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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- Goal: sparse matrix methods from the ground up
- 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
  - relies on `x=L\b`, where `L`, `x`, `b` are all sparse
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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: [          3,                6,                ]
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Ai: [                                   1,  3   ]
Ax: [                                   0.9,1.0]
```

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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end
```

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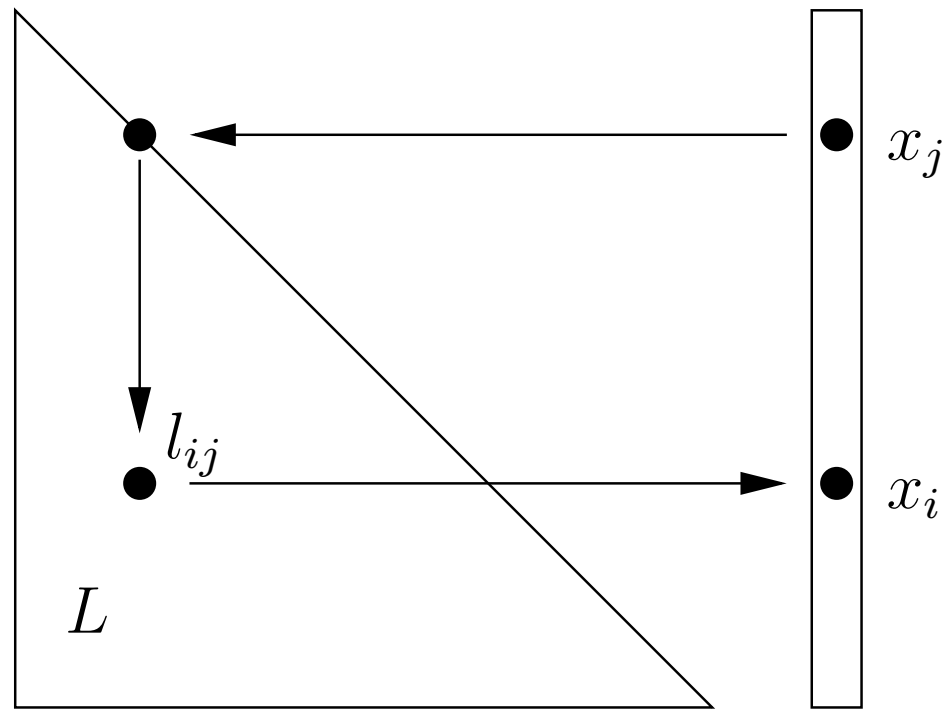
- $b_i \neq 0 \Rightarrow x_i \neq 0$



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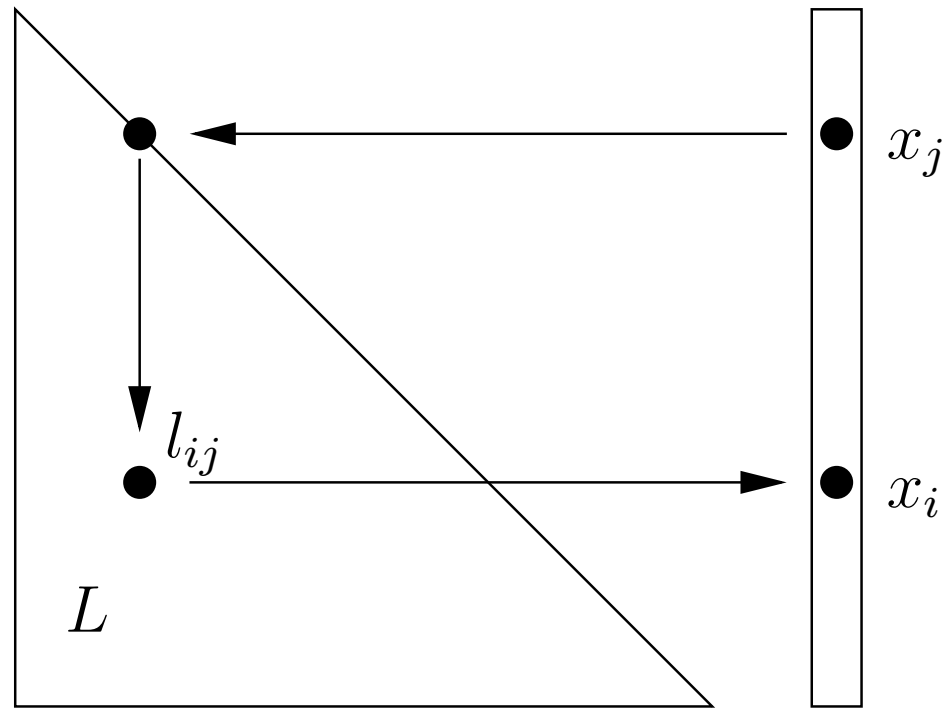

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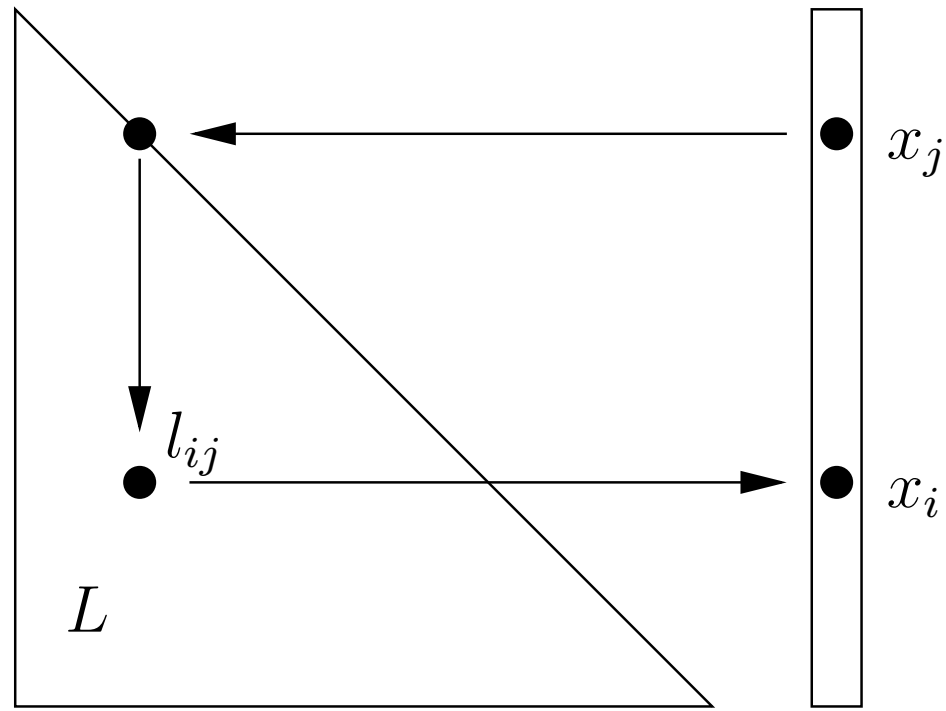
- let $G(L)$ have an edge $j \rightarrow i$ if $l_{ij} \neq 0$



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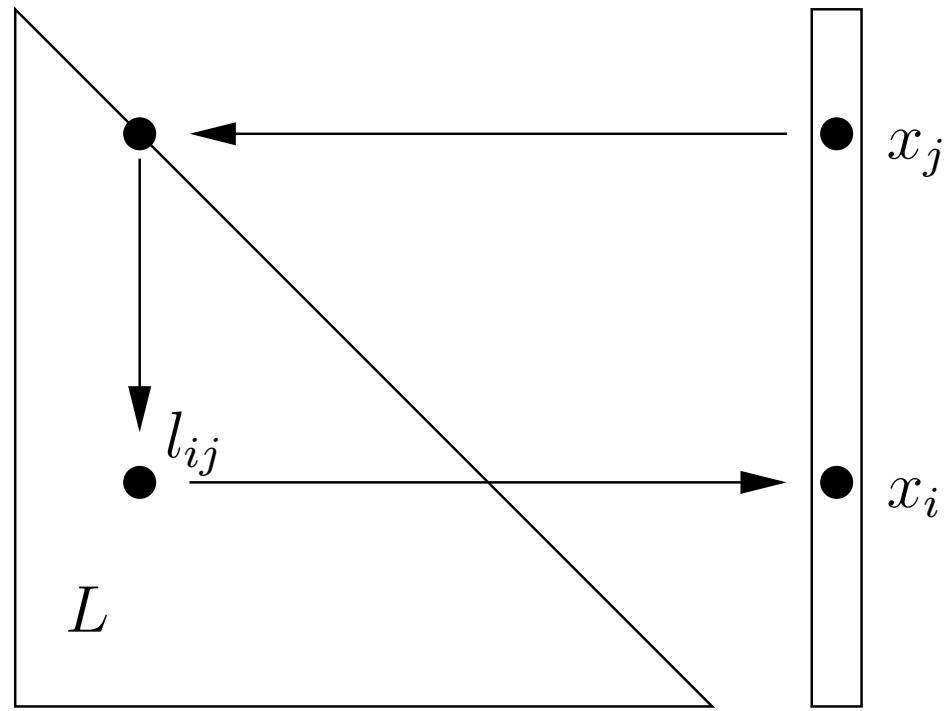
- let $\mathcal{B} = \{i \,|\, b_i \neq 0\}$ and $\mathcal{X} = \{i \,|\, x_i \neq 0\}$



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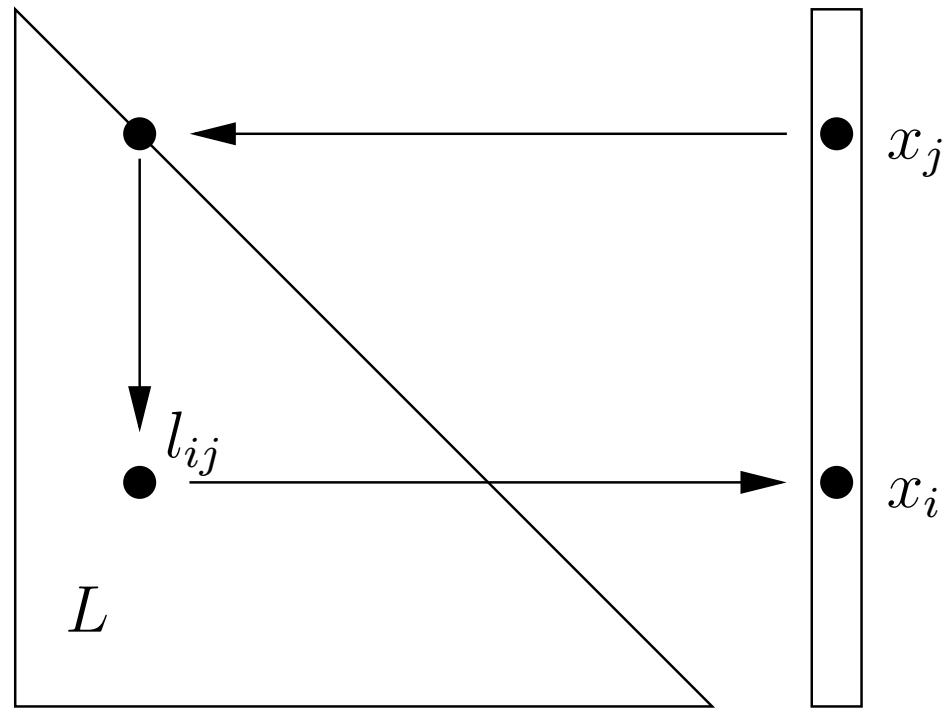
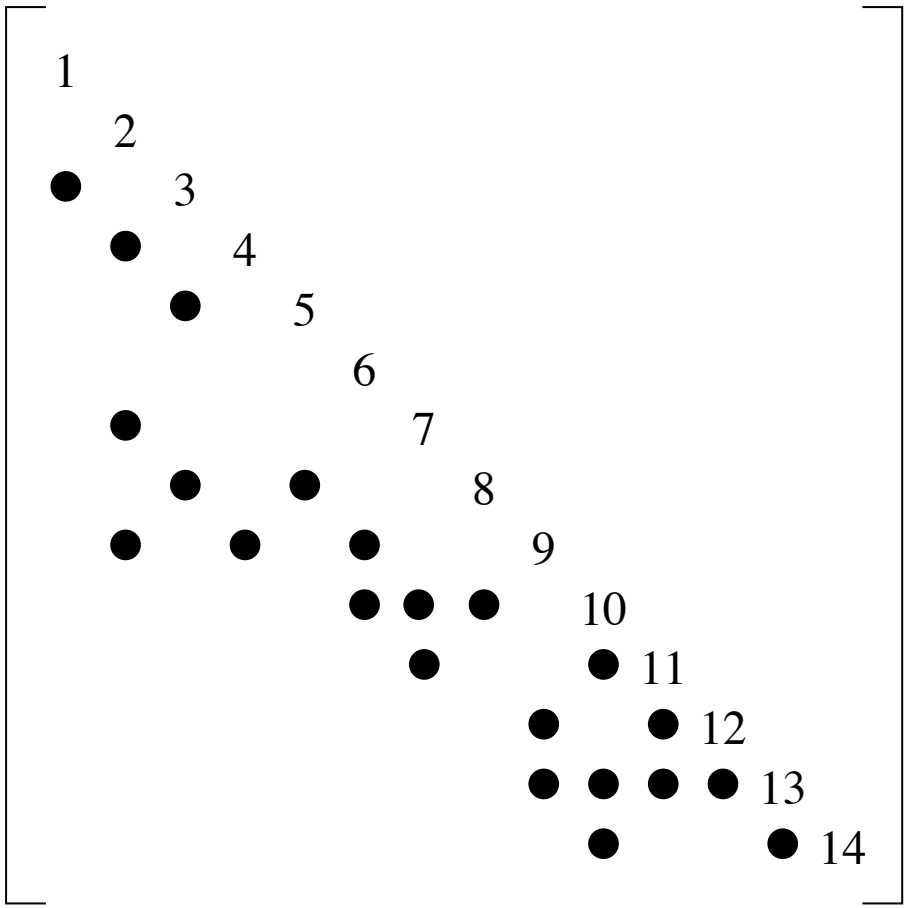
- let $G(L)$ have an edge $j \rightarrow i$ if $l_{ij} \neq 0$
- let $\mathcal{B} = \{i \,|\, b_i \neq 0\}$ and $\mathcal{X} = \{i \,|\, x_i \neq 0\}$
- then $\mathcal{X} = \mathsf{Reach}_{G(L)}(\mathcal{B})$

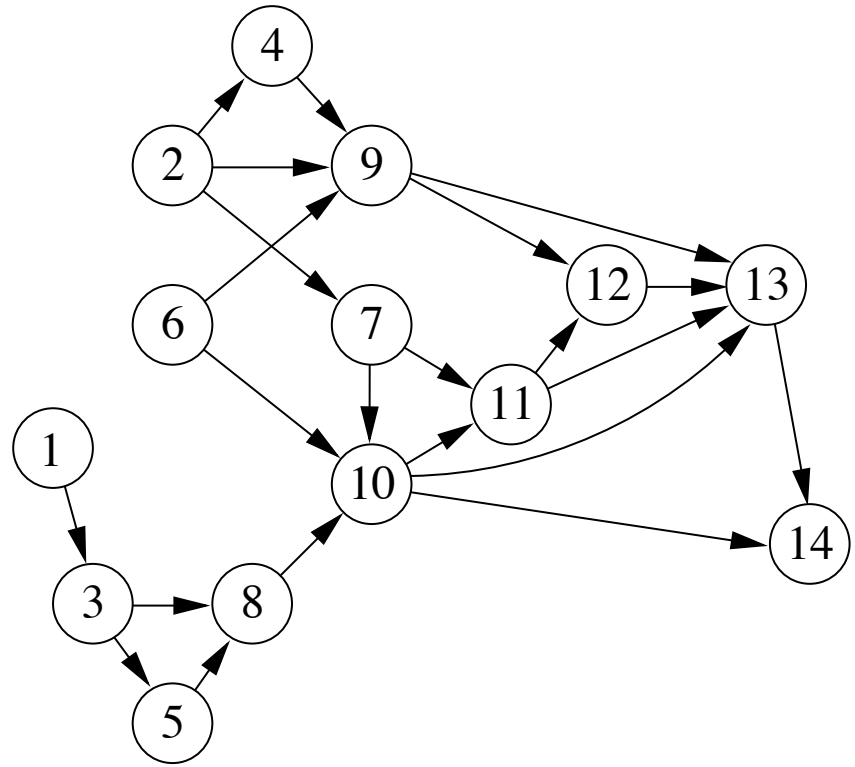


Sparse lower triangular solve, `x=L\b`

Lower triangular matrix L



Graph G_L



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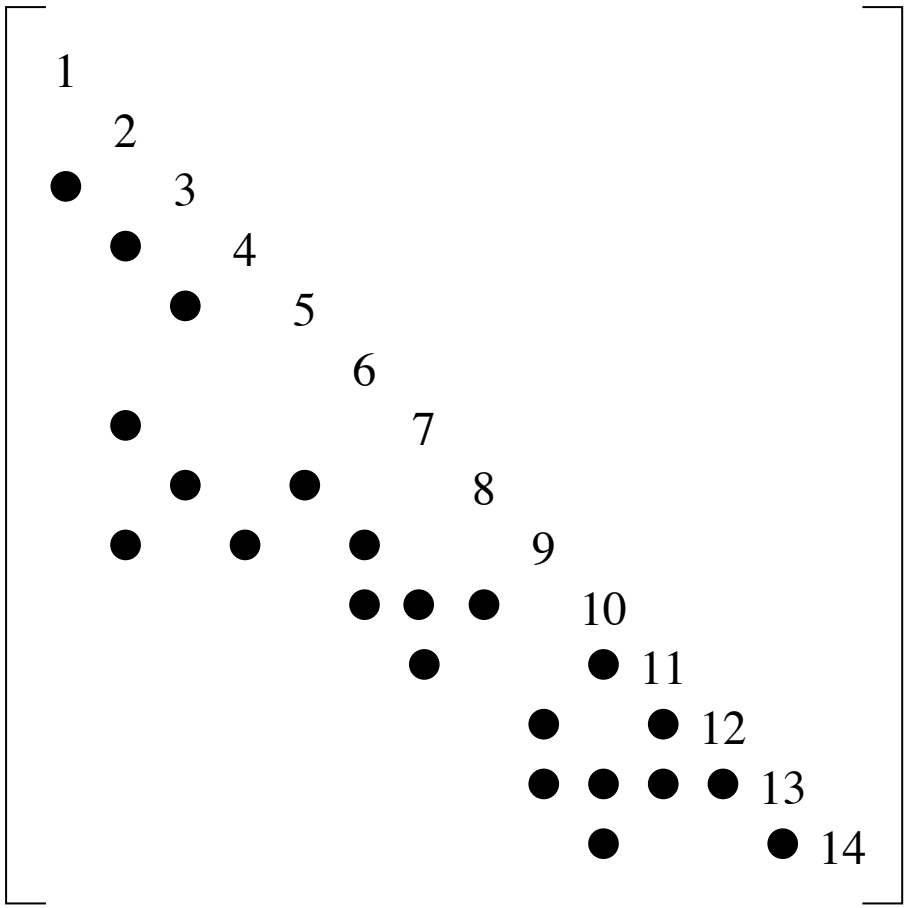

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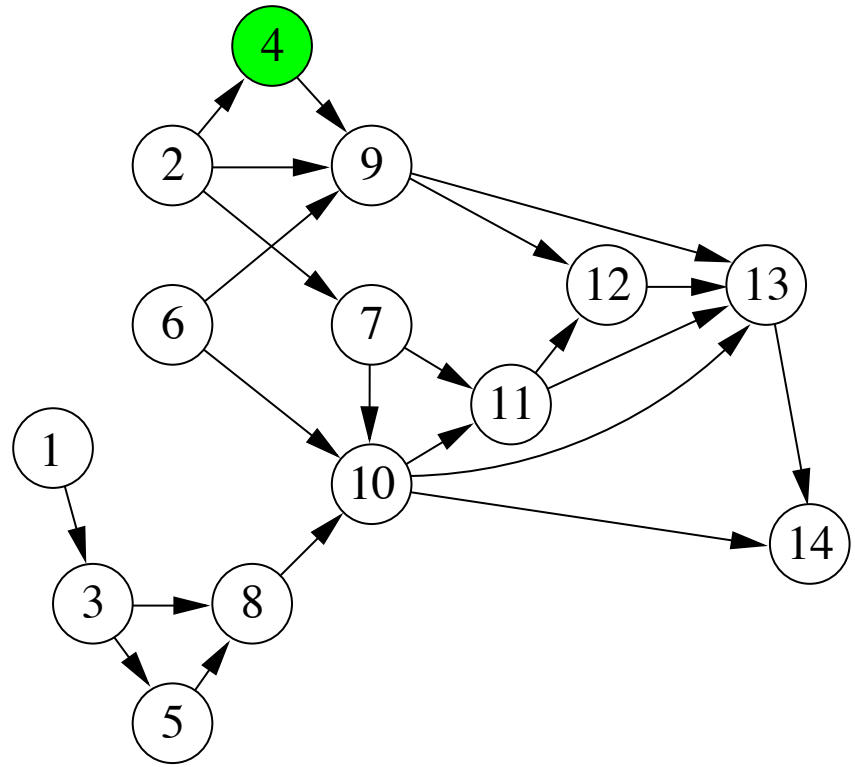
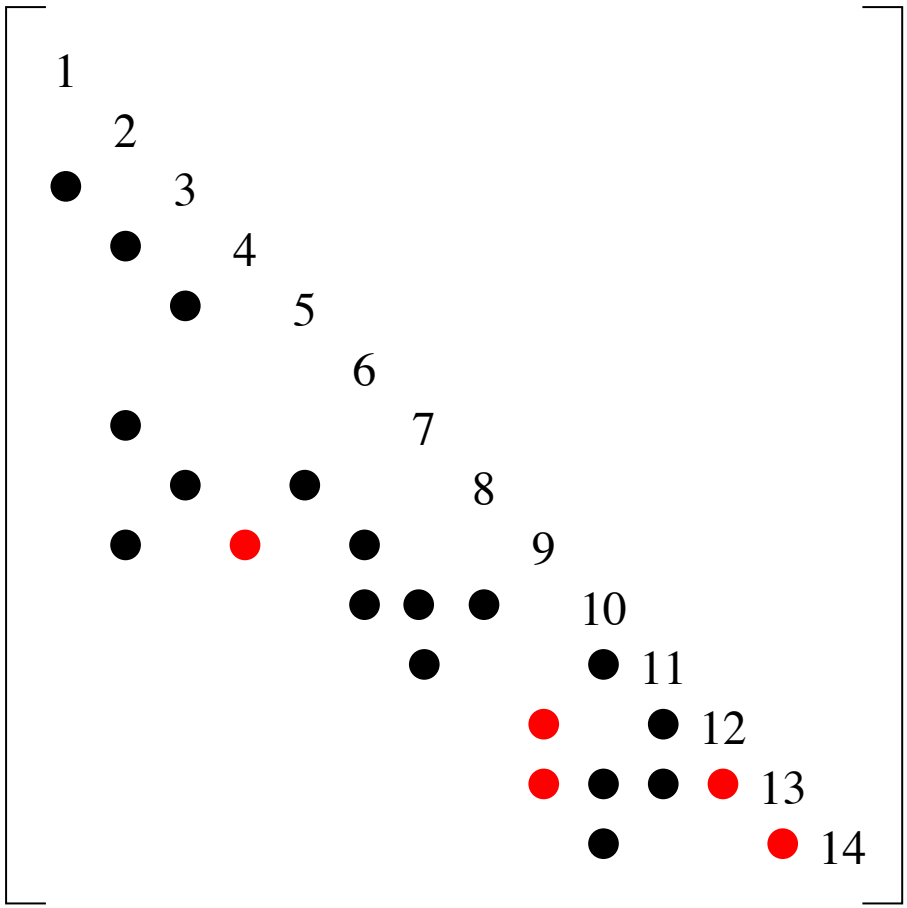


If $\mathcal{B} = \{4\}$

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

Lower triangular matrix L



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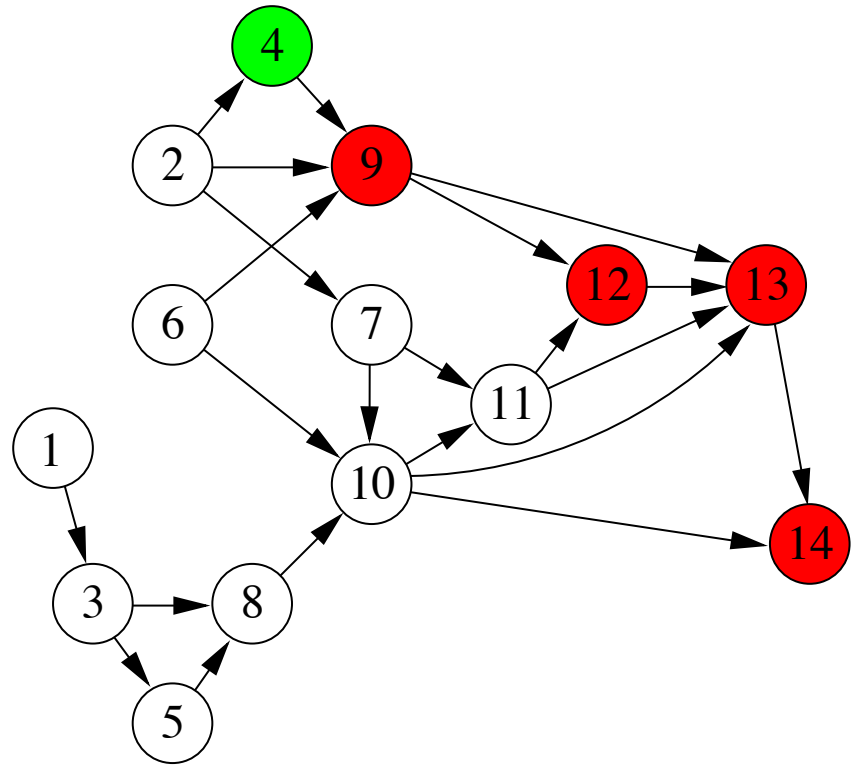
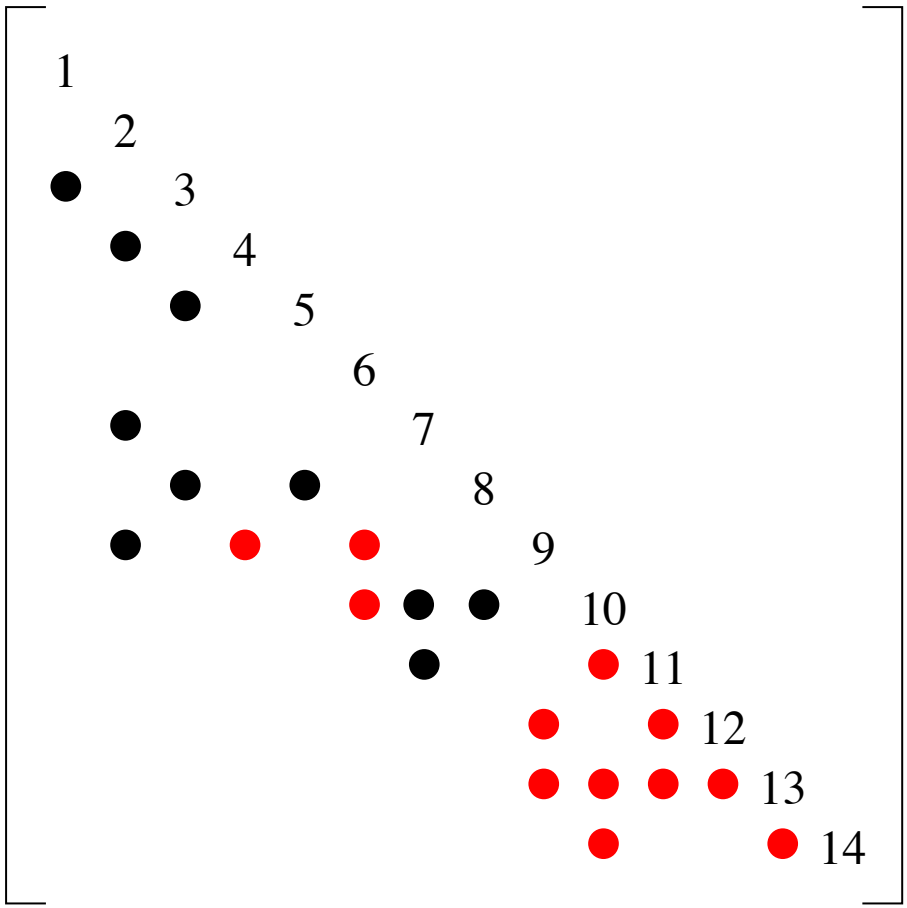


If $\mathcal{B} = \{4\}$
then $\mathcal{X} = \{4, 9, 12, 13, 14\}$

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

Lower triangular matrix L



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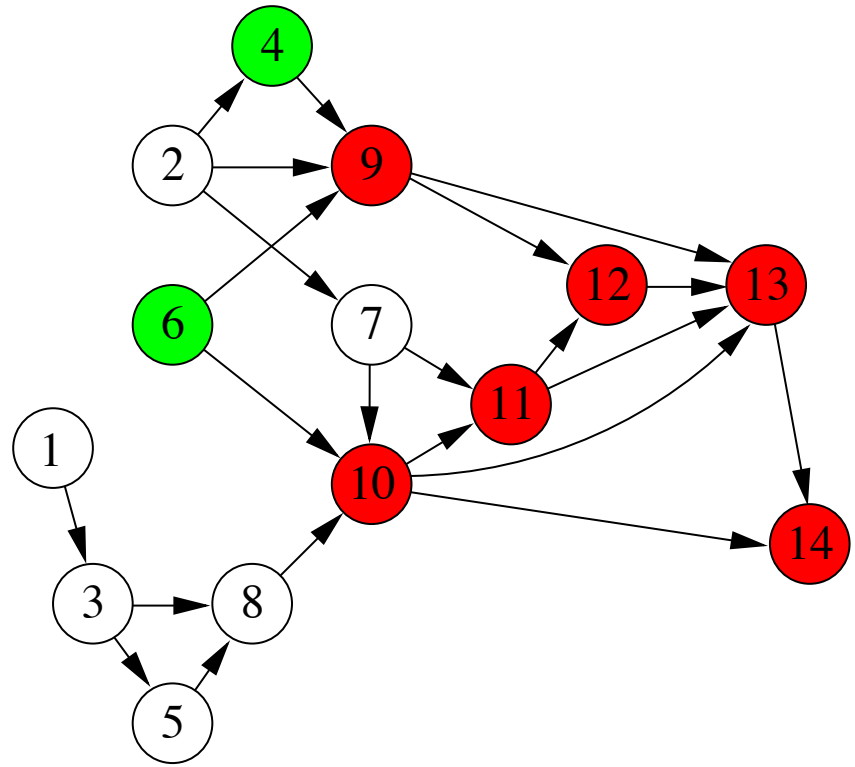

If $\mathcal{B} = \{4, 6\}$

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: $O(n + \text{flops})$, 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 $\mathcal{X}$

```
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function `x = lsolve(L,b)`
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    `x = b`
    for each j in $\mathcal{X}$
        `x(j+1:n) = x(j+1:n) - L(j+1:n,j) * x(j)`

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

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
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    push j onto stack for X
```

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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which can be less than n

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

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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)
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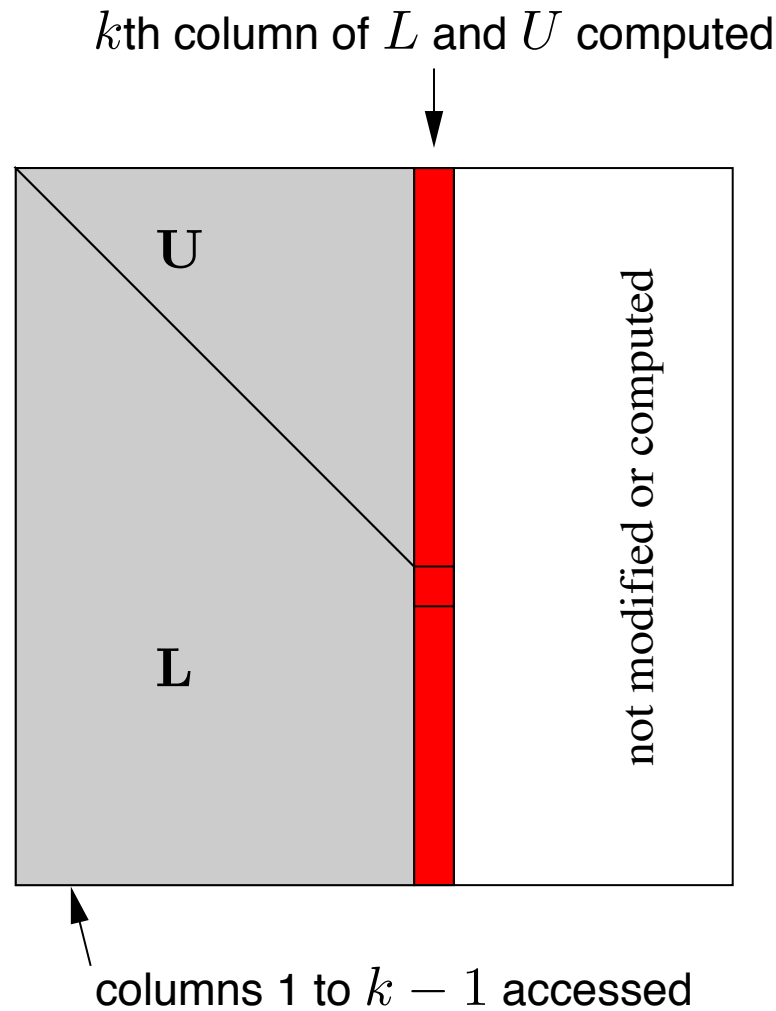

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```
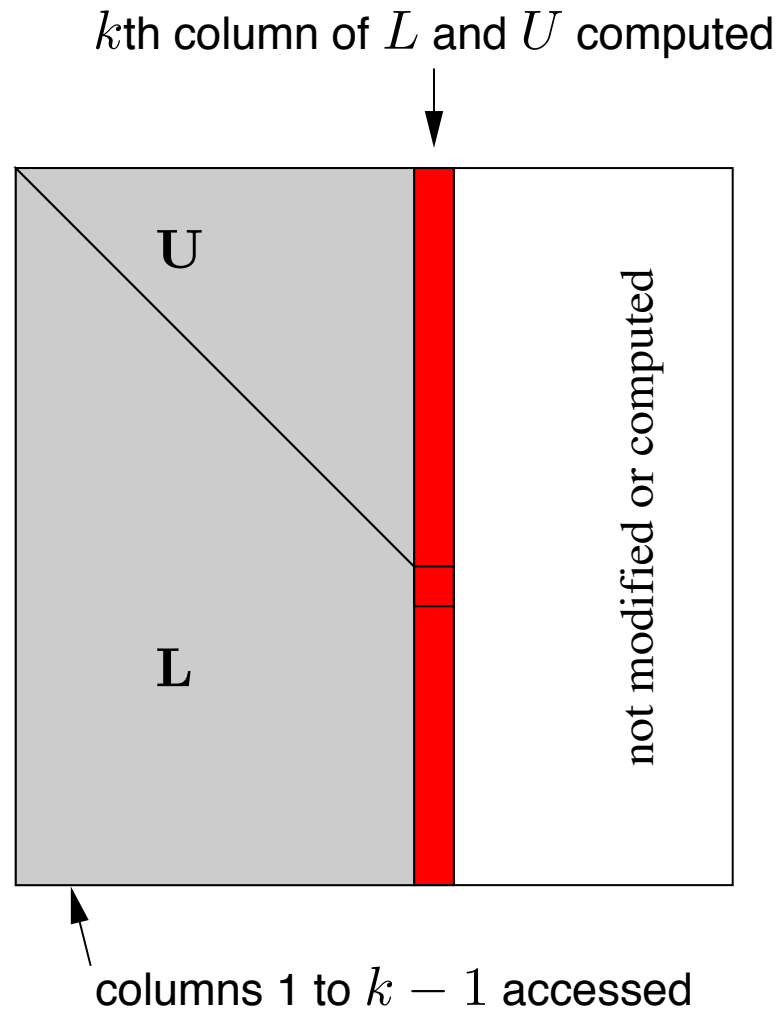

$LU = PAQ$

- 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 $L_{11}L_{11}^T = A_{11}$
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3. $\mathbf{l_{22}} = \sqrt{\mathbf{a_{22}} - \mathbf{l_{12}^T l_{12}}}$

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for k = 1 to n

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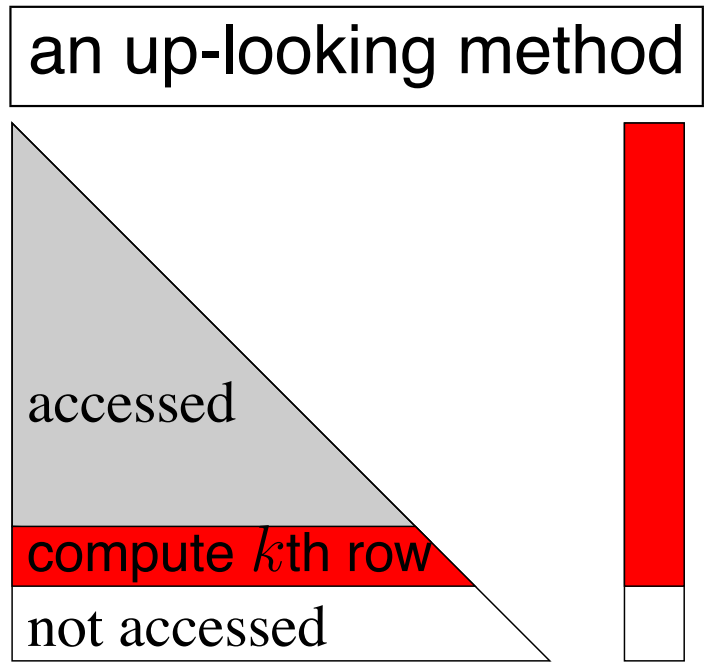
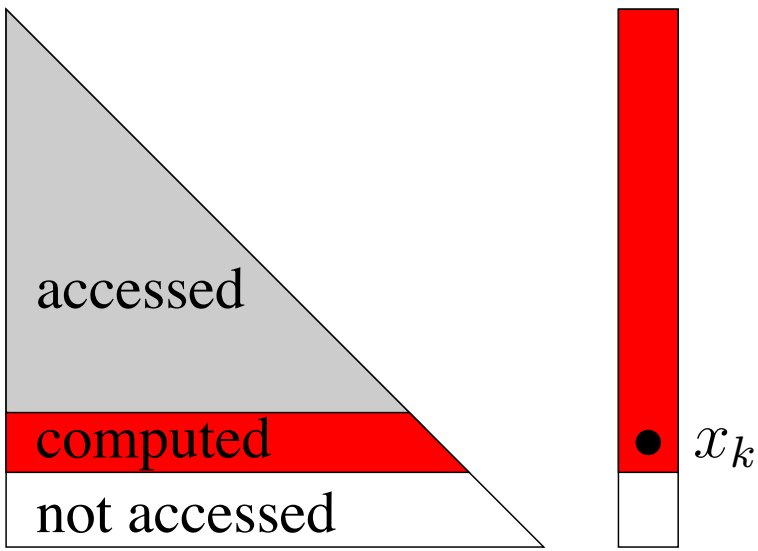


Sparse Cholesky: etree

- 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

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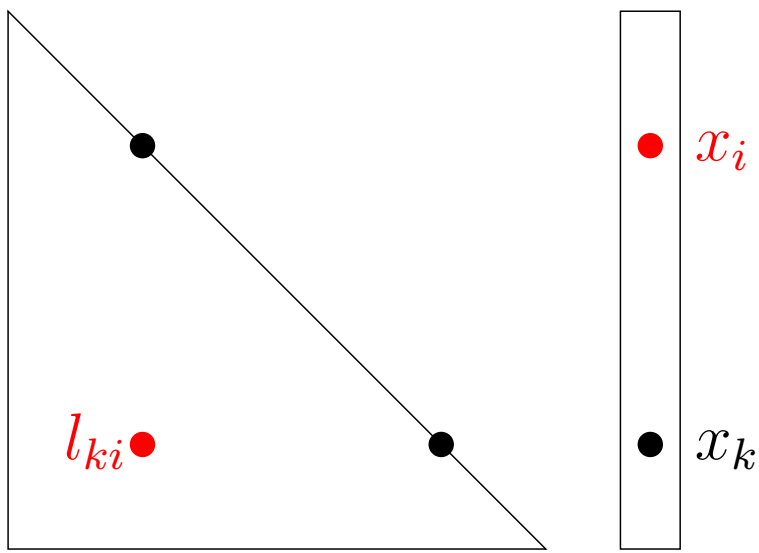

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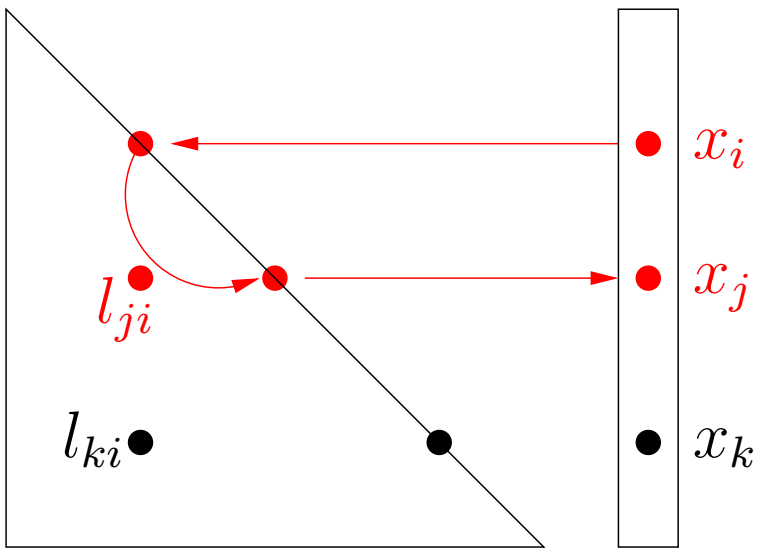

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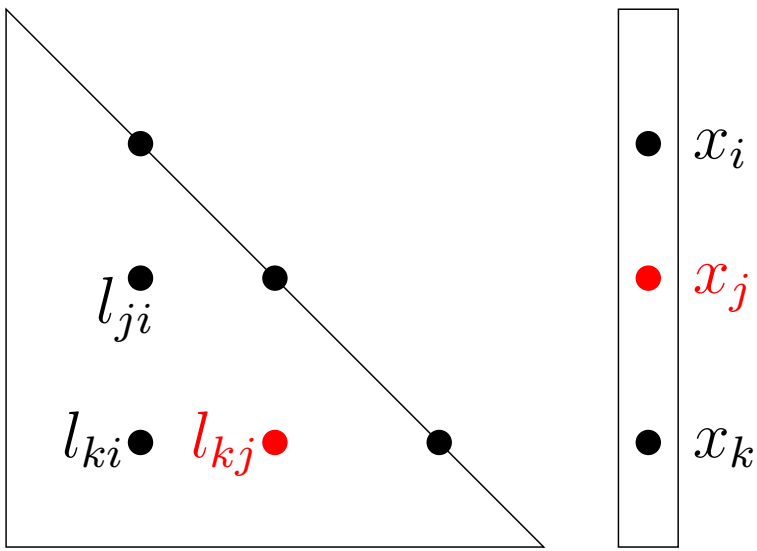

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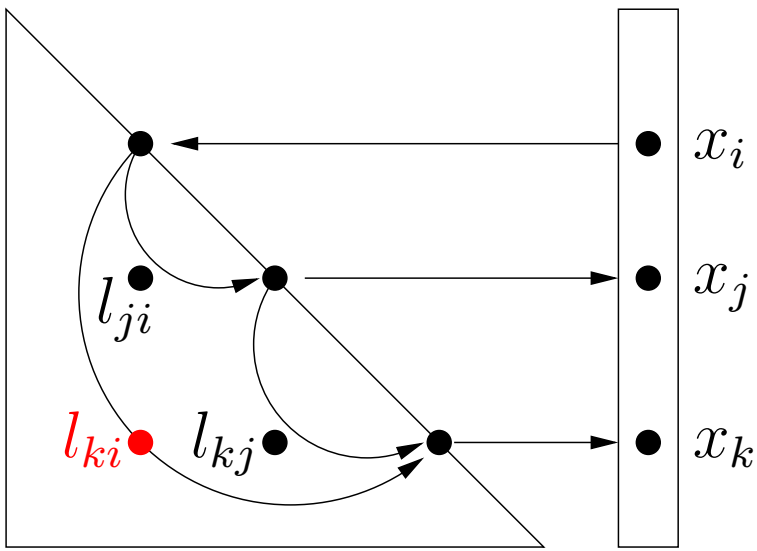

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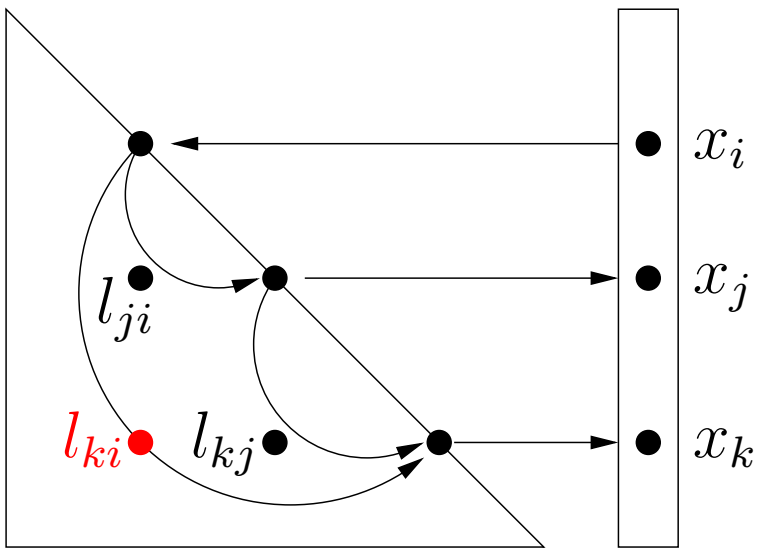

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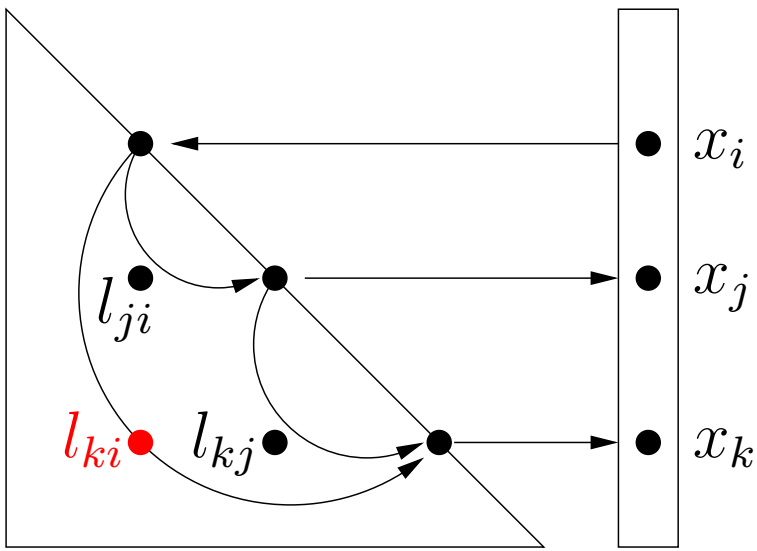

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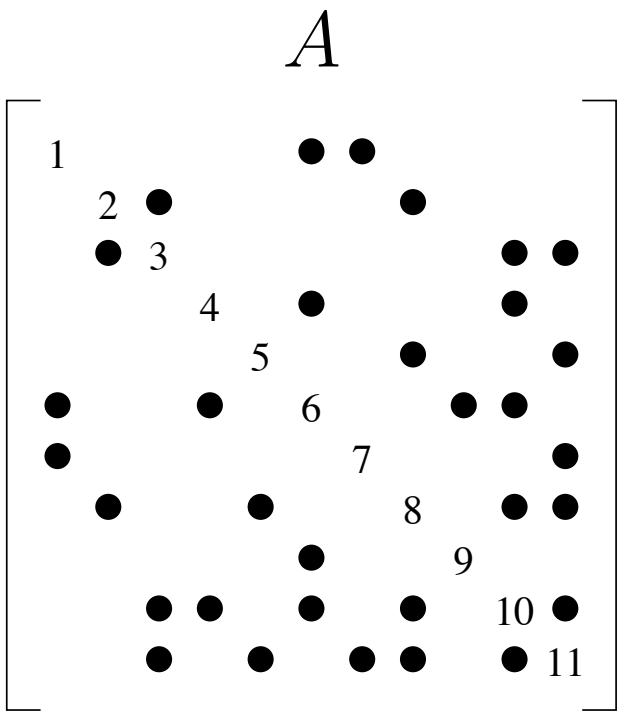

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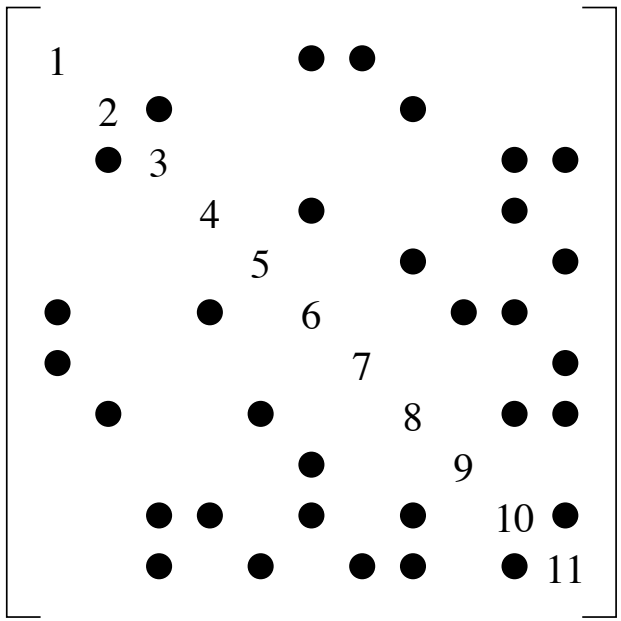

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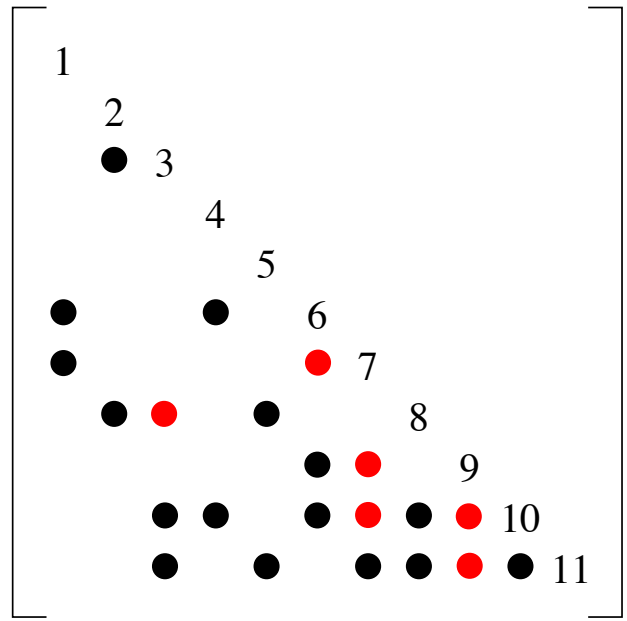

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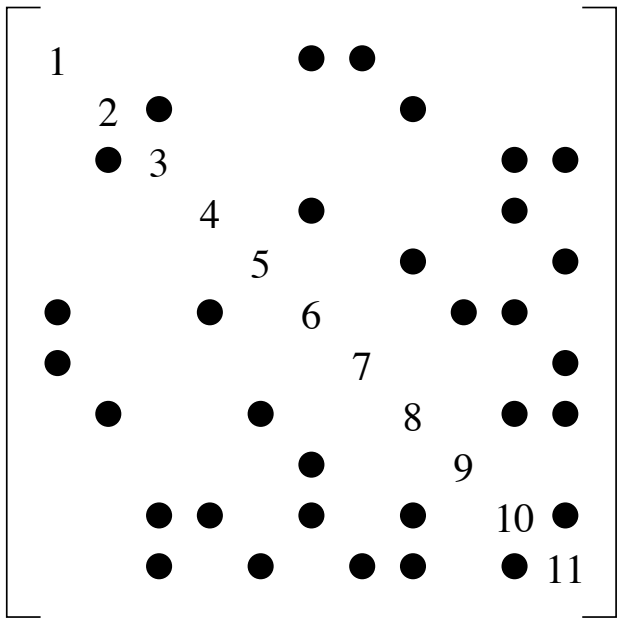

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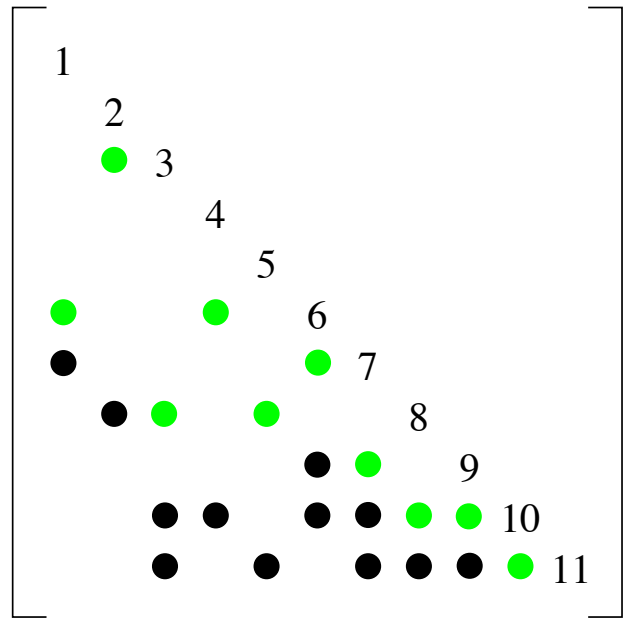
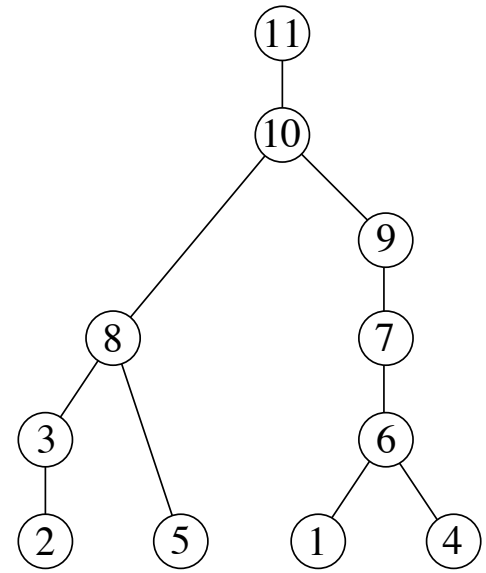


elimination tree



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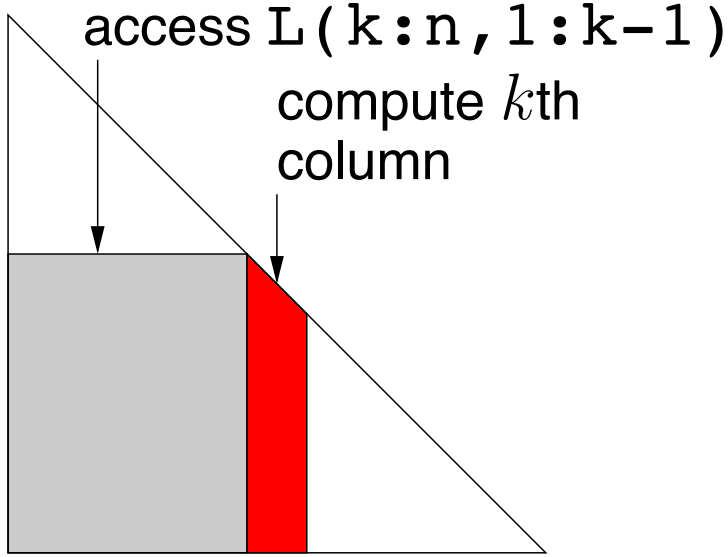
Sparse Cholesky: left-looking



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)
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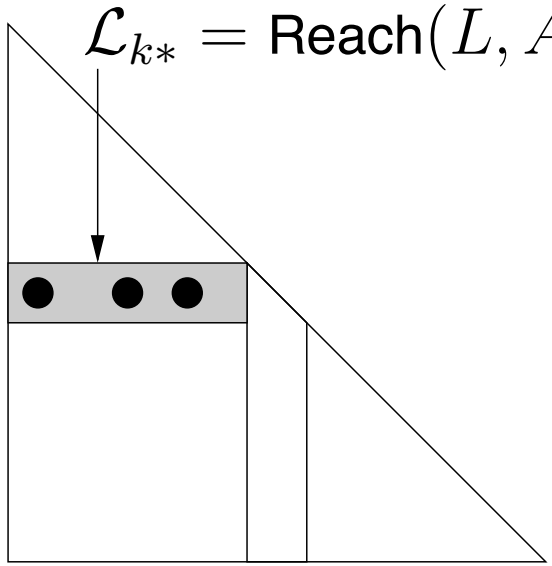
Sparse Cholesky: left-looking



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...

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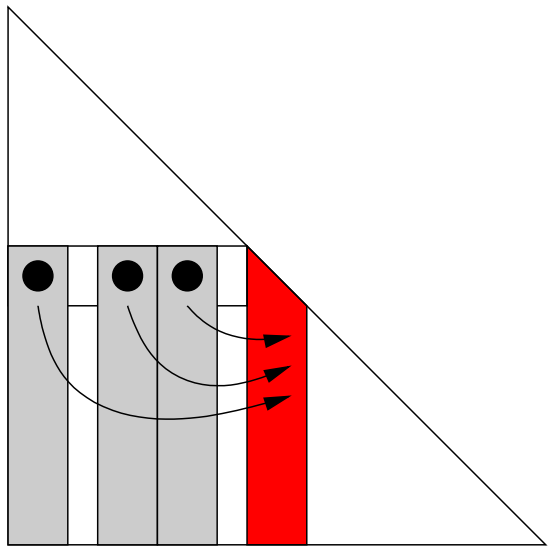

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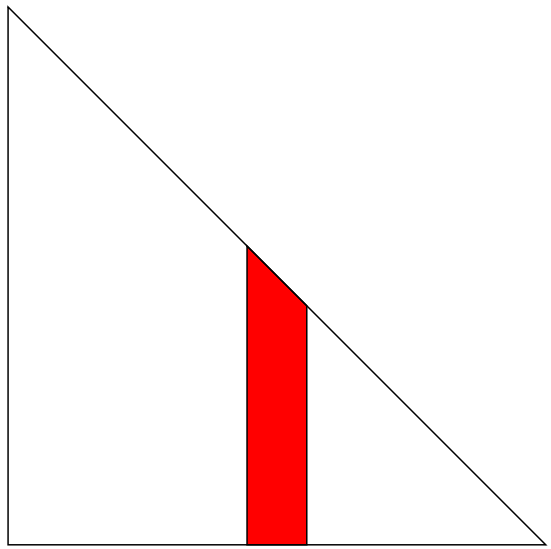

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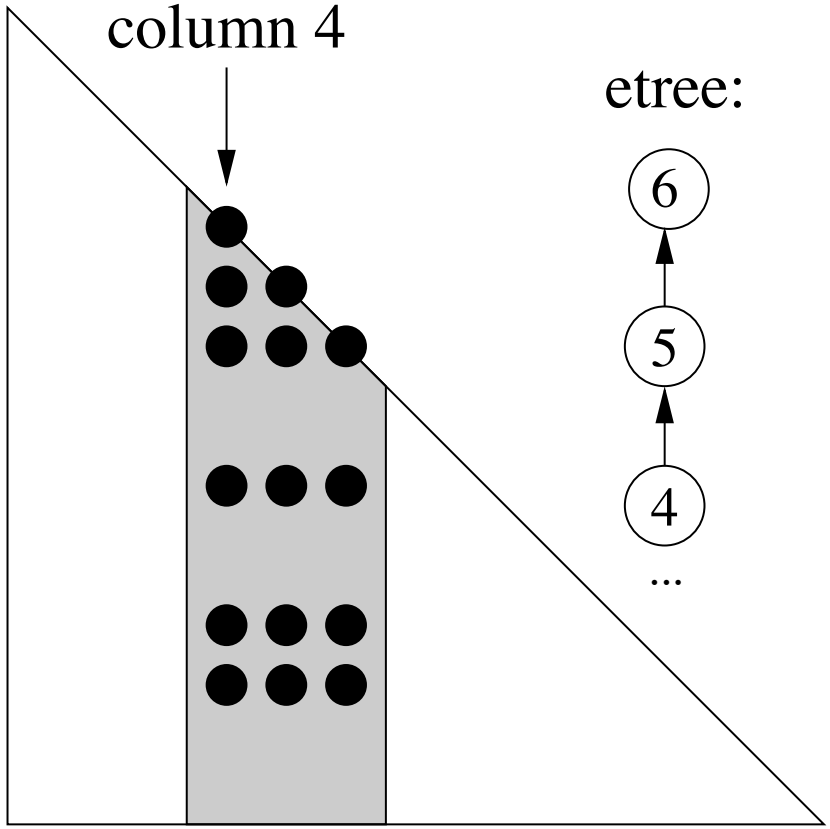
Sparse Cholesky: supernodal



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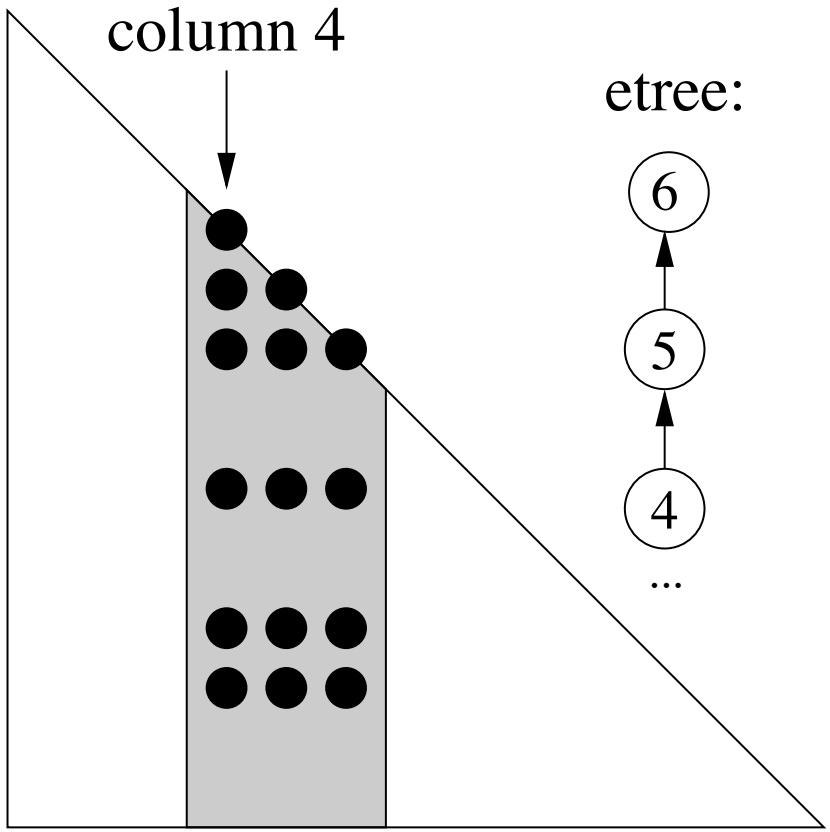

- Adjacent columns of L often have identical pattern

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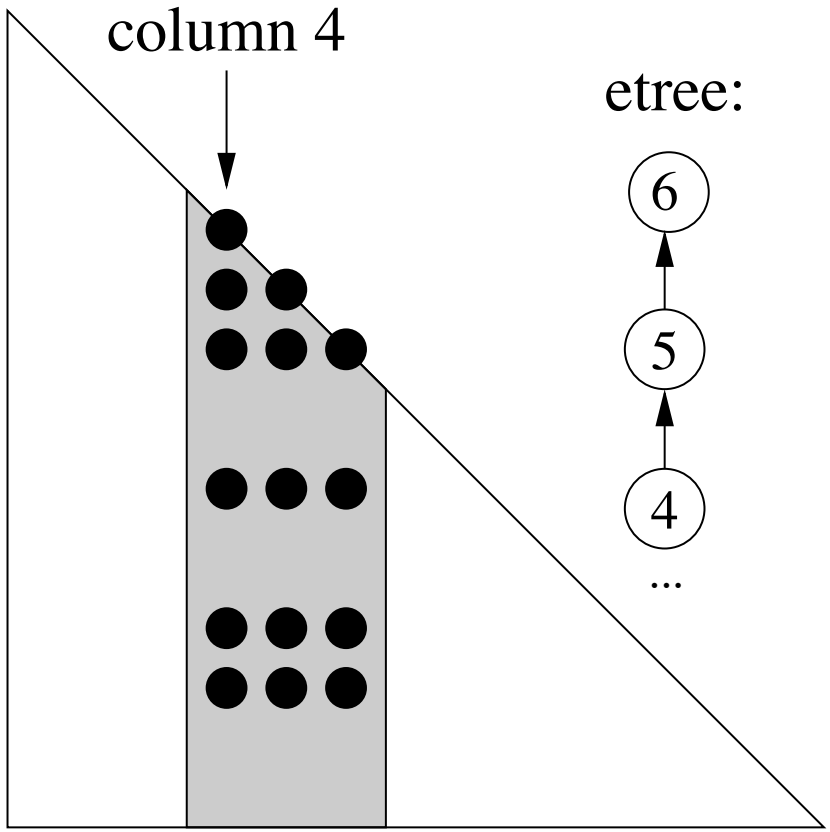

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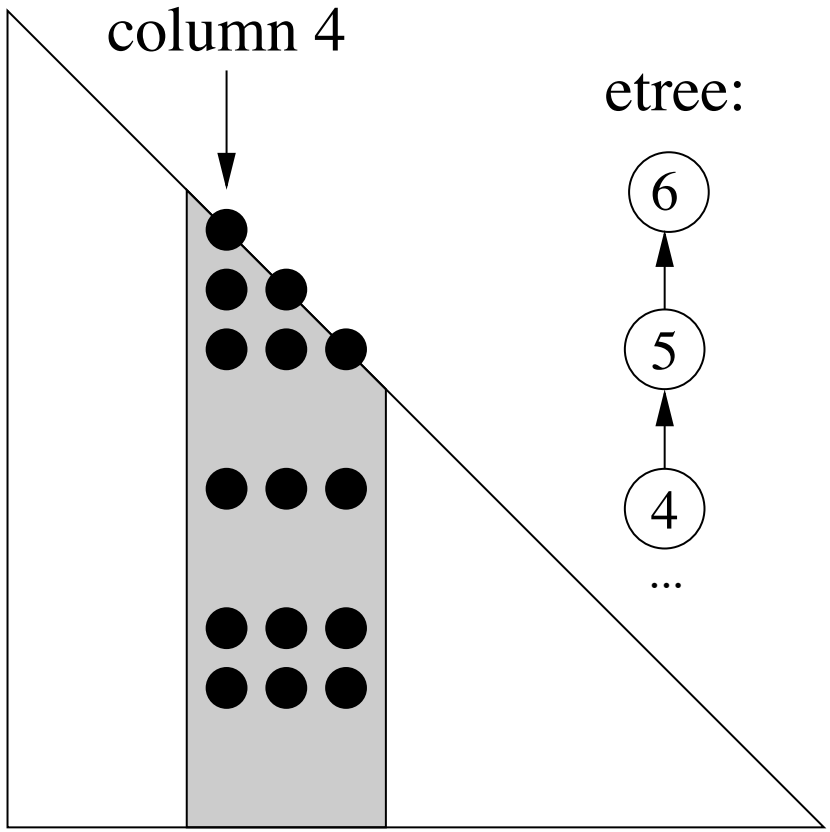

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- can exploit dense submatrix operations

Sparse Cholesky: supernodal

block left-looking

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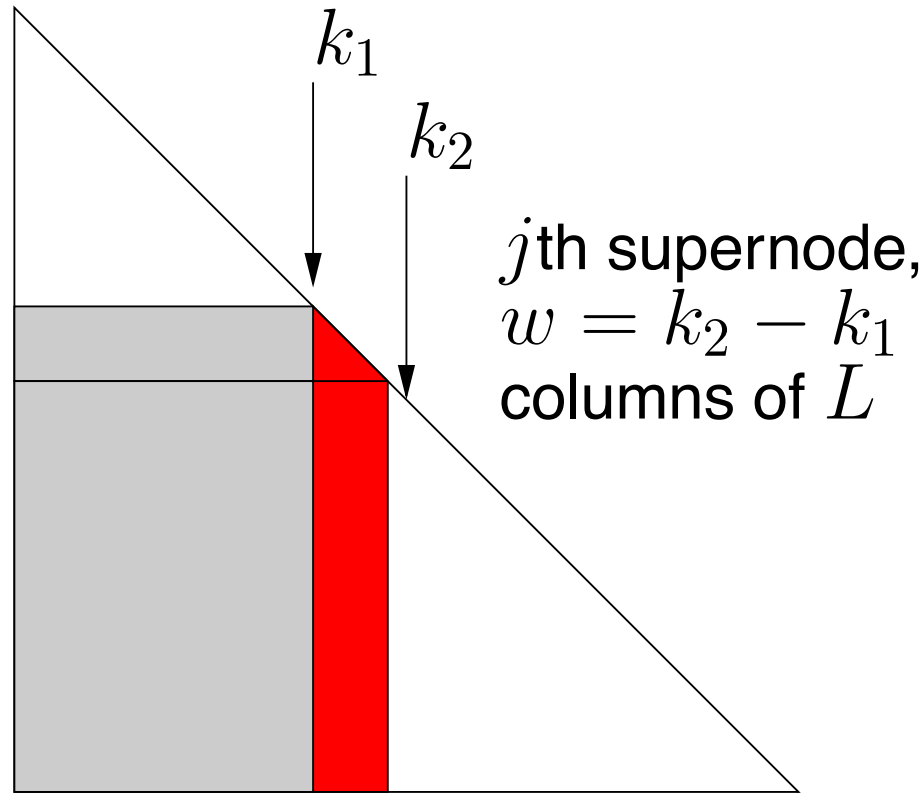

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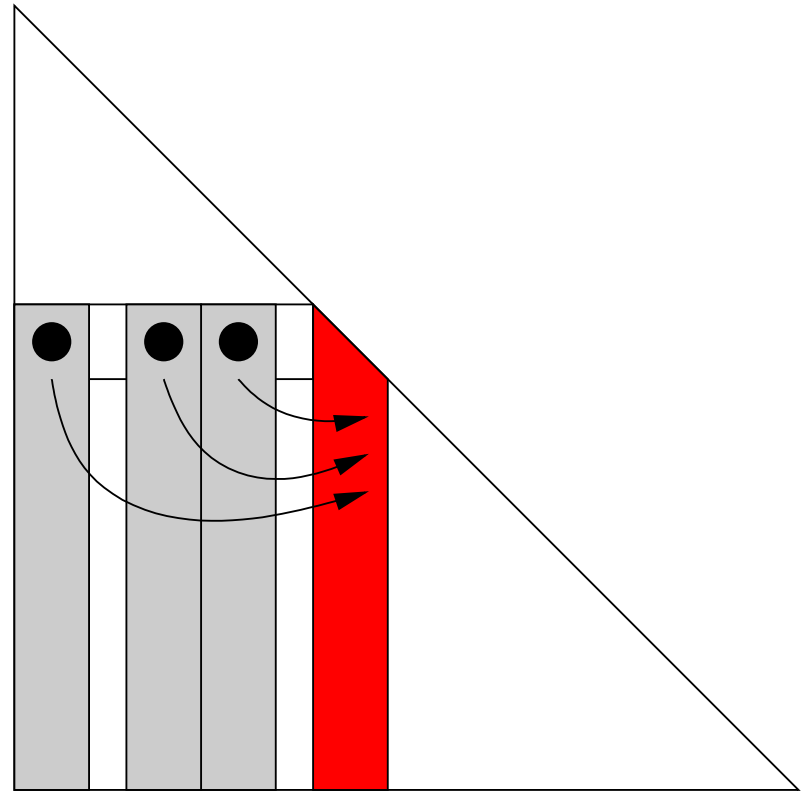

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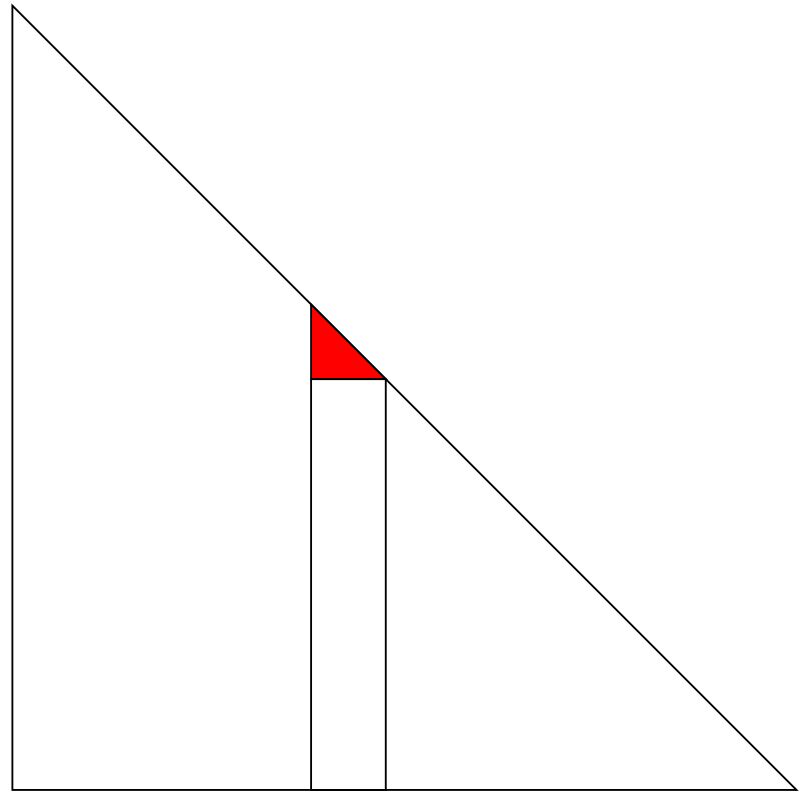

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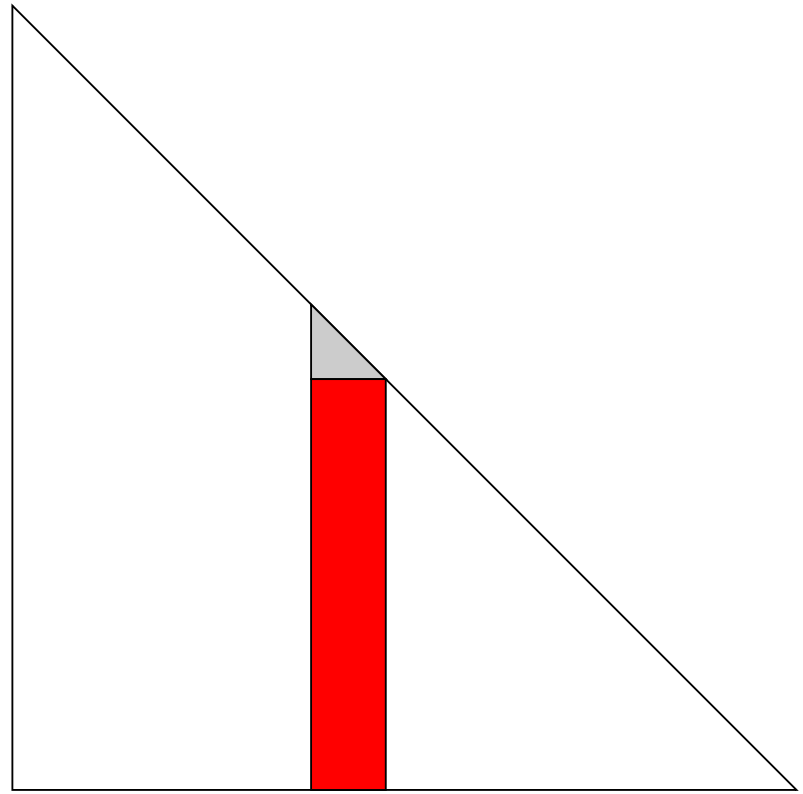
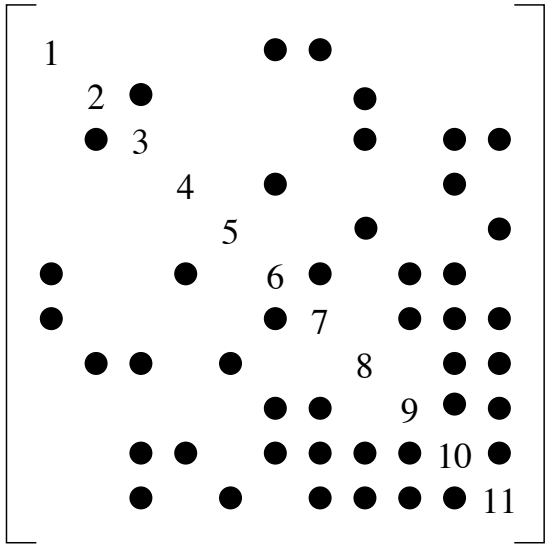
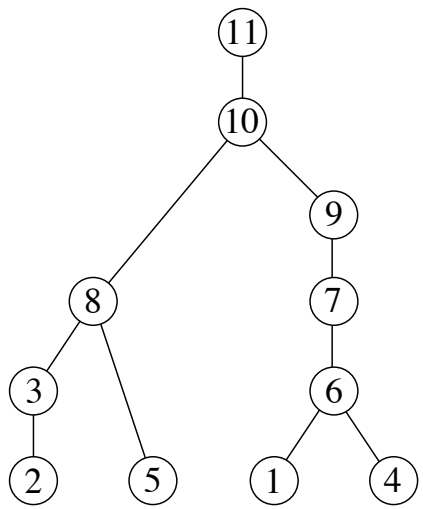
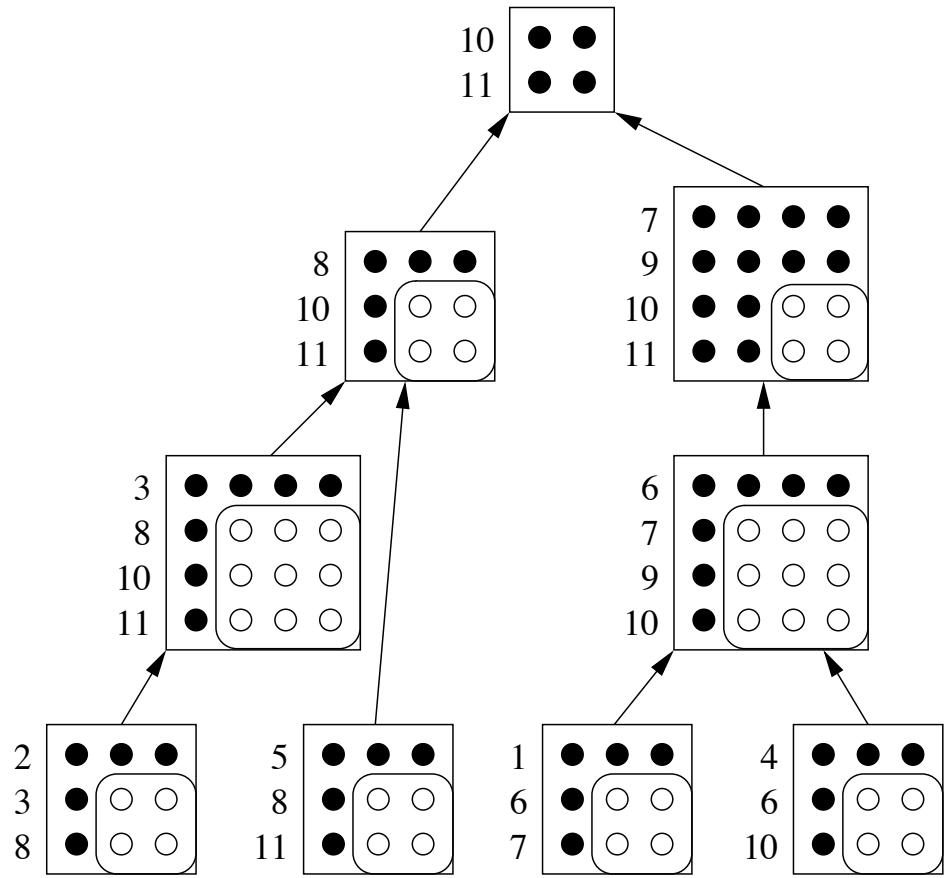


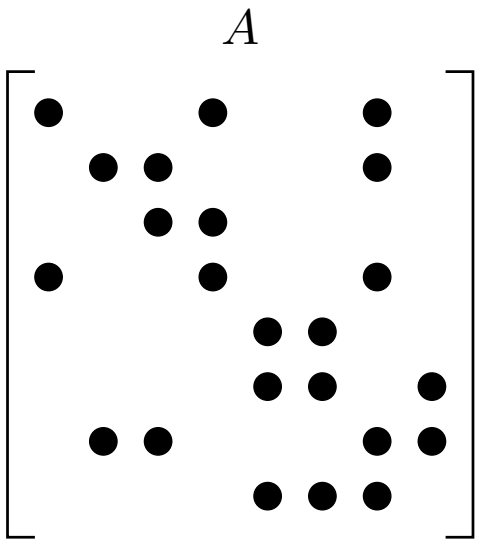
Sparse LU: multifrontal

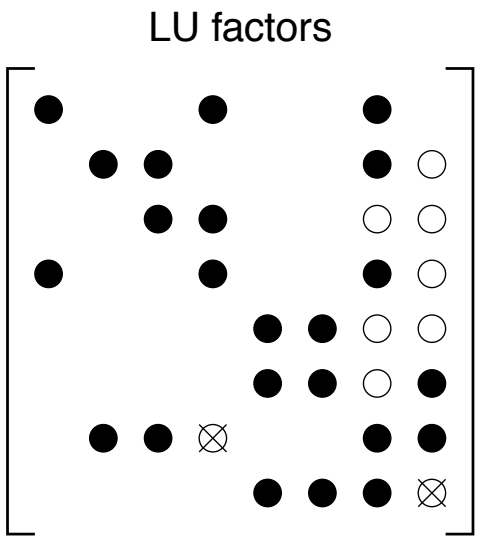


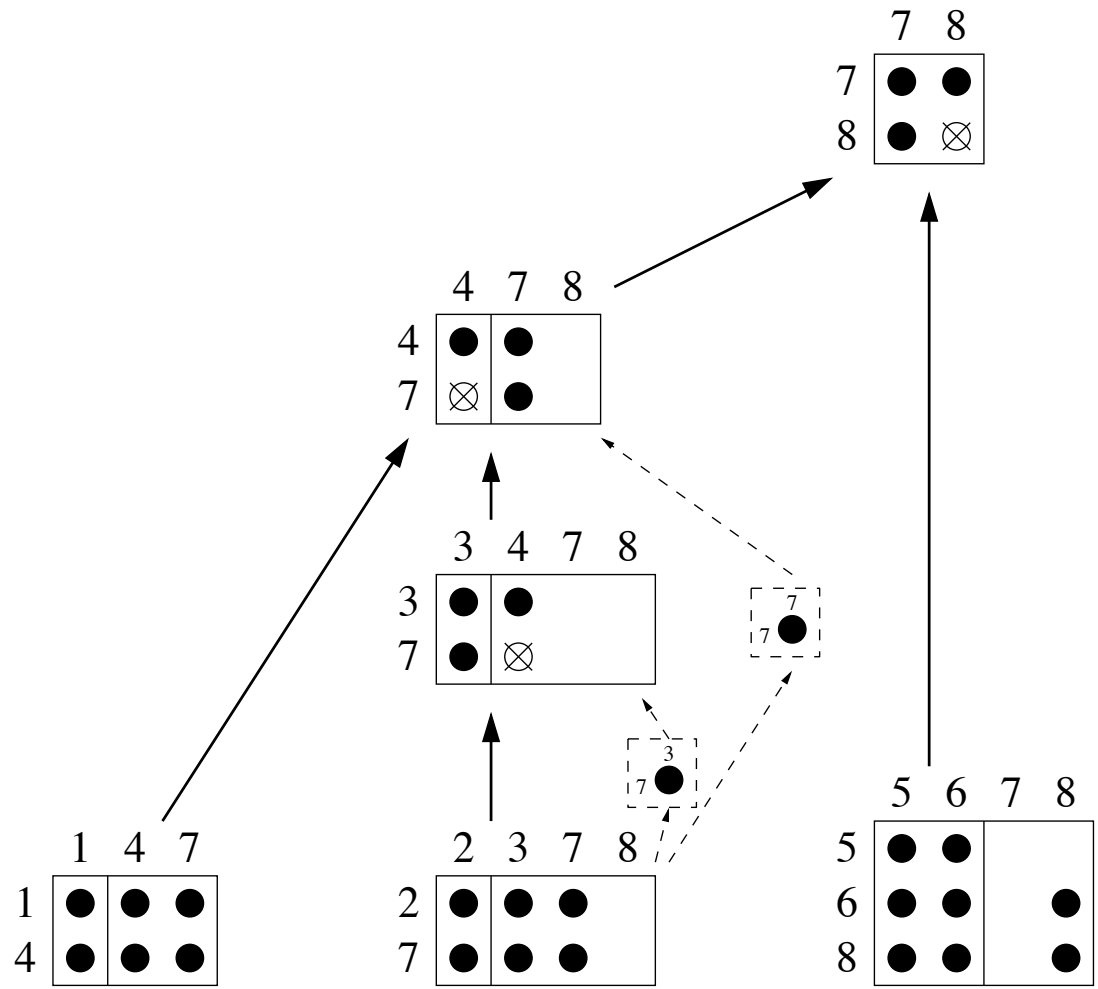




Sparse LU: UMFPACK







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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`

Direct methods for sparse linear systems

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```

- 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