Direct Methods for Sparse Linear Systems:

MATLAB sparse backslash

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So what is a sparse matrix ... ?

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, ...

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  - L, x, b are all sparse
  - must know nonzero pattern of x to compute x efficiently
  - time: O(flops)

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- Lower triangular solve (`x=L\b`)
- Sparse LU factorization (`[L,U,P]=lu(A)`)
  - left-looking, partial pivoting
  - fill-reducing column ordering
  - relies on `x=L\b`, where `L`, `x`, `b` are all sparse
  - time: O(n+flops)

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- Sparse Cholesky factorization (`L=chol(A)'`)
  - up-looking and left-looking
  - fill-reducing symmetric ordering
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- 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 (... many others)

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

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```
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]
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Ap: [0,          3,                                ]
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```
Ap: [                             6,       8,          ]
Ai: [                             0,   2,            ]
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```

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

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

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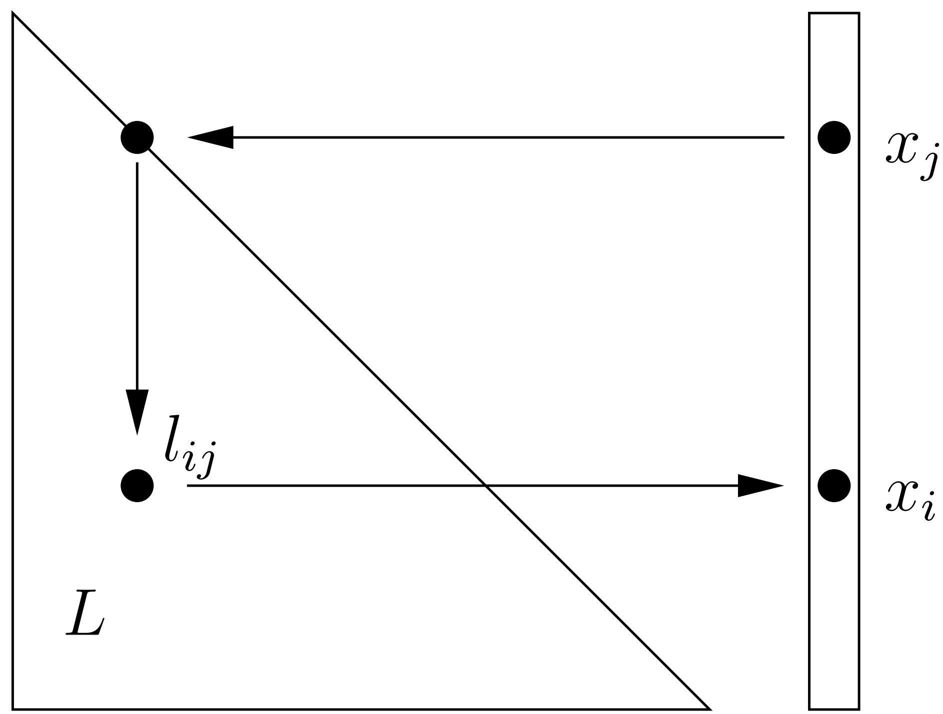
- $b_i \neq 0 \Rightarrow x_i \neq 0$



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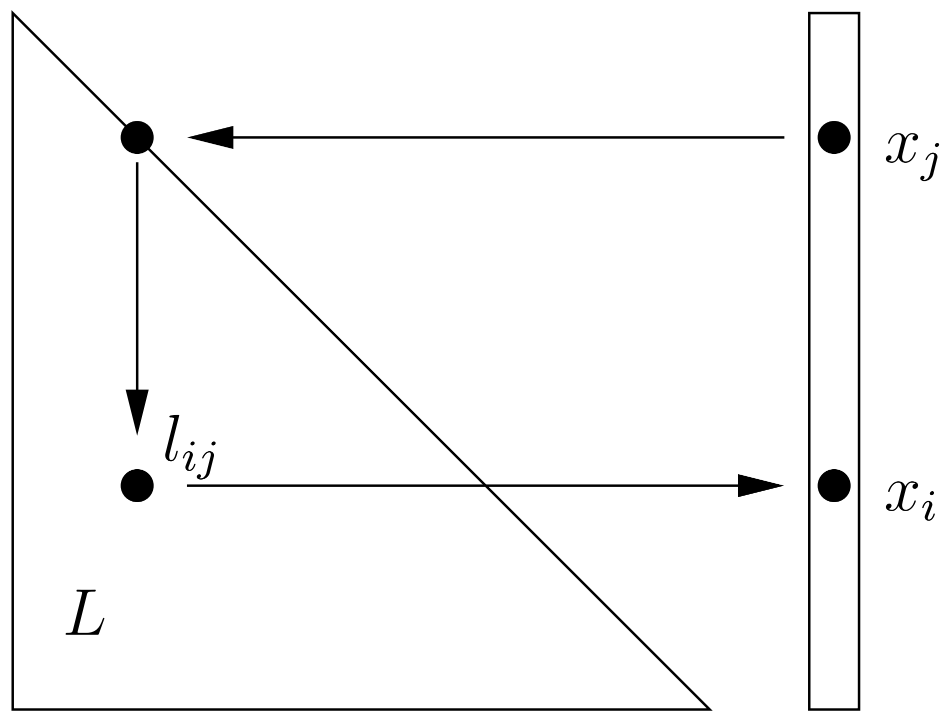

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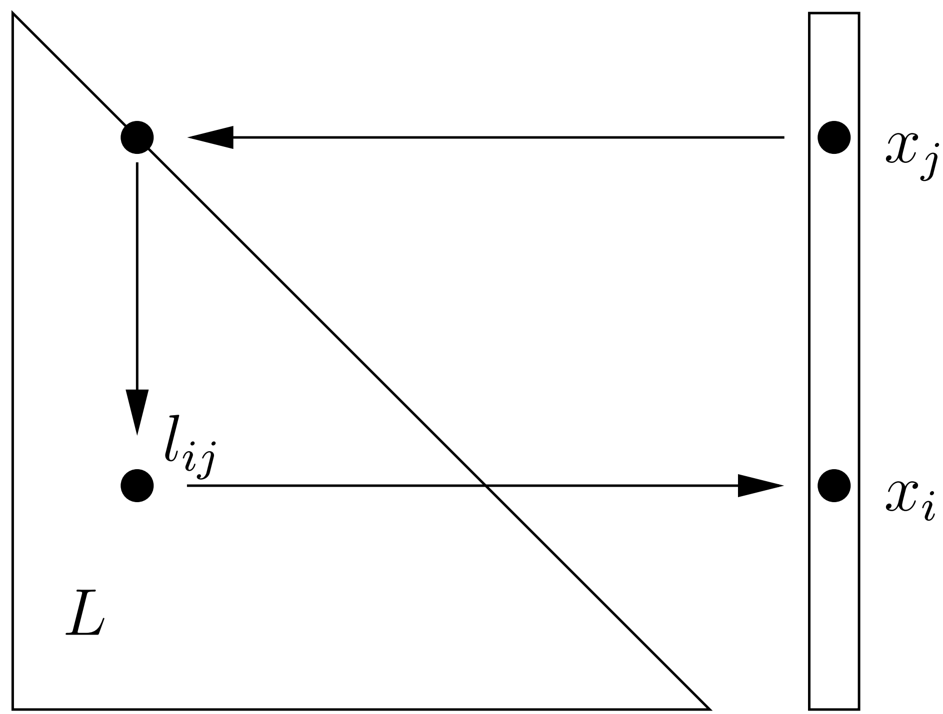
- let $G(L)$ have an edge $j \rightarrow i$ if $l_{ij} \neq 0$



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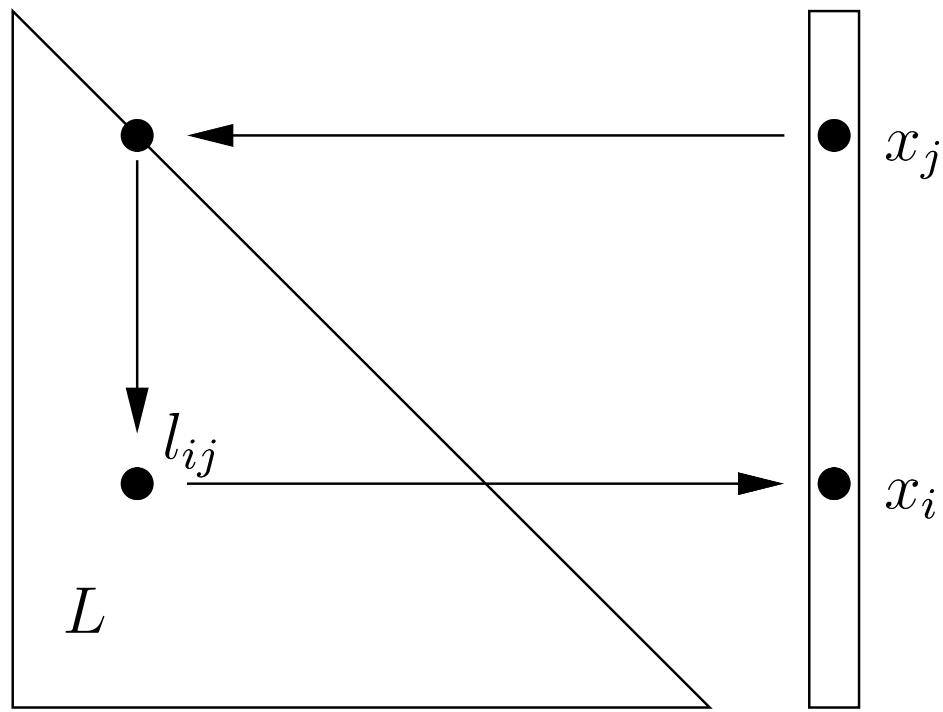
- let $\mathcal{B} = \{i \,|\, b_i \neq 0\}$ and $\mathcal{X} = \{i \,|\, x_i \neq 0\}$



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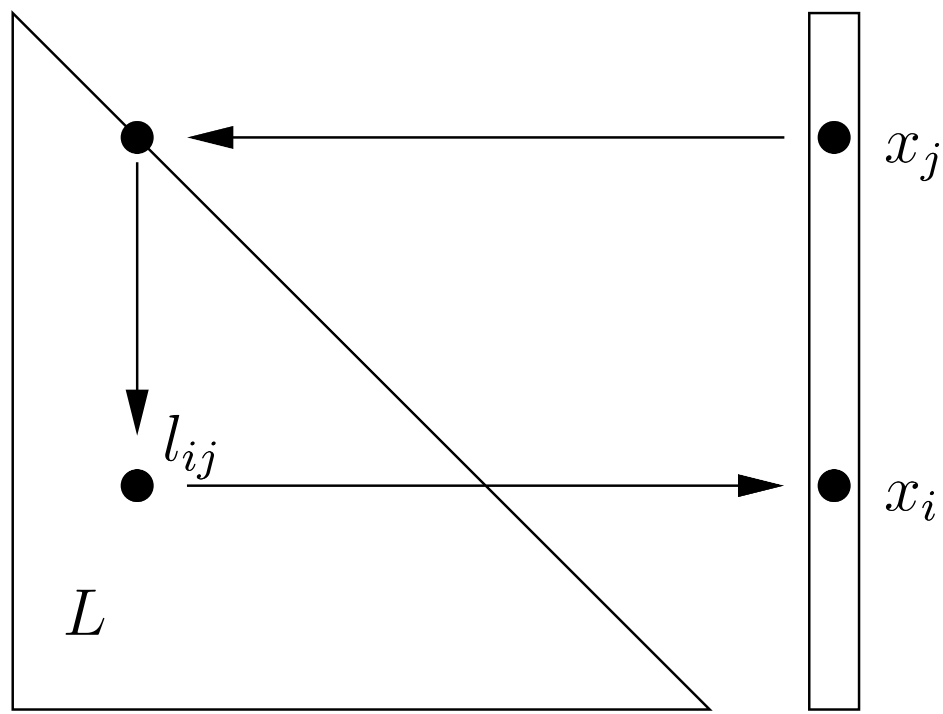
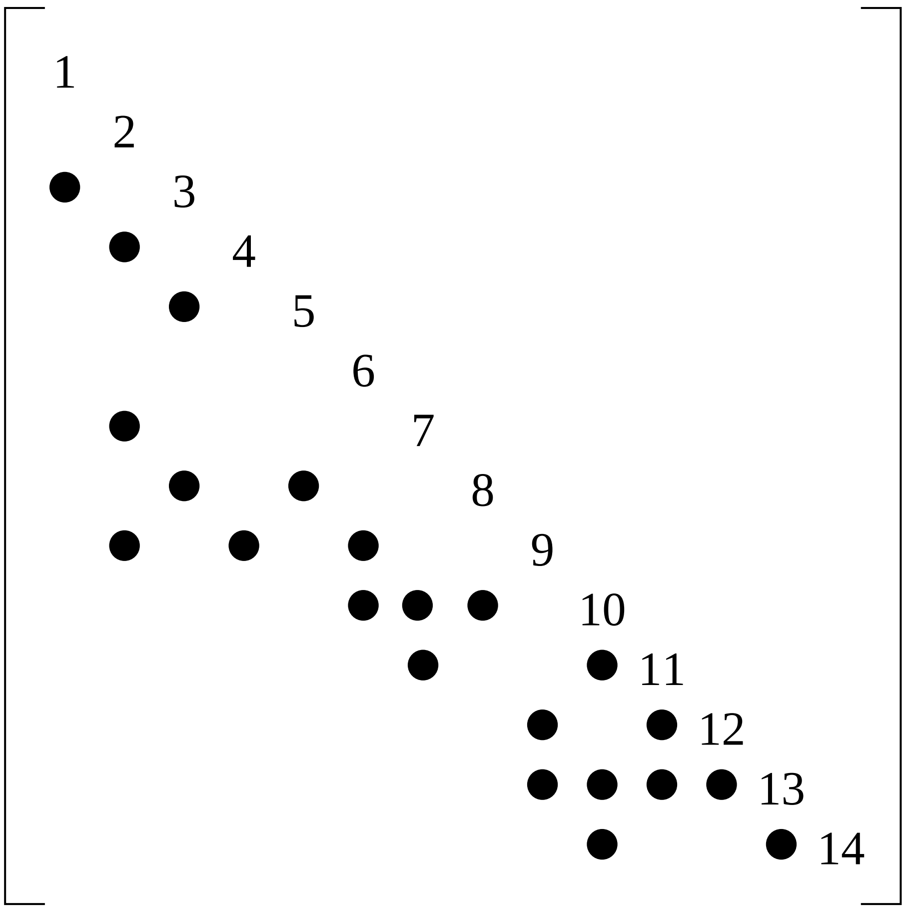
- $x_j \neq 0 \wedge l_{ij} \neq 0 \Rightarrow x_i \neq 0$
- let $G(L)$ have an edge $j \rightarrow i$ if $l_{ij} \neq 0$
- let $\mathcal{B} = \{i \mid b_i \neq 0\}$ and $\mathcal{X} = \{i \mid x_i \neq 0\}$
- then $\mathcal{X} = \text{Reach}_{G(L)}(\mathcal{B})$

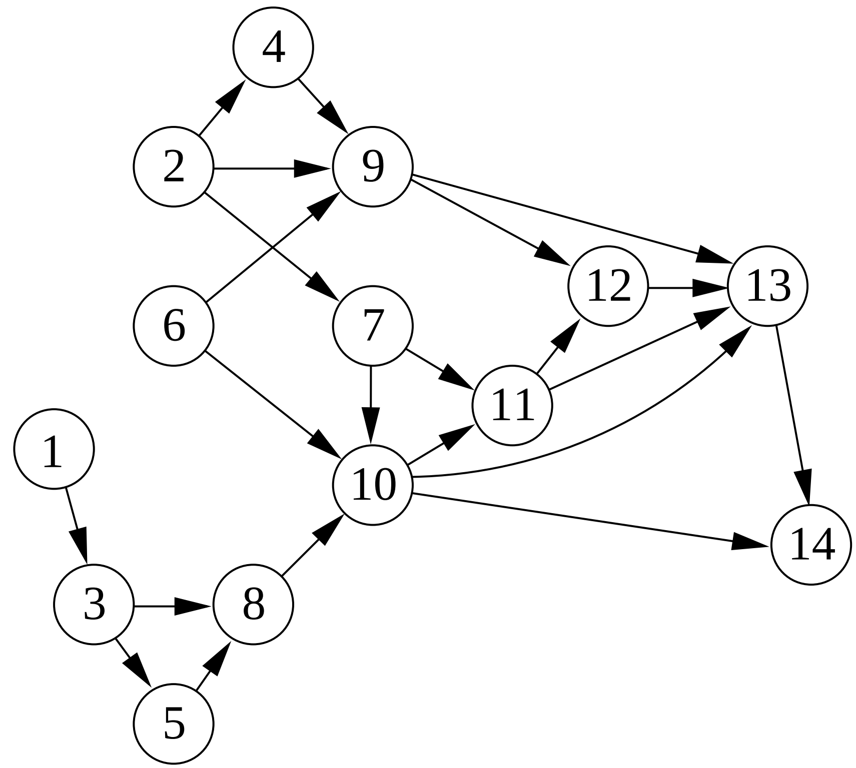


Sparse lower triangular solve, x=L\b

Lower triangular matrix L



Graph G_L



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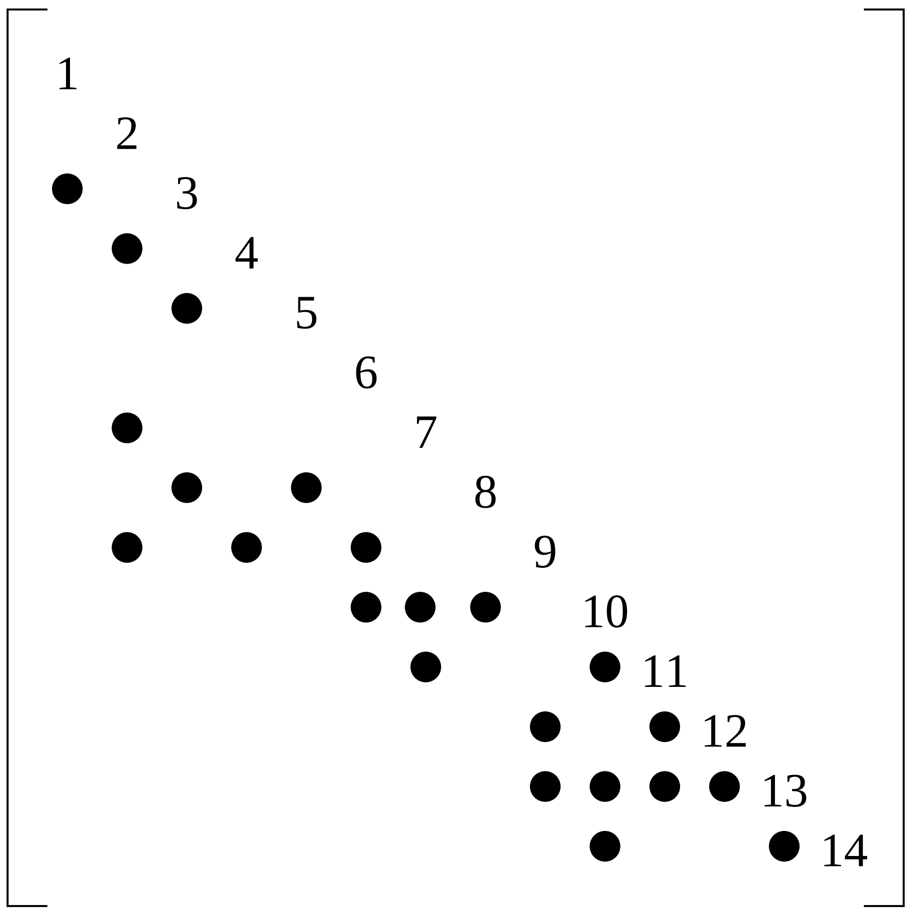

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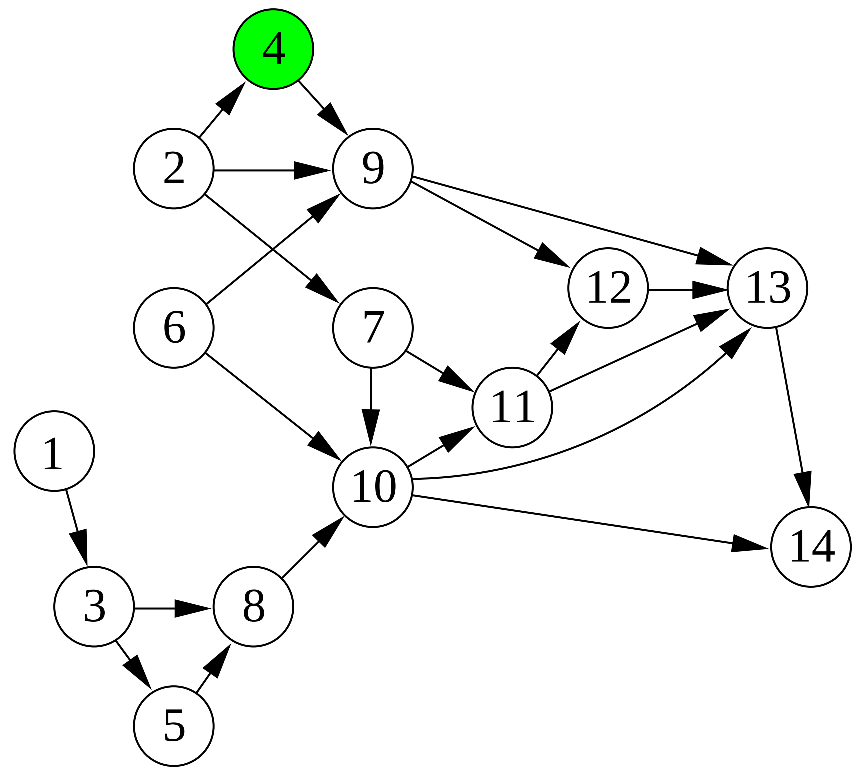
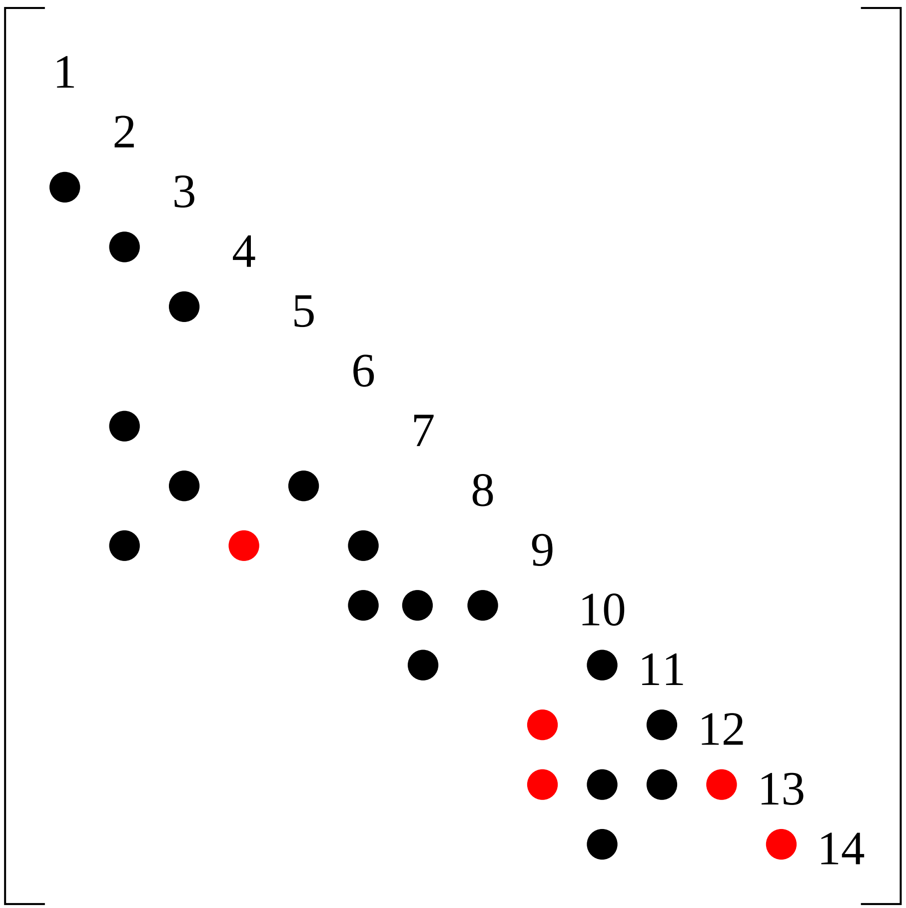


If $\mathcal{B} = \{4\}$

Sparse lower triangular solve, x=L\b

Lower triangular matrix L



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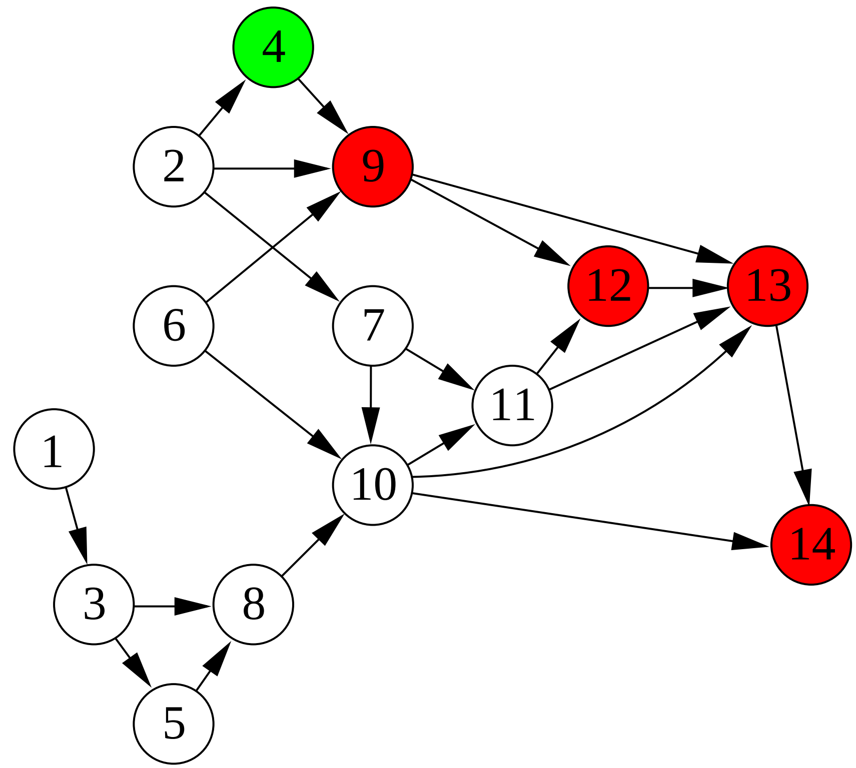
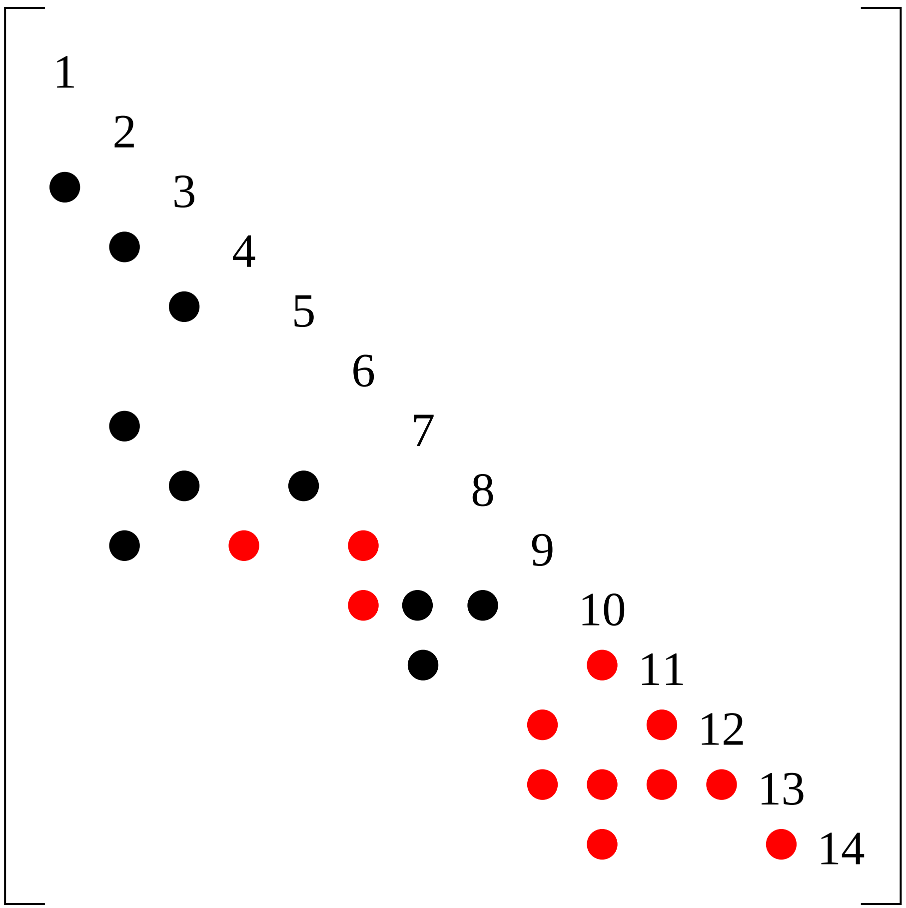


If $\mathcal{B} = \{4\}$
then $\mathcal{X} = \{4, 9, 12, 13, 14\}$

Sparse lower triangular solve, x=L\b

Lower triangular matrix L



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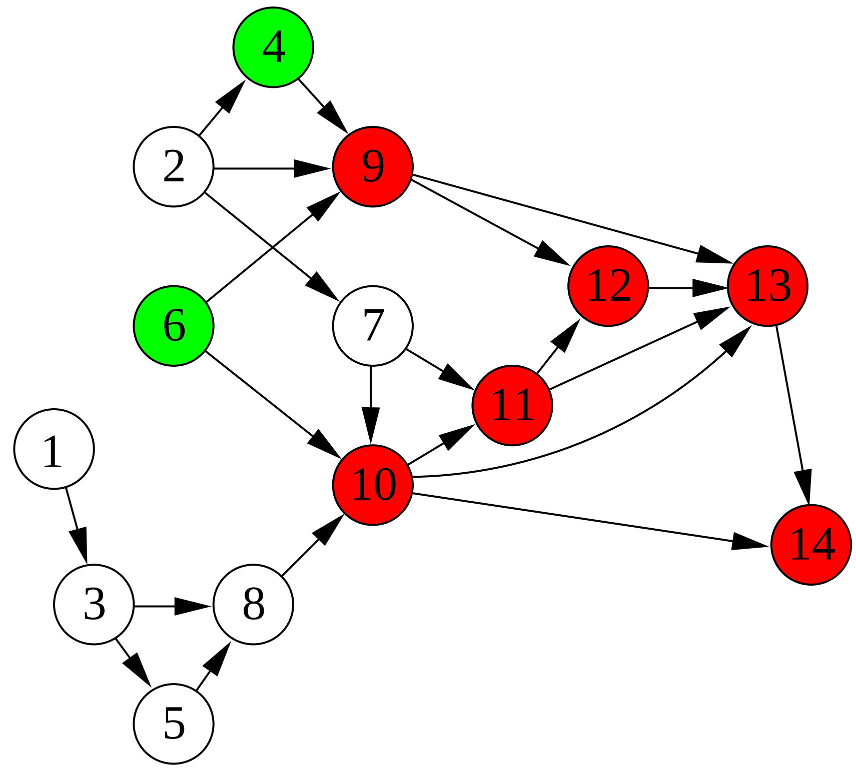

If $\mathcal{B} = \{4, 6\}$
then $\mathcal{X} = \{6, 10, 11, 4, 9, 12, 13, 14\}$

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

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

function `x = lsolve(L,b)`

```
    X = Reach(L, B)
    x = b
    for each j in X
        x(j+1:n) = x(j+1:n) - L(j+1:n,j) * x(j)
```

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

```
    for each i in B do
        if (node i is unmarked) dfs(i)
```

function dfs(j)

```
    mark node j
    for each i in L_j do
        if (node i is unmarked) dfs(i)
    push j onto stack for X
```

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

```
function x = lsolve(L,b)
    𝒳 = Reach(L,ℬ)
    x = b
    for each j in 𝒳
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$\boxed{\text{Total time: } O(\text{flops})}$

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

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    $\mathcal{X} =$ Reach$(L, \mathcal{B})$
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    for each i in $\mathcal{B}$ do
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function dfs(j)
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    for each i in $\mathcal{L}_j$ do
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    push j onto stack for $\mathcal{X}$

$\boxed{\text{which can be less than } n}$

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```
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
```

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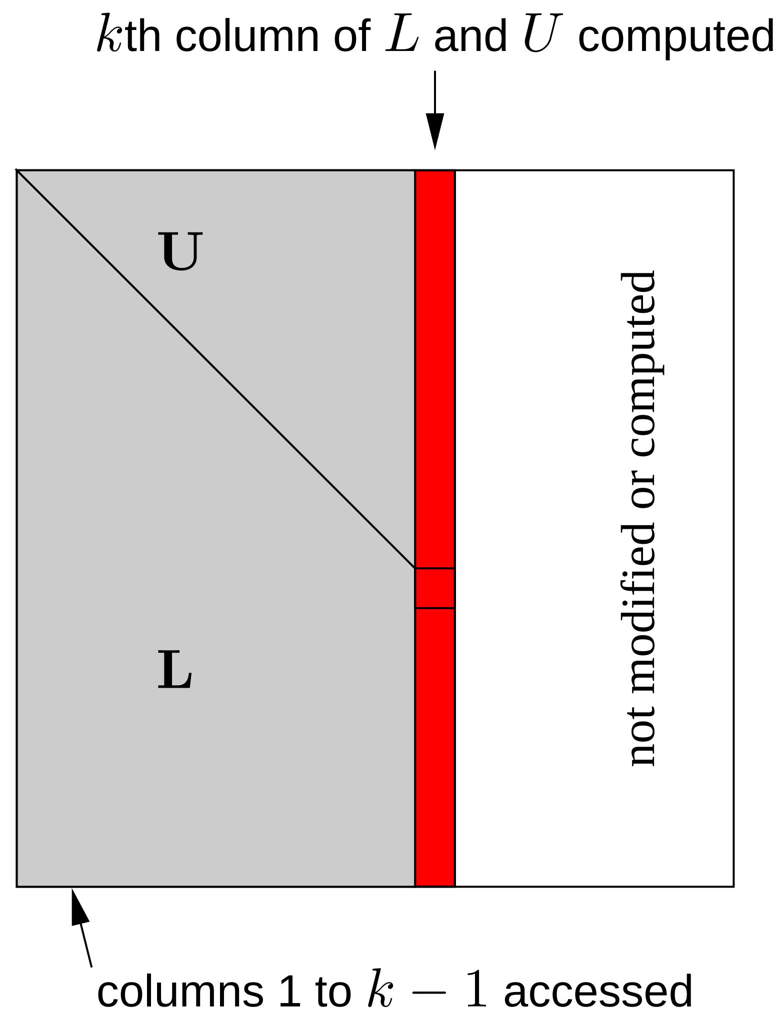

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```
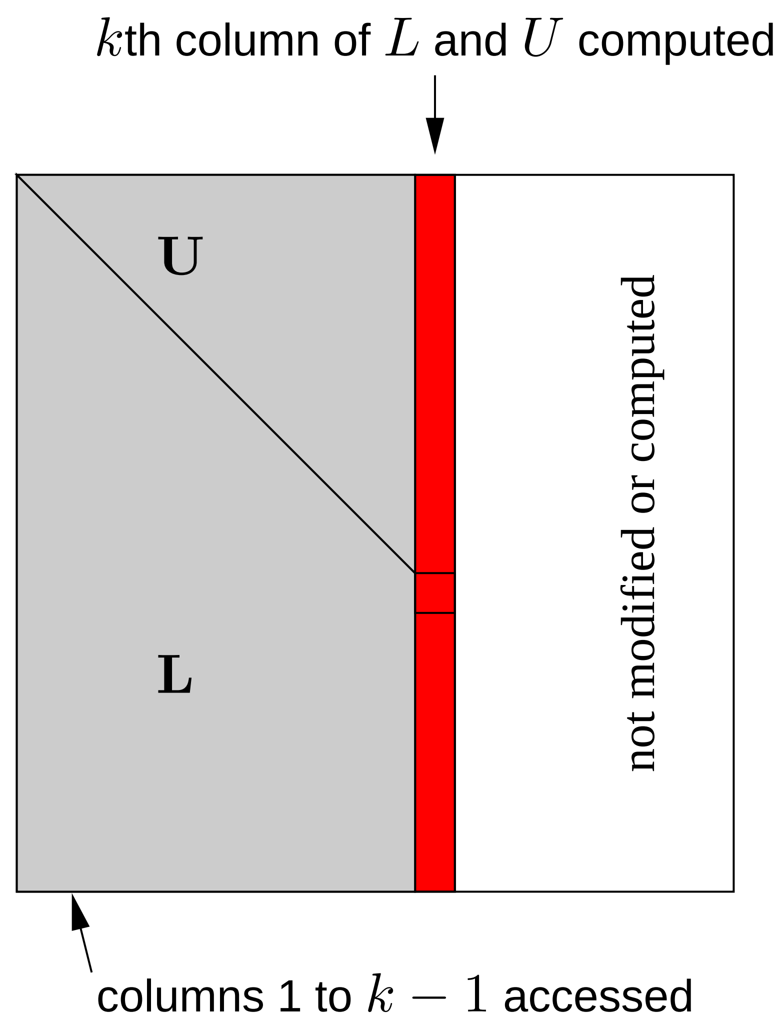

$LU = PAQ$

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



Sparse Cholesky, $LL^T = A$

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

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1. factorize $L_{11} L_{11}^T = A_{11}$
2. solve $\mathbf{L_{11} l_{12}} = \mathbf{a_{12}}$ for l_{12}

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

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for k = 1 to n

solve $L_{11}l_{12} = a_{12}$ for l_{12}

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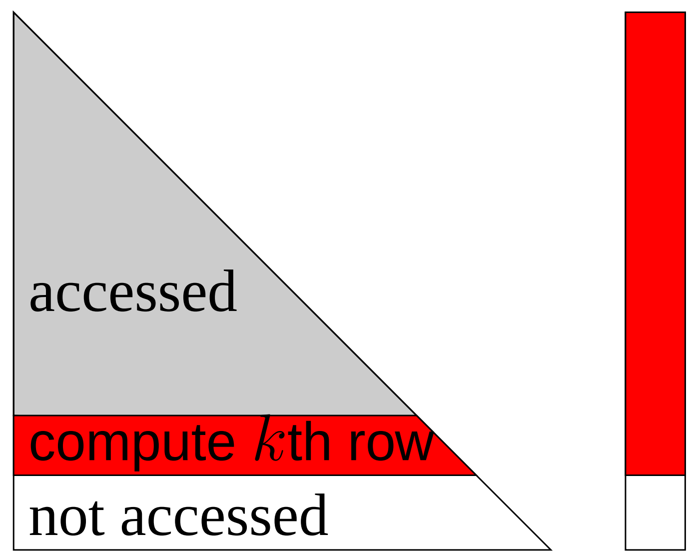
an up-looking method

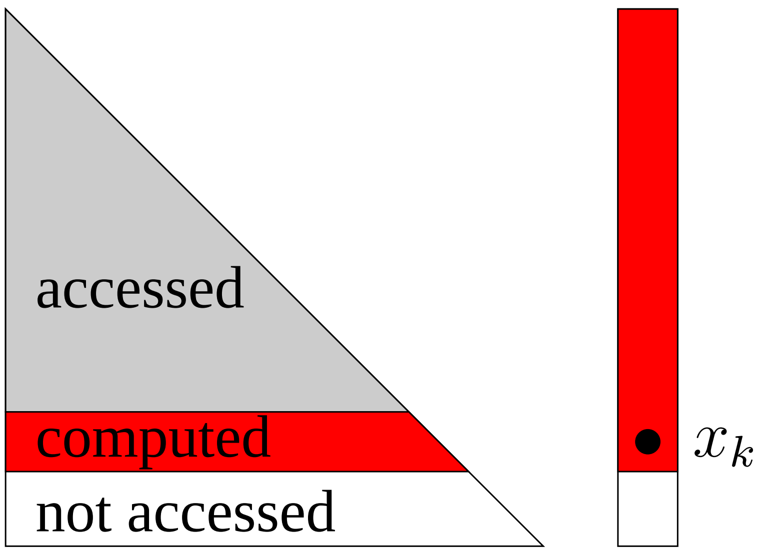


Sparse Cholesky: etree

- 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:



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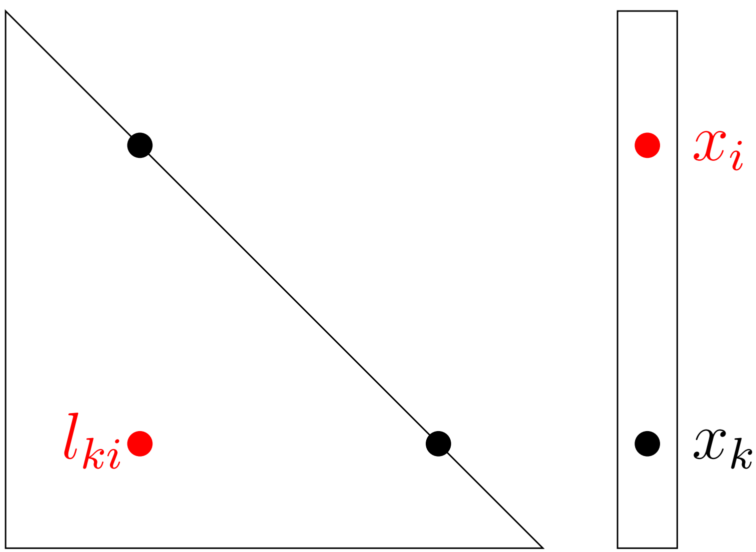

- $l_{ki} \neq 0 \Leftrightarrow x_i \neq 0$

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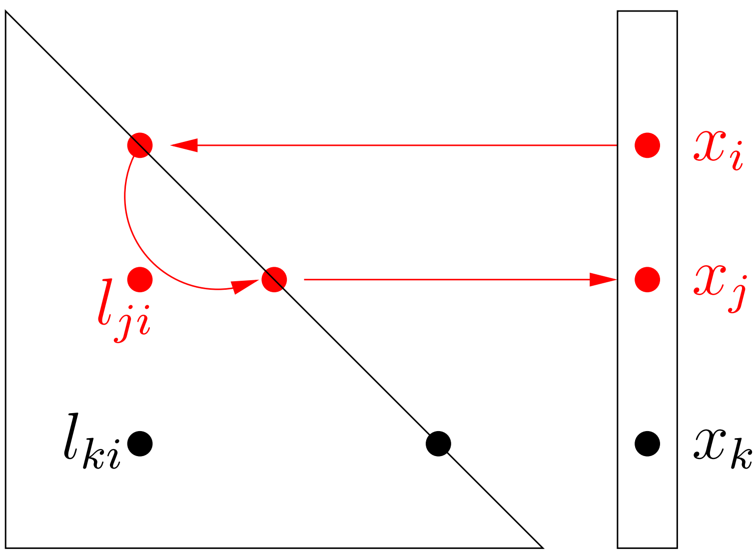

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- ($l_{ji} \neq 0$ and $x_i \neq 0$) $\Rightarrow x_j \neq 0$

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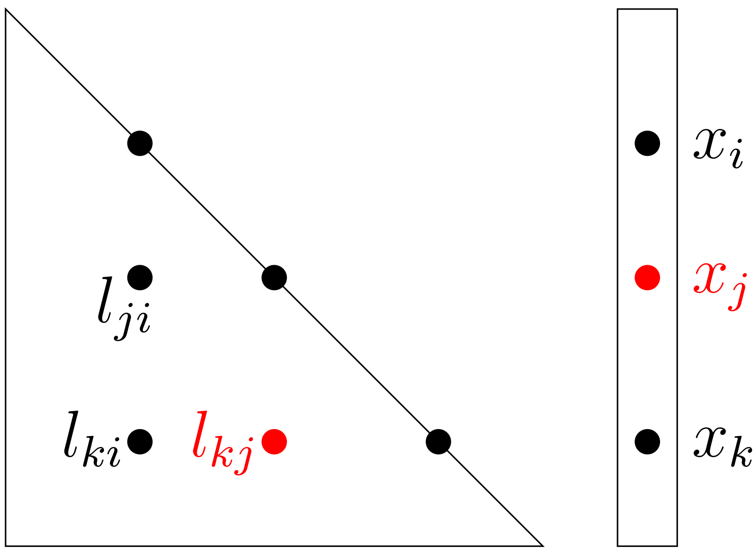

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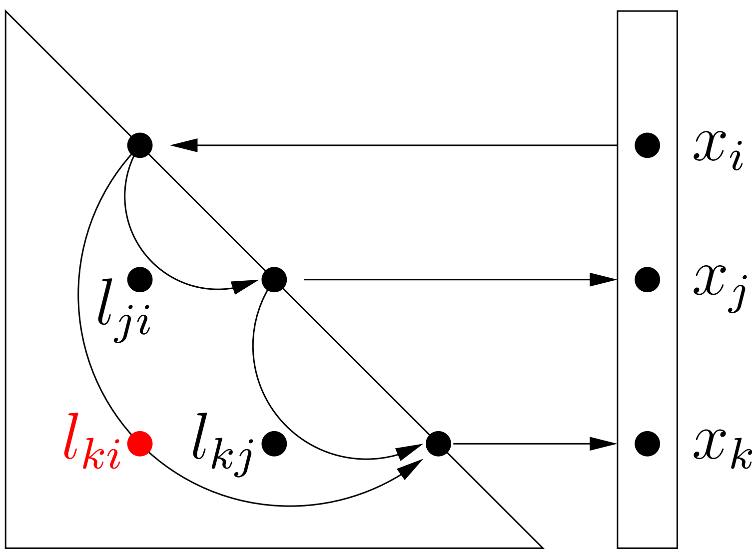
- $l_{kj} \neq 0 \Leftrightarrow x_j \neq 0$

Sparse Cholesky: etree

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



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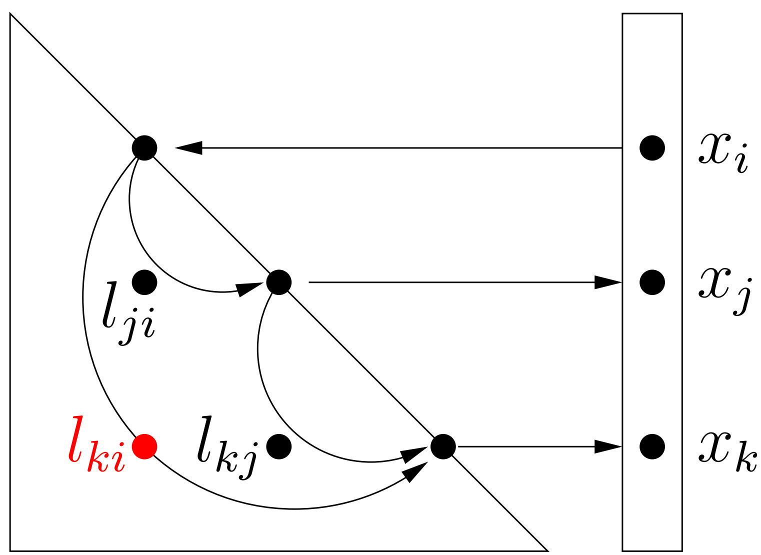

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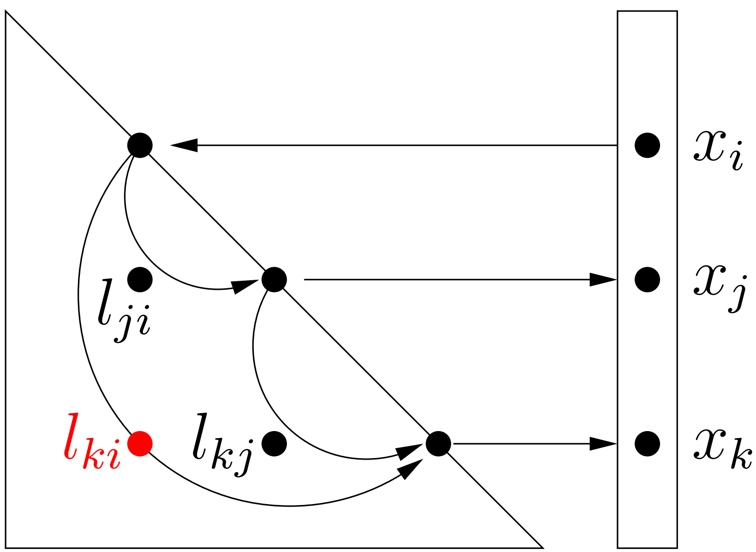

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Sparse Cholesky: etree

$$A$$

$$\begin{bmatrix}
1 & & & & & \bullet & \bullet & & & & \\
& 2 & \bullet & & & & & \bullet & & & \\
& \bullet & 3 & & & & & & & \bullet & \bullet \\
& & & 4 & & \bullet & & & & \bullet & \\
& & & & 5 & & & \bullet & & & \bullet \\
\bullet & & & \bullet & & 6 & & & \bullet & \bullet & \\
\bullet & & & & & & 7 & & & & \bullet \\
& \bullet & & & \bullet & & & 8 & & \bullet & \bullet \\
& & & & & \bullet & & & 9 & & \\
& & \bullet & \bullet & & \bullet & & \bullet & & 10 & \bullet \\
& & \bullet & & \bullet & & \bullet & \bullet & & \bullet & 11
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Cholesky factor L of A

$$\begin{bmatrix}
1 & & & & & & & & & & \\
& 2 & & & & & & & & & \\
& \bullet & 3 & & & & & & & & \\
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& & & & 5 & & & & & & \\
\bullet & & & \bullet & & 6 & & & & & \\
\bullet & & & & & {\color{red}\bullet} & 7 & & & & \\
& \bullet & {\color{red}\bullet} & & \bullet & & & 8 & & & \\
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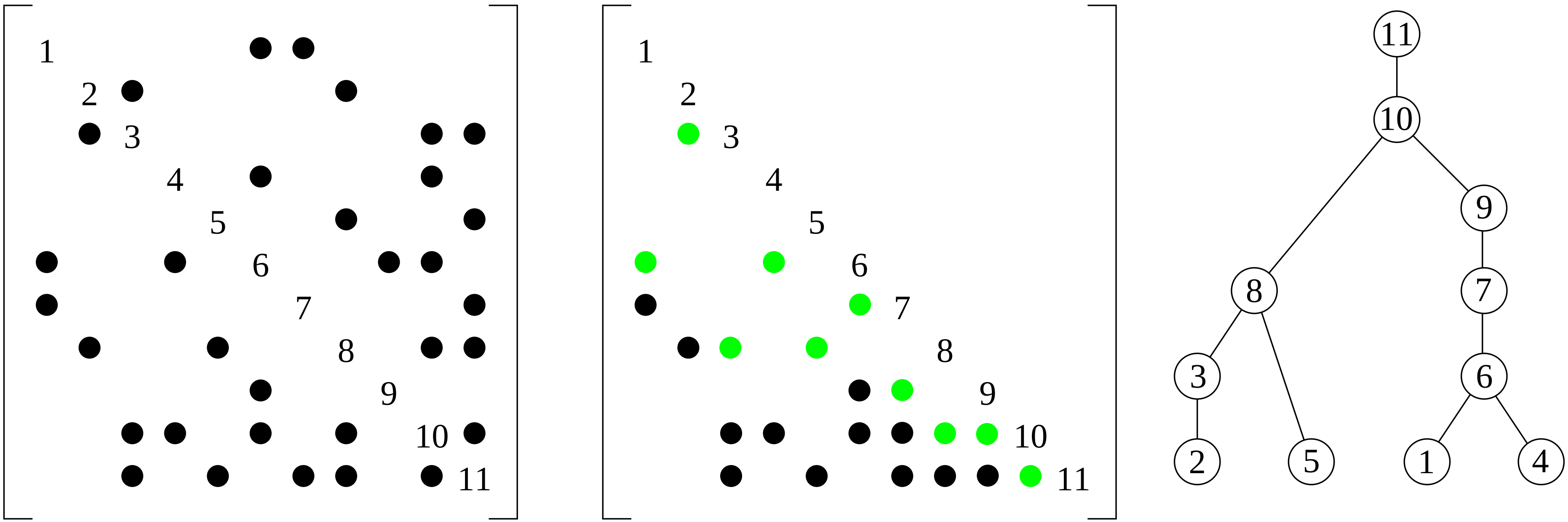
Sparse Cholesky: etree

A | Cholesky factor L of A | elimination tree



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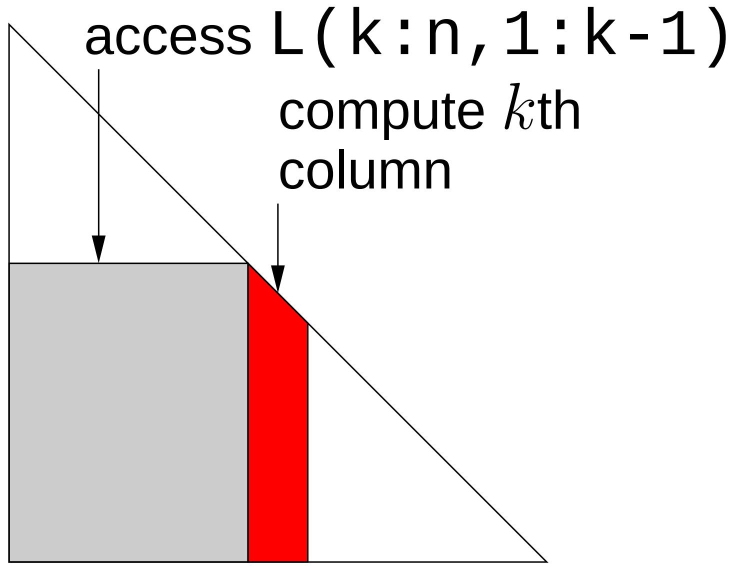
Sparse Cholesky: left-looking



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))
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```
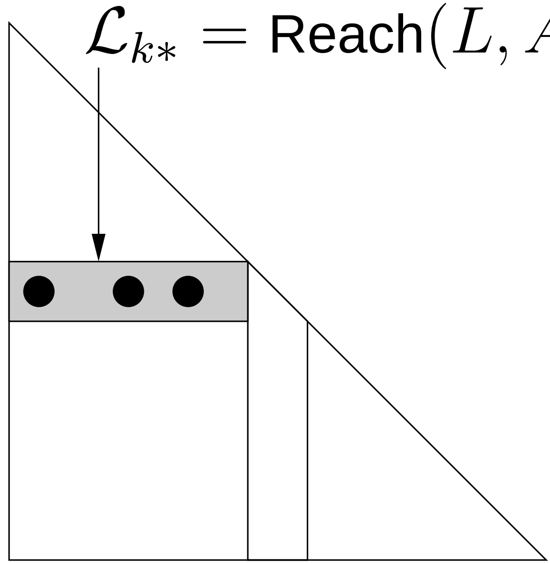

Sparse Cholesky: left-looking

$\mathcal{L}_{k*} = \text{Reach}(L, A(1:k,k))$



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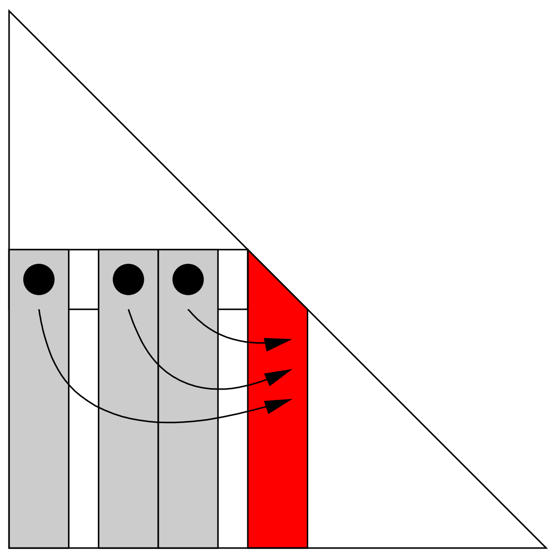
        ...

    ...

    ...

Sparse Cholesky: left-looking



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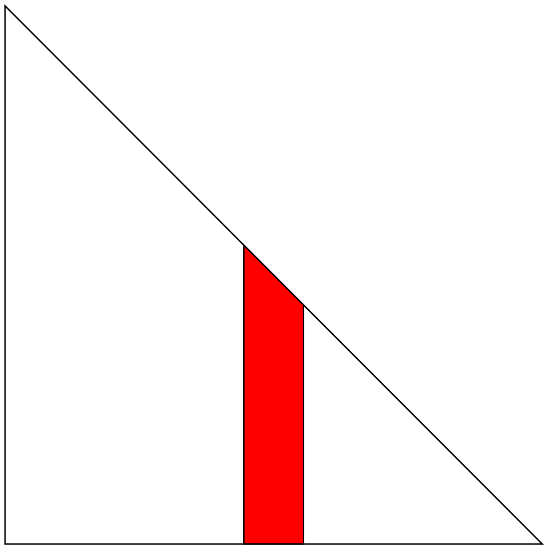

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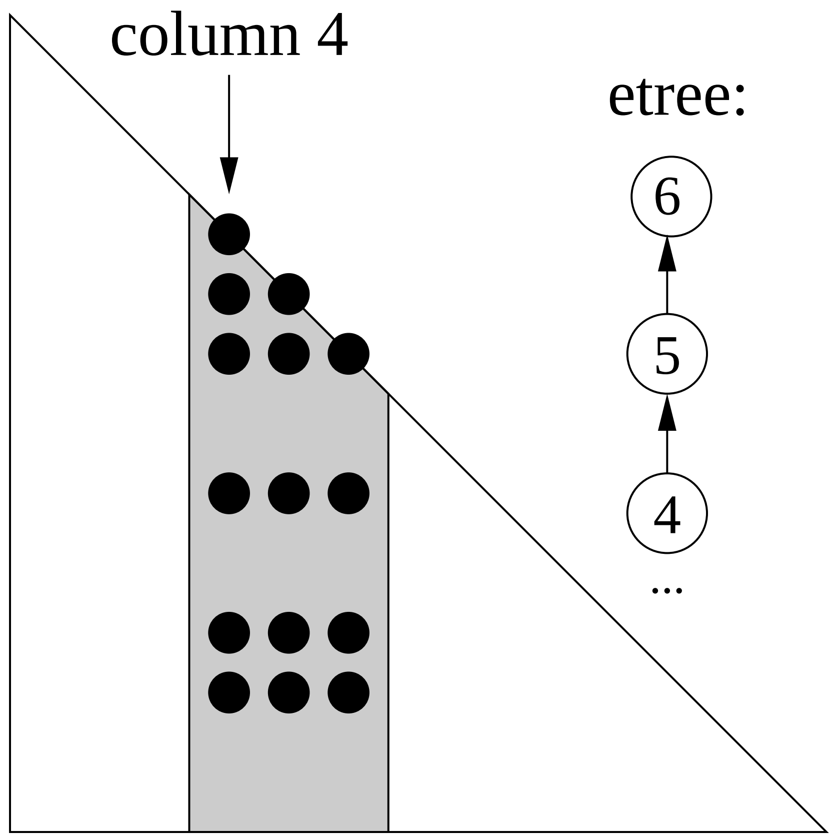
Sparse Cholesky: supernodal



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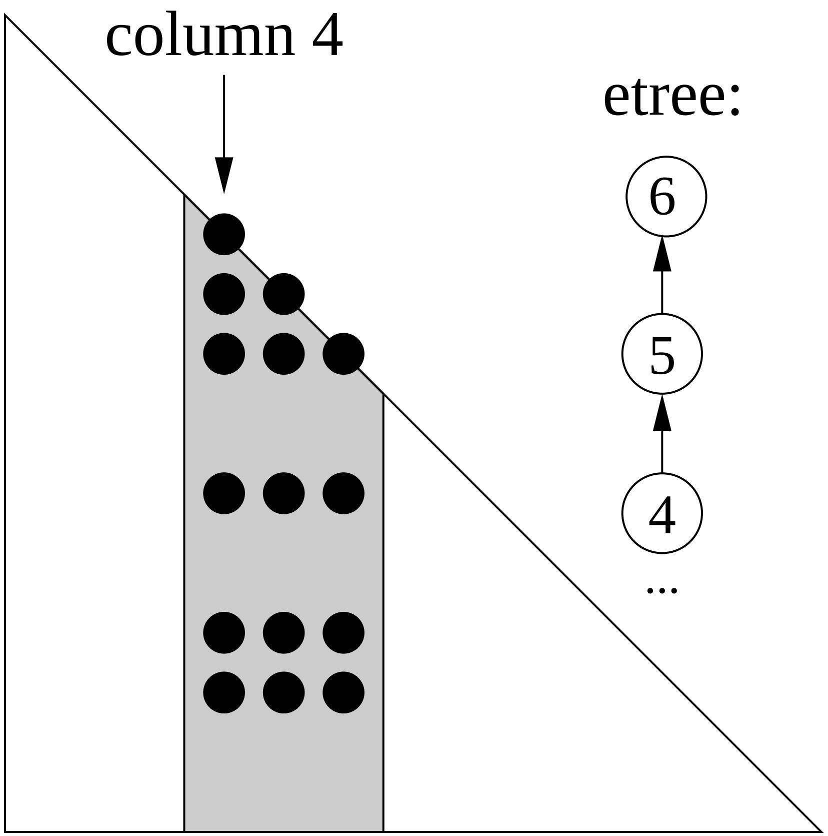
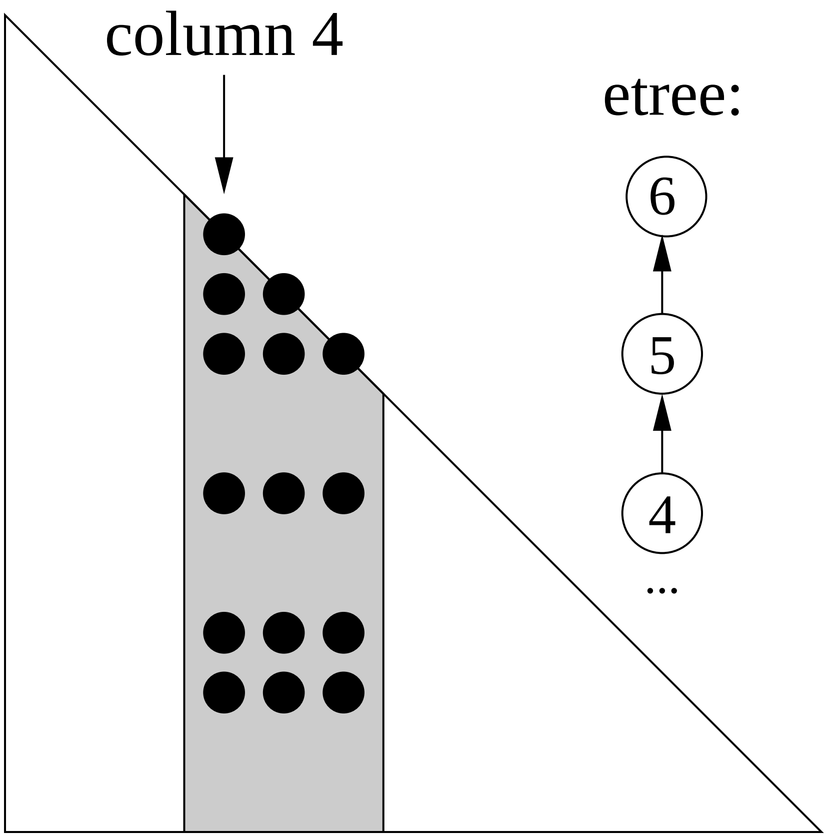


- Adjacent columns of L often have identical pattern

Sparse Cholesky: supernodal



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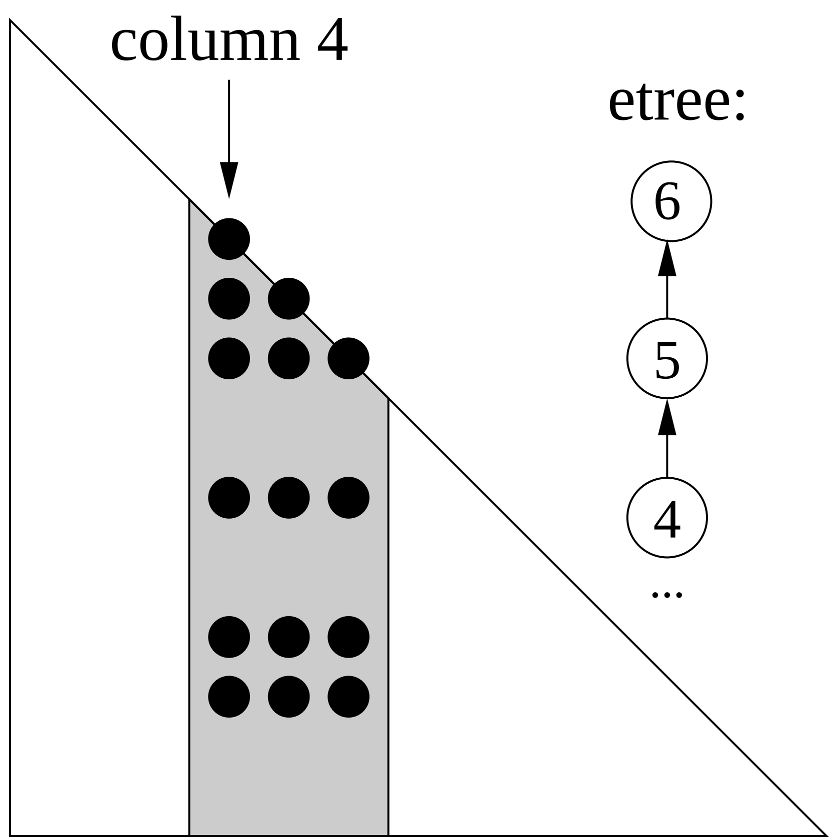
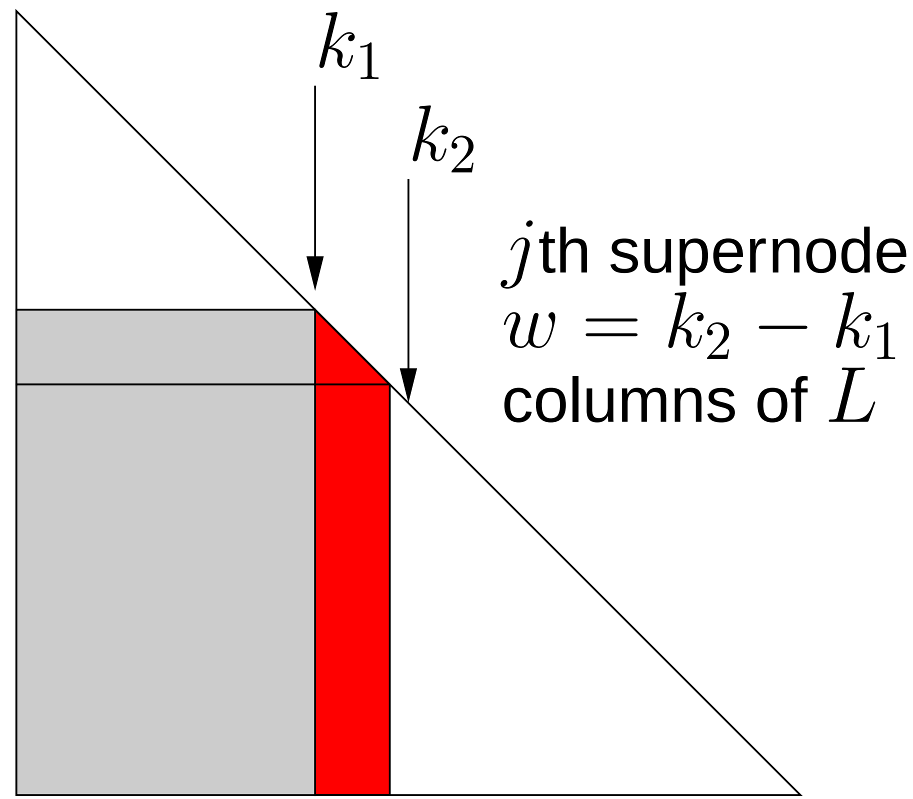


- Adjacent columns of L often have identical pattern
- a chain in the elimination tree
- can exploit dense submatrix operations

Sparse Cholesky: supernodal

block left-looking

- for jth supernode:



Sparse Cholesky: supernodal

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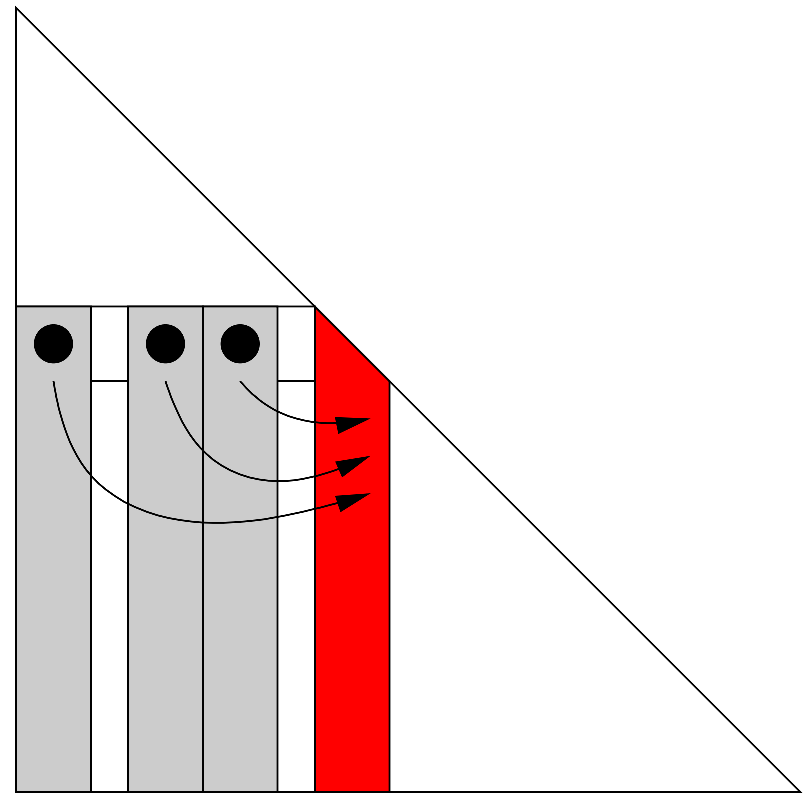

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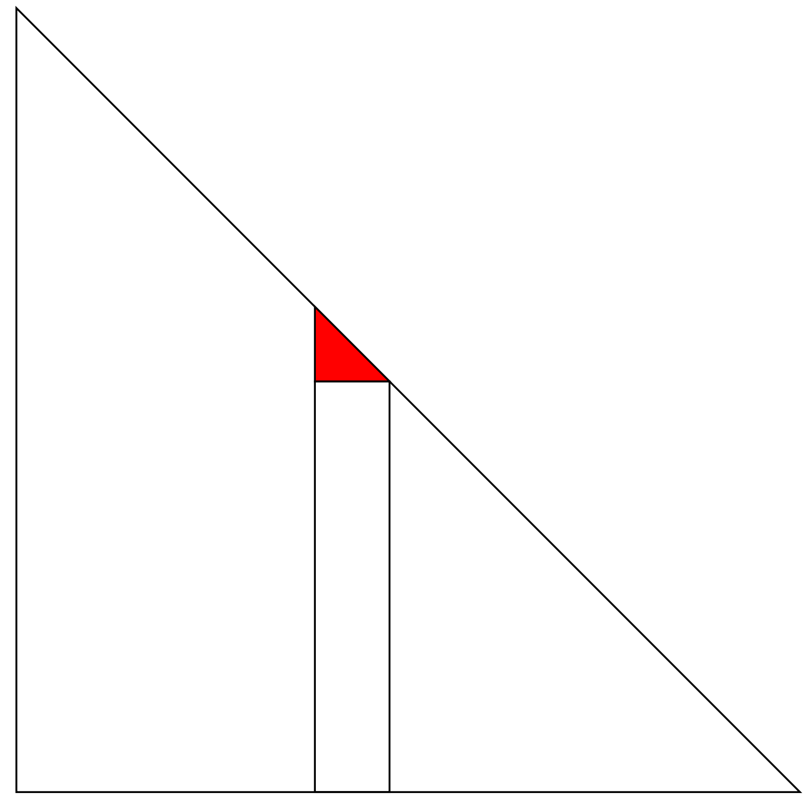

- for jth supernode:
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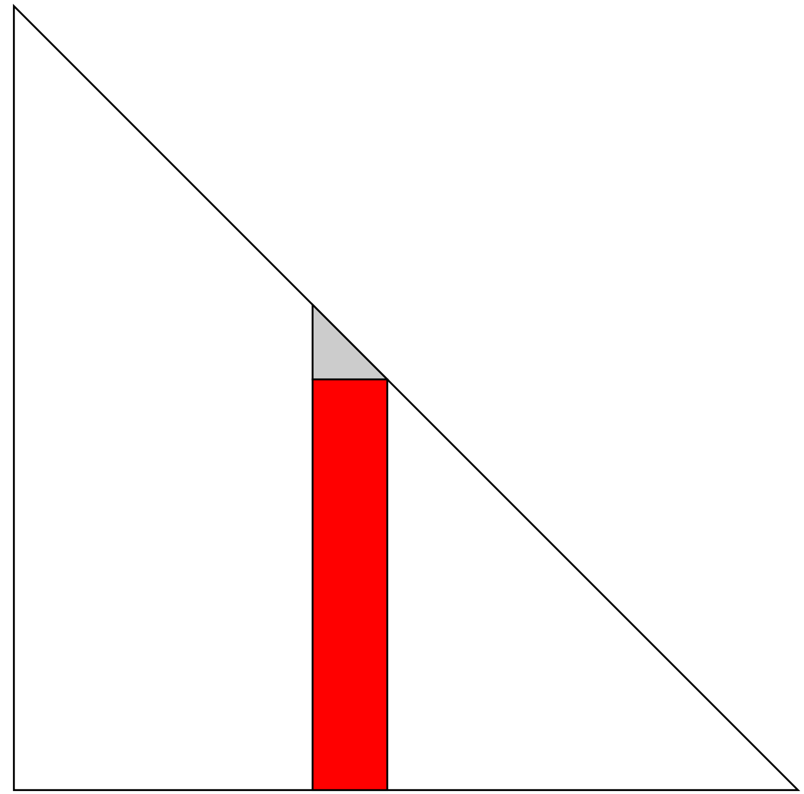
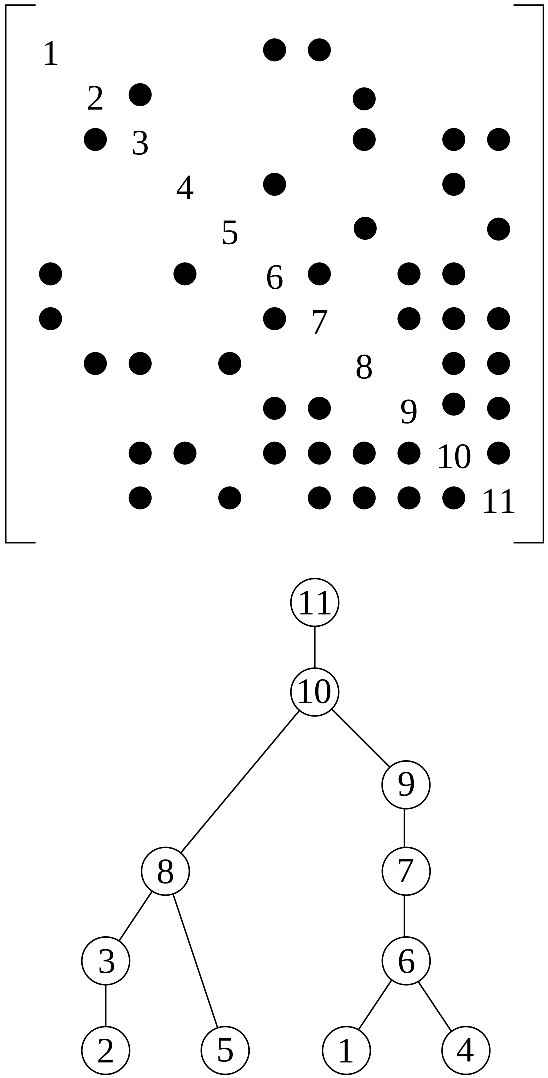
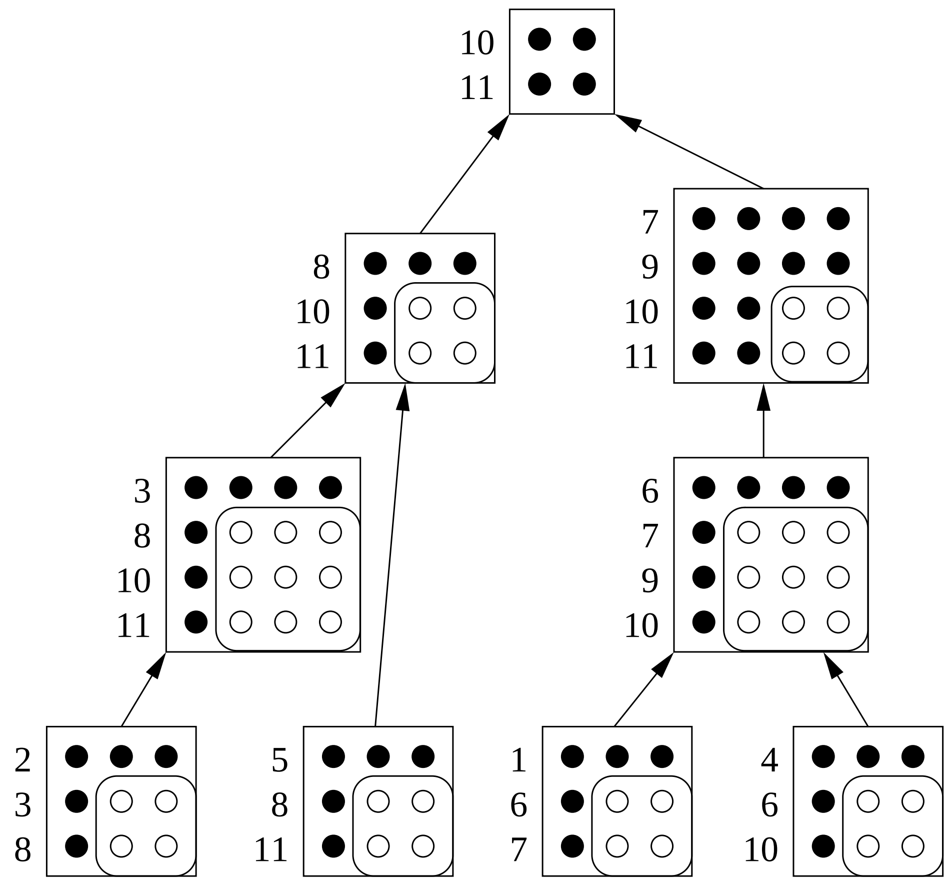


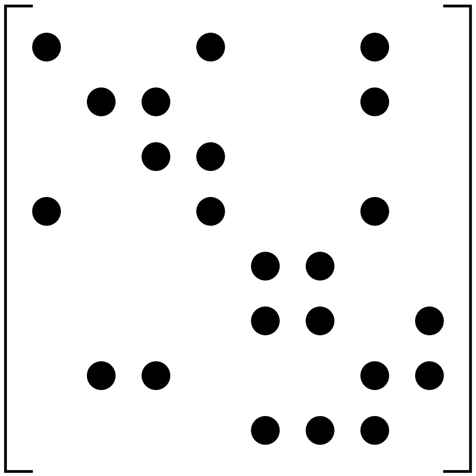
Sparse LU: multifrontal



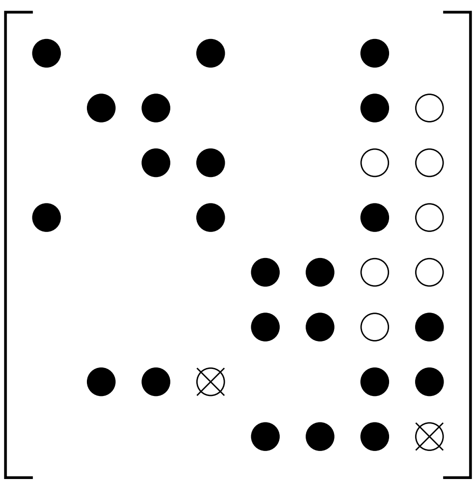


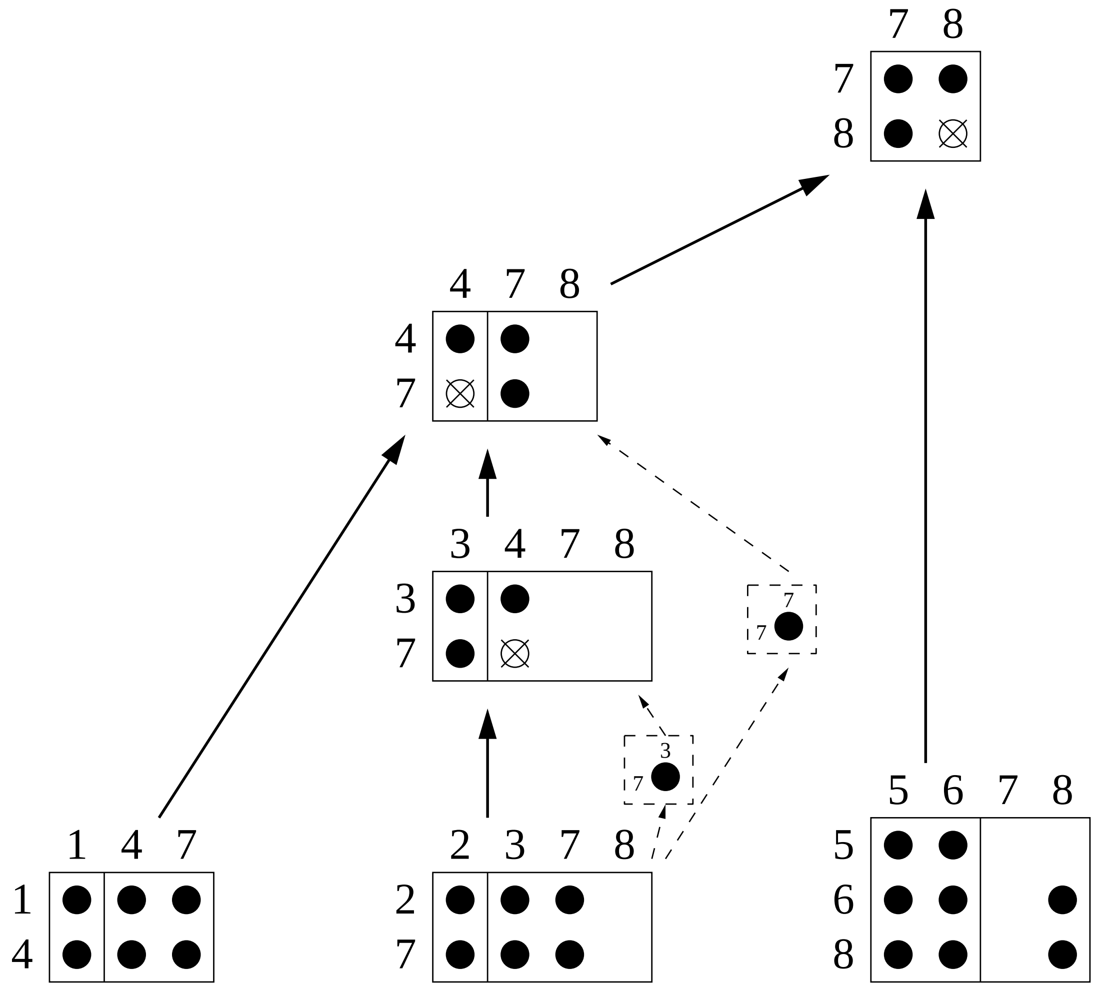
Sparse LU: UMFPACK

A



LU factors





x=A\b **when A is sparse**

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- http://www.cise.ufl.edu/research/sparse

Postscript

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- 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`

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