Unit 1.2 Special Matrices

Numerical Analysis

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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 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 $\mathbf{x} \neq 0$, $\mathbf{x}^T \mathbf{A} \mathbf{x} > 0$, 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} , $\ell_{ij}=0$ if j>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 ${f A}={f L}{f L}^H.$

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Cholesky Decomposition - Algorithm

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

Algorithm 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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$\mathbf{L}\mathbf{D}\mathbf{L}^T$ 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 1's on the diagonal and ${f D}$ is a diagonal matrix.

For example

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

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

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

$\mathbf{L}\mathbf{D}\mathbf{L}^T$ Decomposition, 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:

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

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

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

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

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

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

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

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

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

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

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

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

$$a'_{21} = a_{21}/d_{11}$$

$$a'_{31} = a_{31}/d_{11}$$

$$a'_{31} = a_{31}/d_{11}$$

$$a'_{31} = a_{31}/d_{11}$$

$$a'_{31} = a_{31}/d_{11}$$

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

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

- 5×5 tridiagonal matrix is shown.
 - For large $n \times n$ 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 5×3 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 5×3 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,

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

$$(1.2.8)$$

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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 5×5 tridiagonal matrix we get the following sequence.

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

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

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

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

 a_{44}

 a_{54}

 a_{45}

 a_{55}

 u_{45}

 u_{55}

0

 ℓ_{54}

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;
04
       for (i=0; i<n; i++) {
05
          // copy a[i][j] to u[i][j] needs no action due to in-place LU
          for (j=i+1; j<i+m && j<n; j++) { // form l[j][i]
06
             a[j][i] /= a[i][i];
07
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
11
                a[j][k] -= a[j][i]*a[i][k];
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

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

$$LUx = b (1.2.10)$$

$$Ly = b \tag{1.2.11}$$

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

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

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

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

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

$$\mathbf{A}_{22} = \mathbf{L}_{21}\mathbf{U}_{12} + \mathbf{L}_{22}\mathbf{U}_{22} \tag{1.2.18}$$

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

$$\mathbf{A}_{11} = \begin{bmatrix} a_{11} & a_{12} & a_{13} \\ a_{21} & a_{22} & a_{23} \\ a_{31} & a_{32} & a_{33} \end{bmatrix}, \mathbf{A}_{12} = \begin{bmatrix} a_{14} & a_{15} \\ a_{24} & a_{25} \\ a_{34} & a_{35} \end{bmatrix},$$

$$\mathbf{A}_{21} = \begin{bmatrix} a_{41} & a_{42} & a_{43} \\ a_{51} & a_{52} & a_{53} \end{bmatrix}, \mathbf{A}_{22} = \begin{bmatrix} a_{44} & a_{45} \\ a_{54} & a_{55} \end{bmatrix}.$$

- 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

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

• \mathbf{L}_{ii} and \mathbf{U}_{ii} are the LU factors of submatrices \mathbf{A}_{ii} , $1 \leq i \leq m-1$, and \mathbf{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

$$egin{aligned} \mathbf{A}^{(1)} &= egin{bmatrix} \mathbf{A}_{11} & \mathbf{A}_{1m} \ \mathbf{A}_{m1} & \mathbf{0} \end{bmatrix} \ \mathbf{A}^{(2)} &= egin{bmatrix} \mathbf{A}_{22} & \mathbf{A}_{2m} \ \mathbf{A}_{m2} & \mathbf{0} \end{bmatrix} \ & \cdots \ \mathbf{A}^{(m-1)} &= egin{bmatrix} \mathbf{A}_{(m-1)(m-1)} & \mathbf{A}_{(m-1)m} \ \mathbf{A}_{m(m-1)} & \mathbf{0} \end{bmatrix} \ \mathbf{A}^{(m)} &= [\mathbf{A}_{mm}] \end{aligned}$$

- 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 $\mathcal{O}(n^{1.1-1.5})$
 - ullet 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.
 - \bullet Have been shown to have excellent efficiency, $\mathcal{O}(n^{1.1-1.5}).$

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