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Sparse matrix decompositions and graph characterizations

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ABSTRACT

Zeros in positive definite correlation matrices arise frequently in probability and statistics, and are intimately related to the notion of stochastic independence. The question of when zeros (i.e., sparsity) in a positive definite matrix A are preserved in its Cholesky decomposition, and vice versa, was addressed by Paulsen et al. [V.I. Paulsen, S.C. Power, R.R. Smith, Schur products and matrix completions, *J. Funct. Anal.* 85 (1989) 151–178]. In particular, they prove that for the pattern of zeros in A to be retained in the Cholesky decomposition of A , the pattern of zeros in A has to necessarily correspond to a chordal (or decomposable) graph associated with a specific type of vertex ordering. This result therefore also yields a characterization of chordal graphs in terms of sparse positive definite matrices, and has proved to be extremely useful in probabilistic and statistical analysis of Markov random fields. Now, consider a positive definite matrix A and its Cholesky decomposition given by $A = LDL^T$, where L is lower triangular with unit diagonal entries, and D a diagonal matrix with positive entries. In this paper, we prove that a necessary and sufficient condition for zeros (i.e., sparsity) in a positive definite matrix A to be preserved in its associated Cholesky matrix L , and in addition also preserved in the inverse of the Cholesky matrix L^{-1} , is that the pattern of zeros corresponds to a co-chordal or homogeneous graph associated with a specific type of vertex ordering. We proceed to provide a second characterization of this class of graphs in terms of determinants of submatrices that correspond to cliques

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in the graph. These results add to the growing body of literature in the field of sparse matrix decompositions, and also prove to be critical ingredients in the probabilistic analysis of an important class of Markov random fields.

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1. Introduction

Chordal and co-chordal graphs, and their relationships to sparse matrix decompositions, play an important role in the probabilistic and statistical analysis of Markov random fields (see [8–10, 18]). In these models the above classes of graphs are used to encode zeros in covariance or correlation matrices (or their inverses). The zero entries in these positive definite correlation matrices are intimately related to the notion of stochastic independence.

A characterization of chordal graphs or decomposable graphs, the class of graphs containing no induced cycle of length greater than or equal to 4, in terms of appropriate sub-manifolds of positive definite matrices was provided in [14]. In particular, positive definite matrices with zero entries according to a decomposable graph necessarily preserve these zero entries in their respective Cholesky matrices. The task undertaken in this paper is to find parallel and useful characterizations of co-chordal or homogeneous graphs, the class of graphs containing no induced 4-cycle or 4-path, in terms of appropriate sub-manifolds of positive definite matrices.

Let $G = (V, E)$ denote an undirected graph, where $V = \{1, 2, \dots, |V|\}$ represents the finite vertex set and E denotes the corresponding edge set. We use the notation \mathbb{M}_p to denote the set of $p \times p$ symmetric matrices and \mathbb{M}_p^+ to denote the set of $p \times p$ positive definite matrices. Without loss of generality, the notation used in this paper specifies the permutation or ordering $\sigma \in S_p$, where S_p denotes the symmetric group, by a p -tuple describing where $(1, 2, \dots, p)$ is sent by σ . Thus, $\sigma = (1\ 2\ 5\ 4\ 3)$ means $\sigma(1) = 1, \sigma(2) = 2, \sigma(3) = 5, \sigma(4) = 4$ and $\sigma(5) = 3$. Without ambiguity, in some places in the paper we will denote σ , an element of the symmetric group on p -letters, by a p -tuple describing where (u, v, w, \dots) is sent by σ . As we explain shortly, these orderings play an important role in our results. Given a graph $G = (V, E)$ and an ordering σ of the vertices of the graph, we define

$$P_{G_\sigma} = \left\{ \Sigma \in \mathbb{M}_{|V|}^+ : \Sigma_{ij} = 0 \text{ whenever } (\sigma^{-1}(i), \sigma^{-1}(j)) \notin E \right\},$$

and

$$\mathcal{L}_{G_\sigma} = \left\{ L \in \mathbb{M}_{|V|} : L_{ii} = 1, L_{ij} = 0 \text{ for } i < j \text{ or } (\sigma^{-1}(i), \sigma^{-1}(j)) \notin E \right\}.$$

The space P_{G_σ} is essentially a sub-manifold of the space of $|V| \times |V|$ positive definite matrices where the elements are restricted to be zero whenever the corresponding edge (under the ordering σ) is missing from E . Similarly, the space \mathcal{L}_{G_σ} is a subspace of lower triangular matrices with diagonal entries equal to 1, such that the elements in the lower triangle are restricted to be zero whenever the corresponding edge (under the ordering σ) is missing from E . We now state the main theorem of the paper. It characterizes co-chordal or homogeneous graphs in terms of (1) sparse matrix decompositions and (2) determinants of submatrices of cliques in the graph.

Theorem 1. Consider a graph $G = (V, E)$ together with an ordering of its vertices as denoted by σ . Then the following statements are equivalent.

- (1) G is a homogeneous graph and σ is a Hasse tree based elimination scheme.¹
- (2) If D is an arbitrary diagonal matrix with positive diagonal entries, then

$$L \in \mathcal{L}_{G_\sigma} \Leftrightarrow L^{-1} \in \mathcal{L}_{G_\sigma} \Leftrightarrow \Sigma := LDL^T \in P_{G_\sigma}.$$

¹ A certain type of vertex ordering that will be formally defined later in the paper.

(3) Let $\Sigma \in P_{G_\sigma}$ be arbitrarily chosen. Let $\Sigma = LDL^T$ denote its modified Cholesky decomposition, where L is a lower triangular matrix with unit diagonal entries and D is a diagonal matrix with diagonal entries D_{ii} , $i = 1, 2, \dots, p$. Then for any maximal clique C of the graph G ,

$$|(\Sigma^{-1})_{\sigma(C)}| = \prod_{i \in \sigma(C)} \frac{1}{D_{ii}}.$$

The outline of the remainder of the paper is as follows. Section 2 introduces terminology and notation from both linear algebra and graph theory that is required in subsequent sections. Section 3 provides a first characterization of co-chordal graphs in terms of sparse matrix decompositions. Section 4 provides a second characterization of co-chordal graphs in terms of determinants of submatrices. The results in Sections 3 and 4 are illustrated through examples, which a sophisticated reader can skip.

2. Preliminaries

2.1. Graph theory

This section introduces notation and terminology that is required in subsequent sections. An undirected graph $G = (V, E)$ consists of two sets V and E , with V representing the set of vertices, and $E \subseteq V \times V$ the set of edges satisfying:

$$(u, v) \in E \iff (v, u) \in E$$

When $(u, v) \in E$, we say that u and v are *adjacent* in G . A graph is said to be *complete* if all the vertices are adjacent to each other, i.e., $(u, v) \in E$ for all $u, v \in V$ such that $u \neq v$. A subgraph of V induced by $A \subset V$ is the graph $G' = (A, E \cap (A \times A))$.

Definition 1. A *path* connecting two distinct vertices u and v in G is a sequence of distinct vertices (u_0, u_1, \dots, u_n) where $u_0 = u$ and $u_n = v$, and for every $i = 0, \dots, n - 1$, $(u_i, u_{i+1}) \in E$.

Definition 2. A *cycle* is a path with an additional edge between the two endpoints u_0 and u_n .

Definition 3. A set of vertices $A \subset V$ is said to constitute a *clique* if the graph induced by A is a complete subgraph of V . Equivalently, a clique is a set of vertices in V which are all adjacent to each other.

Definition 4. A set of vertices $A \subset V$ is said to be a *maximal clique* if A is a clique and is not contained in another clique. Equivalently, $A \subset V$ is a maximal clique if it is a clique and the graph induced by $A \cup \{u\}$, for any $u \in V \setminus A$, is no longer a clique.

2.2. Modified Cholesky decomposition

If Σ is a positive definite matrix, then there exists a unique decomposition

$$\Sigma = LDL^T, \tag{1}$$

where L is a lower triangular matrix with unit diagonal entries and D a diagonal matrix with positive diagonal entries. This decomposition of Σ is referred to as the *modified Cholesky decomposition* of Σ (see [16]). The lemma below provides an explicit formulation of the inverse of a lower triangular matrix with unit diagonal entries, and will be useful in subsequent sections.

Lemma 1. Let L be a $p \times p$ lower triangular matrix with diagonal entries equal to 1. Let

$$A = \cup_{r=2}^p \{ \tau : \tau \in \{1, 2, \dots, p\}^r, \tau_i < \tau_{i-1} \ \forall 2 \leq i \leq r \},$$

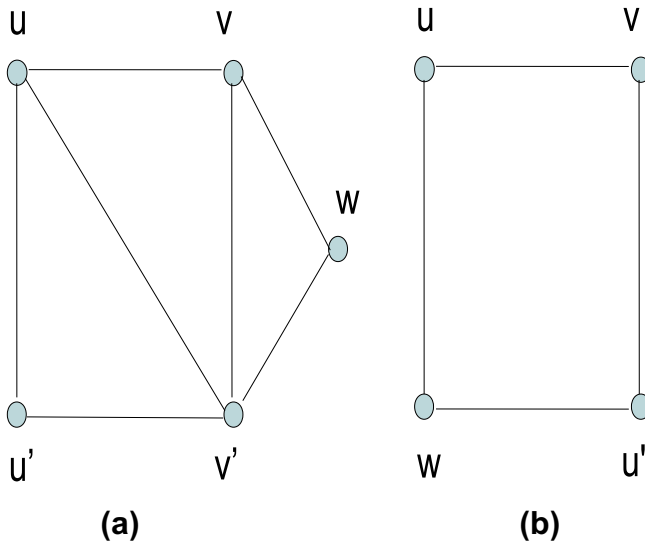


Fig. 1. (a) A decomposable graph, and (b) a non-decomposable graph.

and

$$L_\tau = \prod_{i=2}^{dim(\tau)} L_{\tau_{i-1}\tau_i}, \tau \in \mathcal{A},$$

where $dim(\tau)$ denotes the length of the vector τ . Then $L^{-1} = N$, where

$$N_{ij} = \begin{cases} 0 & \text{if } i < j \\ 1 & \text{if } i = j \\ \sum_{\tau \in \mathcal{A}, \tau_1=i, \tau_{dim(\tau)}=j} (-1)^{dim(\tau)-1} L_\tau & \text{if } i > j. \end{cases}$$

2.3. Decomposable graphs

An undirected graph G is said to be *decomposable* if any induced subgraph does not contain a cycle of length greater than or equal to four. They are also sometimes known as chordal graphs or triangulated graphs. See Fig. 1 for an example of a decomposable graph and a non-decomposable graph. Since their introduction by Chvatal [3], these graphs have been well studied, and are used in various fields such as optimization, computer science, probability and statistics. An important branch of probability and statistics where the class of decomposable graphs has proven to be quite useful is the study of Markov random fields/Graphical models. Decomposable graphs have several characterizations. One such characterization is in terms of vertex orderings. We first introduce notation and terminology that is required in order to formally state this characterization.

Definition 5. For an undirected graph $G = (V, E)$, an ordering σ of V is known as a *perfect vertex elimination scheme* for G if for every triplet i, j, k with $1 \leq i < j < k \leq p$ the following holds.

$$(\sigma^{-1}(j), \sigma^{-1}(i)) \in E, (\sigma^{-1}(k), \sigma^{-1}(i)) \in E \Rightarrow (\sigma^{-1}(k), \sigma^{-1}(j)) \in E.$$

A perfect vertex elimination scheme σ for the decomposable graph G in Fig. 1(a) is given by $\sigma : (u, u', v, v', w) \xrightarrow{\sigma} (3, 4, 2, 5, 1)$.

The existence of such an ordering characterizes decomposable graphs (see Paulsen et al. [14]). More formally, an undirected graph $G = (V, E)$ is decomposable iff there exists an ordering σ of V , which is a

perfect vertex elimination scheme. For a given decomposable graph $G = (V, E)$, there can however be several orderings which gives rise to perfect vertex elimination schemes. A constructive way to obtain such an ordering is given in Lauritzen [11]. There is an interesting and useful connection between decomposable graphs, orderings which give rise to perfect vertex elimination schemes, and the matrix spaces P_{G_σ} and \mathcal{L}_{G_σ} .

Lemma 2 (Paulsen et al. [14]). *Let $G = (V, E)$ be a decomposable graph, and σ an ordering of V which corresponds to a perfect vertex elimination scheme for G . Then for any positive definite matrix Σ with modified Cholesky decomposition given by $\Sigma = LDL^T$, the following holds.*

$$L \in \mathcal{L}_{G_\sigma} \Leftrightarrow \Sigma \in P_{G_\sigma}.$$

Hence, for $\Sigma \in P_{G_\sigma}$, the zeros in Σ are preserved in the lower triangle of the corresponding matrix L obtained from the modified Cholesky decomposition. Moreover for $L \in \mathcal{L}_{G_\sigma}$, the zeros in L are preserved in the matrix Σ obtained by $\Sigma = LDL^T$, for any diagonal matrix D with positive diagonal entries. The converse of Lemma 2 is also true.

Lemma 3 (Paulsen et al. [14]). *Let $G = (V, E)$ be a graph, σ be an ordering of V , and D be an arbitrary diagonal matrix with positive diagonal entries. Suppose*

$$L \in \mathcal{L}_{G_\sigma} \Leftrightarrow \Sigma := LDL^T \in P_{G_\sigma}.$$

Then G is a decomposable graph and σ corresponds to a perfect vertex elimination scheme for G .

Hence, Lemmas 2 and 3 characterize a decomposable graph G and a perfect vertex elimination scheme σ for G in terms of the preservation of zeros in the modified Cholesky decomposition of matrices in P_{G_σ} . These characterizations of decomposable graphs and orderings of vertices of G has proven to be tremendously useful for working with sparse positive definite matrices in probability and statistics (see [7, 10, 12, 17, 18]). Another class of graphs that is also highly useful in this context is the class of co-chordal graphs or homogeneous graphs (see [2, 8–10, 12]). Yet characterizations of homogeneous graphs, similar to the above for decomposable graphs, are not available. These characterizations are the subject of the rest of the paper.

2.4. Homogeneous graphs

A graph $G = (V, E)$ is defined to be co-chordal or homogeneous if for all v, v' such that $(v, v') \in E$, either

$$\{u : u = v' \text{ or } (u, v') \in E\} \subseteq \{u : u = v \text{ or } (u, v) \in E\},$$

or

$$\{u : u = v \text{ or } (u, v) \in E\} \subseteq \{u : u = v' \text{ or } (u, v') \in E\}.$$

Equivalently, a graph G is said to be homogeneous if it is decomposable and does not contain the graph $\bullet^1 - \bullet^2 - \bullet^3 - \bullet^4$, denoted by A_4 , as an induced subgraph. See Fig. 2 for an example of a homogeneous graph, and a non-homogeneous graph which is decomposable. Connected homogeneous graphs have an equivalent representation in terms of directed rooted trees, called *Hasse diagrams*. The reader is referred to [12] for a detailed account of the properties of homogeneous graphs. We write $v \rightarrow w$ whenever

$$\{u : u = w \text{ or } (u, w) \in E\} \subseteq \{u : u = v \text{ or } (u, v) \in E\}.$$

Now denote by R the equivalence relation on V defined by

$$uRv \Leftrightarrow u \rightarrow v \text{ and } v \rightarrow u.$$

Let \bar{v} denote the equivalence class in V/R containing v . The Hasse diagram of G is defined as a directed graph with vertex set $V_H = V/R = \{\bar{v} : v \in V\}$ and edge set E_H consisting of directed edges with $(\bar{u}, \bar{v}) \in E_H$ for $\bar{u} \neq \bar{v}$ if the following holds: $u \rightarrow v$ and $\nexists v'$ such that $u \rightarrow v' \rightarrow v, \bar{v}' \neq \bar{u}, \bar{v}' \neq \bar{v}$.

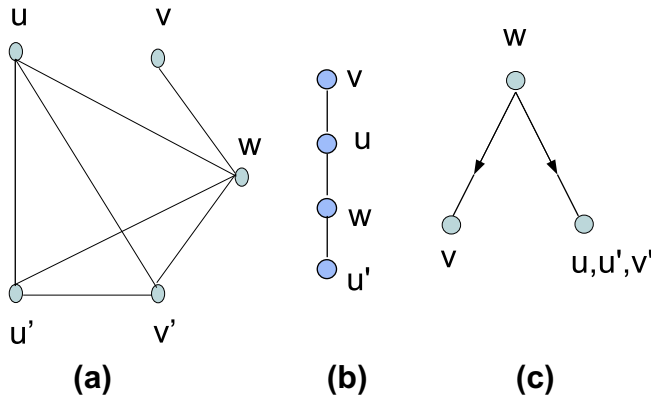


Fig. 2. (a) A homogeneous graph, (b) a non-homogeneous graph which is decomposable, and (c) the Hasse tree corresponding to the homogeneous graph in (a).

If G is a connected homogeneous graph, then the Hasse diagram described above is a directed rooted tree such that the number of children of a vertex is never equal to one. It was proved in [12] that there is a one-to-one correspondence between the set of connected homogeneous graphs and the set of directed rooted trees with vertices weighted by positive integers ($w(\bar{u}) = |\bar{u}|$), such that no vertex has exactly one child. If $u \rightarrow v$ and $\bar{u} \neq \bar{v}$, we say that u is an ancestor of v in the Hasse tree of G . It is easily seen that if G is a disconnected homogeneous graph, then each connected component of G gives rise to a Hasse tree. If $\bar{u} = \bar{v}$, we say that u is a twin of v in the Hasse tree of G .

A subclass of orderings associated with a homogeneous graph, which will be used in subsequent analysis, is defined as follows.

Definition 6. If $G = (V, E)$ is a homogeneous graph, then an ordering σ of V is defined to be a *Hasse tree based elimination scheme* for G if for every pair of vertices u, v , the following holds.

$$u \rightarrow v, \bar{u} \neq \bar{v} \Rightarrow \sigma(u) > \sigma(v).$$

Alternatively, if \bar{u} is an ancestor of \bar{v} in the Hasse diagram of G , then $\sigma(u) > \sigma(v)$.

The lemma below follows easily from the definition of homogeneous graphs.

Lemma 4.

- (a) If $G_i = (V_i, E_i)$ is a homogeneous graph for every $1 \leq i \leq n$, and V_i and V_j are disjoint for every $1 \leq i \neq j \leq n$, then $G = (\cup_{i=1}^n V_i, \cup_{i=1}^n E_i)$ is also a homogeneous graph. Conversely, if $G = (V, E)$ is a homogeneous graph, then any disjoint connected component of G is also a homogeneous graph.
- (b) If $G = (V, E)$ is a connected homogeneous graph, $|V| = m$, and σ is a Hasse tree based elimination scheme for G , then the equivalence class of $\sigma^{-1}(m)$ lies at the root of the Hasse tree of G .

Example 1. Consider the homogeneous graph G in Fig. 2(a) and the corresponding Hasse tree in Fig. 2(c). A Hasse tree based elimination scheme σ for the homogeneous graph G is given by $\sigma(w) = 5, \sigma(v) = 4, \sigma(v') = 3, \sigma(u') = 2, \sigma(u) = 1$. Note that a homogeneous graph is also a decomposable graph, and a Hasse tree based elimination scheme is also a perfect vertex elimination scheme. However, every perfect vertex elimination scheme for a homogeneous graph may not necessarily be a Hasse tree based elimination scheme. For the homogeneous graph G in Fig. 2(a), the ordering σ given by $\sigma(v') = 5, \sigma(w) = 4, \sigma(u') = 3, \sigma(u) = 2, \sigma(v) = 1$ is a perfect vertex elimination scheme, but not a Hasse tree based elimination scheme, since $w \rightarrow v', \bar{w} \neq \bar{v}'$ but $\sigma(w) = 4 < \sigma(v') = 5$.

3. Characterization in terms of sparse matrix decompositions

We now provide the first characterization of homogeneous graphs that yields a parallel result to that of Paulsen et al. [14] for decomposable graphs. We note that antecedents of the results in Paulsen et al. [14] were given in [1,5,6].

Lemma 5 (Khare and Rajaratnam [10]). *Let $G = (V, E)$ be a homogeneous graph, and σ an ordering of V which corresponds to a Hasse tree based elimination scheme for G . Then for any positive definite matrix Σ with modified Cholesky decomposition given by $\Sigma = LDL^T$, the following holds.*

$$\Sigma \in P_{G_\sigma} \Leftrightarrow L \in L_{G_\sigma} \Leftrightarrow L^{-1} \in L_{G_\sigma}.$$

A detailed constructive proof is given in [9]. A proof in a more general context can also be found in [2,13]. One of the main results of this paper is the converse of Lemma 5.

Proposition 1. *Let $G = (V, E)$ be a graph, σ be an ordering of V , and D be an arbitrary diagonal matrix with positive diagonal entries. Suppose*

$$L \in \mathcal{L}_{G_\sigma} \Leftrightarrow L^{-1} \in \mathcal{L}_{G_\sigma} \Leftrightarrow \Sigma := LDL^T \in P_{G_\sigma}.$$

Then G is a homogeneous graph and σ corresponds to a Hasse tree based elimination scheme for G .

Proof. We proceed by induction and prove the result in a series of claims.

Claim 1. The result holds for $|V| = 3$.

Proof of Claim 1. Let $V = \{u, v, w\}$. We consider two cases.

Case I: $E = \phi, \{(u, v)\}, \{(u, w)\}, \{(v, w)\}$ or $\{(u, v), (u, w), (v, w)\}$. See Fig. 3.

G is a homogeneous graph in every case. Also, each disjoint connected component is a complete graph, which means that every ordering corresponds to a Hasse tree based elimination scheme. Hence, the result holds vacuously.

Case II: $E = \{(u, v), (v, w)\}, \{(u, w), (v, w)\}$ or $\{(u, v), (u, w)\}$. See Fig. 4.

Let us first consider the case $E = \{(u, v), (v, w)\}$. Note that G is a homogeneous graph. It remains to be shown that σ is a Hasse tree based elimination scheme. Now if $\sigma(v) = 1$, and

$$L = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 1 & 0 & 1 \end{pmatrix} \in \mathcal{L}_{G_\sigma},$$

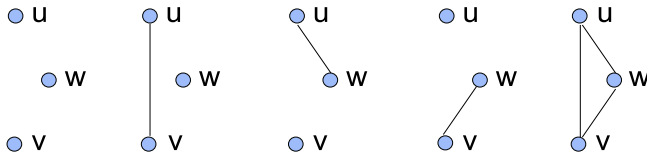


Fig. 3. Case I with $|V| = 3$ for Proposition 1.

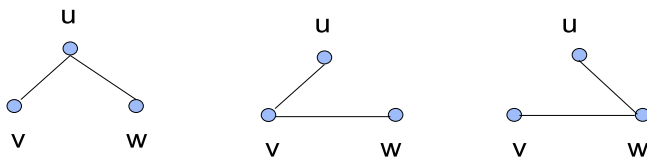


Fig. 4. Case II with $|V| = 3$ for Proposition 1.

then $\Sigma_{32} = (LDL^T)_{32} = d_{11} \neq 0$. Hence, $\Sigma \notin P_{G_\sigma}$, yielding a contradiction. Similarly, if $\sigma(v) = 2$, and

$$L = \begin{pmatrix} 1 & 0 & 0 \\ 1 & 1 & 0 \\ 0 & 1 & 1 \end{pmatrix} \in \mathcal{L}_{G_\sigma},$$

then $L_{31}^{-1} = 1 \neq 0$. Hence, $L^{-1} \notin \mathcal{L}_{G_\sigma}$, once more yielding a contradiction to the assumptions in the proposition. Hence $\sigma(v) = 3$. Note that $v \rightarrow u, v \rightarrow w$ and $\bar{v} \neq \bar{u}, \bar{v} \neq \bar{w}$. Hence, any ordering σ such that $\sigma(v) = 3$ is a Hasse tree based elimination scheme. The other cases when $E = \{(u, w), (v, w)\}$ and $E = \{(u, v), (u, w)\}$ follow by symmetry. Hence, the result for $|V| = 3$ holds true.

As mentioned earlier, we shall use an induction argument on the number of vertices to prove the result. Suppose now that the result holds true for all graphs with $m - 1$ vertices. Let $G = (V, E)$ be a graph with $|V| = m$, and σ be an ordering of V for which

$$L \in \mathcal{L}_{G_\sigma} \Leftrightarrow L^{-1} \in \mathcal{L}_{G_\sigma} \Leftrightarrow \Sigma := LDL^T \in P_{G_\sigma},$$

for an arbitrary diagonal matrix D with positive diagonal entries. We need to show two results: (i) G is homogeneous and (ii) the ordering σ is a Hasse tree based elimination scheme.

Let G' be the subgraph induced by G on the set of vertices $V \setminus \{\sigma^{-1}(m)\}$, and let σ' be the restriction of σ on $V \setminus \{\sigma^{-1}(m)\}$. Note that G' together with the ordering σ' is none other than G with the ordering σ (or G_σ), but with the highest labeled vertex removed.

Claim 2.

$$L^* \in \mathcal{L}_{G'_{\sigma'}} \Leftrightarrow (L^*)^{-1} \in \mathcal{L}_{G'_{\sigma'}} \Leftrightarrow \Sigma^* = L^*D^*(L^*)^T \in P_{G'_{\sigma'}}.$$

where D^* is the upper $(m - 1) \times (m - 1)$ principal submatrix of D .

Proof of Claim 2. Let $L^* \in \mathcal{L}_{G'_{\sigma'}}$. Then

$$\begin{aligned} L &:= \begin{pmatrix} L^* & \mathbf{0} \\ \mathbf{0}^T & 1 \end{pmatrix} \in \mathcal{L}_{G_\sigma} \\ \Rightarrow \begin{pmatrix} L^* & \mathbf{0} \\ \mathbf{0}^T & 1 \end{pmatrix}^{-1} &= \begin{pmatrix} (L^*)^{-1} & \mathbf{0} \\ \mathbf{0}^T & 1 \end{pmatrix} \in \mathcal{L}_{G_\sigma} \\ \Rightarrow (L^*)^{-1} &\in \mathcal{L}_{G'_{\sigma'}}. \end{aligned}$$

By a similar argument $(L^*)^{-1} \in \mathcal{L}_{G'_{\sigma'}} \Rightarrow L^* \in \mathcal{L}_{G'_{\sigma'}}$. Hence $(L^*)^{-1} \in \mathcal{L}_{G'_{\sigma'}} \Leftrightarrow L^* \in \mathcal{L}_{G'_{\sigma'}}$.

Note that,

$$\begin{aligned} L^* &\in \mathcal{L}_{G'_{\sigma'}} \\ \Leftrightarrow L &= \begin{pmatrix} L^* & \mathbf{0} \\ \mathbf{0}^T & 1 \end{pmatrix} \in \mathcal{L}_{G_\sigma} \\ \Leftrightarrow \Sigma &= LDL^T = \begin{pmatrix} L^*D^*(L^*)^T & \mathbf{0} \\ \mathbf{0}^T & D_{mm} \end{pmatrix} \in P_{G_\sigma} \\ \Leftrightarrow \Sigma^* &:= L^*D^*(L^*)^T \in P_{G'_{\sigma'}}. \end{aligned}$$

Hence, we have now established that

$$L^* \in \mathcal{L}_{G'_{\sigma'}} \Leftrightarrow (L^*)^{-1} \in \mathcal{L}_{G'_{\sigma'}} \Leftrightarrow \Sigma^* = L^* D^* (L^*)^T \in P_{G'_{\sigma'}}.$$

By the induction hypothesis, it follows that G' is a homogeneous graph and σ' corresponds to a Hasse tree based elimination scheme for G' , i.e.,

$$\sigma'(v) = \sigma(v) < \sigma'(u) = \sigma(u) \text{ when } u \rightarrow v, \bar{u} \neq \bar{v}, \forall u, v \in V \setminus \{\sigma^{-1}(m)\}. \tag{2}$$

Claim 3. G is a homogeneous graph and σ is a Hasse tree based elimination scheme.

Proof of Claim 3. Now let $V' = \cup_{i=1}^k V_i$, where V_i is the vertex set corresponding to the i th disjoint connected component of G' .

Suppose $(\sigma^{-1}(m), u) \notin E$ for each $u \in V \setminus \{\sigma^{-1}(m)\}$, i.e., the vertex $\sigma^{-1}(m)$ is disconnected from the graph G' . Then by Lemma 4, the graph G is a homogeneous graph with $V = (\cup_{i=1}^k V_i) \cup \{\sigma^{-1}(m)\}$ being the disjoint partition of the vertices corresponding to its disjoint connected components. Also, from (2) and the fact that $\sigma^{-1}(m)$ is disconnected from every vertex in $V \setminus \{\sigma^{-1}(m)\}$, it follows that σ is a Hasse tree based elimination scheme for G .

Suppose $(\sigma^{-1}(m), u) \in E$ for some $u \in V_i$. Let $v_i^* \in V_i$ be such that $\sigma(v_i^*) = \max_{v_i \in V_i} \sigma(v_i)$. Since G' is a homogeneous graph, σ restricted to $V \setminus \{\sigma^{-1}(m)\}$ is a Hasse tree based elimination scheme, and V_i is the vertex set corresponding to a connected component of G' , it follows from Lemma 4 that the equivalence class of v_i^* lies at the top of the Hasse tree of V_i in G' . We therefore deduce that $(v_i^*, v_i) \in E, \forall v_i \in V_i$.

We proceed by claiming that $(\sigma^{-1}(m), v_i^*) \in E$. If $v_i^* = u$, it follows immediately. If $v_i^* \neq u$, then $m > \sigma(v_i^*) > \sigma(u)$. Suppose L is defined by

$$L_{ij} = \begin{cases} 1 & \text{if } i = m, j = \sigma(u) \text{ or } i = \sigma(v_i^*), j = \sigma(u) \text{ or } i = j, \\ 0 & \text{otherwise.} \end{cases}$$

Note that $L \in \mathcal{L}_{G_{\sigma}}$. If $\Sigma := LL^T$, then by assumption $\Sigma \in P_{G_{\sigma}}$, and

$$\Sigma_{m\sigma(v_i^*)} = L_{m\sigma(u)}L_{\sigma(v_i^*)\sigma(u)} + \sum_{v \in V_i, v \neq u} L_{m\sigma(v)}L_{\sigma(v_i^*)\sigma(v)} = 1.$$

Hence, it follows that $(\sigma^{-1}(m), v_i^*) \in E$. Now let $v_i \in V_i, v_i \neq v_i^*$. We also now claim that $(\sigma^{-1}(m), v_i) \in E$. Note that $(v_i^*, v_i) \in E$ from the discussion above. Suppose L is defined by

$$L_{ij} = \begin{cases} 1 & \text{if } i = m, j = \sigma(v_i^*) \text{ or } i = \sigma(v_i^*), j = \sigma(v_i) \text{ or } i = j, \\ 0 & \text{otherwise.} \end{cases}$$

First note that $L \in \mathcal{L}_{G_{\sigma}}$, and hence by assumption $L^{-1} \in \mathcal{L}_{G_{\sigma}}$. Since $L_{m\sigma(v_i)}^{-1} = 1$ (by using the inversion formula in Lemma 1), it follows that $(\sigma^{-1}(m), v_i) \in E$. Hence, we have established that if $(\sigma^{-1}(m), u) \in E$ for some $u \in V_i$, then $(\sigma^{-1}(m), v_i) \in E$ for every $v_i \in V_i$.

Now let $V_{i_1}, V_{i_2}, \dots, V_{i_p}$ be the components of G' which share at least one edge with $\sigma^{-1}(m)$. Since the graph induced by V_{i_r} on G' is a connected homogeneous graph for every $1 \leq r \leq p$, and $\sigma^{-1}(m)$ is connected to every vertex in $V_{i_1}, V_{i_2}, \dots, V_{i_p}$ by the argument above, the introduction of $\sigma^{-1}(m)$ does not give rise to any new 4-cycle or 4-path, due of the following reasoning: Consider an arbitrary collection of 4 vertices in V . If all of them lie in V_{i_r} for some r , and if $\sigma^{-1}(m)$ is not one of the vertices, then these 4 vertices cannot form a 4-cycle or a 4-path as the subgraph induced by V_{i_r} on G is a homogeneous graph. If none of the vertices is $\sigma^{-1}(m)$, and all of them do not lie in V_{i_r} for some r , then the graph induced by these vertices on G is a disconnected graph, which implies that the induced sub-graph cannot be a 4-cycle or a 4-path. Finally, if $\sigma^{-1}(m)$ is one of the vertices, and since it is connected to all the other three vertices, they cannot form an induced 4-cycle or an induced 4-path.

It follows that the graph induced by $\{\sigma^{-1}(m)\} \cup \left(\bigcup_{r=1}^p V_{i_r}\right)$ on G is a connected homogeneous graph. Moreover, since $\sigma^{-1}(m)$ is connected to every vertex in $V_{i_1}, V_{i_2}, \dots, V_{i_p}$, its equivalence class has to lie at the root of the corresponding Hasse tree. Note that the disjoint connected components of G' other than $V_{i_1}, V_{i_2}, \dots, V_{i_p}$ are also connected homogeneous graphs. It follows that G is a homogeneous graph with disjoint connected components $\{\sigma^{-1}(m)\} \cup \left(\bigcup_{r=1}^p V_{i_r}\right)$ and $V_t, t \neq i_1, i_2, \dots, i_p$. Note that σ' (which is the restriction of σ to G') corresponds to a Hasse tree based elimination scheme for G' , and that $\sigma(u) < m$ whenever $u \neq \sigma^{-1}(m)$. Hence, $\sigma(u) < m$ whenever $\sigma^{-1}(m) \rightarrow u, \sigma^{-1}(m) \neq \bar{u}$. Also, since $\sigma^{-1}(m)$ is at the top of the Hasse tree in its connected component, there does not exist $u \in V \setminus \{\sigma^{-1}(m)\}$ such that $u \rightarrow \sigma^{-1}(m)$. This leads us to conclude that σ is a Hasse tree based elimination scheme for G . Hence the result is proved. \square

Remark. A useful alternative probabilistic characterization of homogeneous graphs can be found in [4,15]. This probabilistic result essentially states that G is homogeneous iff “ G is Markov equivalent to a directed acyclic graph (DAG)”. In contrast, the characterization proved in this section is algebraic in nature, and is therefore different from the probabilistic characterization. The algebraic characterization above can be established directly starting from the probabilistic characterization mentioned above, by using the notion of “d-separation”. The proof however is non-trivial and does not seem to offer a simplification over the first principles proof provided here.

We now give a series of examples to illustrate the necessity of the assumptions in the characterization discussed above.

Example 2. Consider the homogeneous graph G in Fig. 2(a). Let σ be a Hasse tree based elimination scheme defined by $\sigma(w) = 5, \sigma(v) = 4, \sigma(v') = 3, \sigma(u') = 2, \sigma(u) = 1$. Let

$$L = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 1 & 1 & 1 & 1 & 1 \end{pmatrix} \in \mathcal{L}_{G_\sigma}.$$

Then,

$$L^{-1} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 & 0 \\ 0 & 0 & -1 & -1 & 1 \end{pmatrix} \in \mathcal{L}_{G_\sigma}, \text{ and } \Sigma = LL^T = \begin{pmatrix} 1 & 1 & 1 & 0 & 1 \\ 1 & 2 & 2 & 0 & 2 \\ 1 & 2 & 3 & 0 & 3 \\ 0 & 0 & 0 & 1 & 1 \\ 1 & 2 & 3 & 1 & 5 \end{pmatrix} \in P_{G_\sigma}.$$

Now consider σ which is a perfect vertex elimination scheme, but not a Hasse tree based elimination scheme, given by $\sigma(v') = 5, \sigma(w) = 4, \sigma(u') = 3, \sigma(u) = 2, \sigma(v) = 1$. Then

$$L = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 \\ 0 & 1 & 1 & 1 & 1 \end{pmatrix} \in \mathcal{L}_{G_\sigma}, \text{ but } L^{-1} = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 & 0 \\ 0 & -1 & 1 & 0 & 0 \\ -1 & 0 & -1 & 1 & 0 \\ 1 & 0 & 0 & -1 & 1 \end{pmatrix} \notin \mathcal{L}_{G_\sigma}.$$

It can be verified that $\Sigma = LL^T \in P_{G_\sigma}$. Now let σ be given by $\sigma(v) = 5, \sigma(u') = 4, \sigma(v') = 3, \sigma(w) = 2, \sigma(u) = 1$. Then, σ is not a perfect vertex elimination scheme, and

$$L = \begin{pmatrix} 1 & 0 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 & 0 \\ 1 & 1 & 1 & 0 & 0 \\ 1 & 1 & 1 & 1 & 0 \\ 0 & 1 & 0 & 0 & 1 \end{pmatrix} \in \mathcal{L}_{G_\sigma}, \text{ but } \Sigma = LL^T = \begin{pmatrix} 1 & 1 & 1 & 1 & 0 \\ 1 & 2 & 2 & 2 & 1 \\ 1 & 2 & 3 & 3 & 1 \\ 1 & 2 & 3 & 4 & 1 \\ 0 & 1 & 1 & 1 & 2 \end{pmatrix} \notin P_{G_\sigma}.$$

Now consider the non-homogeneous graph G in Fig. 2(b). Note that G is however a decomposable graph. The ordering σ given by $\sigma(u') = 4, \sigma(w) = 3, \sigma(u) = 2, \sigma(v) = 1$ is a perfect vertex elimination scheme. However,

$$L = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 1 & 1 & 0 & 0 \\ 0 & 1 & 1 & 0 \\ 0 & 0 & 1 & 1 \end{pmatrix} \in \mathcal{L}_{G_\sigma}, \text{ but } L^{-1} = \begin{pmatrix} 1 & 0 & 0 & 0 \\ -1 & 1 & 0 & 0 \\ 1 & -1 & 1 & 0 \\ -1 & 1 & -1 & 1 \end{pmatrix} \notin \mathcal{L}_{G_\sigma}.$$

4. Characterization in terms of determinants

We now give a second characterization of homogeneous graphs with vertex orderings corresponding to Hasse tree based elimination schemes. Let us first establish some notation, that shall be used throughout this section. If $A \in \mathbb{M}_n$ and $M, M^* \subseteq \{1, 2, \dots, n\}$, then

$$A_M := ((A_{ij}))_{i,j \in M}, \quad A_{MM^*} := ((A_{ij}))_{i \in M, j \in M^*}.$$

The proposition below and its converse, stated and proved subsequently, provide the second characterization of homogeneous graphs.

Proposition 2. *Let $G = (V, E)$ be a homogeneous graph, and σ an ordering of V which corresponds to a Hasse tree based elimination scheme for G . Let $\Sigma \in P_{G_\sigma}$, and $\Sigma = LDL^T$ denote its Cholesky decomposition. Then, for any maximal clique C ,*

$$|(\Sigma^{-1})_{\sigma(C)}| = \prod_{i \in \sigma(C)} \frac{1}{D_{ii}}.$$

Proof. Let $C \subseteq V$ be a maximal clique in G , where $C = \{u_1, u_2, \dots, u_r\}$, with $\sigma(u_1) > \sigma(u_2) > \dots > \sigma(u_r)$. First note that

$$(\Sigma^{-1})_{\sigma(C)} = \left[(L^{-1})_{\sigma(V)\sigma(C)} \right]^T D^{-1} \left[(L^{-1})_{\sigma(V)\sigma(C)} \right]. \tag{3}$$

We will prove that the determinant of the RHS of (3) equals the determinant of $\left[(L^{-1})_{\sigma(C)}^T \right] D_{\sigma(C)}^{-1} \left[(L^{-1})_{\sigma(C)} \right]$, and the result will follow.

We start by first showing that $L_{\sigma(w)\sigma(u_i)}^{-1} = 0$ when $w \notin C$ for $i = 1, 2, \dots, r$. Note that $\sigma(u_i) > \sigma(w)$, $L_{\sigma(w)\sigma(u_i)}^{-1} = 0$, as L^{-1} is a lower triangular matrix. Now let $\sigma(u_i) < \sigma(w)$. Suppose to the contrary that $L_{\sigma(w)\sigma(u_i)}^{-1} \neq 0$. Since $L^{-1} \in \mathcal{L}_{G_\sigma}$ by Lemma 5, we get $(w, u_i) \in E$. Hence, w is an ancestor or twin of u_i in the Hasse tree of G . Now by the very definition of a homogeneous graph, every vertex sharing an edge with u_i also shares an edge with w . Hence, $(w, u_j) \in E$ for $j = 1, 2, \dots, r$, which gives a contradiction to the maximality of C . Hence we conclude that $L_{\sigma(w)\sigma(u_i)}^{-1} = 0$ when $w \notin C$ for $i = 1, 2, \dots, r$.

Now using the Cauchy–Binet identity in (3),

$$\begin{aligned} |(\Sigma^{-1})_{\sigma(C)}| &= \left| \left[(L^{-1})_{\sigma(V)\sigma(C)} \right]^T D^{-1} \left[(L^{-1})_{\sigma(V)\sigma(C)} \right] \right| \\ &= \sum_{A \subseteq V, |A|=r} \left| \left[(L^{-1})_{\sigma(A)\sigma(C)} \right]^T D_{\sigma(A)}^{-1} \left[(L^{-1})_{\sigma(A)\sigma(C)} \right] \right|. \end{aligned}$$

Note that if $A \subseteq V$, $|A| = r$, and $A \neq C$, then there exists w such that $w \in A$ but $w \notin C$. Hence, from the argument above, $L_{\sigma(w)\sigma(u_i)}^{-1} = 0$ for $i = 1, 2, \dots, r$, and for such $A \neq C$,

$$\left| \left[(L^{-1})_{\sigma(A)\sigma(C)} \right]^T D_{\sigma(A)}^{-1} \left[(L^{-1})_{\sigma(A)\sigma(C)} \right] \right| = \left| \left[(L^{-1})_{\sigma(A)\sigma(C)} \right]^T \right| \left| D_{\sigma(A)}^{-1} \right| \left| \left[(L^{-1})_{\sigma(A)\sigma(C)} \right] \right| = 0,$$

since one row in the matrix $(L^{-1})_{\sigma(A)\sigma(C)}$ is zero. Therefore the only non-zero summand in the Cauchy–Binet formula is when $A = C$. Hence

$$|(\Sigma^{-1})_{\sigma(C)}| = \left| \left[(L^{-1})_{\sigma(C)} \right]^T \right| \left| D_{\sigma(C)}^{-1} \right| \left| \left[(L^{-1})_{\sigma(C)} \right] \right| = \prod_{i \in \sigma(C)} \frac{1}{D_{ii}},$$

where the last equality follows from the fact that $(L^{-1})_{\sigma(C)}$ is a lower triangular matrix with all diagonal entries equal to one (and therefore has determinant one), and $D_{\sigma(C)}^{-1}$ is a diagonal matrix. Hence the result is proved. \square

We now proceed to prove the following lemma required in the proof of the converse of Proposition 2.

Lemma 6. *Let $G = (V, E)$ be a 4-cycle or 4-path, and let σ be an ordering of V . Then, irrespective of the way σ orders the vertices of the 4-cycle or the 4-path, there exist $u, v, w \in V$ such that $(u, v), (v, w) \in E$, $(u, w) \notin E$, and $\sigma(v) < \sigma(u) < \sigma(w)$ or $\sigma(u) < \sigma(v) < \sigma(w)$.*

Proof.

- (i) Let G be a 4-cycle. Recall that $u, v \in V$ are said to be *neighbors* in G if $(u, v) \in E$. Consider the two neighbors of $v := \sigma^{-1}(1)$. Let u denote the neighbor with the smaller σ -value, and w denote the remaining neighbor. Note that $(u, v), (v, w) \in E$, but $(u, w) \notin E$. Also, $\sigma(v) = 1 < \sigma(u) < \sigma(w)$.
- (ii) Let G be a 4-path. We consider three possibilities which are exhaustive, and in each case show the existence of three vertices with the required properties.

Case I. $\sigma^{-1}(1)$ **has two neighbors**: Let $v := \sigma^{-1}(1)$. In this case, let u denote the neighbor with the smaller σ -value, and w denote the remaining neighbor. Hence, $\sigma(v) = 1 < \sigma(u) < \sigma(w)$.

Case II. $\sigma^{-1}(1)$ **has one neighbor, and $\sigma^{-1}(2)$ has two neighbors**: Let $v := \sigma^{-1}(2)$. If one of the two neighbors of $v = \sigma^{-1}(2)$ is $u = \sigma^{-1}(1)$, denote the remaining neighbor by w , and observe that $\sigma(w)$ is equal to 3 or 4. Hence, $\sigma(u) = 1 < \sigma(v) = 2 < \sigma(w)$. If the neighbors of $v = \sigma^{-1}(2)$ are $u = \sigma^{-1}(3)$ and $w = \sigma^{-1}(4)$, then $\sigma(v) = 2 < \sigma(u) = 3 < \sigma(w) = 4$.

Case III. $\sigma^{-1}(1)$ **and $\sigma^{-1}(2)$ both have one neighbor**: In this case, $v := \sigma^{-1}(3)$ has two neighbors, one of which has to be $w = \sigma^{-1}(4)$. Let u be the remaining neighbor and observe that $\sigma(u)$ is equal to 1 or 2. Hence, $\sigma(u) < \sigma(v) = 3 < \sigma(w) = 4$.

We now establish the converse of Proposition 2.

Proposition 3. *Let $G = (V, E)$ be a graph, and σ be an ordering of V . Now if G is not a homogeneous graph, or if G is a homogeneous graph and σ does not correspond to a Hasse tree based elimination scheme*

for G , then there exists a maximal clique C , and $\Sigma \in P_{G_\sigma}$ such that

$$|(\Sigma^{-1})_{\sigma(C)}| \neq \prod_{i \in \sigma(C)} \frac{1}{D_{ii}},$$

where $\Sigma = LDL^T$ denotes the modified Cholesky decomposition of Σ .

Proof of Proposition 3. We shall prove the result for each of the two possible cases.

Case I: G is not a homogeneous graph.

As the graph G is not homogenous, it contains a 4-cycle or a 4-path. If G contains a 4-cycle or a 4-path, by Lemma 6, there exist $u, v, w \in V$ such that $(u, v), (v, w) \in E, (u, w) \notin E$, and $\sigma(v) < \sigma(u) < \sigma(w)$ or $\sigma(u) < \sigma(v) < \sigma(w)$. Now define Σ as follows.

$$\Sigma_{ij} = \begin{cases} 5 & \text{if } i = \sigma(v), j = \sigma(v), \\ 1 & \text{if } i = j, i \neq \sigma(v), \\ 1 & \text{if } i = \sigma(v), j = \sigma(u) \text{ or } i = \sigma(v), j = \sigma(w) \\ & \text{or } i = \sigma(u), j = \sigma(v) \text{ or } i = \sigma(w), j = \sigma(v), \\ 0 & \text{otherwise.} \end{cases}$$

Then $\Sigma \in P_{G_\sigma}$. Note that all the diagonal entries of Σ are 1 and all off-diagonal entries are 0 except the 3×3 submatrix for $\sigma(u), \sigma(v), \sigma(w)$. Hence, Σ is a permuted block diagonal matrix with $\sigma(u), \sigma(v), \sigma(w)$ forming one block and every other index forming a block by itself. Using the simple fact that the inverse of a permuted block triangular matrix is permuted block triangular, we get that

$$\Sigma_{ij}^{-1} = \begin{cases} \frac{1}{3} & \text{if } i = \sigma(v), j = \sigma(v), \\ \frac{4}{3} & \text{if } i = \sigma(u), j = \sigma(u) \text{ or } i = \sigma(w), j = \sigma(w), \\ 1 & \text{if } i = j, i \neq \sigma(v) \text{ or } \sigma(u) \text{ or } \sigma(w), \\ -\frac{1}{3} & \text{if } i = \sigma(v), j = \sigma(u) \text{ or } i = \sigma(v), j = \sigma(w), \\ & \text{or } i = \sigma(u), j = \sigma(v) \text{ or } i = \sigma(w), j = \sigma(v), \\ \frac{1}{3} & \text{if } i = \sigma(u), j = \sigma(w) \text{ or } i = \sigma(w), j = \sigma(u), \\ 0 & \text{otherwise.} \end{cases}$$

Let C denote the maximal clique of G containing u and v . Note that $w \notin C$. Let Σ_3 denote the 3×3 submatrix of Σ corresponding to $\sigma(u), \sigma(v), \sigma(w)$. Let $\Sigma_3 = L_3 D_3 L_3^T$ denote the modified Cholesky decomposition of Σ_3 , and $\Sigma = LDL^T$ be the modified Cholesky decomposition of Σ . For $i, j \in \{\sigma(u), \sigma(v), \sigma(w)\}$, let us define for simplicity of notation, $(L_3)_{ij}$ as the entry in the row corresponding to $\sigma^{-1}(i)$ and the column corresponding to $\sigma^{-1}(j)$ in L_3 . Using the property that all the diagonal entries of Σ are 1 and all off-diagonal entries are 0 except for Σ_3 , and the uniqueness of the modified Cholesky decomposition of Σ , it follows that

$$L_{ij} = \begin{cases} (L_3)_{ij} & \text{if } i > j, i, j \in \{\sigma(u), \sigma(v), \sigma(w)\}, \\ 1 & \text{if } i = j, \\ 0 & \text{otherwise,} \end{cases}$$

and

$$D_{ii} = \begin{cases} (D_3)_{ii} & \text{if } i = \sigma(u), \sigma(v) \text{ or } \sigma(w), \\ 1 & \text{otherwise.} \end{cases}$$

The actual values of the elements of L_3 and D_3 however, depends on the relative order of $\sigma(u), \sigma(v), \sigma(w)$. If $\sigma(v) < \sigma(u) < \sigma(w)$, then $D_{\sigma(v)\sigma(v)} = 5, D_{\sigma(u)\sigma(u)} = \frac{4}{5}, D_{\sigma(w)\sigma(w)} = \frac{3}{4}$ and $D_{ii} = 1$ if $i \neq \sigma(v), \sigma(u)$ or $\sigma(w)$. Hence,

$$|(\Sigma^{-1})_{\sigma(C)}| = \frac{1}{3} \neq \prod_{i \in \sigma(C)} \frac{1}{D_{ii}} = \frac{1}{4}.$$

If $\sigma(u) < \sigma(v) < \sigma(w)$, then $D_{\sigma(u)\sigma(u)} = 1$, $D_{\sigma(v)\sigma(v)} = 4$, $D_{\sigma(w)\sigma(w)} = \frac{3}{4}$ and $D_{ii} = 1$ if $i \neq \sigma(u), \sigma(v)$ or $\sigma(w)$. Hence,

$$|(\Sigma^{-1})_{\sigma(C)}| = \frac{1}{3} \neq \prod_{i \in \sigma(C)} \frac{1}{D_{ii}} = \frac{1}{4}.$$

Case II: G is homogeneous but σ is not a Hasse tree based elimination scheme.

Since σ is not a Hasse tree based elimination scheme, there exist vertices $a, b \in V$ such that b is an ancestor of a in the Hasse tree of G , and $\sigma(b) < \sigma(a)$. Since b is an ancestor of a , there exists $c \in V$, such that $(b, c) \in E$ and $(a, c) \notin E$. Now there are three possibilities for the way σ orders a, b, c given that $\sigma(b) < \sigma(a)$, namely, $\sigma(b) < \sigma(a) < \sigma(c)$ or $\sigma(b) < \sigma(c) < \sigma(a)$ or $\sigma(c) < \sigma(b) < \sigma(a)$. Let $v = b$, $u = a$, $w = c$ for the first possibility, and $v = b$, $u = c$, $w = a$ for the latter two possibilities. Then note that $(u, v), (v, w) \in E$, $(u, w) \notin E$, and $\sigma(v) < \sigma(u) < \sigma(w)$ or $\sigma(u) < \sigma(v) < \sigma(w)$. We have thus shown the existence of vertices u, v, w such that $(u, v), (v, w) \in E$, $(u, w) \notin E$, and $\sigma(v) < \sigma(u) < \sigma(w)$ or $\sigma(u) < \sigma(v) < \sigma(w)$. We can therefore use the same Σ and maximal clique C as in Case I above, and reach the desired conclusion. Hence the result is proved. \square

We now illustrate the proposition through an example.

Example 3. Consider the homogeneous graph G in Fig. 2(a). The maximal cliques are given by $C_1 = \{w, v', u', u\}$ and $C_2 = \{w, v\}$. The ordering σ given by $\sigma(w) = 5, \sigma(v) = 4, \sigma(u') = 3, \sigma(u) = 2, \sigma(v') = 1$ is a Hasse tree based elimination scheme. Let

$$\Sigma = \begin{pmatrix} 1 & 1 & 1 & 0 & 1 \\ 1 & 2 & 2 & 0 & 2 \\ 1 & 2 & 3 & 0 & 3 \\ 0 & 0 & 0 & 1 & 1 \\ 1 & 2 & 3 & 1 & 5 \end{pmatrix} \in P_{G_\sigma}.$$

Then,

$$|(\Sigma^{-1})_{\sigma(C_1)}| = 1 = \prod_{i \in \sigma(C_1)} \frac{1}{D_{ii}},$$

and

$$|(\Sigma^{-1})_{\sigma(C_2)}| = 1 = \prod_{i \in \sigma(C_2)} \frac{1}{D_{ii}}.$$

Now consider σ which is a perfect vertex elimination scheme, but not a Hasse tree based elimination scheme, given by $\sigma(v') = 5, \sigma(w) = 4, \sigma(u') = 3, \sigma(u) = 2, \sigma(v) = 1$, then

$$\Sigma = \begin{pmatrix} 1 & 0 & 0 & 1 & 0 \\ 0 & 1 & 1 & 1 & 1 \\ 0 & 1 & 2 & 2 & 2 \\ 1 & 1 & 2 & 4 & 3 \\ 0 & 1 & 2 & 3 & 4 \end{pmatrix} \in P_{G_\sigma},$$

but

$$|\Sigma_{\sigma(C_2)}^{-1}| = 2 \neq \prod_{i \in \sigma(C_2)} \frac{1}{D_{ii}} = 1.$$

Now let σ be given by $\sigma(v) = 5, \sigma(u') = 4, \sigma(v') = 3, \sigma(w) = 2, \sigma(u) = 1$. Then, σ is not a perfect vertex elimination scheme, and

$$\Sigma = \begin{pmatrix} 5 & 1 & 1 & 1 & 0 \\ 1 & 5 & 1 & 1 & 1 \\ 1 & 1 & 5 & 1 & 0 \\ 1 & 1 & 1 & 5 & 0 \\ 0 & 1 & 0 & 0 & 5 \end{pmatrix} \in P_{G_\sigma},$$

but

$$|(\Sigma^{-1})_{\sigma(C_1)}| = 0.002042484 \neq \prod_{i \in \sigma(C_1)} \frac{1}{D_{ii}} = 0.001953125.$$

Consider the non-homogeneous graph G in Fig. 2(b). Note however that G is a decomposable graph. The maximal cliques are given by $C_1 = \{u', w\}, C_2 = \{w, u\}, C_3 = \{u, v\}$. The ordering σ given by $\sigma(u') = 4, \sigma(w) = 3, \sigma(u) = 2, \sigma(v) = 1$ is a perfect vertex elimination scheme. Let

$$\Sigma = \begin{pmatrix} 2 & 1 & 0 & 0 \\ 1 & 2 & 1 & 0 \\ 0 & 1 & 2 & 1 \\ 0 & 0 & 1 & 2 \end{pmatrix} \in P_{G_\sigma}.$$

Note however that

$$|(\Sigma^{-1})_{\sigma(C_3)}| = \frac{3}{5} \neq \prod_{i \in \sigma(C_3)} \frac{1}{D_{ii}} = \frac{1}{3}.$$

The two characterizations in the paper are summarized in the main theorem in the introduction.

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