Sparse Gauss Elimination

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Outline

- A square matrix A is symmetric positive definite (SPD) if A is symmetric, $A = A^T$, and for any nonzero vector x, $x^T Ax > 0$.
- Cholesky factorization decomposes a SPD A as $A = L^T L$, where L is lower trianglular with positive diagonal.
- Cholesky decomposition does not need pivoting.

Problem

Gauss elimination on ($\bullet$ means nonzero, blank means 0)

$$\begin{bmatrix} \bullet & \bullet & \bullet & \bullet \\ \bullet & \bullet & & \\ \bullet & & \bullet & \\ \bullet & & & \bullet \end{bmatrix} \quad \text{vs.} \quad \begin{bmatrix} \bullet & & & \bullet \\ & \bullet & & \bullet \\ & & \bullet & \bullet \\ \bullet & \bullet & \bullet & \bullet \end{bmatrix}$$

produces

$$\begin{bmatrix} \bullet & \bullet & \bullet & \bullet \\ 0 & \bullet & {\color{red}\bullet} & {\color{red}\bullet} \\ 0 & {\color{red}\bullet} & \bullet & {\color{red}\bullet} \\ 0 & {\color{red}\bullet} & {\color{red}\bullet} & \bullet \end{bmatrix} \quad \text{vs.} \quad \begin{bmatrix} \bullet & & & \bullet \\ & \bullet & & \bullet \\ & & \bullet & \bullet \\ 0 & 0 & 0 & \bullet \end{bmatrix}$$

fill: number of nonzeros
fill-in: number of nonzeros introduced during factorization
We want to keep the fill-in small.

Problem cont.

Assume A is SPD.

Let P be a permutation matrix and write $Ax = b$ as

$$(PAP^T)(Px) = Pb.$$

1. Find P
2. Factorize $PAP^T = LL^T$
3. Solve $(LL^T)(Px) = Pb$

Find P such that fill-in in L is as small as possible.

Graphs

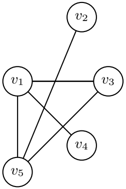
For an $n \times n$ symmetric matrix A, define graph $G = (V, E)$ with

$$V = \{v_1, \ldots, v_n\}, \quad E = \{(v_i, v_j) \mid a_{ij} \neq 0\}.$$

G represents any matrix PAP^T with appropriate relabeling of vertices.

Example 1.

	1	2	3	4	5
1	●		●	●	●
2		●			●
3	●		●		●
4	●			●	
5	●	●	●		●



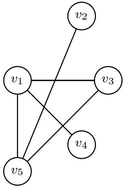
Graphs cont.

Example 1. cont. Consider eliminating with a_{11}.

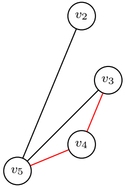
Remove v_1 and its incident edges.

Pairwise connect the vertices adjacent to v_1, i.e. $\{\mathrm{adj}(v_1)\}$

	1	2	3	4	5
1	●		●	●	●
2		●			●
3	●		●		●
4	●			●	
5	●	●	●		●



	1	2	3	4	5
1	●		●	●	●
2		●			●
3	0		●	●	●
4	0		●	●	●
5	0	●	●	●	●



Graph of $A(2:5, 2:5)$

Graphs cont.

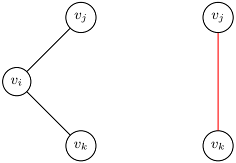
Example 1. cont. Consider eliminating with a_{ii} in

$$
\begin{array}{ccccc}
a_{ii} & \cdots & a_{ij} & \cdots & a_{ik} \\
\vdots & & & & \\
a_{ji} & \cdots & a_{jj} & \cdots & \color{red}{a_{jk}} \\
\vdots & & & & \\
a_{ki} & \cdots & \color{red}{a_{kj}} & &
\end{array}
$$

If $a_{ji} = 0$ (or a_{ki}) nothing to do. Assume $a_{ij} = a_{ji} \neq 0$, $a_{ik} = a_{ki} \neq 0$.

(j, k) and (k, j) entries become structural nonzeros.

If $(v_j, v_k) \notin E$ then becomes an edge in the new graph.



Elimination

Definition 2. Ordering of the vertices of $G = (V, E)$ is
$\alpha : V \to \{1, \dots, n\}$

Denote G with ordering α by $G_\alpha = (V, E, \alpha)$.

Theorem 3. When x_i is eliminated from subsequent equations, the graph of the remaining system is contained in $\bar{G}$, which is obtained from G by

1. *removing v_i*
2. *pair-wise connection of all vertices previously connected to v_i*

Denote G_i the graph obtained by eliminating x_i and denote

$$G_1 = G_{x_1}$$
$$G_i = (G_{i-1})_{x_i}, \quad i = 2, \dots, n-1.$$

Definition 4. Elimination process on $G = (V, E, \alpha)$ is the sequence

$$G = G_0, G_1, G_2, \dots, G_{n-1}.$$

Elimination cont.

For a $V' \subseteq V$, $G(V')$ is the subgraph of G with vertices V' and edges $\in E$ with endpoints in V'.

Definition 5. Elimination process is perfect if

$$G_i = G(V - \cup_{j=1}^{i} \{v_i\}).$$

That is, no new edges, resp. nonzeros are introduced.

Elimination cont.

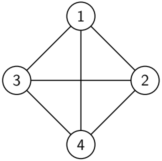
Definition 6. Vertex v is simplificial if the subgraph induced by adj(v) is complete.

Definition 7. An ordering α is perfect elimination ordering, if for all $1 \leq i \leq n$, v_i is simplificial in $G(L_i)$ where

$$L_i = \{v_j \mid \alpha(v_j) > \alpha(v_i)\}$$

Example 8.

Vertex 1 is simplificial as the graph induced by $L_1 = \{2, 3, 4\}$ is complete.

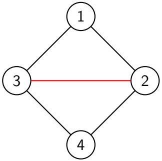


Chordal graphs

Definition 9. Chord is an edge connecting two non-consecutive vertices in a cycle.

Example 10.

Edge $(2, 3)$ is chord.



Definition 11. $G = (V, E)$ is chordal if every cycle of length > 3 has a chord.

Any subgraph of a chordal graph is chordal.

Theorem 12. A graph is chordal iff it has a perfect elimination ordering.

Chordal graphs cont.

Definition 13. Let $G = (V, E)$ be any graph. $G^* = (V, E^*)$, where $E \subseteq E^*$ is a chordal extension of G if G^* is chordal.

The problem is:

Given a sparse SPD A find a chordal extension $G^* = (V, E^*)$ of $G = (V, E)$ obtained form A such that $|E - E^*|$ is minimized.

This is an NP complete problem.

Minimum-degree ordering

Given graph G of a SPD matrix A

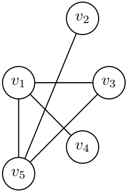
while $|V| > 1$
    select a vertex of minimum degree in and order v next
    eliminate v and connect pairwise the adjacent vertices
    $V = V \setminus \{v\}$

Resolving ties: when several vertices are of the same degree.

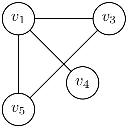
Minimum-degree ordering cont.

Example 14. Select v_2.

	1	2	3	4	5
1	•		•	•	•
2		•			•
3	•		•		•
4	•			•	
5	•	•	•		•



	1	2	3	4	5
1	•		•	•	•
2		•			•
3	•		•		•
4	•			•	
5	•	0	•		•

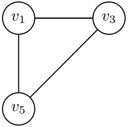


Select v_4

Minimum-degree ordering cont.

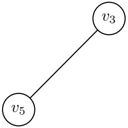
Example 14. cont.

	1	2	3	4	5
1	●		●	0	●
2		●			●
3	●		●		●
4	●			●	
5	●	0	●		●



Select v_1

	1	2	3	4	5
1	●		●	0	●
2		●			●
3	0		●		●
4	●			●	
5	0	0	●		●



Minimum-degree ordering cont.

Example 14. cont.

Select v_3

$$
\begin{array}{c|ccccc}
 & 1 & 2 & 3 & 4 & 5 \\
\hline
1 & \bullet & & \bullet & {\color{red}0} & \bullet \\
2 & & \bullet & & & \bullet \\
3 & {\color{red}0} & & \bullet & & \bullet \\
4 & \bullet & & & \bullet & \\
5 & {\color{red}0} & {\color{red}0} & {\color{red}0} & & \bullet
\end{array}
$$

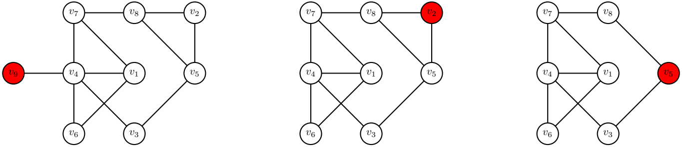
v_5

Eliminate in the order x_2, x_4, x_1, x_3

Minimum-degree ordering cont.

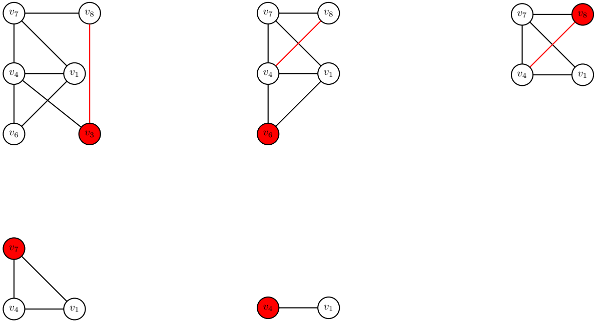
Example 15.

	1	2	3	4	5	6	7	8	9
1	●			●		●	●		
2		●			●			●	
3			●	●	●				
4	●		●	●		●	●		●
5		●	●		●			●	
6	●			●		●			
7	●			●			●	●	
8		●			●		●	●	
9				●					●



Minimum-degree ordering cont.

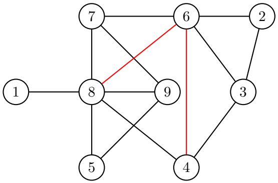
Example 15. cont.



Eliminate in order x_9, x_2, x_5, x_3, x_6, x_8, x_7, x_4

Minimum-degree ordering cont.

$$PAP^T = \begin{array}{cc|ccccccccc}
 & & 1 & 2 & 3 & 4 & 5 & 6 & 7 & 8 & 9 \\
 & & 9 & 2 & 5 & 3 & 6 & 8 & 7 & 4 & 1 \\
\hline
1 & 9 & \bullet & & & & & & & \bullet & \\
2 & 2 & & \bullet & \bullet & & & \bullet & & & \\
3 & 5 & & \bullet & \bullet & \bullet & & \bullet & & & \\
4 & 3 & & & \bullet & \bullet & & {\color{red}\bullet} & & \bullet & \\
5 & 6 & & & & & \bullet & & & \bullet & \bullet \\
6 & 7 & & \bullet & \bullet & {\color{red}\bullet} & & \bullet & \bullet & {\color{red}\bullet} & \\
7 & 8 & & & & & & \bullet & \bullet & \bullet & \bullet \\
8 & 4 & \bullet & & & \bullet & \bullet & {\color{red}\bullet} & \bullet & \bullet & \bullet \\
9 & 1 & & & & & \bullet & & \bullet & \bullet & \bullet
\end{array}$$



Markowitz rule

For general sparse matrices.

Denote

- r_i number of nonzeros in row i
- c_j number of nonzeros in row j

Chose (i, j) to minimize $(r_i - 1)(c_j - 1)$.

$(r_i - 1)(c_j - 1)$ is Markowitz count.

Markowitz rule cont.

Example 16.

	1	2	3	4	5	6
1	•	•	•			•
2			•			•
3	•	•	•	•	•	•
4		•		•		•
5	•		•		•	
6			•			•

Consider $(3,3)$: $r_3 = 6$, $c_i = 5$. Markowitz count is 20: at most 20 nonzeros are introduced.

Consider $(1,1)$: $r_1 = 4$, $c_i = 3$. Markowitz count is 6: at most 6 nonzeros are introduced.

Markowitz rule cont.

Numerical stability

If we chose a pivot only using the Markowitz count we may encounter a very small (compared to the other entries in a column) or a zero pivot.

Consider a pivot as acceptable if

$$|a_{ij}| \geq u \max_k |a_{kj}|, \quad 0 < u \leq 1.$$

If $u = 1$, we have partial pivoting.