



Perfect elimination orderings for symmetric matrices

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Abstract We introduce a new class of structured symmetric matrices by extending the notion of perfect elimination ordering from graphs to weighted graphs or matrices. This offers a common framework capturing common vertex elimination orderings of monotone families of chordal graphs, Robinsonian matrices and ultrametrics. We give a structural characterization for matrices that admit perfect elimination orderings in terms of forbidden substructures generalizing chordless cycles in graphs.

Keywords Chordal graph · Perfect elimination ordering · Unit interval graph · Ultrametric · Shortest path metric · Robinson matrix

1 Introduction

We introduce a new class of structured matrices by ways of *perfect elimination orderings*, an extension to weighted graphs of the classical notion of perfect elimination

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ordering for graphs. This offers a common framework for the study of (adjacency matrices of) chordal graphs (and their metric powers) as well as for ultrametrics and Robinsonian (dis)similarity matrices.

Recall that a graph $G = (V, E)$ is *chordal* when it does not contain a chordless cycle of length at least 4, where a cycle $C = (v_1, \dots, v_p)$ in G is said to be *chordless* if C is an induced subgraph of G , i.e., if none of the pairs $\{v_i, v_j\}$ for $|i - j| \geq 2$ (indices taken modulo p) is an edge of G . Chordal graphs appear as tractable or well-behaved cases in many optimization problems (see, e.g., [15, 16]). This is often due to their equivalent characterization in terms of perfect elimination orderings. A linear order π of V is called a *perfect elimination ordering* of G if, for any vertices $x, y, z \in V$ such that $x <_\pi y <_\pi z$, $\{x, y\}, \{x, z\} \in E$ implies $\{y, z\} \in E$. It is a well known fact that G is chordal if and only if G has a perfect elimination ordering [7, 13].

In this paper we extend this notion of vertex ordering to weighted graphs, aka symmetric matrices. Throughout \mathcal{S}^V is the set of symmetric matrices indexed by the set $V = [n]$. Given a matrix $A = (A_{xy}) \in \mathcal{S}^V$ we say that a linear order π of V is a *perfect elimination ordering of A* if it satisfies the following *three-points condition*

$$A_{yz} \geq \min\{A_{xy}, A_{xz}\} \text{ for all } x, y, z \in V \text{ with } x <_\pi y <_\pi z. \quad (1)$$

Note that the diagonal entries do not play a role in this definition. When $A = A_G$ is the adjacency matrix of a graph G both notions of perfect elimination orderings of A_G and perfect elimination orderings of G coincide.

Given a distance space (V, d) and its associated distance matrix $D \in \mathcal{S}^V$ (with entries $D_{xy} = D_{yx} = d_{xy}$ for $x \neq y$ and $D_{xx} = 0$ for $x, y \in V$), a perfect elimination ordering of the matrix $A = -D$ is a linear order π of V satisfying

$$D_{yz} \leq \max\{D_{xy}, D_{xz}\} \text{ for all } x, y, z \in V \text{ with } x <_\pi y <_\pi z. \quad (2)$$

Recall that (V, d) is an ultrametric if the inequality in (2) holds for *all* elements $x, y, z \in V$. In other words we have the following connection.

Lemma 1 *Let (V, d) be a distance space with distance matrix D . Then (V, d) is an ultrametric if and only if every linear ordering of V is a perfect elimination ordering of the matrix $-D$.*

Another special class of matrices admitting a perfect elimination ordering arises from Robinsonian matrices. A symmetric matrix A is called a *Robinsonian similarity matrix* if there exists a linear order π of V satisfying the following three-points condition:

$$A_{xz} \leq \min\{A_{xy}, A_{yz}\} \text{ for all } x, y, z \in V \text{ with } x <_\pi y <_\pi z; \quad (3)$$

such an ordering is then called a *Robinson ordering* of A . In the context of distances, a matrix D is called a *Robinsonian dissimilarity matrix* when $A = -D$ is a Robinsonian similarity matrix. Robinsonian matrices have a long history and play an important role in classification problems in data science, in particular in ranking problems [12] and in the seriation problem (introduced by the archeologist Robinson [24] for chronological

dating) (see, e.g., [20]). There the goal is to order (seriate) a set of objects, given through their pairwise (dis)similarities, in such a way that two objects are ranked close to each other if they have a large correlation/similarity (or a small dissimilarity).

It is a classical observation by Roberts [22] that the adjacency matrix of a graph G is Robinsonian if and only if G is a unit interval graph, i.e., its vertices can be labeled by unit intervals on a line so that adjacent vertices receive intersecting intervals. Clearly, the condition (3) implies (1) and thus any Robinson ordering of A is a perfect elimination ordering of A . For adjacency matrices of graphs, this corresponds to the fact that unit interval graphs are chordal graphs. So Robinsonian matrices are weighted graph analogues of unit interval graphs and this fact formed the motivation for the present work to investigate weighted analogues of chordal graphs.

There is a well known structural characterization of unit interval graphs in terms of minimal forbidden substructures (namely, claws and asteroidal triples; see [14,22]). An analogous structural characterization was given in [19] for Robinsonian matrices (by extending the notion of asteroidal triple to weighted graphs). For chordal graphs the minimal forbidden substructures are the chordless cycles. This raises the natural question of understanding the minimal forbidden substructures for the class of matrices admitting a perfect elimination ordering. A main contribution of this note is to provide such a structural characterization, in terms of weighted chordless walks, a new key notion which we will introduce below (see Theorem 1).

The paper is organized as follows. Sections 2.1 and 2.2 contain definitions and preliminary results about vertex elimination orderings and simplicial vertices. In Sect. 2.3 we present our main structural result (Theorem 1) for matrices admitting a perfect elimination ordering. In Sect. 2.4 we discuss related notions: common perfect elimination orderings of powers of chordal graphs, distance-preserving elimination orderings of shortest path distance matrices, and conclude with a brief discussion of other graph properties that could be extended to matrices and of related recognition algorithms. The last Sect. 3 is devoted to the proof of our main structural result in Theorem 1.

2 Perfect elimination orderings of matrices

2.1 Perfect elimination orderings and simplicial elements

Given a graph $G = (V, E)$, recall that $v \in V$ is a *simplicial vertex* of G if its neighbors form a clique of G . Then an order π of V is a perfect elimination ordering of G if and only if each vertex v is simplicial in $G[\{x \in V : v \leq_{\pi} x\}]$, the subgraph of G induced by the nodes coming after v in π . In the same way, given a matrix $A \in S^V$, an element $v \in V$ is said to be *simplicial in A* if

$$A_{yz} \geq \min\{A_{vy}, A_{vz}\} \text{ for all distinct } y, z \in V \setminus \{v\}. \tag{4}$$

Then an order π of V is a perfect elimination ordering of A precisely when each $v \in V$ is simplicial in $A[\{x \in V : v \leq_{\pi} x\}]$, the principal submatrix of A indexed by the elements coming after v in π . We next observe that simplicial elements are precisely those coming first in some perfect elimination ordering.

Lemma 2 Assume $A \in S^V$ has a perfect elimination ordering and let $v \in V$. Then, v is simplicial for A if and only if there exists a perfect elimination ordering of A with v as first element.

Proof The ‘if’ part is clear. We show the ‘only if part’ by induction on the size n of A . The case $n = 3$ is clear. Assume now that $n \geq 4$ and a is simplicial for A and consider a perfect elimination ordering π of A starting at $b \neq a$. Then we know that b is simplicial in A . Consider the submatrix A' induced by $V \setminus \{b\}$. Then A' still has a perfect elimination ordering and a is still simplicial in A' . Hence, by the induction assumption, there exists a perfect elimination ordering π' of A' starting at a , say $\pi' = (a, u, \dots, w)$. We consider the ordering $\tilde{\pi} = (a, b, u, \dots, w)$ obtained by inserting b between a and u . We claim that $\tilde{\pi}$ is a perfect elimination ordering of A , that is, $A_{yz} \geq \min\{A_{xy}, A_{xz}\}$ for all $x <_{\tilde{\pi}} y <_{\tilde{\pi}} z$. This is true if $b \notin \{x, y, z\}$ since π' is a perfect elimination ordering. Assume now that $b \in \{x, y, z\}$. Then $b \neq z$ (as b is second in $\tilde{\pi}$). If $b = x$ then the desired inequality follows from the fact that b is simplicial in A . Finally, if $b = y$ then $x = a$ and the desired inequality follows from the fact that a is simplicial in A . \square

2.2 Common perfect elimination orderings

Let $\alpha_0 < \alpha_1 < \alpha_2 < \dots < \alpha_L$ denote the distinct values taken by the entries of a matrix $A \in S^V$ and, for $\ell = 0, 1, \dots, L$, define its *level graph* $G_\ell = (V, E_\ell)$, whose edges are the pairs $\{x, y\}$ with $A_{xy} \geq \alpha_\ell$. Thus, (V, E_0) is the complete graph on V (i.e., A_{G_0} is the all-ones matrix) and $E_L \subseteq \dots \subseteq E_1$. It is easy to check that (up to shifting all entries of A by α_0 and assuming all its diagonal entries are zero) A can be decomposed as a conic combination of the adjacency matrices of its level graphs:

$$A - \alpha_0 A_{G_0} = \sum_{\ell=1}^L (\alpha_\ell - \alpha_{\ell-1}) A_{G_\ell}. \tag{5}$$

As a direct application we have the following characterization.

Lemma 3 A matrix $A \in S^V$ has a perfect elimination ordering if and only if there exists an ordering π of V which is a common perfect elimination ordering of all the level graphs of A .

In other words, a necessary condition for A to have a perfect elimination ordering is that all its level graphs be chordal, however for finding a perfect elimination ordering of A one needs to find an ordering which is a perfect elimination ordering *simultaneously* for all its level graphs.

Clearly we may assume without loss of generality that $\alpha_0 = 0$. Moreover, the exact values of $\alpha_0, \dots, \alpha_L$ are not important (as long as they are strictly increasing). For instance, A has a perfect elimination ordering if and only if the matrix $\tilde{A} = \sum_{\ell=1}^L A_{G_\ell}$ does too. Hence the question whether a matrix has a perfect elimination ordering is equivalent to asking whether a finite *monotone* family of graphs $G_1 \supseteq G_2 \supseteq \dots \supseteq G_L$ admits a common perfect elimination ordering. We will come back to this in Sect. 2.4.1.

Finally observe that any *arbitrary* order of V is a perfect elimination ordering of A precisely when all its level graphs are disjoint unions of cliques. Such (similarity) matrices A correspond thus to distance matrices D of ultrametrics, via the correspondence $A = -D$.

2.3 Structural characterization of matrices with perfect elimination orderings

We now describe the structural obstructions for the symmetric matrices admitting a perfect elimination ordering. First we introduce some notation.

A *walk* is an ordered sequence $W = (v_0, v_1, \dots, v_p)$ of elements of V . Then we set $V(W) = \{v_0, v_1, \dots, v_p\}$, $I(W) = \{v_i : 1 \leq i \leq p - 1\}$ is the set of *internal* elements of W , v_0 and v_p are its *endpoints*. The walk W is said to be *closed* if $v_0 = v_p$ and the walk W is said to be *self-contained* if $I(W) = V(W)$. A closed walk is called a *cycle* if v_0, v_1, \dots, v_{p-1} are all distinct.

The following notions will play a key role in our structural characterization. For a matrix $A \in S^V$, a walk $W = (v_0, v_1, \dots, v_p)$ is said to be *weighted chordless* in A if

$$A_{v_{i-1}v_{i+1}} < \min\{A_{v_{i-1}v_i}, A_{v_{i+1}v_i}\} \text{ for all } 1 \leq i \leq p - 1. \tag{6}$$

In addition, W is said to be a *weighted chordless cycle* in A if W is a cycle which, in addition to (6), also satisfies the inequality

$$A_{v_{p-1}v_1} < \min\{A_{v_{p-1}v_0}, A_{v_0v_1}\}. \tag{7}$$

Hence a walk (y, x, z) is weighted chordless precisely when the triple (x, y, z) violates the inequality in (1) and thus its internal element x cannot come before both y, z in any perfect elimination ordering of A .

It is useful to compare with the notion of chordless cycle in graphs. Let $A = A_G$ be the adjacency matrix of a graph $G = (V, E)$. Then, a walk $W = (v_1, \dots, v_p)$ is *weighted chordless* in A_G precisely when all the 2-chords $\{v_i, v_{i+2}\}$ ($1 \leq i \leq p - 2$) are not edges of G . Therefore, either W is an induced walk in G (i.e., none of the chords $\{v_i, v_j\}$ ($1 \leq i, i + 2 \leq j \leq p$) is an edge of G), or W contains a chordless cycle of G (meaning $V(W)$ contains a subset inducing a chordless cycle in G). In particular, if W is a weighted chordless cycle in A_G then W is equal to or contains a chordless cycle of G .

By definition, chordal graphs are exactly the graphs that have no chordless cycle of length at least 4. It is natural to ask whether a similar structural characterization holds for matrices. We start with some easy observations.

Lemma 4 *Consider a matrix $A \in S^V$. If (i) A has a perfect elimination ordering then (ii) A has no weighted chordless cycle, which in turn implies that (iii) every level graph of A is a chordal graph.*

Proof (i) \implies (ii): Assume π is a perfect elimination ordering of A , W is a weighted chordless cycle in A and v_i is the element of W coming first in π . As (v_{i-1}, v_i, v_{i+1}) is a weighted chordless walk we get a contradiction.

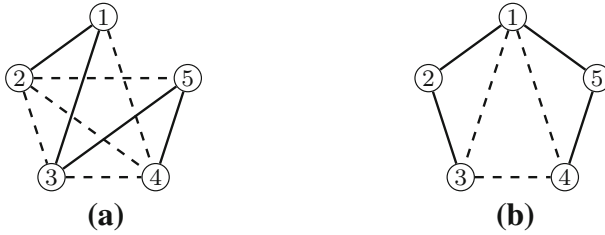


Fig. 1 Visualization of two $\{0, 1, 2\}$ -symmetric matrices of size 5 as weighted graphs, where bold edges have weight 2, dashed edges have weight 1 and non-edges have weight 0: First, an example of a matrix which has no weighted chordless cycle (because $(2, 1, 3)$, $(1, 2, 5)$, $(1, 3, 5)$, $(1, 4, 5)$, $(3, 5, 4)$ are all the chordless 2-walks and they cannot be concatenated to build a weighted chordless cycle) and also no simplicial vertex (and thus no perfect elimination ordering) (a); second, an example where all level graphs are chordal, but $(1, 2, 3, 4, 5)$ is a weighted chordless cycle (b)

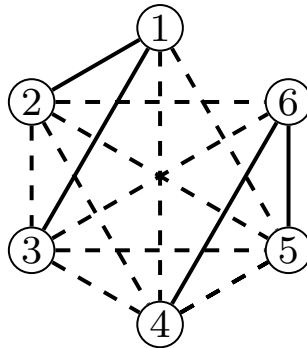


Fig. 2 Visualization of a $\{0, 1, 2\}$ -symmetric matrix of size 6 as a weighted graph, where bold edges have weight 2, dashed edges have weight 1 and non-edges have weight 0. This matrix has no simplicial vertex and no self-contained weighted chordless walk (because $(2, 1, 3)$, $(1, 2, 6)$, $(1, 3, 6)$, $(1, 4, 6)$, $(1, 5, 6)$, $(4, 6, 5)$ are all the chordless 2-walks but they cannot be concatenated to a build a self-contained weighted chordless walk)

(ii) \implies (iii): Assume $C = (v_1, \dots, v_p)$ is a chordless cycle in some level graph $G^{(l)}$ of A , i.e., $A_{v_i v_{i+1}} \geq \alpha_l$ for $i = 1, \dots, p$, while $A_{v_i v_j} < \alpha_l$ whenever $|i - j| \geq 2$. Then C is a weighted chordless cycle in A , contradicting (ii). \square

The reverse implications are not true in general. See Figure 1 for examples.

Although the matrix in Figure 1(a) has no weighted chordless cycle, it yet contains a forbidden structure for perfect elimination orderings, namely $(1, 4, 5, 3, 1, 2, 5)$ is a self-contained weighted chordless walk in the matrix. Recall that a walk W is *self-contained* if $V(W) = I(W)$. More generally, a family $\{W_1, \dots, W_k\}$ of walks is *self-contained* if $\cup_{h=1}^k V(W_h) = \cup_{h=1}^k I(W_h)$. Figure 2 gives an example having no simplicial vertex and also no self-contained weighted chordless walk, so forbidding a single self-contained chordless walk is not sufficient to guarantee a perfect elimination ordering; we need to forbid families of them.

Lemma 5 *If $A \in S^V$ has a self-contained family of weighted chordless walks, then A does not have a perfect elimination ordering.*

Proof Same proof as for the implication (i) \implies (ii) in Lemma 4. □

Lemma 6 *Assume $A \in \mathcal{S}^V$ does not contain any self-contained family of weighted chordless walks. Then A has a simplicial vertex.*

Proof Suppose for contradiction that A does not have a simplicial vertex. That is, for any $x \in V$ there exist $y \neq z \in V \setminus \{x\}$ such that $A_{yz} < \min\{A_{xy}, A_{xz}\}$, i.e., $P_x := (y, x, z)$ is a weighted chordless walk. Then we have a self-contained family $\{P_x : x \in V\}$ of weighted chordless walks in A . □

Corollary 1 *A matrix $A \in \mathcal{S}^V$ has a perfect elimination ordering if and only if there does not exist a self-contained family of weighted chordless walks in A .*

Proof The ‘only if’ part is shown in Lemma 5. We now show the ‘if part’, using induction on the size n of A . The base case $n \leq 3$ is trivial. So let us assume that A has size $n \geq 4$. In view of Lemma 6, A has a simplicial vertex v_1 . Consider now the principal submatrix A_1 of A indexed by $V \setminus \{v_1\}$. By the induction assumption, A_1 has a perfect elimination ordering π_1 . Then, appending v_1 as first element before π_1 , we get the ordering $\pi = (v_1, \pi_1)$ of V , which is a perfect elimination ordering of A . This concludes the proof. □

The argument used in the proof of Lemma 6 is the matrix analogue of the well known fact that a graph has no simplicial vertex if and only if each vertex is the midpoint of an induced P_3 (a path with three vertices). Dirac’s theorem informally says that some of these induced P_3 ’s can be assembled to form a chordless cycle. As a matrix analogue, we will show that it suffices to exclude self-contained *pairs of two* weighted chordless walks. This is our main structural characterization result, which we will prove in Sect. 3 below, since the technical details are more involved.

Theorem 1 *A symmetric matrix A has a perfect elimination ordering if and only if A has no self-contained pair of weighted chordless walks.*

Note that the matrix from Figure 2 has a self-contained pair of two weighted chordless walks, namely $W_1 = (6, 2, 1, 3, 6)$ and $W_2 = (1, 4, 6, 5, 1)$ (note that $6 \in I(W_2)$ and $1 \in I(W_1)$).

2.4 Applications and related concepts

2.4.1 Common perfect elimination orderings of powers of chordal graphs

Given a graph $G = (V, E)$ let d_G be its shortest path metric, with associated distance matrix D_G . For a positive integer k , the k -th power G^k is the graph on V , whose edges are the pairs $\{u, v\}$ with distance $d_G(u, v) \leq k$. So we have a monotone graph family: $G^1 \subseteq \dots \subseteq G^k$. Duchet [9] shows that if G^k is chordal then so is G^{k+2} . Hence if G and G^2 are chordal then all powers of G are chordal. Dragan et al. [8] prove that if G and G^2 are chordal then they admit a common common perfect elimination ordering (see also [2, Thm 5]), and Brandstädt et al. [1] prove that, for any integers $i_1, \dots, i_k, G^{i_1}, \dots, G^{i_k}$ admit a common elimination ordering if they are all chordal. Consequently, the following holds.

Theorem 2 (Brandstädt, Chepoi and Dragan [1]) *If G and G^2 are chordal, then all the powers of G admit a common perfect elimination ordering.*

This theorem has an interesting implication in our context: the reverse direction of Lemma 4 is true for the shortest path distance matrix D_G of a graph.

Corollary 2 *Let G be an undirected graph and let D_G be its shortest path distance matrix. Then the following assertions are equivalent.*

- (i) $-D_G$ has a perfect elimination ordering;
- (ii) $-D_G$ has no weighted chordless cycle;
- (iii) Every level graph of $-D_G$ is chordal;
- (iv) G and G^2 are chordal.

Proof This follows from Lemma 4 and Theorem 2 after observing the correspondence between the adjacency matrices of the powers of G and the level graphs of $-D_G$. \square

This result does not extend to shortest path distance matrices of weighted graphs. For this consider the matrix A from Figure 2 and define the matrix $D = (3 - A_{xy})_{x,y \in [6]}$. Then D is a shortest path distance matrix (for the weights D_{xy}), but $-D$ has no perfect elimination ordering and no weighted chordless cycle.

2.4.2 Distance-preserving elimination orderings

Here we point out a link between perfect elimination orderings and the following notion of distance-preserving ordering considered by Chepoi [5]. For a graph $G = (V, E)$, a linear ordering v_1, \dots, v_n of V is called a *distance-preserving elimination ordering* if for each $i \in [n]$ the subgraph G_i of G induced by $\{v_i, \dots, v_n\}$ is *isometric*, i.e., d_{G_i} coincides with the restriction of d_G to $\{v_i, \dots, v_n\}$. This notion can be naturally generalized to weighted graphs: Given nonnegative edge weights $w \in \mathfrak{N}^E$ the shortest path metric of (G, w) is denoted by $d_{(G,w)}$, and a linear ordering v_1, \dots, v_n of V is a *distance-preserving elimination ordering* of (G, w) if for each $i \in [n]$ the weighted subgraph (G_i, w) is *isometric*, i.e., $d_{(G_i,w)}$ coincides with the restriction of $d_{(G,w)}$ to $\{v_i, \dots, v_n\}$.

We may identify the weighted graph (G, w) with the symmetric matrix $W \in \mathcal{S}^V$ given by $W_{xy} = w_{xy}$ for $\{x, y\} \in E(G)$ and $W_{xy} = M$ for $\{x, y\} \notin E$ for some sufficiently large positive number M .

Proposition 1 *Let (G, w) be a graph with nonnegative edge weights w and corresponding weight matrix $W \in \mathcal{S}^V$. Any perfect elimination ordering of $-W$ is a distance-preserving elimination ordering of (G, w) .*

Proof Let $\pi = (v_1, \dots, v_n)$ be a perfect elimination ordering of $-W$ and assume π is not distance-preserving for (G, w) . Let i be the smallest integer such that $d_{(G_{i+1},w)}$ is not equal to the restriction of $d_{(G,w)}$ to $\{v_{i+1}, \dots, v_n\}$. Then there exist v_j, v_k with $i < j < k$ such that $d_{(G_{i+1},w)}(v_j, v_k) > d_{(G,w)}(v_j, v_k)$ and thus every shortest path P between v_j and v_k in (G_i, w) passes through v_i . Let P be such a path, say $P = (v_j, \dots, v_r, v_i, v_s, \dots, v_k)$. As π is a perfect elimination ordering of $-W$ we have $W_{v_r v_s} \leq \max\{W_{v_i v_r}, W_{v_i v_s}\}$ and thus

$$d_{(G_i,w)}(v_r, v_s) \leq W_{v_r v_s} \leq \max\{W_{v_i v_r}, W_{v_i v_s}\} \leq W_{v_i v_r} + W_{v_i v_s} = d_{(G_i,w)}(v_r, v_s).$$

Hence equality holds throughout and thus the path $P \setminus \{v_i\}$ is again a shortest path from v_j to v_k in (G_i, w) but now not traversing v_i , a contradiction. \square

The reverse direction is not true in general, even for $\{0, 1\}$ matrices.

2.4.3 Outlook about other structured matrices and recognition algorithms

We conclude with some observations about possible further extensions of graph properties to symmetric matrices and about recognition algorithms.

We present in this paper a matrix analogue of chordal graphs, motivated by the fact that Robinsonian matrices give a matrix analogue of unit interval graphs. The key point in both cases is that chordal and unit interval graphs can be defined by a three-points condition on their adjacency matrix. We now mention two more graph classes that would also fit within this pattern: interval and cocomparability graphs.

Recall that a graph $G = (V, E)$ is an *interval graph* if and only if there is a linear ordering π of V such that $\{x, z\} \in E$ implies $\{y, z\} \in E$ for all $x <_\pi y <_\pi z$ [21]. Hence one may define an *interval matrix* A to be a matrix $A \in \mathcal{S}^V$ whose index set V admits a linear ordering π such that

$$A_{xz} \leq A_{yz} \quad \text{for all } x <_\pi y <_\pi z. \tag{8}$$

Similarly G is a *cocomparability graph* if and only if there is a linear ordering π of V such that $\{x, z\} \in E$ implies $\{x, y\} \in E$ or $\{y, z\} \in E$ for all $x <_\pi y <_\pi z$ [17]. Hence one may define a *cocomparability matrix* A to be a matrix $A \in \mathcal{S}^V$ whose index set V admits a linear ordering π such that

$$A_{xz} \leq \max\{A_{xy}, A_{yz}\} \quad \text{for all } x <_\pi y <_\pi z. \tag{9}$$

Clearly relation (3) implies (8), which in turn implies both (1) and (9). In other words, this extends to matrices the well known fact that unit interval graphs are interval graphs, which in turn are chordal and cocomparability graphs.

As shown in [19] the structural characterization of unit interval graphs in terms of minimal forbidden structures extends naturally to the matrix setting and in this paper (Theorem 1) we provide such an extension for chordal graphs. Establishing such extensions for interval and cocomparability matrices, or a more general theory for generalizing structural characterizations from graphs to matrices, is an interesting open problem which we leave for further research.

On the algorithmic side, one has the question of finding a perfect elimination ordering of an $n \times n$ symmetric A (if some exists). Clearly, one can find a simplicial element in A in $O(n^3)$ operations and thus one can find a perfect elimination ordering of A in $O(n^4)$ operations (or decide that none exists). This raises the question of finding a more efficient algorithm.

There are two well-known linear time algorithms for recognizing chordal graphs (and finding perfect elimination orderings): *lexicographic breadth-first search* (Lex-BFS) [23] and *maximum cardinality search* (MCS) [26]. A natural question is whether these algorithmic techniques can be extended to matrices.

Corneil [6] gives an algorithm for recognizing unit interval graphs based on three sweeps of Lex-BFS. In [18] a weighted generalization of Lex-BFS, called *Similarity First Search (SFS)*, is introduced, which applies to symmetric matrices. It is shown in [18] that n sweeps of SFS can recognize Robinsonian matrices of size n by returning a Robinson ordering. It is natural to ask whether SFS can also be used to find perfect elimination orderings.

In [3] it is shown that Lex-BFS can find a common perfect elimination ordering of the powers of a chordal graph G (assuming G^2 is chordal). Hence, in view of Corollary 2, if D is a shortest path distance matrix, then a single sweep of SFS finds a perfect elimination ordering of $-D$. However it is not difficult to construct a symmetric matrix for which a single sweep of SFS does not suffice to find a perfect elimination ordering. This thus raises the question whether one can find perfect elimination orderings of matrices using multiple sweeps of SFS.

A generalization of MCS is proposed in the proof of Theorem 2 in [1], which can be adapted to the matrix setting. But it is not difficult to find a symmetric matrix for which this generalized MCS cannot find a perfect elimination ordering in just one sweep. Again one may ask whether a multi-sweep type variant of MCS can find a perfect elimination ordering.

In this context note that it is shown recently in [10] that n sweeps of Lex-BFS permit to find elimination orderings certifying cocomparability graphs.

Finally, one may also ask to find *all* perfect elimination orderings of a symmetric matrix. In the graph case an efficient algorithm is given in [4] (see also [25]). It is an interesting question whether these methods extend to the general matrix setting.

3 Proof of Theorem 1

In this section we prove Theorem 1. By Lemma 5, if a matrix A contains a self-contained pair of weighted chordless walks then it has no perfect elimination ordering, hence it remains to show the converse implication. A first easy observation is that it in fact suffices to show the existence of a simplicial vertex. Indeed, Theorem 1 follows easily from the next result (using induction on the size of the matrix).

Theorem 3 *If a matrix A has no self-contained pair of weighted chordless walks then A has a simplicial vertex.*

We will in fact prove a stronger result (Theorem 4 below). Before stating this stronger result we introduce some notation and preliminary facts. Throughout we let A be a symmetric matrix indexed by a finite set V .

Definition 1 Set $\min A = \min\{A_{xy} : x \neq y \in V\}$. Given $X, Y \subseteq V$ we say that (X, Y) is a *separation* of A if $X \setminus Y, Y \setminus X \neq \emptyset$ and $A_{xy} = \min A$ for all $x \in X \setminus Y$ and $y \in Y \setminus X$.

Lemma 7 *Let (X, Y) be a separation of A . If $x \in X \setminus Y$ is a simplicial vertex of $A[X]$ then x is a simplicial vertex of A , where $A[X]$ denotes the principal submatrix of A indexed by X .*

Proof Let $u, v \in V$, we show that $A_{uv} \geq \min\{A_{ux}, A_{vx}\}$. This is true when (say) $u \in Y \setminus X$ since then $A_{xu} = \min A$, and also when $u, v \in X$ because x is simplicial in $A[X]$. □

Lemma 8 *There exists a separation (X, Y) of A for which the following property holds for each $Z \in \{X, Y\}$:*

*For all $u \in Z \setminus (X \cap Y)$ and $s \in X \cap Y$, either $A_{su} > \min A$ holds, (P)
or there exists a weighted chordless walk from u to s in $A[Z]$
which is internally vertex-disjoint from $X \cap Y$.*

In addition, given $a, b \in V$ with $A_{ab} = \min A$, there exists a separation (X, Y) of A separating a, b (i.e., $a \in X \setminus Y, b \in Y \setminus X$ or vice versa) and (P) holds for $u \in \{a, b\}$.

Proof Let $G = (V, E)$ be the graph on V whose edges are the pairs $\{x, y\}$ with $A_{xy} > \min A$. If G is not connected and C_1, \dots, C_t ($t \geq 2$) denote its connected components then we may set $X = C_1$ and $Y = V \setminus C_1$.

Assume now that G is connected. Let S be a minimal vertex separator of G and let C_1, \dots, C_t be the connected components of $G[V \setminus S]$. Fix $s \in S$. As $S \setminus \{s\}$ is not a vertex separator of G it follows that s is adjacent to at least one vertex in each component C_i . Hence for any $x \in C_i$ there is a path from x to s in $G[C_i \cup \{s\}]$ and if we choose this path shortest possible then either it consists of a single edge or it provides a weighted chordless walk from x to s in A which is contained in $C_i \cup \{s\}$ and thus internally vertex-disjoint from S . Thus the lemma holds if we set, e.g., $X = C_1$ and $Y = V \setminus C_1$.

Finally if we are given a pair a, b with $A_{ab} = \min A$ then choosing S to be a minimal (a, b) -vertex separator in G and C_1 the component containing a gives the final statement. □

Definition 2 A walk W is said to be a *critical walk* of A if W is a closed weighted chordless walk whose end point v_0 is simplicial in A and there exists an internal element $u \in I(W)$ such that $A_{v_0u} = \min A$.

A walk W is said to be *rooted in a set* $S \subset V$ if the end points of W belong to S and the internal elements of W belong to $V \setminus S$ with $I(W) \neq \emptyset$.

We can now formulate the following stronger result.

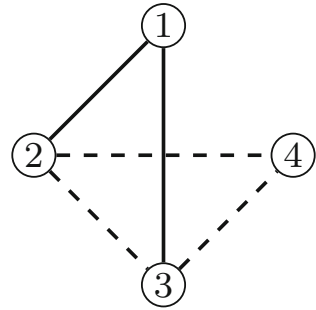
Theorem 4 *If a matrix A has no self-contained pair of weighted chordless walks then it satisfies at least one of the following two properties (A) or (B):*

A has a critical walk, (A)

A has two distinct simplicial vertices u, v such that $A_{uv} = \min A$. (B)

Property (B) is a matrix analogue of a known fact that the diameter of a chordal graph is attained by a pair of simplicial vertices (see, e.g., [11]). This property is no longer true for symmetric matrices, see Figure 3. A weaker well known fact by Dirac [7] is that a chordal graph has at least two simplicial vertices that are not adjacent

Fig. 3 A visualization of a $\{0, 1, 2\}$ -matrix of size four as a weighted graph, where each bold edge has weight two and each dashed edge has weight one. Observe that 4 is the unique simplicial vertex in A



if it is not a complete graph. The example in Figure 3 shows that even this weaker fact fails for general matrices.

Clearly both properties (A) and (B) imply the existence of a simplicial vertex, hence Theorem 4 does indeed imply Theorem 3 (and thus in turn Theorem 1). The following lemma will provide the main technical ingredient for the proof of Theorem 4.

Lemma 9 *Let (X, Y) be a separation of A satisfying the property (P) from Lemma 8. Assume that every proper (i.e., distinct from A) principal submatrix of A satisfies (A) or (B). Then each $Z \in \{X, Y\}$ satisfies at least one of the following two properties (P1), (P2):*

$$A[Z] \text{ has a simplicial vertex belonging to } Z \setminus (X \cap Y), \tag{P1}$$

$$\text{there is a weighted chordless walk in } A[Z] \text{ which is rooted in } X \cap Y. \tag{P2}$$

Proof We show that $A[X]$ satisfies (P1) or (P2) (same reasoning for $A[Y]$). For this we will iteratively construct a sequence of subsets $Z_0 = X, Z_1, \dots, Z_k$ which is strictly monotone: $Z_0 \supset \dots \supset Z_i \supset \dots \supset Z_k$ and satisfies the following two properties (Q1)–(Q2) for all $0 \leq i \leq k$:

$$Z_i \text{ meets } Y \text{ and } V \setminus Y, \tag{Q1}$$

$$\text{if } x \in Z_i \setminus Y \text{ is simplicial in } A[Z_i] \text{ then } x \text{ is also simplicial in } A[X]. \tag{Q2}$$

We first observe that if we can find a set Z_k satisfying (Q1)–(Q2) and $|Z_k \cap Y| = 1$ then we can stop and conclude that (P1) or (P2) holds for $A[X]$. To see this consider the (proper) submatrix $A[Z_k]$, which by assumption satisfies (A) or (B). Assume first $A[Z_k]$ satisfies (B). Then there are distinct simplicial elements u, v in $A[Z_k]$. At least one of them, say u , belongs to $Z_k \setminus Y$. Then by (Q2) we know that u is simplicial in $A[X]$ and thus (P1) holds for $A[X]$. Assume now $A[Z_k]$ satisfies (A). Then there is a critical walk W in $A[Z_k]$. If its end point v_0 belongs to $Z_k \setminus Y$ then v_0 is critical in $A[X]$ (again by (Q2)) and thus (P1) holds for $A[X]$. Assume now $v_0 \in Y$. Then as $|Z_k \cap Y| = 1$ the walk W is in fact a weighted chordless walk rooted in $X \cap Y$ and thus (P2) holds for $A[X]$.

We now proceed to construct the sets Z_i satisfying (Q1)–(Q2) until we can conclude that (P1) or (P2) holds for $A[X]$. We start with $Z_0 = X$ which indeed satisfies (Q1)–

(Q2). Suppose we have Z_{i-1} satisfying (Q1)-(Q2) and $|Z_{i-1} \cap Y| \geq 2$. Consider the matrix $A[Z_{i-1}]$. We claim that if (P1) and (P2) do not hold for $A[X]$ then

$$\min A[Z_{i-1}] = A_{vw} \text{ for some } v, w \in Z_{i-1} \cap Y \text{ with } v \neq w. \tag{10}$$

By assumption $A[Z_{i-1}]$ satisfies (A) or (B). Assume first (B) holds and let v, w be simplicial vertices in $A[Z_{i-1}]$ with $A_{vw} = \min A[Z_{i-1}]$. If at least one of the two vertices belongs to $Z_{i-1} \setminus Y$, then (P1) follows by (Q2). Otherwise, as $A_{uv} = \min A[Z_{i-1}]$, we get (10).

Assume next $A[Z_{i-1}]$ satisfies (A) and let W be a critical walk in $A[Z_{i-1}]$, so its end point v_0 is simplicial in $A[Z_{i-1}]$. If $v_0 \in Z_{i-1} \setminus Y$ then v_0 is simplicial in $A[X]$ (by (Q2)) and thus (P1) holds. Assume now $v_0 \in Z_{i-1} \cap Y$. As W is critical there exists an internal vertex $u \in I(W)$ such that $A_{v_0u} = \min A[Z_{i-1}]$. If $u \in Y$ then (10) holds. Otherwise W contains a subwalk which is a weighted chordless walk rooted in $X \cap Y$ and thus (P2) holds.

So we may now assume (10) holds. Let (C, D) be a separation of $A[Z_{i-1}]$ separating v and w , as in Lemma 8, with (say) $v \in C \setminus D$ and $w \in D \setminus C$. Without loss of generality $C \cap (V \setminus Y) \neq \emptyset$. Set $Z_i = C$. Then $Z_i \subset Z_{i-1}$ (since $w \in Z_{i-1} \setminus C$) and (Q1) holds for Z_i . We claim:

$$\text{If } (Z_{i-1} \setminus Y) \cap (C \cap D) \neq \emptyset \text{ then (P2) holds for } A[X]. \tag{11}$$

For this consider $z \in (Z_{i-1} \setminus Y) \cap (C \cap D)$ and apply Lemma 8 to the separation (C, D) of $A[Z_{i-1}]$ separating $v, w \in Z_{i-1} \setminus (C \cap D)$ and $z \in C \cap D$. Then either $A_{zv} > \min A[Z_{i-1}]$ holds or there exists a weighted chordless walk $W_1 = (z, a, \dots, v)$ from z to v in $A[Z_{i-1}]$ that is internally vertex-disjoint from $C \cap D$; in the former case we set $W_1 = (z, v)$ (i.e., $a = v$). Analogously, either $A_{zw} > \min A[Z_{i-1}]$ holds or there exists a weighted chordless walk $W_2 = (z, b, \dots, w)$ from z to w internally vertex-disjoint from $C \cap D$; in the former case set $W_2 = (z, w)$ (i.e., $b = w$). Then $a \in C \setminus D$ and $b \in D \setminus C$, which implies $A_{ab} = \min A[Z_{i-1}]$. From this it follows that the walk W obtained by traveling first from v to z along the reverse of W_1 and then from z to w along W_2 is a weighted chordless walk in $A[X]$. By $z \notin X \cap Y$ and $v, w \in X \cap Y$ it contains at least one subwalk W_0 which is a weighted chordless walk in $A[X]$ rooted in $X \cap Y$ and thus (P2) holds.

So we may now assume in addition that $(Z_{i-1} \setminus Y) \cap (C \cap D) = \emptyset$, we claim that $Z_i = C$ satisfies (Q2). For this let $x \in C \setminus Y$ simplicial in $A[C]$, we show that x is simplicial in $A[X]$. Indeed, $x \notin D$ and thus x is simplicial in $A[Z_{i-1}]$ (by Lemma 7) and also in $A[X]$ (as $A[Z_{i-1}]$ satisfies (Q2)). Hence $Z_i = C$ satisfies (Q1)-(Q2), which concludes the proof. □

With the help of Lemma 9 we can now prove Theorem 4.

Proof (of Theorem 4) The proof is by induction on the size of the matrix A . So we may assume A has no self-contained pair of weighted chordless walks and every proper principal submatrix of A satisfies (A) or (B). Let (X, Y) be a separation of A satisfying property (P) of Lemma 8.

Assume first $X \cap Y = \emptyset$. By the induction assumption $A[X]$ satisfies (A) or (B), which implies that the same holds for A (since a simplicial vertex of $A[X]$ is also simplicial in A in view of Lemma 7).

Assume now $S = X \cap Y \neq \emptyset$. In view of Lemma 9 both $A[X]$ and $A[Y]$ satisfy (P1) or (P2). We distinguish three cases, depending on these possible combinations.

Case 1: Both $A[X]$ and $A[Y]$ satisfy (P1). Hence there exist $x \in X \setminus S$ which is simplicial in $A[X]$ and $y \in Y \setminus S$ which is simplicial in $A[Y]$. Then x, y are simplicial in A (by Lemma 7) with $A_{xy} = \min A$ and thus (B) holds.

Case 2: $A[X]$ satisfies (P1) and $A[Y]$ satisfies (P2) (or vice versa). So let $x \in X \setminus S$ which is simplicial in $A[X]$ and let $Q = (v_1, v_2, \dots, v_{k-1}, v_k)$ be a chordless walk in $A[Y]$ which is rooted in S (i.e., $v_1, v_k \in S$ and $v_2, \dots, v_{k-1} \in Y \setminus S$ with $k \geq 3$). By property (P) there exist weighted chordless walks $W_1 = (x, \dots, u, v_1)$ from x to v_1 (resp., $W_2 = (x, \dots, v, v_k)$ from x to v_k) in $A[X]$ which are internally vertex-disjoint from S , where we allow a walk $W_1 = (x, v_1)$ (resp., $W_2 = (x, v_k)$) of length one, in which case $A_{xv_1} > \min A$ (resp., $A_{xv_k} > \min A$). Consider the walk W obtained by concatenating the three walks W_1, Q, W_2 in that order, that we may visualize as $W = ([x]W_1[v_1]Q[v_k]W_2[x])$ (where we insert the connection vertices between consecutive walks into brackets just to clarify the definition). Then W is a closed walk whose end point x is indeed simplicial in A (in view of Lemma 7). Moreover W is a weighted chordless walk in A . Indeed the only missing inequalities are $A_{uv_2} < \min\{A_{uv_1}, A_{v_1v_2}\}$ and $A_{vv_{k-1}} < \min\{A_{vv_k}, A_{v_kv_{k-1}}\}$ which do hold since $A_{uv_2} = A_{vv_{k-1}} = \min A$ (as $u, v \in X \setminus S$ and $v_2, v_{k-1} \in Y \setminus S$). Finally, we have $A_{xv_2} = \min A$. Therefore W is a critical walk in A and thus (A) holds.

Case 3: Both $A[X]$ and $A[Y]$ satisfy (P2). So let $P = (u_1, u_2, \dots, u_{l-1}, u_l)$ (resp., $Q = (v_1, v_2, \dots, v_{k-1}, v_k)$) be a chordless walk in $A[X]$ (resp., in $A[Y]$), which are rooted in S (i.e., $u_1, u_l, v_1, v_k \in S, u_2, \dots, u_{l-1} \in X \setminus S$, and $v_2, \dots, v_{k-1} \in Y \setminus S$ with $k, l \geq 3$). By property (P) there exist weighted chordless walks $W_1 = (v_2, \dots, y, u_1)$ from v_2 to u_1 and $W_2 = (v_2, \dots, y', u_l)$ from v_2 to u_l in $A[Y]$ which are internally disjoint from S (where W_1 and W_2 may have length one as in Case 2). Then one can check (as in Case 2) that the concatenated walk $W = ([v_2]W_1[u_1]P[u_l]W_2[v_2])$ is a closed weighted chordless walk with v_2 as only vertex which is not an internal element of W . Analogously, using again (P) we find weighted chordless walks $W_3 = (u_2, \dots, x, v_1)$ and $W_4 = (u_2, \dots, x', v_k)$ in $A[X]$ which are internally disjoint from S . So the walk $W' = ([u_2]W_3[v_1]Q[v_k]W_4[u_2])$ is a weighted chordless walk in A with only u_2 as non-internal element. Finally as v_2 is an internal element of W' and u_2 is an internal element of W , the two walks (W, W') form a self-contained pair of weighted chordless walks in A , which contradicts the assumption on A . So we reach a contradiction and the proof is completed. \square

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