Direct Methods for Sparse Linear Systems:

MATLAB sparse backslash

Tim Davis

davis@cise.ufl.edu

University of Florida

So what is a sparse matrix ... ?

a matrix *“... that allows special techniques to take advantage of the large number of zero elements”* (Wilkinson)

sparse matrices arise in a wide range of applications ...

Sparse matrices arise in ...

computational fluid dynamics, finite-element methods, statistics, time/frequency domain circuit simulation, dynamic and static modeling of chemical processes, cryptography, magneto-hydrodynamics, electrical power systems, differential equations, quantum mechanics, structural mechanics (buildings, ships, aircraft, human body parts...), heat transfer, MRI reconstructions, vibroacoustics, linear and non-linear optimization, financial portfolios, semiconductor process simulation, economic modeling, oil reservoir modeling, astrophysics, crack propagation, Google page rank, 3D computer vision, cell phone tower placement, tomography, multibody simulation, model reduction, nano-technology, acoustic radiation, density functional theory, quadratic assignment, elastic properties of crystals, natural language processing, DNA electrophoresis, ...

Outline

- Sparse matrix algorithms: numerics plus graph theory
- Goal: sparse matrix methods from the ground up
- Lower triangular solve (`x=L\b`)
- Sparse LU factorization (`[L,U,P]=lu(A)`)
- Sparse Cholesky factorization (`L=chol(A)'`)
- Supernodal and multifrontal methods (`x=A\b`)
    - cache-friendly dense matrix kernels (BLAS)
    - supernodal (left-looking)
    - multifrontal (right-looking)

... next: sparse matrix data structures

Sparse data structures

- compressed sparse column format
- column j is `Ai[Ap[j] ...   Ap[j+1]-1]`, ditto in `Ax`
- Thus, `A(:,j)` is easy in MATLAB; `A(i,:)` hard

$$A = \begin{bmatrix} 4.5 & 0 & 3.2 & 0 \\ 3.1 & 2.9 & 0 & 0.9 \\ 0 & 1.7 & 3.0 & 0 \\ 3.5 & 0.4 & 0 & 1.0 \end{bmatrix}$$

```
Ap: [0,               3,              6,        8,       10]
Ai: [0,   1,   3,   1,   2,   3,   0,   2,   1,   3  ]
Ax: [4.5,3.1,3.5,2.9,1.7,0.4,3.2,3.0,0.9,1.0]
```

Sparse lower triangular solve, x=L\b

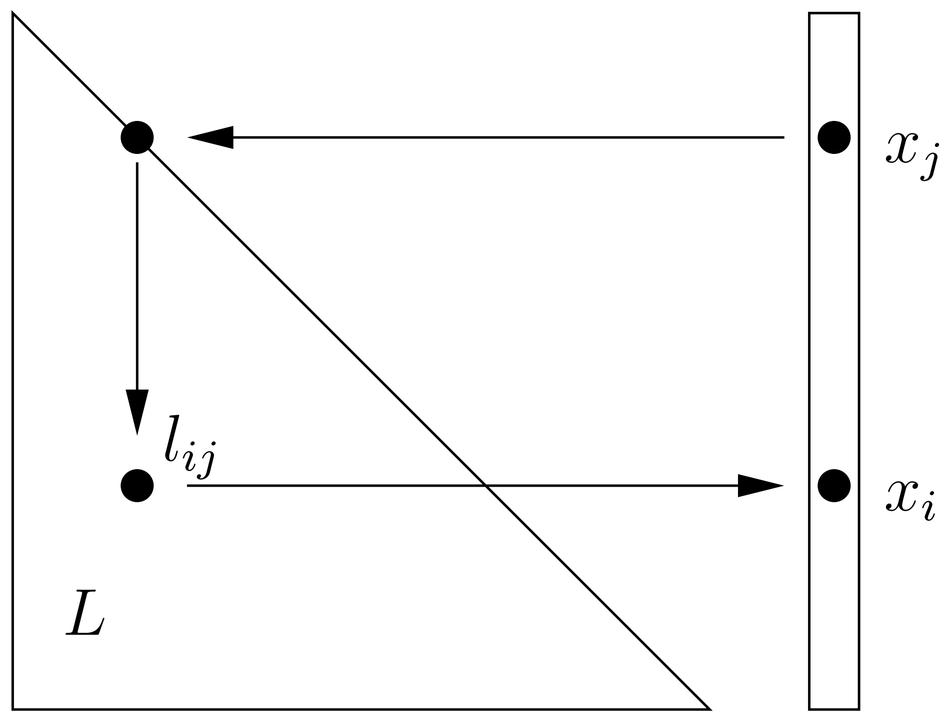
```
x = b
for j = 1:n
    if (x(j) ≠ 0)
        x(j+1:n) = x(j+1:n) - L(j+1:n,j) * x(j)
    end
end
```

- O(n+flops) time too high
- the problem:
  ```
  for j=1:n
    if (x(j) ≠ 0)
  ```
- need pattern of x before computing it

Sparse lower triangular solve, `x=L\b`

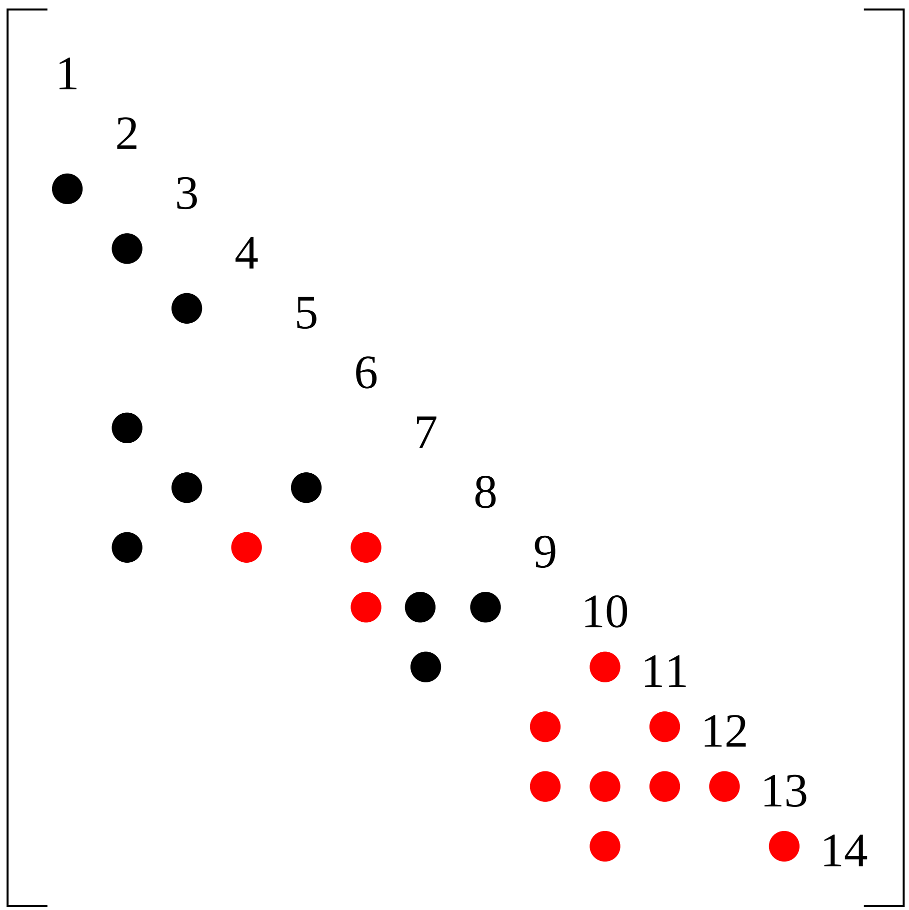
```
x = b
for j = 1:n
    if (x(j) ≠ 0)
        x(j+1:n) = x(j+1:n) - L(j+1:n,j) * x(j)
    end
end
```

- $b_i \neq 0 \Rightarrow x_i \neq 0$
- $x_j \neq 0 \wedge l_{ij} \neq 0 \Rightarrow x_i \neq 0$
- let $G(L)$ have an edge $j \rightarrow i$ if $l_{ij} \neq 0$
- let $\mathcal{B} = \{i \,|\, b_i \neq 0\}$ and $\mathcal{X} = \{i \,|\, x_i \neq 0\}$
- then $\mathcal{X} = \text{Reach}_{G(L)}(\mathcal{B})$

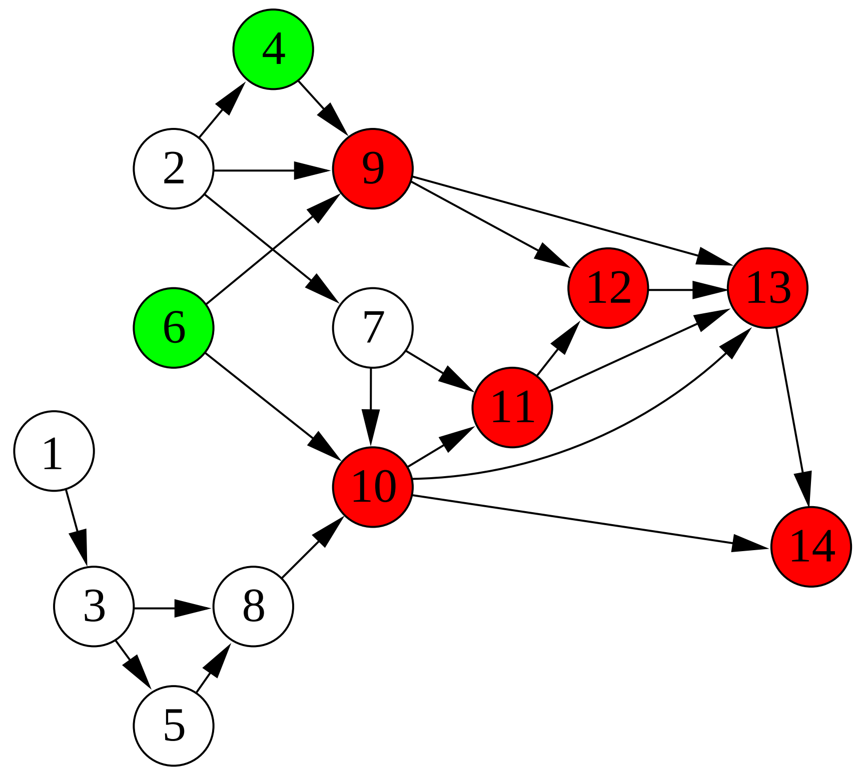


Sparse lower triangular solve, x=L\b

Lower triangular matrix L



Graph G_L



If $\mathcal{B} = \{4, 6\}$
then $\mathcal{X} = \{6, 10, 11, 4, 9, 12, 13, 14\}$

Sparse lower triangular solve, `x=L\b`

```
function x = lsolve(L,b)
    x = b
    for j = 1:n
        if (x(j) ≠ 0)
            x(j+1:n) = x(j+1:n) - L(j+1:n,j)*x(j)
```

Time: $O(n + \text{flops})$, need $\mathcal{X}$ to get $O(\text{flops})$

Sparse lower triangular solve, `x=L\b`

function `x = lsolve(L,b)`

$\mathcal{X} = \text{Reach}(L, \mathcal{B})$

`x = b`

for each j in $\mathcal{X}$

```
x(j+1:n) = x(j+1:n) - L(j+1:n,j) * x(j)
```

function $\mathcal{X} = \text{Reach}(\texttt{L}, \mathcal{B})$

for each i in $\mathcal{B}$ do

if (node i is unmarked) dfs(i)

function dfs(j)

mark node j

for each i in $\mathcal{L}_j$ do

if (node i is unmarked) dfs(i)

push j onto stack for $\mathcal{X}$

Total time: $O(\text{flops})$

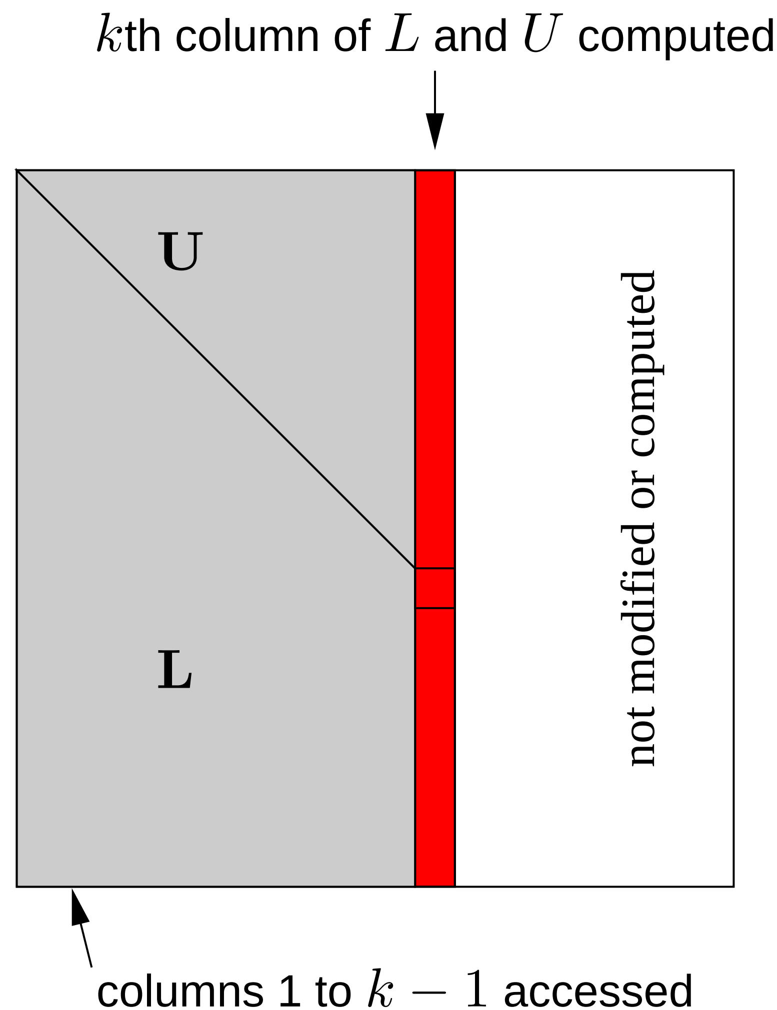
Sparse LU (Gilbert/Peierls)

- left-looking. kth step computes kth column of $\mathbf{L}$ and $\mathbf{U}$

```
L = speye(n)
U = speye(n)
for k = 1:n
    x = L \ A(:,k)
    U(1:k,k) = x(1:k)
    L(k:n,k) = ...
        x(k:n) / U(k,k)
end
```

$LU = PAQ$

- P: partial pivoting on x
- Q: fill-reducing column pre-ordering



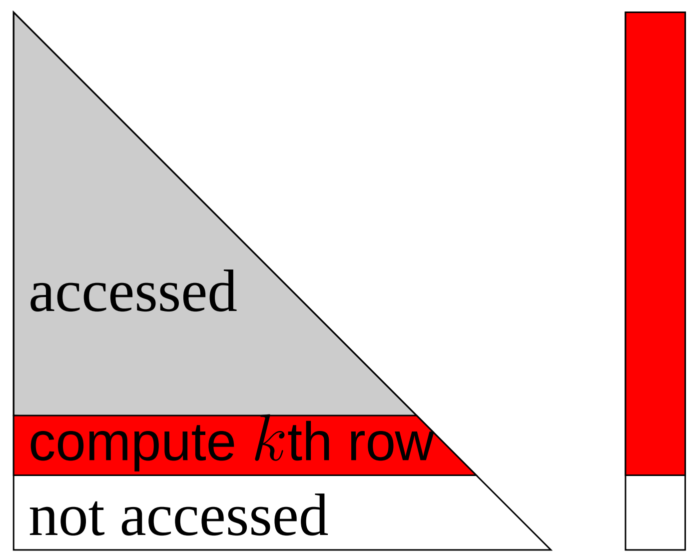
Sparse Cholesky, $LL^T = A$

$$\begin{bmatrix} L_{11} & \\ l_{12}^T & l_{22} \end{bmatrix} \begin{bmatrix} L_{11}^T & l_{12} \\ & l_{22} \end{bmatrix} = \begin{bmatrix} A_{11} & a_{12} \\ a_{12}^T & a_{22} \end{bmatrix}$$

1. factorize $L_{11}L_{11}^T = A_{11}$
2. solve $L_{11}l_{12} = a_{12}$ for l_{12}
3. $l_{22} = \sqrt{a_{22} - l_{12}^T l_{12}}$

for k = 1 to n
    solve $L_{11}l_{12} = a_{12}$ for l_{12}
    $l_{22} = \sqrt{a_{22} - l_{12}^T l_{12}}$

an up-looking method

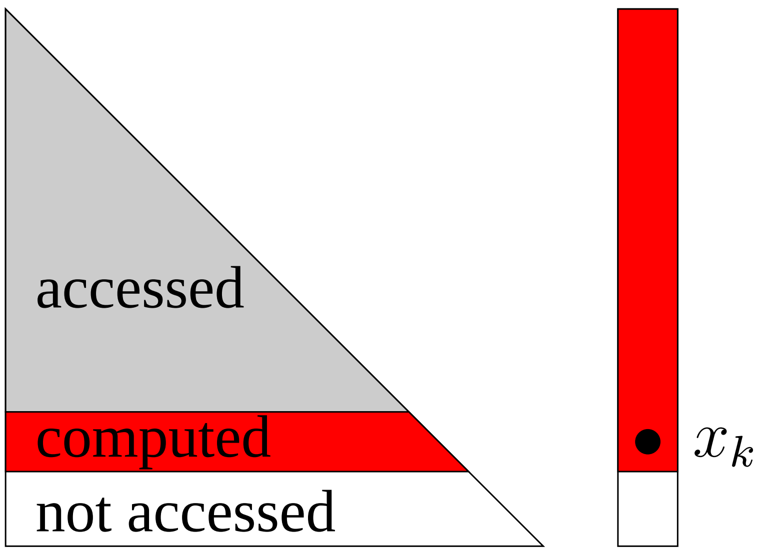


Sparse Cholesky: etree

- elimination tree
- arises in many direct methods
  - Compute nonzero pattern of `x=L\b` for a Cholesky `L` in time $O(|x|)$, the number of nonzeros in `x`
  - ...

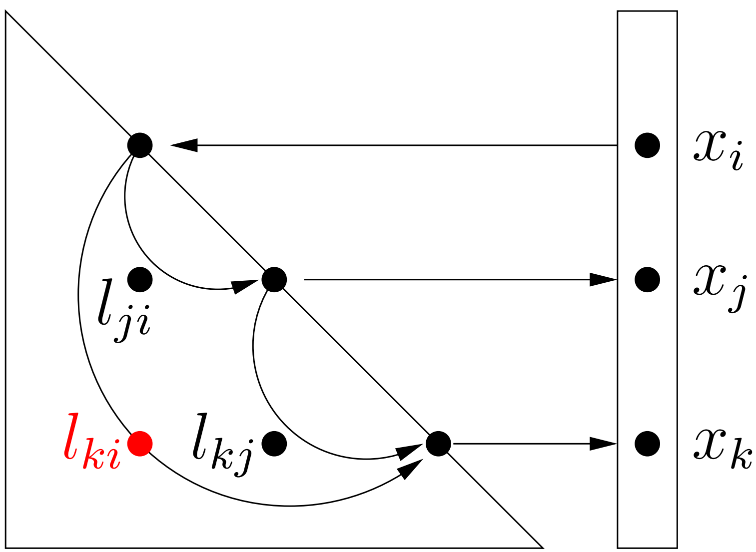
Sparse Cholesky: etree

Elimination tree $\mathcal{T}$: pruning the graph of L.
Consider computing kth row of L:



Sparse Cholesky: etree

Elimination tree $\mathcal{T}$: pruning the graph of L.
Consider computing kth row of L:

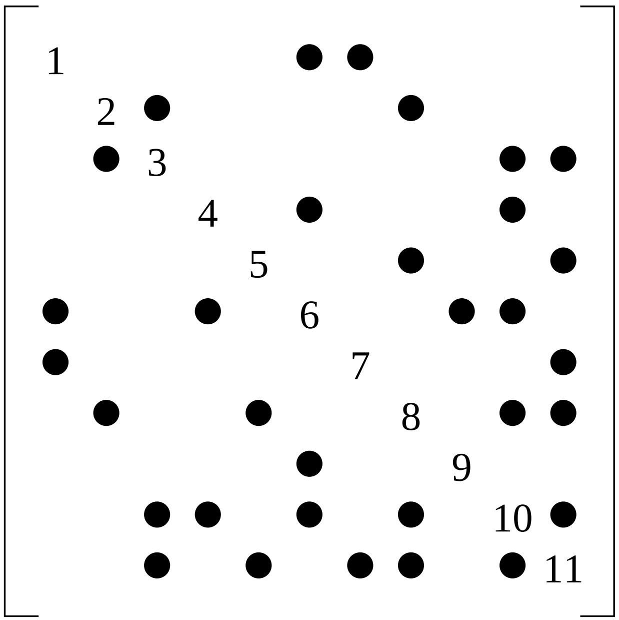


- $l_{ki} \neq 0 \Leftrightarrow x_i \neq 0$
- ($l_{ji} \neq 0$ and $x_i \neq 0$) $\Rightarrow x_j \neq 0$
- $l_{kj} \neq 0 \Leftrightarrow x_j \neq 0$
- Thus, l_{ki} redundant for $\mathcal{X} = \text{Reach}(b)$.

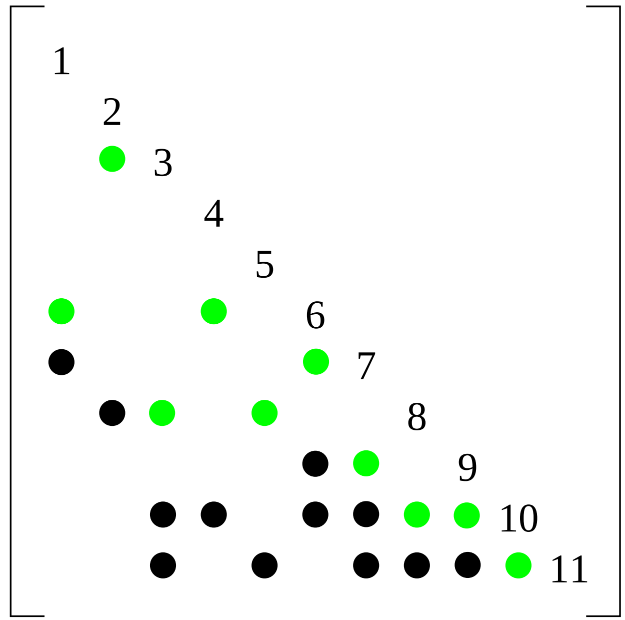
- parent$(i) = \min\{j > i \,|\, l_{ji} \neq 0\}$; other edges redundant
- $\mathcal{L}_{k*} = \text{Reach}(A_{1:k,k})$ in $O(|\mathcal{L}_{k*}|)$ time

Sparse Cholesky: etree

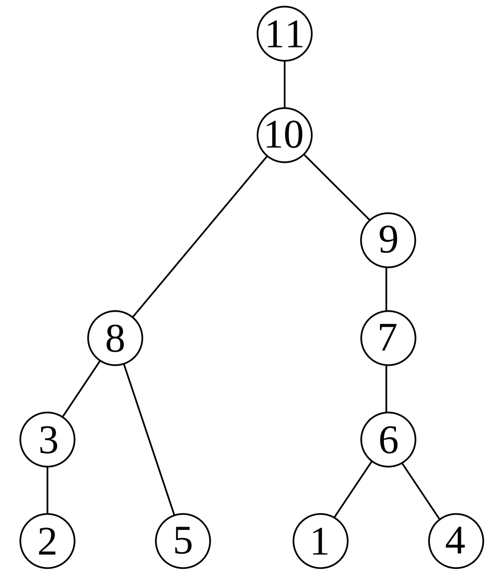
A



Cholesky factor L of A



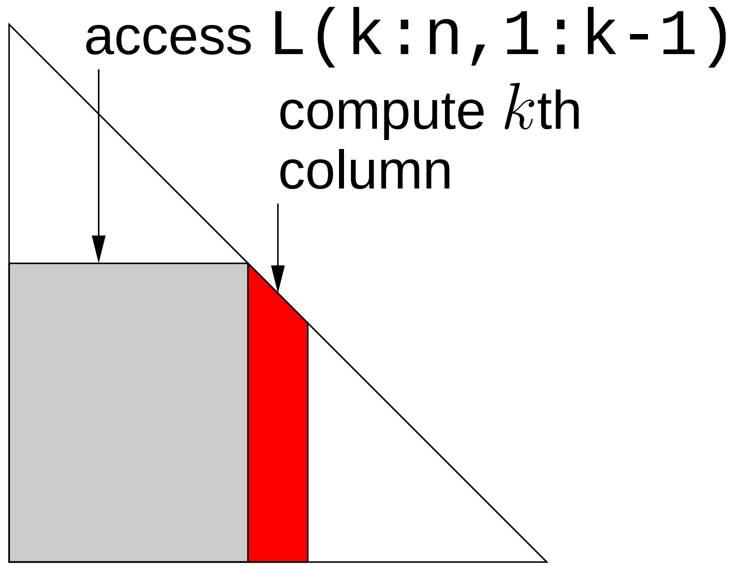
elimination tree



Sparse Cholesky: overview

- Symbolic analysis:
  - fill-reducing ordering, $\bar{A} = PAP^T = LL^T$
  - etree of $\bar{A}$: nearly $O(|A|)$
  - depth-first postordering of etree: $O(n)$
  - column counts of L: nearly $O(|A|)$
  - some methods find $\mathcal{L}$: $O(|L|)$ or less
- Numeric factorization:
  - up-looking
  - left-looking, supernodal
  - right-looking, multifrontal

Sparse Cholesky: left-looking



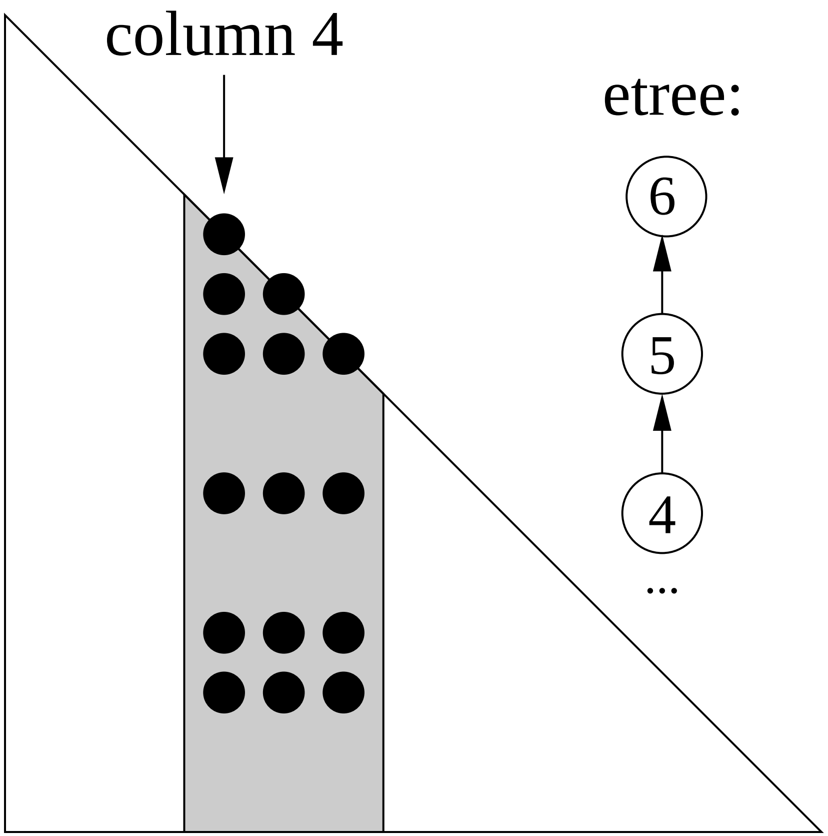
for $k = 1$ to n

```
    x = A(k:n,k)
```

    for each j in Reach$(L, A(1:k,k))$

```
        x(k:n) = x(k:n) - L(k:n,j) * L(k,j)
    L(k,k) = sqrt(x(k))
    L(k+1:n,k) = x(k) / L(k,k)
```

Sparse Cholesky: supernodal

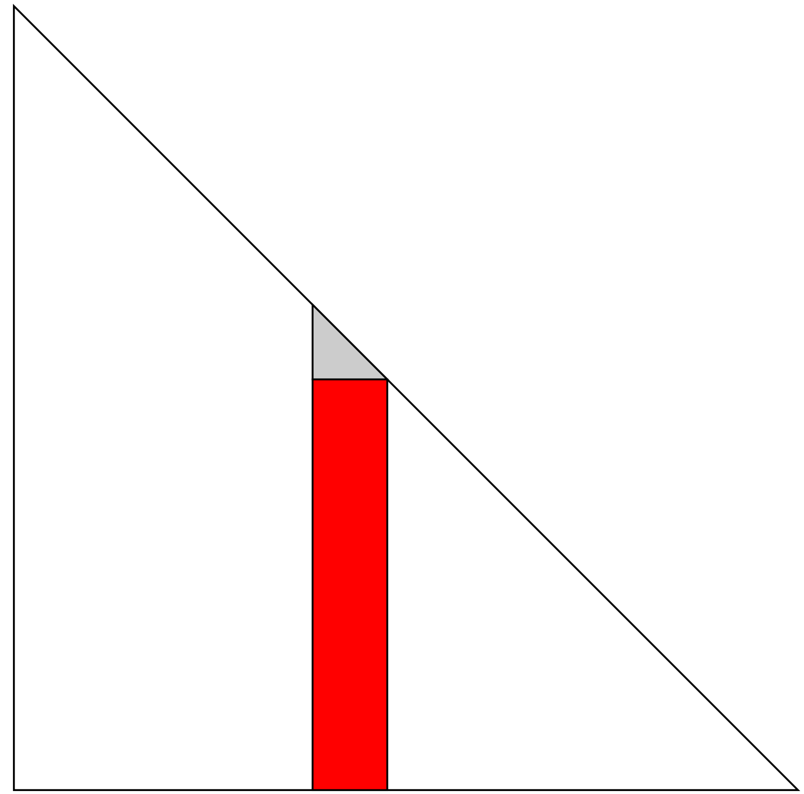


- Adjacent columns of L often have identical pattern
- a chain in the elimination tree
- can exploit dense submatrix operations

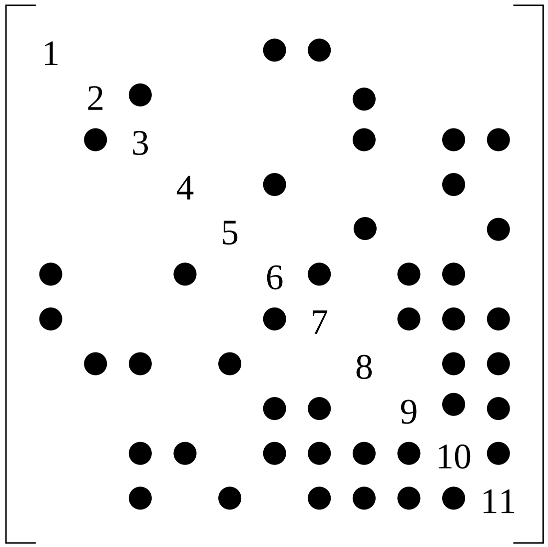
Sparse Cholesky: supernodal

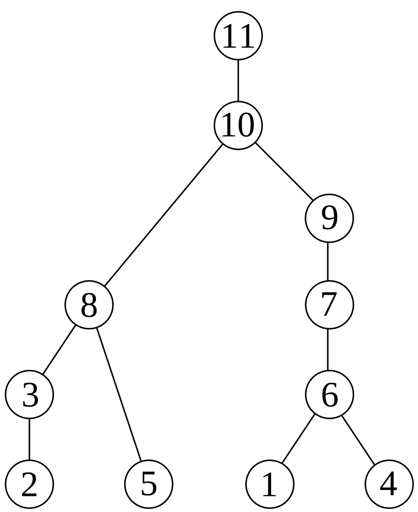
block left-looking

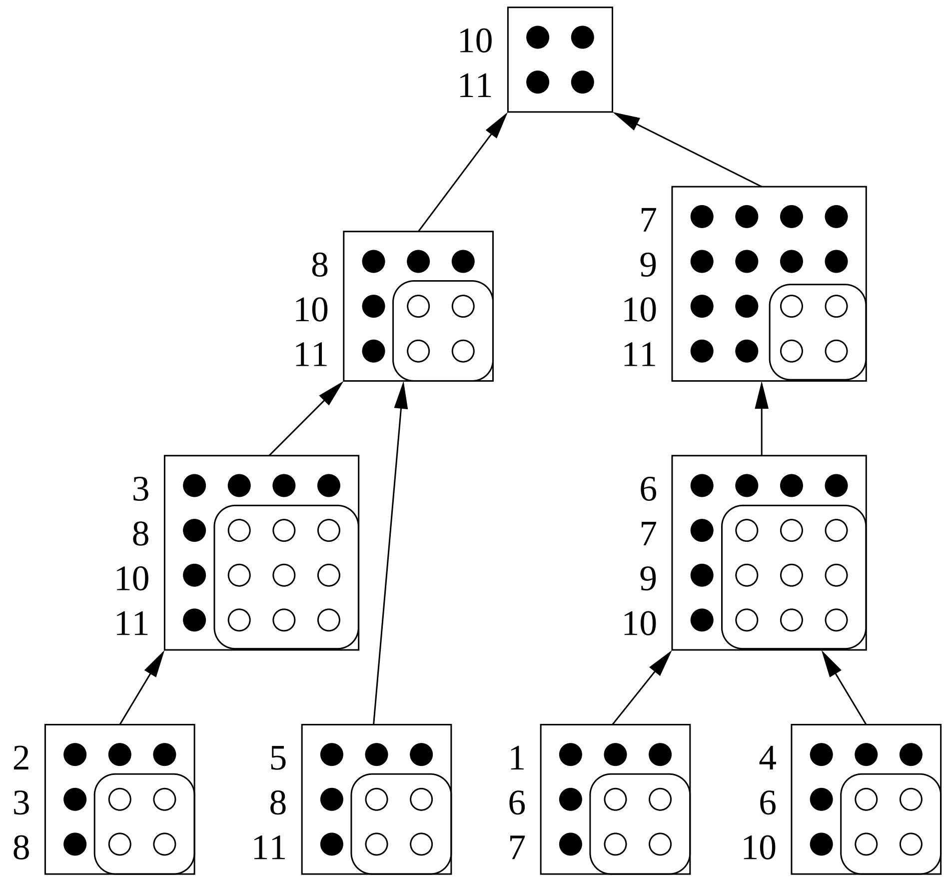
- for jth supernode:
- (1) sparse block matrix multiply
- (2) dense Cholesky
- (3) dense block $Lx = b^T$ solve



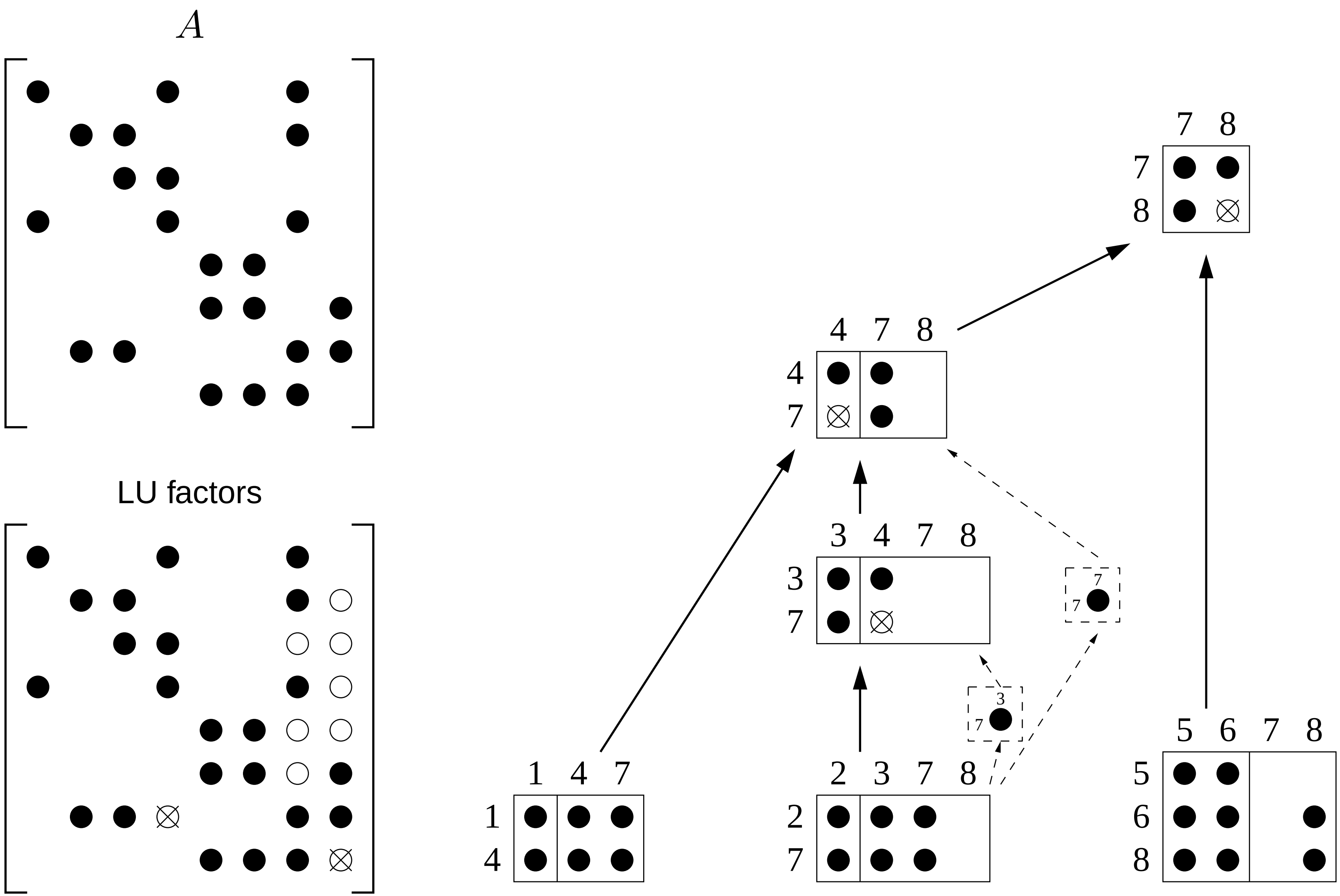
Sparse LU: multifrontal







Sparse LU: UMFPACK



`x=A\b` when A is sparse

- if A diagonal: scale each row
- if A banded: LAPACK
- if A lower or upper triangular: forward/backsolve
- if A rectangular: Givens-based QR
- if `A=A'` and `all(diag(A)>0)`: try `chol`, supernodal or up-looking (CHOLMOD)
- else: `lu`, either multifrontal (UMFPACK) or left-looking (GPLU)
- http://www.cise.ufl.edu/research/sparse

Postscript

- Up-coming book: *Direct Methods for Sparse Linear Systems*, SIAM, Sept. 2006.
- Sparse Cholesky update/downdate
  - Given $A = LL^T$, compute $\overline{LL}^T = A \pm ww^T$
  - *"among the most important algorithms in linear algebra"*, Wilkinson
  - time proportional to number of entries that change
  - columns of L that change: sparsity pattern of `x=L\w`

Direct methods for sparse linear systems

`x = A\b`

- Sparse matrix algorithms: numerics plus graph theory
- Goal: sparse matrix methods from the ground up
- Lower triangular solve (`x=L\b`)
- Sparse LU factorization (`[L,U,P]=lu(A)`)
- Sparse Cholesky factorization (`L=chol(A)'`)
- Supernodal and multifrontal methods (`x=A\b`)
- Sparse Cholesky update/downdate (`cholupdate`)
- Up-coming SIAM book: September 2006