{21} = a_{21}/d_{11}$$

$$\ell_{31} = a_{31}/d_{11}$$

$$d_{22} = a_{22} - d_{11}\ell_{21}^{2}$$

$$\ell_{32} = (a_{32} - \ell_{31}d_{11}\ell_{21})/d_{22}$$

$$d_{33} = a_{33} - d_{11}\ell_{31}^{2} - d_{22}\ell_{32}^{2}$$

#### Two-step process:

$$d_{11} = a_{11}$$

$$\ell_{21} = a_{21}/d_{11}$$

$$\ell_{31} = a_{31}/d_{11}$$

$$a'_{22} = a_{22} - d_{11}\ell_{21}^{2}$$

$$a'_{32} = a_{32} - d_{11}\ell_{31}\ell_{21}$$

$$a'_{33} = a_{33} - d_{11}\ell_{31}^{2}$$

$$d_{22} = a'_{22}$$

$$\ell_{32} = a'_{32}/d_{22}$$

$$a''_{33} = a'_{33} - d_{22}\ell_{32}^{2}$$

$$d_{33} = a_{33}^{"}$$

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#### Banded Matrices

In some applications matrix A is banded

$$a_{ij} = 0,$$
 if  $|i - j| > m.$  (1.2.5)

• For example, m=1

$$\mathbf{A} = \begin{bmatrix} a_{11} & a_{12} & 0 & 0 & 0 \\ a_{21} & a_{22} & a_{23} & 0 & 0 \\ 0 & a_{32} & a_{33} & a_{34} & 0 \\ 0 & 0 & a_{43} & a_{44} & a_{45} \\ 0 & 0 & 0 & a_{54} & a_{55} \end{bmatrix} . \tag{1.2.6}$$

- $\bullet \ 5 \times 5$  tridiagonal matrix is shown.
  - ullet For large n imes n matrices, the elements are mostly zeros
  - Even for m > 1 cases
- We can exploit this property for more efficient solution for both CPU time and matrix storage.

#### Banded Matrices, II

• The matrix shown in Eq. (1.2.6) can be stored using a  $5 \times 3$  array as

$$\mathbf{A}^{T} = \begin{bmatrix} 0 & a_{21} & a_{32} & a_{43} & a_{54} \\ a_{11} & a_{22} & a_{33} & a_{44} & a_{55} \\ a_{12} & a_{23} & a_{34} & a_{45} & 0 \end{bmatrix}.$$
 (1.2.7)

- The storage space reduced to  $5 \times 3$  entries.
- In general, for an m-banded matrix, the storage requirement reduces from  $n \times n$  to  $n \times m$ .
  - When  $n \gg m$ , the saving is very significant.
- The LU factors of a banded matrix is also banded. For example,

$$\begin{bmatrix} a_{11} & a_{12} & 0 & 0 & 0 \\ a_{21} & a_{22} & a_{23} & 0 & 0 \\ 0 & a_{32} & a_{33} & a_{34} & 0 \\ 0 & 0 & a_{43} & a_{44} & a_{45} \\ 0 & 0 & 0 & a_{54} & a_{55} \end{bmatrix} = \begin{bmatrix} 1 & 0 & 0 & 0 & 0 \\ \ell_{21} & 1 & 0 & 0 & 0 \\ 0 & \ell_{32} & 1 & 0 & 0 \\ 0 & 0 & \ell_{43} & 1 & 0 \\ 0 & 0 & 0 & \ell_{54} & 1 \end{bmatrix} \begin{bmatrix} u_{11} & u_{12} & 0 & 0 & 0 \\ 0 & u_{22} & u_{23} & 0 & 0 \\ 0 & 0 & u_{33} & u_{34} & 0 \\ 0 & 0 & 0 & u_{44} & u_{45} \\ 0 & 0 & 0 & 0 & u_{55} \end{bmatrix}$$

$$(1.2.8)$$

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# Banded Matrices, III

- The standard LU decomposition algorithm can be applied to the banded matrices as well.
- Applying in-place LU decomposition to the  $5\times 5$  tridiagonal matrix we get the following sequence.

$$\begin{bmatrix} a_{11} & a_{12} & 0 & 0 & 0 \\ a_{21} & a_{22} & a_{23} & 0 & 0 \\ 0 & a_{32} & a_{33} & a_{34} & 0 \\ 0 & 0 & a_{43} & a_{44} & a_{45} \\ 0 & 0 & 0 & a_{54} & a_{55} \end{bmatrix} \qquad \begin{bmatrix} u_{11} & u_{12} & 0 & 0 & 0 \\ \ell_{21} & u_{22} & u_{23} & 0 & 0 \\ 0 & \ell_{32} & u_{33} & u_{34} & 0 \\ 0 & 0 & 0 & a_{54} & a_{55} \end{bmatrix}$$

$$\begin{bmatrix} u_{11} & u_{12} & 0 & 0 & 0 \\ \ell_{21} & a'_{22} & a_{23} & 0 & 0 \\ 0 & a_{32} & a_{33} & a_{34} & 0 \\ 0 & 0 & a_{43} & a_{44} & a_{45} \\ 0 & 0 & 0 & a_{54} & a_{55} \end{bmatrix} \qquad \begin{bmatrix} u_{11} & u_{12} & 0 & 0 & 0 \\ \ell_{21} & u_{22} & u_{23} & 0 & 0 \\ 0 & \ell_{32} & u_{33} & u_{34} & 0 \\ 0 & 0 & \ell_{43} & u_{44} & u_{45} \\ 0 & 0 & 0 & \ell_{54} & a'_{55} \end{bmatrix}$$

$$\begin{bmatrix} u_{11} & u_{12} & 0 & 0 & 0 \\ \ell_{21} & u_{22} & u_{23} & 0 & 0 \\ 0 & \ell_{32} & a'_{33} & a_{34} & 0 \\ 0 & 0 & a_{43} & a_{44} & a_{45} \\ 0 & 0 & 0 & a_{54} & a_{55} \end{bmatrix} \qquad \begin{bmatrix} u_{11} & u_{12} & 0 & 0 & 0 \\ \ell_{21} & u_{22} & u_{23} & 0 & 0 \\ 0 & \ell_{32} & u_{33} & u_{34} & 0 \\ 0 & 0 & \ell_{43} & u_{44} & u_{45} \\ 0 & 0 & 0 & \ell_{43} & u_{44} & u_{45} \\ 0 & 0 & 0 & \ell_{43} & u_{44} & u_{45} \\ 0 & 0 & 0 & \ell_{43} & u_{44} & u_{45} \\ 0 & 0 & 0 & \ell_{43} & u_{44} & u_{45} \\ 0 & 0 & 0 & \ell_{54} & u_{55} \end{bmatrix}$$

#### Banded Matrices, IV

- Note that the LU decomposition does not change the band structure of the matrix
  - This is a property of the LU decomposition
  - Copying the current row to form U-row does not change any zero entry to nonzero
  - Making L-column does not add any nonzero entry, either
  - Updating submatrix only update within the band
- Taking advantage of the band structure, LU factorization can be more efficient
  - Computation complexity  $\mathcal{O}(m^2n)$
  - Compared to  $\mathcal{O}(n^3)$
  - If  $m \ll n$ , the saving can be very significant
  - A large number of real world applications can apply this method

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#### Banded Matrices, V

#### Algorithm 1.2.4. LU Decomposition - Banded Matrix

```
void LUband(double A[n][n],int m)
01
02
03
       int i,j,k;
       for (i=0; i<n; i++) {
04
          // copy a[i][j] to u[i][j] needs no action due to in-place LU
05
          for (j=i+1; j<=i+m && j<n; j++) { // form l[j][i]
06
07
             a[j][i] /= a[i][i];
80
          for (j=i+1; j<=i+m && j<n; j++) { // update lower submatrix
09
             for (k=i+1; k<=i+m && k<n; k++) {
10
                a[j][k] -= a[j][i]*a[i][k];
11
12
13
          }
       }
14
15 }
```

- Forward and backward substitutions need to be modified accordingly
  - Lower computational complexity,  $\mathcal{O}(n)$

#### **Block Matrices**

ullet The LU factorization of a matrix  $oldsymbol{A}$  is effective in solving the linear system using forward and backward substitutions

$$\mathbf{A}\mathbf{x} = \mathbf{b} \tag{1.2.9}$$

$$\mathbf{LUx} = \mathbf{b} \tag{1.2.10}$$

$$\mathbf{L}\mathbf{y} = \mathbf{b} \tag{1.2.11}$$

$$\mathbf{U}\mathbf{x} = \mathbf{y} \tag{1.2.12}$$

where  $\mathbf{y} = \mathbf{L}^{-1}\mathbf{b}$  is the forward substitution, and  $\mathbf{x} = \mathbf{U}^{-1}\mathbf{y}$  is the backward substitution.

• In some applications, the matrix A is partitioned into blocks of submatrices. Example below shows  $n \times n$  matrix A is partitioned into four submatrices

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{bmatrix} \tag{1.2.13}$$

where  ${\bf A}_{11}$  is an  $n_1 \times n_1$  matrix;  ${\bf A}_{22}$  is an  $n_2 \times n_2$  matrix;  ${\bf A}_{12}$  is  $n_1 \times n_2$  and  ${\bf A}_{21}$ is  $n_2 \times n_1$ , with  $n_1 + n_2 = n$ .

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### Block LU Factorization

LU factorization can also be carried out on the block matrix A

$$\mathbf{A} = \begin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{12} \\ \mathbf{A}_{21} & \mathbf{A}_{22} \end{bmatrix} = \begin{bmatrix} \mathbf{L}_{11} & \mathbf{0} \\ \mathbf{L}_{21} & \mathbf{L}_{22} \end{bmatrix} \begin{bmatrix} \mathbf{U}_{11} & \mathbf{U}_{12} \\ \mathbf{0} & \mathbf{U}_{22} \end{bmatrix}$$
(1.2.14)

where  ${f L}_{11}$  and  ${f L}_{22}$  are lower triangular matrices with dimension of  $n_1 imes n_1$  and  $n_2 \times n_2$ , respectively;  $\mathbf{U}_{11}$  and  $\mathbf{U}_{22}$  are upper triangular matrices with similar dimensions.  ${f L}_{21}$  and  ${f U}_{12}$  are not necessarily triangular matrices. Then

$$\mathbf{A}_{11} = \mathbf{L}_{11} \mathbf{U}_{11} \tag{1.2.15}$$

$$\mathbf{A}_{12} = \mathbf{L}_{11} \mathbf{U}_{12} \tag{1.2.16}$$

$$\mathbf{A}_{21} = \mathbf{L}_{21} \mathbf{U}_{11} \tag{1.2.17}$$

$$\mathbf{A}_{12} = \mathbf{L}_{11}\mathbf{U}_{12}$$
 (1.2.16)  
 $\mathbf{A}_{21} = \mathbf{L}_{21}\mathbf{U}_{11}$  (1.2.17)  
 $\mathbf{A}_{22} = \mathbf{L}_{21}\mathbf{U}_{12} + \mathbf{L}_{22}\mathbf{U}_{22}$  (1.2.18)

- ullet Thus,  ${f L}_{11}$  and  ${f U}_{11}$  are found by LU factorizing  ${f A}_{11}.$
- ullet  $U_{12}$  and  $L_{21}$  are obtained by extending the row-copying and column-normalization operations while performing LU factorization on  $A_{11}$ .
- ullet  ${f L}_{22}$  and  ${f U}_{22}$  are the LU factors of the updated  ${f A}_{22}$  submatrix

$$\mathbf{A}_{22} - \mathbf{L}_{21}\mathbf{U}_{12} = \mathbf{L}_{22}\mathbf{U}_{22}.\tag{1.2.19}$$

## Block Matrix Example

Example of a block matrix

- Partitioning of matrices may help in operation or storage efficiency improvements.
- Many practical linear systems have special matrix forms and those matrices can be exploited using different partitions.

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# Block LU Factorization - Bordered Block Diagonal Form

• The same idea can be extended to bordered-block-diagonal form matrices

$$egin{bmatrix} \mathbf{A}_{11} & \mathbf{0} & \mathbf{0} & \cdots & \mathbf{A}_{1m} \ \mathbf{0} & \mathbf{A}_{22} & \mathbf{0} & \cdots & \mathbf{A}_{2m} \ \mathbf{0} & \mathbf{0} & \mathbf{A}_{33} & \cdots & \mathbf{A}_{3m} \ & \ddots & \ddots & \ddots & \ddots & \ddots & \ddots \ \mathbf{A}_{m1} & \mathbf{A}_{m2} & \mathbf{A}_{m3} & \cdots & \mathbf{A}_{mm} \end{bmatrix}$$

ullet L $_{ii}$  and U $_{ii}$  are the LU factors of submatrices  $old A_{ii}$ ,  $1 \leq i \leq m-1$ , and  $old L_{mm}$  and  $\mathbf{U}_{mm}$  are the LU factors of the updated submatrix:

$$\mathbf{A}_{mm} - \sum_{i=1}^{m-1} \mathbf{L}_{mi} \mathbf{U}_{im} = \mathbf{L}_{mm} \mathbf{U}_{mm}. \tag{1.2.20}$$

#### BBDF, II

ullet Thus, one can organize the matrix  ${f A}$  as m matrices

- The LU decomposition of the submatrices  $\mathbf{A}^{(k)}$ ,  $k=1,\ldots,m-1$ , can be done in parallel, and the LU decomposition is carried out on the diagonal blocks,  $\mathbf{A}_{kk}$ , only.
- The LU decomposition of the last block  $A_{mm}$ , however, can only be performed after all other submatrices have been decomposed and it needs to be performed using Eq. (1.2.20).
- Note that each submatrix needs not to have the same dimension.

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### Sparse Matrices

- ullet In many real applications, the matrix  ${f A}$  is sparse, that is, it has many zero entries.
  - The bordered block diagonal matrix in preceding page is a good example of sparse matrix
- During LU decomposition (and forward and backward substitutions) any operations associated with the zero entries should not be performed at all for better efficiency
  - Even check for zero would take time
  - These entries should not be stored also
- Linked list that stores only nonzero entries should be used
- Need double linked list
  - Two next pointers: one for next in row and one for next in column
- Using double linked list for sparse matrix storage and operation has been shown to speed up linear system solution time
  - Full matrix solution time  $\mathcal{O}(n^3)$
  - Sparse matrix solution time  $\mathcal{O}(n^{1.1-1.5})$
  - Very significant saving when n is large

## Summary

- Cholesky decomposition
  - Much faster for symmetric and positive definite matrices
- Banded matrices
  - Even faster due to large number of zero entries,  $\mathcal{O}(m^2n)$ .
- Block matrices
  - Achieving parallel computations.
- Sparse matrices
  - Need linked list data structure.
  - Have been shown to have excellent efficiency,  $\mathcal{O}(n^{1.1-1.5})$ .