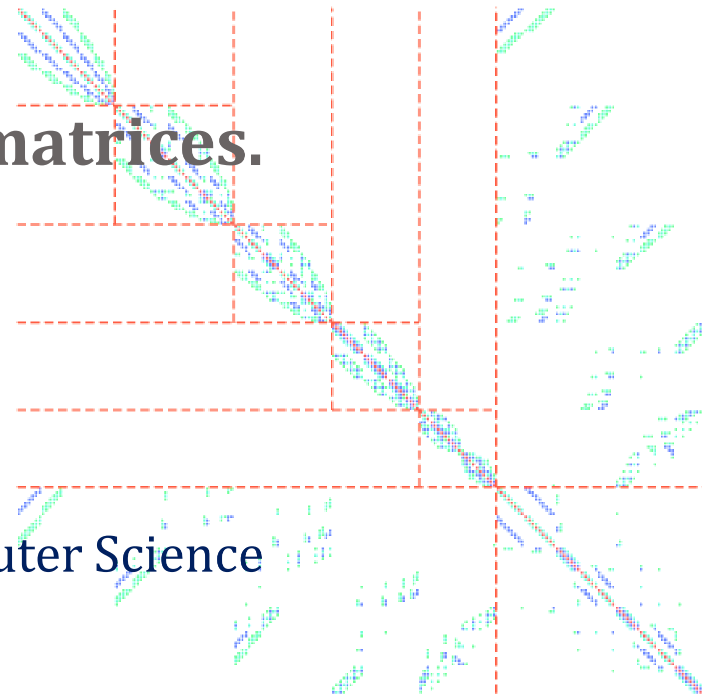
Numerical Methods of Linear Algebra for Sparse Matrices

Lecture 7

Graph representations of sparse matrices. Permutations and reordering



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Structures and graph representations of sparse matrices

Types of sparse matrices

Graph representations

Permutations and reordering

Definition of a sparse matrix

- A sparse matrix is a matrix which has very few nonzero elements.
- Sparsity is the fraction of zero elements in a matrix
- Density is the fraction of non-zero elements in a matrix
- **Example of sparse matrix**: 64 elements, 52 zero elements and 12 nonzero elements (82% sparsity, 18% density)

$$\begin{pmatrix} 1.0 & 0 & 5.0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 3.0 & 0 & 0 & 0 & 0 & 11.0 & 0 \\ 0 & 0 & 0 & 0 & 9.0 & 0 & 0 & 0 \\ 0 & 0 & 6.0 & 0 & 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 7.0 & 0 & 0 & 0 & 0 \\ 2.0 & 0 & 0 & 0 & 0 & 10.0 & 0 & 0 \\ 0 & 0 & 0 & 8.0 & 0 & 0 & 0 & 0 \\ 0 & 4.0 & 0 & 0 & 0 & 0 & 0 & 12.0 \end{pmatrix}$$

Types of sparse matrices

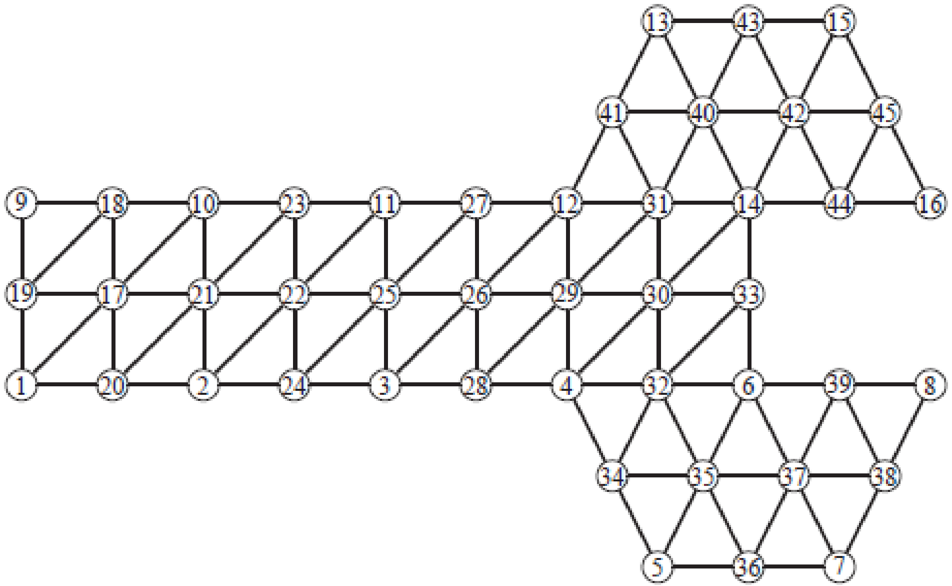
- *Structured matrix*: location of nonzero entries form a regular pattern (block-diagonal, band, several diagonals)
  - Finite difference method (FDM) on rectangular grids produces structured matrices

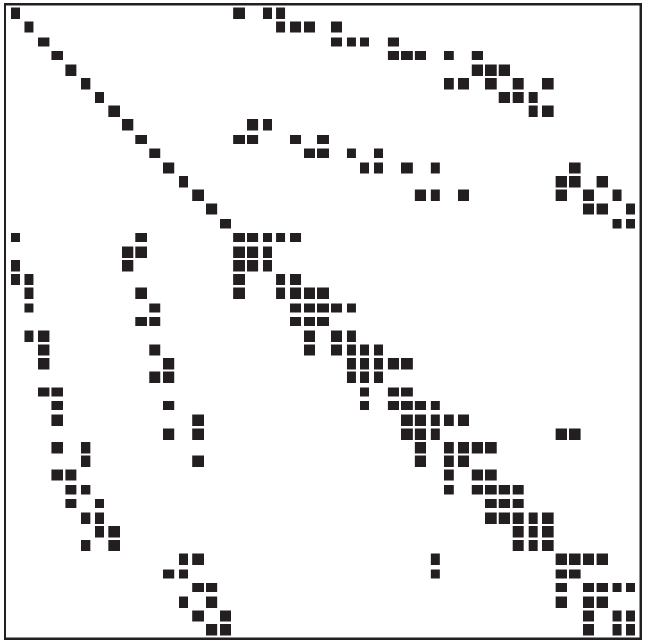
- *Unstructured matrix*: nonzero entries are located irregularly
  - Finite element method (FEM) and finite volume method (FVM) produce unstructured matrices

- The difference between structured and unstructured matrices is important for *iterative* methods that use matrix-by-vector multiplication Av, because of the storage of elements. For *direct* methods, this difference is less important

Example of unstructured matrix

- Finite element mesh and corresponding sparse matrix





Pattern of a sparse matrix

Consider a sparse, in general, rectangular matrix $A \in \mathbb{C}^{n \times m}$

- Pattern of the sparse matrix shows the positions of nonzero elements:

$P_A = \{(i, j) \mid a_{ij} \neq 0\}$, where i is the row number, j is the column number

$$A = \begin{pmatrix} 1 & 0 & 2 \\ 3 & 0 & 0 \\ 0 & 0 & 4 \end{pmatrix}$$

Pattern of A: $\begin{pmatrix} \times & 0 & \times \\ \times & 0 & 0 \\ 0 & 0 & \times \end{pmatrix}$

Types of sparse matrix patterns

- nonsymmetric pattern results from nonsymmetric matrix ($A \neq A^T$):

$\exists\ (i,j) \in P_A:\ (j,i) \notin P_A$. It means that $\exists\ (i,j) \in P_A:\ a_{ij} \neq 0$ and $a_{ji} = 0$.

Example of nonsymmetric pattern: $\begin{pmatrix} \times & 0 & \times \\ 0 & \times & 0 \\ 0 & 0 & \times \end{pmatrix}$

- symmetric pattern can result from either symmetric ($A = A^T$) or nonsymmetric ($A \neq A^T$) matrix

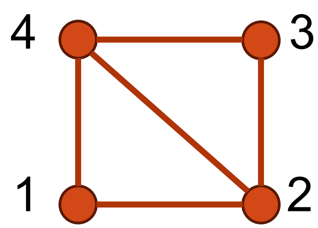
$\exists\ (i,j) \in P_A \iff \exists\ (j,i) \in P_A$. It means that if $a_{ij} \neq 0$, then $a_{ji} \neq 0$

Example of symmetric pattern: $\begin{pmatrix} \times & 0 & \times \\ 0 & \times & 0 \\ \times & 0 & \times \end{pmatrix}$

Graph representations of sparse matrices

- Graph $G=(V,E)$ consists of the set of vertices $V=\{v_1, v_2, ..., v_k\}$ and the set of edges $E=\{(v_i, v_j)\},\ i,j=\overline{1,k},\ E\subseteq V\times V,$ which is the set of binary relations, representing connections between the vertices

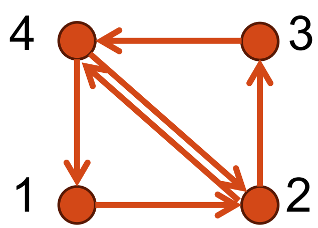
- undirected graph



$\exists\ (v_i, v_j) \Leftrightarrow\ \exists\ (v_j, v_i)$

Edges: (1,4)=(4,1), (4,3)=(3,4), (3,2)=(2,3), (2,1)=(1,2), (4,2)=(2,4)

- directed graph



$\exists\ (v_i, v_j):$ there is no (v_j, v_i)

Edges: (4,1), (1,2), (2,3), (3,4), (4,2) and (2,4)

Adjacency graph and pattern of a sparse matrix

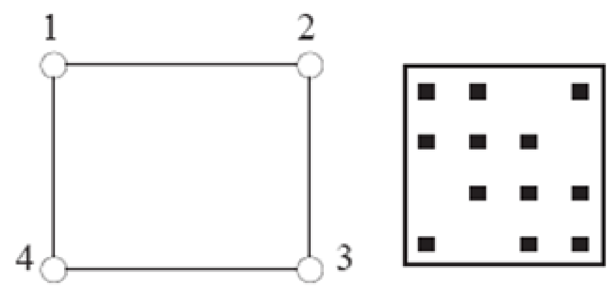
Consider a linear system $Ax = b,\ A \in \mathbb{C}^{n\times n},\ \ b \in \mathbb{C}^n$

- Adjacency graph for a matrix $A \in \mathbb{C}^{n\times n}$

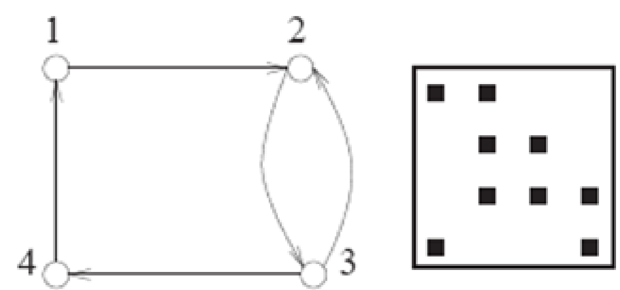
$G = (V, E),$ where the set of vertices $V = \{1, 2, \ldots, n\}$ is the set of n unknowns and the set of edges $E = \{(i, j) \mid a_{ij} \neq 0\},\ \ i, j = \overline{1, n}$

In terms of linear system, an edge exists, if equation i includes unknown j

For undirected graph, the pattern is always symmetric



For directed graph, the pattern is usually nonsymmetric



Linear system of equations and its matrix representation

Consider a linear system $Ax = b$, $A \in \mathbb{C}^{n\times n}$, $b \in \mathbb{C}^n$

$x \in \mathbb{C}^n$ is the vector of unknowns

Matrix representation: $A = \begin{pmatrix} a_{11} & a_{12} & \dots & a_{1n} \\ a_{21} & a_{22} & \dots & a_{2n} \\ \dots & \dots & \dots & \dots \\ a_{n1} & a_{n2} & \dots & a_{nn} \end{pmatrix}$, $b = \begin{pmatrix} b_1 \\ b_2 \\ \dots \\ b_n \end{pmatrix}$, $x = \begin{pmatrix} x_1 \\ x_2 \\ \dots \\ x_n \end{pmatrix}$

System of equations: $\begin{cases} a_{11}\cdot x_1 + a_{12}\cdot x_2 + \dots + a_{1n}\cdot x_n = b_1, \\ a_{21}\cdot x_1 + a_{22}\cdot x_2 + \dots + a_{2n}\cdot x_n = b_2, \\ \dots \\ a_{n1}\cdot x_1 + a_{n2}\cdot x_2 + \dots + a_{nn}\cdot x_n = b_n. \end{cases}$

Rows $i = \overline{1,n}$ of the matrix represent equations $1, 2, \dots., n$

Columns $j = \overline{1,n}$ of the matrix represent unknonws $x_1, x_2, \dots., x_n$

The problem of fill-ins in the direct methods for linear systems

If we apply a *direct* method to solve the linear system $Ax = b$ (i.e. obtain exact solution in a finite number of steps), we can get less sparse matrix as a result of such called *fill - ins* (for example, in Gaussian elimination method)

- Fill-ins are nonzero entries, which appear at the places of zero entries, when solving a linear system

We can reduce the number of fill-ins by relocating the entries in the matrix using permutation of rows and reordering of unknowns

Permutations

- Permutation π of length n is a row-vector $\{1,2,...,n\}$, where every element appears only once: $\pi = \{i_1, i_2, ..., i_n\}$

Example. Initial set $\{1,2,3,4\}$. Permutation $\pi = \{2,4,1,3\}$

π_n is the set of all permutations of the length n

$|\pi_n| = n!$ is the number of such permutations

- Row π-permutation for the matrix $A \in \mathbb{C}^{n \times m}$

$A_{\pi,*} = \{a_{\pi(i),j}\}, \ i = \overline{1,n}, \ j = \overline{1,m}$

- Column π-permutation for the matrix $A \in \mathbb{C}^{n \times m}$

$A_{*,\pi} = \{a_{i,\pi(j)}\}, \ i = \overline{1,n}, \ j = \overline{1,m}$

Interchange and permutation matrices

- Interchange matrix P_{ij} is the identity matrix with permuted rows i and j

Example. $I = \begin{pmatrix} 1 & 0 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \end{pmatrix}, P_{12} = \begin{pmatrix} 0 & 1 & 0 \\ 1 & 0 & 0 \\ 0 & 0 & 1 \end{pmatrix}$

- Permutation matrix P_π is a matrix, where in every row and every column there is only one nonzero entry, which is equal to 1

Example. $I = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}, \pi = \{2,3,1,4\}, \; P_\pi = \begin{pmatrix} 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix}$

Permutation matrix

- Row π-permutation matrix P_π permutes the rows of A:

$A_{\pi,*} = P_\pi A$, where $P_\pi = P_{i_n,j_n} P_{i_{n-1},j_{n-1}} \ldots P_{i_1,j_1}$ is the product of interchange matrices (i.e. successive permutations)

- Column π-permutation matrix Q_π permutes the columns of A:

$A_{*,\pi} = AQ_\pi$, where $Q_\pi = P_{i_1,j_1} P_{i_2,j_2} \ldots P_{i_{n-1},j_{n-1}} P_{i_n,j_n}$

Properties

1) $P_\pi Q_\pi = I,\ Q_\pi = P_\pi^{-1}$

1) P_π and Q_π are orthogonal: $P_\pi^{-1} = P_\pi^{T},\ Q_\pi^{-1} = Q_\pi^{T}$

Permutation: reordering and renumeration

Consider a linear system $Ax = b$, $A \in \mathbb{C}^{n\times n}$, $b \in \mathbb{C}^n$

$x \in \mathbb{C}^n$ is the vector of unknowns

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

Rows $i = \overline{1, n}$ of the matrix represent equations $1, 2, \dots, n$

Columns $j = \overline{1, n}$ of the matrix represent unknonws $x_1, x_2, \dots, x_n$

Permute the rows $\rightarrow$ reorder equations

Permute the columns $\rightarrow$ renumerate unknowns

Example of permutation

Consider a linear system $Ax = b$, $A \in \mathbb{C}^{4\times 4}$, $b \in \mathbb{C}^4$

$$A = \begin{pmatrix} a_{11} & 0 & a_{13} & 0 \\ 0 & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & 0 & 0 \\ 0 & a_{42} & 0 & a_{44} \end{pmatrix}$$

$$\begin{pmatrix} a_{11} & 0 & a_{13} & 0 \\ 0 & a_{22} & a_{23} & a_{24} \\ a_{31} & a_{32} & 0 & 0 \\ 0 & a_{42} & 0 & a_{44} \end{pmatrix} \begin{pmatrix} x_1 \\ x_2 \\ x_3 \\ x_4 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{pmatrix}$$

Consider a permutation $\pi = \{4, 1, 3, 2\}$

Step 1

1. Permute columns with permutation $\pi = \{4,1,3,2\}$: AQ_π

In order to multiply A by Q_π on the right, we can represent

left-hand side of the system $Ax = b$ as $Ax = AIx = AQ_\pi Q_\pi^{-1}x$ (as $Q_\pi Q_\pi^{-1} = I$)

$AQ_\pi Q_\pi^{-1}x = b$

$(AQ_\pi)(P_\pi x) = b,$ as $Q_\pi^{-1} = P_\pi$

AQ_π permutes the columns of A, $P_\pi x$ permutes the vector of unknowns

$$\begin{pmatrix} 0 & a_{11} & a_{13} & 0 \\ a_{24} & 0 & a_{23} & a_{22} \\ 0 & a_{31} & 0 & a_{32} \\ a_{44} & 0 & 0 & a_{42} \end{pmatrix} \begin{pmatrix} x_4 \\ x_1 \\ x_3 \\ x_2 \end{pmatrix} = \begin{pmatrix} b_1 \\ b_2 \\ b_3 \\ b_4 \end{pmatrix}$$

Vector of unknowns is permuted, right-hand side vector is not changed

Step 2

2. Permute rows with the same permutation $\pi = \{4,1,3,2\}$: $P_\pi A$

$(AQ_\pi)(P_\pi x) = b$ from the previous step 1. Now we multiply both sides by P_π

$(P_\pi A Q_\pi)(P_\pi x) = P_\pi b$

$P_\pi A$ permutes the rows of A, $P_\pi b$ permutes the vector of right-hand side

$$\begin{pmatrix} a_{44} & 0 & 0 & a_{42} \\ 0 & a_{11} & a_{13} & 0 \\ 0 & a_{31} & 0 & a_{32} \\ a_{24} & 0 & a_{23} & a_{22} \end{pmatrix} \begin{pmatrix} x_4 \\ x_1 \\ x_3 \\ x_2 \end{pmatrix} = \begin{pmatrix} b_4 \\ b_1 \\ b_3 \\ b_2 \end{pmatrix}$$

Right-hand side vector is permuted, vector of unknowns is not changed

Symmetric permutation

$$\begin{pmatrix} a_{44} & 0 & 0 & a_{42} \\ 0 & a_{11} & a_{13} & 0 \\ 0 & a_{31} & 0 & a_{32} \\ a_{24} & 0 & a_{23} & a_{22} \end{pmatrix} \begin{pmatrix} x_4 \\ x_1 \\ x_3 \\ x_2 \end{pmatrix} = \begin{pmatrix} b_4 \\ b_1 \\ b_3 \\ b_2 \end{pmatrix}$$

Note that after two steps with the same permutation
the diagonal entries are from original matrix, but in a different order

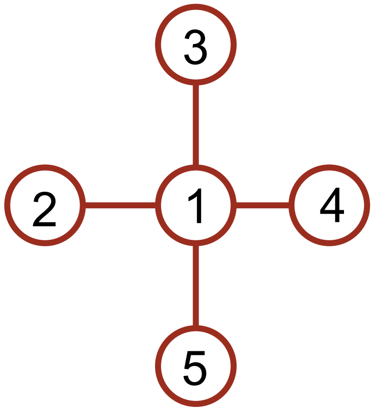
- symmetric permutation of matrix A

$A_{\pi,\pi} = P_\pi A P_\pi^T$ permutes equations and unknowns in the same way
For the adjacency graph, if matrix A had graph G, then matrix $A' = A_{\pi,\pi}$ will have graph G', where G' has the same form as G, but the vertices are renumerated

Importance of renumeration of vertices in the adjacency graph

Consider two examples

- In a star graph, if we enumerate the vertices starting from the center clockwise in ascending order, the pattern of the matrix will look like an arrow pointing up

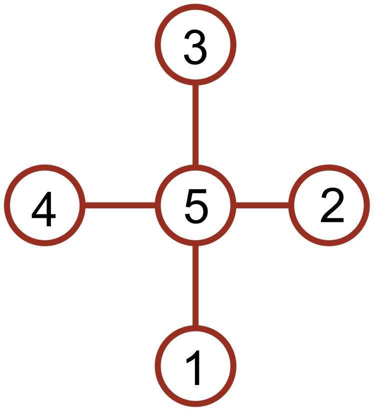


$$\begin{pmatrix} \times & \times & \times & \times & \times \\ \times & \times & 0 & 0 & 0 \\ \times & 0 & \times & 0 & 0 \\ \times & 0 & 0 & \times & 0 \\ \times & 0 & 0 & 0 & \times \end{pmatrix}$$

For the "arrow pointing up" matrix, factorization A=LU does not preserve the pattern of the original matrix, as it produces dense L and U, thus giving **a lot of fill - ins**

Importance of renumeration of vertices in the adjacency graph

- However, if we enumerate the vertices starting from the center clockwise in descending order, the pattern of the matrix will look like an arrow pointing down

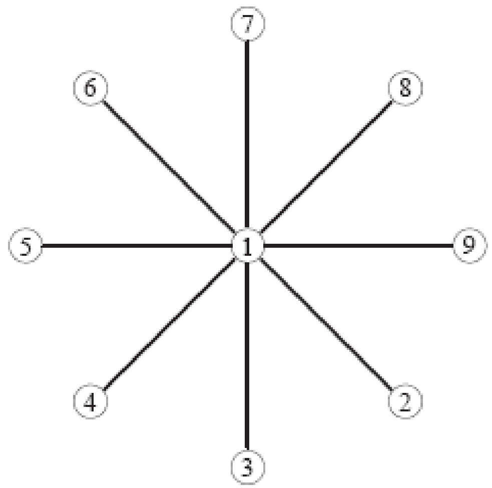


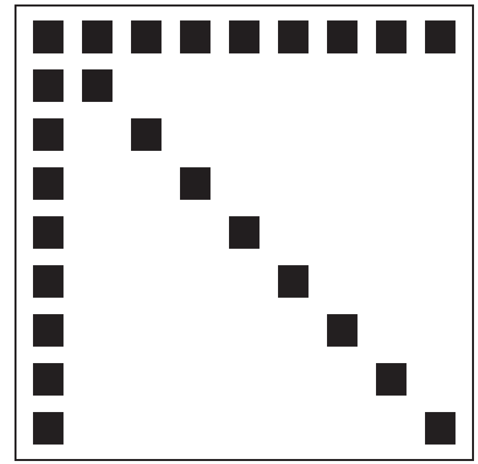
$$\begin{pmatrix} \times & 0 & 0 & 0 & \times \\ 0 & \times & 0 & 0 & \times \\ 0 & 0 & \times & 0 & \times \\ 0 & 0 & 0 & \times & \times \\ \times & \times & \times & \times & \times \end{pmatrix}$$

For the "arrow pointing down" matrix, factorization A=LU preserves the pattern of the original matrix and produces **no fill - ins**

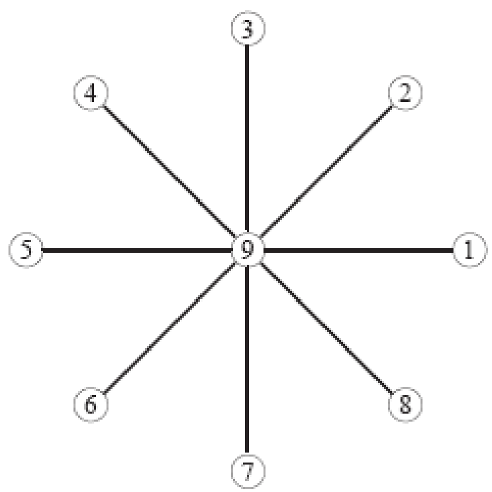
Reordering for star matrices

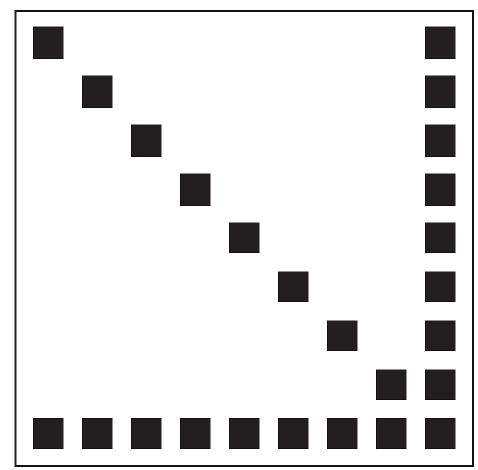
- A lot of fill-ins during Gaussian elimination





- No fill-ins during Gaussian elimination





Examples of reordering algorithms: standard and reverse Cuthill-McKee