SPARSE DIRECT METHODS

- **Building blocks for sparse direct solvers**
- **SPD case. Sparse Column Cholesky/**
- **Elimination Trees - Symbolic factorization**

Direct Sparse Matrix Methods

Problem addressed: Linear systems

$$Ax = b$$

➤ We will consider mostly Cholesky –

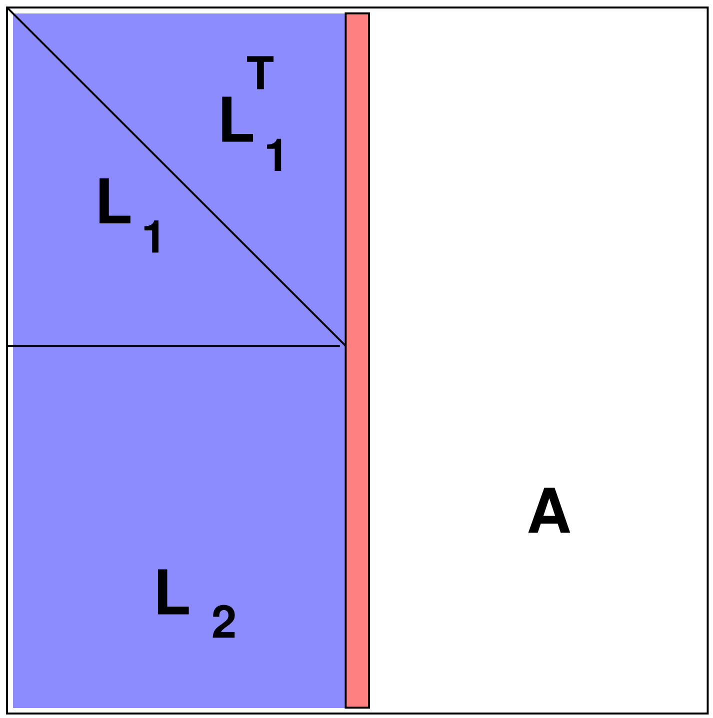
➤ We will consider some implementation details and tricks used to develop efficient solvers

Basic principles:

- Separate computation of structure from rest [symbolic factorization]
- Do as much work as possible statically
- Take advantage of clique formation (supernodes, mass-elimination).

Sparse Column Cholesky

For $j = 1, \ldots, n$ Do:
  $l(j:n, j) = a(j:n, j)$
  For $k = 1, \ldots, j-1$ Do:
    // cmod(k,j):
    $l_{j:n,j} := l_{j:n,j} - l_{j,k} * l_{j:n,k}$
  EndDo
  // cdiv (j) [Scale]
  $l_{j,j} = \sqrt{l_{j,j}}$
  $l_{j+1:n,j} := l_{j+1:n,j} / l_{jj}$
EndDo



The four essential stages of a solve

1. Reordering: $A \quad \longrightarrow \quad A := PAP^T$

➤ Preprocessing: uses graph [Min. deg, AMD, Nested Dissection]

2. Symbolic Factorization: Build static data structure.

➤ Exploits 'elimination tree', uses graph only.

➤ Also: 'supernodes'

3. Numerical Factorization: Actual factorization $A = LL^T$

➤ Pattern of L is known. Uses static data structure. Exploits supernodes (blas3)

4. Triangular solves: Solve $Ly = b$ then $L^T x = y$

ELIMINATION TREES

The notion of elimination tree

- Elimination trees are useful in many different ways [theory, symbolic factorization, etc..]

- For a matrix whose graph is a tree, parent of column $j < n$ is defined by

$$\boxed{Parent(j) = i, \text{ where } a_{ij} \neq 0 \text{ and } i > j}$$

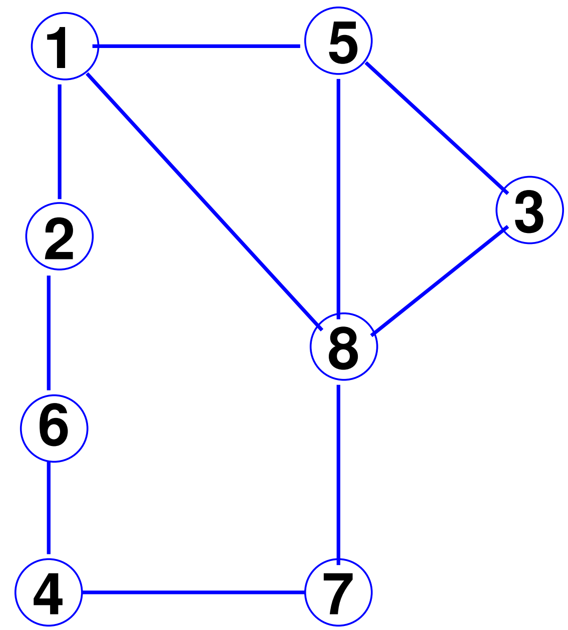
- For a general matrix matrix, consider $A = LL^T$, and $G^F =$ 'filled' graph = graph of $L + L^T$. Then

$$\boxed{Parent(j) = \min(i) \ s.t. \ a_{ij} \neq 0 \text{ and } i > j}$$

- Defines a tree rooted at column n (Elimintion tree).

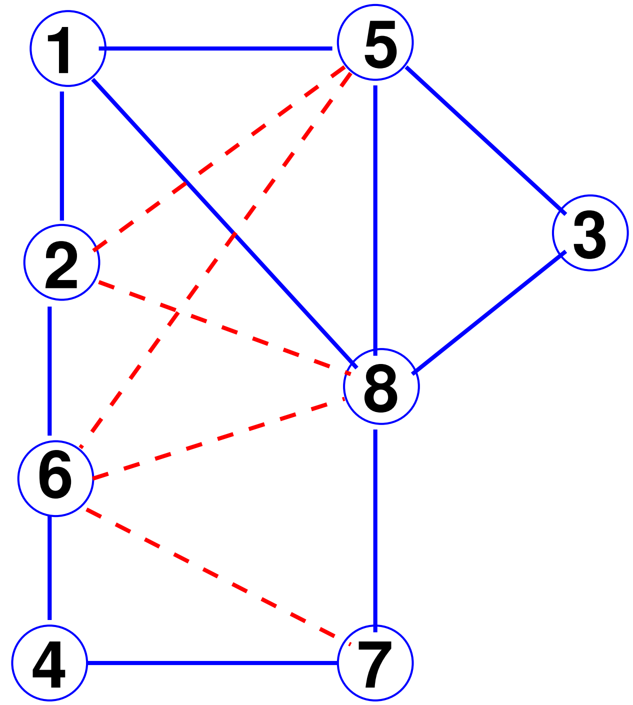
Example: Original matrix and Graph

$$
\begin{bmatrix}
1 & \star & & & \star & & & \star \\
\star & 2 & & & & \star & & \\
& & 3 & & \star & & & \star \\
& & & 4 & & \star & \star & \\
\star & & \star & & 5 & & & \star \\
& \star & & \star & & 6 & & \\
& & & \star & & & 7 & \star \\
\star & & \star & & \star & & \star & 8
\end{bmatrix}
$$

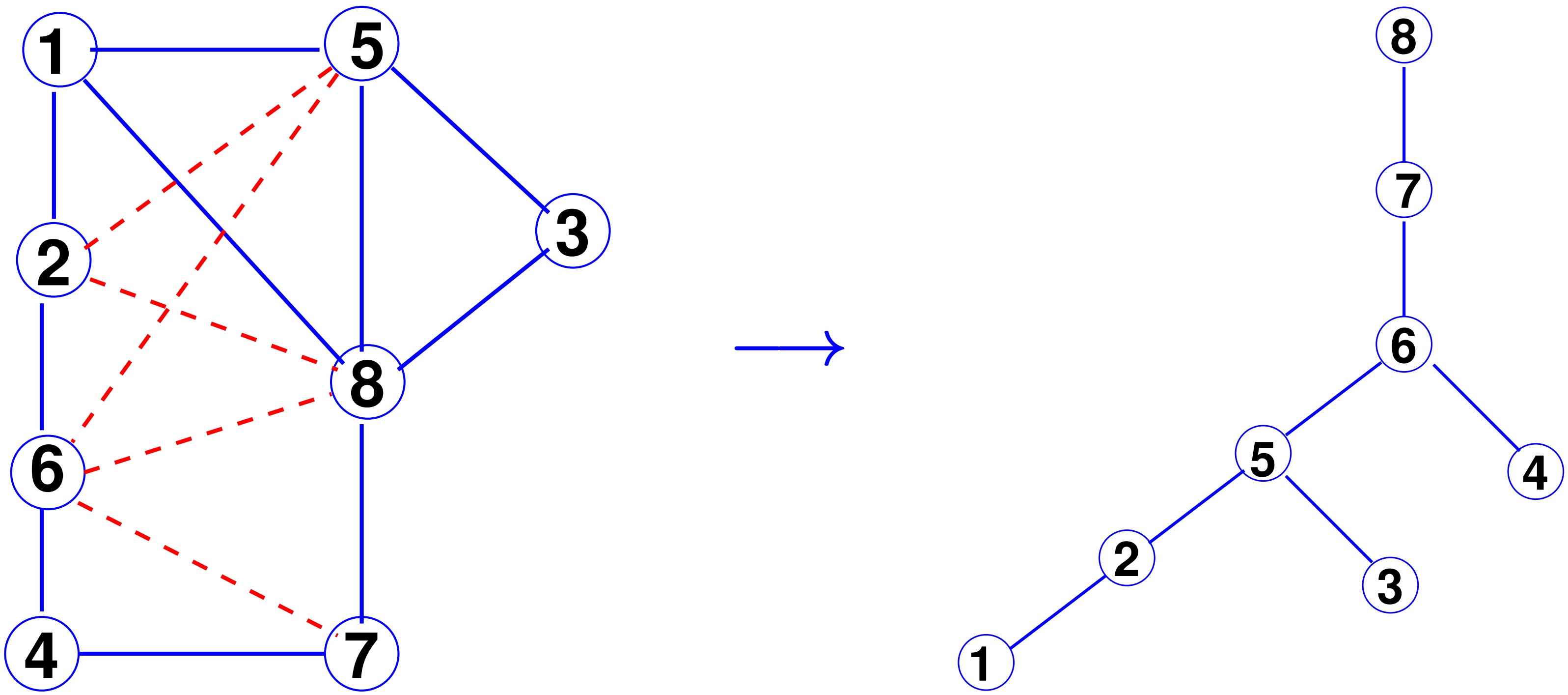


Filled matrix+graph

$$\begin{bmatrix}
1 & \star & & & \star & & & \star \\
\star & 2 & & & \blacksquare & \star & & \blacksquare \\
& & 3 & & \star & & & \star \\
& & & 4 & & \star & \star & \\
\star & \blacksquare & \star & & 5 & \blacksquare & & \star \\
& \star & & \star & \blacksquare & 6 & \blacksquare & \blacksquare \\
& & & \star & & \blacksquare & 7 & \star \\
\star & \blacksquare & \star & & \star & \blacksquare & \star & 8
\end{bmatrix}$$



Corresponding Elimination Tree

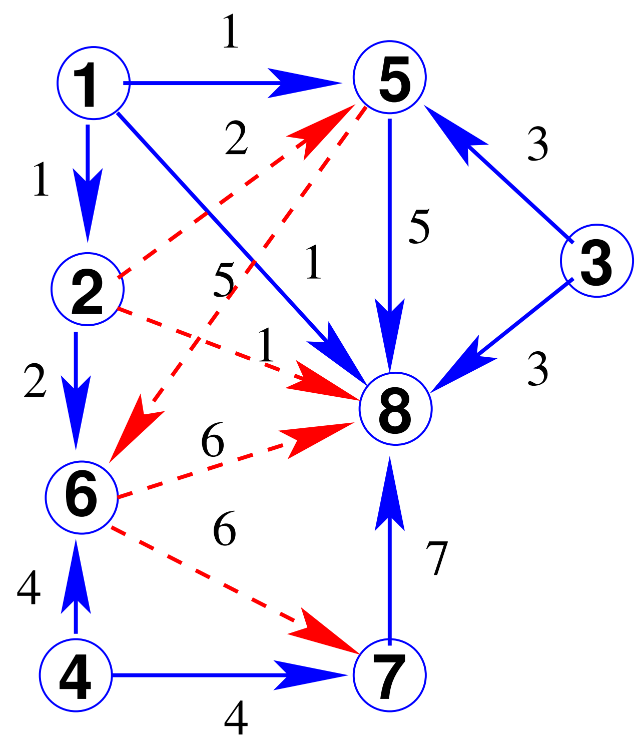


- Parent(i) = 'first nonzero entry in L(i+1:n,i)'
- Parent(i) = min $\{j > i \mid j \in Adj_{G^F}(i)\}$

Where does the elimination tree come from?

- Answer in the form of an excercise.

Consider the elimination steps for the previous example. A directed edge means a row (column) modification. It shows the task dependencies. There are unnecessary dependencies. For example: $\mathbf{1} \longrightarrow \mathbf{5}$ can be removed because it is subsumed by the path $\mathbf{1} \rightarrow \mathbf{2} \rightarrow \mathbf{5}$.



To do: Remove all the redundant dependencies.. What is the result?

Facts about elimination trees

➤ Elimination Tree defines dependencies between columns.

➤ The root of a subtree cannot be used as pivot before any of its descendents is processed.

➤ Elimination tree depends on ordering;

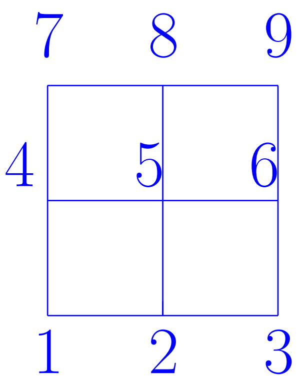
➤ Can be used to define 'parallel' tasks.

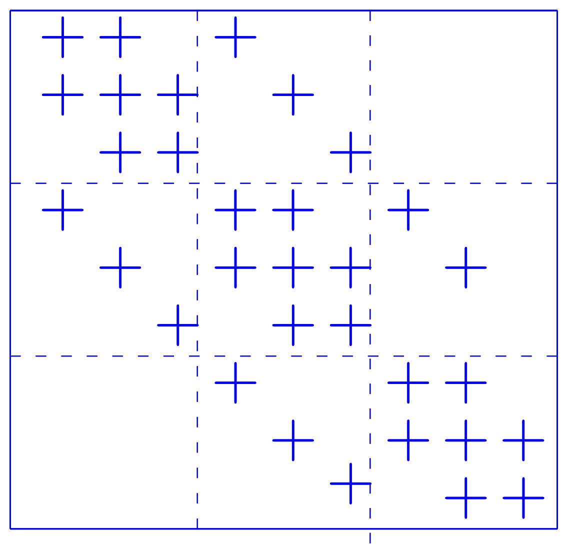
➤ For parallelism: flat and wide trees $\longrightarrow$ good; thin and tall (e.g. of tridiagonal systems) $\longrightarrow$ Bad.

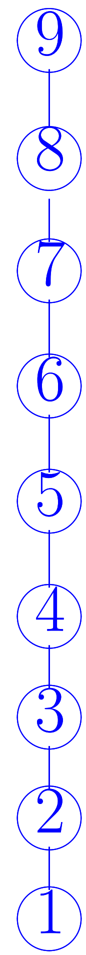
➤ For parallel executions, Nested Dissection gives better trees than Minimun Degree ordering.

Elim. tree depends on ordering (Not just the graph)

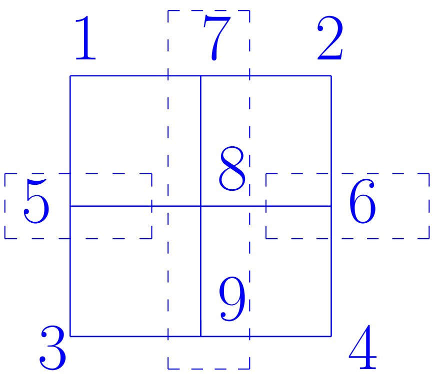
Example: $\mathbf{3} \times \mathbf{3}$ grid for 5-point stencil [natural ordering]

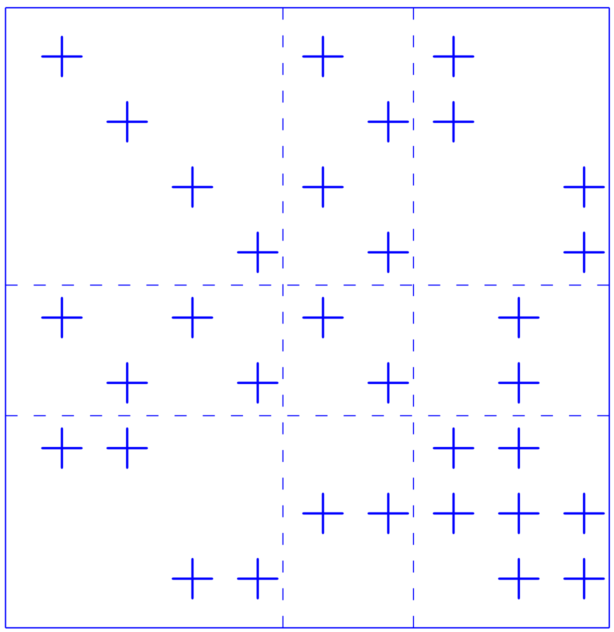


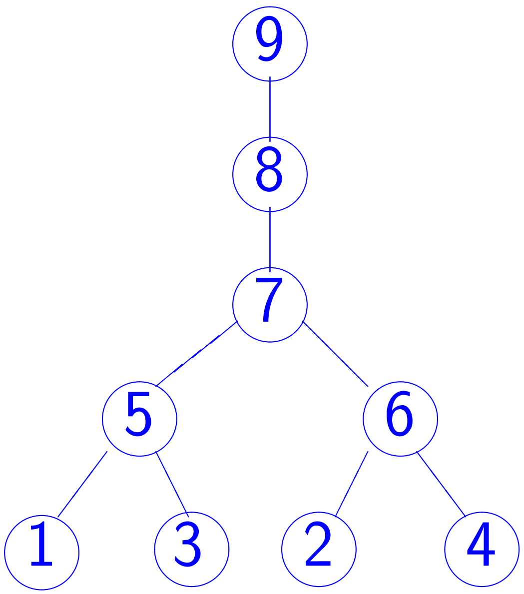




Same example with nested dissection ordering





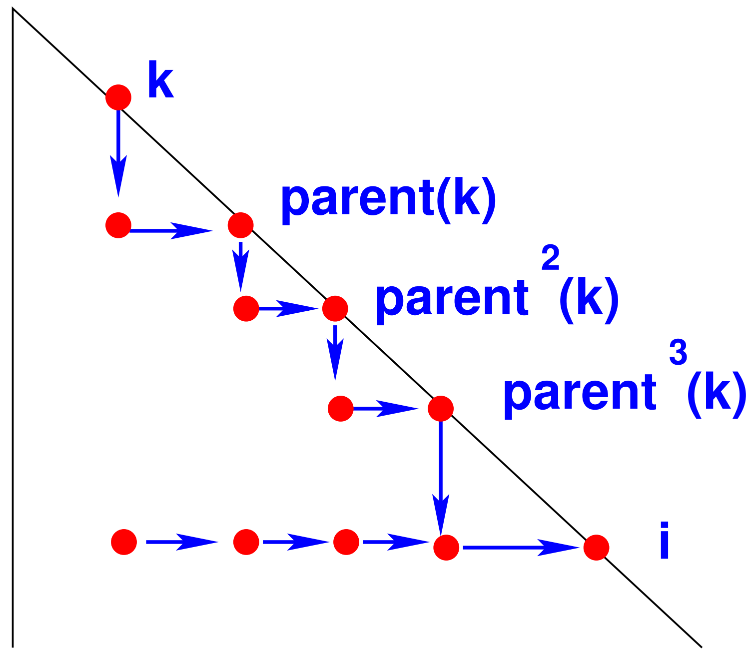


Properties

➤ The elimination tree is a spanning tree of the filled graph [a tree containing all vertices] - obtained by removing edges.

➤ If $l_{ik} \neq 0$ then i is an ancestor of k in the tree

✍1 In the previous example: follow the creation of the fill-in (6,8).

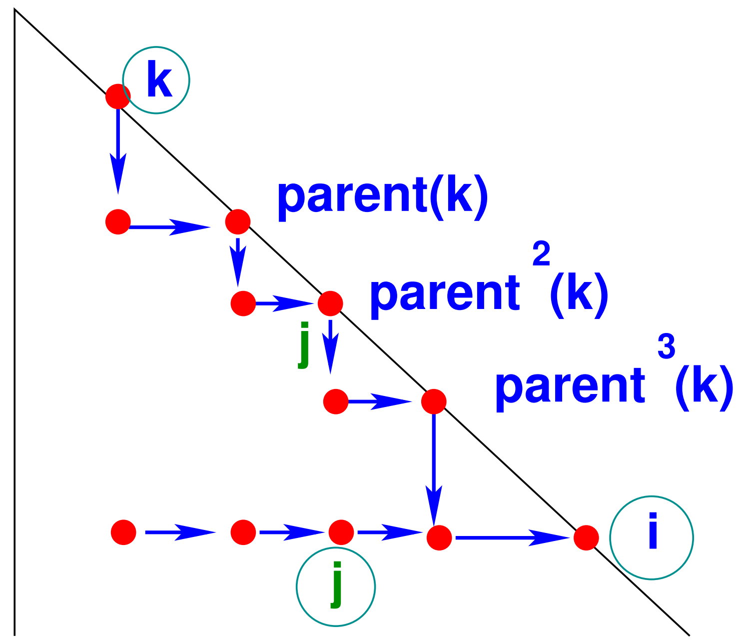


In particular: if $a_{ik} \neq 0, k < i$ then $i \rightsquigarrow k$

➤ Consequence: no fill-in between branches of the same subtree

Elimination trees and the pattern of L

➤ It is easy to determine the sparsity pattern of L because the pattern of a given column is "inherited" by the ancestors in the tree.

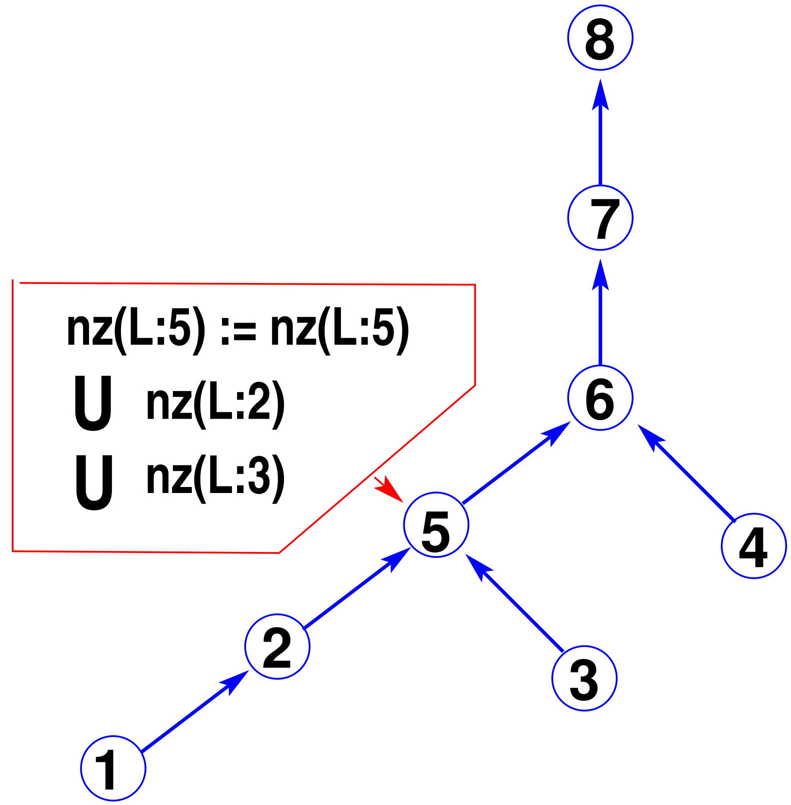


Theorem: For $i > j$, $l_{ij} \neq 0$ iff j is an ancestor of some $k \in Adj_A(i)$ in the elimination tree.

In other words:

$$l_{ij} \neq 0, i > j \ \text{ iff } \ \left| \ \begin{array}{l} \exists k \in Adj_A(i) s.t. \\ j \rightsquigarrow k \end{array} \right.$$

In theory: To construct the pattern of L, go up the tree and accumulate the patterns of the columns. Initially L has the same pattern as $TRIL(A)$.



- However: Let us assume tree is not available ahead of time
- Solution: Parents can be obtained dynamically as the pattern is being built.
- This is the basis of symbolic factorization.

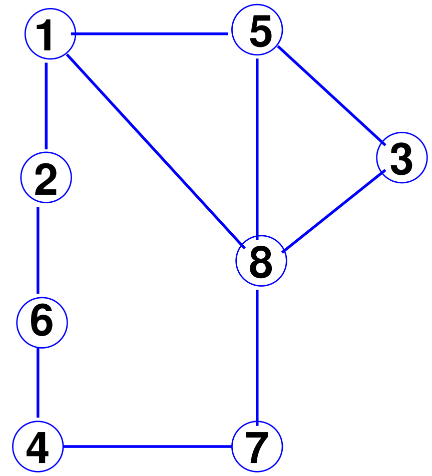
Notation :

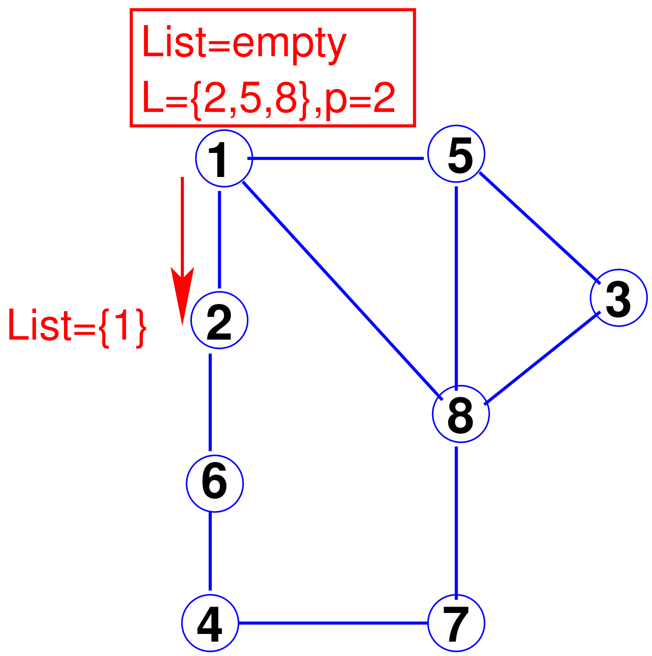
- $nz(X)$ is the pattern of X (matrix or column, or row). A set of pairs (i,j)
- $tril(X)$ = Lower triangular part of pattern [matlab notation] $\{(i,j) \in X \mid i > j\}$
- Idea: dynamically create the list of nodes needed to update $L_{:,j}$.

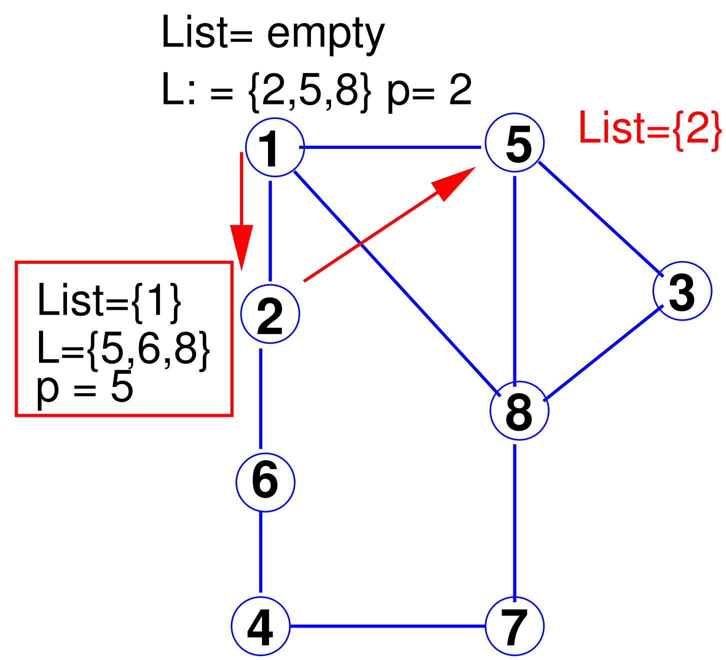
ALGORITHM : 1. *Symbolic factorization*

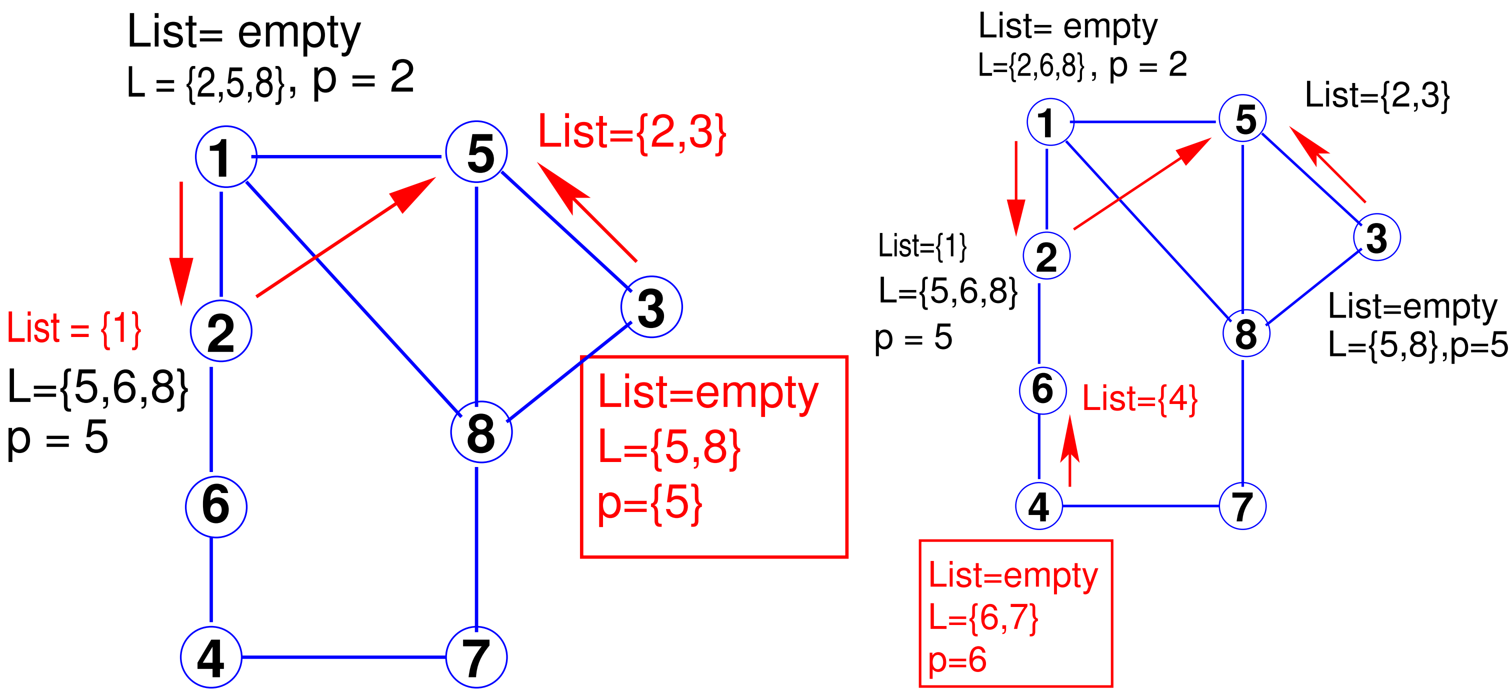
1. Set: $nz(L) = tril(nz(A))$,
2. Set: $list(j) = \emptyset, j = 1, \cdots, n$
3. For $j = 1 : n$
4. for $k \in list(j)$ do
5. $nz(L_{:,j}) := nz(L_{:,j}) \cup nz(L_{:,k})$
6. end
7. $p = \min\{i > j \mid L_{i,j} \neq 0\}$
8. $list(p) := list(p) \cup \{j\}$
9. End

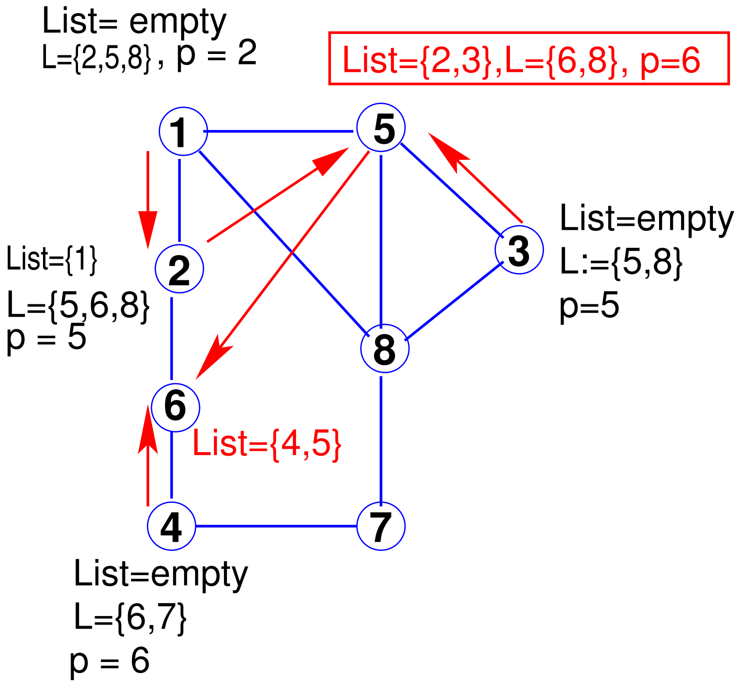
Example: Consider the earlier example:

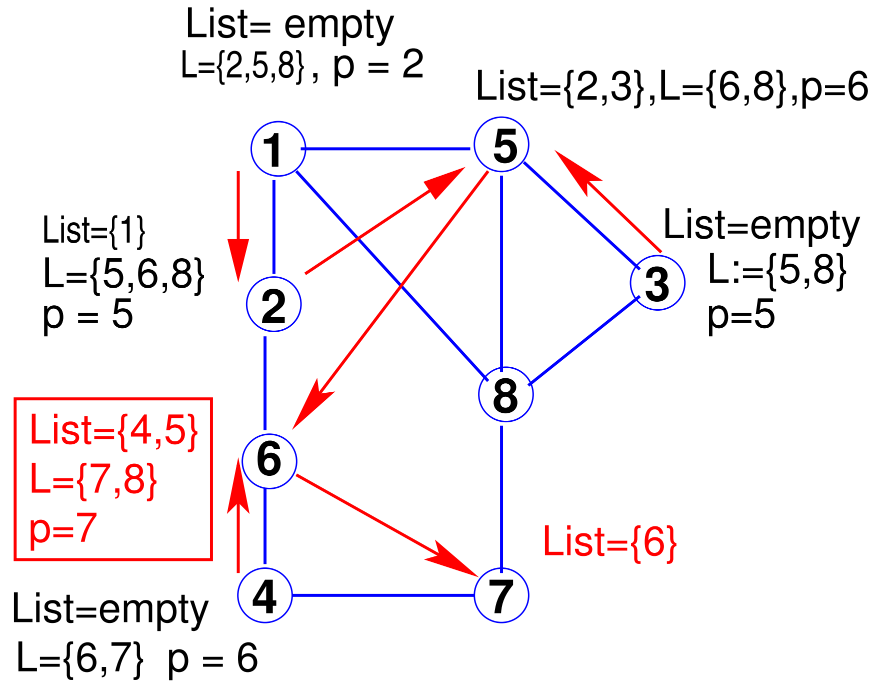







List= empty
L = {2,5,8}, p = 2
1
5
List={2,3}
3
List = {1}
2
L={5,6,8}
p = 5
8
List=empty
L={5,8}
p={5}
6
4
7
List= empty
L={2,6,8}, p = 2
1
5
List={2,3}
3
List={1}
2
L={5,6,8}
p = 5
List=empty
L={5,8},p=5
8
6
List={4}
4
7
List=empty
L={6,7}
p=6


List= empty
L={2,5,8} , p = 2
List={2,3},L={6,8}, p=6
1
5
List=empty
L:={5,8}
p=5
3
List={1}
2
L={5,6,8}
p = 5
8
6
List={4,5}
4
7
List=empty
L={6,7}
p = 6


List= empty
L={2,5,8} , p = 2
List={2,3},L={6,8},p=6
1
5
List={1}
L={5,6,8}
p = 5
List=empty
L:={5,8}
p=5
3
2
8
List={4,5}
L={7,8}
p=7
6
List={6}
4
7
List=empty
L={6,7} p = 6

Multifrontal methods

- Start with the frontal method.
- Recall: Finite element matrix:

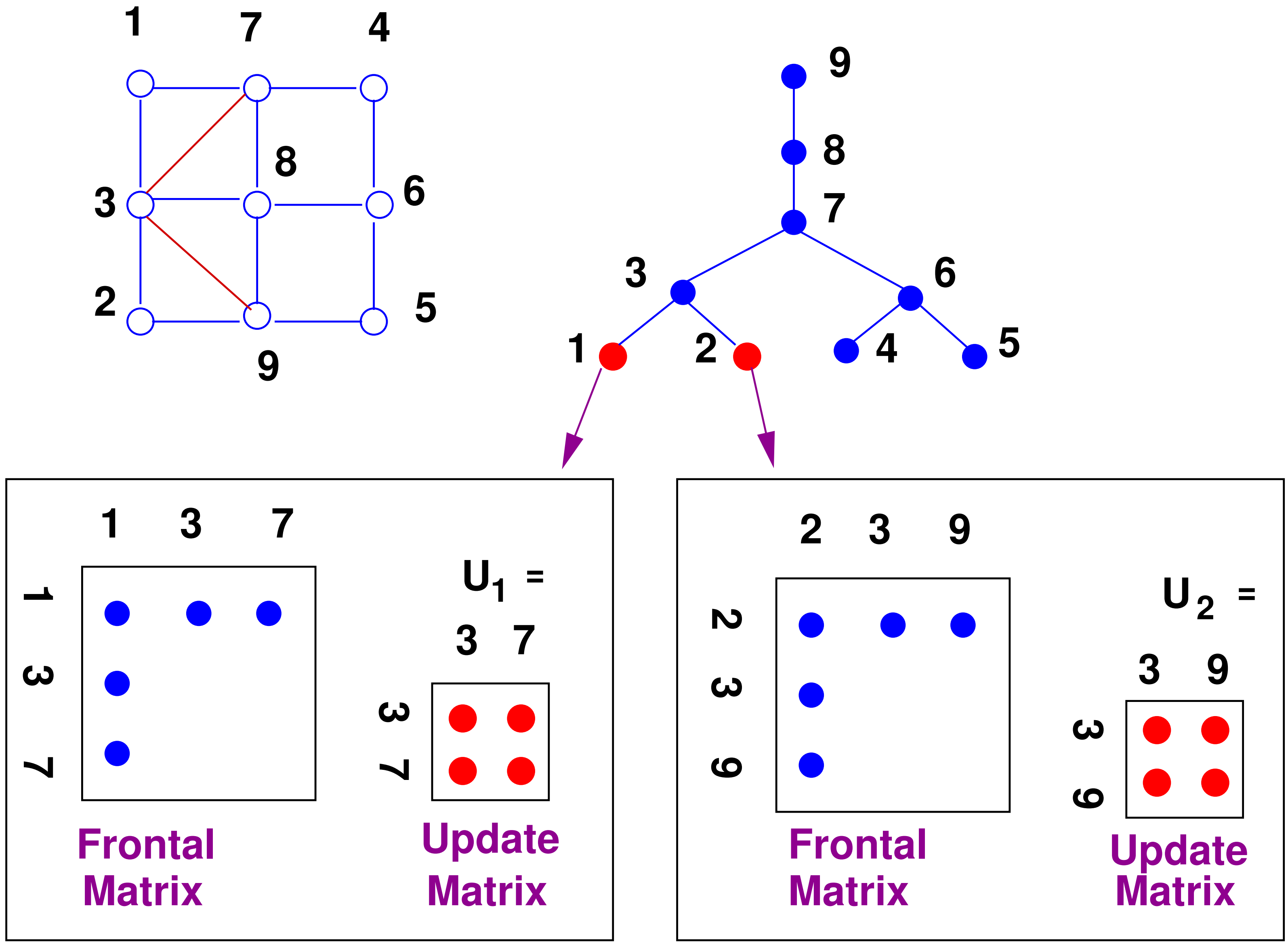
$$\boldsymbol{A} = \sum \boldsymbol{A}^{[e]}$$

$\boldsymbol{A}^{[e]}$ = element matrix associated with element $\boldsymbol{e}$.

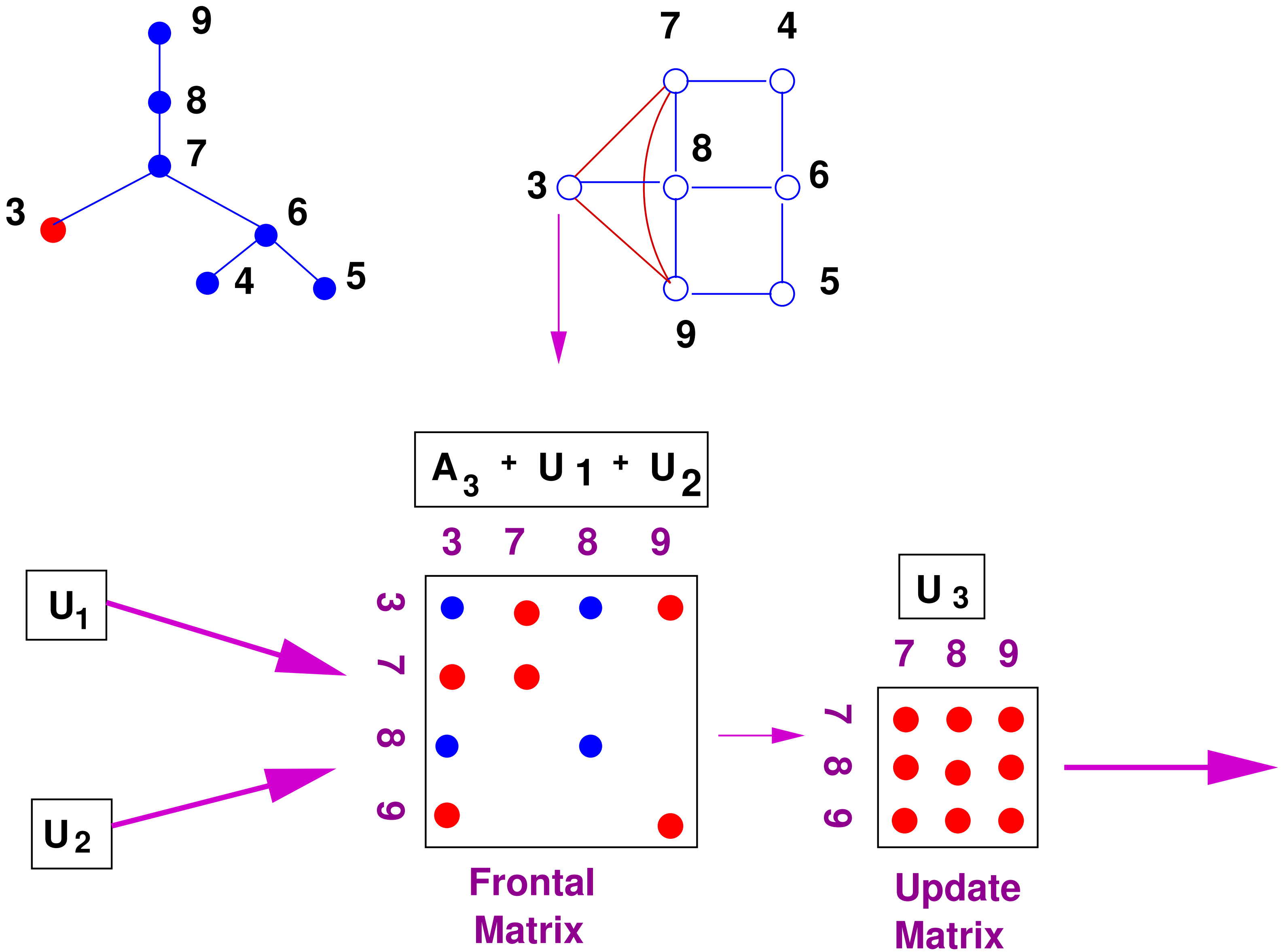
- An old idea: Execute Gaussian elimination as the elements are being assembled
- Dependency: variabes $\leftrightarrow$ elements, creates an assembly tree.
- Method is called *the frontal method*
- Very popular among finite element users: saves storage

Multifrontal methods: extension to general matrices

- Elimination tree replaces assembly tree
- Proceed in post-order traversal of elimination tree in order not to violate task dependencies.
- When a node is eliminated an update matrix is created.
- This matrix is passed to the parent which adds it to its frontal matrix.
- Requires a stack of pending update matrices
- Update matrices popped out as they are needed
- Often implemented with nested dissection-type ordering
- More complex than a left-looking algorithm



1
7
4
8
3
6
2
5
9
9
8
7
3
6
1
2
4
5
1 3 7
1 3 7
Frontal Matrix
U1 =
3 7
3 7
Update Matrix
2 3 9
2 3 9
Frontal Matrix
U2 =
3 9
3 9
Update Matrix



9
8
7
3
6
4
5
7
4
8
3
6
5
9
A3 + U1 + U2
3 7 8 9
U1
U2
U3
7 8 9
Frontal
Matrix
Update
Matrix

Eliminating nodes 1 and 2: What happens on matrix

$$
\left[\begin{array}{c||c||c||ccc||c||c||c}
\mathbf{1} & & \star & & & & \star & & \\ \hline\hline
 & \mathbf{2} & \star & & & & & & \star \\ \hline\hline
\star & \star & \mathbf{3} & & & & \blacksquare & \star & \blacksquare \\ \hline\hline
 & & & \mathbf{4} & & \star & \star & & \\
 & & & & \mathbf{5} & \star & & & \star \\
 & & & \star & \star & \mathbf{6} & & \star & \\ \hline\hline
\star & & \blacksquare & \star & & & \mathbf{7} & \star & \\ \hline\hline
 & & \star & & & \star & \star & \mathbf{8} & \star \\ \hline\hline
 & \star & \blacksquare & & \star & & & \star & \mathbf{9}
\end{array}\right]
\begin{array}{l}
\\
\\
\leftarrow \boldsymbol{U_1(3,:)} \leftarrow \boldsymbol{U_2(3,:)} \\
\\
\\
\\
\leftarrow \boldsymbol{U_1(7,:)} \\
\\
\qquad\qquad\quad \leftarrow \boldsymbol{U_2(9,:)}
\end{array}
$$

Supernodes

➤ Contiguous columns tend to inherit the pattern of the columns from they are updated $\longrightarrow$ Many columns with same sparsity pattern. Supernode $=$ a set of contiguous columns in the Cholesky factor L that have the same sparsity pattern.

➤ The set $\{j, j+1, ..., j+s\}$ is a supernode if

$$NZ(L_{*,k}) = NZ(L_{*,k+1}) \bigcup \{k+1\} \quad j \le k < j+s$$

where $NZ(L_{*,k})$ is nonzero set of column k of L.

➤ Other terms used: Mass elimination, indistinguishible nodes, active variables in front, subscript compression,...

➤ Gain in performance due to savings in Gather-Scatter operations.