Numerical Linear Algebra for Computational Science and Information Engineering

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.

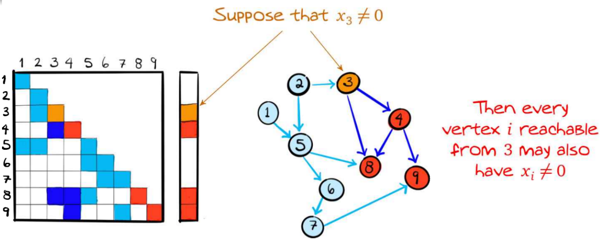
  That is, $X \subset V$ is the minimal set such that:

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

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.



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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

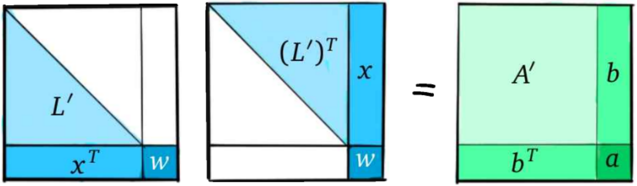
1. Define the set B from the sparsity pattern of b.
2. Find the set X of non-zero x components using DFS on B.
3. Run modified version of the algorithm to solve $Lx = b$ with a sparse L, but compute x_i only if $i \in X$.

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:



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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 $k = 2, \ldots, n$:

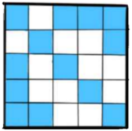
- Let the leading k-by-k block of A be written as $\begin{bmatrix} A' & b \\ b^T & a \end{bmatrix}$ where A' is the $(k-1)$-dimensional leading block, b is $(k-1)$-by-1 and a is a scalar.
- Solve for $x \in \mathbb{R}^{k-1}$ such that $L'x = b$ where L' and b are sparse.
- Compute $w := \sqrt{a - x^T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

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

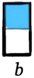
Return $L := L'$

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$_2$

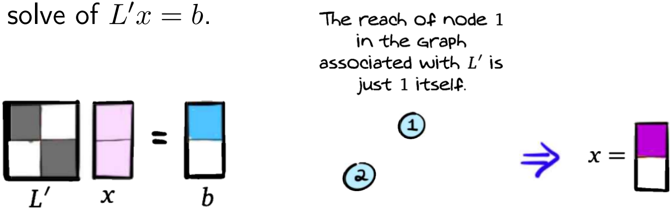
- Consider a matrix A with the following non-zero pattern: 

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

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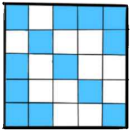
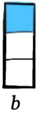
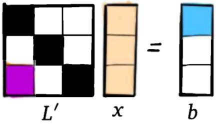
Up-looking Cholesky algorithm, cont'd₃

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

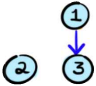
- Let the vector 

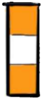
complete the 4-by-4 leading block $\begin{bmatrix} A' & b \\ b^T & a \end{bmatrix}$ of A.

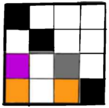
  Then, the up-looking Cholesky algorithm requires that we do the sparse triangular solve of $L'x = b$.



The reach of node 1 in the graph associated with L' is 1 and 3.



$\Rightarrow x =$ 

- 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 .

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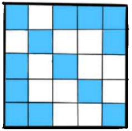
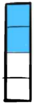
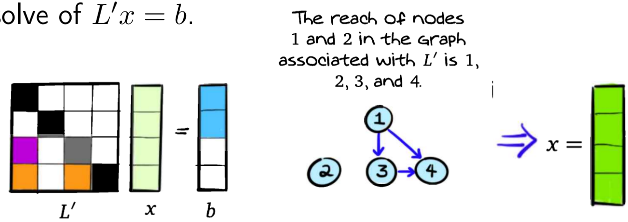
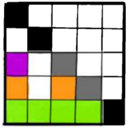
Up-looking Cholesky algorithm, cont'd$_4$

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

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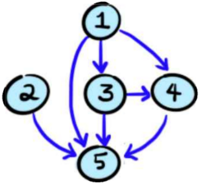
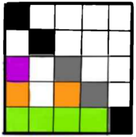
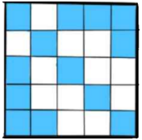
Up-looking Cholesky algorithm, cont'd$_5$

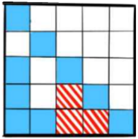
- The up-looking Cholesky algorithm yield a factor with the following non-zero pattern:



$L =$ 

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.

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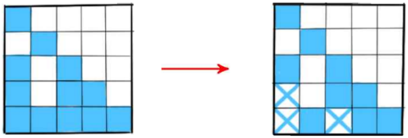
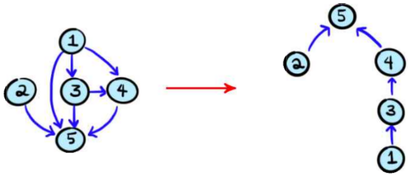
Elimination tree

- 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**:



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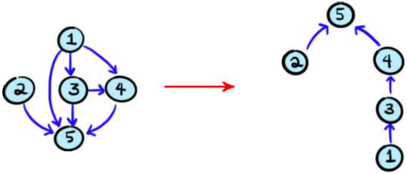
Elimination tree, cont'd



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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.

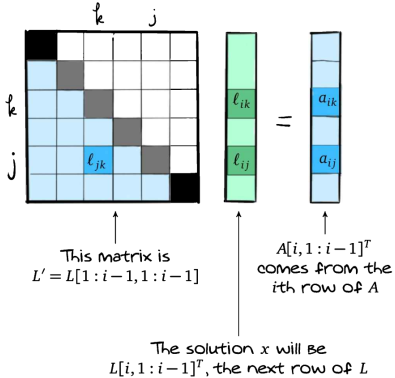
   I.e., **if** the graph is **connected**, then it is a **directed tree**.

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 $L' := L[1:i-1, 1:i-1]$:



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- 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 ℓ_{ij} is non-zero if

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

(b) there is a column index $k < j$ such that ℓ_{jk} and ℓ_{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 ℓ_{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.

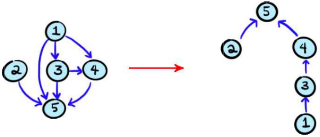
The elimination tree is obtained as follows.

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:



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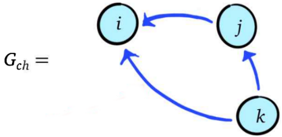
Properties of the elimination tree

- 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:



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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.

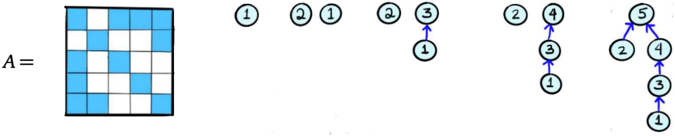
  For that, we need to figure out how to efficiently compute the elimination tree from the given sparsity pattern of A.
- The idea behind computing the elimination tree of A is to proceed one vertex at a time, maintaining a forest which contains all the vertices added so far. The elimination tree shall 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:



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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:

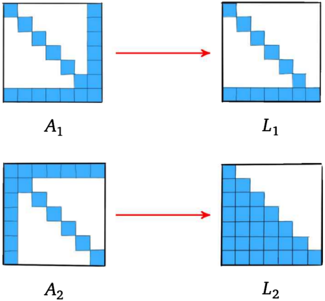
1. $L[k, 1:k] := A[k, 1:k]$
2. For each $j < k$ such that $\ell_{kj} \neq 0$:
3. $\quad \ell_{kj} \leftarrow \ell_{kj} / \ell_{jj}$
4. $\quad$ For each $i > j$ such that $\ell_{ij} \neq 0$:
5. $\qquad \ell_{ki} \leftarrow \ell_{ki} - \ell_{ij} / \ell_{kj}$

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., $P_rAP_c \cdot P_c^T x = P_r b$), they can have a significant impact on the sparsity pattern, i.e., the graph G_{ch} of the Cholesky factor:



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  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.

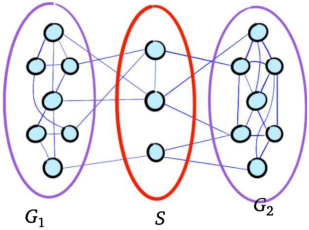
- **How should a matrix be ordered to reduce the number of fill-ins in the Cholesky factor L?**

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



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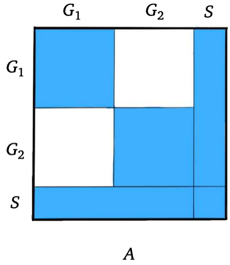
where S is referred to as a **separator**.

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



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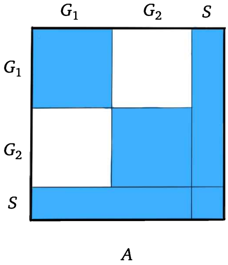
which is structurally close to the A_1 matrix with small number of fill-ins.

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



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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:

- **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
```

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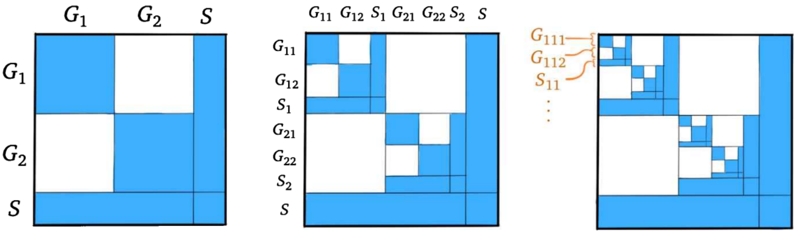
- The description of `find_separator_set` is beyond the scope of this class. A good separator set has as few nodes as possible, and it decomposes the graph in roughly equally sized subgraphs. Finding a good separator set is actually a NP-hard problem.

Nested dissection, cont'd

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



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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.