

The Elimination Tree of an Unsymmetric Matrix: Theory and Applications

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CSC05 — 21 June 2005

BASIC ASSUMPTIONS

A is a large, sparse, unsymmetric, and irreducible matrix with nonzero diagonal entries

Factorization $A = LU$ exists, where L is unit lower triangular and U is upper triangular

No accidental cancellation during factorization

No use of supernodes for efficiency

No pivoting for stability {will be relaxed later}

ELIMINATION TREE FOR SYMMETRIC A [Schreiber]

Parent Function Defines $T(A)$

$$\rho(k) \equiv \min\{x \mid x > k \text{ and } x \xrightarrow{L} k \xrightarrow{L^t} x\}$$

$\{\rho(k)$ is the row index of the first nonzero
below the diagonal in the k -th column of $L\}$

Property: The vertices in the subtree $\mathcal{T}[k]$ rooted at k form a connected component of the subgraph of the undirected graph $G(A)$ induced by $\{1, 2, \dots, k\}$

ELIMINATION TREE FOR UNSYMMETRIC A [E+L]

Parent Function Defines $T(A)$

$$\rho(k) \equiv \min\{x \mid x > k \text{ and } x \xrightarrow{L} k \xrightarrow{U} x\}$$

$\{\text{reduces to the previous definition if } A \text{ is symmetric}\}$

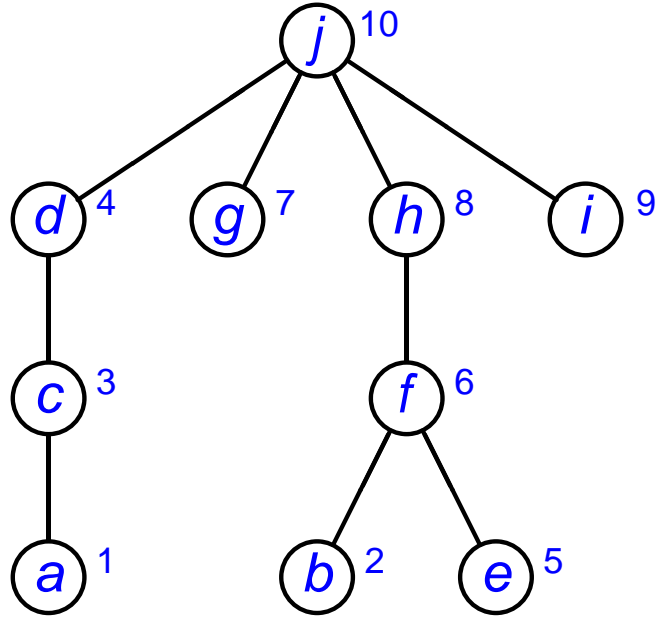
Property: The vertices in $\mathcal{T}[k]$ form a **strongly** connected component of the subgraph of the **directed** graph $G(A)$ induced by $\{1, 2, \dots, k\}$

CANONICAL EXAMPLE

Filled Matrix

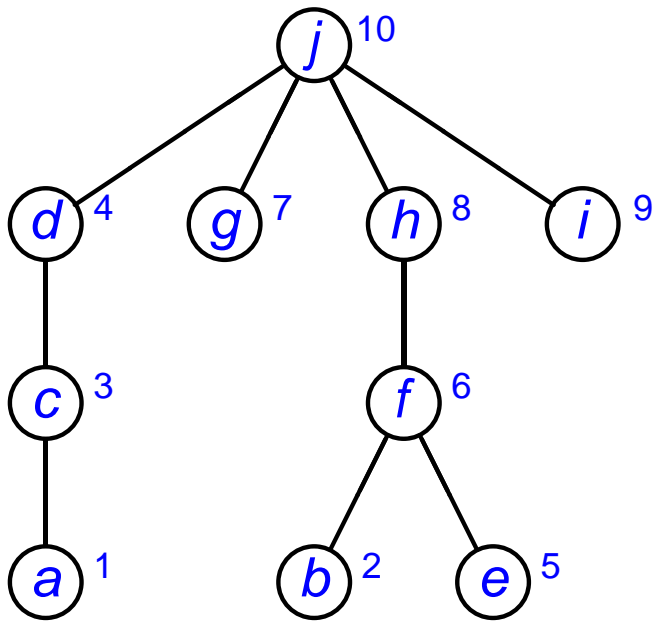
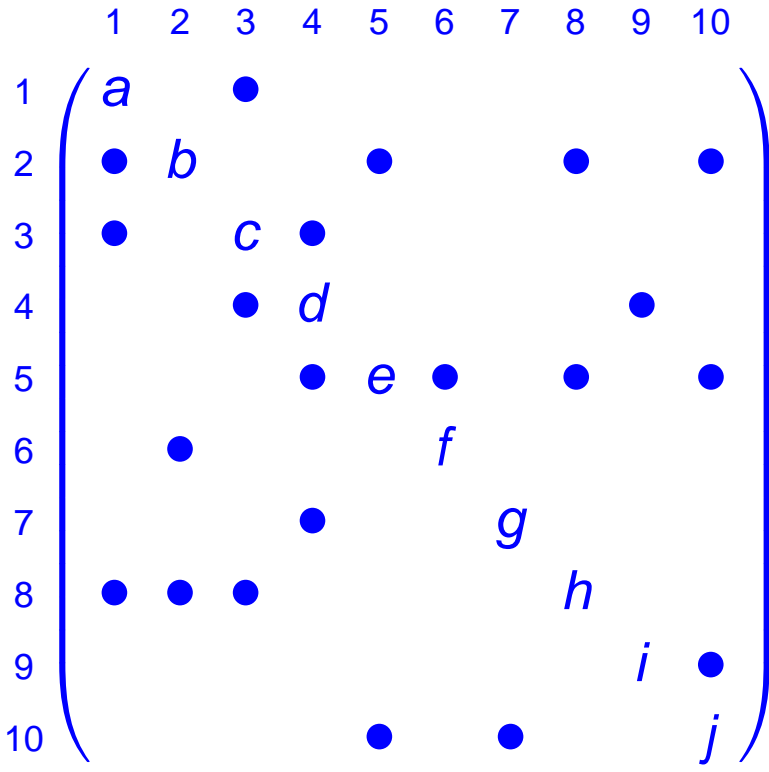
$$A^+ \equiv L + U - I = \begin{matrix} & \begin{matrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \end{matrix} & \left(\begin{array}{cccccccccc} a & & \bullet & & & & & & & \\ \bullet & b & \circ & & \bullet & & & \bullet & & \bullet \\ \bullet & & c & \bullet & & & & & & \\ & & \bullet & d & & & & & \bullet & \\ & & & \bullet & e & \bullet & & \bullet & \circ & \bullet \\ & & \bullet & \circ & \circ & \circ & f & \circ & \circ & \circ \\ & & & \bullet & & & & g & \circ & \\ \bullet & \bullet & \bullet & \circ & \circ & \circ & & h & \circ & \circ \\ & & & & & & & & i & \bullet \\ & & & & \bullet & \circ & \bullet & \circ & \circ & j \end{array} \right) \end{matrix}$$

Elimination Tree

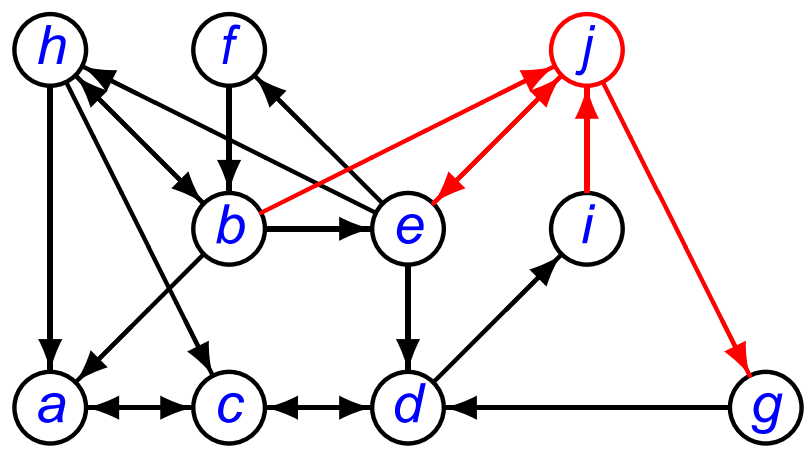


$j \xrightarrow{L} d \xrightarrow{U} j$ but neither $j \xrightarrow{L} d$ nor $d \xrightarrow{U} j$

CANONICAL EXAMPLE (continued)

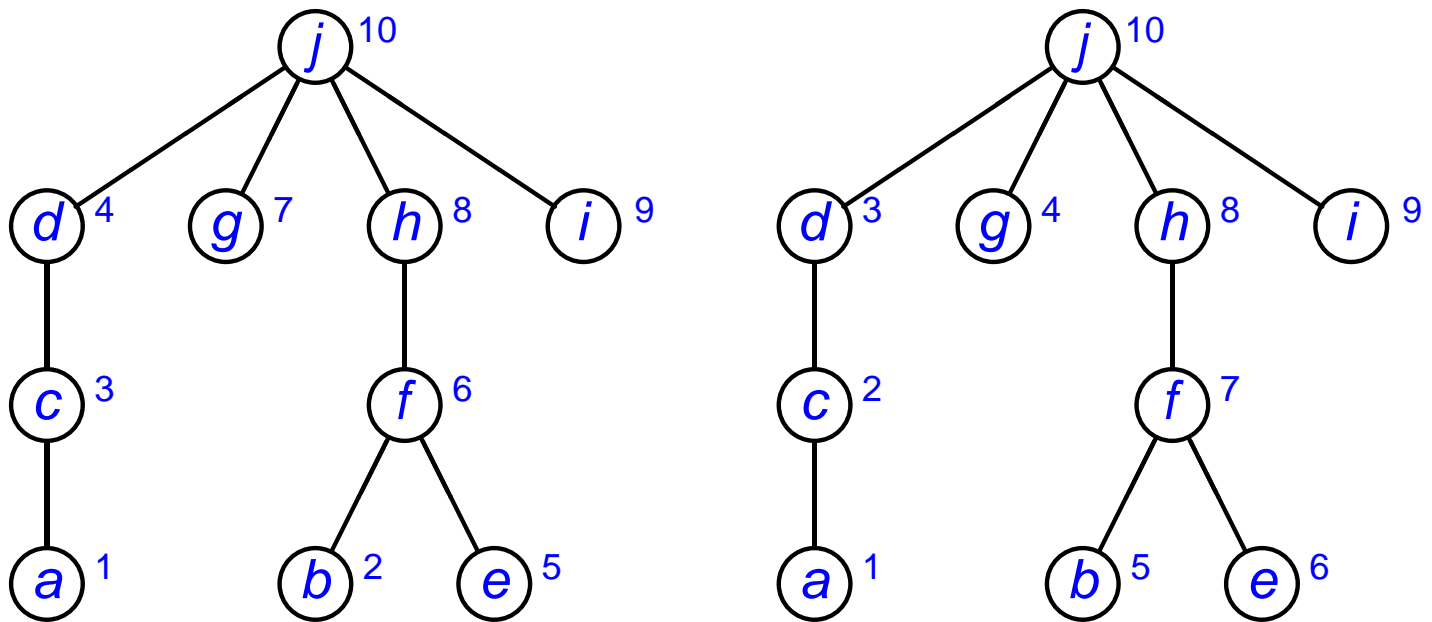


Property: The vertices in $\mathcal{T}[k]$ form a strongly connected component of the subgraph of the directed graph $G(A)$ induced by **any** set of vertices that contains $\mathcal{T}[k]$ but **no** ancestors of k in $T(A)$



POSTORDERING OF $T(A)$

If c_1, \dots, c_t are the children of k in $T(A)$, then number the vertices within each subtree $T[c_i]$ consecutively and number k immediately after its descendants



Postordering does **not** preserve the filled graph
{ more fill and work in practice? }

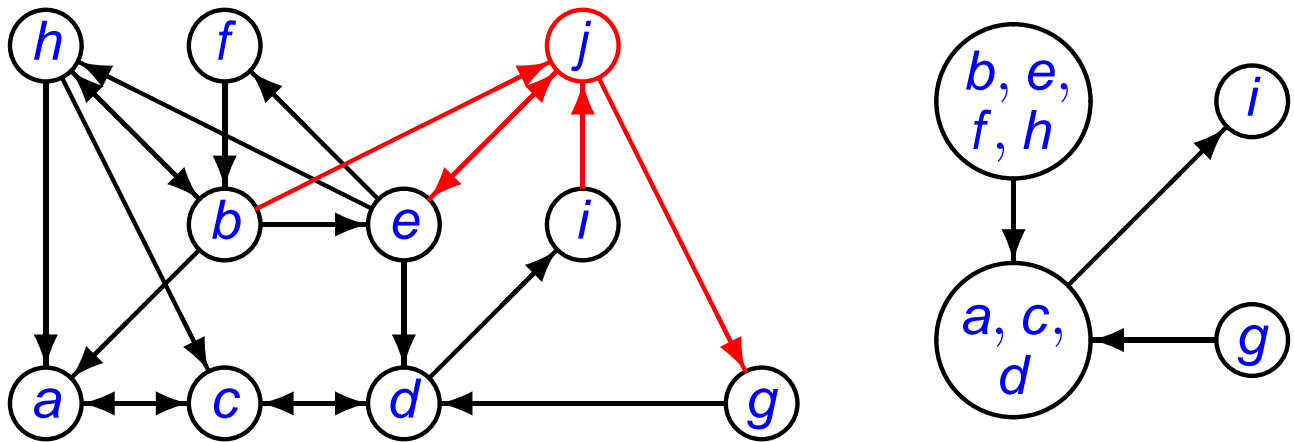
Postordering **does** preserve the structure of $T(A)$; i.e.,
 $T(PAP^t)$ is isomorphic to $T(A)$

Postordering **does** preserve the values of the diagonal elements of U ; i.e., $\text{diag}(U) = P^t \text{diag}(U(PAP^t)) P$
{ impact on numerical stability? }

UPPER BBT POSTORDERING

Postordering does **not** specify the order in which the subtrees $\mathcal{T}[c_i]$ themselves are numbered

From the subgraph of $G(A)$ induced by the vertices in $\mathcal{T}[k] \setminus \{k\} = \cup_{i=1, t} \mathcal{T}[c_i]$, form the **quotient graph** $Q_k(A)$ by coalescing the vertices in each $\mathcal{T}[c_i]$

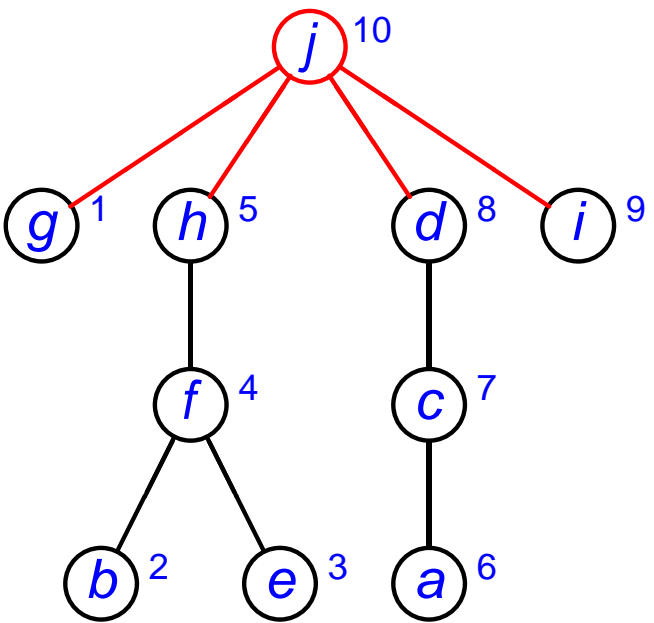
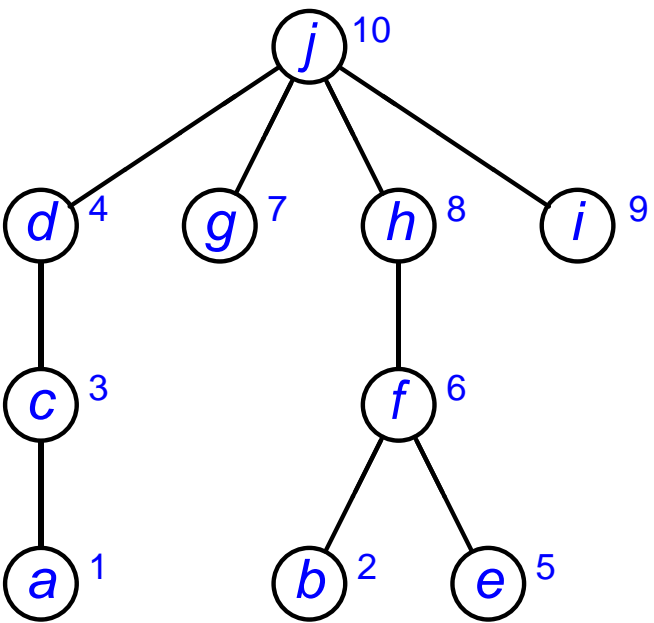


$Q_k(A)$ is **acyclic** {since each $\mathcal{T}[c_i]$ is a component}

If we use a **topological sort** of $Q_k(A)$ to order the $\mathcal{T}[c_i]$ during the postordering, every edge in $G(A)$ from a vertex in $\mathcal{T}[c_i]$ to a vertex in $\mathcal{T}[c_j]$ ($j \neq i$) goes from the lower-numbered to the higher-numbered vertex

Thus the permuted matrix is in **upper bordered block triangular (BBT)** form

UPPER BBT POSTORDERING (continued)



$(PAP^t)^+ =$

g									
	b	•		•	•				•
		e	•	•				•	•
	•		f	•	•	•	•	•	•
	•			h	•	•	•	•	•
					a	•			
						c	•		
							d	•	
									i
	•	•	•	•	•	•	•	•	j

{the bordered block triangular structure is recursive}

UPWARD-LOOKING LU FACTORIZATION

Algorithm

```
for  $k := 1$  to  $n$  do
   $z = A_{k*}$ 
  for  $i := 1$  to  $k - 1$  do {sparsely}
    if  $z_i \neq 0$  then
       $l_{ki} = z_i / u_{ii}; z = z - l_{ki} \times U_{i*}$ 
    end if
  end for
   $U_{k*} = z$ 
end for
```

If $l_{ki} \neq 0$, then the k -th row of L and U depends on the i -th row of U (and, indirectly, the i -th row of L)

Therefore $G(L)$ captures the data dependencies among the rows of A^+ {i.e., the potential parallelism}

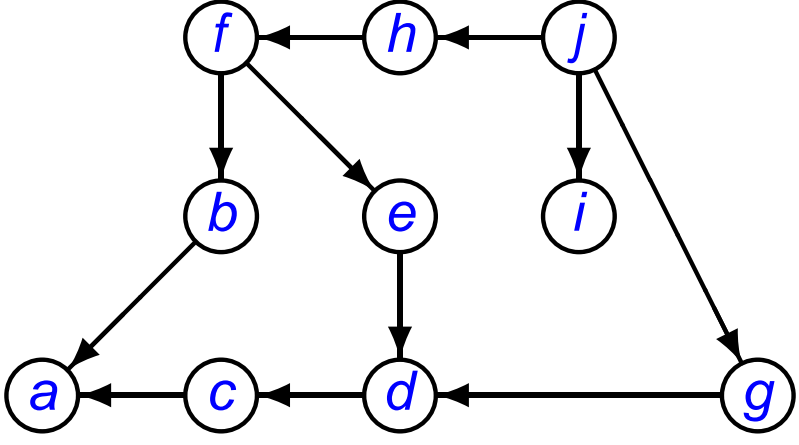
Its transitive reduction $G(L^\circ)$ preserves paths and thus is a minimal representation of these dependencies
{ $G(L^\circ)$ is one of the elimination dags [Gilbert+L]}

UPWARD-LOOKING FACTORIZATION (continued)

Filled Matrix

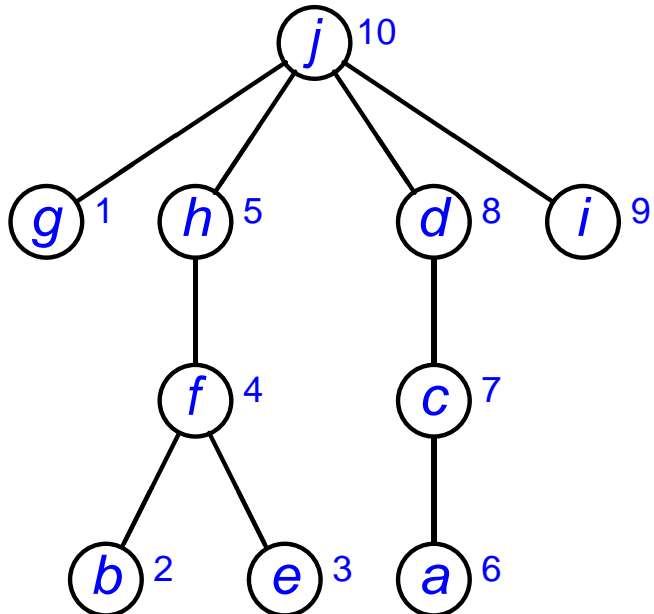
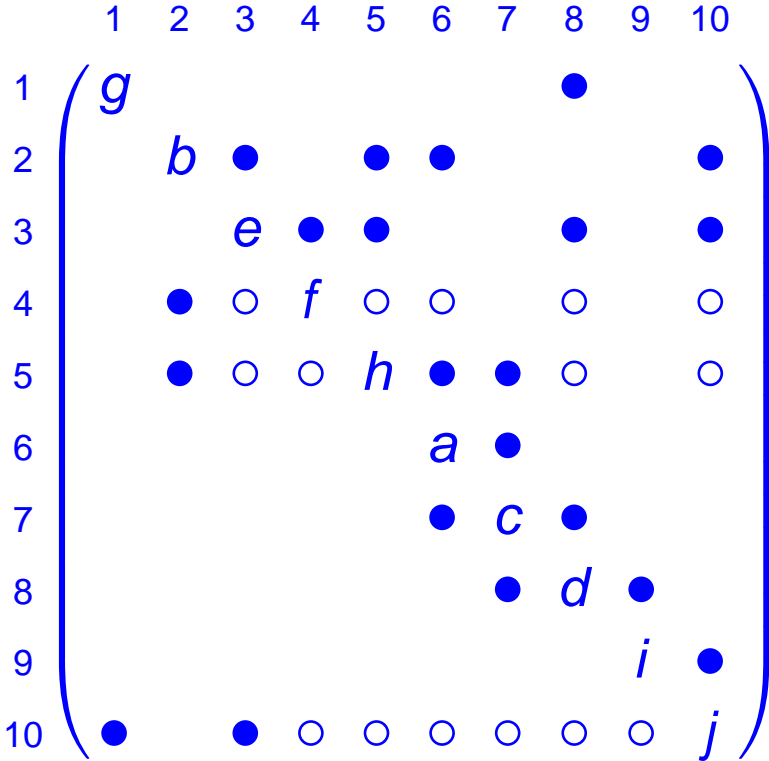
$$A^+ = \begin{matrix} & \begin{matrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \end{matrix} & \begin{pmatrix} a & & \bullet & & & & & & & \\ \bullet & b & \circ & & \bullet & & & \bullet & & \bullet \\ \bullet & & c & \bullet & & & & & & \\ & & \bullet & d & & & & & \bullet & \\ & & & \bullet & e & \bullet & & \bullet & \circ & \bullet \\ & & \bullet & \circ & \circ & f & & \circ & \circ & \circ \\ & & & \bullet & & & g & & \circ & \\ \bullet & \bullet & \bullet & \circ & \circ & \circ & & h & \circ & \circ \\ & & & & & & & & i & \bullet \\ & & & & \bullet & \circ & \bullet & \circ & \circ & j \end{pmatrix} \end{matrix}$$

Elimination DAG $G(L^0)$

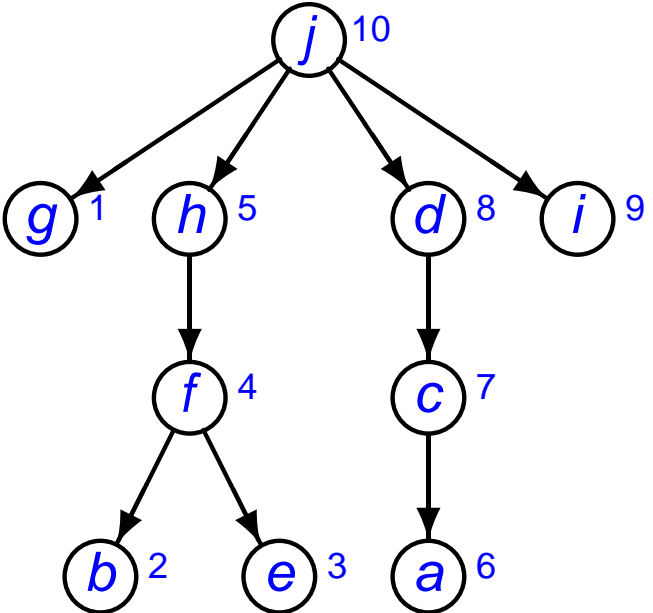


UPWARD-LOOKING FACTORIZATION (continued)

Definition: A is **upper BBT ordered** if the natural ordering is an upper BBT postordering of $T(A)$.



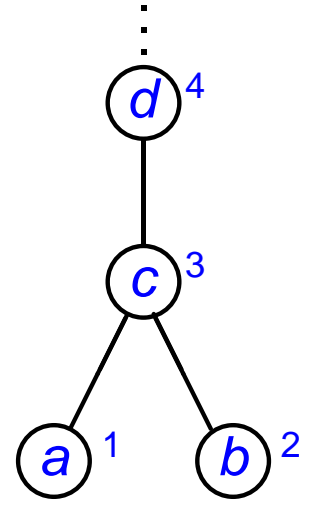
Theorem: If A is upper BBT ordered, then $G(L^0)$ is $T(A)$ with edges directed from parent to child.



SYMMETRIC MULTIFRONTAL [Speelpenning]

Goal: Use dense matrices as much as possible

$$A^+ \equiv \begin{matrix} & \begin{matrix} 1 & 2 & 3 & 4 & 5 & 6 \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \end{matrix} & \begin{pmatrix} a & & \bullet & & & \bullet \\ & b & \bullet & \bullet & & \\ \bullet & \bullet & c & \circ & \bullet & \circ \\ & \bullet & \circ & d & \bullet & \circ \\ & & \bullet & \bullet & e & \bullet \\ \bullet & & \circ & \circ & \bullet & f \end{pmatrix} \end{matrix}$$



$$\mathcal{F}_1 \equiv \begin{matrix} & \begin{matrix} 1 & 3 & 6 \end{matrix} \\ \begin{matrix} 1 \\ 3 \\ 6 \end{matrix} & \begin{pmatrix} a & \bullet & \bullet \\ \bullet & & \\ \bullet & & \end{pmatrix} \end{matrix},$$

$$\mathcal{U}_1 \equiv \begin{matrix} & \begin{matrix} 3 & 6 \end{matrix} \\ \begin{matrix} 3 \\ 6 \end{matrix} & \begin{pmatrix} \circ & \circ \\ \circ & \circ \end{pmatrix} \end{matrix}$$

$$\mathcal{F}_2 \equiv \begin{matrix} & \begin{matrix} 2 & 3 & 4 \end{matrix} \\ \begin{matrix} 2 \\ 3 \\ 4 \end{matrix} & \begin{pmatrix} b & \bullet & \bullet \\ \bullet & & \\ \bullet & & \end{pmatrix} \end{matrix},$$

$$\mathcal{U}_2 \equiv \begin{matrix} & \begin{matrix} 3 & 4 \end{matrix} \\ \begin{matrix} 3 \\ 4 \end{matrix} & \begin{pmatrix} \circ & \circ \\ \circ & \circ \end{pmatrix} \end{matrix}$$

$$\mathcal{F}_3 \equiv \begin{matrix} & \begin{matrix} 3 & 4 & 5 & 6 \end{matrix} \\ \begin{matrix} 3 \\ 4 \\ 5 \\ 6 \end{matrix} & \begin{pmatrix} \bullet & \circ & \bullet & \circ \\ \circ & \circ & & \\ \bullet & & & \\ \circ & & & \circ \end{pmatrix} = \begin{matrix} & \begin{matrix} 3 & 5 \end{matrix} \\ \begin{matrix} 3 \\ 5 \end{matrix} & \begin{pmatrix} c & \bullet \\ \bullet & \end{pmatrix} \end{matrix} \leftrightarrow \mathcal{U}_1 \leftrightarrow \mathcal{U}_2$$

{ \leftrightarrow denotes the extend-add operator}

SYMMETRIC MULTIFRONTAL (continued)

Algorithm

for $k := 1$ to n do

Assemble **frontal matrix** \mathcal{F}_k from the nonzeros in

$[a_{ik}]_{k \leq i \leq n}$ and all **updates** \mathcal{U}_c with $\rho(c) = k$

$$\text{Factor } \mathcal{F}_k = \begin{pmatrix} l_{kk} & & \\ [l_{ik}]_{k < i \leq n, l_{ik} \neq 0} & & I \end{pmatrix} \times \begin{pmatrix} 1 & & \\ & & \\ & & \mathcal{U}_k \end{pmatrix} \\ \times \begin{pmatrix} l_{kk} & [l_{jk}]_{k < j \leq n, l_{jk} \neq 0}^t & \\ & & \\ & & I \end{pmatrix}$$

end for

Why It Works

$\rho(k)$ is the **first** row/column to which \mathcal{U}_k contributes;
and (nesting property)

$$\text{struct}(l_{pk}, \dots, l_{nk}) \subseteq \text{struct}(l_{pp}, \dots, l_{np}),$$

with $p = \rho(k)$, so $\mathcal{F}_{\rho(k)}$ can accommodate all of \mathcal{U}_k
{ entries not in row/column $\rho(k)$ are added to $\mathcal{U}_{\rho(k)}$ }

UNSYMMETRIC MULTIFRONTAL?

Algorithm

for $k := 1$ to n do

Assemble frontal matrix \mathcal{F}_k from nonzeros in

$[a_{ik}]_{k \leq i \leq n}$, $[a_{kj}]_{k \leq j \leq n}$, and all **unassembled**

updates \mathcal{U}_m that contribute to row or column k

$$\text{Factor } \mathcal{F}_k = \begin{pmatrix} l_{kk} & & \\ [l_{ik}]_{k < i \leq n, l_{ik} \neq 0} & & \\ & & I \end{pmatrix} \times \begin{pmatrix} 1 & & \\ & & \\ & & \mathcal{U}_k \end{pmatrix} \\ \times \begin{pmatrix} u_{kk} & [u_{kj}]_{k < j \leq n, u_{kj} \neq 0} & \\ & & \\ & & I \end{pmatrix}$$

end for

Implicit Assumptions

- Rows (resp., columns) of \mathcal{F}_k correspond to rows i where $l_{ik} \neq 0$ (resp., columns j with $u_{kj} \neq 0$)
- Each update matrix \mathcal{U}_m can be assembled into a *single* frontal matrix

EXAMPLE

$$A^+ = \begin{matrix} & \begin{matrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \end{matrix} & \left(\begin{array}{cccccccccc} a & & \bullet & & & & & & & \\ \bullet & b & \circ & & \bullet & & & \bullet & & \bullet \\ \bullet & & c & \bullet & & & & & & \\ & & \bullet & d & & & & & \bullet & \\ & & & \bullet & e & \bullet & & \bullet & \circ & \bullet \\ & \bullet & \circ & \circ & \circ & f & & \circ & \circ & \circ \\ & & & \bullet & & & g & & \circ & \\ \bullet & \bullet & \bullet & \circ & \circ & \circ & & h & \circ & \circ \\ & & & & & & & & i & \bullet \\ & & & & \bullet & \circ & \bullet & \circ & \circ & j \end{array} \right) \end{matrix}$$

$$\mathcal{F}_1 = \begin{matrix} & \begin{matrix} 1 & 3 \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 8 \end{matrix} & \left(\begin{array}{cc} a & \bullet \\ \bullet & \\ \bullet & \\ \bullet & \end{array} \right), & \mathcal{U}_1 = \begin{matrix} & \begin{matrix} 3 \end{matrix} \\ \begin{matrix} 2 \\ 3 \\ 8 \end{matrix} & \left(\begin{array}{c} \circ \\ \circ \\ \circ \end{array} \right), & \mathcal{F}_2 = \begin{matrix} & \begin{matrix} 2 & 3 & 5 & 8 & 10 \end{matrix} \\ \begin{matrix} 2 \\ 6 \\ 8 \end{matrix} & \left(\begin{array}{ccccc} b & \circ & \bullet & \bullet & \bullet \\ \bullet & & & & \\ \bullet & & & & \end{array} \right)$$

\mathcal{U}_1 contains a contribution to row 2 but \mathcal{F}_2 cannot accommodate the (3, 3) entry of \mathcal{U}_1

Thus conditions (a) and (b) are incompatible in general
 {but both are valid when A is structurally symmetric}

(b) BUT NOT (a) APPROACH [Duff+Reid]

Assume every nonzero entry in $A + A^t$ is structurally nonzero in A {i.e., make A structurally symmetric}

Expanded frontal matrix $\tilde{\mathcal{F}}_k$ has the symmetric row/column set $\{i \mid i \geq k \text{ and } \tilde{\ell}_{ik} \neq 0\}$, where $A + A^t = \tilde{L}\tilde{L}^t$

The updates come from the children of k in $T(A + A^t)$

Improvement: [Amestoy+Puglisi] Suppress the rows and columns of $\tilde{\mathcal{F}}_k$ that are structurally zero, e.g.,

$$\tilde{\mathcal{F}}_2 \equiv \begin{matrix} & \begin{matrix} 2 & 3 & 5 & 8 & 10 \end{matrix} \\ \begin{matrix} 2 \\ 3 \\ 6 \\ 8 \end{matrix} & \begin{pmatrix} b & \circ & \bullet & \bullet & \bullet \\ & \circ & & & \\ \bullet & & & & \\ \bullet & \circ & & & \end{pmatrix} \end{matrix} = \begin{matrix} & \begin{matrix} 2 & 5 & 8 & 10 \end{matrix} \\ \begin{matrix} 2 \\ 6 \\ 8 \end{matrix} & \begin{pmatrix} b & \bullet & \bullet & \bullet \\ \bullet & & & \\ \bullet & & & \end{pmatrix} \end{matrix} \leftrightarrow \mathcal{U}_1$$

{rows 5 and 10 and column 6 are structurally zero}

Since the entries in row/column k can still be structurally zero, some entries in corresponding columns/rows of the update can also be zero

(possibly extra storage and work)

(a) BUT NOT (b) APPROACH [Hadfield+Davis; Gupta]

Decompose \mathcal{U}_1 as

$$\mathcal{U}_1 \equiv \begin{matrix} & & 3 \\ & 2 & \\ & 3 & \\ & 8 & \end{matrix} \begin{pmatrix} \circ \\ \circ \\ \circ \end{pmatrix} = \begin{matrix} & & 3 \\ & 2 & \\ & 3 & \end{matrix} \begin{pmatrix} \circ \\ \circ \end{pmatrix} \leftrightarrow \begin{matrix} & & 3 \\ & 3 & \\ & 8 & \end{matrix} \begin{pmatrix} \circ \\ \circ \\ \circ \end{pmatrix} \equiv \mathcal{U}_1^2 \leftrightarrow \mathcal{U}_1^3$$

and assemble row \mathcal{U}_1^2 into \mathcal{F}_2 and column \mathcal{U}_1^3 into \mathcal{F}_3

Decompose \mathcal{U}_k by repeatedly removing the row/column of **lowest** index i and assembling it into \mathcal{F}_i

Improvement: Stop when \mathcal{F}_i can accommodate **all** entries in what remains of \mathcal{U}_k , i.e., (nesting property)

$$\text{struct}(\ell_{ik}, \dots, \ell_{nk}) \subseteq \text{struct}(\ell_{ii}, \dots, \ell_{ni})$$

$$\text{struct}(u_{ki}, \dots, u_{kn}) \subseteq \text{struct}(u_{ii}, \dots, u_{in})$$

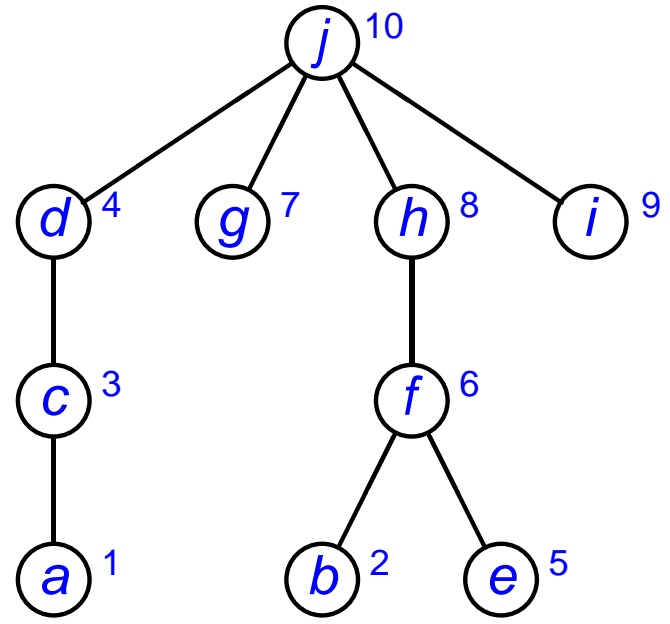
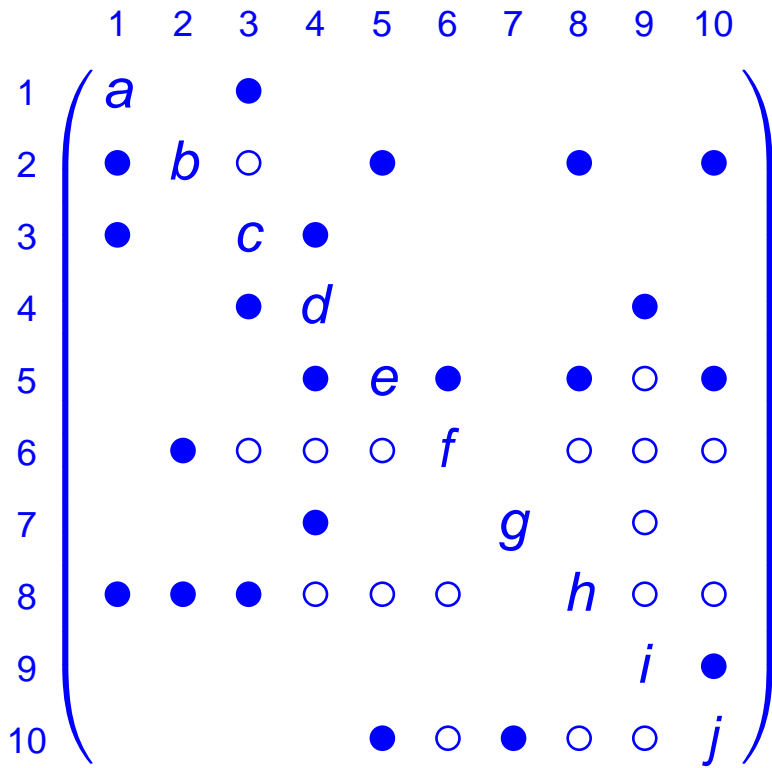
Theorem: [E+L]

$$\text{struct}(\ell_{pk}, \dots, \ell_{nk}) \subseteq \text{struct}(\ell_{pp}, \dots, \ell_{np})$$

$$\text{struct}(u_{kp}, \dots, u_{kn}) \subseteq \text{struct}(u_{pp}, \dots, u_{pn})$$

if $p = \rho(k) \equiv \min\{x \mid x > k \text{ and } x \xrightarrow{L} k \xrightarrow{U} x\}$.

EXAMPLE



$$\mathcal{F}_2 \equiv \begin{matrix} & & 2 & 3 & 5 & 8 & 10 \\ 2 & & \left(\begin{matrix} b & \circ & \bullet & \bullet & \bullet \end{matrix} \right) \\ 6 & & \left(\begin{matrix} \bullet \\ \bullet \\ \bullet \end{matrix} \right) \\ 8 & & \left(\begin{matrix} \bullet \end{matrix} \right) \end{matrix} = \begin{matrix} & & 2 & 5 & 8 & 10 \\ 2 & & \left(\begin{matrix} b & \bullet & \bullet & \bullet \end{matrix} \right) \\ 6 & & \left(\begin{matrix} \bullet \\ \bullet \\ \bullet \end{matrix} \right) \\ 8 & & \left(\begin{matrix} \bullet \end{matrix} \right) \end{matrix} \leftrightarrow \mathcal{U}_1^2$$

$$\mathcal{U}_2 \equiv \begin{matrix} & & 3 & 5 & 8 & 10 \\ 6 & & \left(\begin{matrix} \circ & \circ & \circ & \circ \end{matrix} \right) \\ 8 & & \left(\begin{matrix} \circ & \circ & \circ & \circ \end{matrix} \right) \end{matrix} = \begin{matrix} & & 3 \\ 6 & & \left(\begin{matrix} \circ \\ \circ \end{matrix} \right) \\ 8 & & \left(\begin{matrix} \circ \end{matrix} \right) \end{matrix} \leftrightarrow \begin{matrix} & & 5 \\ 6 & & \left(\begin{matrix} \circ \\ \circ \end{matrix} \right) \\ 8 & & \left(\begin{matrix} \circ \end{matrix} \right) \end{matrix} \leftrightarrow \begin{matrix} & & 8 & 10 \\ 6 & & \left(\begin{matrix} \circ & \circ \end{matrix} \right) \\ 8 & & \left(\begin{matrix} \circ & \circ \end{matrix} \right) \end{matrix}$$

$$\equiv \mathcal{U}_2^3 \leftrightarrow \mathcal{U}_2^5 \leftrightarrow \mathcal{U}_2^{\rho(2)}$$

EXAMPLE (continued)

$$\mathcal{F}_3 \equiv \begin{matrix} & 3 & 4 \\ 3 & \bullet & \bullet \\ 4 & \bullet & \\ 6 & \circ & \\ 8 & \bullet & \end{matrix} = \begin{matrix} & 3 & 4 \\ 3 & c & \bullet \\ 4 & \bullet & \\ 8 & \bullet & \end{matrix} \leftrightarrow \mathcal{U}_1^3 \leftrightarrow \mathcal{U}_2^3$$

$$\mathcal{U}_3 = \begin{matrix} & 4 \\ 4 & \circ \\ 6 & \circ \\ 8 & \circ \end{matrix} \equiv \mathcal{U}_3^{\rho(3)}$$

$$\mathcal{F}_4 \equiv \begin{matrix} & 4 & 9 \\ 4 & \bullet & \bullet \\ 5 & \bullet & \\ 6 & \circ & \\ 7 & \bullet & \\ 8 & \circ & \end{matrix} = \begin{matrix} & 4 & 9 \\ 4 & d & \bullet \\ 5 & \bullet & \\ 7 & \bullet & \end{matrix} \leftrightarrow \mathcal{U}_3^4$$

$$\mathcal{U}_4 \equiv \begin{matrix} & 9 \\ 5 & \circ \\ 6 & \circ \\ 7 & \circ \\ 8 & \circ \end{matrix} = \begin{matrix} & 9 \\ 5 & \circ \end{matrix} \leftrightarrow \begin{matrix} & 9 \\ 6 & \circ \end{matrix} \leftrightarrow \begin{matrix} & 9 \\ 7 & \circ \end{matrix} \leftrightarrow \begin{matrix} & 9 \\ 8 & \circ \end{matrix}$$

$$\equiv \mathcal{U}_4^5 \leftrightarrow \mathcal{U}_4^6 \leftrightarrow \mathcal{U}_4^7 \leftrightarrow \mathcal{U}_4^8$$

$\{\mathcal{U}_4^{\rho(4)} \text{ is the null matrix}\}$

EXAMPLE (continued)

$$\mathcal{F}_5 \equiv \begin{matrix} & 5 & 6 & 8 & 9 & 10 \\ \begin{matrix} 5 \\ 6 \\ 8 \\ 10 \end{matrix} & \begin{pmatrix} e & \bullet & \bullet & \circ & \bullet \\ \circ & & & & \\ \circ & & & & \\ \bullet & & & & \end{pmatrix} \end{matrix} = \begin{matrix} & 5 & 6 & 8 & 10 \\ \begin{matrix} 5 \\ 10 \end{matrix} & \begin{pmatrix} e & \bullet & \bullet & \bullet \\ \bullet & & & \end{pmatrix} \end{matrix} \leftrightarrow \mathcal{U}_2^5 \leftrightarrow \mathcal{U}_4^5$$

$$\mathcal{U}_5 = \begin{matrix} & 6 & 8 & 9 & 10 \\ \begin{matrix} 6 \\ 8 \\ 10 \end{matrix} & \begin{pmatrix} \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ \end{pmatrix} \end{matrix} \equiv \mathcal{U}_5^{\rho(5)}$$

$$\mathcal{F}_6 \equiv \begin{matrix} & 6 & 8 & 9 & 10 \\ \begin{matrix} 6 \\ 8 \\ 10 \end{matrix} & \begin{pmatrix} f & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ \\ \circ & \circ & \circ & \circ \end{pmatrix} \end{matrix} = \begin{matrix} & 6 \\ \begin{matrix} 6 \end{matrix} & \begin{pmatrix} f \end{pmatrix} \end{matrix} \leftrightarrow \mathcal{U}_2^6 \leftrightarrow \mathcal{U}_4^6 \leftrightarrow \mathcal{U}_5^6$$

$$\mathcal{U}_6 = \begin{matrix} & 8 & 9 & 10 \\ \begin{matrix} 8 \\ 10 \end{matrix} & \begin{pmatrix} \circ & \circ & \circ \\ \circ & \circ & \circ \end{pmatrix} \end{matrix} \equiv \mathcal{U}_6^{\rho(6)}$$

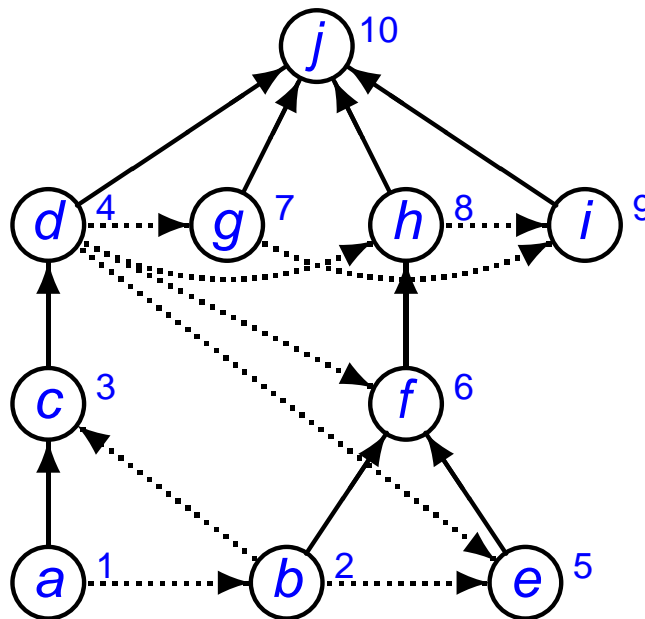
{nonzeros in \mathcal{U}_2^6 and \mathcal{U}_5^6 are not limited to the leftmost column and topmost row of \mathcal{F}_6 }

DATAFLOW GRAPH $D(A)$

Each vertex k corresponds to a frontal matrix / update

Each **solid** edge is a tree edge and corresponds to a
{possibly null} update $\mathcal{U}_k^{\rho(k)}$ to frontal matrix $\mathcal{F}_{\rho(k)}$

Each **dotted** cross edge corresponds to a nonnull
update \mathcal{U}_k^s to frontal matrix \mathcal{F}_s with $k < s < \rho(k)$



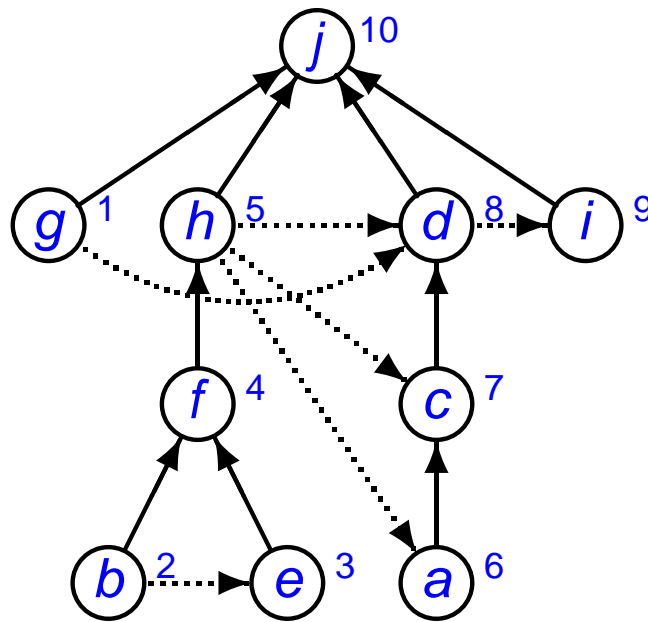
The dataflow graph for the “(b) but not (a)” approach is

$T(A + A^t)$ {a chain for the example above}

Theorem: If $x \mapsto y$ is an edge in $D(A)$, then y is an ancestor of x in $T(A + A^t)$.

{possibly more exploitable parallelism}

UPPER BBT POSTORDERING REVISITED



Theorem: When A is upper BBT ordered,

$$\rho(k) = \min\{x \mid x > k \text{ and } x \xrightarrow{L} k \xrightarrow{U} x\};$$

the decomposition of \mathcal{U}_k is by **columns**; and all cross edges lead to **older siblings and their descendants**.

Advantages

- simplifies the implementation
- enables a stack-based approach that reduces the storage required for updates

Disadvantages

- increased work and fill?

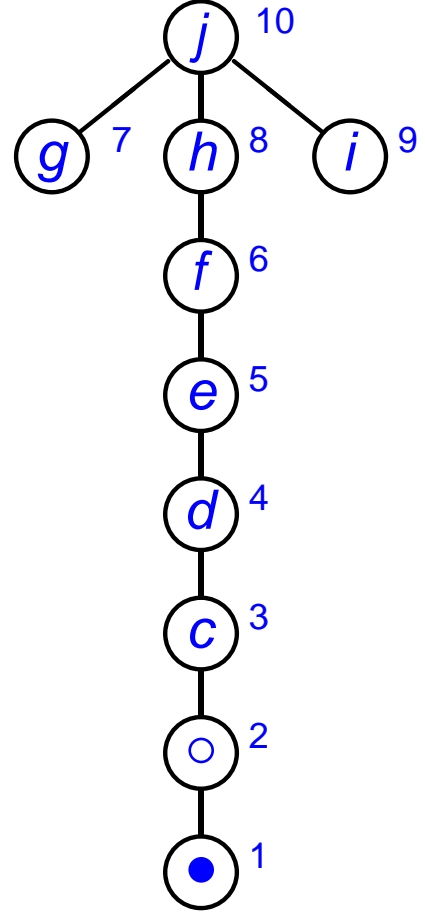
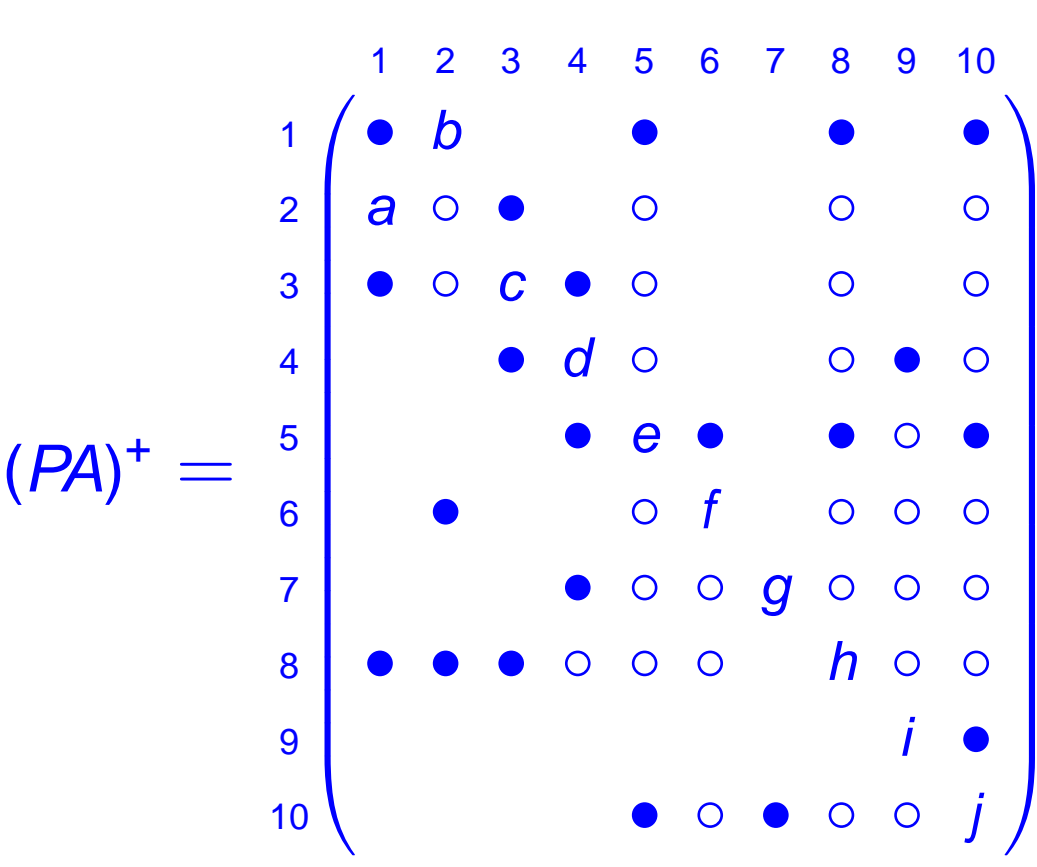
PIVOTING FOR STABILITY

SuperLU Approach {= No Pivoting} [Demmel+Li]:

Replace any pivot of magnitude less than $\sqrt{\epsilon} \|A\|_1$ by $\sqrt{\epsilon} \|A\|_1$ and use an extra stage of iterative refinement to compensate for the perturbation

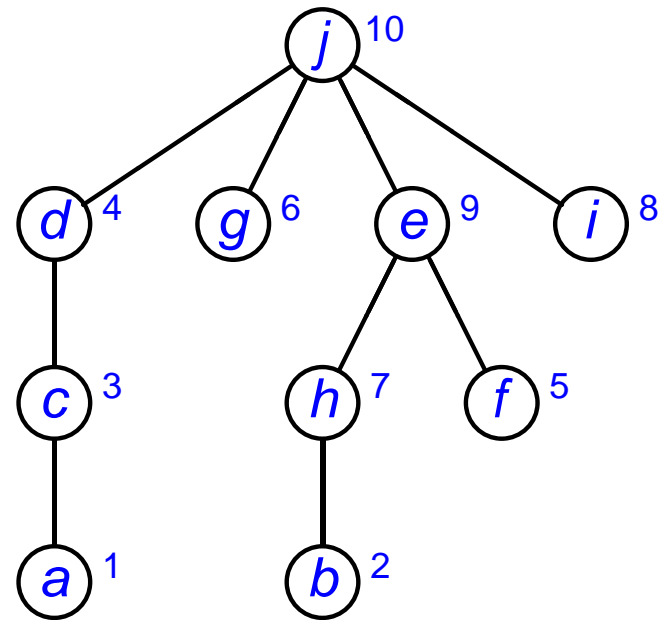
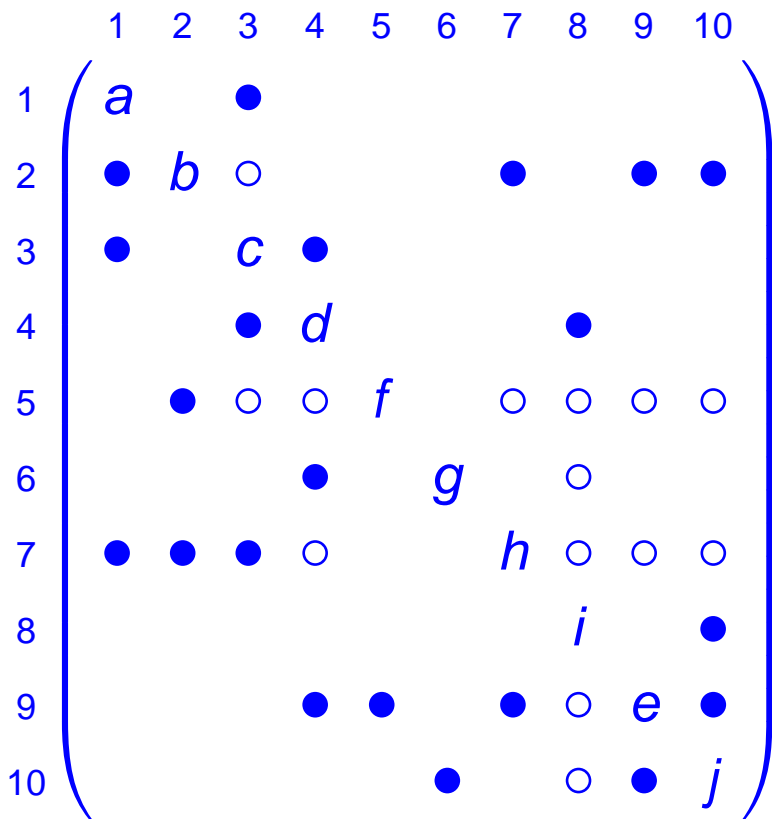
Unrestricted Pivoting

A **single** row or column interchange can completely destroy the structure of $T(A)$ and $D(A)$



PIVOTING FOR STABILITY (continued)

Delayed elimination: Symmetrically permute A so that row/column k immediately follows row/column m ; e.g., delaying e after i ,



Theorem: Let

$$S = \{k\} \cup \{x \mid k < x \leq m \text{ and } x \text{ ancestor of } k\}.$$

If $x \notin S$ and $\rho(x) \notin S$, then x has the same parent in $T(PAP^t)$.

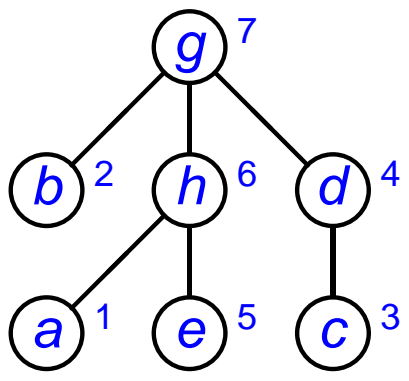
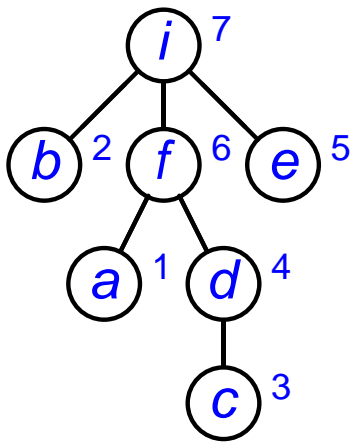
{Local effect on $T(A)$; insufficient alone in general}

PIVOTING FOR STABILITY (continued)

Pivoting within diagonal blocks (e.g., supernodes):

Exchange rows within a diagonal block; e.g.,

$$A = \begin{pmatrix} & 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ 1 & a & & & & & \bullet & \\ 2 & & b & & & & & \bullet \\ 3 & & & c & \bullet & & & \\ 4 & & & \bullet & d & & \bullet & \\ 5 & & & & & e & \bullet & \bullet \\ 6 & \bullet & & & \bullet & & f & g \\ 7 & \bullet & \bullet & & & \bullet & h & i \end{pmatrix}, \quad QA = \begin{pmatrix} & 1 & 2 & 3 & 4 & 5 & 6 & 7 \\ 1 & a & & & & & \bullet & \\ 2 & & b & & & & & \bullet \\ 3 & & & c & \bullet & & & \\ 4 & & & \bullet & d & & \bullet & \\ 5 & & & & & e & \bullet & \bullet \\ 6 & \bullet & \bullet & & & & h & i \\ 7 & \bullet & & & \bullet & & f & g \end{pmatrix}$$



Theorem: Let $S = \{k, k + 1, \dots, m\}$ and let Q be the permutation matrix that exchanges rows k and m . If $a_{ij} \neq 0$ for $i, j \in S$, then $T(QA)$ is the same as $T(A)$, except that the parent of each child $s \notin S$ in $T(A)$ of a vertex in S can now be any vertex in S .

{Local effect on $T(A)$; insufficient alone in general}

PIVOTING FOR STABILITY (continued)

Combined Approach [Duff+Reid]

If pivot k is unacceptable, delay that step of elimination until after the parent $p = \rho(k)$ of k is eliminated
{there is no change to the pivot value until then}

If pivot p is also unacceptable, then treat $\{p, k\}$ as a “supernode” and pivot within the supernodal block
{any extra fill is restricted to rows/columns p and k }

The effect on the elimination tree of each delayed elimination or row exchange is local

PIVOTING IN UNSYMMETRIC MULTIFRONTAL

Problem: \mathcal{F}_k has already been assembled when pivot k is evaluated and deemed unacceptable so the dataflow graph $D(PAP^t)$ or $D(QA)$ of the permuted matrix does **not** capture all flows

PIVOTING IN MULTIFRONTAL (continued)

Solution: Keep the **original** dataflow graph $D(A)$ but make k an assembly-only vertex at which we

- Assemble all updates contributing to row/column k into frontal matrix \mathcal{F}_k
- Permute row k immediately after row $p = \rho(k)$
{ $p \xrightarrow{L} k$ since A is upper BBT ordered }
- Permute column k either immediately after column p (if present) or to where column p would be (otherwise)
- Treat the **entire** \mathcal{F}_k as the update; that is, decompose it in the usual way with the pieces sent along edges in the dataflow graph to vertices between k and p in the original order

{ approach works when A is upper BBT ordered }

PIVOTING IN MULTIFRONTAL (continued)

$$(PAP^t)^+ = \begin{matrix} & \begin{matrix} 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 & 10 \end{matrix} \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \\ 6 \\ 7 \\ 8 \\ 9 \\ 10 \end{matrix} & \begin{pmatrix} g & & & & & & & \bullet & & \\ & b & \bullet & & \bullet & \bullet & & & & \bullet \\ & & e & \bullet & \bullet & & & \bullet & & \bullet \\ & \bullet & \circ & f & \circ & \circ & & \circ & & \circ \\ & \bullet & \circ & \circ & h & \bullet & \bullet & \circ & & \circ \\ & & & & & a & \bullet & & & \\ & & & & & \bullet & c & \bullet & & \\ & & & & & & \bullet & d & \bullet & \\ & & & & & & & & i & \bullet \\ \bullet & & \bullet & \circ & \circ & \circ & \circ & \circ & \circ & j \end{pmatrix} \end{matrix}$$

Delaying elimination of vertex 5 until after its parent 10,

$$\mathcal{U}_5 \equiv \begin{matrix} & \begin{matrix} 6 & 7 & 8 & 10 & 5 \end{matrix} \\ \begin{matrix} 10 \\ 5 \end{matrix} & \begin{pmatrix} \circ & \cdot & \circ & \circ & \circ \\ \bullet & \bullet & \circ & \circ & h \end{pmatrix} \end{matrix} = \mathcal{U}_5^6 \leftrightarrow \mathcal{U}_5^7 \leftrightarrow \mathcal{U}_5^8 \leftrightarrow \mathcal{U}_5^{10}$$

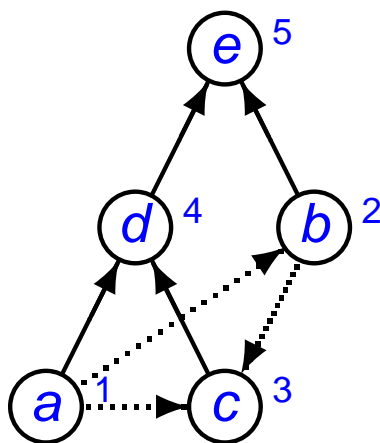
where \cdot denotes an entry that would have filled in and

$$\mathcal{U}_5^s = \begin{matrix} & s \\ \begin{matrix} 10 \\ 5 \end{matrix} & \begin{pmatrix} \circ \\ \bullet \end{pmatrix} \end{matrix}, \quad 6 \leq s \leq 8; \quad \mathcal{U}_5^{10} = \begin{matrix} & \begin{matrix} 10 & 5 \end{matrix} \\ \begin{matrix} 10 \\ 5 \end{matrix} & \begin{pmatrix} \circ & \circ \\ \circ & h \end{pmatrix} \end{matrix}$$

The recipient of \mathcal{U}_5^s expects an update to row 10; and vertex 10 (= supernode {10, 5}) can accommodate an update to column 5

WHAT IF A IS NOT BBT ORDERED?

$$\begin{matrix} & 1 & 2 & 3 & 4 & 5 \\ \begin{matrix} 1 \\ 2 \\ 3 \\ 4 \\ 5 \end{matrix} & \begin{pmatrix} a & \bullet & & \bullet & \\ & b & & & \bullet \\ \bullet & \circ & c & \circ & \circ \\ & & \bullet & d & \circ \\ & & & \bullet & e \end{pmatrix} \end{matrix}$$



$$\begin{matrix} & 2 & 3 & 4 & 1 & 5 \\ \begin{matrix} 2 \\ 3 \\ 4 \\ 1 \\ 5 \end{matrix} & \begin{pmatrix} b & & & & \bullet \\ & c & & \bullet & \\ & \bullet & d & \circ & \\ \bullet & & \bullet & a & \circ \\ & \bullet & \circ & e \end{pmatrix} \end{matrix}$$

Delaying elimination of vertex 1 until after its parent 4,

$$\begin{aligned}
 \mathcal{U}_1 &\equiv \begin{matrix} & 2 & 4 & 1 \\ \begin{matrix} 3 \\ 1 \end{matrix} & \begin{pmatrix} \cdot & \cdot & \bullet \\ \bullet & \bullet & a \end{pmatrix} \end{matrix} = \begin{matrix} & 2 \\ \begin{matrix} 3 \\ 1 \end{matrix} & \begin{pmatrix} \cdot \\ \bullet \end{pmatrix} \end{matrix} \leftrightarrow \begin{matrix} & 4 & 1 \\ \begin{matrix} 3 \end{matrix} & \begin{pmatrix} \cdot & \bullet \end{pmatrix} \end{matrix} \leftrightarrow \begin{matrix} & 4 & 1 \\ \begin{matrix} 1 \end{matrix} & \begin{pmatrix} \bullet & a \end{pmatrix} \\
 &\equiv \mathcal{U}_1^2 \leftrightarrow \mathcal{U}_1^3 \leftrightarrow \mathcal{U}_1^4
 \end{aligned}$$

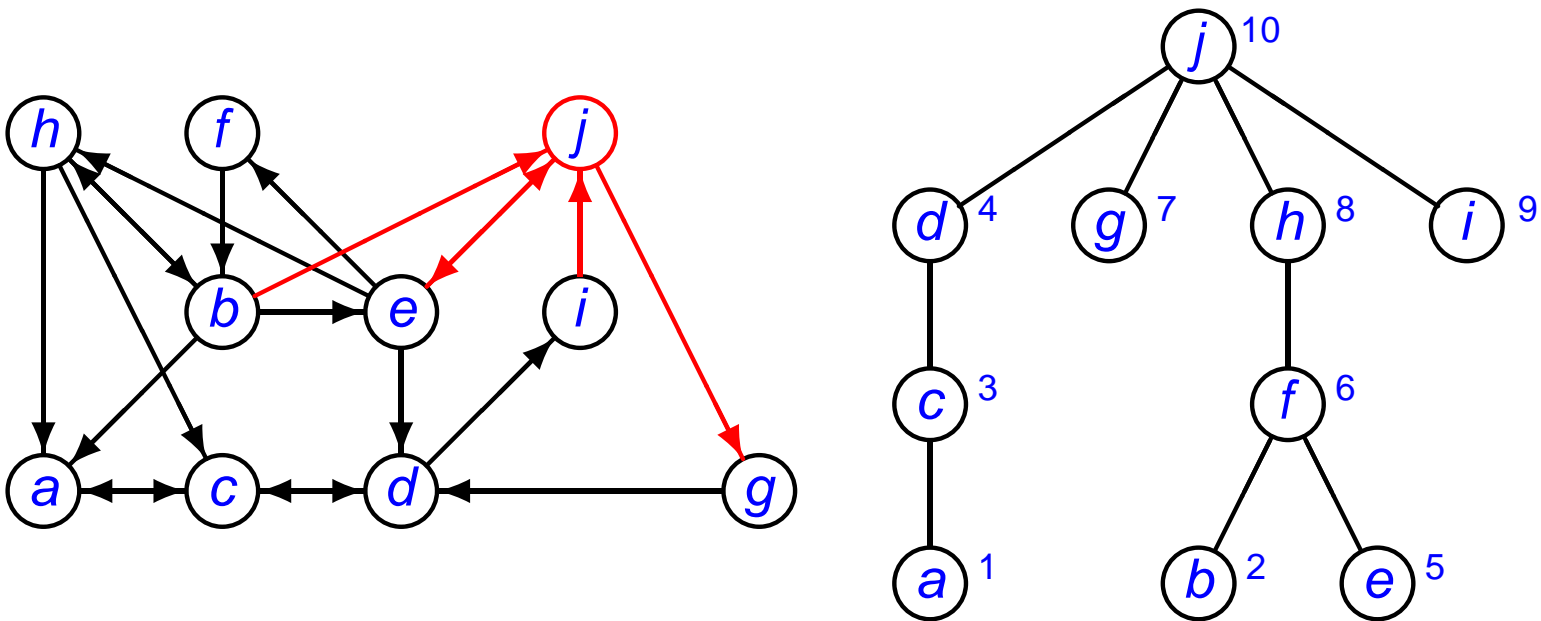
$$\mathcal{F}_2 \equiv \begin{matrix} & 2 & 5 \\ \begin{matrix} 2 \\ 3 \\ 1 \end{matrix} & \begin{pmatrix} b & \bullet \\ \cdot \\ \bullet \end{pmatrix} \end{matrix} = \begin{matrix} & 2 & 5 \\ \begin{matrix} 2 \end{matrix} & \begin{pmatrix} b & \bullet \end{pmatrix} \end{matrix} \leftrightarrow \mathcal{U}_1^2$$

$$\mathcal{U}_2 \equiv \begin{matrix} & 5 \\ \begin{matrix} 3 \\ 1 \end{matrix} & \begin{pmatrix} \circ \\ \circ \end{pmatrix} \end{matrix} = \begin{matrix} & 5 \\ \begin{matrix} 3 \end{matrix} & \begin{pmatrix} \circ \end{pmatrix} \end{matrix} \leftrightarrow \begin{matrix} & 5 \\ \begin{matrix} 1 \end{matrix} & \begin{pmatrix} \bullet \end{pmatrix} \end{matrix} \equiv \mathcal{U}_2^3 \leftrightarrow \mathcal{U}_2^4,$$

There is no edge from vertex 2 to vertex 4 (into which vertex 1 was coalesced) over which to send \mathcal{U}_2^4

FINDING THE ELIMINATION TREE $T(A)$

Theorem: k is the parent of c if and only if k is the **first** vertex after c such that k and c belong to the same strongly connected component of the subgraph $G_k(A)$ of $G(A)$ induced by $\{1, 2, \dots, k\}$.



Algorithm *eTree* {computes $\rho(k) \equiv \text{fpnz}(k)$ }

for $k = 1$ **to** n **do**

Find the component \mathcal{X} of $G_k(A)$ that contains k

for each $x \in \mathcal{X} \setminus \{k\}$ **do**

if $\text{fpnz}(x) = \infty$ **then** $\text{fpnz}(x) = k$

end for

$\text{fpnz}(k) = \infty$

end for

FINDING THE ELIMINATION TREE (continued)

Time = $O(ne)$, where e = the number of edges in $G(A)$
{ Finding the strongly connected components of
 $G_k(A)$ takes time $O(e_k)$, where e_k is the number of
vertices and edges in $G_k(A)$ reachable from k
[Tarjan; Gabow; ...] }

REDUCING THE EFFECTIVE SIZE

The strongly connected components of $G_k(A)$ induce
an **acyclic** quotient graph $G(Q_k)$ that succinctly
represents its connectivity [Pagallo+Maulino]:

Let x and y belong to components \mathcal{X} and \mathcal{Y} ;
then $x \Rightarrow y$ if and only if $\mathcal{X} = \mathcal{Y}$ or $\mathcal{X} \Rightarrow \mathcal{Y}$

Theorem: If \mathcal{X} is a component of $G_k(A)$, and m is the
highest-numbered vertex in \mathcal{X} , then $\mathcal{X} = \mathcal{T}[m]$.

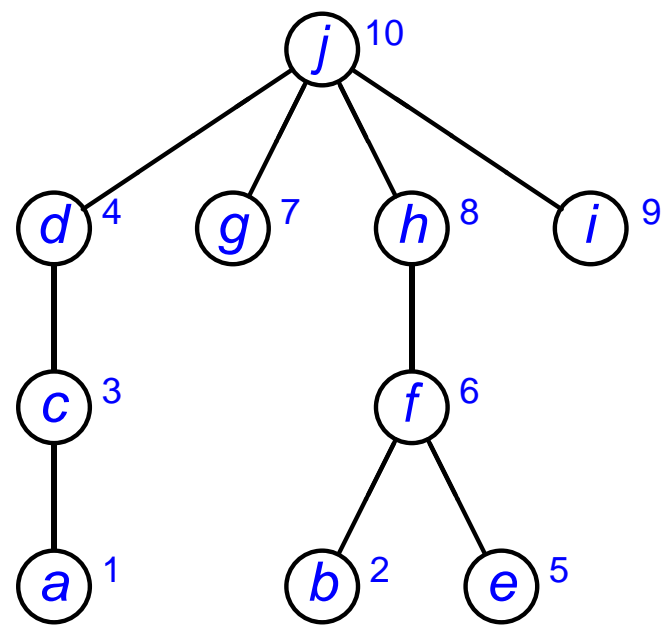
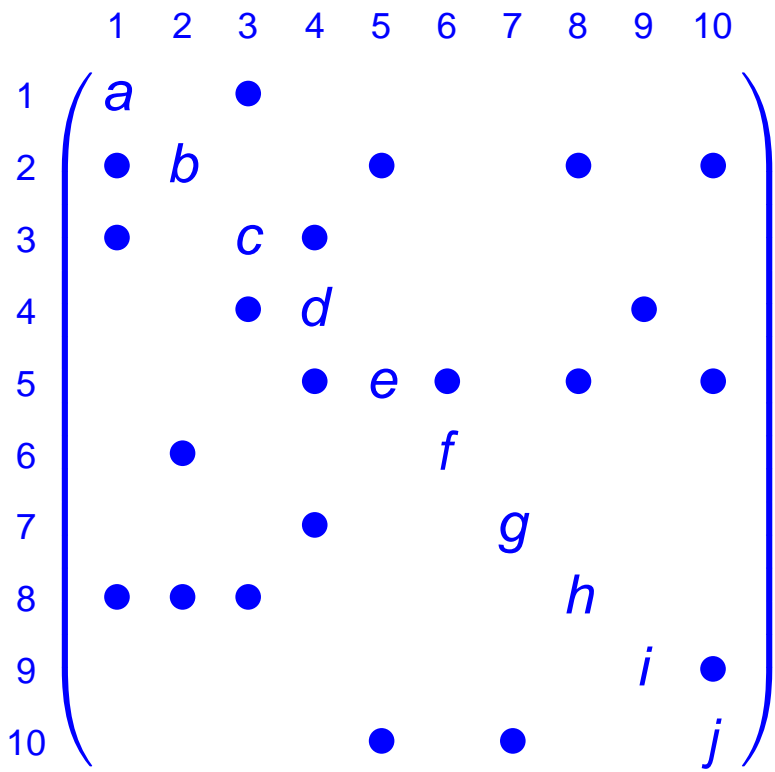
REDUCING THE EFFECTIVE SIZE (continued)

$G_k(A)$ can be obtained from $G_{k-1}(A)$ by

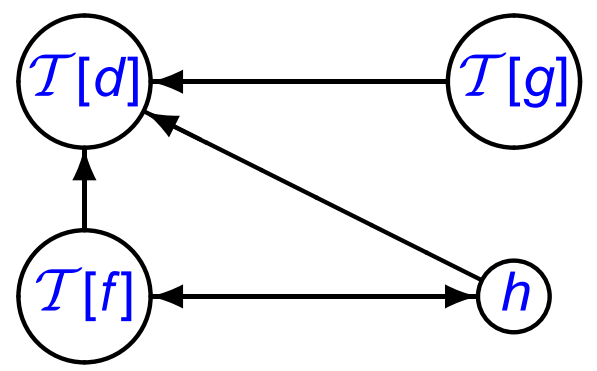
- adding vertex k ;
- adding all edges $u \xrightarrow{A} k$ with $u < k$
- adding all edges $k \xrightarrow{A} v$ with $v < k$

$G(Q_k)$ can be obtained from $G(Q_{k-1})$ in two steps:

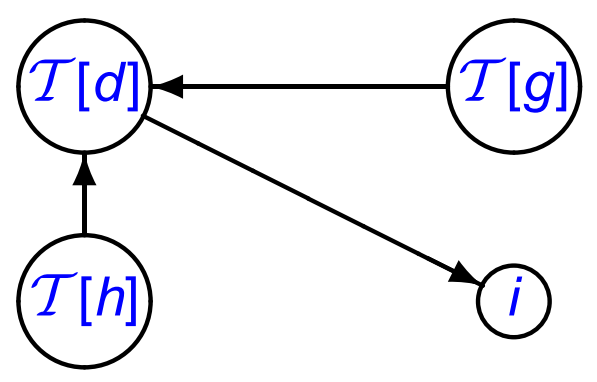
1. Form intermediate graph $G(Q'_k)$ from $G(Q_{k-1})$ by
 - adding vertex k ;
 - for each vertex $\mathcal{T}[u]$, adding edge $\mathcal{T}[u] \mapsto k$ if $x \xrightarrow{A} k$ for some $x \in \mathcal{T}[u]$; and
 - for each vertex $\mathcal{T}[v]$, adding edge $k \mapsto \mathcal{T}[v]$ if $k \xrightarrow{A} y$ for some $y \in \mathcal{T}[v]$
2. Form $G(Q_k)$ from $G(Q'_k)$ by coalescing k and all vertices in the strongly connected component of $G(Q'_k)$ that contains it into the new vertex $\mathcal{T}[k]$



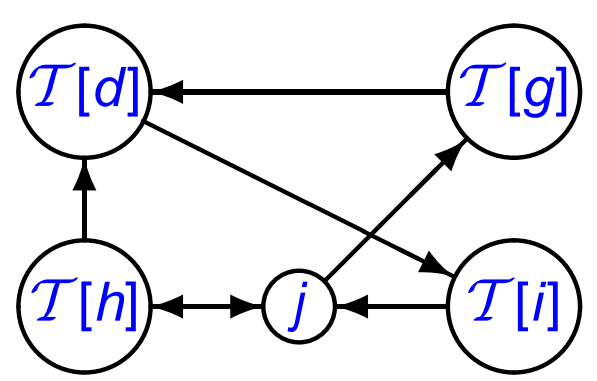
$$Q'_8 = \left(\begin{array}{ccc|c} \mathcal{T}[d] & & & \\ \bullet & \mathcal{T}[f] & & \bullet \\ \bullet & & \mathcal{T}[g] & \\ \hline \bullet & \bullet & & h \end{array} \right)$$



$$Q'_9 = \left(\begin{array}{ccc|c} \mathcal{T}[d] & & & \bullet \\ \bullet & \mathcal{T}[g] & & \\ \bullet & & \mathcal{T}[h] & \\ \hline & & & i \end{array} \right)$$



$$Q'_{10} = \left(\begin{array}{ccc|c} \mathcal{T}[d] & & & \bullet \\ \bullet & \mathcal{T}[g] & & \\ \bullet & & \mathcal{T}[h] & \bullet \\ \hline & & & \mathcal{T}[i] \\ & \bullet & \bullet & j \end{array} \right)$$



FINDING THE ELIMINATION TREE (continued)

Theorem: If $\mathcal{T}[c]$ is a vertex of $G(Q'_k)$ that is coalesced into $\mathcal{T}[k]$, then c is a child of k .

Algorithm *eTreeQ* {computes $\rho(k) \equiv \text{fpnz}(k)$ }

$G(Q_0) =$ empty graph

for $k = 1$ **to** n **do**

 Create $G(Q'_k)$ from $G(Q_{k-1})$ by adding k and its incident edges

 Find the component \mathcal{X} of $G(Q'_k)$ that contains k

for each $\mathcal{T}[c] \in \mathcal{X} \setminus \{k\}$ **do**

$\text{fpnz}(c) = k$

end for

 Create $G(Q_k)$ from $G(Q'_k)$ by coalescing

 the vertices in \mathcal{X} into the new vertex $\mathcal{T}[k]$

$\text{fpnz}(k) = \infty$

end for

{We can take advantage of the fact that $G(Q_{k-1})$ is an acyclic subgraph of $G(Q'_k)$ to find the component \mathcal{X} of $G(Q'_k)$ that contains k }

FINDING THE ELIMINATION TREE (continued)

{ Initialization prior to first call to $scc(k)$ }

for each v in $G(A)$ **do**

$visited[v] = inSC[v] = 0$

end for

Algorithm $scc(k)$

$inSC[k] = k$

$SC = \{k\}$

$dfs(k)$

return SC { = component of $G(Q'_k)$ containing k }

procedure $dfs(v)$

$visited[v] = k$

for each w adjacent to v in $G(Q'_k)$ **do**

if $visited[w] \neq k$ **then** $dfs(w)$

if $inSC[w] = k$ **then** $inSC[v] = k$

{ $inSC[w] = k$ if and only if $w \Rightarrow k$ in $G(Q'_k)$ }

end for

if $inSC[v] = k$ **then** $SC = SC \cup \{v\}$

end procedure

FINDING AN UPPER BBT ORDERING (continued)

Name	n	$\frac{nz(A)}{n}$	$symm$	$t_s(A)$ (ms)	$\frac{t_t(A)}{t_s(A)}$
Averous/epb1	14734	6.45	72.94	15.7	.47
Bai/rw5151	5146	3.92	0.01	5.5	.49
Goodwin/goodwin	7319	44.37	26.68	37.8	.48
Graham/graham1	8398	36.59	29.47	38.3	.49
Grund/bayer02	11710	4.63	7.44	7.2	1.24
Grund/bayer10	10803	5.76	8.86	6.2	1.24
HB/gemat11	4578	6.86	70.96	1.4	1.50
Hamrle/Hamrle2	5952	3.72	12.18	1.5	1.87
Hohn/fd12	6787	3.90	2.98	5.7	.74
Hohn/fd15	10645	3.92	3.03	10.5	.67
Hohn/fd18	15367	3.94	2.51	17.2	.66
Hohn/sinc12	6974	38.43	22.65	262.8	.07
Hollinger/g7jac040	11194	9.36	8.81	63.0	.85
Lucifora/cell1	7055	4.26	79.63	4.1	.71
Lucifora/cell2	7055	4.26	79.63	4.3	.67
Nasa/barth	5711	3.49	13.66	1.8	1.56
Nasa/barth4	5826	3.90	11.11	2.4	1.58
Nasa/barth5	12960	3.93	7.61	6.2	1.90
Shen/e40r0100	17281	32.03	88.69	39.3	.68
Shen/shermanACd	6042	6.99	61.65	3.2	.88
TOKAMAK/utm5940	5794	14.35	28.94	17.0	.31

FINDING AN UPPER BBT ORDERING

Let c_1, \dots, c_t be the children of k in $T(A)$

The subtrees $\mathcal{T}[c_1], \dots, \mathcal{T}[c_t]$ are the vertices of $G(Q_{k-1})$ that are coalesced into $\mathcal{T}[k]$ during the formation of $G(Q_k)$

For an upper BBT postordering c_i must be numbered before c_j if $x \mapsto y$ for some $x \in \mathcal{T}[c_i]$ and $y \in \mathcal{T}[c_j]$; i.e., $\mathcal{T}[c_i] \mapsto \mathcal{T}[c_j]$

In Algorithm **scc**, vertices are added to **SC** in the following order:

- Add vertex k first
- If $\mathcal{T}[c_i] \mapsto \mathcal{T}[c_j]$ in $G(Q'_k)$ and $\mathcal{T}[c_j] \in \mathbf{SC}$, then add $\mathcal{T}[c_i]$ to **SC** {i.e., **after** $\mathcal{T}[c_j]$ }

That is, ignoring vertex k , the reverse of this order satisfies the condition for an upper BBT postordering

{The additional runtime is negligible}

OTHER APPLICATIONS

Diagonal Markowitz Ordering [Amestoy+Li+Ng]

The algorithm for finding $T(A)$ can be extended to maintain a compact and efficient representation of the nonzero structure of the reduced matrix, which can be used to select diagonal pivots that locally minimize the work

Finding Supernodes

Supernodes (i.e., dense diagonal blocks) form chains in $T(A)$, which suggests both how to find them (via postordering) and how to relax their definition (cf. [Ashcraft+Grimes])

Symbolic Factorization

Using $\rho(k)$ and the nesting property, more edges can be pruned, making the algorithm more efficient
{path-symmetric symbolic factorization [E+L]}

SUMMARY

- The elimination tree $T(A)$ of an unsymmetric matrix
 - Properties of upper BBT postorderings of $T(A)$
 - A dataflow graph for unsymmetric multifrontal
 - The impact of pivoting for stability
 - Algorithms for finding $T(A)$
 - Other applications
-

CONCLUSION

$$\rho(k) \equiv \min\{x \mid x > k \text{ and } x \xrightarrow{L} k \xrightarrow{U} x\}$$

is the right generalization of elimination tree to
unsymmetric matrices

REFERENCES

The theory of elimination trees for sparse unsymmetric matrices, SIAM Journal on Matrix Analysis and Applications, 26(3):686–705, 2005

A tree-based dataflow model for the unsymmetric multifrontal method (to appear in *Electronic Transactions on Numerical Analysis*)

Algorithmic aspects of elimination trees for sparse unsymmetric matrices (in progress)