Chordal graphs and sparse semidefinite optimization

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Semidefinite program (SDP)

$$\begin{array}{ll} \text{minimize} & \mathbf{tr}(CX) \\ \text{subject to} & \mathbf{tr}(A_k X) = b_k, \quad k = 1, \ldots, m \\ & X \succeq 0 \end{array}$$

variable X is symmetric matrix; $X \succeq 0$ means X is positive semidefinite

- used in convex modeling systems (CVX, YALMIP, CVXPY, . . .)
- relaxations of nonconvex quadratic and polynomial optimization

Sparse semidefinite optimization

- in many applications the coefficients A_k, C are sparse
- optimal X is typically dense, even for sparse A_k, C

Exploiting sparsity

1. Symmetric primal-dual interior-point methods

exploit sparsity when forming 'Schur complement' equations

2. Non-symmetric interior-point methods (matrix completion methods)

(Fukuda et al. 2000, Burer 2003, Srijuntongsiri et al. 2004, Andersen et al. 2010)

3. Decomposition (combined with interior-point or first-order methods)

(Fukuda et al. 2000, Nakata et al. 2003, Kim et al. 2011, Sun et al. 2014, . . .)

we will discuss approaches 2 and 3

Chordal graphs

chordal graphs have been studied in many fields since the 1960s

- linear algebra (sparse factorization, completion problems)
- combinatorial optimization (a class of 'perfect' graphs)
- machine learning (graphical models, Euclidean distance matrices)
- nonlinear optimization (partial separability)
- computer science (database theory)

first used in semidefinite optimization by Fujisawa, Kojima, Nakata (1997)

Overview

Lecture 1

I. Chordal graphs

II. Sparse matrices

Lecture 2

III. Non-symmetric interior-point methods

IV. Decomposition

V. Semidefinite relaxations

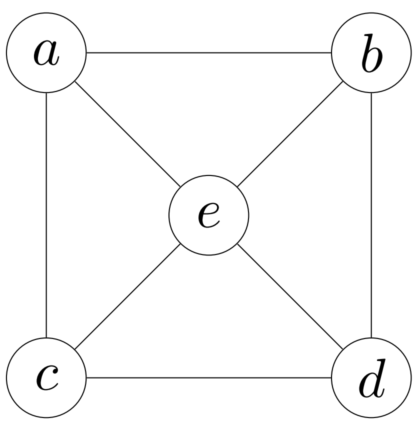
I. Chordal graphs

- definition, fundamental theorems
- perfect elimination
- triangularization

Undirected graph

$$G = (V, E)$$

- V is set of **vertices**
- $E \subseteq \{\{v, w\} \mid v, w \in V\}$ is set of **edges**
- v and w are **adjacent** if $\{v, w\} \in E$
- **neighborhood** $\text{adj}(v)$ of vertex v is set of vertices adjacent to v



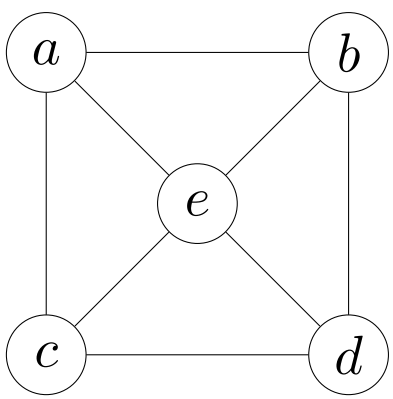
- vertices: $V = \{a, b, c, d, e\}$
- edges: $E = \{\{a, b\}, \{a, c\}, \{a, e\}, \ldots\}$
- $\text{adj}(a) = \{b, c, e\}$

Subgraphs and cliques

Definition: subgraph (induced by) $W \subset V$

$$G(W) = (W, E(W)), \qquad E(W) = \{\{v,w\} \in E \mid v,w \in W\}$$

- subgraph is **complete** if $E(W) = \{\{v,w\} \mid v,w \in W\}$
- a **clique** is a **maximal** complete subgraph



- subgraph (induced by) $W = \{a,b,c,d\}$:

$$E(W) = \{\{a,b\},\{b,d\},\{c,d\},\{a,c\}\}$$

- $W = \{a,b,e\}$ is a clique
- $W = \{a,b\}$ is complete but not a clique

Example: symmetric sparsity pattern

Definition: undirected graph $G = (V, E)$ with $V = \{1, 2, \ldots, n\}$

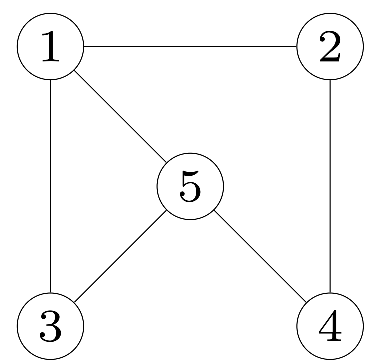
- symmetric matrix A of order n has this sparsity pattern ($A \in \mathbf{S}^n_E$) if

$$i \neq j, \quad \{i, j\} \notin E \qquad \Longrightarrow \qquad A_{ij} = A_{ji} = 0$$

  entries A_{ij} with $i = j$ or $\{i, j\} \in E$ may or may not be zero

- not unique (unless all off-diagonal entries of A are nonzero)
- cliques of G correspond to maximal 'dense' principal submatrices

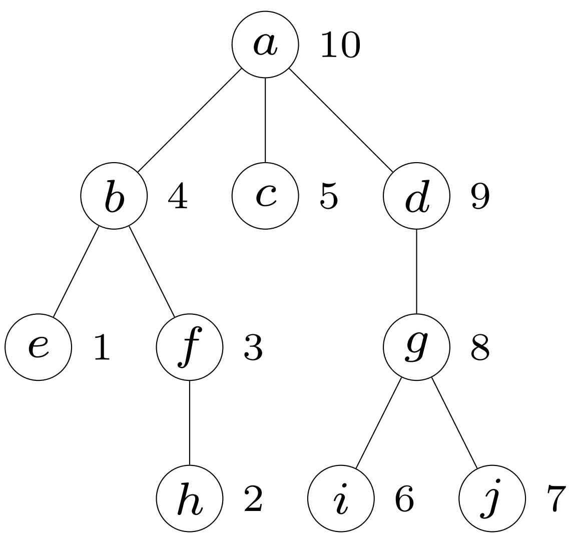
$$A = \begin{bmatrix} A_{11} & A_{12} & A_{13} & 0 & A_{15} \\ A_{21} & A_{22} & 0 & A_{24} & 0 \\ A_{31} & 0 & A_{33} & 0 & A_{35} \\ 0 & A_{42} & 0 & A_{44} & A_{45} \\ A_{51} & 0 & A_{53} & A_{54} & A_{55} \end{bmatrix}$$



Rooted tree

connected, acyclic graph with one vertex designated as root

- parent of vertex v is denoted $p(v)$
- ancestors of higher degree denoted $p^k(v)$, $k = 1, 2 \ldots$
- topological ordering: visits child before parent
- postordering: descendants of each vertex numbered consecutively

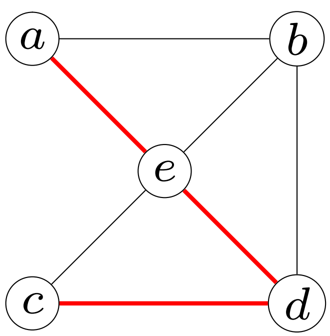


$$p(h) = f, \quad p^2(h) = b, \quad p^3(h) = a, \quad \ldots$$

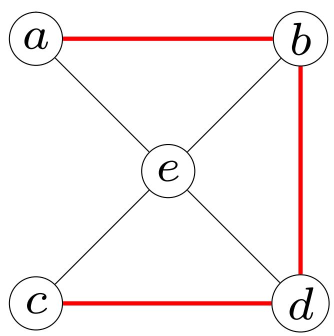
Chorded paths and cycles

a **chord** is an edge between non-consecutive vertices in a path or cycle

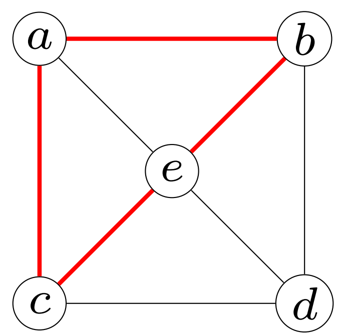
- a one-edge 'shortcut' in a path or cycle
- all shortest paths are chordless



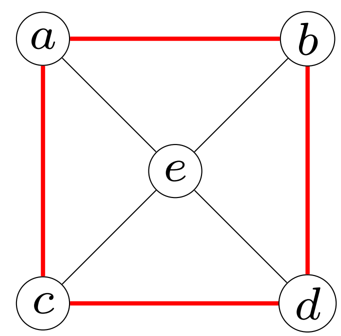
chorded path



chordless path



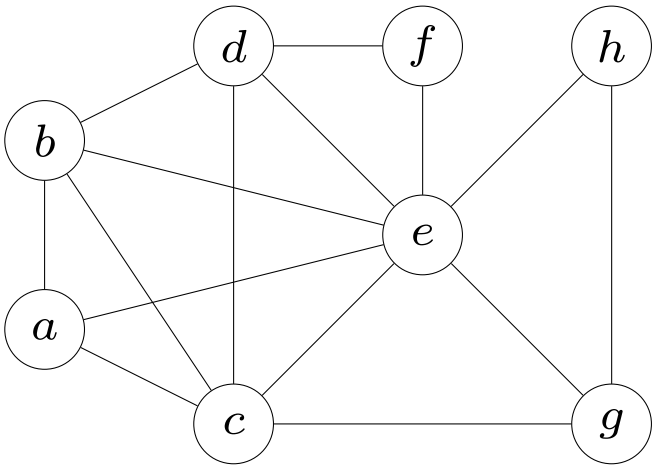
chorded cycle



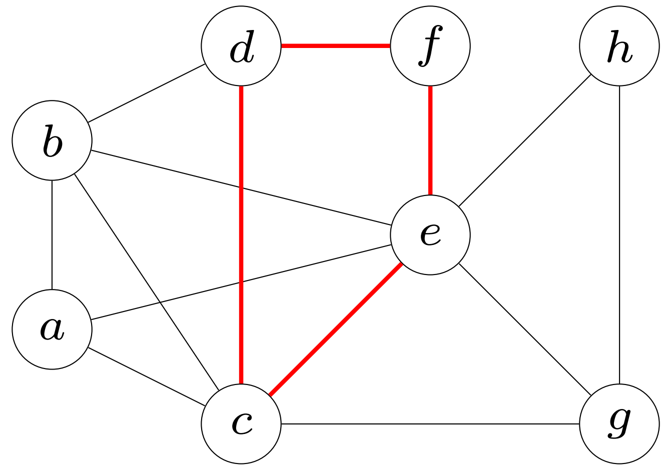
chordless cycle

Chordal graph

Chordal graph: every cycle of length greater than three has a chord



chordal



not chordal

- using chords to take 'shortcuts', all cycles can be reduced to triangles
- subgraphs of chordal graphs are chordal

also known as rigid circuit graphs, triangulated, decomposable graphs, . . .

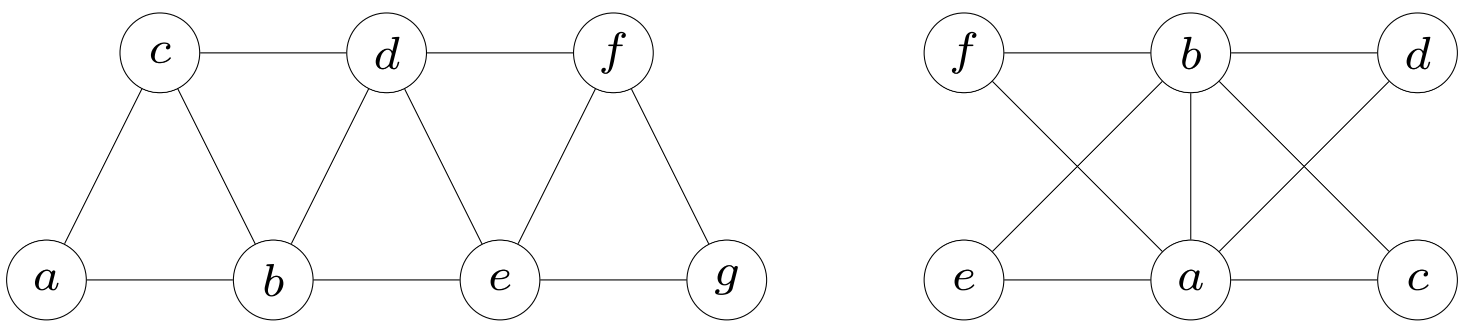
Examples

Trivial: complete graphs, trees, cactus graphs (no cycles of length > 3)

k-**Trees:** constructed recursively

- k-tree with k vertices is complete graph
- to construct k-tree with $n + 1$ vertices from k-tree with n vertices:

  make new vertex adjacent to a complete subgraph of k vertices

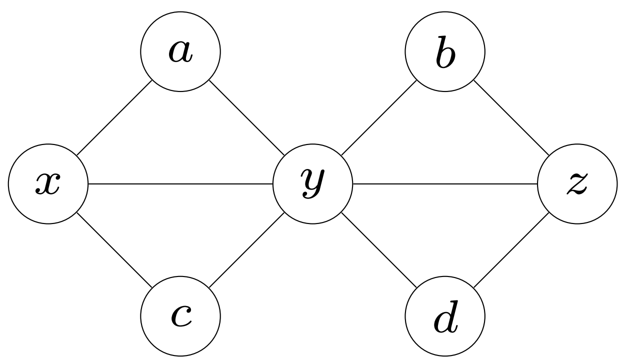


two 2-trees

Minimal vertex separator

Definition: $S \subset V$ is a minimal vw-separator if

- v and w are in different connected components of $G(V \setminus S)$
- no strict subset of S is a vw-separator

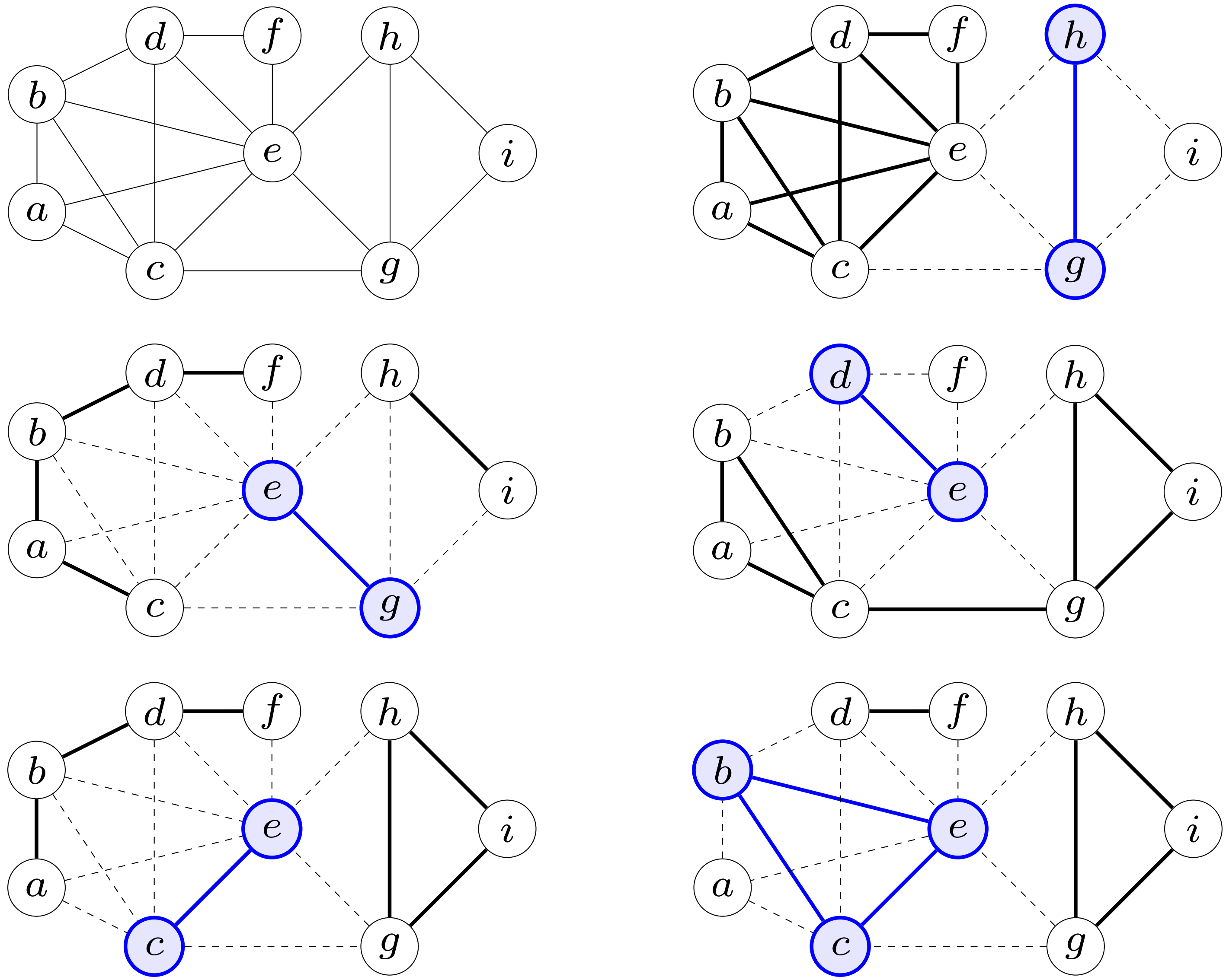


- $\{x, y\}$ is a minimal ac-separator
- $\{y\}$ is a minimal ad-separator

Chordal graphs (Dirac 1961, Buneman 1974)

- graph is chordal if and only if all minimal vertex separators are complete
- every minimal vertex separator is a subset of at least two cliques

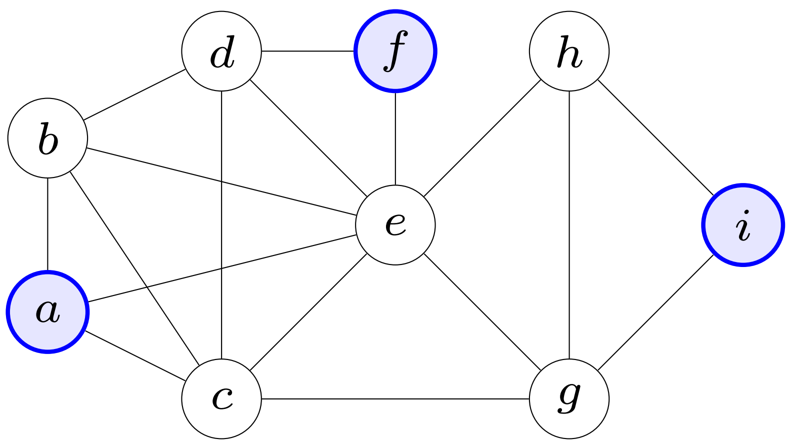
Example



Simplicial vertices

Definition: v is a simplicial vertex if $\mathrm{adj}(v)$ is complete

- closed neighborhood $\{v\} \cup \mathrm{adj}(v)$ is a clique
- $\{v\} \cup \mathrm{adj}(v)$ is the only clique that contains v



three simplicial vertices

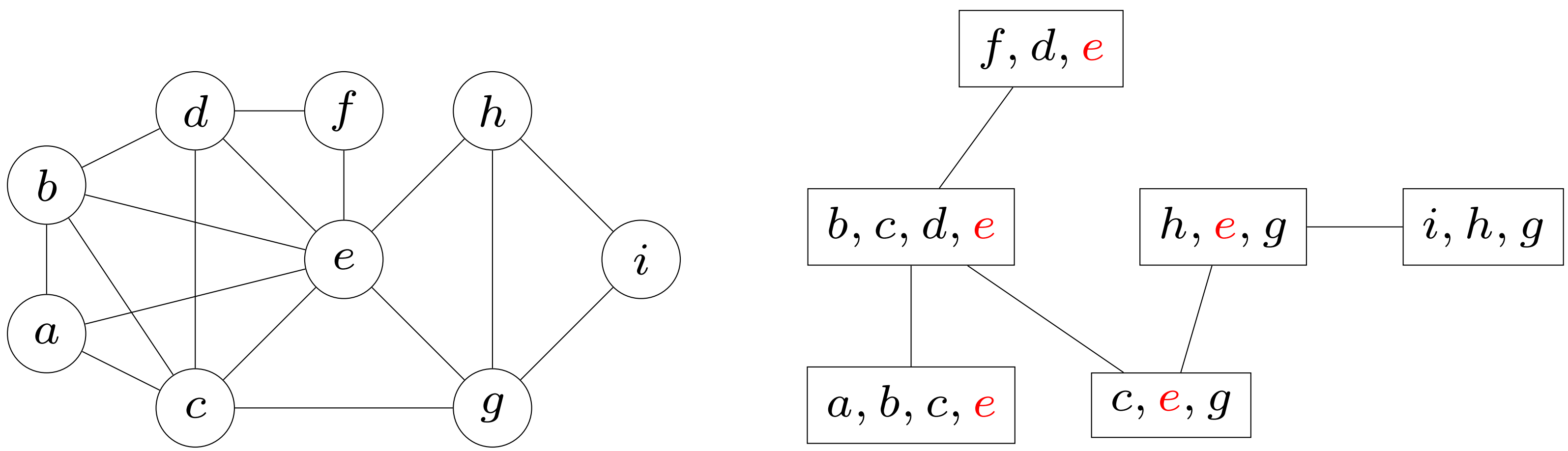
Chordal graphs (Dirac 1961)

a non-complete chordal graph has at least 2 non-adjacent simplicial vertices

Clique tree

Definition: clique tree with the induced subtree property for $G = (V, E)$

- vertices of clique tree are the cliques of G
- for every $v \in V$, cliques that contain v form subtree of clique tree

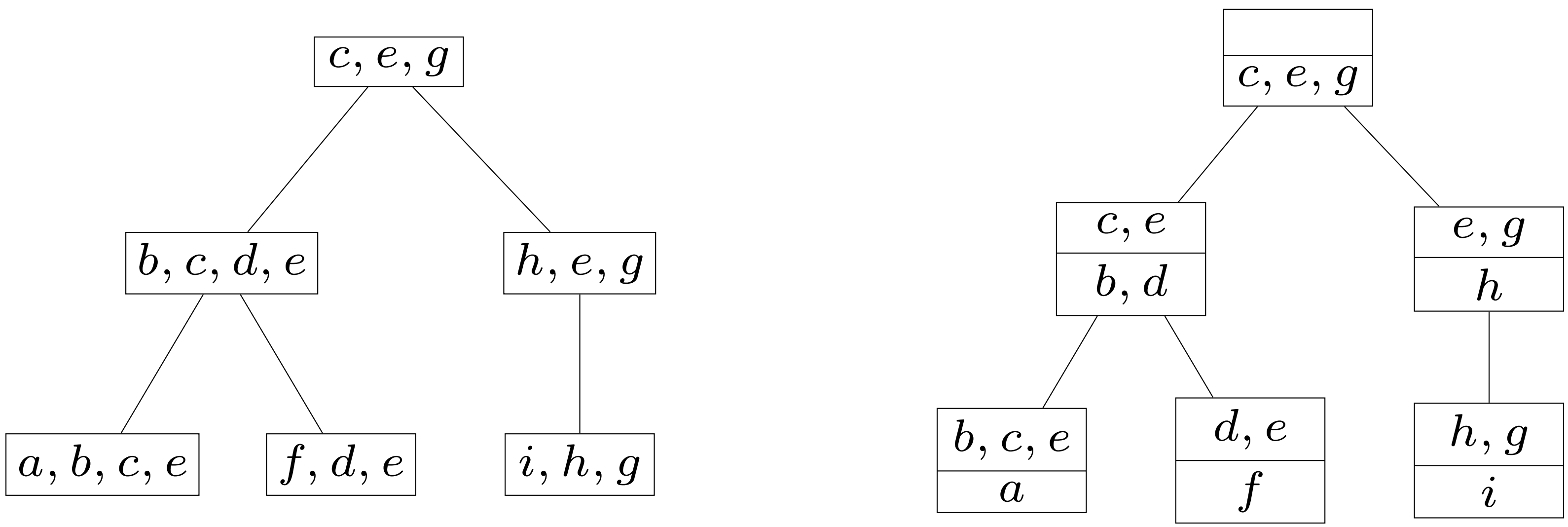


Chordal graphs (Buneman 1974, Gavril 1974)

G is chordal if and only it has a clique tree with induced subtree property

Clique separators and residuals

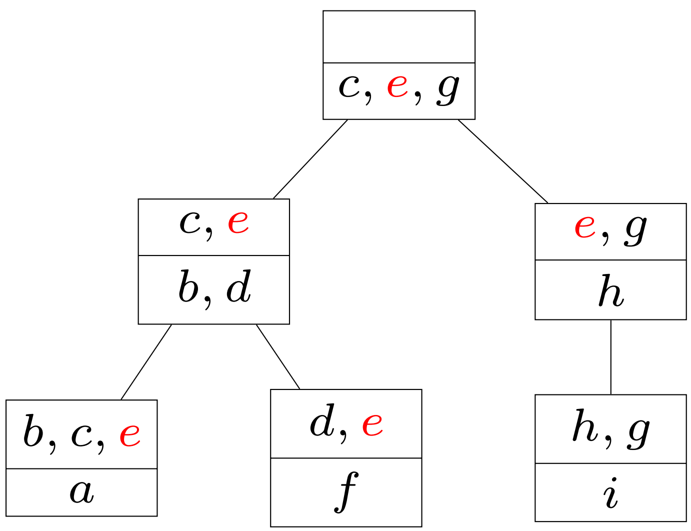
- choose any clique as root; denote parent function as $p(W)$
- clique **separator** of non-root clique W is $\mathrm{sep}(W) = W \cap p(W)$
- clique **residual** is $\mathrm{res}(W) = W \setminus \mathrm{sep}(W)$ (and $\mathrm{res}(W) = W$ for root)

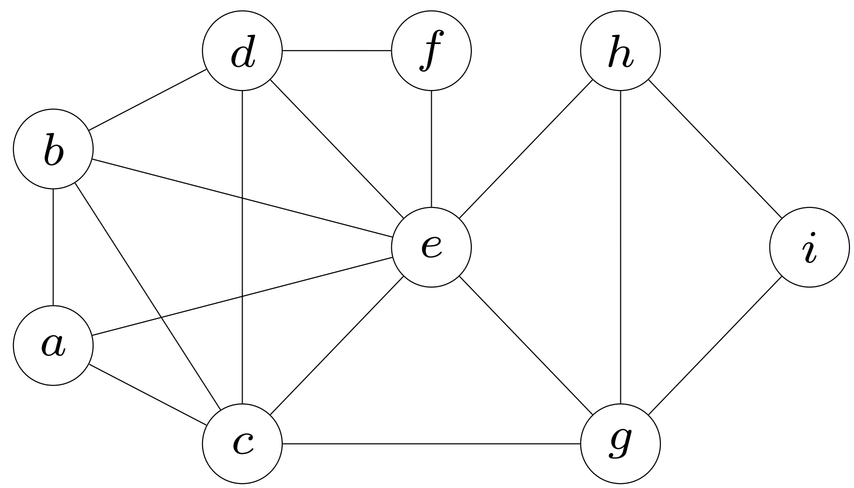


$$W = \{b, c, d, e\}, \qquad \mathrm{res}(W) = \{b, d\}, \qquad \mathrm{sep}(W) = \{c, e\}$$

Graph structure from rooted clique tree

- every vertex v belongs to exactly one clique residual $\mathrm{res}(W)$
- if $v \in \mathrm{res}(W)$ then W is the root of the subtree of cliques that contain v
- the clique separators $\mathrm{sep}(W)$ are the minimal vertex separators
- a vertex is simplicial if it does not belong to any clique separator





chordal graph has at most $n = |V|$ cliques, $n - 1$ minimal vertex separators

Tree intersection graphs

Definition: given a family of subtrees $\{R_v \mid v \in V\}$ of a tree T

- tree intersection graph $G = (V, E)$ has vertex set V
- $\{v, w\} \in E$ if and only if R_v and R_w intersect

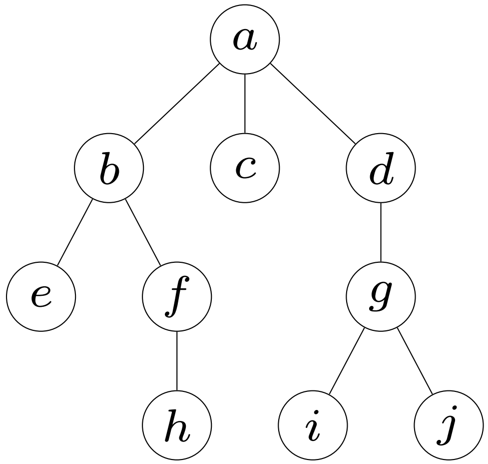
Chordality (Gavril 1974, Buneman 1974)

- a tree intersection graph is chordal
- every chordal graph can be represented as a tree intersection graph

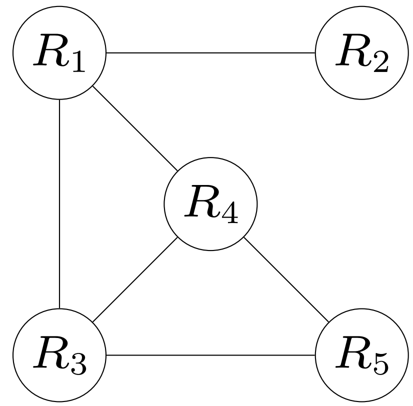
  (for example, T is the clique tree, R_v subtree of cliques that contain v)

Example

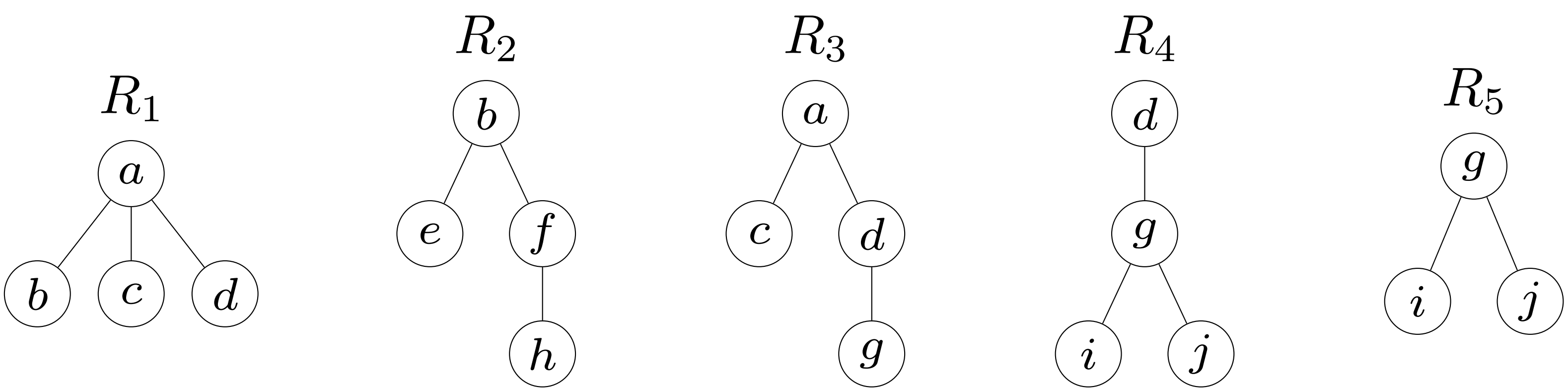
tree T



tree intersection graph



five subtrees of T



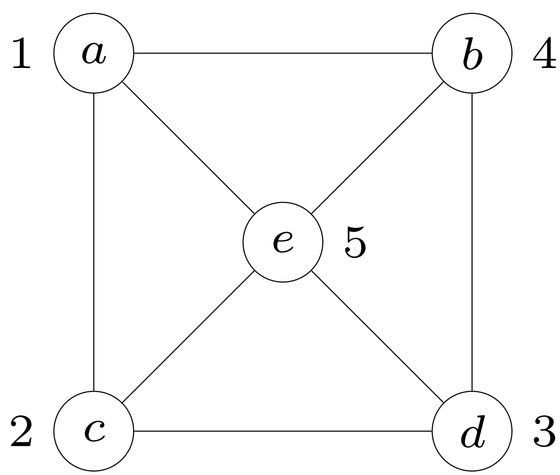
I. Chordal graphs

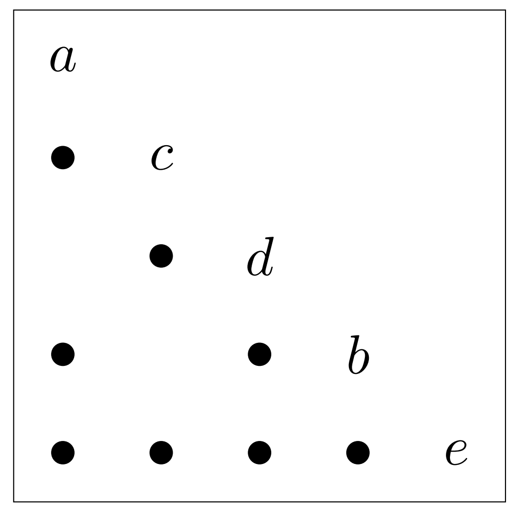
- definition, fundamental theorems
- **perfect elimination**
- triangularization

Ordered undirected graphs

$$G_\sigma = (V, E, \sigma)$$

- σ is a bijection from $\{1, 2, \ldots, |V|\}$ to V
- ordering notation: $v \prec w$ means $\sigma^{-1}(v) < \sigma^{-1}(w)$





can be represented as annotated graph or triangular array

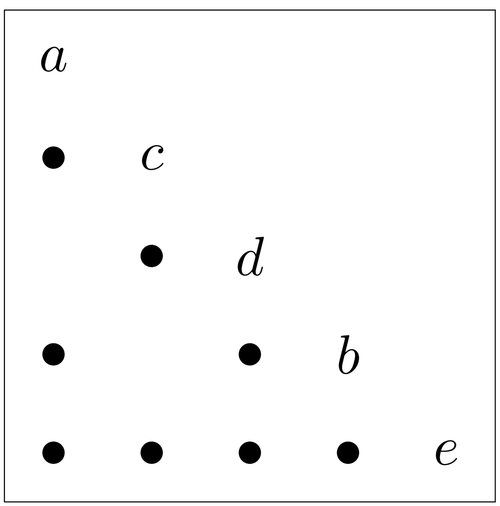
Monotone neighborhoods

- higher and lower (monotone) neighborhoods

$$\mathrm{adj}^+(v) = \mathrm{adj}(v) \cap \{w \mid w \succ v\}, \qquad \mathrm{adj}^-(v) = \mathrm{adj}(v) \cap \{w \mid w \prec v\}$$

- closed higher and lower neighborhoods

$$\mathrm{col}(v) = \{v\} \cup \mathrm{adj}^+(v), \qquad \mathrm{row}(v) = \{v\} \cup \mathrm{adj}^-(v)$$



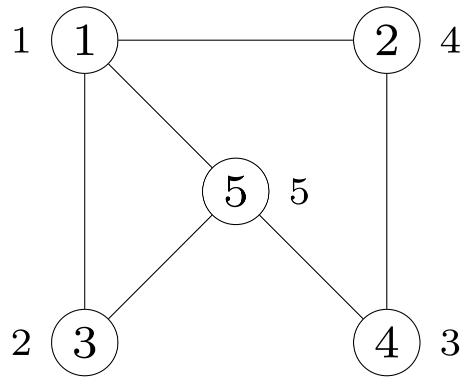
monotone neighborhoods of c:

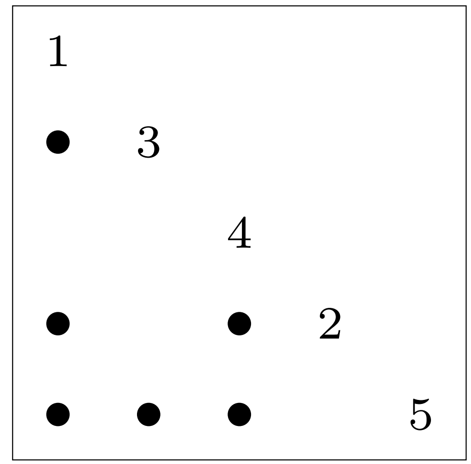
$$\mathrm{adj}^+(c) = \{d, e\}, \quad \mathrm{adj}^-(c) = \{a\}$$

$$\mathrm{col}(c) = \{c, d, e\}, \quad \mathrm{row}(c) = \{c, a\}$$

Example: ordered symmetric sparsity pattern

- ordered sparsity pattern (V, E, σ) of order 5 with $\sigma = (1, 3, 4, 2, 5)$





- represents symmetric reordering (P_σ is permutation matrix defined by σ)

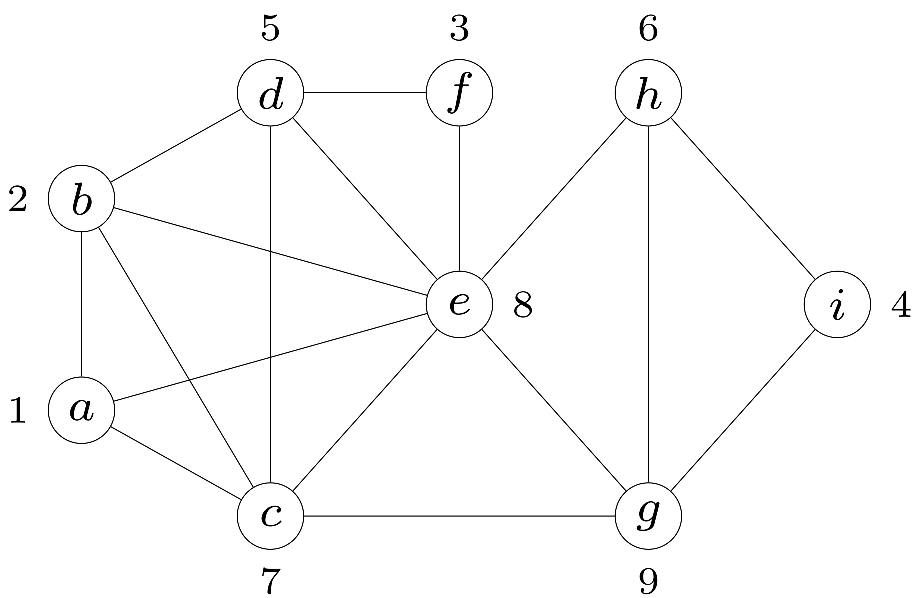
$$P_\sigma A P_\sigma^T = \begin{bmatrix} A_{11} & A_{31} & 0 & A_{21} & A_{51} \\ A_{31} & A_{33} & 0 & 0 & A_{53} \\ 0 & 0 & A_{44} & A_{42} & A_{54} \\ A_{21} & 0 & A_{42} & A_{22} & 0 \\ A_{51} & A_{53} & A_{54} & 0 & A_{55} \end{bmatrix}$$

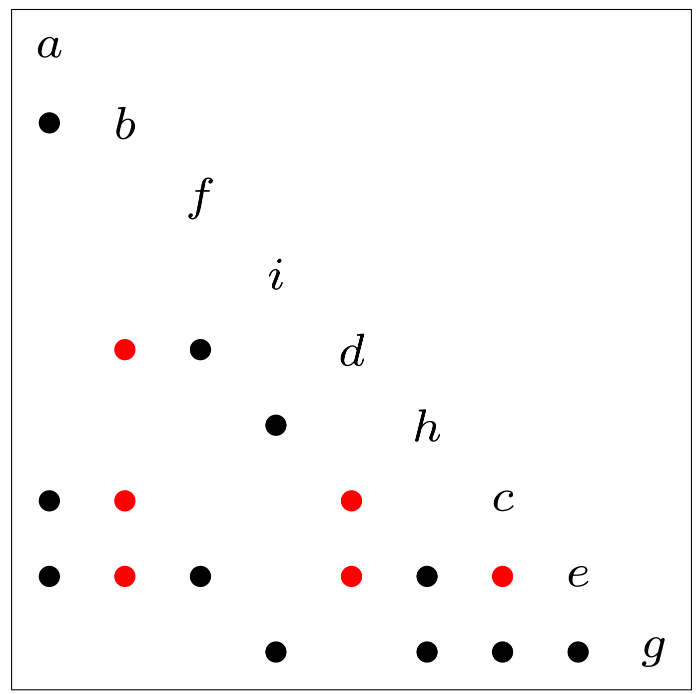
Filled graph

an ordered graph is **filled** or **monotone transitive** if

$$w, z \in \mathrm{adj}^+(v) \quad \Longrightarrow \quad \{w, z\} \in E$$

higher neighborhood of every vertex is complete



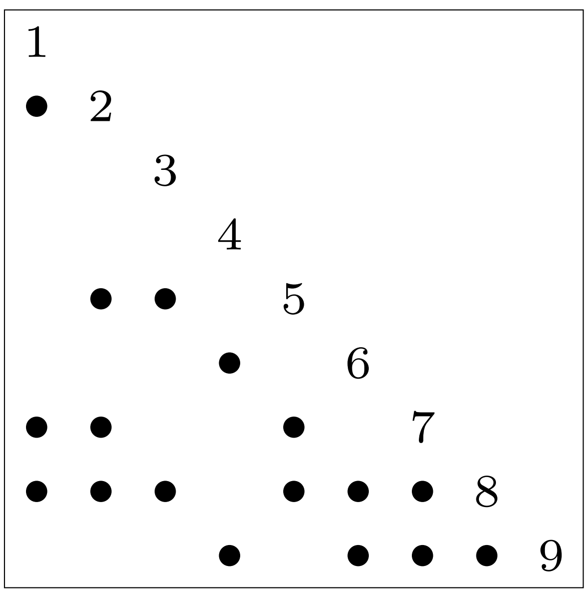


Example: pattern of Cholesky factor

Cholesky factorization of positive define $A \in \mathbf{S}^n$

$$A = LDL^T$$

- L unit lower triangular, D positive diagonal
- $L + L^T$ has a filled sparsity pattern, with $\sigma = (1, 2, \ldots, n)$



$$i > j > k, \qquad \{i, j\} \in E, \qquad \{i, k\} \in E$$

$$\Downarrow$$

$$\{j, k\} \in E$$

Perfect elimination ordering

σ is a **perfect elimination ordering** for (V, E) if (V, E, σ) is filled

Chordal graphs (Fulkerson and Gross 1965)

a graph is chordal if and only if it has a perfect elimination ordering

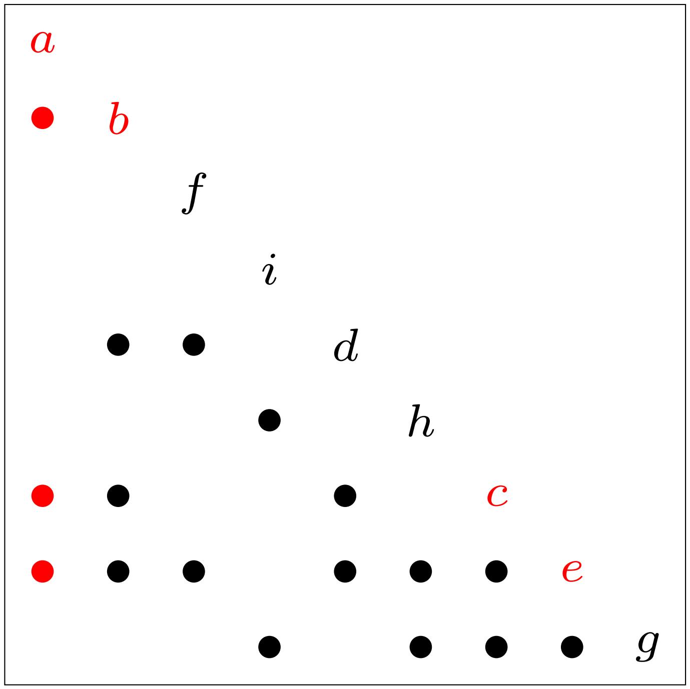
Simplicial elimination

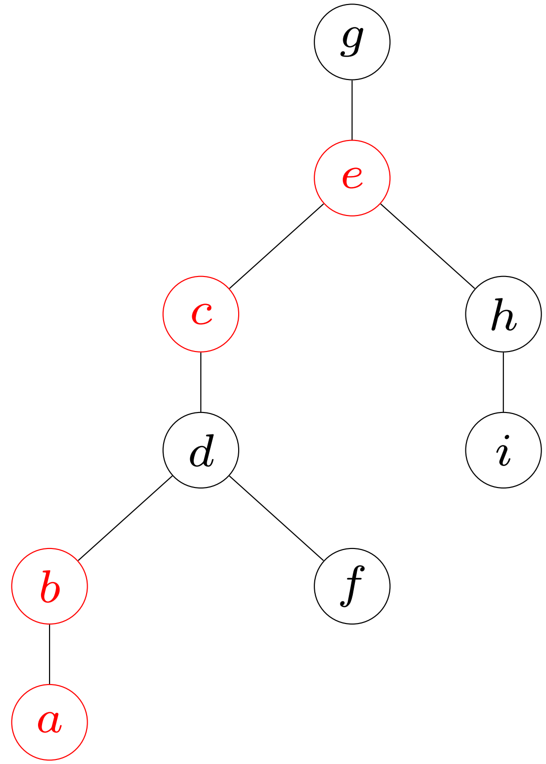
- find a simplicial vertex v and take $\sigma(1) = v$
- let $\sigma(2), \ldots, \sigma(n)$ be a perfect elimination ordering of $G(V \setminus \{v\})$

Practical algorithms

- find perfect elimination ordering in $O(|V| + |E|)$ time
- can be used to test chordality

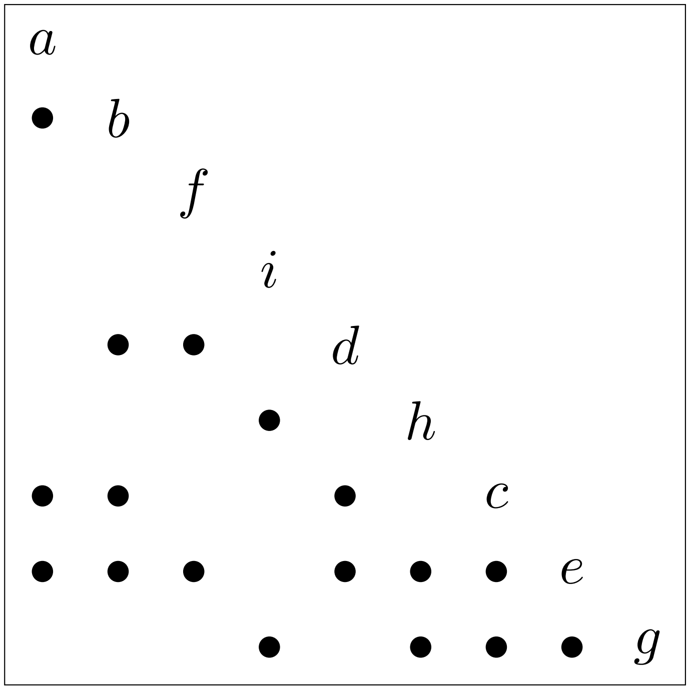
Elimination tree for filled graph

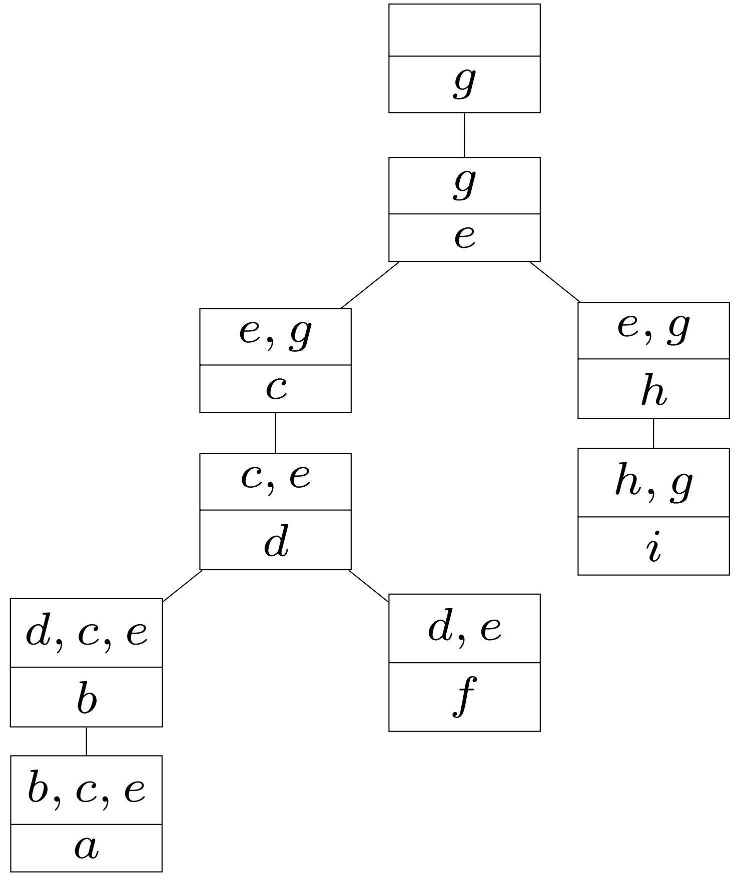




- parent $p(v)$ of vertex v is first vertex in $\mathrm{adj}^+(v)$
- elements of $\mathrm{adj}^+(v)$ are ancestors of v (not necessarily contiguous)

Expanded elimination tree

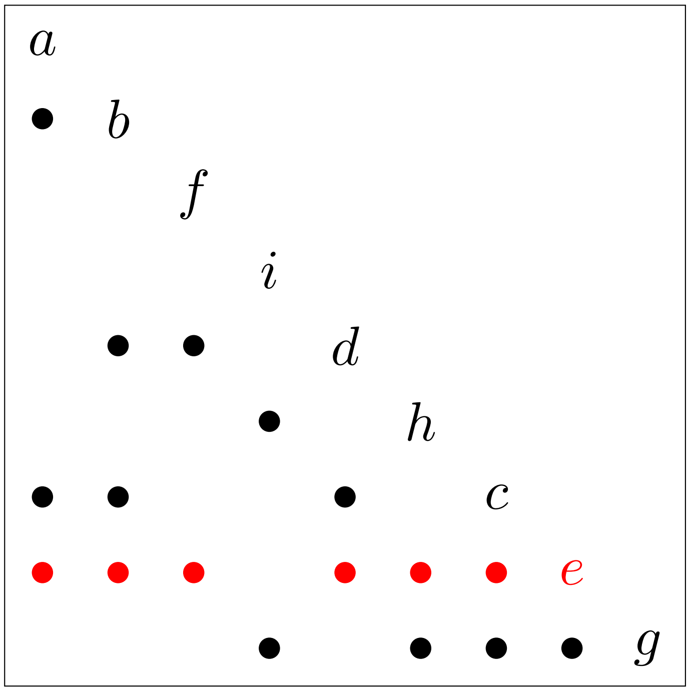


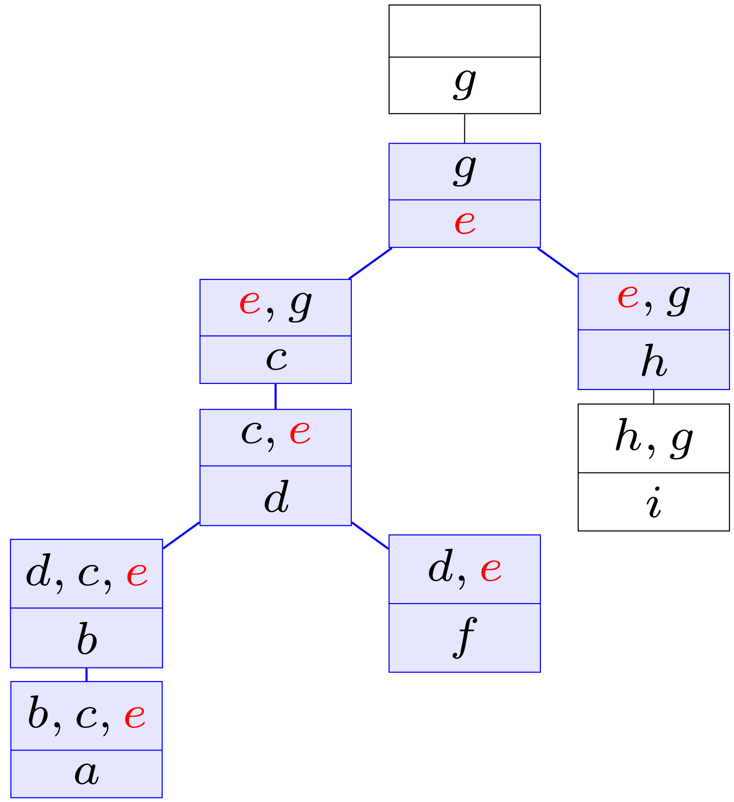


- row above vertex v is $\mathrm{adj}^+(v)$
- monotone transitivity: $\mathrm{adj}^+(v) \subset \mathrm{col}(p(v))$ for every (non-root) v

Induced subtree property

$\mathrm{row}(v) = \{w \mid v \in \mathrm{col}(w)\}$ forms a subtree of elimination tree





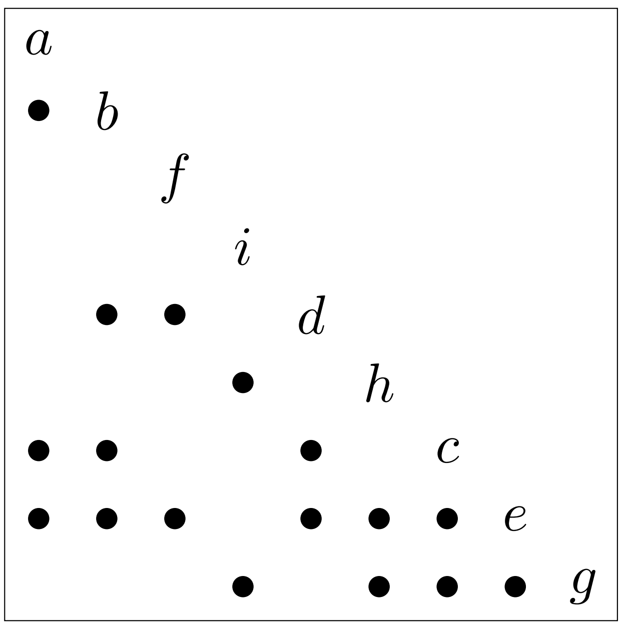
$$\mathrm{row}(e) = \{a, b, f, d, h, c, e\}$$

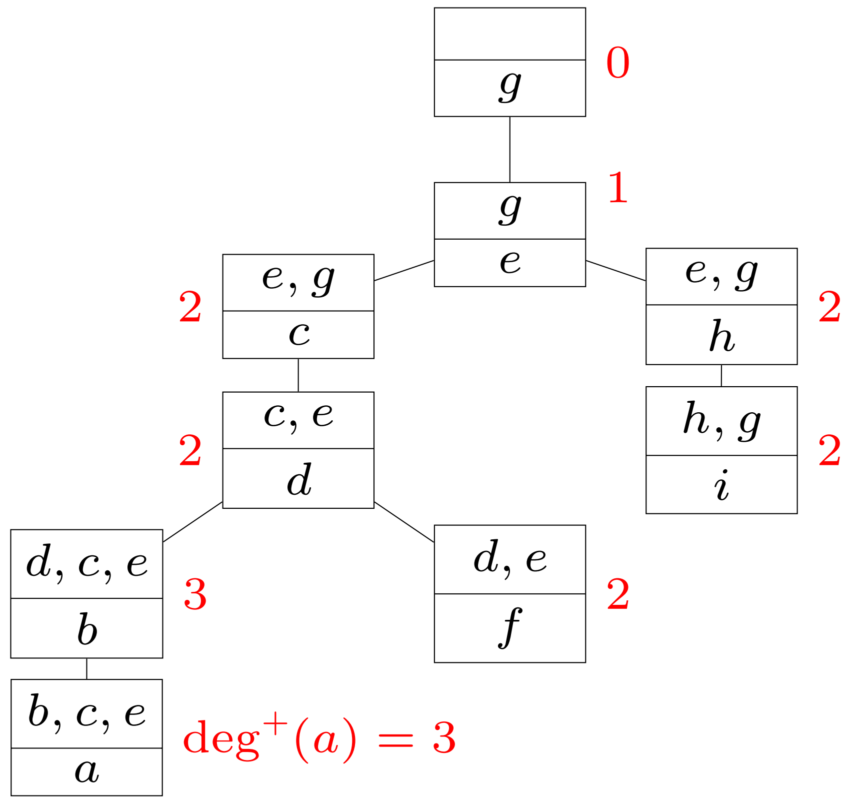
gives another representation of chordal graph as tree intersection graph

Higher degrees

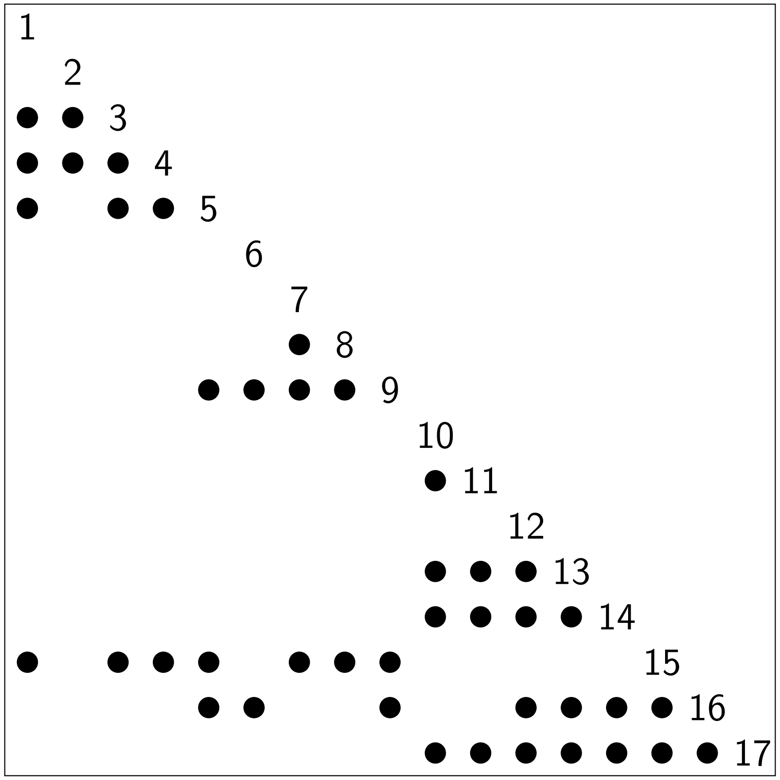
Definition: higher degree of vertex v is $\deg^+(v) = |\text{adj}^+(v)|$

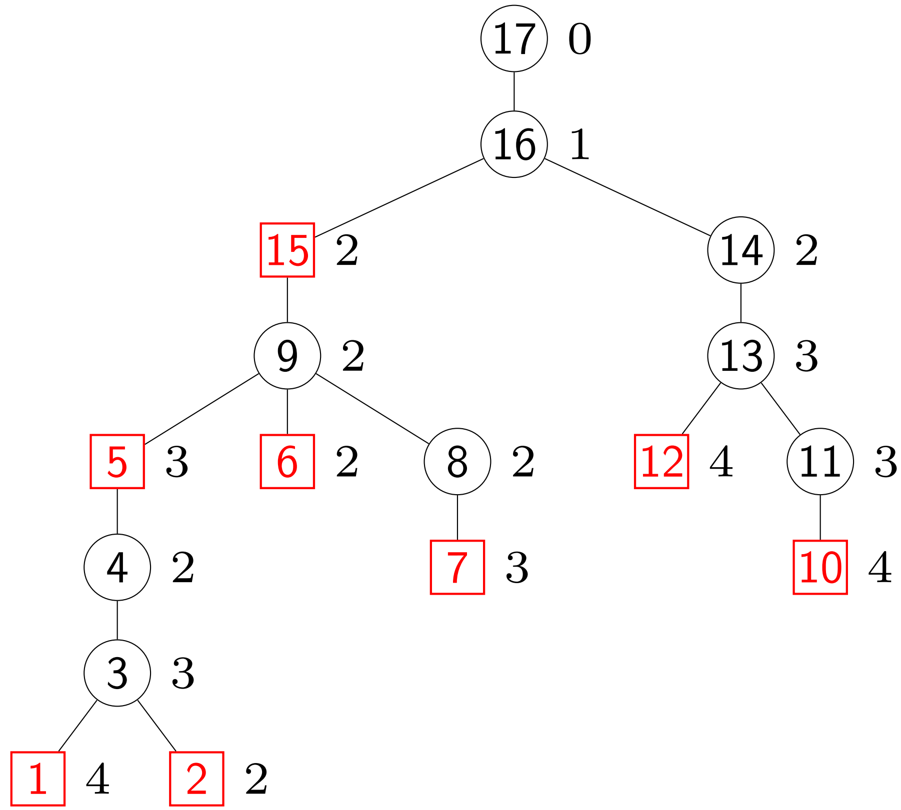
- higher degrees satisfy $\deg^+(v) \leq \deg^+(p(v)) + 1$
- $\deg^+(v) = \deg^+(p(v)) + 1$ holds only if $\text{adj}^+(v) = \text{col}(p(v))$





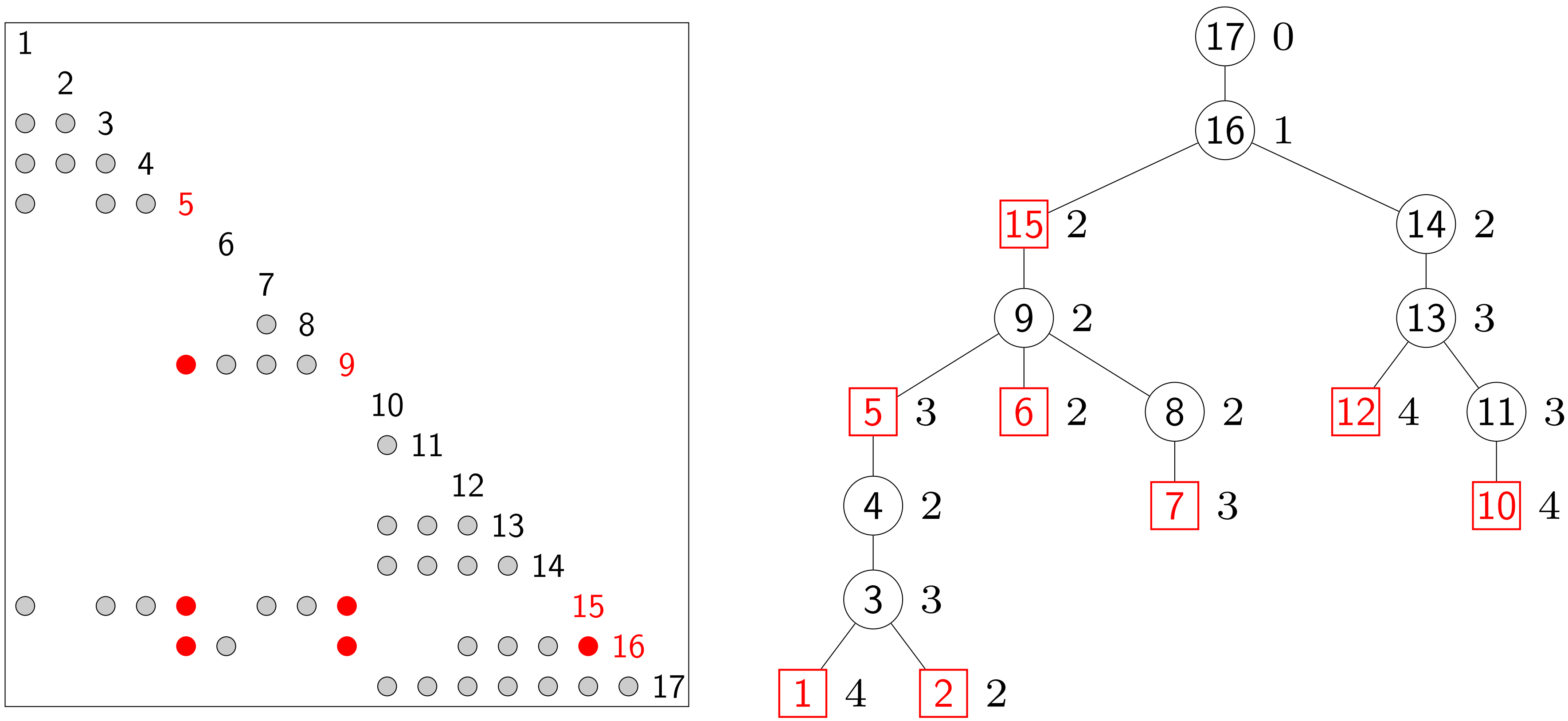
Cliques from elimination tree





- cliques are sets $\mathrm{col}(v)$ with v the **representative vertex** of the clique
- v is clique representative if $\deg^+(w) < \deg^+(v) + 1$ for all its children w

Cliques from elimination tree

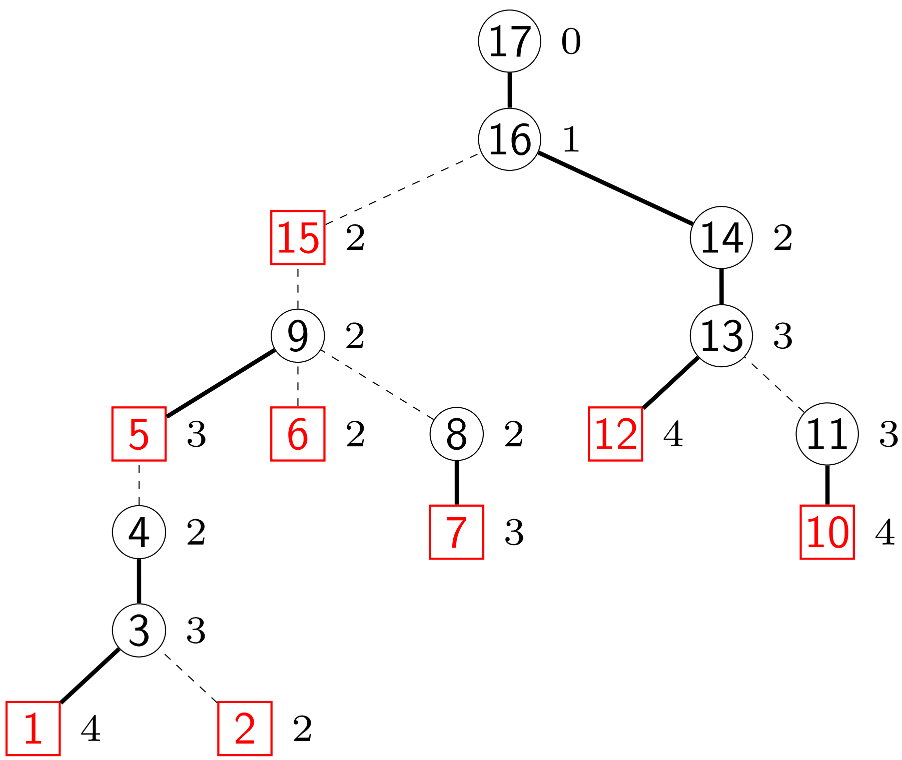


- test only needs elimination tree, higher degrees, not entire graph
- implies that a chordal graph has at most n cliques

Maximal supernodes

Definition: sets $\mathrm{sn}(v) = \{v, p(v), p^2(v), \ldots, p^{n_v}(v)\}$ that partition V

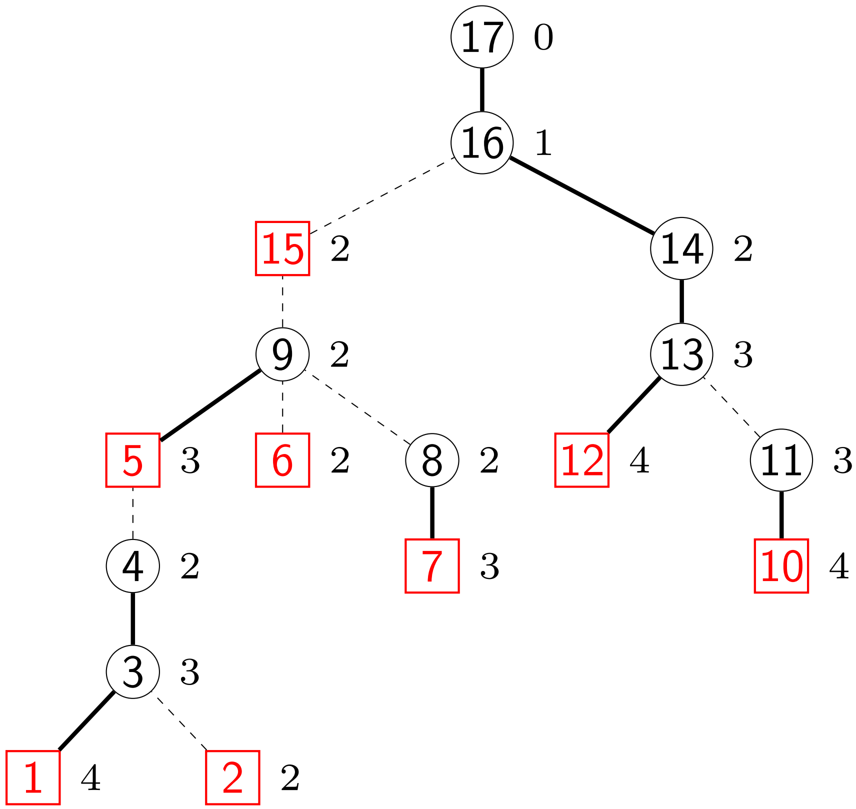
- v is a clique representative vertex
- $\deg^+(p^k(v)) = \deg^+(v) - k$ for $k = 1, \ldots, n_v$

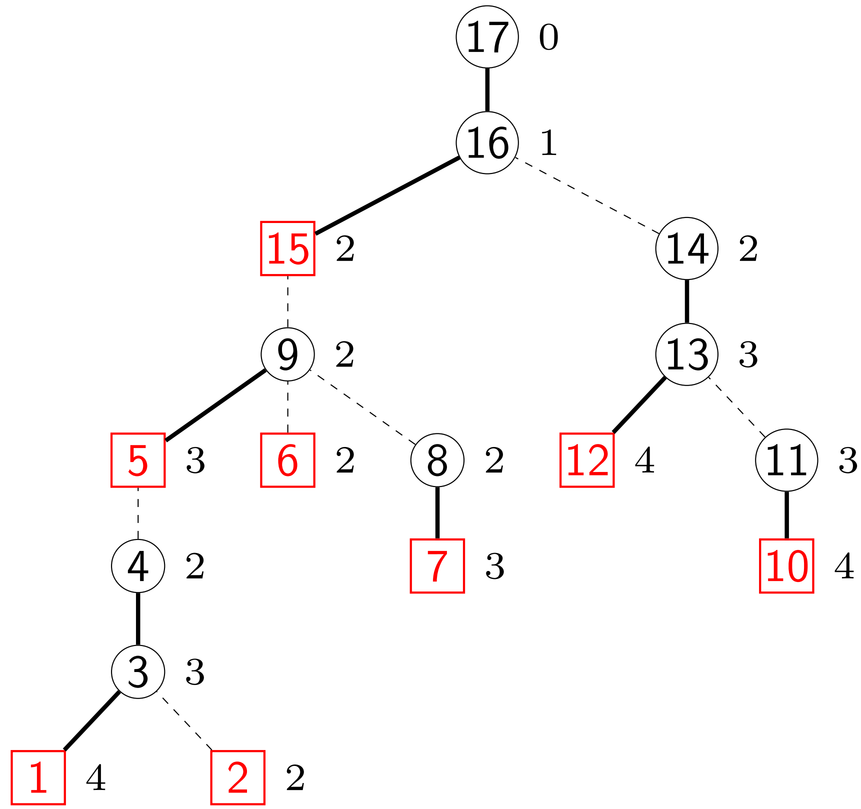


$$
\begin{aligned}
\mathrm{sn}(1) &= \{1, 3, 4\} \\
\mathrm{sn}(2) &= \{2\} \\
\mathrm{sn}(5) &= \{5, 9\} \\
\mathrm{sn}(6) &= \{6\} \\
\mathrm{sn}(7) &= \{7, 8\} \\
\mathrm{sn}(10) &= \{10, 11\} \\
\mathrm{sn}(12) &= \{12, 13, 14, 16, 17\} \\
\mathrm{sn}(15) &= \{15\}
\end{aligned}
$$

(Lewis, Peyton, Pothen 1998, Pothen and Sun 1990)

Nonuniqueness of maximal supernode partition



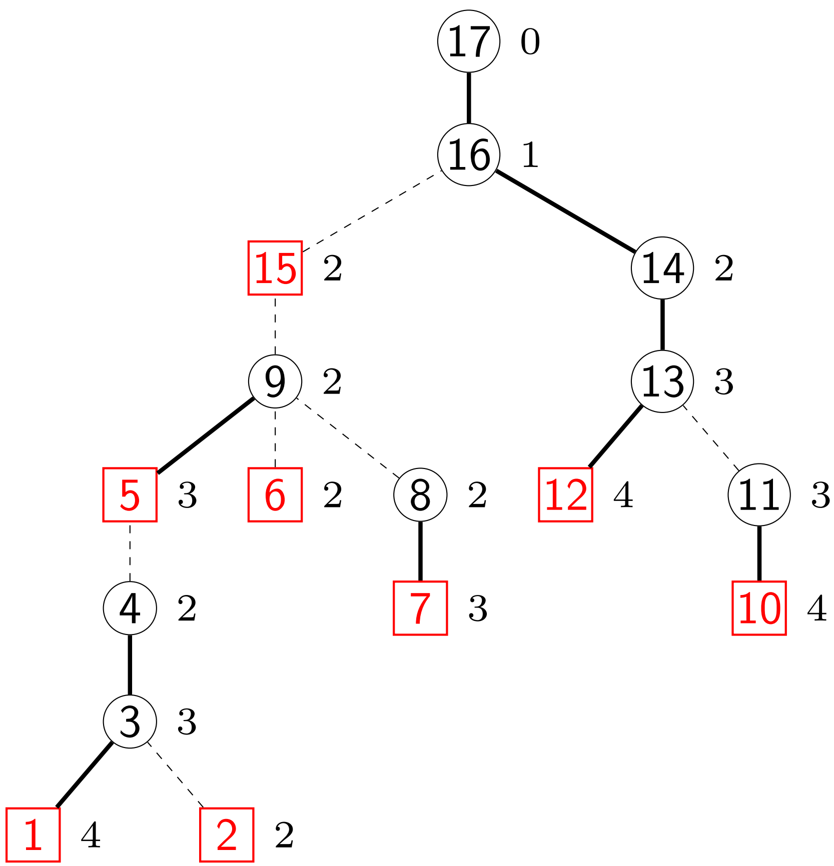


$$\begin{aligned} \mathrm{sn}(15) &= \{15\} \\ \mathrm{sn}(12) &= \{12, 13, 14, 16, 17\} \end{aligned}$$

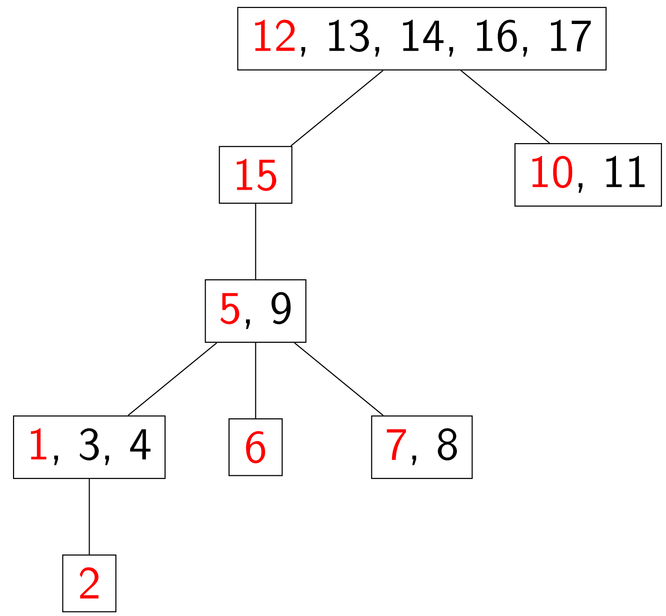
$$\begin{aligned} \mathrm{sn}(15) &= \{15, 16, 17\} \\ \mathrm{sn}(12) &= \{12, 13, 14\} \end{aligned}$$

Supernodal elimination tree

elimination tree

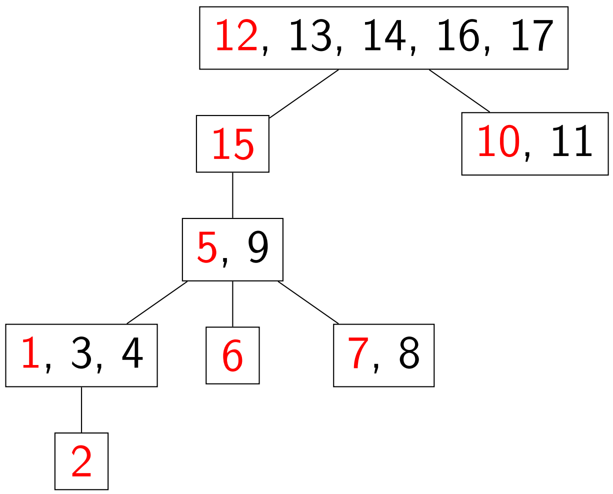


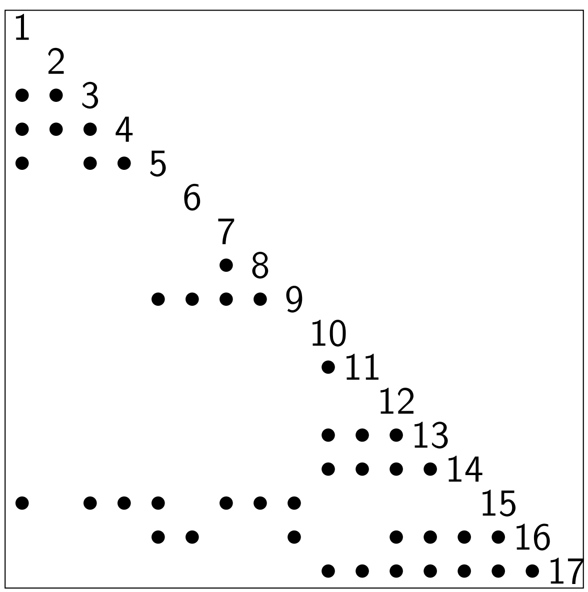
supernodal elimination tree

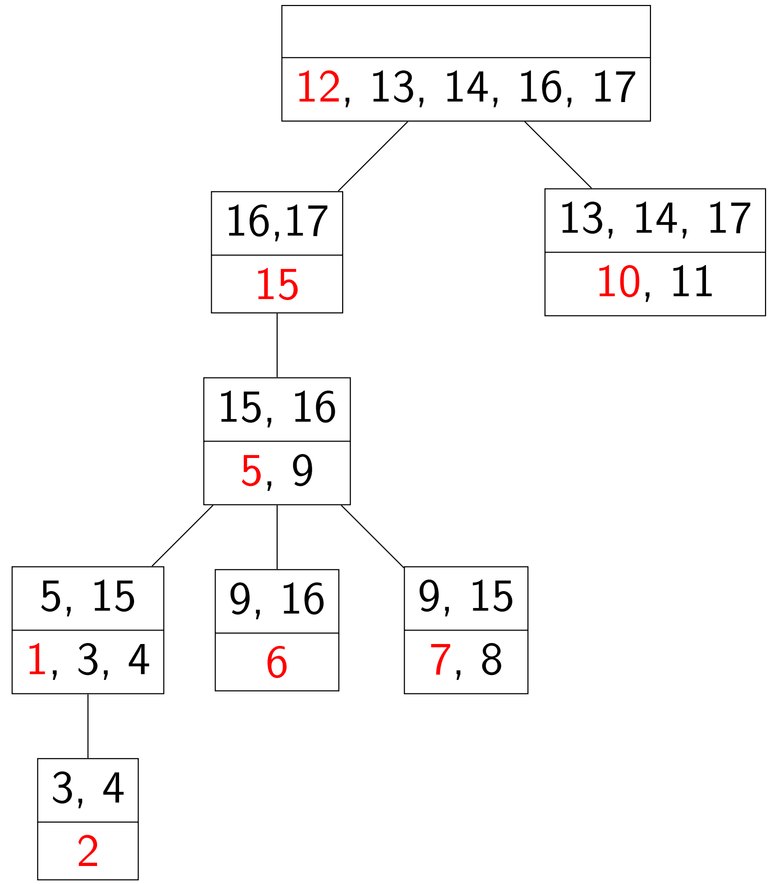


- vertices are supernodes $\mathrm{sn}(v)$
- parent of $\mathrm{sn}(v)$: supernode that contains parent (in etree) of last element of $\mathrm{sn}(v)$

Clique tree from supernodal elimination tree







- $\mathrm{sn}(v)$ is residual of clique $\mathrm{col}(v)$
- separator is $\mathrm{col}(v) \setminus \mathrm{sn}(v)$

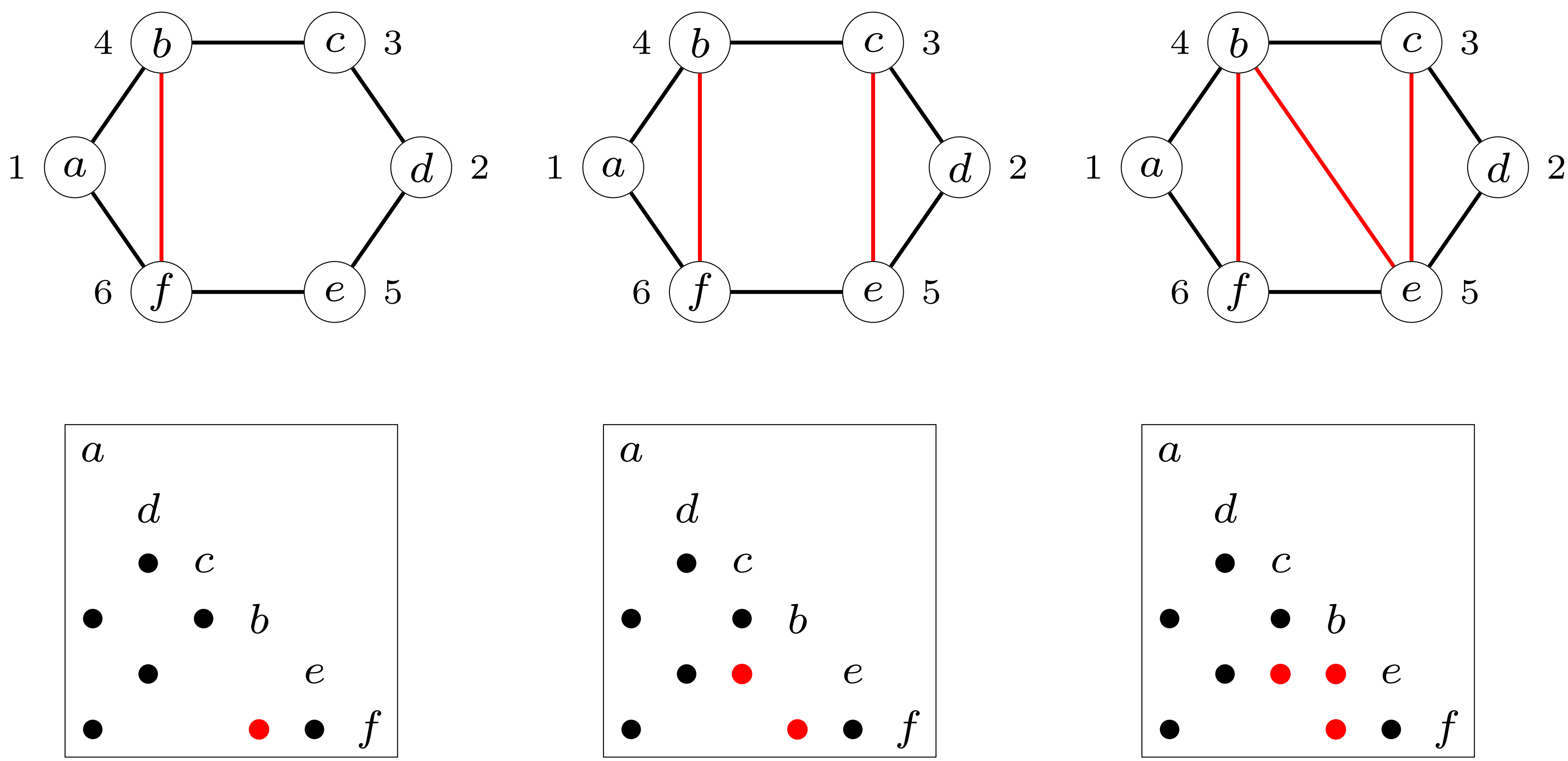
I. Chordal graphs

- chordal graphs
- perfect elimination
- **triangularization**

Triangularization

construct filled graph from ordered graph $G_\sigma = (V, E, \sigma)$:

- enumerate vertices $v = \sigma(i)$ for $i = 1, \ldots, |V|$
- in cycle i, add edges to make higher neighborhood $\mathrm{adj}^+(v)$ complete

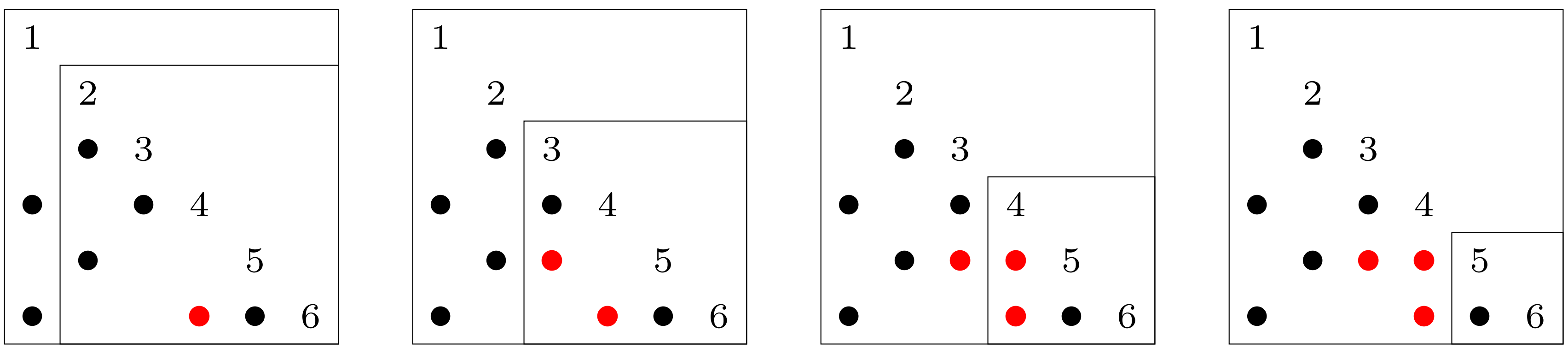


Example: Cholesky factorization

to factor A as $A = LDL^T$, factor A as

$$
\begin{aligned}
A = \begin{bmatrix} a & b^T \\ b & C \end{bmatrix} &= \begin{bmatrix} 1 & 0 \\ (1/a)b & I \end{bmatrix} \begin{bmatrix} a & 0 \\ 0 & C - (1/a)bb^T \end{bmatrix} \begin{bmatrix} 1 & (1/a)b^T \\ 0 & I \end{bmatrix} \\
&= \hat{L}\hat{D}\hat{L}^T
\end{aligned}
$$

and factor $C - (1/a)bb^T$



pattern of $\hat{L} + \hat{D} + \hat{L}^T$ during iteration

Fill-in

- the added edges during triangularization are called fill-in F_σ
- ordering σ is a perfect elimination ordering for (V, E) if $F_\sigma = \emptyset$
- the graph $(V, E \cup F_\sigma)$ is a chordal extension of (V, E)

Minimum ordering: minimizes fill-in $|F_\sigma|$; NP-complete (Yannakakis 1981)

Minimal ordering: there exists no ordering σ' with $F_{\sigma'} \subset F_\sigma$

- perfect elimination ordering if graph is chordal
- several algorithms with linear complexity (in $|V| + |E|$)
- maximum cardinality search (Tarjan and Yannakakis 1984), several others

Non-minimal heuristics: often give smaller $|F_\sigma|$ than minimal ordering

Analysis of filled graph

algorithms for analyzing filled graph of (V, E, σ) without constructing it:

- constructing elimination tree
- calculating monotone (higher and lower) degrees
- calculating number of filled edges
- finding clique representatives
- finding supernodes, supernodal elimination tree

complexity is linear or nearly linear in $|V| + |E|$ ($i.e.$, size of original graph)

(Liu 1990, Gilbert, Ng, Peyton 1994, Davis 2006)

Overview

Lecture 1

I. Chordal graphs

II. Sparse matrices

Lecture 2

III. Non-symmetric interior-point methods

IV. Decomposition

V. Semidefinite relaxations

II. Sparse matrices

- sparse matrix cones
- chordal decomposition
- logarithmic barriers

Sparse matrix cones

two matrix cones in $\mathbf{S}^n_E$ (symmetric of order n with sparsity pattern E)

- positive semidefinite matrices

$$\mathbf{S}^n_{E,+} = \{X \in \mathbf{S}^n_E \mid X \succeq 0\}$$

- matrices with a positive semidefinite completion

$$\mathbf{S}^n_{E,\mathrm{c}} = \{\Pi_E(X) \mid X \succeq 0\}$$

Π_E is projection on $\mathbf{S}^n_E$:

$$\Pi_E(X)_{ij} = \begin{cases} X_{ij} & \text{if } i = j \text{ or } \{i,j\} \in E \\ 0 & \text{otherwise} \end{cases}$$

Example

for general E, cones are not equal

Example: tridiagonal matrices of order 3 ($\mathbf{S}^3_E = \{A \in \mathbf{S}^3 \mid A_{31} = 0\}$

$$A = \begin{bmatrix} 1 & 1 & 0 \\ 1 & 1 & 1 \\ 0 & 1 & 1 \end{bmatrix}$$

- A is not positive semidefinite ($A \notin \mathbf{S}^n_{E,+}$)
- A has a positive semidefinite completion ($A \notin \mathbf{S}^n_{E,\mathrm{c}}$)

$$A = \Pi_E(\begin{bmatrix} 1 & 1 & 1 \\ 1 & 1 & 1 \\ 1 & 1 & 1 \end{bmatrix})$$

Properties

the two cones are convex, closed, pointed, with nonempty interior

Positive semidefinite cone

$$\mathbf{S}^n_{E,+} = \mathbf{S}^n_+ \cap \mathbf{S}^n_E$$

- intersection of closed convex cone and subspace, hence closed convex
- identity matrix is in the interior
- pointed: $X \in \mathbf{S}^n_{E,+}$ and $-X \in \mathbf{S}^n_{E,+}$ only if $X = 0$

Positive semidefinite completable cone

$$\mathbf{S}^n_{E,\mathrm{c}} = \Pi_E(\mathbf{S}^n_+)$$

- projection on a subspace of a convex cone with nonempty interior
- closed and pointed because $\Pi_E(X) = 0$, $X \succeq 0$ only if $X = 0$

Two cones are dual cones

- dual of positive semidefinite completable cone is p.s.d. cone

$$\begin{aligned}
(\mathbf{S}^n_{E,\mathrm{c}})^* &= \{Y \in \mathbf{S}^n_E \mid \mathbf{tr}(XY) \geq 0 \ \ \forall X \in \mathbf{S}^n_{E,\mathrm{c}}\} \\
&= \{Y \in \mathbf{S}^n_E \mid \mathbf{tr}\left(Y \Pi_E(W)\right) \geq 0 \ \ \forall W \succeq 0\} \\
&= \{Y \in \mathbf{S}^n_E \mid \mathbf{tr}(YW) \geq 0 \ \ \forall W \succeq 0\} \\
&= \mathbf{S}^n_{E,+}
\end{aligned}$$

- dual of p.s.d. cone is positive semidefinite completable cone

$$(\mathbf{S}^n_{E,+})^* = \mathrm{cl}(\mathbf{S}^n_{E,\mathrm{c}}) = \mathbf{S}^n_{E,\mathrm{c}}$$

II. Sparse matrices

- sparse matrix cones
- **chordal decomposition**
- logarithmic barriers

Notation

Index set: ordered list of distinct elements of $V = \{1, 2, \ldots, n\}$

Selection matrix: if β is an index set, P_β is 0-1 matrix of size $|\beta| \times n$

$$(P_\beta)_{ij} = 1 \quad \text{if } j = \beta_i, \qquad (P_\beta)_{ij} = 0 \quad \text{otherwise}$$

a permutation matrix if $|\beta| = n$

- used to select subvectors or principal submatrices:

$$P_\beta x = x_\beta, \qquad P_\beta X P_\beta^T = X_{\beta\beta}$$

- adjoint defines subvector or submatrix in otherwise zero vector or matrix

$$(P_\beta^T y)_i = \begin{cases} y_j & j = \beta_i \\ 0 & j \notin \beta \end{cases} \qquad (P_\beta^T Y P_\beta)_{kl} = \begin{cases} Y_{ij} & i = \beta_k, j \in \beta_l \\ 0 & (i,j) \notin \beta \times \beta \end{cases}$$

Cholesky factorization and chordal sparsity

$$P_\sigma A P_\sigma^T = LDL^T$$

P_σ a permutation, L unit lower triangular, D positive diagonal

- if $A \in \mathbf{S}_E^n$ and σ is a perfect elimination ordering for E, then

$$P_\sigma^T (L + L^T) P_\sigma \in \mathbf{S}_E^n$$

  A has a 'zero fill' Cholesky factorization

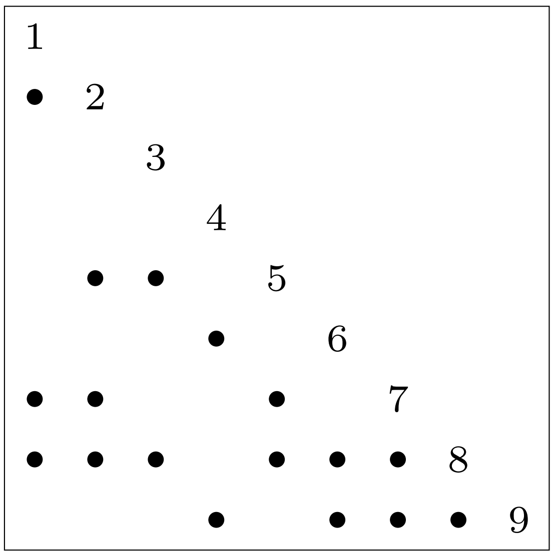
- if E is not chordal, then for every σ there exist p.d. $A \in \mathbf{S}_E^n$ for which

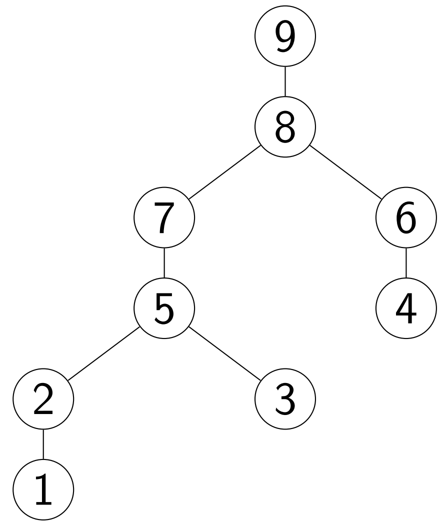
$$P_\sigma^T (L + L^T) P_\sigma \notin \mathbf{S}_E^n$$

(Rose 1070)

Assumptions and notation

E is chordal with perfect elimination ordering $\sigma = (1, 2, \ldots, n)$





- γ_j, η_j: index sets with elements of $\mathrm{col}(j)$, $\mathrm{adj}^+(j)$; for example,

$$\gamma_2 = (2, 5, 7, 8), \qquad \eta_2 = (5, 7, 8)$$

- hence, $\eta_k \subseteq \gamma_j$ if if j is the parent of k in elimination tree
- $V_\mathrm{r} \subseteq V$ is set of clique representative vertices (i for which γ_i is a clique)

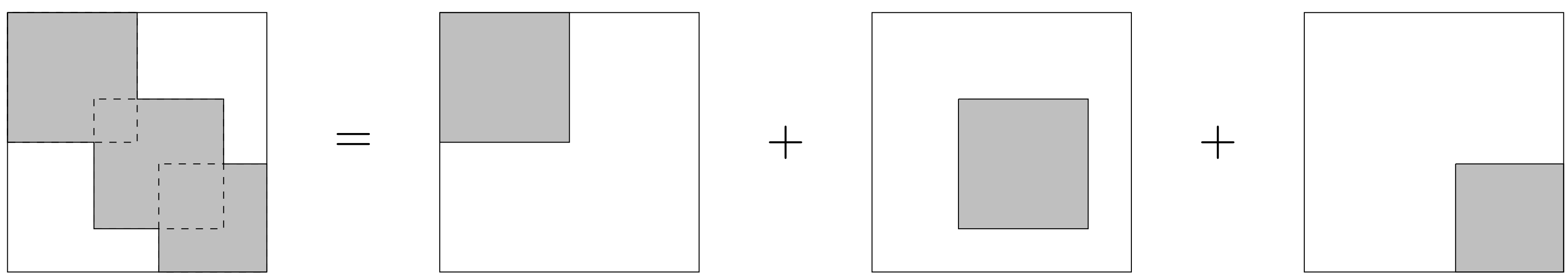
Decomposition of chordal p.s.d. cone

$A \in \mathbf{S}^n_E$ is positive semidefinite if and only if it can be expressed as

$$A = \sum_{i \in V_\mathrm{r}} P_{\gamma_i}^T B_i P_{\gamma_i} \quad \text{with} \quad B_i \succeq 0, \quad i \in V_\mathrm{r}$$

(Griewank and Toint 1984, Agler, Helton, McCullough, Rodman 1988)

Example (three cliques γ_1, γ_j, γ_k)



$A \succeq 0$ $\qquad$ $P_{\gamma_1}^T B_1 P_{\gamma_1} \succeq 0$ $\qquad$ $P_{\gamma_j}^T B_j P_{\gamma_j} \succeq 0$ $\qquad$ $P_{\gamma_k}^T B_k P_{\gamma_k} \succeq 0$

Decomposition from Cholesky factorization

$$A = LDL^T = \sum_{j=1}^{n} D_{jj} L_j L_j^T$$

- use maximal supernode partition $\mathrm{sn}(i)$ to group outer products

$$A = \sum_{i \in V_\mathrm{r}} \sum_{j \in \mathrm{sn}(i)} D_{jj} P_{\gamma_j}^T L_{\gamma_j j} L_{\gamma_j j} P_{\gamma_j}$$

- use property $\gamma_j \subset \gamma_i$ for $j \in \mathrm{sn}(i)$

$$A = \sum_{i \in V_\mathrm{r}} P_{\gamma_i}^T \left(\sum_{j \in \mathrm{sn}(i)} D_{jj} L_{\gamma_i j} L_{\gamma_i j} \right) P_{\gamma_i} = \sum_{i \in V_\mathrm{r}} P_{\gamma_i}^T B_i P_{\gamma_i}$$

where $B_i = \sum_{j \in \mathrm{sn}(i)} D_{jj} L_{\gamma_i j} L_{\gamma_i j}^T$

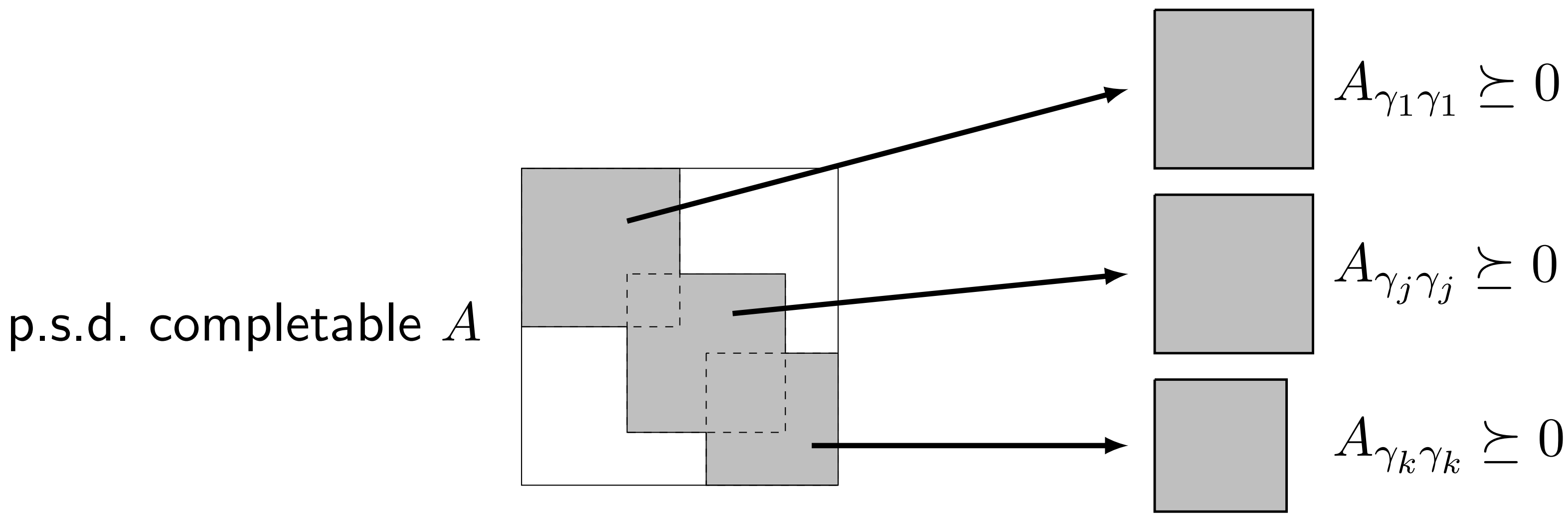
Decomposition of chordal p.s.d. completable cone

$A \in \mathbf{S}^n_E$ has a positive semidefinite completion if and only if

$$A_{\gamma_i\gamma_i} \succeq 0, \quad i \in V_\mathrm{r}$$

(Grone, Johnson, Sá, Wolkowicz, 1984)

Example (three cliques γ_1, γ_j, γ_k)



Proof from duality

- duality of the p.s.d. cone and p.s.d. completable cone

$$A \in \mathbf{S}^n_{E,\mathrm{c}} \qquad \Longleftrightarrow \qquad \mathbf{tr}(AY) \geq 0 \quad \forall Y \in \mathbf{S}^n_{E,+}$$

- use chordal decompositionn of p.s.d. cone

$$\begin{aligned} A \in \mathbf{S}^n_{E,\mathrm{c}} \quad &\Longleftrightarrow \quad \sum_{i \in V_\mathrm{r}} \mathbf{tr}\left(A P_{\gamma_i}^T B_i P_{\gamma_i}\right) \quad \forall B_i \succeq 0 \\ &\Longleftrightarrow \quad \sum_{i \in V_\mathrm{r}} \mathbf{tr}\left(P_{\gamma_i} A P_{\gamma_i}^T B_i\right) \quad \forall B_i \succeq 0 \\ &\Longleftrightarrow \quad P_{\gamma_i} A P_{\gamma_i}^T \succeq 0 \quad \forall i \in V_\mathrm{r} \end{aligned}$$

Positive semidefinite completion

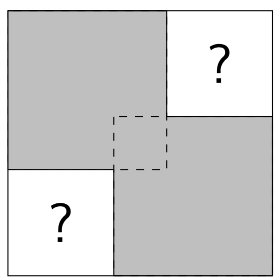
given $A \in \mathbf{S}^n_{E,\mathrm{c}}$ find X such that

$$A = \Pi_E(X), \qquad X \succeq 0$$

(Grone, Johnson, Sá, Wolkowicz, 1984)

Algorithms

- recursion on clique tree or (supernodal) elimination tree
- at each step, consider simple two-block completion problem



Euclidean distance matrices

Definition: $A \in \mathbf{S}^n$ is a Euclidean distance matrix if it can be written as

$$A_{ij} = \|x_i - x_j\|_2^2$$

for a set of vectors $x_1, \ldots, x_n$

Semidefinite parameterization: A is EDM if and only if and

$$A_{ij} = G_{ii} - 2G_{ij} + G_{jj}, \quad G \succeq 0$$

for some G (the Gram matrix with elements $G_{ij} = x_i^T x_j$)

Euclidean distance matrix completion

given $A \in \mathbf{S}^n_E$ find an EDM X such that

$$A = \Pi_E(X)$$

EDM completion with chordal pattern E

$A \in \mathbf{S}^n_E$ has an EDM completion if

$$A_{\gamma_i \gamma_i} \text{ is a Euclidean distance matrix,} \quad \text{for all cliques } \gamma_i$$

and completion can be constructed by a recursion over the elimination tree

(Bakonyi and Johnson 1995)

II. Sparse matrices

- sparse matrix cones
- chordal decomposition
- **logarithmic barriers**

References

- M.S. Andersen, J. Dahl, L. Vandenberghe, "Logarithmic barriers for sparse matrix cones", *Optimization Methods and Software* (2013)
- CHOMPACK Library for chordal matrix computations. `cvxopt.github.io/chompack`

Logarithmic barrier for p.s.d. cone

$$\phi(X) = -\log\det X, \qquad \mathbf{dom}\,\phi = \mathbf{int}\,\mathbf{S}^n_{E,+}$$

Gradient

$$\nabla\phi(X) = -\Pi_E(X^{-1})$$

- Π_E is projection on $\mathbf{S}^n_E$
- evaluation requires entries of X^{-1} on diagonal and for $\{i,j\} \in E$

Hessian: for arbitrary $Y \in \mathbf{S}^n_E$,

$$\nabla^2\phi(X)[Y] = \frac{d}{dt}\phi(x+tY)\bigg|_{t=0} = \Pi_E\left(X^{-1}YX^{-1}\right)$$

Logarithmic barrier for p.s.d. completable cone

Dual of log-det barrier

$$\phi_*(S) = \sup_X \left(-\,\mathbf{tr}(SX) - \phi(X)\right)$$

- optimal $\widehat{X}$ satifies $\Pi_E(\widehat{X}^{-1}) = S$
- $Z = \widehat{X}^{-1}$ solves

$$\begin{array}{ll} \text{maximize} & \log\det Z \\ \text{subject to} & \Pi_E(Z) = S \end{array}$$

$\widehat{X}^{-1}$ is maximum determinant positive definite completion of S

Gradient and Hessian

$$\nabla\phi_*(S) = -\widehat{X}, \qquad \nabla^2\phi_*(S) = \nabla^2\phi(\widehat{X})^{-1}$$

Multifrontal Cholesky factorization

computes factorization $X = LDL^T$ by recursion on elimination tree

- for each vertex i, (temporarily) store a dense **update matrix**

$$U_i = -\sum_{\text{descendants } k \text{ of } i} D_{kk} L_{\eta_i k} L_{\eta_i k}^T$$

(η_i is index set for nonzeros in column i of L below diagonal)

- U_j and column j of factorization (D_{jj}, $L_{\eta_j j}$) computed recursively from

$$\begin{bmatrix} X_{jj} & X_{\eta_j j}^T \\ X_{\eta_j j} & -U_j \end{bmatrix} + P_{\gamma_j} \left(\sum_{i \text{ is child of } j} P_{\eta_i}^T U_i P_{\eta_i} \right) P_{\gamma_j}^T = D_{jj} \begin{bmatrix} 1 \\ L_{\eta_j j} \end{bmatrix} \begin{bmatrix} 1 \\ L_{\eta_j j} \end{bmatrix}^T$$

(Duff and Reid 1983)

Multifrontal algorithm

iterate over etree in topological order (children visited before their parents)

- at vertex j, first form **frontal matrix**

$$\left[\begin{array}{cc} F_{11} & F_{12} \\ F_{21} & F_{22} \end{array}\right] = \left[\begin{array}{cc} X_{jj} & X_{\eta_j j}^T \\ X_{\eta_j j} & 0 \end{array}\right] + P_{\gamma_j} \left(\sum_{\text{children } i \text{ of } j} P_{\eta_i}^T U_i P_{\eta_i} \right) P_{\gamma_j}^T$$

- then execute a **pivoting step**

$$D_{jj} := F_{11}, \qquad L_{\eta_j j} := \frac{1}{D_{jj}} F_{21}, \qquad U_j := F_{22} - D_{jj} L_{\eta_j j} L_{\eta_j j}^T$$

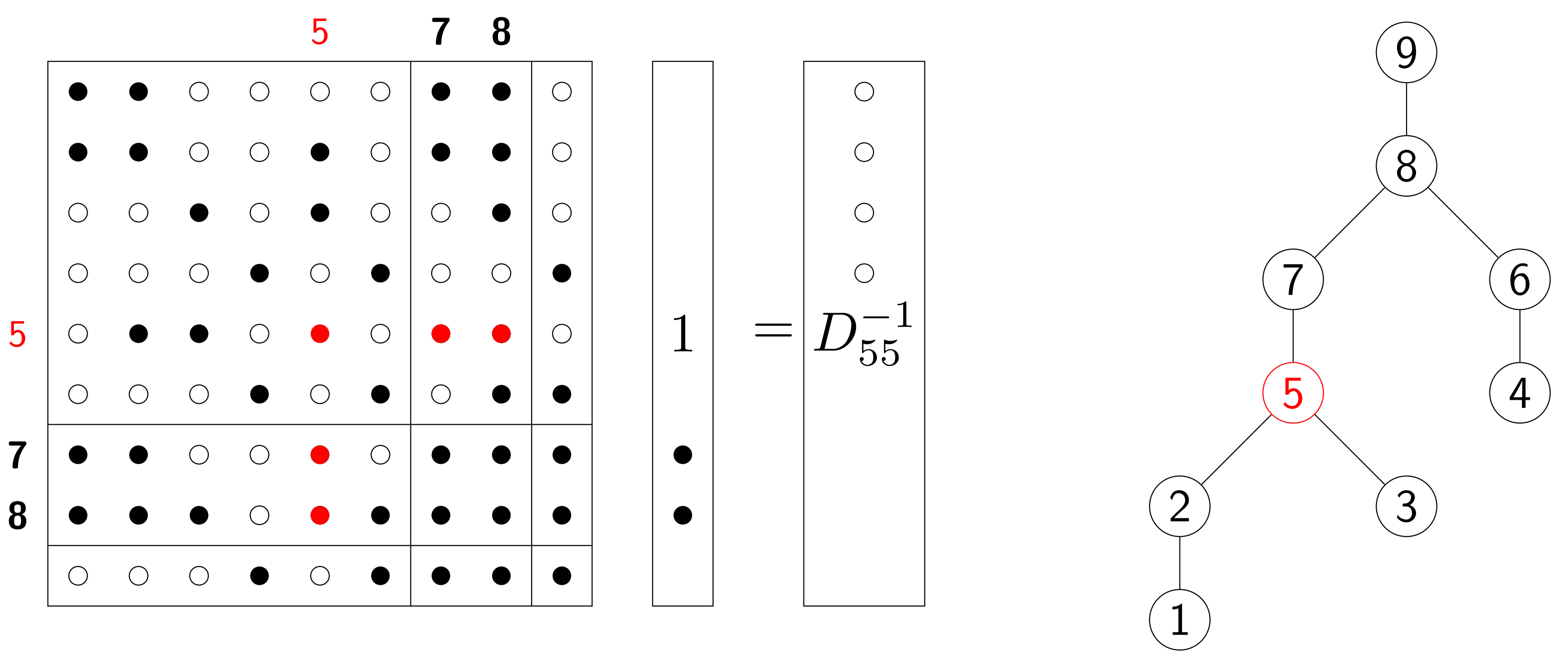
pivoting step is a dense level 2 BLAS operation (matrix-vector operation)

Partial inverse $\Pi_E(X^{-1})$

inverse $S = X^{-1}$ satisfies $SL = L^{-T}D^{-1}$:

$$\left[\begin{array}{cc} S_{jj} & S_{\eta_j j}^T \\ S_{\eta_j j} & S_{\eta_j \eta_j} \end{array}\right] \left[\begin{array}{c} 1 \\ L_{\eta_j j} \end{array}\right] = \left[\begin{array}{c} 1/D_{jj} \\ 0 \end{array}\right], \qquad j = 1, \ldots, n$$

this allows us to compute $S_{\eta_j j}$, S_{jj} from $S_{\eta_j \eta_j}$ (and L, D)



Algorithm for partial inverse

iterate over vertices of elimination tree in reverse topological order

- at vertex j, compute

$$S_{\eta_j j} := -V_j L_{\eta_j j}, \qquad S_{jj} := \frac{1}{D_{jj}} - S_{\eta_j j}^T L_{\eta_j j}$$

  $V_j = S_{\eta_j \eta_j}$ is dense 'update matrix'

- for each child i of j, form

$$V_i := P_{\eta_i} P_{\gamma_j}^T \begin{bmatrix} S_{jj} & S_{\eta_j j}^T \\ S_{\eta_j j} & V_j \end{bmatrix} P_{\gamma_j} P_{\eta_i}^T$$

  (multiplications with $P_{\eta_i} P_{\gamma_j}^T$ extract a principal submatrix)

main operation is dense matrix-vector multiplication $V_j L_{\eta_j j}$

Matrix completion

given $S \in \mathbf{S}^n_E$, solve nonlinear equation

$$\Pi_E(X^{-1}) = S$$

with variable $X \in \mathbf{S}^n_E$

- solution $\widehat{X}$ is inverse of maximum determinant completion of S
- $\widehat{X} = -\nabla \phi_*(S)$ (barrier of p.s.d. completable cone)
- factorization $\widehat{X} = LDL^T$ follows from equation used for partial inverse:

$$\begin{bmatrix} S_{jj} & S_{\eta_j j}^T \\ S_{\eta_j j} & S_{\eta_j \eta_j} \end{bmatrix} \begin{bmatrix} 1 \\ L_{\eta_j j} \end{bmatrix} = \begin{bmatrix} 1/D_{jj} \\ 0 \end{bmatrix}, \qquad j = 1, \ldots, n$$

Algorithm for completion

iterate over vertices of elimination tree in reverse topological order

- at vertex j, compute

$$L_{\eta_j j} := -V_j^{-1} S_{\eta_j j}, \qquad D_{jj} := (S_{jj} - S_{\eta_j j}^T L_{\eta_j j})^{-1}$$

  $V_j = S_{\eta_j \eta_j}$ is dense 'update matrix'

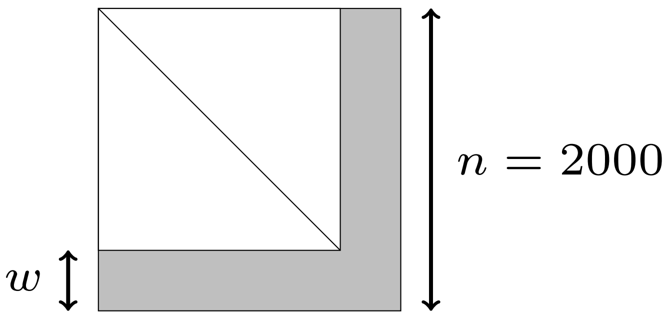
- for each child i of j, form

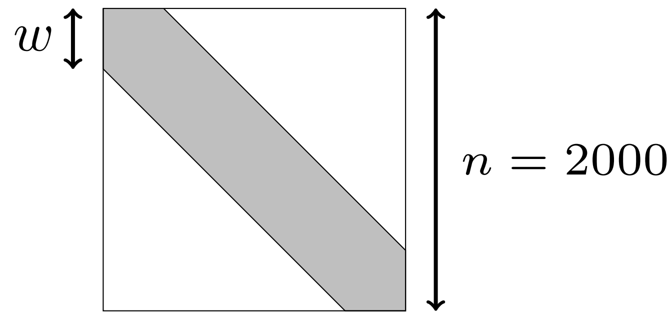
$$V_i := P_{\eta_i}^T P_{\gamma_j}^T \begin{bmatrix} S_{jj} & S_{Jj}^T \\ S_{Jj} & V_j \end{bmatrix} P_{\gamma_j} P_{\eta_i}^T$$

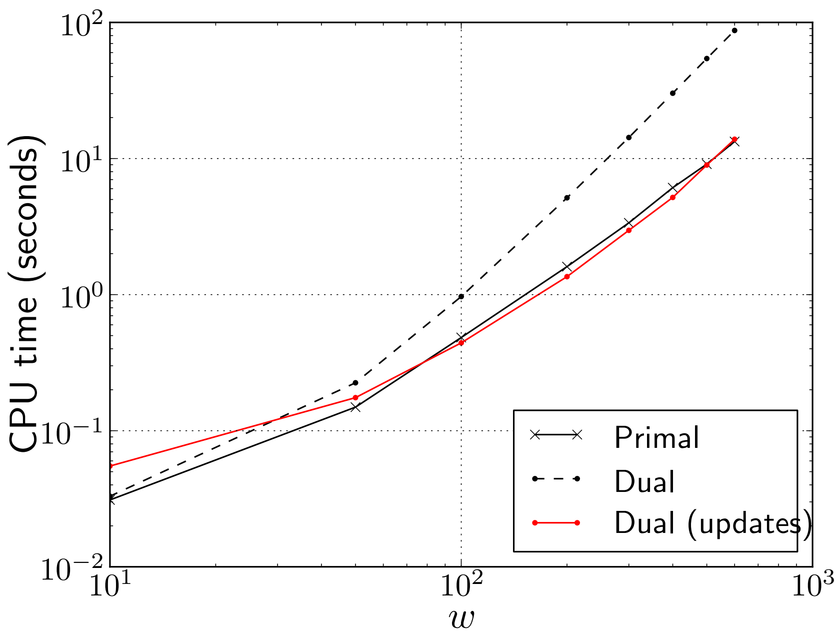
main step is solution of dense system $V_j L_{\eta_j j} = -S_{\eta_j j}$

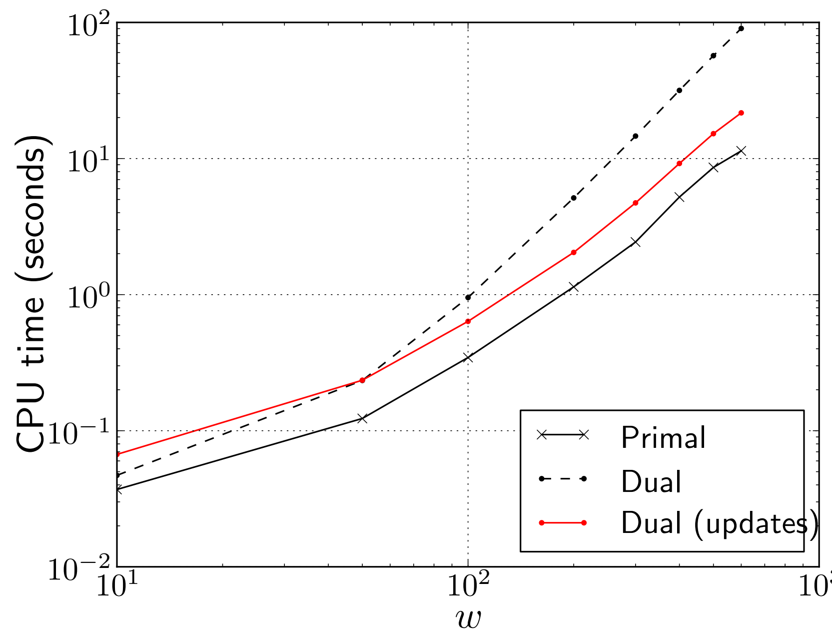
improvement: propagate factorization of V_j, make low-rank updates

Primal/dual gradients for arrow and band patterns







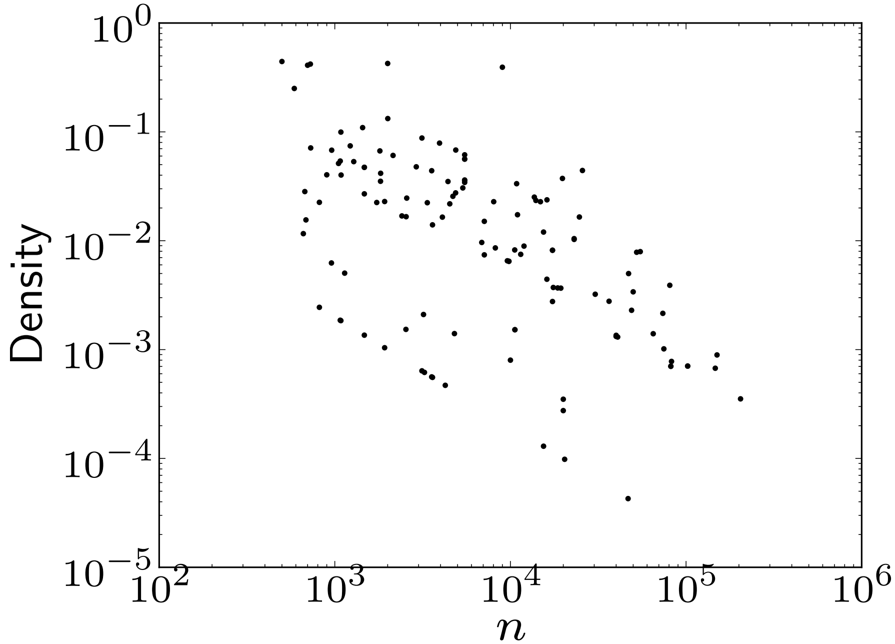


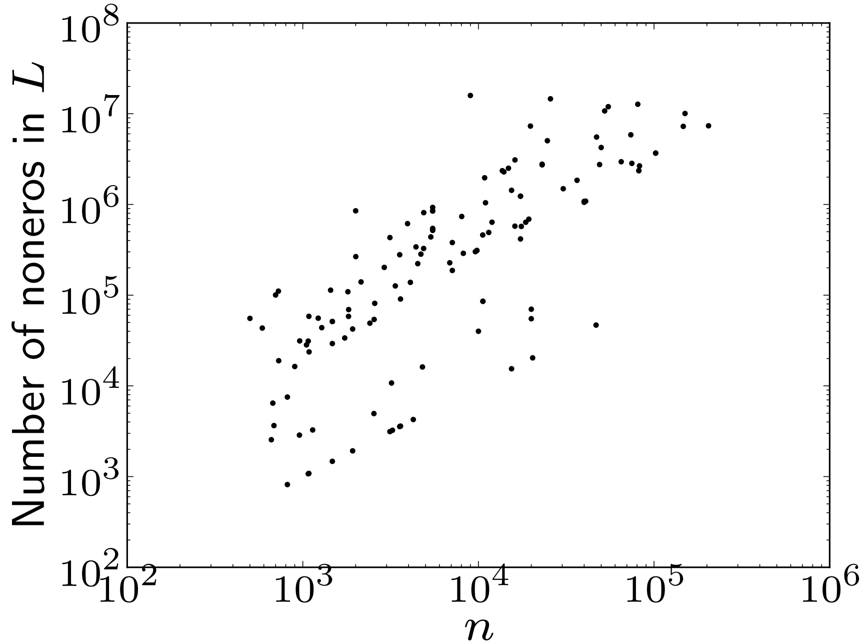
cost is $O(nw^2)$ for primal gradient, dual gradient with low-rank updates

General patterns

128 sparsity patterns from University of Florida sparse matrix collection

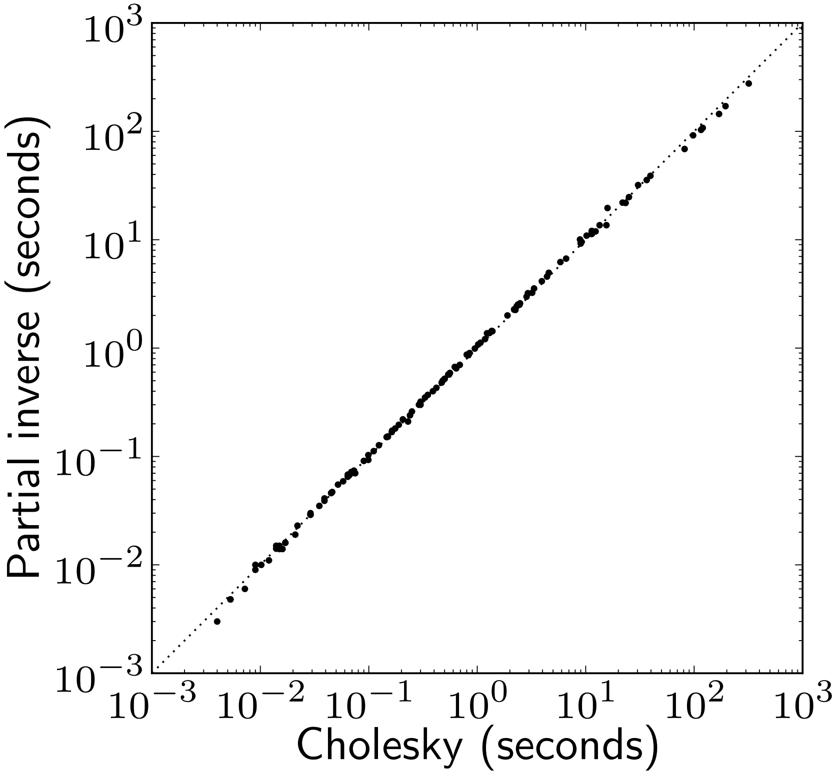
- n ranges between 500 and 204,316
- between 817 and 15,894,180 nonzeros in L



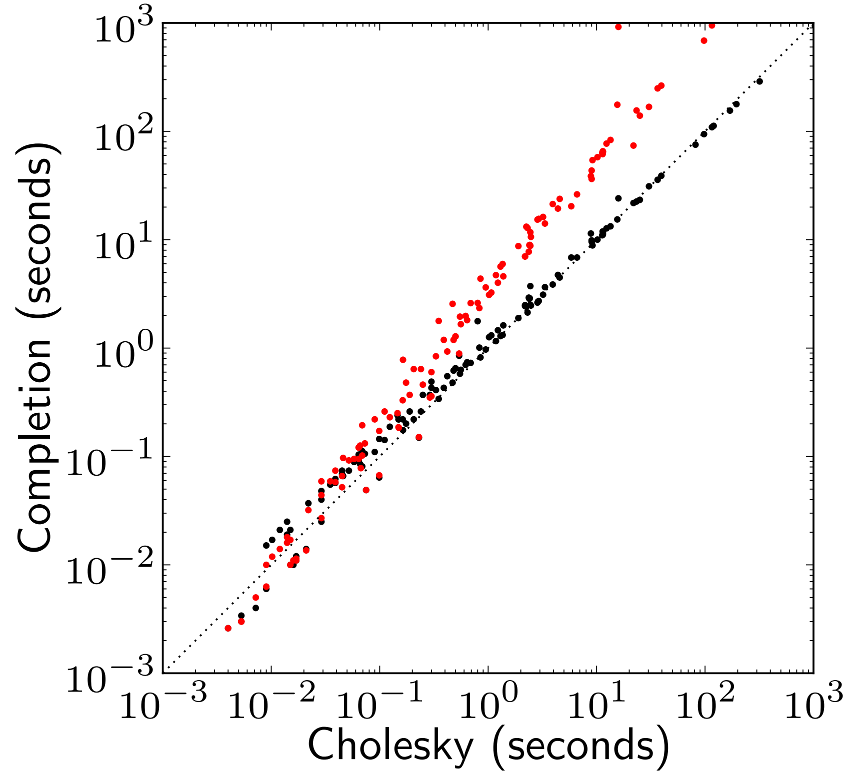


Primal/dual gradient versus Cholesky factorization

primal gradient (partial inverse)



dual gradient (completion)



dual gradient with/without
low-rank updates

Hessian

computing $\nabla\phi(X) = -\Pi_E(X^{-1})$ requires two iterations over etree:

- Cholesky factorization $X = LDL^T$ (iteration in topological order)
- partial inverse from D, L (iteration in reverse topological order)

Hessian evaluation: linearize the two recursions in the gradient algorithm

$$\nabla^2\phi(X)[Y] = \Pi_E(X^{-1}YX^{-1}) = -\frac{d}{dt}\Pi_E(X+tY)^{-1}\bigg|_{t=0}$$

- linearized recursions are adjoints: factorization $\nabla^2\phi(X) = \mathcal{R}_X^{\mathrm{adj}} \circ \mathcal{R}_X$
- factored Hessian useful in interior-point methods to form

$$\mathbf{tr}\left(A_i \nabla^2\phi(X)[A_j]\right) = \mathbf{tr}\left(\mathcal{R}_X(A_i)\mathcal{R}_X(A_j)\right), \quad i,j = 1,\ldots,m$$

Hessian evaluation with sparse arguments

- sparsity patterns from U. Florida sparse matrix collection
- Y dense (w.r.t. E) or sparse (2 randomly chosen nonzero positions)

cost of evaluating $\mathcal{R}_X(Y)$

Sparsity pattern	n	Y dense (seconds)	Y sparse (seconds)	Ratio
HB/plat1919	1919	0.17	0.05	3.7
HB/bcsstk13	2003	1.40	0.36	3.9
HB/lshp3025	3025	0.21	0.05	4.6
Boing/nasa4704	4704	1.05	0.27	4.0
TKK/g3rmt3m3	5357	1.43	0.35	4.1
Schenk_IBMNA/c-36	7479	0.37	0.06	6.1
Wang/swang1	10800	7.05	1.72	4.1
ACUSIM/Pres_Poisson	14822	17.65	4.35	4.1
GHS_psdef/wathen100	30401	6.05	1.38	4.4

Supernodal multifrontal algorithms

- process columns in each supernode $\mathrm{sn}(j)$ as one block column
- iteration over elimination tree replaced by iteration over clique tree or supernodal elimination tree

Advantages

- level 3 BLAS (matrix-matrix) operations replace level 2 BLAS
- fewer frontal matrices to construct

Supernodal factorization and primal gradient

128 sparsity patterns from U. Florida collection