# Numerical Linear Algebra for Computational Science and Information Engineering

## Lecture 06
## Introduction to Direct Methods for Sparse Linear Systems

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# Outline I

# Solving sparse triangular linear systems

Section 9.3 in Darve & Wotters (2021)

# When $L$ is sparse and $b$ is dense

- We want to solve $Lx = b$ where $L$ is a **sparse lower-triangular** matrix with **non-zero diagonal** entries.
- Remember how to proceed when $L$ is dense:

1. $x_1 = b_1/l_{11}$
2. $x_2 = (b_2 - l_{21}x_1)/l_{22}$

$\vdots$

$i$. $x_i = \left(b_i - \sum_{j=1}^{i-1} l_{ij}x_j\right)/l_{ii}$

$\vdots$

$n$. $x_n = \left(b_n - \sum_{j=1}^{n-1} l_{nj}x_j\right)/l_{nn}$

- When $L$ is sparse, we simply need to **skip** the **zero components** $l_{ij}$ **in each summand**.
- We will see in practice session that this can easily be implemented.
- The **final form of** the **implementation depends on** the sparse matrix **data structure** used to store $L$.

# When both $L$ and $b$ are sparse

- **When $L$ and $b$ are sparse**, then **the solution $x$ may be sparse**.
- Ideally, we would like to solve for $x$ as follows:

1. for $i = 1, \ldots, n$ :
2. if $x_i \neq 0$ :
3. $x_i \leftarrow b_i / \ell_{ii}$
4. for $j = 1, \ldots, i-1$ :
5. if $\ell_{ij} \neq 0$ :
5. $x_i \leftarrow x_i - \ell_{ij} x_j / \ell_{ii}$

- But iterating over the non-zero components of $x$ **requires to know the structure of $x$**.
- For any non-zero $x_i$, we have either or both

(a) $b_i \neq 0$

(b) there is some $j < i$ such that $\ell_{ij} \neq 0$ and $x_j \neq 0$.

# When both $L$ and $b$ are sparse, cont'd$_1$

- Let $G = (V, E)$ be the graph associated with $L$, then we denote by $X \subset V$ the minimal set of vertices so that either or both (a) and (b) hold.

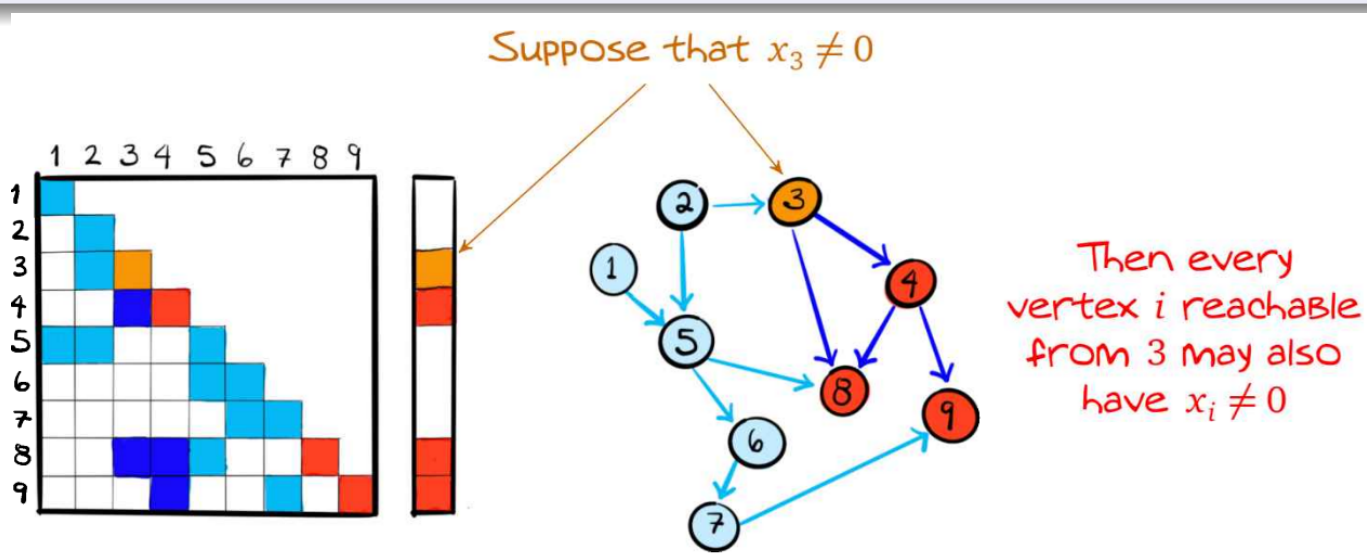
  That is, $X \subset V$ is the minimal set such that:

$$b_i \neq 0 \implies i \in X \text{ and } \ell_{ij} \neq 0 \text{ and } j \in X \implies i \in X.$$

## Definition (Reachability & Reach)

- A vertex $i \in V$ in a directed graph $G = (V, E)$ is **reachable from a vertex** $j \in V$, if there is a directed path from $j$ to $i$ in $G$. That is, if there is a sequence of edges $(j, i_1), (i_1, i_2), \ldots, (i_{k-1}, i_k), (i_k, i)$ where all the edges are in $E$.
- The set of vertices $i \in V$ reachable from a vertex $j \in V$ is the **reach** of $j$.

- If $j \in X$, then every vertex in the reach of $j$, is also in $X$.



# When both $L$ and $b$ are sparse, cont'd$_2$

- Then, if we let $B \subset V$ be the set of vertices $i \in V$ such that $b_i \neq 0$, then $X$ is the **set of vertices reachable from** $B$.
- Consequently, the set $X$ can be found by operating on the graph $G = (V, E)$ associated with $L$.

  Namely, the set $X$ can be found using a **depth-first traversal** (**DFS**, i.e., for depth-first search) from every vertex in $B$.
- Depth-first traversal starts from some node $j$, and explores as far as possible along each branch in the graph before backtracking.
- We will see an implementation of depth-first traversal in the practice session.
- Procedure to solve $Lx = b$ where both $L$ and $b$ are sparse is as follows:

## Linear solve of $Lx = b$ where both $L$ and $b$ are sparse

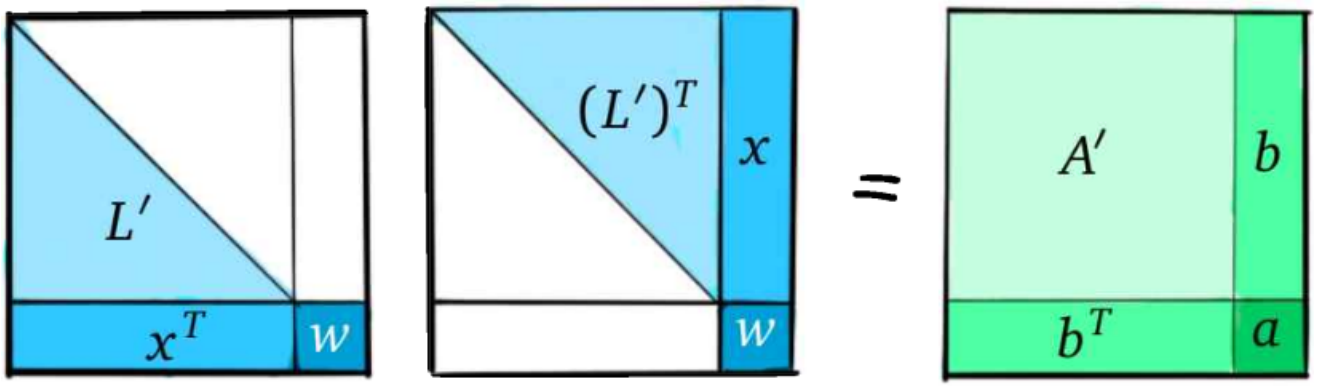
1. Define the set $B$ from the sparsity pattern of $b$.
2. Find the set $X$ of non-zero $x$ components using DFS on $B$.
3. Run modified version of the algorithm to solve $Lx = b$ with a sparse $L$, but compute $x_i$ only if $i \in X$.

# Cholesky factorization

Section 9.4 in Darve & Wotters (2021)

# Up-looking Cholesky algorithm

- Now that we know how to solve sparse triangular systems, we can use this to obtain a sparse Cholesky factorization.
- In particular, the **up-looking Cholesky** algorithm performs a Cholesky factorization by doing a **series of sparse triangular solves**.
- Proceeding by construction, assume the $(n-1)$-dimensional leading block $L'$ of the Cholesky factor $L$ of $A$ is already known, leading the following structure of the $LL^T = A$ factorization:




First, we have $[L', 0_{(n-1)\times 1}] \begin{bmatrix} x \\ w \end{bmatrix} = b$ which simplifies to $L'x = b$.

Second, we have $[x^T\, w] \begin{bmatrix} x \\ w \end{bmatrix} = a$ and $w > 0$ so that $w = \sqrt{a - x^T x}$.

# Up-looking Cholesky algorithm, cont'd$_1$

- This leads to the following algorithm:

## Up-looking Cholesky algorithm

Given a sparse SPD matrix $A \in \mathbb{R}^{n \times n}$, initialize $L' := \sqrt{a_{11}}$.

For $k = 2, \ldots, n$:

- Let the leading $k$-by-$k$ block of $A$ be written as $\begin{bmatrix} A' & b \\ b^T & a \end{bmatrix}$ where $A'$ is the $(k-1)$-dimensional leading block, $b$ is $(k-1)$-by-1 and $a$ is a scalar.
- Solve for $x \in \mathbb{R}^{k-1}$ such that $L'x = b$ where $L'$ and $b$ are sparse.
- Compute $w := \sqrt{a - x^T x}$, and update

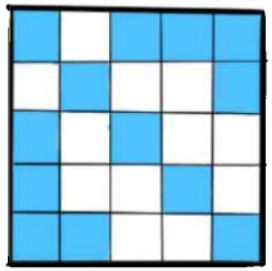
$$L' := \begin{bmatrix} L' & 0 \\ x^T & w \end{bmatrix}$$

Return $L := L'$

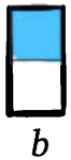
Consequently, the sparse Cholesky factor $L$ of the sparse matrix $A$ is formed by performing $n-1$ sparse triangular solves of sizes $1, \ldots, n-1$.

# Up-looking Cholesky algorithm, cont'd$_2$

- Consider a matrix $A$ with the following non-zero pattern:

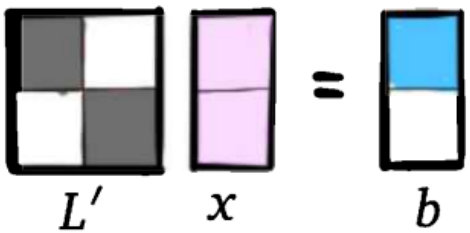


- Since the 2-by-2 leading block $A'$ of $A$ is diagonal, so is the corresponding 2-by-2 Cholesky factor $L'$ such that $L'L'^T = A'$.

  Let the vector 
  
  complete the 3-by-3 leading block $\begin{bmatrix} A' & b \\ b^T & a \end{bmatrix}$ of $A$.

  Then, the up-looking Cholesky algorithm requires that we do the sparse triangular solve of $L'x = b$.

The reach of node 1 in the graph associated with $L'$ is just 1 itself.

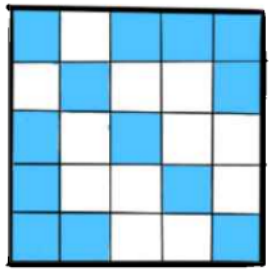


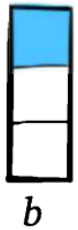


- The Cholesky factor $L' := \begin{bmatrix} L' & 0 \\ x^T & w \end{bmatrix}$ of $\begin{bmatrix} A' & b \\ b^T & a \end{bmatrix}$ has structure  .

# Up-looking Cholesky algorithm, cont'd$_3$

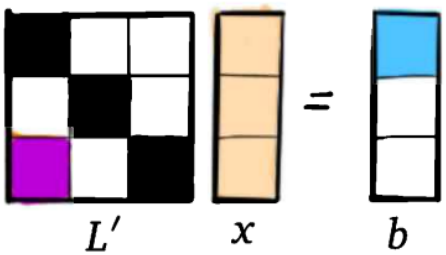
- Consider a matrix $A$ with the following non-zero pattern:

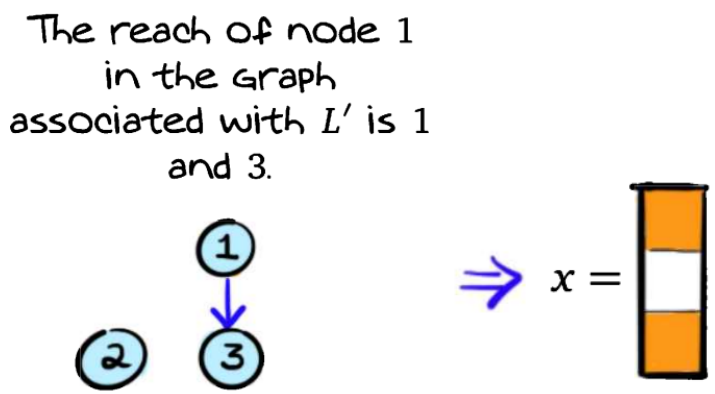


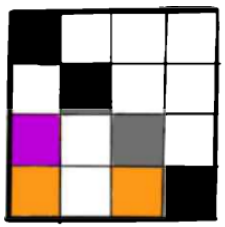
- Let the vector 

complete the 4-by-4 leading block $\begin{bmatrix} A' & b \\ b^T & a \end{bmatrix}$ of $A$.

Then, the up-looking Cholesky algorithm requires that we do the sparse triangular solve of $L'x = b$.

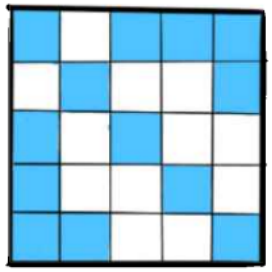


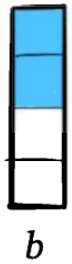




- The Cholesky factor $L' := \begin{bmatrix} L' & 0 \\ x^T & w \end{bmatrix}$ of $\begin{bmatrix} A' & b \\ b^T & a \end{bmatrix}$ has structure  .

# Up-looking Cholesky algorithm, cont'd$_4$

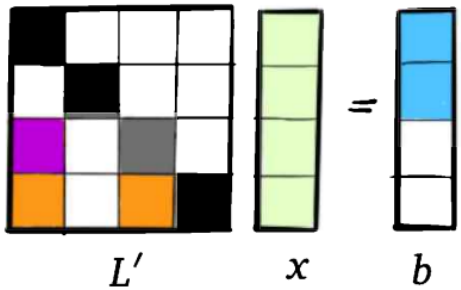
- Consider a matrix $A$ with the following non-zero pattern:



- Let the vector  complete the decomposition $\begin{bmatrix} A' & b \\ b^T & a \end{bmatrix}$ of $A$.

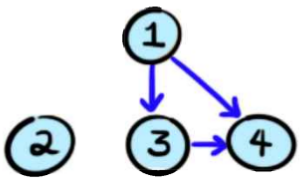


Then, the up-looking Cholesky algorithm requires that we do the sparse triangular solve of $L'x = b$.

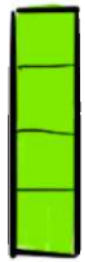


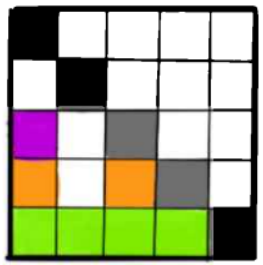


The reach of nodes 1 and 2 in the graph associated with $L'$ is 1, 2, 3, and 4.



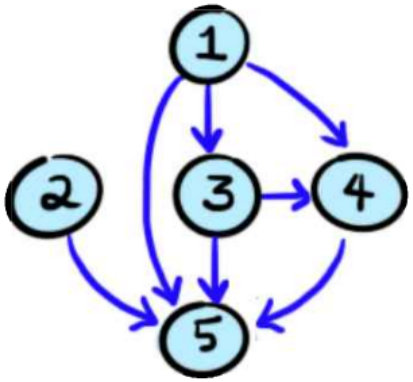


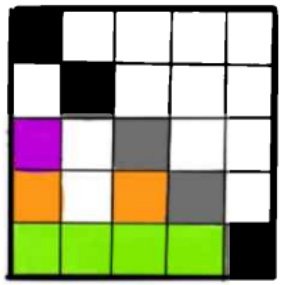
$\Rightarrow x =$ 

- The Cholesky factor $L' := \begin{bmatrix} L' & 0 \\ x^T & w \end{bmatrix}$ of $\begin{bmatrix} A' & b \\ b^T & a \end{bmatrix}$ has structure  .

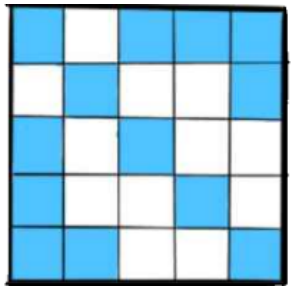
# Up-looking Cholesky algorithm, cont'd$_5$

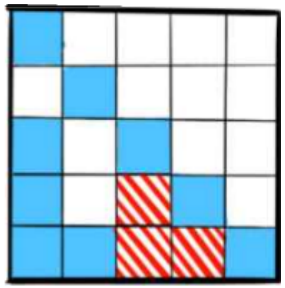
- The up-looking Cholesky algorithm yield a factor with the following non-zero pattern:




$L =$ 

Note that the sparsity of $L$ resembles that of $A$, with additional **fill-ins**:

$A =$ 

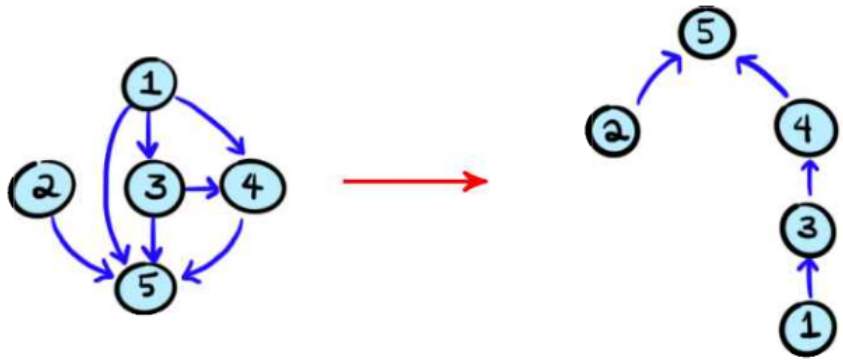
$L =$ 

- While the up-looking algorithm is better than performing a dense Cholesky factorization, it does **require many DFS** in graphs.
- We'll now try to do better than the up-looking algorithm.

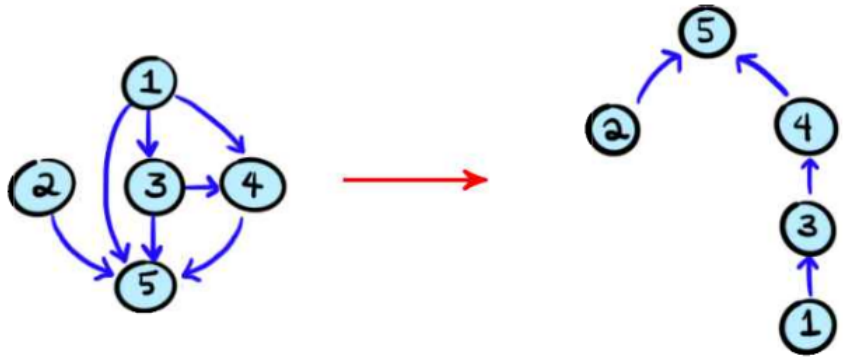
# Elimination tree

- The **graph associated with** the sparsity pattern of **a Cholesky factor** $L$ has a special property which allows to **ignore many of its edges** and **retain the same reach**.
- Consider what happens when we **ignore all the non-zero entries of** $L$ **below the first subdiagonal non-zero component**. E.g.,

Removing these entries results in a **sparsification of the associated graph**:



# Elimination tree, cont'd




**Two general properties** are observed:

1. The **reach** of every vertex remains **unchanged** by sparsification.
2. **Every vertex** of the sparsified graph **has at most one edge** leading **out** of it.

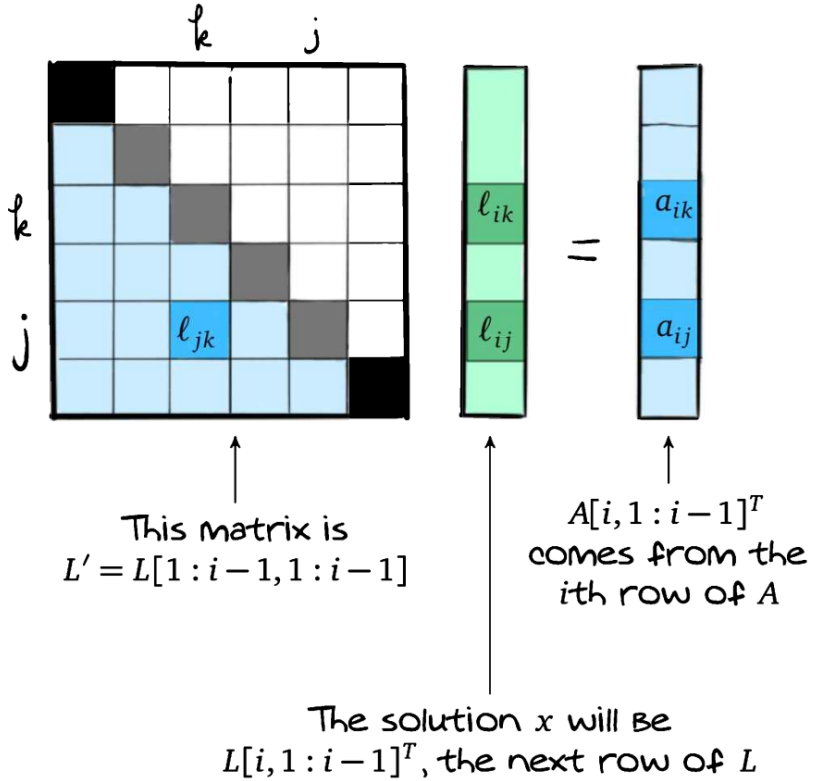
   I.e., **if** the graph is **connected**, then it is a **directed tree**.

Remarks:

- The sparsified graph is called an **elimination tree**.
- The elimination tree **may be disconnected**, in which case it is a forest, but even then, it will be called an elimination tree.
- The elimination tree is an important data structure that **can be used to simplify** all **reach calculations** in a sparse Cholesky factorization.

# Non-zero pattern of $L$

- Say we aim to compute the $i$-th line of the Cholesky factor $L$ of an SPD $A$.
- We are equipped with $L' := L[1 : i-1, 1 : i-1]$:




- We saw the non-zero entries of $L[i, 1 : i-1]$ are the non-zero entries of the solution $x$ of the above system with right-hand side $b := A[1 : i-1, i]$.
- Remember from our sparse triangular solves, $x_j = \ell_{ij}$ is non-zero either if (a) $b_j = a_{ij} \neq 0$, or if (b) $\exists\, k < j$ so that both $\ell_{jk} \neq 0$ and $x_k = \ell_{ik} \neq 0$.

# Non-zero pattern of $L$, cont'd

- Therefore, the pattern of non-zero values of $L$ is characterized as follows:

## Graph of (possible) non-zero entries of $L$

Let $j < i$, then $\ell_{ij}$ is non-zero if

(a) $a_{ij} \neq 0$, or

(b) there is a column index $k < j$ such that $\ell_{jk}$ and $\ell_{ik}$ are non-zero.

We denote by $G_{ch}$ the graph with fewest edges that respect (a) and (b).

That is, $G_{ch}$ is the minimal graph such that $a_{ij} \neq 0 \implies (j,i) \in G_{ch}$ and $(j,k), (i,k) \in G_{ch} \implies (j,i) \in G_{ch}$.

- The graph $G_{ch}$ is a superset of the non-zero pattern of the Cholesky factor $L$ of $A$.

  It can be that $(j,i) \in G_{ch}$ but $\ell_{ij}$ numerically cancels out. However, if so, a tiny perturbation of $A$ with fixed sparsity is enough to make $\ell_{ij} \neq 0$.

  Therefore, the graph $G_{ch}$ is best referred to as the graph of possible non-zero entries of the Cholesky factor $L$.

# Definition of the elimination tree

- The elimination tree can be defined as follows:

## Elimination tree

Let $A$ be an SPD matrix, and $G_{ch}$ be the graph representing the non-zero entries of the Cholesky factor $L$ of $A$.

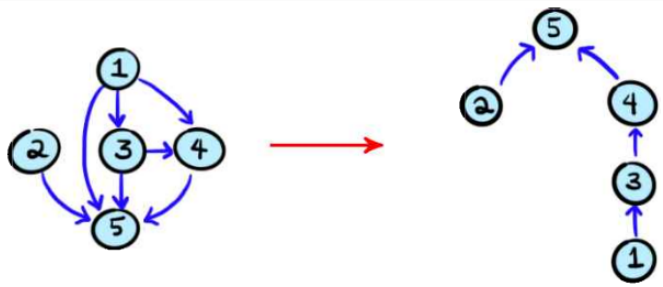
The elimination tree is obtained as follows.

For each node $i$ in $G_{ch}$:

- Let $V_i$ be the set of nodes $j$ of $G_{ch}$ for which there is an edge $(i, j) \in G_{ch}$, i.e., $V_i$ is the set of out-neighbors of $i$. Let $p_i = \min V_i$ be the smallest-indexed node in $V_i$.
- Remove the edges $(i, j)$ for all $j \in V_i \setminus \{p_i\}$ from $G_{ch}$, i.e., remove all the the edges leaving $i$ except for $(i, p_i)$.

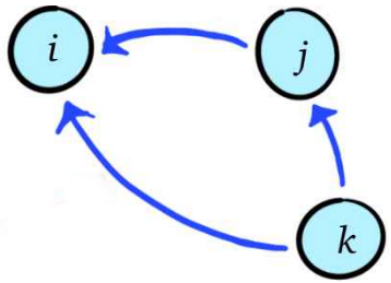
The **elimination tree is** what's **left** of $G_{ch}$.

Example:



# Properties of the elimination tree

- Since for each vertex $i$ in $G_{ch}$, the elimination tree is formed by removing all but one out-neighbors, each vertex is left with at most one single out-neighbor, and the elimination tree is indeed a tree, or at least a forest.
- Consider the following example for a graph $G_{ch}$ of non-zero entries of the Cholesky factor $L$:

$G_{ch} =$ 


As $G_{ch}$ is, the reach of $k$ is $j, i$.

If $k < j < i$, the elimination tree is formed by removing the edge $(k, i)$.

Then, the reach of $k$ in the elimination tree is still $j, i$.

## Theorem (Conservation of reach)

*For a given graph $G_{ch}$ of non-zero entries of a Cholesky factor $L$ of $A$, for any $1 \leq i \leq n$, the reach of the corresponding elimination tree is the same as the reach of $i$ in $G_{ch}$.*

# Computing the elimination tree from $A$

- Since the elimination tree has the same reach as $G_{ch}$, but is sparser than $G_{ch}$, it can be used to more efficiently identify the non-zero entries of the Cholesky factor.

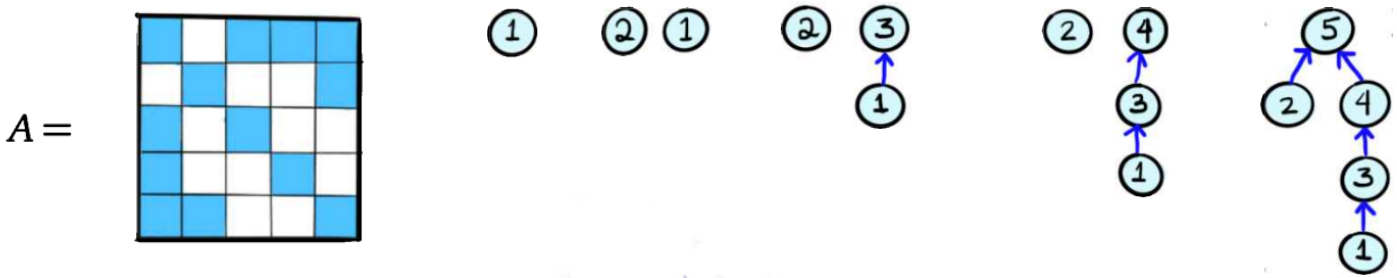
  For that, we need to figure out how to efficiently compute the elimination tree from the given sparsity pattern of $A$.
- The idea behind computing the elimination tree of $A$ is to proceed one vertex at a time, maintaining a forest which contains all the vertices added so far. The elimination tree shall be obtained once all the vertices are added.
- Suppose we have a forest which has all the vertices $1, \ldots, i-1$ at the correct place. To proceed with the $i$-th vertex, if $a_{ik} \neq 0$ for some $k < i$, then we'll want $i$ to be in the reach of $k$. In order to avoid potential redundant edges, we should then connect $i$ to whichever vertex $j$ which is at the leaf of the tree containing $k$.

# Computing the elimination tree from $A$, cont'd

- The pseudocode of the algorithm to build the elimination tree from the sparsity pattern of $A$ is given by

1. Initialize a forest $\mathcal{F} = \emptyset$ :
2. For $i = 1, \ldots, n$ :
3. Add vertex $i$ to $\mathcal{F}$
4. For all $k < i$ such that $a_{ik \neq 0}$ :
5. Find vertex $j$ at the leaf of $k$'s tree
6. Add the edge $(j, i)$ to $\mathcal{F}$

Taking the same sparse matrix $A$ as earlier, the elimination tree is then built as follows:




We see that the same elimination tree is obtained as before.

# Summary

To compute a sparse Cholesky factor $L$ of a sparse matrix $A$, we

1. Build the elimination tree of $A$, at cost $\mathcal{O}(|A|)$, where $|A|$ is the number of non-zero entries in $A$.
2. Find the graph $G_{ch}$ of possible non-zero entries of $L$ using reaches of the elimination tree.
3. Perform the up-looking Cholesky factorization to build $L$.

Pseudocode of the up-looking Cholesky factorization to build row $k$ of $L$:

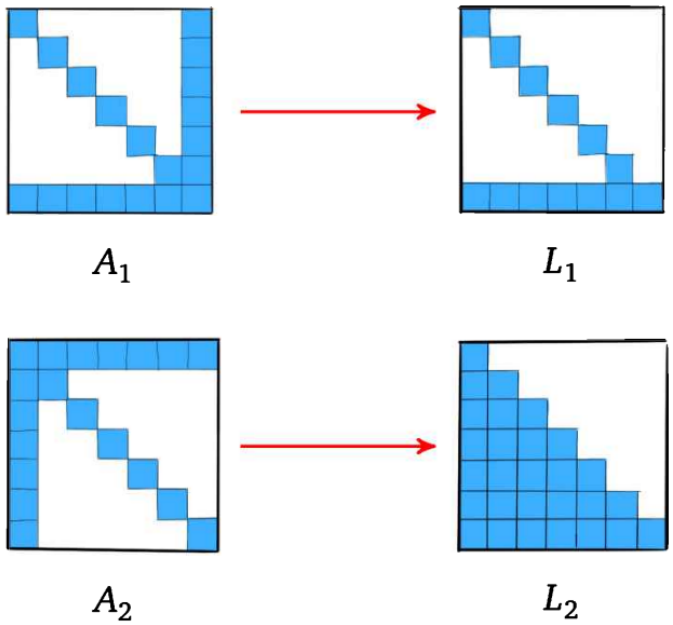
1. $L[k, 1:k] := A[k, 1:k]$
2. For each $j < k$ such that $\ell_{kj} \neq 0$:
3. $\quad \ell_{kj} \leftarrow \ell_{kj}/\ell_{jj}$
4. $\quad$ For each $i > j$ such that $\ell_{ij} \neq 0$ :
5. $\quad\quad \ell_{ki} \leftarrow \ell_{ki} - \ell_{ij}/\ell_{kj}$

# Nested dissesction

Section 9.5 in Darve & Wotters (2021)

# Reducing fill-ins in $L$

- While the row and column permutations of a matrix do not really impact the solution of a linear system (i.e., $P_r A P_c \cdot P_c^T x = P_r b$), they can have a significant impact on the sparsity pattern, i.e., the graph $G_{ch}$ of the Cholesky factor:




  Even though only one row and one column are permuted between $A_1$ and $A_2$, the difference between the numbers of fill-ins in $L_1$ and $L_2$ is very significant.

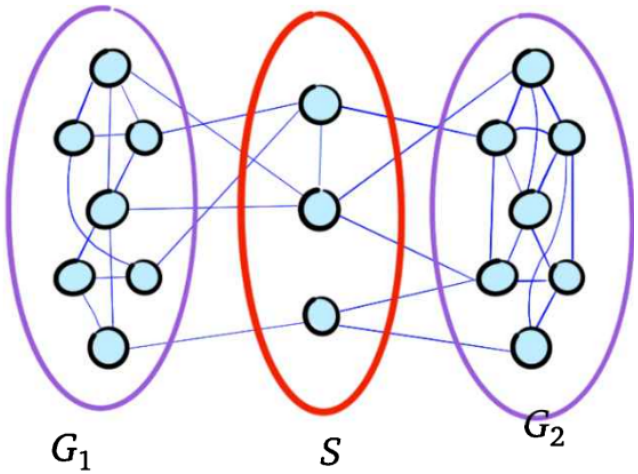
- **How should a matrix be ordered to reduce the number of fill-ins in the Cholesky factor $L$?**

# One step of nested dissection

- **Nested dissection** is a strategy for ordering a matrix $A$ in a way that **closely minimizes** the number of **fill-ins** in $L$.
- **Nested dissection** is a **recursive method based on graph partitioning**.
- Consider the symmetric matrix $A$ with an associated graph $G$.

  Let the vertices of $G$ be decomposed in the disjoint union of $V_1, V_2$ and $S$, so that there are no edges between vertices of $V_1$ and $V_2$.

  If $G_1$ and $G_2$ are the induced graph on $V_1$ and $V_2$, respectively, then we have



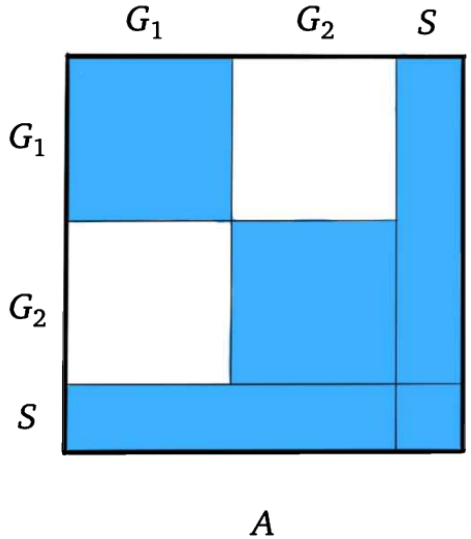

  where $S$ is referred to as a **separator**.

# One step of nested dissection, cont'd$_1$

- A **node separator set** $S$ partitions the graph $G$ of $A$ into three disjoint sets of vertices $V_1, V_2$ and $S$ such that none of the nodes of $V_1$ are connected to any of the nodes of $V_2$, and vice-versa.
- The removal of $S$ from the graph $G$ leads to two subgraphs $G_1$ and $G_2$, disconnected from each other.
- Consider what happens when we order the vertices as

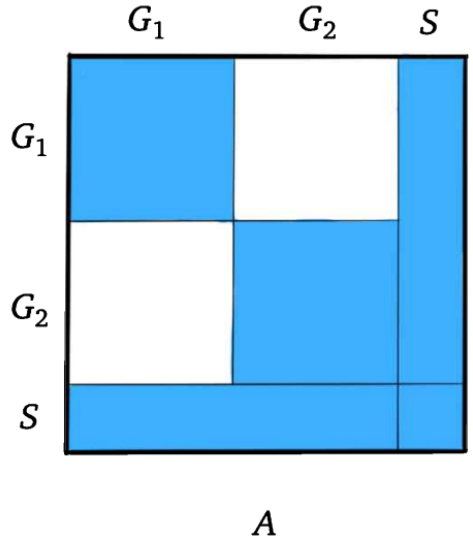
$$(\text{vertices of } G_1, \text{vertices of } G_2, S)$$

we obtain the matrix




which is structurally close to the $A_1$ matrix with small number of fill-ins.

# One step of nested dissection, cont'd$_2$




As a result of the block diagonal structure due to $G_1$ and $G_2$, the Cholesky factor $L$ of the reordered matrix will preserve a block diagonal structure.

If the blue blocks are dense, the sparsity of $L$ is exactly given by that of $A$.

In general, each block of $L$ will be sparse.

From here, we will proceed as follows:

- **Entries in $S$.** For these entries, we give up and accept whatever fill-ins happen. Thus we want $S$ to be as small as possible.
- **Entries in $G_1$ and $G_2$.** For these entries, we will recurse on the blocks $G_1 \times G_1$ and $G_2 \times G_2$, i.e., find small separators $S_1$ and $S_2$ for $G_1$ and $G_2$, respectively, and so on.

# Nested dissection

- The basic idea of **nested dissection** is to **recursively** apply the procedure we just described, and yield a **nested dissection ordering** of the graph nodes.

**Pseudocode for the nested dissection algorithm**

```
function nested_dissection(G::Graph)
    # returns a nested dissection ordering of the nodes of G
    if size(G) < threshold
        # This is the base case of the recursion
        return nodes(G) # nodes of graph G
    end
    [G1, G2, S] = find_separator_set(G)
    # G1 and G2 are two disconnected subgraphs
    # S is the node separator set
    P1 = nested_dissection(G1)
    P2 = nested_dissection(G2)
    return [P1; P2; S]
end
```

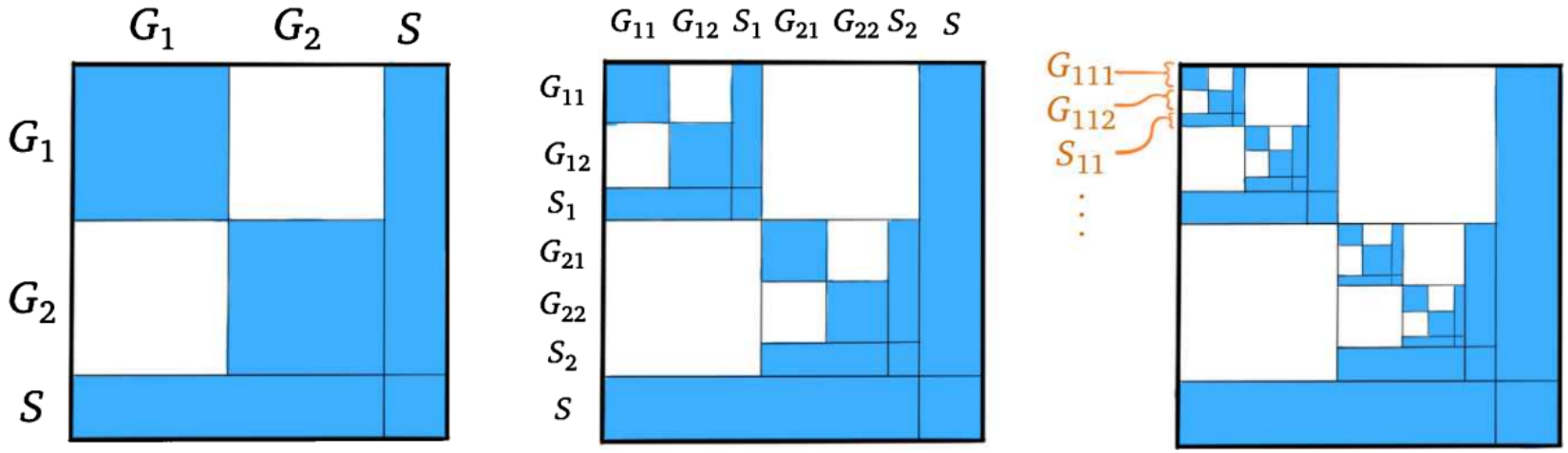
- The description of `find_separator_set` is beyond the scope of this class.

  A good separator set has as few nodes as possible, and it decomposes the graph in roughly equally sized subgraphs.

  Finding a good separator set is actually a NP-hard problem.

# Nested dissection, cont'd

- In the matrix, the recursive process of nested dissection looks like this:




As we can see, if good separators are chosen, the "down-and-right-arrow" patterns shows up at all scales, and we can guarantee that more and more entries of $L$ will be zero.

# Homework problems

# Homework problem

Turn in **your own** solution to the following problem:

**Pb. 16** Find the non-zero pattern of the Cholesky factor $L$ for the following matrix:

$$A = \begin{bmatrix} a_{11} & a_{12} & 0 & a_{14} \\ a_{12} & a_{22} & 0 & a_{24} \\ 0 & 0 & a_{33} & 0 \\ a_{14} & a_{24} & 0 & a_{44} \end{bmatrix}.$$

Show your work using the up-looking Cholesky factorization algorithm.