

ON A PARAMETRIZATION OF POSITIVE SEMIDEFINITE MATRICES WITH ZEROS

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ABSTRACT. We study a class of parametrizations of convex cones of positive semidefinite matrices with prescribed zeros. Each such cone corresponds to a graph whose non-edges determine the prescribed zeros. Each parametrization in this class is a polynomial map associated with a simplicial complex supported on cliques of the graph. The images of the maps are convex cones, and the maps can only be surjective onto the cone of zero-constrained positive semidefinite matrices when the associated graph is chordal and the simplicial complex is the clique complex of the graph. Our main result gives a semi-algebraic description of the image of the parametrizations for chordless cycles. The work is motivated by the fact that the considered maps correspond to Gaussian statistical models with hidden variables.

1. INTRODUCTION

For a positive integer m , let $[m] = \{1, \dots, m\}$. Denote the power set of $F \subseteq [m]$ by 2^F . A collection of subsets $\Delta \subseteq 2^{[m]}$ is a simplicial complex if $2^F \subseteq \Delta$ for all $F \in \Delta$. The elements of Δ are called faces and the inclusion-maximal faces are the facets. The ground set of Δ is the union of its faces. The underlying graph $G(\Delta)$ is the simple undirected graph with the ground set as vertex set and the 2-element faces as edges. All simplicial complexes appearing in this paper are assumed to have ground set $[m]$ and, thus, all underlying graphs have vertex set $[m]$. We make this assumption explicit by speaking of a simplicial complex on $[m]$.

Let \mathbb{S}^m be the $m(m+1)/2$ dimensional vector space of symmetric $m \times m$ matrices. For an undirected graph G with vertex set $V(G) = [m]$ and edge set $E(G)$, define the $|E(G)| + m$ dimensional subspace

$$\mathbb{S}^m(G) = \{ \Sigma = (\sigma_{ij}) \in \mathbb{S}^m : \sigma_{ij} = 0 \text{ if } i \neq j \text{ and } \{i, j\} \notin E(G) \}$$

containing the symmetric matrices with zeros at the non-edges of G . Let $\mathbb{S}_{\geq 0}^m \subset \mathbb{S}^m$ be the convex cone of positive semidefinite matrices and $\mathbb{S}_{\geq 0}^m(G) = \mathbb{S}_{\geq 0}^m \cap \mathbb{S}^m(G)$ the convex subcone of matrices with zeros prescribed by the graph.

This paper is concerned with particular parametrizations of the graphical cone $\mathbb{S}_{\geq 0}^m(G)$. For a subset $\Delta \subseteq 2^{[m]}$, define the polynomial map

$$\phi_{\Delta} : \prod_{F \in \Delta} \mathbb{R}^{|F|} \rightarrow \mathbb{S}_{\geq 0}^m$$

given by

$$\phi_{\Delta}(\gamma) = \Gamma(\gamma)\Gamma(\gamma)^T,$$

where, for $\gamma = (\gamma_{i,F} : F \in \Delta, i \in F)$, the $[m] \times \Delta$ matrix $\Gamma(\gamma)$ has entries

$$(1.1) \quad \Gamma(\gamma)_{i,F} = \begin{cases} \gamma_{i,F} & \text{if } i \in F, \\ 0 & \text{otherwise.} \end{cases}$$

The coordinates of the map are

$$(1.2) \quad \phi_\Delta(\gamma)_{ij} = \sum_{F \in \Delta : i, j \in F} \gamma_{i,F} \gamma_{j,F}, \quad i, j \in [m].$$

In particular, the diagonal coordinates

$$(1.3) \quad \phi_\Delta(\gamma)_{ii} = \sum_{F \in \Delta : i \in F} \gamma_{i,F}^2, \quad i \in [m],$$

are sums of squares, which implies that ϕ_Δ is a proper map, that is, compact sets have compact preimages under ϕ_Δ .

We will be interested in the situation when Δ is a simplicial complex on $[m]$. In this case, the map ϕ_Δ is never injective. It has fibers (preimages) of positive dimension unless the underlying graph is the empty graph.

Lemma 1.1. *For any simplicial complex Δ on $[m]$ with underlying graph $G = G(\Delta)$, the image of ϕ_Δ is a closed full-dimensional semi-algebraic subset of $\mathbb{S}_{\geq 0}^m(G)$.*

Proof. If $i \neq j$ and $\{i, j\}$ is not an edge of G , then no face of Δ contains both i and j . Hence, by (1.2), the image is a subset of $\mathbb{S}_{\geq 0}^m(G)$. The image is semi-algebraic because ϕ_Δ is a polynomial map, and it is closed because ϕ_Δ is proper.

If $\Delta' \subset \Delta$ is another simplicial complex with the same underlying graph then the image of $\phi_{\Delta'}$ is contained in the image of ϕ_Δ . To show full dimension, we may thus assume that Δ is the complex whose facets are the edges of G . Using the shorthand $\gamma_i = \gamma_{i, \{i\}}$ and $\gamma_{ij} = \gamma_{i, \{i, j\}}$ in this special case, the non-zero coordinates of ϕ_Δ are

$$\phi_\Delta(\gamma)_{ij} = \begin{cases} \gamma_i^2 + \sum_{k \in [m] : \{i, k\} \in \Delta} \gamma_{ik}^2 & \text{if } i = j, \\ \gamma_{ij} \gamma_{ji} & \text{if } i \neq j. \end{cases}$$

It is evident that there are no algebraic relations among these coordinates and, thus, the image is full-dimensional. \square

Example 1.2. Let Δ be the simplicial complex whose facets are the edges $\{1, 2\}$ and $\{2, 3\}$ of a three-chain. We have that

$$\Gamma(\gamma) = \begin{pmatrix} \gamma_1 & 0 & 0 & \gamma_{12} & 0 \\ 0 & \gamma_2 & 0 & \gamma_{21} & \gamma_{23} \\ 0 & 0 & \gamma_3 & 0 & \gamma_{32} \end{pmatrix}$$

and

$$\phi_\Delta(\gamma) = \begin{pmatrix} \gamma_1^2 + \gamma_{12}^2 & \gamma_{12} \gamma_{21} & 0 \\ \gamma_{12} \gamma_{21} & \gamma_2^2 + \gamma_{21}^2 + \gamma_{23}^2 & \gamma_{23} \gamma_{32} \\ 0 & \gamma_{23} \gamma_{32} & \gamma_3^2 + \gamma_{32}^2 \end{pmatrix}.$$

It can be shown that ϕ_Δ is a surjective map onto the entire cone $\mathbb{S}_{\geq 0}^3(G)$, which here comprises the tridiagonal positive semidefinite matrices. The surjectivity claim holds as a special case of Corollary 3.2. \square

As we describe in more detail in Section 6, the motivation for considering the parametrization ϕ_Δ comes from statistics. The graphical cones $\mathbb{S}_{\geq 0}^m(G)$ correspond to statistical models for the multivariate normal distribution; see [DP07, §2] and references therein. The parametrization ϕ_Δ is particularly useful for tackling statistical problems in covariance graph models, which treat the cone $\mathbb{S}_{\geq 0}(G)$ as a set of covariance matrices. The parametrization can be regarded as arising from constructions involving hidden or latent variables [CW96, RS02]. This connection can be exploited in particular for computation of maximum likelihood estimates and construction of prior distributions for Bayesian inference [Bar08, PDB07]. It also allows one to simplify the study of algebraic properties of graphical models based on mixed graphs; see [STD08].

In Example 1.2, the map ϕ_Δ is surjective. However, it is known that surjectivity need not always hold. The following example has been given in the literature.

Example 1.3. Let Δ be the simplicial complex with facets $\{1, 2\}$, $\{1, 3\}$ and $\{2, 3\}$, and the complete graph K_3 as underlying graph. Now,

$$\phi_\Delta(\gamma) = \begin{pmatrix} \gamma_1^2 + \gamma_{12}^2 + \gamma_{13}^2 & \gamma_{12}\gamma_{21} & \gamma_{13}\gamma_{31} \\ \gamma_{12}\gamma_{21} & \gamma_2^2 + \gamma_{21}^2 + \gamma_{23}^2 & \gamma_{23}\gamma_{32} \\ \gamma_{13}\gamma_{31} & \gamma_{23}\gamma_{32} & \gamma_3^2 + \gamma_{31}^2 + \gamma_{32}^2 \end{pmatrix}.$$

Suppose we are given a positive definite matrix $\Sigma = (\sigma_{ij})$ in $\mathbb{S}_{\geq 0}^3(K_3) = \mathbb{S}_{\geq 0}^3$. Define the correlation matrix $R = (\rho_{ij})$ with entries $\rho_{ij} = \sigma_{ij}/\sqrt{\sigma_{ii}\sigma_{jj}}$. The matrix R is obtained by multiplying Σ from the left and right with the diagonal matrix that has the entries $1/\sqrt{\sigma_{ii}}$ on the diagonal. It follows that Σ is in the image of ϕ_Δ if and only if R is in the image. For R to be in the image, however, it needs to hold that

$$(1.4) \quad \min\{\rho_{12}, \rho_{13}, \rho_{23}\} \leq \frac{1}{\sqrt{2}};$$

see [SRM⁺98]. Clearly, there are positive definite matrices in $\mathbb{S}_{\geq 0}^3$ whose correlation matrices do not obey this condition.

Our Theorem 5.3 applies to this example and gives a semi-algebraic description of the image of ϕ_Δ . This description reveals that a positive definite matrix is in the image only if its correlation matrix R satisfies

$$(1.5) \quad 1 - \rho_{12}^2 - \rho_{13}^2 - \rho_{23}^2 - 2\rho_{12}\rho_{13}\rho_{23} \geq 0.$$

If $\rho_{12}, \rho_{13}, \rho_{23} > 1/2$, then the left hand side in (1.5) is smaller than $1 - 3/4 - 2/8 = 0$. Hence, one may replace $1/\sqrt{2}$ by $1/2$ in the necessary condition in (1.4). \square

This paper explores in detail the images of the maps ϕ_Δ , which we denote by $\text{im}(\phi_\Delta)$. In Section 2, we show that the image is always a convex cone and we describe its extreme rays. In Section 3, we prove that surjectivity of the map can only be achieved if Δ is the clique complex of a chordal (or decomposable) graph. Section 4 collects results relevant for passing to submatrices and Schur complements. In Section 5, we derive the semi-algebraic description of the image when the underlying graph is a chordless cycle. The connection to statistical models is reviewed in Section 6.

2. CONVEXITY

The set $\mathbb{S}_{\geq 0}^m$ of positive semidefinite $m \times m$ matrices forms a full-dimensional convex cone in the $m(m+1)/2$ dimensional vector space of $m \times m$ symmetric matrices. A ray of $\mathbb{S}_{\geq 0}^m$ is the set of nonnegative scalar multiples of some non-zero matrix in $\mathbb{S}_{\geq 0}^m$. An extreme ray is a ray that cannot be written as a positive linear combination of two distinct rays. The extreme rays of $\mathbb{S}_{\geq 0}^m$ are given by the positive semidefinite matrices of rank 1. Hence, $\mathbb{S}_{\geq 0}^m$ is the convex hull of its rank 1 elements.

For $F \subset [m]$, let $\mathbb{S}_{\geq 0}^m(F)$ be the convex cone of positive semidefinite matrices that have zeros outside the $F \times F$ submatrix.

Theorem 2.1. *For any simplicial complex Δ on $[m]$, the image of ϕ_Δ is a convex cone. The matrices on the extreme rays of the image are the rank one matrices that are in $\mathbb{S}_{\geq 0}^m(F)$ for some face $F \in \Delta$.*

Proof. Elements of the image of the map ϕ_Δ are of the form

$$\sum_{F \in \Delta} \Gamma(\gamma)_F \Gamma(\gamma)_F^T,$$

where $\Gamma(\gamma)_F$ is the column of $\Gamma(\gamma)$ corresponding to face F . This column can be any vector in \mathbb{R}^m that has i -th entry zero for each $i \notin F$. It is clear that the image of ϕ_Δ is closed under positive scaling. We will show that it is closed under addition, by induction on the maximal cardinality of a face in Δ .

If all faces have size 1 then the image ϕ_Δ consists of all positive semidefinite diagonal matrices and is convex. Let F be a facet of Δ and suppose it has cardinality at least 2. Consider the matrix

$$\Sigma = \Gamma(\gamma)_F \Gamma(\gamma)_F^T + \Gamma(\gamma')_F \Gamma(\gamma')_F^T$$

and its Cholesky decomposition $\Sigma = LL^T$, where L is a lower triangular matrix. Since $\Sigma \in \mathbb{S}_{\geq 0}^m(F)$, the Cholesky factor L is also in $\mathbb{S}_{\geq 0}^m(F)$. Moreover, only the first column of L may have support F ; denote this column by L_1 . All other columns of L have support strictly smaller than F . These smaller supports correspond to subfaces of F , so they are in Δ . Hence, Σ is the sum of $L_1 L_1^T$ and an element in the image of $\phi_{\Delta \setminus \{F\}}$. (Removing a facet leaves us with another simplicial complex.) Repeating this process for all other faces of maximal cardinality in Δ and using the inductive hypothesis, we see that the image of ϕ_Δ is closed under addition.

Suppose a non-zero matrix Σ is on an extreme ray of the convex cone $\text{im}(\phi_\Delta)$. Then $\Sigma = \Sigma_1 + \Sigma_2$ for some non-zero and distinct matrices Σ_1, Σ_2 in the same cone implies that both Σ_1 and Σ_2 are scalar multiples of Σ . From the definition, any element in the image of ϕ_Δ is a sum of rank one matrices in it, so only rank one matrices can be on the extreme rays. Moreover, any rank one positive semidefinite matrix is on an extreme ray of $\mathbb{S}_{\geq 0}^m$, so it is also on an extreme ray of the convex subcone $\text{im}(\phi_\Delta)$ that contains it. A rank one matrix in $\text{im}(\phi_\Delta)$ is of the form vv^T for some vector $v \in \mathbb{R}^m$ whose support F is a face of Δ . Hence, $vv^T \in \mathbb{S}_{\geq 0}^m(F)$. \square

A clique in an undirected graph G with vertex set $[m]$ is a subset $F \subseteq [m]$ such that for any pair of distinct vertices $i, j \in F$, $\{i, j\}$ is in $E(G)$. The set of all cliques in G forms a simplicial complex on $[m]$ and is called the *clique complex* of G .

Corollary 2.2. *Let Δ be a simplicial complex on $[m]$ with underlying graph G . Then the extreme rays of the image of ϕ_Δ consist of all rank one matrices in $\mathbb{S}_{\geq 0}^m(G)$ if and only if Δ consists of all the cliques in G .*

3. SURJECTIVITY

The maximal rank of a matrix lying on an extreme ray of $\mathbb{S}_{\geq 0}^m(G)$ is called the *sparsity order* of the graph G and denoted $\text{ord}(G)$. A subgraph H of G is called an *induced subgraph* if for all pairs of vertices i, j in H , $\{i, j\} \in E(H) \iff \{i, j\} \in E(G)$. A graph is called *chordal* if it does not contain any chordless cycle of size more than three as an induced subgraph. The following results are known in the literature [AHMR88, HPR89, Lau01].

Theorem 3.1. *For a graph G with m vertices,*

- (i) $1 \leq \text{ord}(G) \leq m - 2$,
- (ii) $\text{ord}(G) = 1$ if and only if G is chordal,
- (iii) $\text{ord}(G) = m - 2$ if and only if $m \leq 3$ or G is a chordless cycle, and
- (iv) if H is an induced subgraph of G , then $\text{ord}(H) \leq \text{ord}(G)$.

These results readily allow one to characterize when the parametrization ϕ_Δ fills all of the graphical cone $\mathbb{S}_{\geq 0}^m(G)$.

Corollary 3.2. *Let Δ be a simplicial complex and G a graph on $[m]$. The map ϕ_Δ is surjective onto $\mathbb{S}_{\geq 0}^m(G)$ if and only if G is chordal and Δ is its clique complex.*

Proof. (Sufficiency) If Δ contains all cliques in G , then $\text{im}(\phi_\Delta)$ contains all rank one matrices in $\mathbb{S}_{\geq 0}^m(G)$. If G is chordal, then its sparsity order is one, so $\mathbb{S}_{\geq 0}^m(G)$ is generated by rank one matrices in it. Hence $\text{im}(\phi_\Delta) = \mathbb{S}_{\geq 0}^m(G)$ and ϕ_Δ is surjective.

(Necessity) First note that the image of ϕ_Δ is a subset of $\mathbb{S}_{\geq 0}^m(G)$ only if all sets in Δ are cliques of G .

Let Δ be the clique complex of G . If G is not chordal, then there is an induced subgraph that is a chordless cycle of size at least 4. So $\text{ord}(G) \geq 2$, and there is an extreme ray of $\mathbb{S}_{\geq 0}^m(G)$ containing matrices of rank at least two. This ray is not in the convex cone $\text{im}(\phi_\Delta)$, so ϕ_Δ is not surjective. It follows that $\phi_{\Delta'}$ is not surjective for any (arbitrary) subset Δ' of Δ .

Suppose Δ does not contain a clique F in G . Let $v \in \mathbb{R}^m$ be a vector with support F . Then vv^T is a rank one element of $\mathbb{S}_{\geq 0}^m(G)$. It lies in an extreme ray of $\mathbb{S}_{\geq 0}^m(G)$ because it lies in an extreme ray of the larger cone $\mathbb{S}_{\geq 0}^m$. Hence, it cannot be written as a sum of other elements in $\mathbb{S}_{\geq 0}^m(G)$, so it is not in $\text{im}(\phi_\Delta)$, and ϕ_Δ is not surjective. \square

Remark 3.3. The sufficiency of the condition in Corollary 3.2 can also be proved by using the Cholesky decomposition to compute a point in the fiber $\phi_\Delta^{-1}(\Sigma)$ of a matrix $\Sigma \in \mathbb{S}_{\geq 0}^m(G)$. The vertices of a chordal graph G can be brought into a perfect elimination ordering, which ensures sparsity of the lower-triangular Cholesky factor; see for example [PPS89, Thm. 2.4]. Suppose the original vertices $1, \dots, m$ are already in such an order. Then $\Sigma = LL^T$ for a lower-triangular matrix $L = (l_{ij})$ with $l_{ij} = 0$ when $i \neq j$ and $\{i, j\}$ is not an edge of G . The support of each column of L is thus a clique in G . It follows that $\Sigma \in \text{im}(\phi_\Delta)$.

The necessity of the chordality condition in Corollary 3.2 also follows from our semi-algebraic characterization of $\text{im}(\phi_\Delta)$ when Δ is the clique complex of a chordless cycle; see Section 5 that also gives an example of a matrix not in the image. \square

In the statistical literature, the parametrization ϕ_Δ is most commonly considered for a simplicial complex Δ given by the edges of a graph. The parametrization for

such an edge complex is surjective only for chordal graphs whose cliques are of cardinality at most two. This means that there may not be any cycles.

Corollary 3.4. *The edge complex Δ of a graph G yields a surjective parametrization ϕ_Δ of $\mathbb{S}_{\geq 0}^m(G)$ if and only if G is a forest (has no cycles).*

4. SUBMATRICES AND SCHUR COMPLEMENTS

For a simplicial complex Δ on $[m]$ and a subset $A \subset [m]$, define the induced subcomplex $\Delta_A = \{F \in \Delta : F \subseteq A\}$.

Lemma 4.1. *Let Δ be a simplicial complex on $[m]$. If Σ is a matrix in the image of ϕ_Δ , then all proper principal submatrices $\Sigma_{A,A}$, $A \subset [m]$, are in the image of the respective induced subcomplex ϕ_{Δ_A} .*

Proof. Write $\Sigma = \Gamma(\gamma)\Gamma(\gamma)^T$. Let $\Gamma_A(\gamma)$ be the submatrix of $\Gamma(\gamma)$ obtained by removing all rows with index not in A . Then $\Sigma_{A,A} = \Gamma_A(\gamma)\Gamma_A(\gamma)^T + \text{diag}(\gamma')$ where $\gamma'_i = \sum_{F \in \Delta \setminus \Delta_A} \gamma_{i,F}^2$. The matrix $\Gamma_A(\gamma)\Gamma_A(\gamma)^T$ is in the image of ϕ_{Δ_A} , and so is the diagonal matrix $\text{diag}(\gamma')$. By convexity (Theorem 2.1), $\Sigma_{A,A} \in \text{im}(\phi_{\Delta_A})$. \square

The converse of the lemma does not hold. If Δ is the edge complex of a chordless cycle, then any matrix in $\mathbb{S}_{\geq 0}^m(G)$ has all of its proper principal submatrices in the image of the corresponding map ϕ_{Δ_A} , but $\text{im}(\phi_G) \subsetneq \mathbb{S}_{\geq 0}^m(G)$ by Corollary 3.2.

For a square matrix M partitioned as

$$M = \begin{pmatrix} A & B \\ C & D \end{pmatrix},$$

the *Schur complement* of a nonsingular submatrix D in M is defined as $M/D := A - BD^{-1}C$. If M is symmetric positive semidefinite, then so is M/D . If D is further partitioned as

$$D = \begin{pmatrix} E & F \\ G & H \end{pmatrix},$$

and H and D/H are non-singular, then the following *quotient formula* holds: $M/D = (M/H)/(D/H)$. Proofs can be found in textbooks on matrix theory.

For a graph $G = (V, E)$ and a proper subset of vertices $U \subset V$, define a new graph G/U on vertex set $V \setminus U$ as follows. A pair $\{i, j\} \subset V \setminus U$ is an edge in G/U if either $\{i, j\}$ is an edge in G or there is a path between i and j in G through vertices in U . For a simplicial complex Δ on ground set V , define a new simplicial complex Δ/U on $V \setminus U$ where a set $A \subset V \setminus U$ forms a face if either it is a face in Δ or there exists a sequence of distinct elements $u_1, u_2, \dots, u_k \in U$ and distinct faces $B_1, \dots, B_{k+1} \in \Delta$ such that $u_i \in B_i \cap B_{i+1}$ and $A = \bigcup_{i=1}^{k+1} B_i \setminus U$. If faces of Δ form cliques in G , then faces of Δ/U form cliques in G/U .

Proposition 4.2. *Let Δ be a simplicial complex on $[m]$ and $U \subsetneq [m]$ a proper subset of nodes. If Σ is in the image of ϕ_Δ and $\Sigma_{U,U}$ is non-singular, then the Schur complement $\Sigma/\Sigma_{U,U}$ is in the image of $\phi_{\Delta/U}$.*

Proof. By the quotient formula, it suffices to prove the assertion when U consists of only one vertex u . Let $\Sigma = \Gamma(\gamma)\Gamma(\gamma)^T$ be in the image of ϕ_Δ . Define as follows a new matrix $\Gamma_{\Delta/u}(\gamma') = [\gamma'_{v,F}]$ whose rows and columns are indexed by vertices and faces of Δ/u . Fix an arbitrary total order “ \leq ” on faces of Δ . For every pair

distinct faces $F_1 < F_2$ of Δ , both containing u , we get a face $F = (F_1 \cup F_2) \setminus \{u\}$ of Δ/u . Let

$$\gamma'_{iF} = (\gamma_{iF_1} \gamma_{uF_2} - \gamma_{iF_2} \gamma_{uF_1}) / \sqrt{\sigma_{uu}},$$

where γ_{iF_j} is shorthand for γ_{i, F_j} and $\gamma_{iF_j} = 0$ if $i \notin F_j$.

Let $A = V \setminus \{u\}$, and define $\Gamma_{\Delta_A}(\gamma)$ to be the submatrix of $\Gamma(\gamma)$ with rows and columns indexed by vertices and edges of the induced subcomplex Δ_A . We now show the following

$$(4.1) \quad \begin{aligned} \Sigma / \Sigma_{u,u} &:= \Sigma_{A,A} - \frac{1}{\sigma_{uu}} \Sigma_{A,u} \Sigma_{u,A} \\ &= \Gamma_{\Delta_A}(\gamma) \Gamma_{\Delta_A}(\gamma)^T + \Gamma_{\Delta/u}(\gamma') \Gamma_{\Delta/u}(\gamma')^T. \end{aligned}$$

Using $\sigma_{ij} = \sum_{F \in \Delta} \gamma_{iF} \gamma_{jF}$, the ij -entry on the right hand side is

$$\begin{aligned} & \sum_{\substack{F \in \Delta \\ u \notin F}} \gamma_{iF} \gamma_{jF} + \sum_{F \in \Delta/u} \gamma'_{iF} \gamma'_{jF} \\ &= \sum_{\substack{F \in \Delta \\ u \notin F}} \gamma_{iF} \gamma_{jF} + \frac{1}{\sigma_{uu}} \sum_{\substack{F_1 < F_2 \in \Delta \\ u \in F_1 \cap F_2}} (\gamma_{iF_1} \gamma_{uF_2} - \gamma_{iF_2} \gamma_{uF_1}) (\gamma_{jF_1} \gamma_{uF_2} - \gamma_{jF_2} \gamma_{uF_1}) \\ &= \sum_{\substack{F \in \Delta \\ u \notin F}} \gamma_{iF} \gamma_{jF} + \frac{1}{\sigma_{uu}} \sum_{\substack{F_1 \neq F_2 \in \Delta \\ u \in F_1 \cap F_2}} (-\gamma_{iF_1} \gamma_{jF_2} \gamma_{uF_1} \gamma_{uF_2} + \gamma_{iF_1} \gamma_{jF_1} \gamma_{uF_2}^2) \\ &= \sum_{\substack{F \in \Delta \\ u \notin F}} \gamma_{iF} \gamma_{jF} + \frac{1}{\sigma_{uu}} \sum_{\substack{F_1, F_2 \in \Delta \\ u \in F_1 \cap F_2}} (-\gamma_{iF_1} \gamma_{jF_2} \gamma_{uF_1} \gamma_{uF_2} + \gamma_{iF_1} \gamma_{jF_1} \gamma_{uF_2}^2) \\ &= \sum_{\substack{F \in \Delta \\ u \notin F}} \gamma_{iF} \gamma_{jF} + \frac{1}{\sigma_{uu}} \sum_{\substack{F_1 \in \Delta \\ u \in F_1}} \gamma_{iF_1} \gamma_{jF_1} \sum_{\substack{F_2 \in \Delta \\ u \in F_2}} \gamma_{uF_2}^2 - \frac{1}{\sigma_{uu}} \sum_{\substack{F_1, F_2 \in \Delta \\ u \in F_1 \cap F_2}} \gamma_{iF_1} \gamma_{jF_2} \gamma_{uF_1} \gamma_{uF_2} \\ &= \sum_{F \in \Delta} \gamma_{iF} \gamma_{jF} - \frac{1}{\sigma_{uu}} \sum_{\substack{F_1, F_2 \in \Delta \\ u \in F_1 \cap F_2}} \gamma_{iF_1} \gamma_{jF_2} \gamma_{uF_1} \gamma_{uF_2}, \end{aligned}$$

which is equal to the ij -entry on the left hand side. From (4.1) and the convexity of $\text{im}(\phi_{\Delta/u})$ shown in Theorem 2.1, it follows that Schur complement $\Sigma / \Sigma_{u,u}$ is in the image of $\phi_{\Delta/u}$. \square

The converse of Proposition 4.2 cannot hold in general. Let G be a 3-cycle and consider ϕ_G given by the edge complex of G . Then any Schur complement $\Sigma / \Sigma_{u,u}$ of $\Sigma \in \mathbb{S}_{\geq 0}^m(G)$ is in $\text{im}(\phi_{G/\{u\}})$, but not every such matrix Σ is in $\text{im}(\phi_G)$.

5. CHORDLESS CYCLES

Let C_m be the chordless m -cycle with edges $\{1, 2\}, \{2, 3\}, \dots, \{1, m\}$. Excluding trivial cases, assume that $m \geq 3$. Let Δ be the simplicial complex whose facets are the edges of C_m , and define $\phi_{C_m} = \phi_\Delta$. For $m \geq 4$, there is no other simplicial complex Δ' that gives a parametrization $\phi_{\Delta'}$ whose image is a full-dimensional subset of $\mathbb{S}_{\geq 0}^m(C_m)$. In this section we give a semi-algebraic description of $\text{im}(\phi_{C_m})$.

We begin with a simple yet important observation. For a symmetric matrix $\Sigma \in \mathbb{S}^m$ and two distinct indices $i, j \in [m]$, define $\Sigma^{(ij)}$ to be the symmetric matrix obtained by negating the (i, j) and (j, i) entries of Σ .

Lemma 5.1. *Suppose $\Sigma \in \mathbb{S}_{\geq 0}^m$ is a positive semidefinite matrix, and Δ is the edge complex of a graph. If $i \neq j$ and $\{i, j\} \in \Delta$, then Σ is in the image of ϕ_Δ if and only if $\Sigma^{(ij)}$ is in $\text{im}(\phi_\Delta)$.*

Proof. If $\Sigma = \phi_{\Delta}(\gamma)$, then $\Sigma^{(ij)} = \phi_{\Delta}(\bar{\gamma})$, where $\bar{\gamma}$ is identical to γ except for the single entry $\gamma_{ij} = \gamma_{i,\{i,j\}}$ that is replaced by its negative $-\gamma_{ij}$. The entry γ_{ji} remains unchanged. \square

Note that Lemma 5.1 immediately yields the necessary condition stated in (1.5) in Example 1.3 about $C_3 = K_3$, the complete graph on 3 nodes. The lemma can also be used to give an explicit example of a matrix not in the image of the parametrization for C_m , $m \geq 3$.

Example 5.2. For $m \geq 3$, define the symmetric $m \times m$ matrix

$$\Sigma(\rho) = \begin{pmatrix} 1 & \frac{1}{2} & & & & \frac{1}{2}\rho \\ \frac{1}{2} & 1 & \frac{1}{2} & & & \\ & & \ddots & \ddots & \ddots & \\ & & & \frac{1}{2} & 1 & \frac{1}{2} \\ \frac{1}{2}\rho & & & & \frac{1}{2} & 1 \end{pmatrix},$$

where all omitted entries are zero such that $\Sigma(\rho) \in \mathbb{S}^m(C_m)$. Omitting the m -th row and column of $\Sigma(\rho)$ yields a positive definite tridiagonal matrix. Hence, $\Sigma(\rho)$ is in the graphical cone $\mathbb{S}_{\geq 0}^m(C_m)$ if and only if $\det(\Sigma(\rho)) \geq 0$. Using Laplace expansions and the recursive formula for the determinant of a tridiagonal matrix, one can show that

$$\det \Sigma(\rho) = \begin{cases} \frac{1}{2^m} [m+1 - (m-1)\rho](1+\rho) & \text{if } m \text{ is odd,} \\ \frac{1}{2^m} [m+1 + (m-1)\rho](1-\rho) & \text{if } m \text{ is even.} \end{cases}$$

If m is odd, choose $\rho \in (1, 1 + 2/(m-1))$. If m is even, choose $\rho \in (-1 - 2/(m-1), -1)$. Then the determinant of $\Sigma(\rho)$ is positive but the determinant of $\Sigma(-\rho)$ is negative. Since $\Sigma(\rho)^{(1m)} = \Sigma(-\rho)$, it follows from Lemma 5.1 that $\Sigma(\rho)$ is in $\mathbb{S}_{\geq 0}^m(C_m)$ but not in the image of ϕ_{C_m} .

We now state the main result of this section, a semi-algebraic description of the image of ϕ_{C_m} . Let $\mathcal{E}_{\text{dis}}(C_m)$ be the collection of all subsets Θ of the edge set of C_m that comprise only pairwise disjoint edges, that is, for which $\{i, j\}, \{k, l\} \in \Theta$ implies that $\{i, j\} \cap \{k, l\} = \emptyset$. For $\Theta \in \mathcal{E}_{\text{dis}}(C_m)$, we write $[m] \setminus \Theta$ to denote the set of nodes not incident to any edge in Θ . If $\Sigma = (\sigma_{ij})$ is a matrix in $\mathbb{S}_{\geq 0}^m(C_m)$ then its determinant can be expanded as

$$(5.1) \quad \det(\Sigma) = (-1)^{m+1} \cdot 2 \prod_{i=1}^m \sigma_{i,i+1} + \sum_{\Theta \in \mathcal{E}_{\text{dis}}(C_m)} (-1)^{|\Theta|} \prod_{\{i,j\} \in \Theta} \sigma_{ij}^2 \prod_{i \in [m] \setminus \Theta} \sigma_{ii};$$

compare [CDS95, §1.4, eqn. (1.42)]. In the first term, which corresponds to the entire cycle C_m , the indices are read modulo m such that $\rho_{m,m+1} \equiv \rho_{1m}$. The following theorem is the main result of this section.

Theorem 5.3. *A matrix $\Sigma = (\sigma_{ij}) \in \mathbb{S}_{\geq 0}^m(C_m)$ is in the image of ϕ_{C_m} if and only if*

$$\sum_{\Theta \in \mathcal{E}_{\text{dis}}(C_m)} (-1)^{|\Theta|} \prod_{\{i,j\} \in \Theta} \sigma_{ij}^2 \prod_{i \in [m] \setminus \Theta} \sigma_{ii} \geq 2 \prod_{i=1}^m |\sigma_{i,i+1}|.$$

TABLE 1. Spherical volume of the image of ϕ_{C_m} as a fraction of the spherical volume of the cone $\mathbb{S}_{\geq 0}(C_m)$.

m	3	4	5	6	7
Vol	0.78	0.90	0.95	0.98	0.99

Proof. (Necessity) A matrix $\Sigma \in \text{im}(\phi_{C_m})$ is positive semidefinite and thus has a nonnegative determinant. Pick any edge in C_m , say $\{1, 2\}$. Then, by Lemma 5.1, $\Sigma^{(12)}$ is positive semidefinite. Hence,

$$\min \left\{ \det(\Sigma), \det(\Sigma^{(12)}) \right\} = -2 \prod_{i=1}^m |\sigma_{i,i+1}| + \sum_{\Theta \in \mathcal{E}_{\text{dis}}(C_m)} (-1)^{|\Theta|} \prod_{\{i,j\} \in \Theta} \sigma_{ij}^2 \prod_{i \in [m] \setminus \Theta} \sigma_{ii} \geq 0.$$

(Sufficiency) We need to show that under the assumed condition on $\Sigma \in \mathbb{S}_{\geq 0}(C_m)$, the equation system $\phi_{C_m}(\gamma) = \Sigma$ has a feasible solution (γ) in $(\mathbb{R})^V \times (\mathbb{R}^2)^E$. Our proof will show that $\gamma_{i,\{i\}}$ does not play an important role and can simply be set to zero. Since $\text{im}(\Delta)$ is closed and full-dimensional in $\mathbb{S}_{\geq 0}(G)$, it suffices to show that a dense (Zariski open) subset of points Σ satisfying the necessity condition is contained in $\text{im}(\Delta)$. We show that for positive definite Σ , any complex solution γ (with $\gamma_{i,\{i\}} = 0$ for all $i = 1, \dots, m$) is in fact real and thus feasible (Lemma 5.5). The proof is completed by demonstrating the existence of complex solutions for generic Σ using Bernstein's theorem (Lemma 5.6). \square

The following is an immediate consequence of Theorem 5.3.

Corollary 5.4. *For a positive definite matrix $\Sigma = (\sigma_{ij})$ in $\mathbb{S}_{\geq 0}(C_m)$ the following are equivalent:*

- (1) Σ is in the image of ϕ_{C_m} .
- (2) $\Sigma^{(ij)}$ is positive definite for some edge $ij \in C_m$.
- (3) $\Sigma^{(ij)}$ is positive definite for all edges $ij \in C_m$.

The semi-algebraic condition from Theorem 5.3 is easily verified, and we can use it to compute the spherical volume of the cone $\text{im}(\phi_{C_m})$ by Monte Carlo integration. Table 1 shows which fraction of the cone $\mathbb{S}_{\geq 0}(C_m)$ is covered by the image of ϕ_{C_m} , when quantifying this by the ratio of the spherical volumes of the two cones. The rounded ratios were computed by simulating 100,000 matrices in $\mathbb{S}_{\geq 0}(C_m)$. In terms of the ratio of spherical volumes, the difference between $\text{im}(\phi_{C_m})$ and $\mathbb{S}_{\geq 0}(C_m)$ is largest for $m = 3$ and becomes rather minor for $m = 6, 7$.

The remainder of the section is devoted to the details of the proof of the sufficiency of the condition in Theorem 5.3. As mentioned above, our approach is study the equation system $\phi_{\Delta}(\gamma) = \Sigma$ for a given matrix $\Sigma = (\sigma_{ij}) \in \mathbb{S}_{\geq 0}(G)$, which is treated as a parameter to the system. For $\Delta = E(C_m)$, the equations take the form:

$$(5.2a) \quad \gamma_{i,\{i\}}^2 + \gamma_{i,i-1}^2 + \gamma_{i,i+1}^2 = \sigma_{ii}, \quad i = 1, \dots, m,$$

$$(5.2b) \quad \gamma_{i-1,i} \gamma_{i,i-1} = \sigma_{i-1,i}, \quad i = 1, \dots, m.$$

where $\gamma_{i,j}$ denotes $\gamma_{i,\{i,j\}}$ and indices are read modulo m such that $0 \equiv m$ and $1 \equiv m + 1$. The $2m$ equations in (5.2a) and (5.2b) involve $3m$ unknowns and have

an m -dimensional solution set in \mathbb{C}^{3m} . In the sequel we simply omit the unknowns $\gamma_{i,\{i\}}$ from the system. In other words, we study the $2m$ equations in $2m$ unknowns:

$$(5.3a) \quad \gamma_{i,i-1}^2 + \gamma_{i,i+1}^2 = \sigma_{ii}, \quad i = 1, \dots, m,$$

$$(5.3b) \quad \gamma_{i-1,i} \gamma_{i,i-1} = \sigma_{i-1,i}, \quad i = 1, \dots, m.$$

We will show that system (5.3a)-(5.3b) has a real solution if Σ satisfies the condition from Theorem 5.3, which will imply that the system (5.2a)-(5.2a) has a real solution, too. Somewhat surprisingly it suffices to argue that they have a complex solution, as is made precise in the next lemma.

Lemma 5.5. *If a positive definite matrix $\Sigma \in \mathbb{S}_{\geq 0}(C_m)$ satisfies the necessary condition from Theorem 5.3, then all complex solutions to the equations (5.3a)-(5.3b) are in fact real.*

Proof. Suppose the vector $\gamma \in (\mathbb{C}^2)^E$ provides a solution to (5.3a)-(5.3b). Fill the $2m$ unknowns in a matrix $\Gamma(\gamma) \in \mathbb{C}^{V \times E} \simeq \mathbb{C}^{m \times m}$ as in (1.1). Note that we are setting $\gamma_{i,\{i\}} = 0$ for all $i = 1, \dots, m$, so the columns in $\Gamma(\gamma)$ corresponding to the singleton faces $\{1\}, \dots, \{m\}$ are zero and can be omitted. Augment $\Gamma(\gamma)$ to an $(m+1) \times m$ matrix $\Gamma_{(12)}$ by adding the vector $(\gamma_{12}, 0, \dots, 0)$ as a first row. Based on the equations (5.3a)-(5.3b),

$$(5.4) \quad \Gamma_{(12)} \Gamma_{(12)}^T = \begin{pmatrix} \gamma_{12}^2 & \gamma_{12}^2 & \sigma_{12} & & & & & & & & \\ \gamma_{12}^2 & \sigma_{11} & \sigma_{12} & & & & & & & & \sigma_{1m} \\ \sigma_{12} & \sigma_{12} & \sigma_{22} & \sigma_{23} & & & & & & & \\ & & & \sigma_{23} & \sigma_{33} & & & & & & \ddots \\ & & & & \ddots & \ddots & & & & & \\ & & & & & & \ddots & \ddots & & & \sigma_{m-1,m} \\ & \sigma_{1m} & & & & & & \sigma_{m-1,m} & & & \sigma_{mm} \end{pmatrix}$$

with blank entries being zero. The $(m+1) \times (m+1)$ matrix $\Gamma_{(12)} \Gamma_{(12)}^T$ has rank at most m , and thus its determinant vanishes. Therefore, γ_{12} has to satisfy the quartic equation

$$(5.5) \quad \det\left(\Gamma_{(12)} \Gamma_{(12)}^T\right) = a\gamma_{12}^4 + b\gamma_{12}^2 + c = 0.$$

By expanding the determinant of (5.4) along the first row (or column), the coefficients in (5.5) are found to be:

$$\begin{aligned} a &= -\det\left(\Sigma_{[m]\setminus\{1\}, [m]\setminus\{1\}}\right), \\ b &= \det(\Sigma) + 2\sigma_{12}^2 \det\left(\Sigma_{[m]\setminus\{1,2\}, [m]\setminus\{1,2\}}\right) + (-1)^m \cdot 2 \prod_{i=1}^m \sigma_{i-1,i}, \\ c &= -\sigma_{12}^2 \det\left(\Sigma_{[m]\setminus\{2\}, [m]\setminus\{2\}}\right). \end{aligned}$$

Note that the third term in b cancels out a term in $\det(\Sigma)$; recall (5.1). It remains to argue that under the assumption on Σ , the quartic in (5.5) has only real solutions. Define $\Sigma^{(12)}$ by negating σ_{12} as in Lemma 5.1. Then the assumption on Σ implies that both $\det(\Sigma)$ and $\det(\Sigma^{(12)})$ are positive.

First, we claim that the discriminant $b^2 - 4ac$ is positive because

$$(5.6) \quad b^2 - 4ac = \det(\Sigma) \det(\Sigma^{(12)}).$$

Since

$$(5.7) \quad \det(\Sigma) + (-1)^m \cdot 2 \prod_{i=1}^m \sigma_{i-1,i} = \det(\Sigma^{(12)}) - (-1)^m \cdot 2 \prod_{i=1}^m \sigma_{i-1,i}$$

we can write

$$b^2 = \left[\det(\Sigma) + 2\sigma_{12}^2 \det(\Sigma_{[m]\setminus\{1,2\},[m]\setminus\{1,2\}}) + (-1)^m \cdot 2 \prod_{i=1}^m \sigma_{i-1,i} \right] \times \\ \left[\det(\Sigma^{(12)}) + 2\sigma_{12}^2 \det(\Sigma_{[m]\setminus\{1,2\},[m]\setminus\{1,2\}}) - (-1)^m \cdot 2 \prod_{i=1}^m \sigma_{i-1,i} \right].$$

Multiplying out the product, and using (5.7) once more, yields that

$$(5.8) \quad b^2 = \det(\Sigma) \det(\Sigma^{(12)}) + 4\sigma_{12}^4 \det(\Sigma_{[m]\setminus\{1,2\},[m]\setminus\{1,2\}})^2 + 4 \prod_{i=1}^m \sigma_{i-1,i}^2 + \\ 2\sigma_{12}^2 \det(\Sigma_{[m]\setminus\{1,2\},[m]\setminus\{1,2\}}) \left(\det(\Sigma) + \det(\Sigma^{(12)}) \right).$$

Expansion of determinants shows that

$$\det(\Sigma) = \sigma_{11} \det(\Sigma_{[m]\setminus\{1\},[m]\setminus\{1\}}) - \sigma_{12}^2 \det(\Sigma_{[m]\setminus\{1,2\},[m]\setminus\{1,2\}}) \\ - \sigma_{1m}^2 \det(\Sigma_{[m-1]\setminus\{1\},[m-1]\setminus\{1\}}) - (-1)^m \cdot 2 \prod_{i=1}^m \sigma_{i-1,i}.$$

Hence,

$$(5.9) \quad \det(\Sigma) + \det(\Sigma^{(12)}) = 2\sigma_{11} \det(\Sigma_{[m]\setminus\{1\},[m]\setminus\{1\}}) \\ - 2\sigma_{12}^2 \det(\Sigma_{[m]\setminus\{1,2\},[m]\setminus\{1,2\}}) - 2\sigma_{1m}^2 \det(\Sigma_{[m-1]\setminus\{1\},[m-1]\setminus\{1\}}).$$

Moreover, we find from another expansion that

$$(5.10) \quad \det(\Sigma_{[m]\setminus\{2\},[m]\setminus\{2\}}) = \\ \sigma_{11} \det(\Sigma_{[m]\setminus\{1,2\},[m]\setminus\{1,2\}}) + \sigma_{1m}^2 \det(\Sigma_{[m-1]\setminus\{1,2\},[m-1]\setminus\{1,2\}}).$$

Combining (5.8), (5.9) and (5.10), we obtain that our claim (5.6) holds if

$$(5.11) \quad \sigma_{12}^2 \sigma_{1m}^2 \det(\Sigma_{[m]\setminus\{1\},[m]\setminus\{1\}}) \det(\Sigma_{[m-1]\setminus\{1,2\},[m-1]\setminus\{1,2\}}) = \\ \sigma_{12}^2 \sigma_{1m}^2 \det(\Sigma_{[m]\setminus\{1,2\},[m]\setminus\{1,2\}}) \det(\Sigma_{[m-1]\setminus\{1\},[m-1]\setminus\{1\}}) - \prod_{i=1}^m \sigma_{i-1,i}^2.$$

However, all determinants appearing in (5.11) are determinants of tri-diagonal matrices and thus (5.11) can be shown to hold by an induction on m .

As just established, $b^2 - 4ac > 0$. Moreover, since we assume that both $\det(\Sigma)$ and $\det(\Sigma^{(12)})$ are positive it holds that $b > 0$; see e.g. (5.8). In addition, a and c are both negative, and it follows from the usual formula for the solutions of a quadratic equation that all four solutions to the quartic equation in (5.5) are real. Hence, γ_{12} is real and, by symmetry, the same is true for all other components of a solution to (5.3a)-(5.3b). \square

Below we will use a classic result from algebraic geometry to argue that the equations (5.3a)-(5.3b) indeed have complex solutions. For the argument, we are able to restrict attention to generic choices of the entries of Σ because $\text{im}(\Delta)$ is closed and full-dimensional in $\mathbb{S}_{\geq 0}(G)$.

In the final step that completes the proof of sufficiency of the condition in Theorem 5.3, we need to show that for a generic choice of Σ , the equations (5.3a)-(5.3b) have at least one complex solution. In particular, we may assume that $\sigma_{i-1,i} \neq 0$ for all $i \in [m]$. This implies that a solution of (5.3a)-(5.3b) has all components non-zero. Moreover, the solution set of (5.3a)-(5.3b) is identical, up to sign, to that of the rational system

$$\gamma_{i,i+1}^2 + \frac{\sigma_{i-1,i}^2}{\gamma_{i-1,i}^2} = \sigma_{ii}, \quad i = 1, \dots, m.$$

Or simpler yet, setting $x_i = \gamma_{i-1,i}$ (in particular, $x_0 \equiv x_m$), the solution set corresponds exactly to the solution set of the polynomial system

$$(5.12) \quad x_{i+1}^2 x_i^2 - \sigma_{ii} x_i^2 + \sigma_{i-1,i}^2 = 0, \quad i = 1, \dots, m,$$

in the torus $(\mathbb{C}^*)^m = (\mathbb{C} \setminus \{0\})^m$.

Lemma 5.6. *For generic choices of the coefficients σ_{ij} , the equations (5.12) have 2^{m+1} solutions in the torus $(\mathbb{C}^*)^m$.*

Proof. By Bernstein's Theorem [Ber75], for generic choices of the coefficients, the number of roots of a system of polynomial equations is equal to the *mixed volume* of the Newton polytopes of the polynomials. In [HS95], Huber and Sturmfels gave a new proof of this statement and a practical method for computing the mixed volume using mixed subdivisions. We will outline this method here.

Let P_1, P_2, \dots, P_m be polytopes in \mathbb{R}^m with vertex sets A_1, A_2, \dots, A_m respectively. Choose a *lifting function* $w_i : A_i \rightarrow \mathbb{R}$ for each i , and let $\hat{A}_i = \{(v, w_i(v)) \in \mathbb{R}^{m+1} : v \in A_i\}$. Let Q be the convex hull of Minkowski sum $\hat{A}_1 + \hat{A}_2 + \dots + \hat{A}_m$. The *lower hull* of Q consists of the facets whose inward pointing normal vectors have positive last coordinate. The projection of the lower hull of Q forms a subdivision of $P_1 + \dots + P_m$. For a generic choice of lifting function which lies in the complement a certain hyperplane arrangement, the induced subdivision is a *fine mixed subdivision*. For such a fine mixed subdivision, any facet in the lower hull of Q is the convex hull of a set of the form $B_1 + B_2 + \dots + B_m$ where $B_i \subset \hat{A}_i$, $\dim(\text{conv}(B_i)) = |B_i| - 1$, and $\sum_{i=1}^m (|B_i| - 1) = m$. Moreover, the choice of B_1, \dots, B_m is unique for each lower facet. A *mixed cell* is the projection of a lower facet for which $\dim(\text{conv}(B_i)) = 1$ for all i . The mixed volume of the tuple (A_1, A_2, \dots, A_m) is the sum of m -dimensional volumes of the mixed cells that are induced by a generic lifting function. See [HS95] for details and proofs.

Now we will compute the mixed volume of the Newton polytopes of polynomials in (5.12), which are $P_1, P_2, \dots, P_m \subset \mathbb{R}^m$ where P_i is the triangle with vertices $A_i = \{\mathbf{0}, 2e_i, 2e_i + 2e_{i+1}\}$ and the index i is taken modulo m . For each P_i , choose a generic lifting function w_i such that $w_i(\mathbf{0}) > 0$, $w_i(2e_i + 2e_{i+1}) > 0$, and $w_i(2e_i) = 0$. Translating a lifting function w_i by a constant does not affect the mixed subdivision, so such a generic choice is possible.

Suppose a lower facet $\text{conv}(B_1 + \dots + B_m)$ of Q has inward pointing normal vector $(c_1, c_2, \dots, c_m, 1) \in \mathbb{R}^{m+1}$ and $|B_i| = 2$ for all i . Each set B_i is the subset of \hat{A}_i that minimizes the scalar product with the normal vector $(c_1, c_2, \dots, c_m, 1)$.

Suppose $B_1 = \{(\mathbf{0}, a), (2e_1 + 2e_2, b)\}$ where $a = w_1(\mathbf{0})$ and $b = w_1(2e_1 + 2e_2)$. Since the inner product with the normal vector is minimized on the edge B_1 of \hat{A}_1 , we must have $a = 2c_1 + 2c_2 + b < 2c_1$, so $c_1 > a/2 > 0$ and $c_2 < -b/2 < 0$. Then we must have $c_3 < 0$; otherwise B_2 would only contain one point $(2e_2, 0)$. By repeating this argument, we get $c_m < 0$, and finally $c_1 < 0$, contradicting the earlier requirement that $c_1 > 0$. Hence B_1 cannot be of the form $\{(\mathbf{0}, a), (2e_1 + 2e_2, b)\}$. Similarly, for every $i = 1, \dots, m$ the edge $\{\mathbf{0}, 2e_i + 2e_{i+1}\} \subset P_i$ cannot be in any mixed cell.

A mixed cell is a Minkowski sum of m edges, one from each A_i . Since we know that the edges $\{\mathbf{0}, 2e_i + 2e_{i+1}\}$ do not participate in any mixed cell induced by our lifting function, we need to choose either the edge $\{\mathbf{0}, 2e_i\}$ or $\{2e_i, 2e_i + 2e_{i+1}\}$ from each A_i . These edges are in the directions e_i and e_{i+1} respectively. Therefore, unless we choose all edges to be of the first kind or all the second kind, the Minkowski sum is not full dimensional. Both of the two candidates are in fact mixed cells because they are projections of facets of Q with respective inward pointing normal vectors

$$(w_1(\mathbf{0}), w_2(\mathbf{0}), \dots, w_m(\mathbf{0}), 1) \text{ and} \\ (-w_m(2e_m + 2e_1), -w_1(2e_1 + 2e_2), \dots, -w_{m-1}(2e_{m-1} + 2e_m), 1).$$

Each of these two mixed cells is an m -dimensional cube with length 2 and has volume 2^m , so the mixed volume of (P_1, \dots, P_m) is 2^{m+1} . \square

Lemma 5.7. *For any positive definite matrix $\Sigma = (\sigma_{ij})$ in image of ϕ_{C_m} , the fiber $\{\gamma : \phi_{C_m}(\gamma) = \Sigma \text{ and } \gamma_{i,\{i\}} = 0 \text{ for all } i = 1, \dots, m\}$ consists of exactly 2^{m+1} elements, or two elements up to sign.*

Proof. First consider the case when all $\sigma_{i,i+1}$ are nonzero. Since elements of the fiber are in bijection with the solutions of (5.12) under setting $x_i = \gamma_{i-1,i}$, it suffices to show that (5.12) has 2^{m+1} solutions. For generic Σ , this was done in Lemma 5.6. For an arbitrary Σ , let Σ_n be a sequence of generic matrices in $\text{im}(\phi_{C_m})$ that converges to Σ . Each of the 2^{m+1} solutions for Σ_n can be expressed in terms of radicals using (5.5) and (5.12), and each of these 2^{m+1} sequences converge to solutions of (5.12) for Σ by continuity. Moreover the limit points are distinct because the discriminant $b^2 - 4ac$ in (5.5) is positive for Σ as shown the proof of Lemma 5.5 and all x_i in a solution must be nonzero.

Now suppose $\sigma_{12} = 0$. In this case Lemma 5.5 still holds but Lemma 5.6 does not apply. We will now show that the system (5.3a)-(5.3b) still has 2^{m+1} complex solutions. Since $\sigma_{12} = 0$, we have either $\gamma_{12} = 0$ or $\gamma_{21} = 0$. If $\gamma_{21} = 0$, then we can determine $\gamma_{23}, \gamma_{32}, \gamma_{34}, \gamma_{43}, \dots, \gamma_{1,m}, \gamma_{12}$ in that order along the cycle, using (5.3a) and (5.3b) alternately. These equations show that the sequence of γ_{ij} obtained this way is unique up to sign unless we get $\gamma_{i,i+1} = 0$ for some i . However, if $\gamma_{i,i+1} = 0$, then the principal submatrix of Σ indexed by $\{2, 3, \dots, i\}$ would be equal to $\Gamma(\gamma)\Gamma(\gamma)^T$ where $\Gamma(\gamma)$ is defined as in the introduction for the subgraph on vertices $2, 3, \dots, i$ and edges $\{2, 3\}, \dots, \{i-1, i\}$. Then $\Gamma(\gamma)$ would have more rows than nonzero columns since $\gamma_{i,\{i\}} = 0$ for all i , so $\Gamma(\gamma)\Gamma(\gamma)^T$ would not have full rank, contradicting the hypothesis that Σ is positive definite. Hence $\gamma_{i,i+1} \neq 0$ for all i , and setting $\gamma_{21} = 0$ determines all other γ_{ij} up to sign. There are two choices of signs for each pair $\gamma_{i,i+1}$ and $\gamma_{i+1,i}$, even if $\sigma_{i,i+1} = 0$, so there are 2^m solutions with $\gamma_{21} = 0$.

By symmetry, if $\gamma_{12} = 0$, then we can determine $\gamma_{1,m}, \gamma_{m,1}, \gamma_{m,m-1}, \dots, \gamma_{23}, \gamma_{21}$ in that order (going around the cycle in the other direction, with $\gamma_{i,i-1} \neq 0$ in this

case), so there are 2^m solutions when $\gamma_{12} = 0$ also. We cannot have both $\gamma_{21} = 0$ and $\gamma_{12} = 0$ because that would imply that $\Gamma(\gamma)\Gamma(\gamma)^T$ is singular. So there are 2^{m+1} distinct solutions (two solutions up to sign) to the system (5.3a)-(5.3b) when $\sigma_{12} = 0$. By symmetry, there are 2^{m+1} solutions for every $\Sigma \in \text{im}(\phi_{C_m})$. \square

6. STATISTICAL MODELS AND BIPARTITE ACYCLIC DIGRAPHS

In probability theory, positive semidefinite matrices arise as covariance matrices of random vectors. When the random vector $Y = (Y_1, \dots, Y_m)$ is Gaussian (has a multivariate normal distribution) with covariance matrix $\Sigma = (\sigma_{ij})$, then $\sigma_{ij} = 0$ is equivalent to the stochastic independence of the two random variables Y_i and Y_j . Hence, the convex cone $\mathbb{S}_{\Sigma=0}^m(G)$ of positive semidefinite matrices with zeros at the non-edges of a graph G collects all covariance matrices for which the components of Y exhibit a pattern of independences.

For a simplicial complex Δ on $[m]$ with underlying graph G , the map ϕ_Δ traces out a full-dimensional subset of $\mathbb{S}_{\Sigma=0}^m(G)$. This subset arises quite naturally for random vectors whose components are linear combinations of a set of independent random variables. We review this construction next.

Let Δ_2 the set of all faces in Δ that have cardinality at least two. Introduce the random variables ε_i , $i \in [m]$, and H_F , $F \in \Delta_2$. Suppose the random variables H_F are mutually independent with a standard normal distribution, denoted $\mathcal{N}(0, 1)$. Suppose further that the ε_i are mutually independent, independent of the H_F , and distributed as $\varepsilon_i \sim \mathcal{N}(0, \gamma_{i, \{i\}}^2)$ where $\gamma_{i, \{i\}}^2$ is the variance. Define new random variables Y_1, \dots, Y_m as linear combinations:

$$(6.1) \quad Y_i = \sum_{F \in \Delta_2: i \in F} \gamma_{i, F} H_F + \varepsilon_i, \quad i \in [m].$$

Proposition 6.1. *The random vector $Y = (Y_1, \dots, Y_m)$ defined by (6.1) has the positive semidefinite matrix $\phi_\Delta(\gamma)$ as covariance matrix.*

Proof. Write I for the identity matrix (of the appropriate size). Let $\varepsilon = (\varepsilon_1, \dots, \varepsilon_m)$ and $H = (H_F : F \in \Delta_2)$. The concatenation (ε, H) is a random vector with the diagonal $|\Delta| \times |\Delta|$ covariance matrix

$$(6.2) \quad \Omega = \begin{pmatrix} \text{diag}(\gamma_{i, \{i\}}^2) & 0 \\ 0 & I \end{pmatrix}.$$

Let $\Gamma_2(\gamma)$ be the submatrix of $\Gamma(\gamma)$ obtained by retaining only the columns corresponding to faces in Δ_2 ; recall (1.1). Define the $|\Delta| \times |\Delta|$ matrix

$$(6.3) \quad \Lambda = \begin{pmatrix} I & -\Gamma_2(\gamma) \\ 0 & I \end{pmatrix}.$$

Multiplying Λ with $(Y, H)^T$ gives the vector $(\varepsilon, H)^T$. By standard results about linear combinations of random variables, it follows that the Gaussian random vector (Y, H) has covariance matrix $\Lambda^{-1}\Omega\Lambda^{-T}$. The covariance matrix of Y alone is the principal submatrix given by the first m rows and columns of $\Lambda^{-1}\Omega\Lambda^{-T}$. The inverse Λ^{-1} is obtained by negating the upper right block, which becomes simply $\Gamma_2(\gamma)$. It follows that, as claimed,

$$\text{diag}(\gamma_{i, \{i\}}^2) + \Gamma_2(\gamma)\Gamma_2(\gamma)^T = \Gamma(\gamma)\Gamma(\gamma)^T = \phi_\Delta(\gamma). \quad \square$$

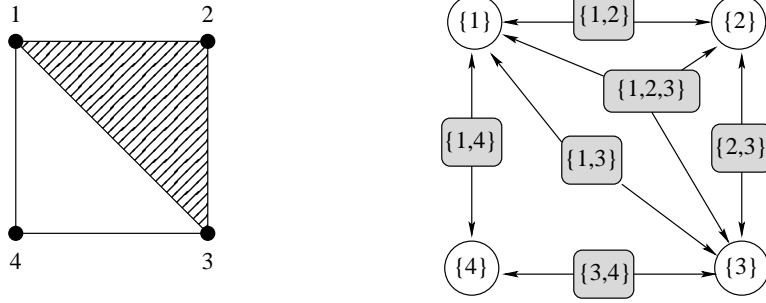


FIGURE 1. A simplicial complex (left) and the acyclic bipartite digraph corresponding to it (right).

In the field of graphical statistical modelling, it is customary to visualize an equation system such as (6.1) by means of an acyclic digraph; see for instance [DSS09, Chap. 3]. Here, we draw the digraph D_Δ that has vertex set Δ and the edges $F \rightarrow \{i\}$ for all pairs of an index $i \in [m]$ and a face $F \in \Delta_2$ with $i \in F$. Note that D_Δ is bipartite with respect to the partitioning $\Delta = \Delta_1 \cup \Delta_2$, where $\Delta_1 = \{\{i\} : i \in [m]\}$ are the singleton faces and Δ_2 was defined above. See Figure 1 for an example.

In the setup of Proposition 6.1, the random variables Y_i are functions of the hidden variables H_F , up to the noise given by the ε_i . There is a dual construction in which the hidden variables \bar{Y}_i are functions of the observed variables. Suppose that the random variables \bar{Y}_i are mutually independent and normally distributed as $\bar{Y}_i \sim \mathcal{N}(0, 1/\gamma_{i,\{i\}}^2)$ with variance $\gamma_{i,\{i\}}^2 \neq 0$. Suppose further that ν_F , $F \in \Delta_2$, are mutually independent $\mathcal{N}(0, 1)$ random variables that are also independent of the \bar{Y}_i . Define random variables \bar{H}_F as linear combinations:

$$(6.4) \quad \bar{H}_F = \sum_{i \in [m]: i \in F} \gamma_{i,F} \bar{Y}_i + \nu_F, \quad F \in \Delta_2.$$

Note that this equation system is associated with the bipartite acyclic digraph obtained by reversing the direction of all edges in D_Δ .

Proposition 6.2. *If the random vector $\bar{H} = (\bar{H}_F : F \in \Delta_2)$ is defined by (6.4), then the positive definite matrix $\phi_\Delta(\gamma)$ is the inverse of the covariance matrix of the conditional distribution of \bar{Y} given \bar{H} .*

Proof. Concatenating \bar{Y} and \bar{H} yields a Gaussian random vector with covariance matrix

$$\Lambda^{-T} \Omega^{-1} \Lambda^{-1} = \begin{pmatrix} \text{diag}(1/\gamma_{i,\{i\}}^2) & \text{diag}(1/\gamma_{i,\{i\}}^2) \Gamma_2(\gamma) \\ \Gamma_2(\gamma)^T \text{diag}(1/\gamma_{i,\{i\}}^2) & I + \Gamma_2(\gamma)^T \text{diag}(1/\gamma_{i,\{i\}}^2) \Gamma_2(\gamma) \end{pmatrix},$$

where we have reused the matrices appearing in (6.2) and (6.3). By standard results about conditional distributions of Gaussian random vectors, the covariance matrix

of the conditional distribution of \bar{Y} given \bar{H} is the Schur complement

$$\text{diag}(\gamma_{i,\{i\}}^2)^{-1} - \text{diag}(\gamma_{i,\{i\}}^2)^{-1} \Gamma_2(\gamma) \left(I + \Gamma_2(\gamma)^T \text{diag}(\gamma_{i,\{i\}}^2)^{-1} \Gamma_2(\gamma) \right)^{-1} \Gamma_2(\gamma)^T \text{diag}(\gamma_{i,\{i\}}^2)^{-1}.$$

It follows from the matrix inversion lemma that the inverse of the conditional covariance matrix is

$$\text{diag}(\gamma_{i,\{i\}}^2) + \Gamma_2(\gamma) \Gamma_2(\gamma)^T = \phi_\Delta(\gamma). \quad \square$$

According to Proposition 6.2, positive definite matrices in $\text{im}(\phi_\Delta)$ also arise as inverses of conditional covariance matrices. Zeros in the inverse of the covariance matrix of a Gaussian random vector have an appealing interpretation in terms of conditional independence; see again [DSS09, Chap. 3].

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