Multicore and Multiprocessor Systems: Part V

Algorithm 4: Conjugate Gradient Method

Input: $A \in \mathbb{R}^{n\times n}, b \in \mathbb{R}^n, x_0 \in \mathbb{R}^n$
Output: $x = A^{-1}b$

$p_0 = r_0 = b - Ax_0,\ \alpha_0 = \|r_0\|_2^2$;
for $m = 0, \ldots, n-1$ **do**
  if $\alpha_m \neq 0$ **then**
    $v_m = Ap_m$;
    $\lambda_m = \frac{\alpha_m}{(v_m, p_m)}$;
    $x_{m+1} = x_m + \lambda_m p_m$;
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CG uses

- one matrix vector product (performing the main work),

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CG uses

- one `dot`,

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CG uses

- two `axpy`,

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CG uses

- one `nrm2`,

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CG uses

- and a nonstandard `axpy` operation with result in `x`.

The key ingredient in the CG method is the sparse matrix vector product (SpMVP).

We learned in part 1 of the lecture that sparse matrix operations are *bandwidth limited*, i.e., the crucial point is always the data transfer for matrix pattern and entries to the processing units.

On the other hand, the SpMVP is trivially parallel due to data parallelism. On multicore architectures the obvious questions are:

- What is the optimal number of threads to use?
- How should the data be distributed among the threads?

First question $\rightsquigarrow$ treated in the exercises.

The second questions is investigated a lot in the literature. We will only sketch a small selection of approaches considering $x = Ab$ for $x, b \in \mathbb{R}^n$ and $A \in \mathbb{R}^{n \times n}$ sparse with properties specified separately in the method descriptions.

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Naive row blocking. (e.g., using OpenMP `parallel for`)

If the matrix A is banded with moderate bandwidth and the number of entries per row is almost the same for all rows, simply grouping the rows in blocks of rows will likely do a good job.

The bandwidth limitations guarantee data locality on b.

Furthermore, the similar lengths of the sparse rows will automatically provide a proper load balancing.

This provides the easiest form of 1d-partitioning.

The simplest form of 2d-partitioning of the matrix A uses (blocks of) columns and (blocks of) rows at the same time. It is usually referred to as hypergraph partitioning since the choice fits the following definition.

Definition (Hypergraph)

A *hypergraph* is an ordered pair $(\mathcal{V}, \mathcal{E})$ of sets. It is a generalization of a graph that consists of vertices (in the set $\mathcal{V}$) and *hyperedges* in the set $\mathcal{E}$. In contrast to an edge in a graph a hyperedge can be an arbitrary subset of $\mathcal{V}$ and not just a pair.

Example

Schematic representation of a hypergraph with seven vertices and four hyperedges.

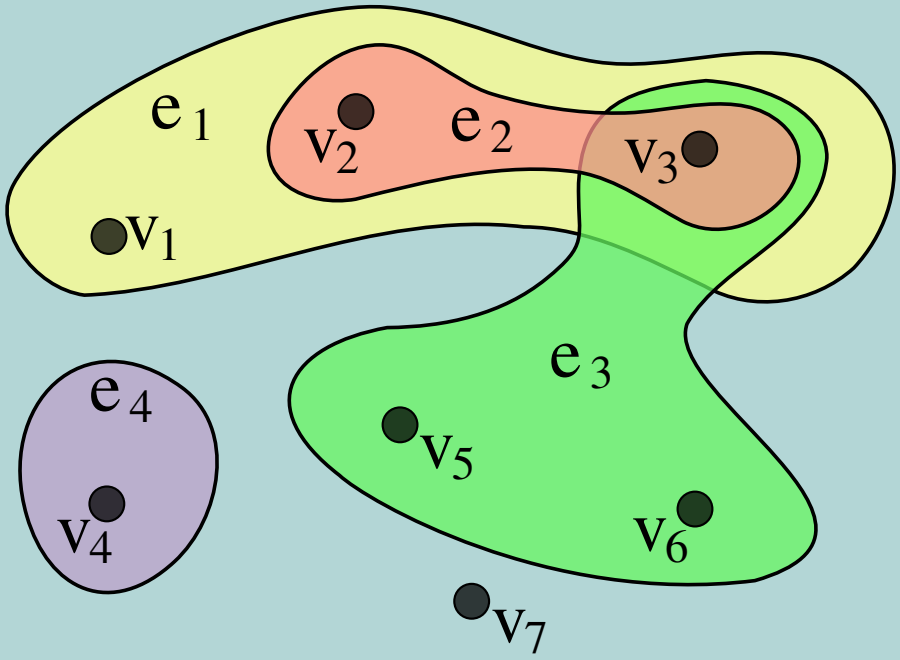


Image source: https://commons.wikimedia.org/wiki/File:Hypergraph-wikipedia.svg

The idea of hypergraph partitioning is to use the hyperedges to find the optimal partitioning of the vertices into k equal sets for optimal balancing of the workload and data communication.

The problem of finding the optimal partition is however np-hard. Therefore cheap heuristics are employed to approximate the optimal partition.

An interesting variant especially for symmetric patterns is the corner symmetric partitioning.

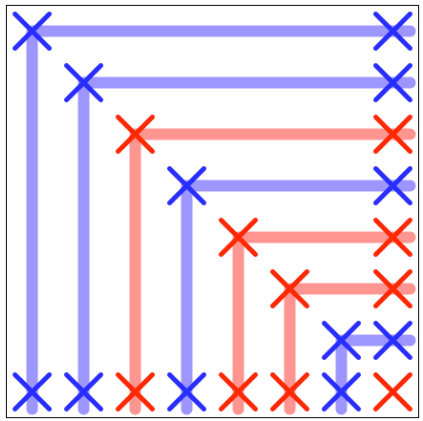


Figure: Corner symmetric partitioning of the arrowhead matrix with 2 partitions.

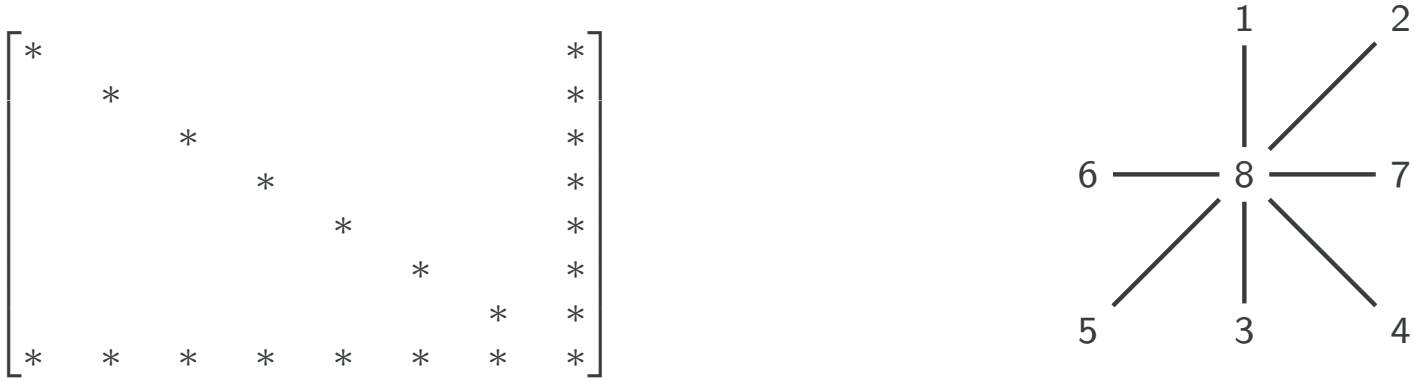
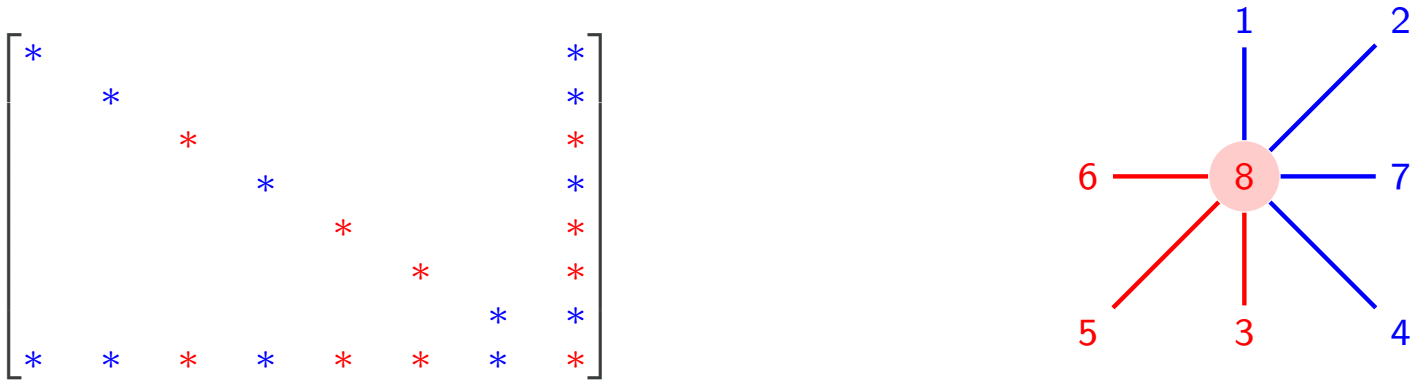


Figure: arrowhead matrix pattern and connectivity graph.

The central node 8 is called *vertex separator*. The identification of such a (group of) node(s) is the central question in the graph model based partitioning. Successive application of this idea leads to the nested dissection scheme.



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Recall:

A *preconditioner* is an invertible linear operator P that approximates the action of A^{-1} for a linear system $Ax = b$.

- Invertibility required to ensure proper preservation of solution,
- preconditioner need not be formed as a matrix, as long as its action on a vector can be provided as a function,
- main purpose of the preconditioner is the grouping of eigenvalues, ideally in a single cluster at $+1$.

Algorithm 5: Preconditioned Conjugate Gradient Method

Input: $A \in \mathbb{R}^{n\times n}$, $b \in \mathbb{R}^n$, $x_0 \in \mathbb{R}^n$, $A^{-1} \approx P \in \mathbb{R}^{n\times n}$
Output: $x = A^{-1}b$

$r_0 = b - Ax_0$, $p_0 = z_0 = Pr_0$, $\alpha_0 = (r_0, p_0)$;
for $m = 0 : n-1$ **do**
  if $\alpha_m \neq 0$ **then**
    $v_m = Ap_m$;
    $\lambda_m = \frac{\alpha_m}{(v_m, p_m)_2}$;
    $x_{m+1} = x_m + \lambda_m p_m$;
    $r_{m+1} = r_m - \lambda_m v_m$;
    $z_{m+1} = Pr_{m+1}$;
    $\alpha_{m+1} = (r_{m+1}, z_{m+1})_2$;
    $p_{m+1} = z_{m+1} + \frac{\alpha_{m+1}}{\alpha_m} p_m$;
  else
    STOP;

Let $D \in \mathbb{R}^{n \times n}$ be a diagonal matrix containing the diagonal of A. Then $P = D^{-1}$ is called Jacobi or diagonal preconditioner.

Properties

- \+ embarrassingly parallel in computation and application,
- \+ storage requirement n `double` numbers,
- − only useful for diagonally dominant systems.

The basic idea of SPAI is to find the best matrix P approximating A^{-1}, while maintaining the sparsity pattern of A.

$$\min_{\mathcal{P}(P)=\mathcal{P}(A)} \|AP - I\|_F^2 = \min_{\mathcal{P}(P)=\mathcal{P}(A)} \underbrace{\sum_{j=1}^{n} \|Ap_j - e_j\|_F^2}_{n \text{ independent least squares problems}}$$

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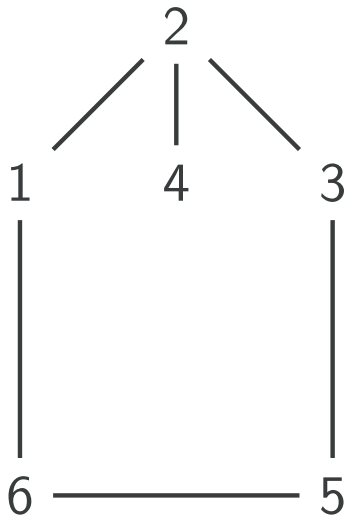
+ only SpMVP needed for the application,
+ n independent least squares problems allow two multicore approaches:
  - rely on threaded BLAS when solving the least squares problems sequentially via `dgeqrs()` from LAPACK,
  - use sequential BLAS with OpenMP for parallel solution of the least squares problems.
– efficient preconditioning requires additional fill-in, which leads to extra storage demands and increased computational complexity.

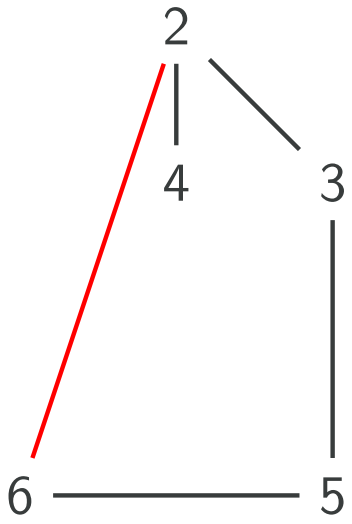


(a) initial graph $\mathcal{G}_0$

$$H_0 = \begin{bmatrix} 1 & * & & & & * \\ * & 2 & * & * & & \\ & * & 3 & & * & \\ & * & & 4 & & \\ & & * & & 5 & * \\ * & & & & * & 6 \end{bmatrix}$$

(b) corresponding submatrix 0

Figure: Basic graph elimination procedure for a symmetric matrix and the Cholesky decomposition



(a) elimination graph $\mathcal{G}_1$

$$H_1 = \begin{bmatrix} 2 & * & * & & * \\ * & 3 & & * & \\ * & & 4 & & \\ & * & & 5 & * \\ * & & & * & 6 \end{bmatrix}$$

(b) corresponding submatrix 1

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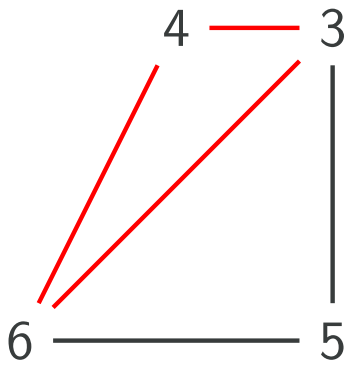
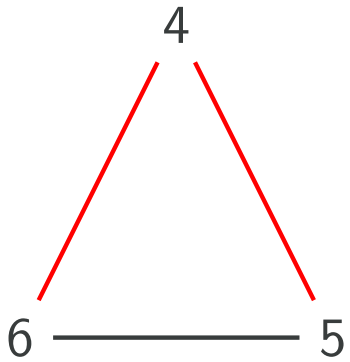


(a) elimination graph $\mathcal{G}_2$

$$H_2 = \begin{bmatrix} 3 & * & * & * \\ * & 4 & & * \\ * & & 5 & * \\ * & * & * & 6 \end{bmatrix}$$

(b) corresponding submatrix 2

Figure: Basic graph elimination procedure for a symmetric matrix and the Cholesky decomposition

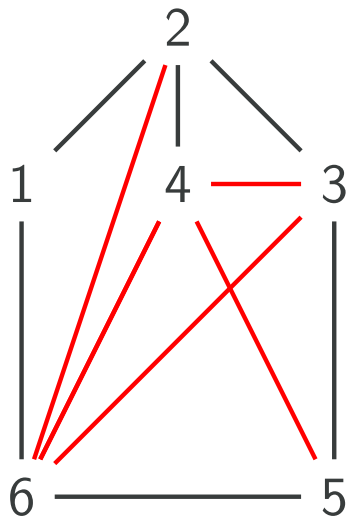


(a) elimination graph $\mathcal{G}_3$

$$H_3 = \begin{bmatrix} 4 & * & * \\ * & 5 & * \\ * & * & 6 \end{bmatrix}$$

(b) corresponding submatrix 3

Figure: Basic graph elimination procedure for a symmetric matrix and the Cholesky decomposition



(a) The filled graph $\mathcal{G}^+(A) = \mathcal{G}(F)$

$$F = \begin{bmatrix} 1 & * & & & & * \\ * & 2 & * & * & & * \\ & * & 3 & * & * & * \\ & * & * & 4 & * & * \\ & & * & * & 5 & * \\ * & * & * & * & * & 6 \end{bmatrix}$$

(b) The final matrix $F = L + L^T$ with fill.

Figure: The filled graph and matrix of a Cholesky decomposition example.

Now

$$L = \begin{bmatrix} 1 & & & & & \\ * & 2 & & & & \\ & * & 3 & & & \\ & * & * & 4 & & \\ & & * & * & 5 & \\ * & * & * & * & * & 6 \end{bmatrix}$$

and thus, the forward elimination is purely sequential. Are we lost?

Consider the Cholesky factor:

$$L = \begin{bmatrix} 1 & & & & & & & & & \\ * & 2 & & & & & & & & \\ & & 3 & & & & & & & \\ & & * & 4 & & & & & & \\ & & * & * & 5 & & & & & \\ & & & & & 6 & & & & \\ & & * & * & * & & 7 & & & \\ & * & * & * & * & & * & 8 & & \\ & & & & & * & & & 9 & \\ & * & * & * & * & & * & * & * & 10 \end{bmatrix}$$

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Definition (column pattern)

The j-th *column pattern* $\mathcal{P}_{*j}$ is the set of row indices of all non-diagonal nonzero entries in the j-th column.

Definition (Supernode)

A *supernode* is a set of contiguous column indices

$$\mathcal{I}(p) = \{p, p+1, \ldots, p+q-1\},$$

such that for all columns $i \in \mathcal{I}(p)$ we have

$$\mathcal{P}_{*i} = \mathcal{P}_{*(p+q-1)} \cup \{i+1, \dot{;} p+q-1\}$$

- Supernodes, thus are special dense diagonal blocks that have the identically same pattern in each column below the diagonal block.

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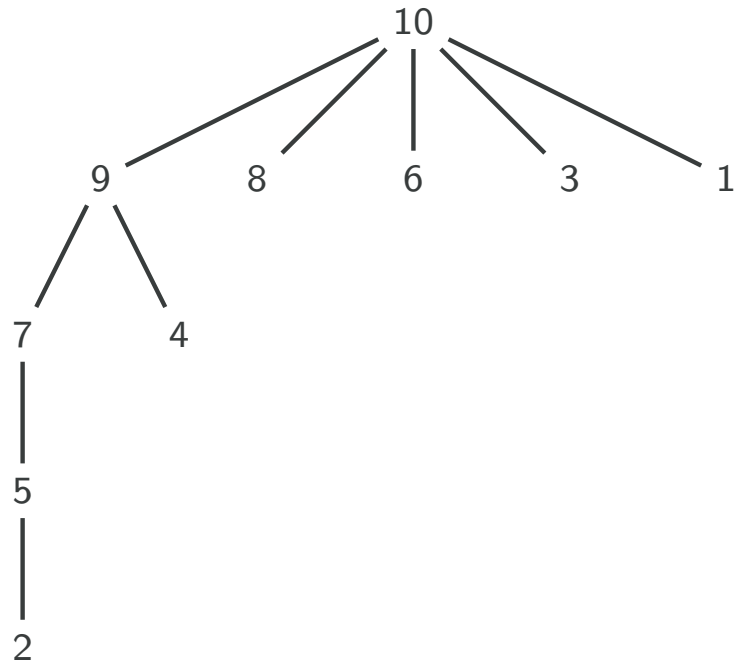
- Column modifications in forward substitution can be expressed in terms of supernodes rather than single diagonal entries.
- Inside the supernode block operations we can exploit parallelism.

Consider the Cholesky factor and corresponding elimination tree

$$L = \begin{bmatrix} 1 & & & & & & & & & \\ & 2 & & & & & & & & \\ & & 3 & & & & & & & \\ & & & 4 & & & & & & \\ & * & & & 5 & & & & & \\ & & & & & 6 & & & & \\ & & & & * & & 7 & & & \\ & & & & & & & 8 & & \\ & * & & * & * & & * & & 9 & \\ * & * & * & * & * & * & * & * & * & 10 \end{bmatrix}$$



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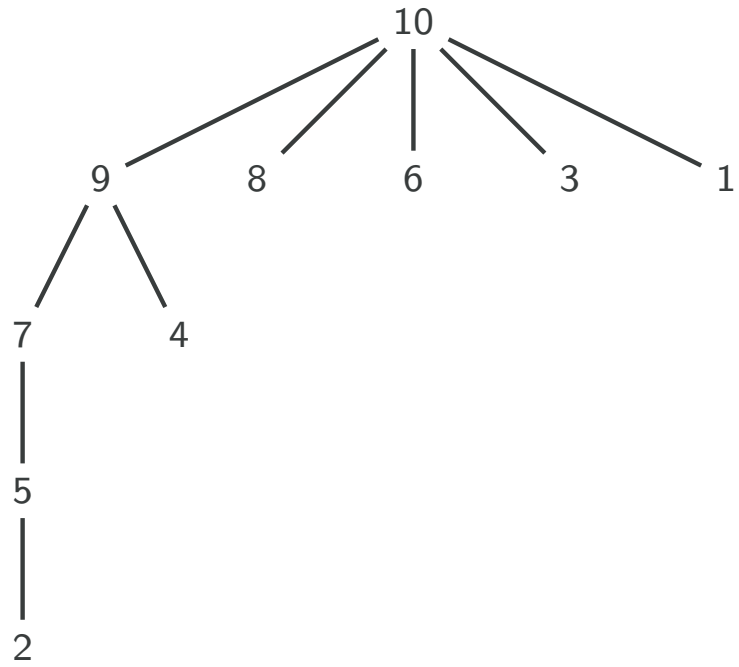

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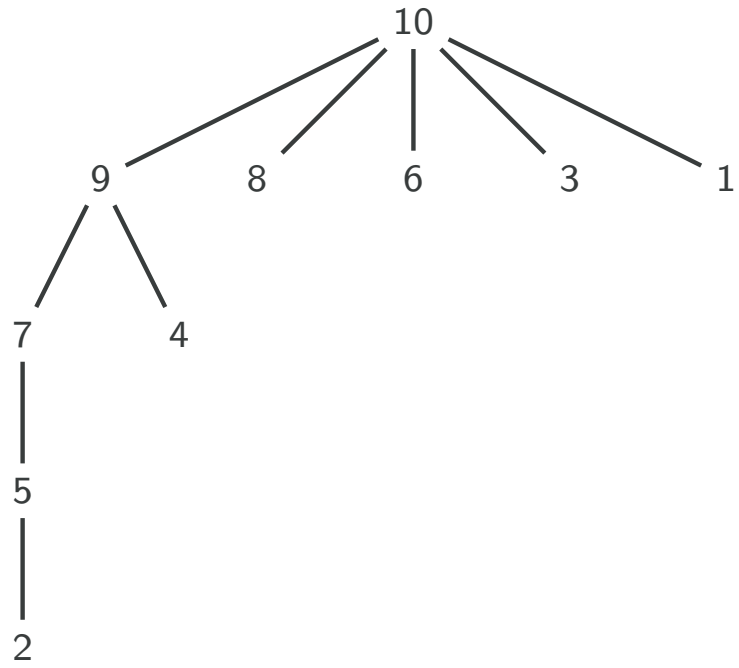

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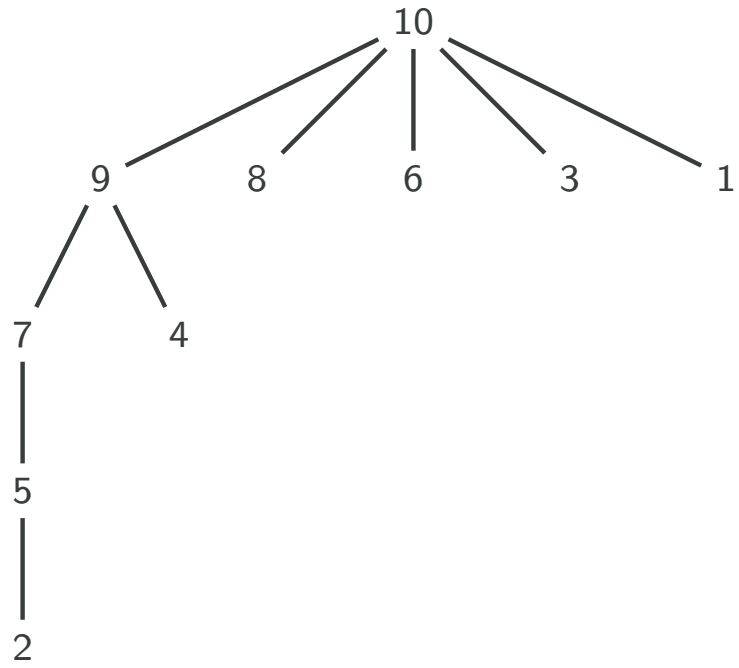

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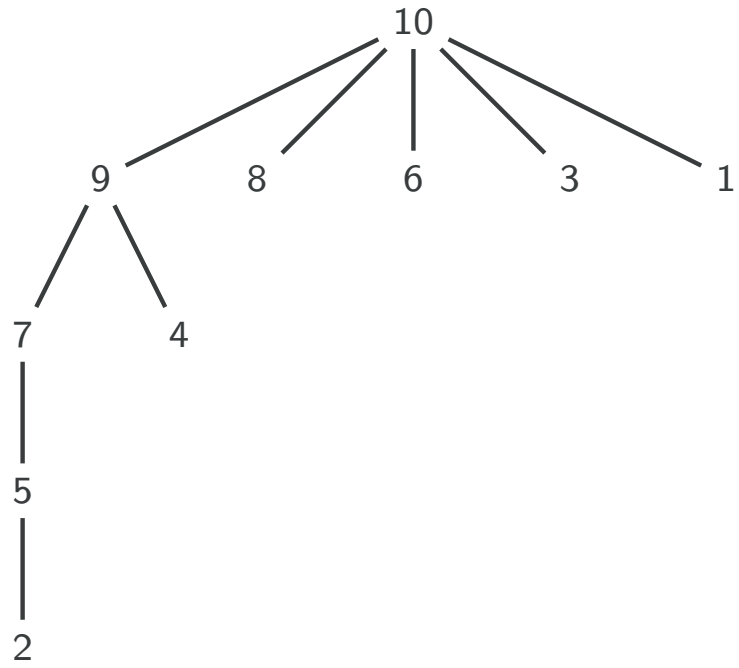

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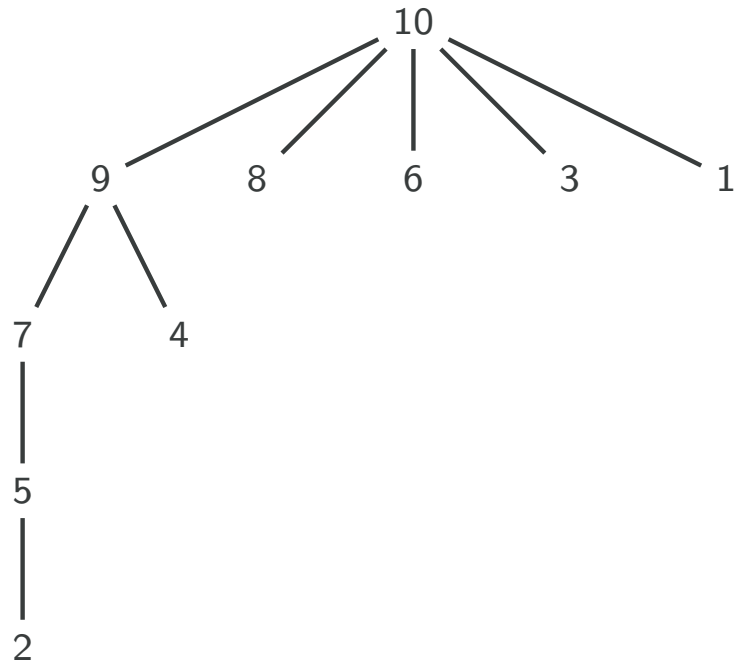

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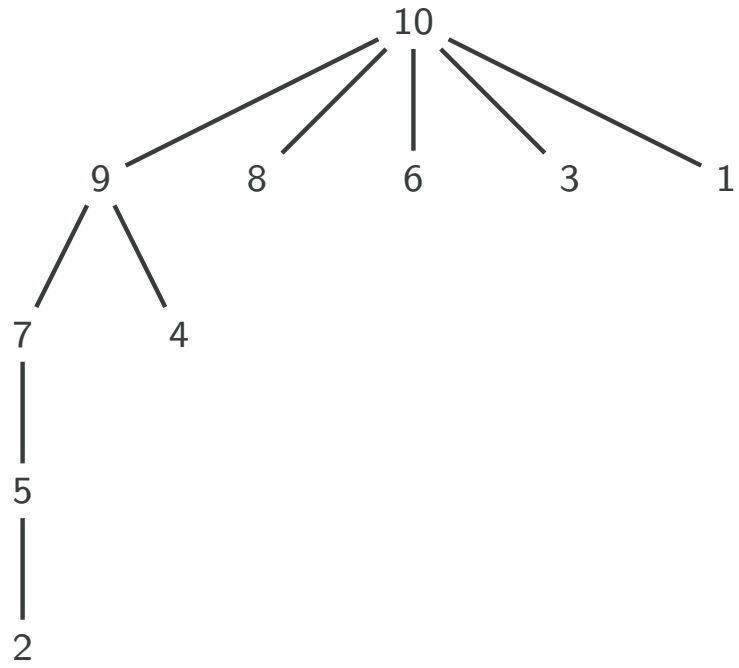

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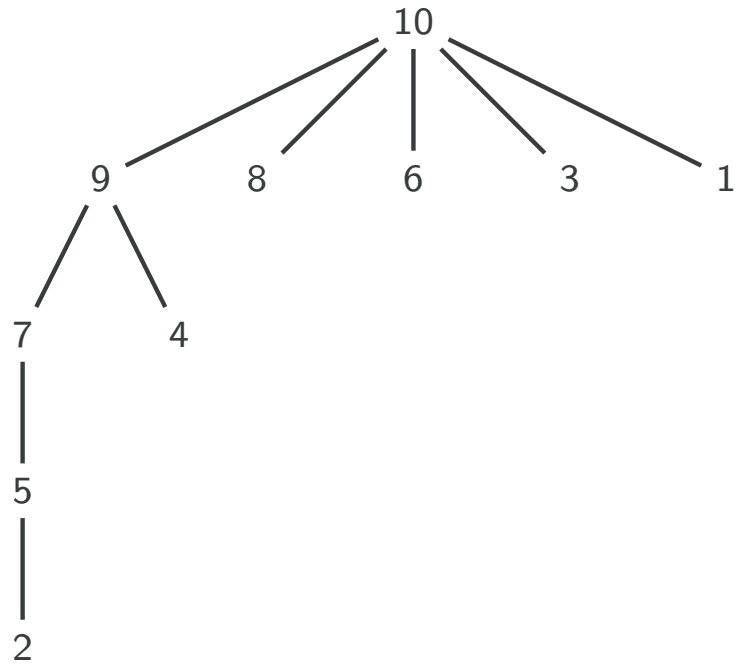

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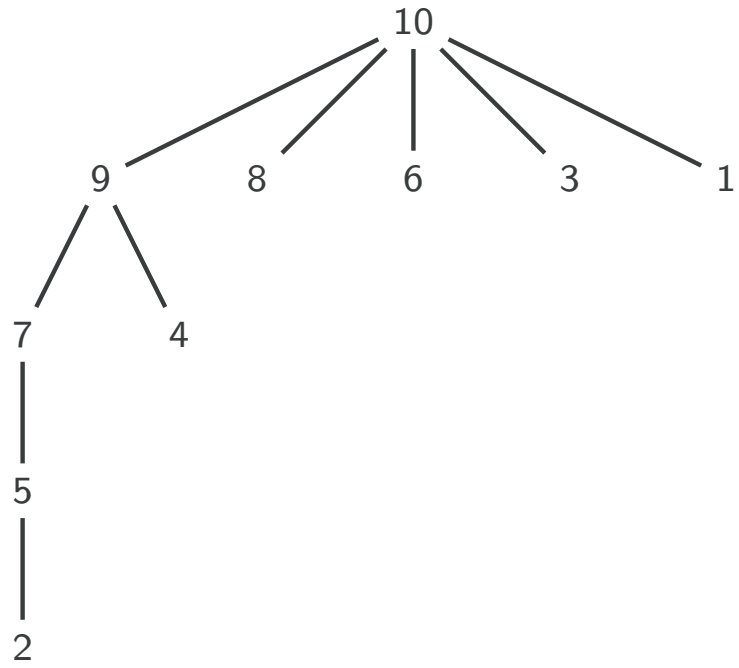
$$L = \begin{bmatrix} 1 & & & & & & & & & \\ & 2 & & & & & & & & \\ & & 3 & & & & & & & \\ & & & 4 & & & & & & \\ & * & & & 5 & & & & & \\ & & & & & 6 & & & & \\ & & & & * & & 7 & & & \\ & & & & & & & 8 & & \\ & * & & * & * & & * & & 9 & \\ * & * & * & * & * & * & * & * & * & 10 \end{bmatrix}$$



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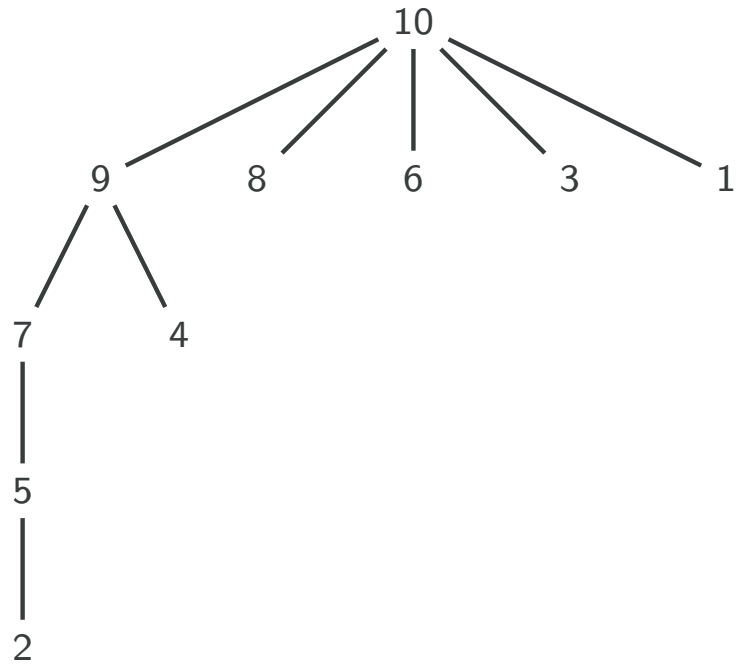

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Remark

Note that elimination trees can be computed without computing the filled graph or the Cholesky factor first.

Relevant Software and Libraries

Dense Linear Algebra

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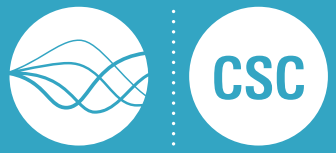

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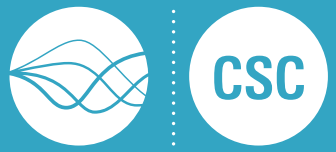

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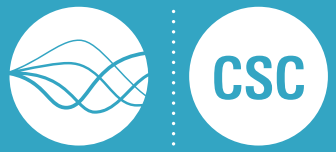

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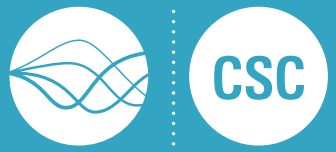

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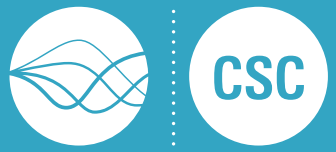

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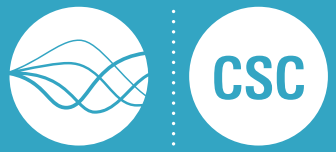

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3. **numactl** referred to as libnuma by several Linux distributions, numactl is a small program/library that can be used to control placement of process memory in NUMA environments. The library version seems to be preferred by the Linux kernel policies. [19]

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