Partial correlation graphs and the neighborhood lattice*

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Abstract

We define and study partial correlation graphs (PCGs) with variables in a general Hilbert space and their connections to generalized neighborhood regression, without making any distributional assumptions. Using operator-theoretic arguments, and especially the properties of projection operators on Hilbert spaces, we show that these neighborhood regressions have the algebraic structure of a lattice, which we call a neighborhood lattice. This lattice property significantly reduces the number of conditions one has to check when testing all partial correlation relations among a collection of variables. In addition, we generalize the notion of perfectness in graphical models for a general PCG to this Hilbert space setting, and establish that almost all Gram matrices are perfect. Under this perfectness assumption, we show how these neighborhood lattices may be “graphically” computed using separation properties of PCGs. We also discuss extensions of these ideas to directed models, which present unique challenges compared to their undirected counterparts. Our results have implications for multivariate statistical learning in general, including structural equation models, subspace clustering, and dimension reduction. For example, we discuss how to compute neighborhood lattices efficiently and furthermore how they can be used to reduce the sample complexity of learning directed acyclic graphs. Our work demonstrates that this abstract viewpoint via projection operators significantly simplifies existing ideas and arguments from the graphical modeling literature, and furthermore can be used to extend these ideas to more general nonparametric settings.

1 Introduction

Graphical models are a popular tool for representing complex joint distributions and have found numerous applications in computational biology, computer vision, signal processing, and natural language processing, just to name a few [KF09; WJ08; Fri04; LMP01]. Undirected graphical models, also known as Markov networks, encode conditional independence statements satisfied by a joint distribution, via separation in an undirected graph [Lau96]. In this sense, we can refer to the corresponding graphs as conditional independence graphs, or CIGs. In general, it is difficult to estimate conditional independence without specific distributional assumptions. Common assumptions include Gaussianity and various closely related extensions (e.g. nonparanormal and elliptical distributions, Gaussian copulas [HD12; HD13; LLW09]). On the other hand, it is fairly straightforward to estimate second-order information, for example covariances and partial correlations among variables, even if the data is non-Gaussian. In fact,

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sample covariances and estimated partial correlations, via node-wise regression, are among the most common practical tools for measuring dependence among variables. In the absence of any distributional assumptions, these quantities are what we can reliably estimate.

In this paper, we study partial correlation graphs, or PCGs, as the minimal-assumption counterparts of CIGs. In the context of PCGs, independence is replaced with orthogonality, and conditional independence is replaced with a corresponding notion of partial (or conditional) orthogonality. We show that the theory for PCGs can be developed in parallel with that of CIGs, by interpreting PCGs as describing partial orthogonality statements among families of projection operators associated with the underlying variables. This algebraic viewpoint allows us to define generalized versions of the Markov property—which we call $L^2$ Markov properties—and derive many of the related properties via independent arguments not relying on properties of CIGs. In doing so, we extend the “classical” theory of conditional independence in graphical models to the weaker notion of partial orthogonality in an abstract Hilbert space, which as we will show applies to problems of general interest to statisticians. It is worth noting that while partial correlation coefficients are well-known from regression analysis, even the “usual” notion of a PCG, as a stand-alone concept, is little known, despite having appeared in the literature before (e.g., [WKR13]).

Studying partial orthogonality is naturally related to the so-called neighborhood regression problem, which has been leveraged with great success in the context of graphical models. More specifically, given a random vector $X = (X_1, \ldots, X_d)$, one can often reconstruct a Markov network for $X$ by regressing each node $X_j$ onto the rest of the nodes $X_{-j} = \{X_1, \ldots, X_d\} \setminus \{X_j\}$. This procedure is valid for several classes of distributions including joint Gaussian models [MB06], Ising models [RWLO10], and exponential random families [YRAL15], as well as semiparametric families [LLW09]. We note that each of these examples requires strong distributional assumptions.

In this paper, we extend the notion of neighborhood regression (Section 4) in two important aspects. First, we do not restrict our analysis to any specific family of distributions; in fact, our analysis extends well beyond the traditional setting of random variables to include vectors in any separable Hilbert space, where there may be no concept of a distribution. Second, we study regression of a single variable $X_j$ onto an arbitrary subset of the rest of the variables: $S \subset \{X_1, \ldots, X_d\} \setminus \{X_j\}$. This generality is needed to verify general partial orthogonality statements involving a pair of variables, as discussed in Section 4. One of the main contributions of this paper is to show that these neighborhood regression problems have a rich algebraic structure, namely that they have the structure of a complete, convex lattice (Theorem 1). This is developed in Section 4.2 and is linked to the separation properties of the PCG in Section 5.2. The lattice property could potentially lead to substantial savings when evaluating all possible conditional statements implied by a PCG for a particular node (Section 4.2). In addition, neighborhood regression onto a general neighborhood $S$ has a natural connection to directed graphical models and structural equation modeling, as discussed in Section 6. Our results have direct implications for the computational and sample complexity of learning directed acyclic graphs (Section 6.2).

We also develop the notion of $L^2$ (Markov) perfectness, the counterpart of the more familiar notion of perfectness (or faithfulness) in the context of CIGs. Under $L^2$ perfectness, there is a one-to-one correspondence between separation in the PCG and partial orthogonality statements implied by the variables. As a result of independent interest, we establish a substantial generalization of a result due to [LM07] that implies the existence of an $L^2$ perfect
covariance matrix (or Gram matrix in general) for every possible graph structure (Theorem 2). We strengthen this result, in Section 5, to show that almost all covariance matrices respecting a graph structure are $L^2$ perfect for it. Similar results are already known for other classes of graphical models [SGS00; Peñ11] and our result thus provides a corresponding extension to the case of undirected graphical models and their $L^2$ extensions described herein.

As far as we know, the lattice property of neighborhood regression has not been noted before in the literature. This useful property has far-reaching implications in terms of the sample complexity needed in recovering “independence” structures from high-dimensional data; see the discussion in Section 6.2. In order to derive this property, we also develop the theory of PCGs in maximum generality, by assuming the variables to be elements of a separable Hilbert space. This includes the special case of random variables with finite second moments, but also covers other objects such as random (or deterministic) vectors, functions and data matrices, once an appropriate inner product, i.e., a similarity measure, is defined; see examples in Section 3.1.

We give largely self-contained proofs of all the results in this theory using operator-theoretic arguments. The perfectness result of Section 5 uses a fairly technical extension of the arguments in [LM07] that invokes ideas from geometric measure theory, and could be of independent interest.

2 Preliminaries

In this section, we review some preliminaries and background material that is useful for setting the stage of our general theory. The material on projections in Section 2.3 in particular is essential for the definitions and results in the sequel.

2.1 Notation

Graph notation. In an undirected graphical model for a random vector $X = (X_1, \ldots, X_d)$, we identify each random variable $X_j$, $j = 1, \ldots, d$, with a node in an undirected graph $G = ([d], E)$, where $[d] = \{1, \ldots, d\}$. Two nodes $i$ and $j$ are adjacent, or neighbors, if $(i, j) \in E$, in which case we write $i \sim j$, otherwise $i \nabla j$. A path from $i$ to $j$ is a sequence $i = k_1, k_2, \ldots, k_{n-1}, k_n = j \in [d]$ of distinct elements with $(k_l, k_{l+1}) \in E$ for each $l = 1, \ldots, n - 1$.

Given two subsets $A, B \subset [d]$, a path connecting $A$ to $B$ is any path with $k_1 \in A$ and $k_n \in B$. A subset $C \subset [d]$ separates $A$ from $B$, denoted by $A - C - B$, if all paths connecting $A$ to $B$ intersect $C$ (i.e. $k_l \in C$ for some $1 < l < n$), otherwise we write $\neg(A - C - B)$. Implicit in this definition is that $A, B$ and $C$ are disjoint.

Subset notation. For any $A \subset [d]$, we denote $X_A = \{X_i : i \in A\}$. We also use the shorthand notations: $\{i\} = i$ and $\{i, j\} = ij$, $A \cup \{i\} = Ai$, $A \cup B = AB$ and so on. In addition, we let $[d]_S = [d] \setminus S = \{1, \ldots, d\} \setminus S$. Common uses of these notational conventions are: $[d]_j = [d] \setminus \{j\}$ and $[d]_{ij} = [d] \setminus \{i, j\}$. For a matrix $\Sigma \in \mathbb{R}^{d \times d}$, and subsets $A, B \subset [d]$, we use $\Sigma_{A,B}$ for the submatrix on rows and columns indexed by $A$ and $B$, respectively. Single index notation is used for principal submatrices, so that $\Sigma_A = \Sigma_{A,A}$. For example, $\Sigma_{ij}$ is the $(i, j)$th element of $\Sigma$ (using the singleton notation), whereas $\Sigma_{ij} = \Sigma_{ij,ij}$ is the $2 \times 2$ submatrix on $\{i, j\}$ and $\{i, j\}$. Similarly, $\Sigma_{Ai,Bj}$ is the submatrix indexed by rows $A \cup \{i\}$ and columns $B \cup \{j\}$.
2.2 Graphical models

For completeness, we recall here some of the traditional definitions from the graphical modeling literature. This is mainly to provide a basis for comparison, and is not needed for most of the results we prove. A more thorough treatment can be found in [KF09; Lau96].

In the context of undirected graphs, there are three so-called Markov properties of interest: A graph $G$ satisfies the

- **pairwise Markov property** if $(i, j) \notin E$ implies that $X_i \perp \perp X_j \mid X_{\{d_{ij}\}}$,
- **local Markov property** if each node is conditionally independent of all other variables given its neighbours,
- **global Markov property** if $A - C - B$ implies that $X_A \perp \perp X_B \mid X_C$.

The notation $X_1 \perp \perp X_2 \mid X_3$ means $X_1$ is (probabilistically) independent of $X_2$ conditioned on $X_3$. In general, these conditions are not equivalent and we have global $\implies$ local $\implies$ pairwise, however, for positive distributions, these conditions are in fact equivalent [KF09]. A graph $G$ satisfying the pairwise Markov property is sometimes called a conditional independence graph (CIG) for the distribution of $X$.

The Markov properties go in one direction: The graphical criterion (i.e. separation) implies a probabilistic conclusion (i.e. conditional independence). The converse is not true in general; when it is, the graph $G$ is called perfect with respect to the joint distribution of $X$. Specifically, $G$ is called perfect if

$$A - C - B \iff X_A \perp \perp X_B \mid X_C.$$  

**Remark 1.** In the literature on graphical models, there are two related notions of perfectness (as defined above) and faithfulness. Conceptually, these terms mean the same thing—namely that there is a one-to-one correspondence between properties of a graph and conditional independence—and the only distinction regards what kind of graphical model is being used. The term “perfect” is more commonly used in reference to undirected graphs, whereas “faithful” is more common with directed acyclic graphs (DAGs). To add to the confusion, faithfulness is sometimes called DAG perfectness. The key difference to remember is that in undirected graphical models, graph separation corresponds to conditional independence, whereas in directed graphical models, the more complicated notion of $d$-separation corresponds to conditional independence. Indeed, the graphical modeling literature distinguishes even more general types of graphs—each with their own Markov properties—such as chain graphs [Fry90; CW93], ancestral graphs [RS02], and other mixed graphs [LS16]. For more details on the relationship between directed and undirected graphs, see [KF09].

2.3 The lattice of projections

We will assume the reader is familiar with the basic theory of Hilbert spaces and their projections; a detailed introduction to these topics can be found in [FW10; Bla06]. For a (separable) Hilbert space $\mathcal{H}$, let $B(\mathcal{H})$ be the space of bounded linear operators on $\mathcal{H}$. For an operator $P \in B(\mathcal{H})$, let $\text{ran}(P) := P\mathcal{H} := \{Px : x \in \mathcal{H}\}$ denote its range and $P^*$ its adjoint, defined via the relation $\langle x, P^*y \rangle = \langle Px, y \rangle$ for all $x, y \in \mathcal{H}$. Here and in the sequel, we use $\langle \cdot, \cdot \rangle_\mathcal{H}$ or the shorthand $\langle \cdot, \cdot \rangle$ to denote the inner product of $\mathcal{H}$.
We recall that $P \in B(H)$ is an orthogonal projection iff it is self-adjoint and idempotent: $P^* = P = P^2$. The set of orthogonal projections in $B(H)$, denoted as $\mathcal{P}(H)$, is of particular importance in this paper. $\mathcal{P}(H)$ can be partially ordered as follows:

**Lemma 1.** For $P, Q \in \mathcal{P}(H)$, the following are equivalent:

(a) $P = PQ$,  
(b) $P = QP$,  
(c) $\text{ran}(P) \subset \text{ran}(Q)$.

**When any of these conditions hold we write $P \leq Q$.**

The equivalence of (a) and (b) follows from self-adjointness of orthogonal projections. Note that when $P$ and $Q$ are both projections, $PQ$ is not necessarily a projection (unless $P$ and $Q$ commute). The above ordering makes $\mathcal{P}(H)$ into a complete lattice, that is, a partially ordered set $S$ in which each subset has both a supremum (join) and an infimum (meet) in $S$. For $P, Q \in \mathcal{P}(H)$, we denote the supremum with $P \lor Q$ and the infimum with $P \land Q$. We have

$$P \land Q = \text{the projection onto } \text{ran}(P) \cap \text{ran}(Q)$$

$$P \lor Q = \text{the projection onto the closed linear span of } \text{ran}(P) \cup \text{ran}(Q).$$

We also let $P^\perp := I - P$, the orthogonal complement of $P$. Note that $P \lor P^\perp = I$ (the identity operator) and $P \land P^\perp = \{0\}$. Also, $P \leq Q$ iff $P^\perp \geq Q^\perp$. See for example [FW10, Section 5, p. 24] and [Bla06, Section II.3.2, p. 78] and the references therein.

We often consider the concrete example where $H = L^2(P)$, the space of random variables (on a probability space with measure $P$) with finite second moments. When applied to a random variable $X$, $P^\perp X = X - PX$ may be interpreted as the residual between $X$ and its projection $PX$. For this reason, when $x$ is a vector in an arbitrary Hilbert space $H$ we will refer to $P^\perp x$ as the *residual* of the projection $PX$ in the sequel. We will also need the following notion of orthogonality of operators:

**Lemma 2.** For $P, Q \in B(H)$, the following are equivalent:

(a) $\langle Px, Qy \rangle = 0$, $\forall x, y \in H$,  
(b) $P^*Q = Q^*P = 0$,  
(c) $\text{ran}(P) \perp \text{ran}(Q)$.

**When any of the conditions above hold, we call $P$ and $Q$ orthogonal and denote this by $P \perp Q$.**

### 3 Partial orthogonality

In contrast to the classical theory of graphical models which works with random variables, we will develop our theory in the abstract setting of a general Hilbert space $H$. We begin by generalizing the usual notion of a PCG to this setting, and then extend the Markov properties defined in Section 2.2 based on this extension. The notion of partial orthogonality (cf. (5))—which is well-defined in any Hilbert space—will play a prominent role here and in the rest of the paper.

#### 3.1 Abstract partial correlation graphs

We start with an abstract generalized definition of PCGs which applies to vectors with elements in a general Hilbert space $H$, and can be considered a minimal-assumption version of conditional independence graphs (CIGs). We then discuss how by specializing to the $L^2$ space of random
variables (as a concrete Hilbert space), we can recover the usual definition of PCGs familiar from regression analysis. Throughout, we write $\mathcal{H}^d = \{(x_1, \ldots, x_d) : x_i \in \mathcal{H}, i \in [d]\}$ for some positive integer $d$, and a separable Hilbert space $\mathcal{H}$. We recall that $[d]_{ij} = \{1, \ldots, d\} \setminus \{i, j\}$.

Fix a vector $x = (x_1, \ldots, x_d) \in \mathcal{H}^d$, and for any $S \subset [d]$, let $P_S \in \mathcal{P}(\mathcal{H})$ denote the projection onto the span of $x_S = \{x_i, i \in S\}$.

**Definition 1** (Pairwise $L^2$ Markov, PCG). We say that $x$ satisfies the pairwise $L^2$ Markov property w.r.t. $G$ if

$$i \sim j \text{ in } G \iff P_i P_S^⊥ P_j = 0, \text{ for } S = [d]_{ij},$$

in which case $G$ is called a partial correlation graph (PCG) of $x$.

For $\mathcal{H} = L^2(\mathbb{P})$, we recover the usual notion of PCG for random variables:

**Example 1.** For a probability measure $\mathbb{P}$, let $\mathcal{H} = L^2(\mathbb{P})$, the space of square-integrable random variables: $X_i \in L^2(\mathbb{P})$ iff $\mathbb{E}X_i^2 < \infty$. The inner product is $\langle X, Y \rangle_{L^2} = \mathbb{E}XY$. Consider zero-mean random variables $X_1, \ldots, X_d \in L^2(\mathbb{P})$. In this case, $P_S$ corresponds to the $L^2$ projection on the span of $X_S$, or regressing on (covariates) $X_i, i \in S$ in statistical terms. Similarly, $P_S^⊥ X_i$ is the residual after regressing $X_i$ on $X_S$.

Now, fix some $S \subset [d]$. The usual partial correlation between $X_i$ and $X_j$ given $X_S$ is the correlation between the residuals $P_S^⊥ X_i$ and $P_S^⊥ X_j$, that is, $\langle P_S^⊥ X_i, P_S^⊥ X_j \rangle_{L^2}$. Thus, the partial correlation is zero iff $P_S^⊥ X_i \perp P_S^⊥ X_j$ (orthogonality in the $L^2$ sense). Since $\text{span}\{P_S^⊥ X_j\} = \text{ran}(P_S^⊥ P_j)$, using Lemma 2(c), the partial correlation is zero iff $P_S^⊥ P_i \perp P_S^⊥ P_j$. This in turn is equivalent to $P_i P_S^⊥ P_j = 0$, by Lemma 2(b). Thus, in this case Definition 1 defines the PCG as the graph where the missing edges between a pair of nodes $(i, j)$ correspond to zero partial correlation between $X_i$ and $X_j$ given the rest of the variables $X_k, k \in [d]_{ij}$. This is the usual notion of the PCG for a collection of random variables.

In Example 1, it is well-known that if $X = (X_1, \ldots, X_d)$ has a Gaussian distribution, then the PCG defined above is in fact a CIG. However, the PCG is defined for any (joint) distribution on $X$ whose marginals have finite second moments, and in general it may not correspond to a CIG. (It is usually sparser than a CIG.)

Going back to the general setup of Definition 1, let $\Sigma = (\langle x_i, x_j \rangle_\mathcal{H}) \in \mathbb{R}^{d \times d}$ be the Gram matrix of the underlying variables $x = (x_j, j \in [d])$. Although the PCG is defined using projection operators, we now show that it is completely determined by the Gram matrix. Unless otherwise stated, we will assume the following from now on:

$$\Sigma := (\langle x_i, x_j \rangle_\mathcal{H}) > 0. \quad (A1)$$

The following result is proved in Appendix A.2:

**Lemma 3.** $|\Sigma_{Si,Sj}| = 0$ is equivalent to $P_i P_S^⊥ P_j = 0$, for all $i, j$ and $S \subset [d]_{ij}$.

It is worth noting that the lemma is not restricted to random variables and holds in the general Hilbert space setup of Definition 1. Since PCGs are preserved under Hilbert space isometries (Appendix A.5), by passing to the case where $x$ is a zero-mean Gaussian random vector with covariance $\Sigma$ (i.e., a special case of Example 1), and using the known results on Gaussian

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1We assume $d < \infty$ for simplicity, though most of our results hold also for $d = \infty$. 6
usual Euclidean inner product and take \( \{ H \} \) define PCGs for purely deterministic objects. For example, let us take Example 2 (PCG for deterministic objects).

abstract PCG of Definition 1, which go beyond the familiar case of Example 1, and also show establishes the equivalence for any \( S \) recovers this well-known result. Note, however, that Lemma 3 is stronger than (2), since it establishes the equivalence for any \( S \subset \{ d \} \). Let us now give more concrete examples of the abstract PCG of Definition 1, which go beyond the familiar case of Example 1, and also show the utility of Lemma 3.

**Example 2** (PCG for deterministic objects). The general setup of Definition 1 allows us to define PCGs for purely deterministic objects. For example, let us take \( \mathcal{H} = \mathbb{R}^n \) with the usual Euclidean inner product and take \( \{ x_j, j \in [d] \} \) to be a collection of vectors in \( \mathbb{R}^n \). The resulting PCG encodes a form of partial orthogonality among these vectors. For example, let \( \{ e_1, \ldots, e_n \} \) be an orthonormal basis of \( \mathbb{R}^n \) and let \( x_j = e_1 + e_j \) for \( j \in [d] \), assuming \( n \geq d \). It is clear that for \( j \neq 1 \) and any subset \( A \subset [d] \) containing 1, \( P_A x_j = P_1 x_j \) and \( P_1^\perp x_j = e_j \). Hence, for distinct \( i, j \neq 1 \) and \( 1 \in A \subset [d] \), we have \( x_i^T P_A^\perp x_j = x_i^T P_1^\perp x_j = 0 \). In other words, “conditional” on any subset \( [d] \) containing 1, \( i \) and \( j \) are orthogonal, i.e., there is no edge between them in the PCG. One can argue with some more work that all the other edges (i.e., between 1 and any other node) are present. Hence the PCG is star-shaped with node 1 at the center. The corresponding Gram matrix and its inverse are

\[
\Sigma = \frac{1}{\gamma - \|u\|^2} \left( \begin{array}{c} 1 \\ u \end{array} \right) \left( \begin{array}{c} u \\ (\gamma - \|u\|^2)I + uu^T \end{array} \right), \quad \Sigma^{-1} = \left( \begin{array}{c} \gamma \\ -u \\ -u^T \\ I \end{array} \right),
\]

where \( \gamma = d/4 \) and \( u = \frac{1}{2} 1_{d-1} \). Here, \( 1_{d-1} \) is the all ones vector in \( \mathbb{R}^{d-1} \), and we have \( \gamma - \|u\|^2 = 1/4 \). The star shape of the PCG is immediately clear from (3) in view of (2), or equivalently Lemma 3.

Similarly, one can take \( \mathcal{H} = \mathcal{F} \) for a Hilbert space of functions and let \( \{ x_j \} \) be functions in \( \mathcal{F} \). For example, take \( \mathcal{H} = H^1([0,1]) \), the Sobolev space of order 1, defined as the space of absolutely continuous functions \( f : [0,1] \to \mathbb{R} \) with derivative \( f' \in L^2([0,1]) \), and \( f(0) = 0 \). The inner product is \( \langle f, g \rangle_{\mathcal{H}} := \langle f', g' \rangle_{L^2([0,1])} = \int_0^1 f'(t)g'(t)dt \), and the corresponding norm is a measure of smoothness of the functions. An orthonormal basis for this space is \( e_k(t) = \mu_k \sin(t/\mu_k) \) for \( k = 1, 2, \ldots \), where \( \mu_k = 2/(2k - 1)\pi \). The exact same construction used earlier, namely \( x_j(t) = e_1(t) + e_j(t), t \in [0,1], j \in [d], \) can be used to obtain a star PCG for
the underlying functions, since one gets the exact same Gram matrix as in (3). In this case, in contrast to the finite-dimensional setting, we can even take $d = \infty$ to have a star PCG with infinitely many leaves. The top row in Figure 1 shows the functions in this construction for $d = 6$. Also shown as the second row is the collection $x_j(t) = e_0(t) + e_j(t), j = 1, \ldots, 6$ which has the same star-shaped PCG with $e_6$ as the central node.

**Example 3** (PCG for random vectors). For a probability measure $\mathbb{P}$, and $n \in \mathbb{N}$, let $\mathcal{H} = (L^2(\mathbb{P}))^n$, the $L^2$ space of random vectors $X \in \mathbb{R}^n$ with bounded second moments: $\mathbb{E}\|X\|_2^2 < \infty$. The inner product here is given by $\langle X, Y \rangle_{\mathcal{H}} = \mathbb{E}\langle X, Y \rangle_{\mathbb{R}^n} = \sum_{i=1}^n \mathbb{E}(X_iY_i)$ where $\langle \cdot, \cdot \rangle_{\mathbb{R}^n}$ is the usual Euclidean inner product in $\mathbb{R}^n$. Fix integers $d$ and $m$, and take a sequence $\{u_{kj}, k \in [m], j \in [d]\} \subset \mathbb{R}^n$ of deterministic vectors, a sequence $\{Z^{kj}, k \in [m], j \in [d]\} \subset L^2(\mathbb{P})$ of zero-mean (scalar) random variables, and let $X_j = \sum_{k=1}^m Z^{kj}u_{kj} \in \mathbb{R}^n$ for $j = 1, \ldots, d$. Clearly each $X_j \in (L^2(\mathbb{P}))^n$ and we have

$$
\langle X_i, X_j \rangle_{\mathcal{H}} = \sum_{k=1}^m \sum_{k'=1}^m \mathbb{E}[Z^{ki}Z^{kj'}] \langle u_{ki}, u_{k'} \rangle_{\mathbb{R}^n}, \quad i, j \in [d]
$$

which can model complex correlations both via the covariance matrices $S_{k,k'} = (\mathbb{E}[Z^{ki}Z^{kj}]) \in \mathbb{R}^{d \times d}$ and the relative positions of $\{u_{kj}\}$ in $\mathbb{R}^n$. Letting $V_j = \text{span}\{u_{1j}, \ldots, u_{mj}\}$, we observe that $X_j \in V_j$, that is $X_j$ is a random element of $V_j$. Thus, we can use this setup to simultaneously model subspace clustering and dimension reduction, especially when assuming $m \ll n$ so that $V_j$s are of much lower dimension than the ambient space, and when some pairs of subspaces are either identical or have large intersections. For example, to see the application to clustering, consider the case where $V_j = V^{(1)}$ for some $j$s and $V_j = V^{(2)}$ for others, with $V^{(1)} \neq V^{(2)}$. Then, the vectors $\{X_j\}$ are naturally divided into two clusters, and their PCG will contain information about the two clusters.

The PCG of Definition 1 for $X = (X_1, \ldots, X_d)$ has a random vector, $X_j$, on each node. The geometry of the subspaces $V_1, \ldots, V_d$ affects this PCG of $X$. For example, when the subspaces are mostly orthogonal, there will be a lot of missing edges in the PCG: $V_i \perp V_j$ for $i \in A$ and $j \in B$, then, $\langle X_i, X_j \rangle_{\mathcal{H}} = 0$ for all $i \in A$, $j \in B$, irrespective of the correlation structure of $Z$. Lemma 3 (with $S = [d]_{ij}$), then, implies that there is no edge between $A$ and $B$ in the PCG (since the inverse Gram matrix has a zero block on indices $A \times B$).

**Example 4** (PCG for random functions). In the setup of Example 3, we can replace $\mathbb{R}^n$ with a Hilbert space $\mathcal{F}$ of real-valued functions on domain $\mathcal{X}$, that is, $\mathbb{R}^X$. We take $\mathcal{H} = (L^2(\mathbb{P}))^\mathcal{X}$, a space of random functions (or random processes) on domain $\mathcal{X}$, with $\langle F, G \rangle_{\mathcal{H}} = \mathbb{E}\langle F, G \rangle_{\mathcal{F}}$. Similar to Example 3, take a deterministic sequence $\{f_{kj} \in \mathcal{F}, k \in [m], j \in [d]\}$, (with $m = \infty$ a possibility when $\mathcal{F}$ is an infinite-dimensional space) and let $F_j = \sum_{k=1}^m Z^{kj}f_{kj}$. All the discussions of the Example 3 go through. The PCG in this case has random functions $\{F_j\}$ as its nodes. Depending on what the inner product of $\mathcal{F}$ measures, the absence of an edge could have different meanings. For example, if $\mathcal{F}$ is a Sobolev space where the norm measures some form of smoothness of the function, an absence of an edge between $F_i$ and $F_j$ includes some information about the relative smoothness of the pair of functions.

For example, let $\mathcal{F}$ be the Sobolev space of Example 2 with basis functions $e_1, e_2, \ldots$, given there. Consider the star construction with $e_1$ at the center but with random weights: $x_j = Z^{1j}e_1 + Z^{2j}e_j$ for $j \in [d]$. Let $S_{k,k'} = (\mathbb{E}[Z^{ki}Z^{kj}]) \in \mathbb{R}^{d \times d}$ for $k, k' = 1, 2$. Note that
$S_{2,1} = S_{1,2}^T$. Let $\delta_{i,j} = 1\{i \neq j\}$ be the Kronecker delta function. It is not hard to see that

$$\Sigma_{i,j} := \langle x_i, x_j \rangle = [S_{1,1} + S_{1,2}^T \delta_{i,1} + S_{1,2} \delta_{i,j} + S_{2,2} \delta_{i,j}]_{i,j}, \quad i,j \in [d].$$

Thus, the off-diagonal elements of the first row of $\Sigma$ ($\Sigma_{1,i}, i \neq 1$) are determined by the corresponding elements of $S_{1,1} + S_{1,2}^T$, while the off-diagonal elements of $\Sigma$ outside the first row and column are determined by those of $S_{1,1}$ alone. It is clear for example, that elements of $S_{2,2}$ besides $[S_{2,2}]_{1,1}$ have no effect on the Gram matrix. The deterministic case of Example 2 corresponds to $S_{1,1} = S_{1,2} = \text{all-ones} \ d \times d \ matrix$. The other extreme $S_{1,1} = S_{1,2} = I_d$ leads to the empty PCG. Many other possibilities exist between these two extremes.

We note that Examples 3 and 4 provide useful statistical frameworks for modeling multivariate dependencies among random functions or other high-dimensional objects, while retaining some familiar aspects of regression analysis and PCGs. In this sense, they provide avenues for extending classical multivariate statistical analysis to collections of higher-order objects (vectors, matrices, functions, etc.).

### 3.2 Global Markov property

Let us now extend Definition 1. In analogy with the global Markov property in the context of CIGs, we can define a global notion of the $L^2$ Markov property with respect to a graph:

**Definition 2** (Global $L^2$ Markov). Given the setup of Definition 1, we say that $x \in \mathcal{H}$ satisfies global $L^2$ Markov property w.r.t. $G$ if

$$S \text{ separates } A \text{ and } B \text{ in } G \implies P_A P_S^\perp P_B = 0. \quad (4)$$

In the special case $\mathcal{H} = L^2(\mathbb{P})$, this reduces to the global Markov property for an undirected graphical model, and hence Definition 2 provides a natural generalization of this property to general Hilbert spaces.

**Remark 2.** In contrast to Definition 1, the one-sided implication in (4) is in line with the usual definition for CIGs in the literature. This way, in the Gaussian case, the usual global Markov property matches the $L^2$ version defined here. The two-sided version of this property then corresponds to the notion of “perfectness” which will be discussed in detail in Section 5. Comparing with Definition 1, we could have used a one-sided implication in defining the pairwise property as well, however, this would introduce some unnecessary technicalities involved with nonuniqueness of the PCG. Our choice of the two-sided implication in the pairwise case leads to a well-defined PCG (i.e. a unique PCG for any given vector $x$), which simplifies the arguments in the sequel.

Since $P_A P_S^\perp P_B = P_B P_S^\perp P_A$ due to self-adjointness of projections, Definition 2 is symmetric in $A$ and $B$. We will use the following notational convention

$$P_A \perp P_B \mid P_S \quad \text{means} \quad P_A P_S^\perp P_B = 0. \quad \text{(partial orthogonality)} \quad (5)$$

Note the use of $\perp$ here to denote orthogonality in $\mathcal{H}$, as opposed to $\perp$ which is reserved for probabilistic independence as usual. This ternary relation among projections is also completely characterized by the Gram matrix $\Sigma$:
Lemma 4. \( \Sigma_{B,A} - \Sigma_{B,S} \Sigma_{S,A}^{-1} \Sigma_{S,A} = 0 \) is equivalent to \( P_A P_S^\perp P_B = 0 \), for disjoint \( A, S, B \subset [d] \).

This lemma will be proved as part of Proposition 1 (Section 4). We refer to (5) as \textit{partial orthogonality}, or \textit{conditional orthogonality}, a generalization of the notion of partial uncorrelatedness of random variables. Clearly the global \( L^2 \) Markov property implies the pairwise version as a special case. The following result, proved in Appendix A.5, establishes the equivalence of the pairwise and global \( L^2 \) Markov properties when the covariance matrix is non-degenerate. Note that this is the \( L^2 \) analogue of a similar well-known result for CIGs [Lau96, Thm. 3.9, p. 35].

Lemma 5. Assuming \( \Sigma \succ 0 \), the pairwise \( L^2 \) Markov property implies the global \( L^2 \) Markov property.

The PCG, as well as the pairwise and global \( L^2 \) Markov properties, can be thought of as being defined based on (1) a vector \( x \in \mathcal{H}^d \) with a particular Gram matrix \( \Sigma \), or more abstractly based on (2) a family of projection operators on the subspaces generated by \( x \). We have implicitly taken the first viewpoint, in which case we can characterize the PCG in terms of \( \Sigma \). There are however subtle differences between (1) and (2). A vector \( x \) uniquely identifies both a Gram matrix \( \Sigma \) and a collection of subspaces, or equivalently a collection of projection operators \( \{P_A\} \). However, neither \( \Sigma \) nor \( \{P_A\} \) uniquely identifies the other. Nevertheless both are useful in encoding \( L^2 \) Markov properties as illustrated in Lemma 3. For example, it is clear from the projection viewpoint, that rescaling any of the components of \( x \) does not change the subspaces and hence the \( L^2 \) Markov properties. This implies the following:

Lemma 6. \( D \Sigma D \) has the same \( L^2 \) Markov properties as \( \Sigma \) for any diagonal matrix \( D \), with nonzero diagonal entries.

Although this can be verified directly in terms of \( \Sigma \), using the characterization of Lemma 4, the projection viewpoint makes this immediately clear. A major theme of this paper is showing the usefulness of the projection interpretation in understanding the algebraic features of the \( L^2 \) Markov property.

Remark 3. Let us say a few words about the terminology. Throughout, we have used the term \( L^2 \) Markov property, while the results hold for any (separable) Hilbert space. Perhaps a more appropriate name would have been “\( \mathcal{H} \) Markov”. However, since all separable Hilbert spaces are isomorphic to \( \ell^2 \) and all infinite-dimensional separable Hilbert spaces are isomorphic to \( \ell^2 = \ell^\infty_2 \), the space of square-integrable sequences. Both correspond to \( L^2 \) spaces associated with counting measures on \([n]\) and \(\mathbb{N}\), respectively.

4 Neighborhood regression

The well-known concept of neighborhood regression provides an alternative characterization of the partial orthogonality relation (5). As will be shown in this section, we can verify the relation \( P_i \perp P_j \mid P_S \), by looking at the coefficients of the regression of \( x_j \) onto \( \{x_k, k \in Si\} \), as opposed to the residuals.

\footnote{In fact, all \( n \)-dimensional Hilbert spaces are isomorphic to \( \ell^n_2 = \mathbb{R}^n, \|\cdot\|_2 \) and all infinite-dimensional separable Hilbert spaces are isomorphic to \( \ell_2 = \ell^\infty_2 \), the space of square-integrable sequences. Both correspond to \( L^2 \) spaces associated with counting measures on \([n]\) and \(\mathbb{N}\), respectively.}
4.1 SEM coefficients

In the literature on undirected graphical models, the neighborhood of a fixed node \( x_j \) is implicitly understood to be the set of all other variables, namely the collection \( x_{-j} \). Here, we extend the notion of neighborhood to any subset \( S \subset [d]_j \), which is necessary for evaluating general conditional orthogonality statements, such as \( x_i \perp x_j \mid x_S \). (See Section 6 for a discussion of how this general setup is needed for learning directed extensions of the PCG.) At a high-level, the neighborhood regression problem for the node \( x_j \) and a subset \( S \subset [d]_j \) is the problem of finding the linear projection of \( x_j \) onto \( x_S \):

**Definition 3.** For any \( S \subset [d]_j \), let

\[
\beta_j(S) := \arg \min_{\beta \in \mathbb{R}^d, \text{supp}(\beta) \subset S} \| x_j - \beta^T x \|^2_H. \tag{6}
\]

We call \( \beta_j(S) \) the structural equation model (SEM) coefficients for variable \( j \) regressed on the variables \( S \).

Here, \( \beta^T x = \sum_{j=1}^d \beta_j x_j \) for any \( \beta \in \mathbb{R}^d \) and \( x \in H^d \). It is not hard to see that \( [\beta_j(S)]_S = \Sigma_{S,j}^{-1} \Sigma_{S,j} \) (Appendix A.3). In addition, it is possible to write the condition \( P_A P_S^\perp P_B = 0 \) directly in terms of the SEM coefficients, and also in terms of the Gram matrix \( \Sigma \). We have the following generalization of Lemma 3 (proved in Appendix A.3):

**Proposition 1.** Under (A1), the following are equivalent:

(a) \( P_A P_S^\perp P_B = 0 \),

(b) \[ [\beta_j(A)]_i = \sum_{k \in S} [\beta_j(S)]_k [\beta_k(A)]_i, \quad \forall i \in A, j \in B, \]

(c) \( \Sigma_{B,A} - \Sigma_{B,S} \Sigma_S^{-1} \Sigma_{S,A} = 0 \) (replaced with \( \Sigma_{B,A} = 0 \) if \( S = \emptyset \)),

(d) \[ [\beta_j(Si)]_i = 0, \quad \forall i \in A, j \in B. \]

Moreover, for any \( i, j \in [d] \) and \( S \subset [d]_{ij} \), we have

\[
[\beta_j(Si)]_i = \frac{\langle x_i, P_{S}^\perp x_j \rangle_H}{\langle x_i, P_S^\perp x_i \rangle_H}. \tag{7}
\]

We note that (d) can be equivalently written as \( [\beta_j(Si)]_i = [\beta_i(Sj)]_j = 0, \forall i \in A, j \in B \), due to symmetry. Most assertions in Proposition 1 are colloquially known (perhaps except part (b)). For example, expressions similar to (7) have appeared before [Tia12], going back to the work of [Cra46] and [Dem69]. Recalling our definition of partial orthogonality in (5), the equivalence \( (a) \iff (d) \) established in Proposition 1 shows that to study partial orthogonality relations it is enough to study neighborhood regression problems:

**Corollary 1.** To test \( P_i \perp P_j \mid P_S \) for all \( S \subset [d]_{ij} \), it is enough to have \( \{\beta_j(T) : T \subset [d]_j\} \).

Corollary 1 motivates studying the collections \( \{\beta_j(T) : T \subset [d]_j\} \), and it turns out that these neighborhood regression problems have rich algebraic properties which will be explored in the next section.
4.2 Neighborhood lattice

We now introduce the main object of study in the rest of the paper.

**Definition 4** (Neighborhood lattice). For any $S \subset [d]$, define a collection of subsets by

$$\mathcal{T}_j(S) = \{ T \subset [d] : P_T P_j = P_S P_j \}. \quad (8)$$

In other words, for any $j$, $\mathcal{T}_j(S)$ is the collection of candidate sets $T \subset [d]$ such that the projection of $x_j$ onto $\{x_i, i \in T\}$ is invariant. Definition 4 is somewhat abstract, though it highlights the algebraic nature of the collection $\mathcal{T}_j(S)$ and the sufficiency of the projection operators $\{P_S, S \subset [d]\}$ in defining it. Note that $\mathcal{T}_j(S)$ as given in (8) is well-defined even when the Gram matrix $\Sigma$ is rank deficient. In order to see the usefulness of this definition, assume in addition that $\Sigma$ is (strictly) positive definite. Then we have the following alternative representations of $\mathcal{T}_j(S)$:

$$\mathcal{T}_j(S) = \{ T \subset [d] : \beta_j(T) = \beta_j(S) \} = \{ T \subset [d] : \text{supp}(\beta_j(T)) = \text{supp}(\beta_j(S)) \}. \quad (9)$$

To see the first equality in (9), note that $\beta_j(S)^T x = P_S x_j$. Since the Gram matrix of $x$ is positive definite, $\beta_j(S) = \beta_j(T)$ is equivalent to $\beta_j(S)^T x = \beta_j(T)^T x$, and hence to $P_S x_j = P_T x_j$. The result follows since for any operator $L$, $L x_j = 0$ is equivalent to $L P_j = 0$. (We have $L P_j y = \langle x_j, y \rangle L x_j$ for all $y$, assuming $\|x_j\|_H = 1$.) The second equality in (9) follows from the first equality, and positive definiteness of Gram matrix. Note that by definition $\text{supp}(\beta_j(S)) \subset S$. We are primarily interested in cases where $\text{supp}(\beta_j(S))$ is much smaller than $S$, and all the other sets $T$ for which $\text{supp}(\beta_j(T))$ is the same as this small set.

Our goal in this paper is to study the algebraic properties of $\mathcal{T}_j(S)$, for which representation (8) is very helpful. Throughout, we fix $j \in [d]$ and $S \subset [d]$. Our next result shows that, $\mathcal{T}_j(S)$ is indeed a lattice, as suggested by the name. Recall that a complete lattice is a partially ordered set, or poset for short, in which all subsets have both a supremum (join) and an infimum (meet) [Sta97, Section 3.3]. We also need the following definition: Let $(\mathcal{P}, \leq)$ be a poset and $\mathcal{C}$ a subposet of $\mathcal{P}$. We say that $\mathcal{C}$ is convex (in $\mathcal{P}$) if $z \in \mathcal{C}$ whenever $x < z < y$ and $x, y \in \mathcal{C}$. A closed interval $[x, y] := \{ z \in \mathcal{P} : x \leq z \leq y \}$ is an example of a convex subposet [Sta97, Section 3.1].

**Theorem 1.** Under (A1), $\mathcal{T}_j(S)$, ordered by inclusion, is a complete lattice. In particular, $\mathcal{T}_j(S)$ has unique minimal and maximal elements, which we denote by $m_j(S)$ and $M_j(S)$, respectively. Moreover, $\mathcal{T}_j(S)$ is convex as a subposet of $2^{[d]}$.

Any finite nonempty lattice is in fact complete. However, the proof we give in Section 8.1 also establishes the result for an infinite collection of variables $\{x_i\}$. $\mathcal{T}_j(S)$ being convex in $2^{[d]}$ means the following: for every two subsets $S_1, S_2 \in \mathcal{T}_j(S)$, and any $S' \subset [d]$, if $S_1 \subset S' \subset S_2$, then $S' \in \mathcal{T}_j(S)$. Thus, using the interval notation, we can represent the neighborhood lattice as

$$\mathcal{T}_j(S) = [m_j(S), M_j(S)] = \{ A \in 2^{[d]} : m_j(S) \subset A \subset M_j(S) \}. \quad (10)$$

In other words, to specify $\mathcal{T}_j(S)$, it is enough to specify its minimum and maximum elements. In Section 5.2, we describe the abstract sets $m_j(S)$ and $M_j(S)$ in terms of the PCG $G$ (Theorems 3 and 4), which gives a useful semantic interpretation in terms of separation properties of a graph. Theorem 1 is in fact a special case of a much more abstract result discussed in Appendix B.
An alternative way to view $\mathcal{T}_j(S)$ is as a collection of subsets of $\{x_i : i \in [d]_j\}$ that have the same explaining power as $S$ for $x_j$. This view can be further advanced by removing the reference to the set $S$. A node $j$ defines an equivalence relation among subsets of $[d]_j$, where $S, T \subset [d]_j$ are equivalent iff $P_S P_j = P_T P_j$. We then say that $S$ and $T$ have the same explaining power for $\{j\}$. This relation partitions $2^{[d]_j}$ into equivalence classes, each of which is a complete lattice according to Theorem 1.

Example 5. Consider the covariance matrix $\Sigma$ shown in Figure 2(a), with dimension $d = 15$. The corresponding PCG is plotted in Figure 2(c). For $j = 3$ and $S = \{9, 8, 11, 12, 14\}$, the minimal set is $m_j(S) = \{9, 12, 14\}$, and maximal set is $M_j(S) = \{4, 5, 7, 8, 9, 10, 11, 12, 13, 14, 15\}$. These can be easily read from the graph as will be described in Section 5.2. Since the lattice can be represented as $\mathcal{T}_j(S) = [m_j(S), M_j(S)]$, we know for example that $\{9, 12, 14, 5\}$ and $\{9, 12, 14, 10, 13\}$ both belong to $\mathcal{T}_j(S)$. Note that these two sets are not comparable in $2^{[d]_j}$, i.e., $\mathcal{T}_j(S)$ is not a chain (or totally ordered set) in $2^{[d]_j}$. In this case, $\mathcal{T}_j(S)$ contains $2^{|M_j(S)|} = 2^8 = 256$ subsets, out of a total possible $2^{|[15]|} = 2^{14}$. Regressing $j = 3$ onto any of these 256 subsets results in the same SEM coefficients.

Remark 4. It is not hard to see that $m_j(S) = \text{supp}(\beta_j(S))$, that is, $m_j(S)$ represents the so-called active set when regressing $x_j$ onto $x_S$, which is of course of interest in regression and graphical models. Thus, there is a one-to-one correspondence between the neighbourhood lattices $\mathcal{T}_j(S)$, the equivalence classes defined above, and the possible active sets for predicting $x_j$. Furthermore, a consequence of Theorem 1 is that there will be a largest set $M_j(S)$ possibly larger than the $S$ we started with, regressing onto which has the same active set. Regressing onto any set strictly larger than $M_j(S)$ will change the active set.

4.3 Computational complexity

Theorem 1, combined with the observations in Remark 4, suggests an intuitive algorithm for efficiently computing the entire neighborhood lattice $\mathcal{T}_j(S)$. Once we have the active set $m_j(S)$, it is enough to compute $M_j(S)$, by sequentially adding the rest of the nodes and either include or reject them based on whether the active set is changed. Once $m_j(S)$ and $M_j(S)$ are computed, the entire lattice is given by (10). This procedure is outlined formally in Algorithm 1. Since this algorithm only requires $d - 1 - |m_j(S)| = O(d)$ projections, we have the following perhaps surprising result:
Proposition 2. For any \( j \) and \( S \subset [d]_j \), it is possible to compute \( T_j(S) \) with \( O(d) \) projections.

Since each projection can be computed in polynomial time (in \( d \)), a consequence of Proposition 2 is that \( T_j(S) \) can be computed in polynomial time. In graphical modeling, it is of significant interest to learn all possible conditional independence statements of the form \( X_i \perp X_j \mid X_S \). Likewise, in our more general setting, it is of interest to learn all partial orthogonality statements of the form \( P_j \perp P_i \mid P_S \) for any \( i \in [d]_j \) and \( S \subset [d]_j \). By Corollary 1, for this it is enough to compute the collection \( \{ T_j(S) : j \in [d], S \subset [d]_j \} \). Let \( T_{(1)}, T_{(2)}, \ldots, T_{(N)} \) be an enumeration of these lattices. Starting from an arbitrary subset \( S \subset [d]_j \), say \([d]_j \) itself, we can compute \( T_j(S) \) in \( O(d - |S| - 1) = O(d) \) projections, using for example Algorithm 1. This gives us \( T_{(1)} \). Then, we pick another \( S \not\subset T_{(1)} \), and repeat the process to obtain \( T_{(2)} \). Thus, we can compute the entire partition into lattice equivalence classes in \( O(Nd) \) projections. This provides answers to all partial orthogonality statements of the form \( P_j \perp P_i \mid P_S \) for any \( i \in [d]_j \) and \( S \subset [d]_j \).

Since \( N \) could potentially be much smaller than \( 2^{d-1} \), this procedure could result in substantial savings relative to the naive approach of checking all the \( 2^{d-1} \) possible subsets. For example, we have the following special case:

Lemma 7. If \( |m_j(S)| \leq k \) for all \( S \subset [d]_j \), then all partial orthogonality statements for the \( j \)th node can be computed in polynomial time, with at most \( O(d^k) \) projections.

In other words, as long as no active set for \( x_j \) has more than \( k \) elements, this computation is polynomial in \( d \). The proof of this lemma follows from the fact that under the assumptions we have \( N \leq \binom{d}{k} \leq d^k \). Whether there are other assumptions, besides that of Lemma 7, that could guarantee a polynomial number \( N \) of lattice equivalence classes is an interesting open question.

In addition to providing direct answers to arbitrary partial orthogonality queries, these computational results also have important implications for the sample complexity of learn-
ing directed graphical models. See Section 6 for more details. Finally, R code implementing Algorithm 1 and more, including the graphical computation of Section 5.2, is available at [Reg].

5 PCGs under Markov perfectness

We now introduce the notion of $L^2$ Markov perfectness, which is the PCG counterpart of the notion of Markov perfectness in undirected graphical models (or faithfulness in the directed case). Recall from Definition (4), that under global $L^2$ Markov property, graph separation implies partial orthogonality. Perfectness upgrades this implication to hold both ways.

**Definition 5.** We say that $x$ is $L^2$ globally Markov perfect w.r.t. $G$ if

$$S \text{ separates } A \text{ and } B \text{ in } G \iff P_A P_S^\perp P_B = 0.$$ 

This notion of perfectness is closely related to the notion of faithfulness in DAGs; see Remark 1. We often abbreviate “$L^2$ globally Markov perfect w.r.t. $G$” and just refer to $x$ as perfect or imperfect. Note that there is no need to specify $G$ either, since it is implied by $x$, due to the uniqueness of PCGs according to Definition 1 (see also Remark 2). Since PCGs and $L^2$ Markov properties can be equivalently characterized by the Gram matrix $\Sigma = (\langle x_i, x_j \rangle_H)$ as discussed in Section 3, we can equivalently talk about perfectness of a Gram matrix $\Sigma$. The corresponding graph is also (uniquely) implied in this case, given by the sparsity pattern of $\Sigma^{-1}$; see (2) and Lemma 3. In this section, we will focus on the Gram matrix interpretation and ask whether a given $\Sigma$ is perfect or not.

5.1 Prevalence of perfectness

One could ask how prevalent $L^2$ Markov perfectness is. This boils down to the prevalence of the (usual) Markov perfectness among Gaussian distributions (see the discussion after Lemma 3). [LM07] shows that for any graph $G$, there is a regular Gaussian distribution which is Markov perfect w.r.t. $G$; this implies that for any potential PCG, there is at least one Gram matrix $\Sigma$ and a corresponding random vector which is perfect w.r.t. that PCG. Here, we extend the argument in [LM07] to show that almost all covariance matrices are $L^2$ Markov perfect. As discussed earlier, given any positive definite matrix $\Sigma$, we can ask whether it is perfect or not, with the graph $G$ being implicit from the support of $\Sigma^{-1}$. This is the language we use throughout this section. Our main result on $L^2$ perfectness is the following:

**Theorem 2.** Let $G$ be an undirected graph on $[d]$, and let $A \in \mathbb{R}^{d \times d}$ be drawn from a continuous distribution (w.r.t. the Lebesgue measure) on positive definite matrices with support $G$. Then, $\Sigma = A^{-1}$, as a Gram matrix, is perfect w.r.t to $G$, with probability one.

Theorem 2 is proved in Section 8.4. The theorem shows that almost all Gram matrices are $L^2$ Markov perfect, justifying making that assumption in some of the results to follow. Compared with [LM07], this is a significant strengthening. Theorem 2 is a consequence of a more technical result, namely, Theorem 5 discussed in Section 8.4, a result which could be of independent interest. One needs a fair amount of technical work to make the notion of “almost all” precise. This is done in Section 8.4 by constructing appropriate measures on a suitable parametrization of the set of Gram matrices that are $L^2$ Markov w.r.t. a given graph $G$. Once done, the same techniques in [LM07] can be extended to show the stronger result as illustrated
in the proof of Theorem 5. In addition, Theorem 2 further strengthens this result by showing that the notion of “almost all” is independent of the particular parametrization of Theorem 5.

**Remark 5.** A corresponding result for linear DAG models appears as Theorem 3.2 in [SGS00], and similarly for chain graphs in [Peñ11]. Although undirected graphs can be viewed as special cases of chain graphs, our results are much stronger compared to the one found in [Peñ11]. The latter result only applies to a very particular parametrization of chain graphs, whereas our results apply to essentially any parametrization of undirected graphs via Theorem 2. Moreover, our proof technique is somewhat more intuitive and applies to PCGs defined over general Hilbert spaces, i.e. not just collections of random variables.

Markov perfectness is useful when making statements regarding the separation of nodes in the PCG, in which case there is a one-to-one correspondence between separation on the graph and the relation $P_A \perp P_B \mid P_S$ among projections. This will be helpful in the next section, where we discuss how the neighborhood lattice $T_j(S)$ can be read off from the separation properties of the PCG.

### 5.2 Graphical computation of the lattice

Under the perfectness assumption, let us now characterize the elements of $T_j(S)$ in terms of the separation in the underlying PCG. For any set $S \subset [d]_j$, define a new set by

$$S^* := \bigcap \{T \subset S : T \text{ separates } j \text{ and } S \setminus T\}.$$  \hfill (11)

Thus, $S^*$ is the smallest subset of $S$ that separates $j$ and $S \setminus S^*$. Our next result gives the following characterization of the minimal set $m_j(S)$, the maximal set $M_j(S)$, and the entire lattice, via graph separation:

**Theorem 3.** Assume $L^2$ Markov perfectness. Fix $j \in [d]$, $S \subset [d]_j$, and define $S^*$ by (11). Let $E_j(S^*) = \{k : S^* \text{ separates } k \text{ and } j\}$. Then,

(a) $m_j(S) = S^*$.

(b) $M_j(S) = S^* \cup E_j(S^*)$.

(c) $T_j(S) = \{S^* \cup T : T \subset E_j(S^*)\}$.

We next provide a characterization of the minimal and maximal sets of the neighborhood lattice of $j$ via connected components of the graph resulting from the removal of $j$:

**Theorem 4.** Under $L^2$ Markov perfectness, suppose that removing node $j$ and the edges connected to it breaks the PCG into $K$ connected components defined by the vertex subsets $G_1, G_2, \ldots, G_K \subset [d]_j$. Let $S_k = S \cap G_k$. Then,

(a) $m_j(S) = \bigcup_k m_j(S_k)$,

(b) $M_j(S) = \bigcup_k M_j(S_k) = \bigcup_k M_j(S_k; G_k)$, where $M_j(S_k; G_k)$ is the largest element of $T_j(S_k; G_k) := \{T \subset G_k : P_T P_j = P_{S_k} P_j\}$.
Figure 3: The graphical computation in Example 6 of the neighborhood lattice $T_j(S)$ for $j = 3$ and $S = \{9, 8, 11, 12, 14\}$. (a) Original PCG with $j$ and $S$ specified with different colors. From this figure, it is easy to see that $S^* = \{9, 12, 14\}$ is the smallest subset of $S$ that separates $j$ from $S \setminus S^*$, hence $m_j(S) = S^*$. (b) Illustration of the three connected components which result after removing node $j = 3$. As a result of Theorem 4, we can work in each component separately. For example, restricted to the left component $G_1 = \{1, 2, 8, 9, 13\}$, the minimal subset of $S \cap G_k = \{8, 9\}$ that separates $j = 3$ from the rest of $S \cap G_k$ is $S_k^* = \{9\}$. Within $G_1$, $S_k^*$ separates $\{8, 13\}$ from $j = 3$. Hence, the restricted lattice $T_j(S \cap G_1; G_1) = \langle \{9\}, \{8, 9, 13\} \rangle$.

In these statements $\emptyset$ denotes the disjoint union. Note that $T_j(S_k^*; G_k)$ is the lattice restricted to the ground set $G_k \cup \{j\}$ (i.e. instead of $[d]$). The original lattice given in Definition 4 can be thought of as $T_j(S_k^*; [d])$. For illustrative purposes, some simple consequences of Theorems 3 and 4 are as follows:

(i) $m_j(S) = \emptyset$ iff there is no path between $j$ and $S$. (Separation by the empty set.)

(ii) If the PCG decomposes into two disjoint components, say $G$ and $H$, then $M_j(S)$ contains $H$ for any $j \in G$ and any $S$.

Both (i) and (ii) hold without the prefectness assumption, and can be shown directly. However, the graphical view of Theorems 3 and 4 makes them immediately clear.

**Example 6.** Continuing with Example 5, let $j = 3$ and $S = \{9, 8, 11, 12, 14\}$. It is clear from Figure 3(a) that the smallest subset $S^*$ of $S$, separating $j$ from $S \setminus S^*$ is $\{9, 12, 14\}$. Hence, $m_j(S) = S^*$ according to Theorem 3. Similarly, $E_j(S^*) = \{4, 5, 7, 8, 10, 11, 13, 15\}$ and $M_j(S) = S^* \cup E_j(S^*)$. To verify Theorem 4, note that removing $j$ breaks the PCG into three connected components $G_1 = \{1, 2, 8, 9, 13\}$, $G_2 = \{7, 10\}$ and $G_3 = \{4, 5, 6, 11, 12, 14, 15\}$, as illustrated in Figure 3(b). Applying Theorem 3, we can compute the restricted lattices $T_j(S \cap G_k; G_k), k = 1, 2, 3$. Using the notation $[m, M]$ to represent a lattice with minimum and maximum elements $m$ and $M$, respectively, the three lattices are: $\langle \{9\}, \{8, 9, 13\} \rangle$, $\langle \{12, 14\}, \{4, 5, 11, 12, 14, 15\} \rangle$ and $\emptyset, \{7, 10\}$. It is clear that the minimal and maximal elements of the original lattice are the disjoint union of the corresponding elements of these three lattices.

As can be seen from Example 6, graphical computation (assuming prefectness holds) is much more computationally efficient than direct computation. The PCG can be constructed from the sparsity pattern of the inverse Gram matrix, $\Sigma^{-1}$, after which all the lattice computations reduce to establishing certain connectivity criteria on the graph. In contrast, direct computation requires evaluating at least some of the SEM coefficients, $\beta_j(S)$, which requires
calculating inverses $\Sigma_S^{-1}$ for different $S$. This task becomes computationally intensive when the model is high-dimensional (and $|S|$ is large) and when $\Sigma_S$ is relatively dense.

6 Directed models

Just as the undirected PCG defined in Definition 1 is the $L^2$ analogue of undirected conditional independence graphs, it is possible to extend the general $L^2$ concepts to directed graphs in a way that mirrors the theory of Bayesian networks (BNs) and structural equation models. In this section, we discuss such extensions and illustrate how these ideas are closely related to neighborhood regression and the neighborhood lattice introduced in Section 4.

6.1 Directed PCGs

There are several equivalent ways to define the notion of a directed PCG, which we describe here. Let $G$ be a directed acyclic graph (DAG) on $[d]$, and let $\Pi_j$ denote the parent set of node $j$ in $G$. Similarly, let $N_j$ be the set of non-descendants of $j$ in $G$ (i.e., $i \in N_j$ if no directed path exists from $j$ to $i$), which is a well-defined notion due to the acyclicity assumption.

Definition 6. We say that $x = (x_1, \ldots, x_d) \in \mathcal{H}^d$ satisfies a directed PCG w.r.t. $G$ if

$$P_i P_{\Pi_j} P_j = 0, \quad \forall j \in [d], \ i \in N_j.$$  \hfill (12)

This condition is modeled after the local Markov properties of BNs. Intuitively, (12) says that the residual after projecting $x_j$ onto its parents is orthogonal to any of $x_j$’s non-descendants. Alternatively, we could require that the residuals after projecting $x_i$ and $x_j$ onto their respective parent sets are orthogonal, which gives a condition which is symmetric in $i$ and $j$:

$$P_i P_{\Pi_i} P_{\Pi_j} P_j = 0, \quad \text{for all distinct } i, j \in [d].$$  \hfill (13)

A common way to rewrite these conditions is to require that there exists a vector $e \in \mathcal{H}^d$, and a matrix $B \in \mathbb{R}^{d \times d}$ with zero diagonal entries, whose associated graph is $G$ (that is, $\{(k, j) : B_{kj} \neq 0\}$ is the edge set of $G$) such that

$$\begin{array}{ll}
(a) \ x = B^T x + e, & (b) \ (B^T x)_i \perp e_i, \quad (c) \ e_i \perp e_j, \quad \forall i, j \in [d].
\end{array}  \hfill (14)
$$

Here, $B^T x$ is interpreted as an element of $\mathcal{H}^d$ with entries $(B^T x)_j = \sum_k B_{kj} x_k$. The model (14) is often called a (recursive) structural equation model (SEM) for $x$.

We have opted to define a directed PCG via (12) owing to its familiarity from the literature on directed graphical models. The following lemma, however, establishes the equivalence of conditions (12-14):

Lemma 8. Let $x = (x_1, \ldots, x_d) \in \mathcal{H}^d$ be a vector satisfying (A1) and $G$ a directed acyclic graph. Then conditions (12), (13), and (14) are equivalent.

The equivalence of (12) and (13) is proved in Appendix A.6. The equivalence of (13) and (14) is established via the following correspondences: $(B^T x)_j = P_{\Pi_j} x_j$ and $e_j = P_{\Pi_j} \perp x_j$. We note that $B$ will not be unique unless the Gram matrix $\Sigma = (\langle x_i, x_j \rangle)$ is nonsingular. Assuming that $\Sigma$ is nonsingular, the $j$th column of $B$ is $\beta_j(\Pi_j)$ as given by Definition 3.
It is always possible to obtain a directed PCG for a given $x \in \mathcal{H}^d$ by fixing an ordering of the elements of $x$ and performing recursive projection, i.e., projecting each element onto those that come before it in the ordering. More precisely, fix a $d \times d$ permutation matrix $P$, and let $\tilde{x} = P x$. Then, we set $e_1 = \tilde{x}_1$ and proceed by projecting $\tilde{x}_j$ onto $\tilde{x}_1, \ldots, \tilde{x}_{j-1}$ for $j \geq 2$, and calling the residual $e_j$. It is easy to see that this procedure leads to an SEM of the form $\tilde{x} = \tilde{B}^T \tilde{x} + e$ where $\tilde{B}^T$ is upper triangular. In terms of the original vector $x$, we obtain an SEM of the form (14) with $B = B(P) = P^T \tilde{B}$, hence a directed PCG as defined above. In the other direction any directed PCG is obtained in this way, i.e. if (14) holds, one can obtain a permutation matrix $P$ such that $P B P^T$ is lower triangular (due to acyclicity assumption). Furthermore, letting $\pi_P : [d] \to [d]$ be the permutation associated with $P$ and defining $S_j = S_j(P) = \pi_P^{-1}(\{1, \ldots, j\})$, the $j$th column of the matrix $B$ obtained in this way corresponds to the coefficients $\beta_j(S_j)$ as given by Definition 3. More interestingly, the support of $\beta_j(S_j)$ could be smaller than $S_j$ (the original candidate parent set used in the recursive projection). This support will be the minimal element of the corresponding neighborhood lattice, $T_j(S_j)$, and will act as the (actual) parent set of $j$ in the constructed PCG: that is, $\Pi_j = m_j(S_j)$ and $\beta_j(S_j) = \beta_e(\Pi_j)$. The recursive projection procedure thus establishes an interesting connection between undirected PCGs, directed PCGs, SEM coefficients, and the neighborhood lattice which can be exploited when learning graphs from data (Section 6.2).

From the above discussion, it is clear that for any $x \in \mathcal{H}^d$, there are in fact many potential directed PCGs: One for each possible ordering of its elements (note that some orderings might lead to the same directed PCG). The corresponding SEM coefficients $B$ can be related to the Cholesky factors of the inverse Gram matrix, after proper permutation: Assume that (14) holds, $P$ is a permutation matrix that makes $P B P^T$ lower triangular (always possible for a DAG), and $D$ is the diagonal Gram matrix of $e$. Letting $\Sigma$ be the Gram matrix of $x$, it is not hard to see that $\Sigma^{-1} = (I - B)D^{-1} (I - B)^T$ and $P(I - B)D^{-1/2} P^T = L$ for the Cholesky decomposition $P \Sigma^{-1} P^T = LL^T$. From this interpretation, it is clear that the SEM in (14)—alternatively a directed PCG—is not unique, i.e., for every permutation $P$ of the elements of $x$, there is a corresponding SEM obtained from the Cholesky decomposition of $P \Sigma^{-1} P^T$. This distinguishes directed PCGs from undirected PCGs, which are always unique.

### 6.2 Learning directed PCGs

The SEM model (14) provides a useful, interpretable way to describe how the variables in $x = (x_1, \ldots, x_d)$ relate to one another that is commonly used in applications such as biology, social science, and machine learning. Given its apparent utility in practice, it is of significant interest to learn the coefficient matrix $B$ from data. Furthermore, since the matrix $B$ can be interpreted as a weighted adjacency matrix for the underlying DAG $G$, learning $B$ also implies learning the structural relations encoded by the graph $G$.

Unfortunately, since directed PCGs are not unique these models are unidentifiable. In the previous subsection we illustrated how the notion of a directed PCG is naturally related to an implicit ordering on the variables, represented by a permutation $P$. To circumvent identifiability issues, one often seeks permutations that result in the sparsest DAGs, as these represent parsimonious explanations of the variables that are simple to interpret in practice. If we know the order of the variables that leads to the sparsest possible directed graph $G$, then we can use the recursive projection procedure outlined in Section 6.1 to estimate $G$. More specifically, we can use (6) with the neighborhoods $S_j$ defined previously to estimate the
support of each $\beta_j(S_j)$ and hence the graph $G$.

In practice, of course, we do not know this ordering. Thus, we must consider all possible $d!$ orderings of the variables. A naive algorithm would compute $\beta_j(S)$ for all possible neighborhoods $S \subset [d]$, and check all possible permutations to find the sparsest graph $G$. This is clearly computationally infeasible. In considering all possible neighborhoods, however, one implicitly encounters the neighborhood lattices $T(S_j)$ (Definition 4) for every possible $S \subset [d]$ and $j \in [d]$. These lattices encode how much “redundancy” exists in the different neighborhoods, and suggests that we can reduce the total number of neighborhoods one must consider by exploiting the algebraic structure of these lattices. This leads one to wonder: Is it possible to exploit this redundancy in order to learn directed PCGs more efficiently?

Without sparsity or other simplifying assumptions, there are $2^{d-1}d$ neighborhood problems to consider, which is intractable when $d$ is large. By imposing a natural sparsity assumption on the neighborhood lattices, however, the total number of neighborhood problems reduces substantially owing to the redundancies encoded by the neighborhood lattices. For example, if we assume that $|m_j(S)| \leq k \ll d$, for all $S \subset [d]$ and $j \in [d]$, the total number of neighborhood problems reduces to at most $\binom{d}{k}d \leq d^{k+1} \ll 2^{d-1}d$. This is an immediate consequence of the lattice construction in Section 4.2. By Remark 4, we have $m_j(S) = \text{supp}(\beta_j(S))$, so that this assumption amounts to assuming that the parent sets are sparse, which is a natural assumption to make in practice. This suggests that one can learn all possible SEM representations of the variables using a much smaller sample size, relative to the naive approach of solving all possible regressions. This has been successfully exploited for Gaussian models [AAZ16] to achieve optimal sample complexity $n = \Omega(k \log d)$ in learning recursive structural equation models [GH17]. The results presented in the current work suggest that these ideas can be extended much further to non-Gaussian models, a direction we intend to pursue in the future.

7 Discussion

In this paper, we explored PCGs as counterparts to conditional independence graphs (CIGs), when no assumptions are made about the distribution beyond the knowledge of the second moments. We investigated the notion of partial orthogonality as the counterpart of conditional independence and its natural relation to the general neighborhood regression problem. We also investigated the algebraic structure of neighborhood regressions, motivated by the problem of enumerating all partial orthogonality relations efficiently. Finally, we also discussed some subtleties and complications in extending these ideas to directed models. Studying these extensions in more depth is left for future work. Below, we discuss an additional avenue for future work regarding the estimation of partial orthogonality relations from a finite sample.

From a statistical perspective, all the discussions in this paper have been at the population level. In practical statistical applications, one has to estimate partial orthogonality relations from a sample of size $n$. To be precise, consider the cases where the underlying Hilbert space $\mathcal{H}$ has a stochastic component, that is, its inner product is defined as $\langle x_1, y_1 \rangle_\mathcal{H} = \mathbb{E}(x_1, y_1)_\mathcal{H}_0$ for $x_1, y_1$ random elements from a base Hilbert space $\mathcal{H}_0$, e.g., $\mathcal{H}_0 = \mathbb{R}$ or $\mathcal{H}_0 = H^1([0,1])$; see examples in Section 3.1. Now, assume that we observe independent copies $x^{(1)}, \ldots, x^{(n)}$ of $x \in \mathcal{H}^d$, a stochastic vector in $\mathcal{H}_0^d$. Based on this sample, we wish to estimate some or all of the partial orthogonality relations (5).

Under the perfectness assumption, according to the theorems of Section 5.2, the problem reduces to estimating the support of $\Sigma^{-1}$. If $d$ is fixed and $n \to \infty$, thresholding the inverse of
the sample Gram matrix, given by

\[ \hat{\Sigma} = (\hat{\Sigma}_{i,j}) \in \mathbb{R}^{d \times d}, \quad \hat{\Sigma}_{i,j} = \frac{1}{n} \sum_{k=1}^{n} \langle x^{(k)}_i, x^{(k)}_j \rangle_{\mathcal{H}_0}, \]

may be sufficient without many assumptions on the distribution. For high-dimensional data \((d \gg n)\), however, it would be interesting to see if some of the well-known penalized estimators such as the graphical lasso [FHT08] can be used to estimate the PCG without the Gaussian assumptions. Much of the previous work in this area has been focused on the Gaussian case [MB06; YL07; BEGd08; Uhl12]. Note that to recover the PCG, we need to have consistent support recovery, perhaps the strongest form of consistency in high-dimensional problems.

Without the perfectness assumption, we have to consistently estimate the support of \(\beta_j(S)\) for all \(j\) and \(S \subset [d]\), simultaneously (Corollary 1). This can be done, at least in theory, by solving all the neighborhood regression problems:

\[ \hat{\beta}_j(S) := \arg \min_{\beta \in \mathbb{R}^d, \text{supp}(\beta) \subset S} \frac{1}{n} \sum_{k=1}^{n} \| x^{(k)}_j - \beta^T x^{(k)} \|_{\mathcal{H}_0}^2, \]

and asking whether the support of \(\hat{\beta}_j(S)\), after thresholding or adding regularization, is consistent for that of \(\beta_j(S)\) for all \(j\) and \(S\). This is a very challenging problem, as there are \(a \text{ priori} a\) super-exponential number of these neighborhood regressions. Here is where the lattice property from Section 4.2 comes into play: By exploiting the lattice property, we can reduce the total number of neighborhood regression problems that we need to look at, as detailed in Section 6.2.

Finally, we note that the results presented here offer an interesting connection between undirected and directed graphs via the well-understood and intuitive notion of neighborhood regression. While such connections have appeared in passing in previous work, our results confirm and extend these ideas in the very general setting of an abstract Hilbert space. While there is much interest in using undirected graphs to simplify learning directed graphs, we emphasize that these results also offer a way to go in the opposite direction. Namely, given a DAG, how can we interpret the relationships encoded in the model in terms of the perhaps more familiar undirected PCG? Theorems 3 and 4 provide an explicit description of how the connections in \(B\)—given by \(m_j(S)\)—can be characterized in terms of the underlying PCG. Thus, our results provide an intuitive bridge between SEM and PCGs in a very general setting.

8 Proofs of the main results

Let us start with some preliminary lemmas. Recall the lattice of projections, \(\mathcal{P}(\mathcal{H})\), introduced in Section 2.3 and its meet and join operations. We have:

**Lemma 9.** For \(P, Q \in \mathcal{P}(\mathcal{H})\), \(Py = 0\) and \(Qy = 0 \iff (P \vee Q)y = 0\).

In addition, for the collection of projection operators \(\{P_S, S \subset [d]\}\) introduced in Definition 1, we have: For any \(T_1, T_2 \subset [d]\), \(P_{T_1} \vee P_{T_2} = P_{T_1 \cup T_2}\) and \(P_{T_1} \wedge P_{T_2} = P_{T_1 \cap T_2}\). In particular, \(S \subset T\) implies \(P_S \leq P_T\). All these statements extend to any number of operators and can be argued by considering bases for the underlying subspaces. For example, for the statement in Lemma 9, a basis for the range of \(P \vee Q\) can be built in such a way that it consists of the
union of bases for the range of $P$ and the range of $Q$, from which the statement follows. The following lemma is also key in the proofs:

**Lemma 10.** For $S \subset T$, $R = T \setminus S$ and any $L \in B(\mathcal{H})$,

$$P_T L = P_S L \iff P_R P_S^\perp L = 0.$$  

**Proof.** Since $P_S \leq P_T$, we have $P_T P_S = P_S$, hence $(P_T - P_S)L = P_T(I - P_S)L = P_T P_S^\perp L$. That is, the LHS is equivalent to $P_T P_S^\perp L = 0$. Multiplying by $P_R$ and using $P_R \leq P_T$ gives the RHS, i.e., $P_R P_S^\perp L = 0$. Now assume that the RHS is true; since in addition we have $P_S P_S^\perp L = 0$, it follows that $(P_R \lor P_S) P_S^\perp L = 0$ by Lemma 9, from which we get the LHS by noting that $P_R \lor P_S = P_{S \cup R}$. \hfill \qed

### 8.1 Proof of Theorem 1

**Closure under intersections:** Let $Q$ be the projection onto the range of $P_S P_j$, so that we have $Q \leq P_S$. Assume that $T_1, T_2, \ldots \in T_j(S)$ and let $R = \bigcap_k T_k$. Note that $Q$ is also the projection onto the range of $P_{T_k} P_j = P_S P_j$ for all $k$. Hence, $Q \leq P_{T_k}$ (and also $Q P_{T_k} P_j = P_{T_k} P_j$). Since $P_R = \bigwedge_k P_{T_k}$, it follows that $Q \leq P_R \leq P_{T_k}$ for all $k$. This last statement is equivalent to $P_R Q = Q$ and $P_R P_{T_k} = P_R$ for all $k$. Now, we have

$$P_R P_j = P_R P_{T_k} P_j = P_R(Q P_{T_k} P_j) = Q P_{T_k} P_j = P_{T_k} P_j = P_S P_j,$$

hence $R \in T_j(S)$. The first equality follows from $P_R \leq P_{T_k}$, the second and fourth since $Q$ projects onto range $P_{T_k} P_j$, and the third since $Q \leq P_R$. Thus, we have shown that $T_j(S)$ is closed under intersections.

**Closure under unions:** Let $S^*$ be the minimal element of $T_j(S)$ which exists by the previous argument. Note that

$$T \in T_j(S) \iff T \supset S^* \text{ and } P_T P_S^\perp P_j = 0.$$  

To see this, it is enough to note that for $T \supset S^*$, we have $(P_T - P_S^*) P_j = P_T(I - P_S^*) P_j = P_T P_S^\perp P_j$, where the first equality is by $P_S^* \leq P_T$. Now, assume that $T_1, T_2, \ldots \in T_j(S)$ and let $M = \bigcup_k T_k$. Since $T_k \in T_j(S)$, we have $T_k \supset S^*$ and $P_{T_k} P_S^\perp P_j = 0$ for all $k$. It follows that $(\bigvee_k P_{T_k}) P_S^\perp, P_j = 0$ (Lemma 9). But $P_M = \bigvee_k P_{T_k}$, that is, $P_M P_S^\perp, P_j = 0$, hence $M \in T_j(S)$ by (16).

**Convexity:** Let $S_1, S_2 \in T_j(S)$ and $S' \subset [d]_j$. Assume that $S_1 \subset S' \subset S_2$, so that $P_{S_1} \leq P_{S'} \leq P_{S_2}$. We have $P_{S_1} P_j = P_{S_2} P_j$. Multiply on the left by $P_{S'}$ and note that $P_{S'} P_{S_1} = P_{S_1}$, and $P_{S'} P_{S_2} = P_{S'}$. Thus, $P_{S_1} P_j = P_{S'} P_j$ showing that $S' \in T_j(S)$. The proof is complete.

### 8.2 Proof of Theorem 3

Throughout the proof of this theorem, we work under the assumption of $L^2$ Markov perfectness, i.e., all the lemmas in this subsection are stated under that assumption. We note that

$$S' \in T_j(S) \iff T_j(S) = T_j(S') \iff S \in T_j(S').$$  

**Lemma 11.** Let $A \subset S \subset [d]_j$. Then, $A \in T_j(S)$ iff $A$ separates $j$ from $S \setminus A$.  

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Lemma 13. Separation has these properties:

- Additive property: \( A - C_1 - B_1 \) and \( A - C_2 - B_2 \) implies \( A - (C_1 \cup C_2) - (B_1 \cup B_2) \).
• Reduction property: $A - C_1 \uplus C_2 - B$ and $C_2 - A - B$ implies $A - C_1 - B$.

**Proof.** We only show the reduction property, for which it is enough to show that there is no path from $A$ to $B$ that passes through $C_2$ and not $C_1$. If so, a portion of it gives a path from $C_2$ to $B$ that does not pass through $C_1$, and clearly not $A$ since the paths do not self-cross. But then $A$ does not separate $C_2$ and $B$, a contradiction. Figure 4 illustrates the argument. □

**Proof of Theorem 4.** By induction we can reduce to the case where the nodes are partitioned into two disjoint components $G_1$ and $G_2$, after the removal of $j$. This implies $G_1 - j - G_2$. For any set $A$, let $A_k := A \cap G_k, k = 1, 2$. We have

$$j - A - (S \setminus A) \iff j - A_1 - (S_1 \setminus A_1) \text{ and } j - A_2 - (S_2 \setminus A_2)$$

(19)

To see this, note that the RHS implies $j - A - (S_1 \setminus A_1) \cup (S_2 \setminus A_2)$ by the additive property. But $(S_1 \setminus A_1) \cup (S_2 \setminus A_2) = S \setminus A$ since $G_1$ and $G_2$ are disjoint.

Now assume the LHS. Then, clearly $j - A - (S_1 \setminus A_1)$. But we also have $A_2 - j - (S_1 \setminus A_1)$. Applying the reduction property, we get $j - A_1 - (S_1 \setminus A_1)$. The other implication is similar, hence we get the RHS.

Equipped with (19), we can prove part (a). Let $S^* = \text{the smallest subset of } S \text{ separating } j$ and $S \setminus S^*$ (see (11)), and let $S^*_1$ and $S^*_2$ be its components (i.e., $S^*_k = S^* \cap G_k, k = 1, 2$). Then, by (19) $S^*_k$ separates $j$ and $S_k \setminus S^*_k$, for $k = 1, 2$. It remains to show that $S^*_k$ is the smallest such set (for each $k$). Suppose that there is a proper subset $S'_k$ of $S^*_k$ that separates $j$ and $S \setminus S'_k$. Then, applying (19) with $A_1 = S'_1$ and $A_2 = S'_2$ and $A = S' := S'_1 \cup S'_2$, we conclude that $S'$ separates $j$ and $S \setminus S'$. But $S'$ is a proper subset of $S^*$, violating the assumption that $S^*$ is the minimal set with such property. It follows that we should have $m_j(S_1) = S_1^*$ and $m_j(S_2) = S_2^*$ which proves part (a).

For part (b), let $S_k^* = m_j(S_k), k = 1, 2$ and $S^* = m_j(S)$. From part (a), we have $S^* = S_1^* \cup S_2^*$. Fix $r \in [d]_j$. We claim that

$$r - S^* - j \iff r - S_1^* - j \text{ or } r - S_2^* - j$$

(20)

The $\Leftarrow$ implication is clear. For the other direction, assume that $r$ is separated from $j$ by $S^*$, i.e., all the paths from $r$ to $j$ pass through $S^*$. WLOG, assume that $r \in G_1$ (the case $r \in G_2$ is similar). Suppose that there is a path from $r$ to $j$ that passes through $S_2^*$. A portion of this path gives a path from $r$ to $S_2^*$, hence to $G_2$, that does not pass through $j$, contradicting $G_1 - j - G_2$. Hence all the paths from $r$ to $j$ should pass through $S_1^*$, i.e., $r - S_1^* - j$, proving (20).

From (20), we conclude that $E_j(S^*) = E_j(S_1^*) \cup E_j(S_2^*)$. Combined with characterization of $M_j(S)$ in Theorem 3(b), this proves the first equality in part (b).

To see the second equality in (b), recall that $T_j(S_k; G_k)$ is the lattice with ground set restricted to $G_k \cup \{j\}$. First, the minimal element of $T_j(S_k; G_k)$ is the same as that of $T_j(S_k)$. This is true since a subset $A$ of $S_k$ separates $j$ and $S_k \setminus A$ in $G_k \cup \{j\}$ iff it does so in $G$. (If the separation happens in $G_k \cup \{j\}$ but not in $G$, there will be a path from $S_k \setminus A$ to $j$ passing through some $G_r, r \neq k$ contradicting disjointness of $G_k$ and $G_r$.) Even more directly, a minimal subset of $T_j(S_k)$ is a subset of $S_k$, hence $G_k$, and the restriction in $T_j(S_k; G_k)$ is automatically satisfied. Knowing that the minimal element of $T_j(S_k; G_k)$ is $S_k^*$, we invoke Theorem 3(b) restricted to $G_k \cup \{j\}$ to conclude that $M_j(S_k; G_k) = S_k^* \cup E_j(S_k^*; G_k)$ where $E_j(S_k^*; G_k) = \{i \in G_k : S_k^* \text{ separates } i \text{ and } j\}$. Going through the argument leading to (20), it is clear that we can replace (20) with

$$r - S^* - j \iff [r - S_1^* - j \text{ and } r \in G_1] \text{ or } [r - S_2^* - j \text{ and } r \in G_2]$$

(21)
showing that $E_j(S^*) = E_j(S_1^*; G_1) \cup E_j(S_2^*; G_2)$. Combined with the expression for $M_j(S_k; G_k)$, the desired result follows.

\[ \square \]

### 8.4 Proof of Theorem 2

For simplicity, let us introduce some notation and terminology. Let $S^d$ be the set of symmetric $d \times d$ matrices, $S^d_{++}$ the set of $d \times d$ positive definite matrices, and $S^d_{++1} = \{ \Gamma \in S^d_{++} : \Gamma_{i,i} = 1, \ i \in [d] \}$. Matrices in $S^d_{++1}$ are often called correlation matrices. To avoid confusion, we will call them Cor matrices. According to Lemma 6, $L^2$ Markov properties are invariant to arbitrary rescaling of the Gram matrix $\Sigma$. Thus, it is enough to focus on the case where $(\Sigma^{-1})_{i,i} = 1$ for all $i \in [d]$. We will call a matrix $\Sigma$ such that $\Sigma^{-1} \in S^d_{++1}$, an inverse-Cor matrix.

Given any graph $G$ on nodes $[d]$, our goal is to construct a collection of random inverse-Cor matrices that are $L^2$ Markov w.r.t. $G$. We then show that with probability one, such inverse-Cor matrices are perfect. The class of inverse-Cor matrices that are $L^2$ Markov w.r.t. $G$ can be written as

$$\Psi^{-1}_G := \{ \Gamma^{-1} : \Gamma \in \Psi_G \}, \quad \text{where} \quad \Psi_G := \{ \Gamma \in S^d_{++1} : \Gamma_{i,j} \neq 0 \ \text{iff} \ i,j \in G \}.$$

Note that $\Psi_G$ is the set of Cor matrices with support $G$. The first step in our approach is to put a distribution on $\Psi^{-1}_G$ as the push-forward of a distribution on $\Psi_G$ which we construct. Our construction is not uniform w.r.t. the Lebesgue measure, however, in Theorem 2, we extend the result to any distribution on $\Psi_G$ which is absolutely continuous w.r.t. the Lebesgue measure.

Before describing our construction of a random inverse-Cor matrix, let us set up some more notation. We let $L^n$ and $H^s$ ($s > 0$) denote, respectively, the Lebesgue measure and the $s$-dimensional Hausdorff measure on $\mathbb{R}^n$. The dimension of the ambient space of $H^s$ will be clear from the context. For the graph $G$, let $g = |G|$ be the number of edges. We often identify $\Psi_G$ with a subset of $\mathbb{R}^G$, and often identify $\mathbb{R}^G$ with $\mathbb{R}^g$, after ordering the edges, the particular order being unimportant. For example, if $G$ is $1 - 2 - 3$, with $g = |G| = 2$, and $\Gamma \in \Psi_G$ is

$$\Gamma = \begin{pmatrix} 1 & \delta_{12} & 0 \\ \delta_{12} & 1 & \delta_{23} \\ 0 & \delta_{23} & 1 \end{pmatrix},$$

we either view $\Gamma$ as $\{\delta_{12}, \delta_{23}\} = (\delta_{ij}, i,j \in G)$, as an element of $\mathbb{R}^G$, or as the ordered pair $(\delta_{12}, \delta_{23})$ as an element of $\mathbb{R}^g = \mathbb{R}^2$.

For $\delta = (\delta_{ij}, i,j \in G) \in \mathbb{R}^G$ and $\varepsilon > 0$, define $A^{G,\delta,\varepsilon} = (a_{ij}^{G,\delta,\varepsilon}) \in \mathbb{R}^{d \times d}$ by setting

$$a_{ii}^{G,\delta,\varepsilon} = 1, \ \forall i \quad \text{and} \quad a_{ij}^{G,\delta,\varepsilon} = \delta_{ij} \varepsilon 1\{i,j \in G\}, \ \forall i \neq j. \quad (22)$$

For a fixed $\delta \in \mathbb{R}^G$, let $\varepsilon_G(\delta)$ be the largest $\varepsilon > 0$ such that $A^{G,\delta,\varepsilon}$ is positive definite, that is, $\varepsilon_G(\delta) := \sup\{\varepsilon > 0 : A^{G,\delta,\varepsilon} \in S^d_{++} \}$. Let $[-1,1]_* := [-1,1] \setminus \{0\}$ and consider

$$\mathcal{M}^G := \{ (\delta, \varepsilon) : \ \delta \in [-1,1]^G, \ \varepsilon \in (0, \varepsilon_G(\delta)) \}.$$

The set $\{(A^{G,\delta,\varepsilon})^{-1} : (\delta, \varepsilon) \in \mathcal{M}^G \}$ is (a parametrization of) the set of all inverse-Cor matrices that are $L^2$ Markov w.r.t. $G$. In other words, with the map $\zeta$ given by

$$\zeta : \mathbb{R}^G \times \mathbb{R} \rightarrow S^d, \quad \zeta(\delta, \varepsilon) = (A^{G,\delta,\varepsilon})^{-1}, \quad (23)$$

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we have \( \zeta(\mathcal{M}^G) = \Psi_G^{-1} \). We note that \( \mathcal{M}^G \) is a subset of \([-1, 1]^G \times (0, \infty) \subset \mathbb{R}^G \times \mathbb{R} \simeq \mathbb{R}^{g+1} \). We will equip \( \mathcal{M}^G \) with the Lebesgue measure (i.e., \( \mathcal{L}^{g+1} \)).

Alternatively, we can work with the normalized Lebesgue measure to obtain a uniform probability distribution. For technical reasons, we will work with the subset of \( \mathcal{M}^G \) for which \( \delta \) has unit \( \ell_\infty \) norm. Let \( \mathbb{S}_\infty^G := \{ \delta \in \mathbb{R}^G : \|\delta\|_\infty = 1 \} \), \( \mathbb{S}_{\infty,*}^G = [-1, 1]_*^G \cap \mathbb{S}_\infty^G \), and

\[
\mathcal{M}_\infty^G := \mathcal{M}^G \cap (\mathbb{S}_\infty^G \times \mathbb{R}) = \{ (\delta, \varepsilon) : \delta \in \mathbb{S}_{\infty,*}^G, \varepsilon \in (0, \varepsilon_G(\delta)) \}.
\]

The function \( \varepsilon_G \), restricted to \( \mathbb{S}_{\infty,*}^G \), is continuous and bounded. In fact, sup \( \varepsilon_G(\mathbb{S}_{\infty,*}^G) = 1 \) so that \( \mathcal{M}_\infty^G \subset [-1, 1]^G \times (0, 1) \). Hence \( \mathcal{M}_\infty^G \) has finite and positive \( \mathcal{H}^g \)-measure (on \( \mathbb{R}^{g+1} \)), where \( g := |G| \). We equip \( \mathcal{M}_\infty^G \) with the normalized \( \mathcal{H}^g \)-measure, to get a uniform probability distribution. The uniform distribution on \( \mathcal{M}_\infty^G \) can also be described as follows: Pick \( \delta' \) by drawing each entry uniformly from \([-1, 1]_* \), and given \( \delta' \), set \( \delta = \delta' / \|\delta'\|_\infty \) and draw \( \varepsilon \) uniformly from \([0, \varepsilon_G(\delta)]\); the vector \((\delta, \varepsilon)\) has the desired distribution. We will use \( \mu_G \) to refer to the uniform distribution on \( \mathcal{M}_\infty^G \). See Figure 5. The map \( \zeta \) defined earlier is also well-behaved over \( \mathcal{M}_\infty^G \): It is one-to-one, and onto \( \Psi_G^{-1} \), that is, \( \zeta : \mathcal{M}_\infty^G \rightarrow \Psi_G^{-1} \) is a bijection. We can now put a distribution on inverse-Cor matrices, \( \Psi_G^{-1} \), as the push-forward of \( \mu_G \) by \( \zeta \).

Let us now consider the subclass of \( \Psi_G^{-1} \) which is non-perfect. It is enough to work with the corresponding subsets in \( \mathcal{M}^G \) and \( \mathcal{M}_\infty^G \):

\[
\mathcal{N}^G = \{(\delta, \varepsilon) \in \mathcal{M}^G : (A^G,\delta,\varepsilon)^{-1} \text{ is not perfect}\},
\]

\[
\mathcal{N}_\infty^G = \{(\delta, \varepsilon) \in \mathcal{M}_\infty^G : (A^G,\delta,\varepsilon)^{-1} \text{ is not perfect}\} = \mathcal{N}^G \cap (\mathbb{S}_\infty^G \times \mathbb{R})
\]

The following result is the key component on which Theorem 2 is based:

**Theorem 5.** For \( \delta \in [-1, 1]^G \), let \( B_\delta := \{ \varepsilon : (\delta, \varepsilon) \in \mathcal{N}^G \} \), and let \( g := |G| \geq 2 \). There exists a set \( \mathcal{D} \subset [-1, 1]^G \) such that

(a) \( \mathcal{D}^c \) is an \( \mathcal{L}^g \)-null set,

(b) \( \mathbb{S}_\infty^G \cap \mathcal{D}^c \) is an \( \mathcal{H}^{g-1} \)-null set, and

(c) for every \( \delta \in \mathcal{D} \), \( B_\delta \) is finite, that is, \( \mathcal{H}^0(B_\delta) < \infty \).
In particular, (d) the set \( N^G \) is \( \mathcal{H}^{g+1} \)-null set, and \( N^G_\infty \) is \( \mathcal{H}^g \)-null set.

Since \( \mathcal{H}^{g+1} = \mathcal{L}^{g+1} \) on \( \mathbb{R}^{g+1} \), we can equivalently say that \( N^G \) has Lebesgue measure zero. Theorem 5 is proved in Section 8.5. To get an intuition for this result, consider the example \( G = 1 - 2 - 3 \) illustrated in Figure 5. Theorem 5 says that there is a “good” set \( \mathcal{D} \) of \( (\delta_{12}, \delta_{23}) \in [-1,1]^2 \) which has full 2-dimensional measure, and its boundary (i.e., the intersection with the perimeter of the square \([-1,1]^2\)) has full 1-dimensional measure, and such that for any \((\delta_{12}, \delta_{23}) \in \mathcal{D} \) at most finitely many \( \varepsilon \) are problematic, i.e. lead to a nonperfect Gram matrix. Equipped with this result, we can finish the proof of Theorem 2:

\[ N = \{ \Gamma \in \Psi_G : \Gamma^{-1} \text{ is not perfect} \}. \]  

Proof of Theorem 2. Recall the identification of \( \Psi_G \) with a subset of \( \mathbb{R}^G \simeq \mathbb{R}^g \). The cases \( g = 0 \) and \( g = 1 \) are trivial, so we will assume \( g \geq 2 \). We proceed in two steps:

**Step 1.** We first show that for any distribution on Cor matrices, \( \Psi_G \), that is absolutely continuous w.r.t \( \mathcal{H}^g = \mathcal{L}^g \) on \( \Psi_G \), the result holds. Consider the map \( F : \mathbb{R}^G \times \mathbb{R} \to \mathbb{R}^G \) given by \( F(\delta, \varepsilon) = (\delta_{ij} \varepsilon, ij \in G) \). Since \( F \) is a \( C^1 \) map, it is locally Lipschitz. In fact, \( F \) is Lipschitz over \( \mathcal{M}^G_\infty \). It is well-known that a Lipschitz map (between two metric spaces) maps \( \mathcal{H}^s \)-null sets to \( \mathcal{H}^s \)-null sets, for any \( s > 0 \); see for example [KP08, Proposition 2.4.7]. Since \( \mathcal{H}^g(\mathcal{N}^G_\infty) = 0 \) according to Theorem 5, it follows that \( \mathcal{H}^g(F(\mathcal{N}^G_\infty)) = 0 \). Let

\[ N = \{ \Gamma \in \Psi_G : \Gamma^{-1} \text{ is not perfect} \}. \]  

Recalling the identification of \( \Psi_G \) with a subset of \( \mathbb{R}^G \), and that \( F : \mathcal{M}^G_\infty \to \Psi_G \) is a bijection, we have \( F(\mathcal{N}^G_\infty) \simeq N \), that is, \( \mathcal{H}^g(N) = 0 \).

**Step 2.** Now consider the map \( \xi \) on \( \mathbb{R}^d_+ \times \mathbb{R} \to \mathbb{R}^G \) given by

\[ \xi : (x_k, k \in [d]; y_{ij}, ij \in G) \mapsto \left( \frac{y_{ij}}{\sqrt{x_i x_j}}, ij \in G \right), \]  

which should be thought of as mapping a general PD matrix, with support \( G \), to its corresponding Cor matrix (ignoring the diagonal of all ones). We claim that the push-forward of \( \mathcal{L}^{g+d} \) by \( \xi \) is absolutely continuous w.r.t. to \( \mathcal{H}^g = \mathcal{L}^g \) on \( \mathbb{R}^G \simeq \mathbb{R}^g \). This follows since \( \xi \) is \( C^1 \), hence locally Lipschitz on \( \Omega := \mathbb{R}^d_+ \times \mathbb{R}^g \); see Lemma 16 in Appendix A.4 for details. Combined with the result of Step 1, this implies \( \mathcal{L}^{g+d}(\xi^{-1}(N)) = 0 \). But \( \xi^{-1}(N) \) is the set of all PD matrices with support \( G \) that are not perfect. The proof is complete.

It is worth noting that the measure \( \mu_G \), constructed in this section, is itself interesting. It gives a practical device to generate a random sample (albeit with non-uniform distribution) from the set of all (properly normalized) Gram matrices that are \( L^2 \) Markov w.r.t. to any given graph \( G \). The only computational burden is computing \( \varepsilon_G(\delta) \), which can be obtained by solving a convex optimization problem. We expect this approach to be much more efficient in practice than, say, rejection sampling.

### 8.5 Proof of Theorem 5

Let us introduce some notation, most of which are borrowed from [LM07] with minor modifications. We assume familiarity with the arguments in [LM07] and keep the discussion of the notation to a minimum. An \( ij \)-path on \([d]\) is an ordered sequence \( i_0 \to i_1 \to i_2 \cdots \to i_t \to i_{t+1} \),
where \( i_j, j = 0, \ldots, t + 1 \) are distinct elements of \([d]\), \( i_0 = i \) and \( i_{t+1} = j \). We represent such a path as an ordered subset \( \Pi = \{i_0, i_1, \ldots, i_{t+1}\} \) of \([d]\). An \( i_0 \)-cycle on \([d]\) is a \( i_0 \)-path; that is, an ordered sequence of the form \( i_0 \rightarrow i_1 \rightarrow i_2 \rightarrow \cdots \rightarrow i_t \rightarrow i_0 \), where \( i_j, j = 0, \ldots, t \) are distinct elements of \([d]\). We will represent such a cycle as an ordered subset \( C = \{i_0, i_1, \ldots, i_t\} \) of \([d]\).

Ultimately, the \( ij \)-paths and \( i_0 \)-cycles will be used to represent non-intersecting paths and cycles on a graph \( G \) on nodes \([d]\). The graph \( G \) will be viewed as set of unordered pairs from \([d]\) representing the edges of \( G \). We say that an \( ij \)-path \( \Pi = \{i = i_0, i_1, \ldots, i_{t+1} = j\} \) belongs to \( G \), denoted as \( \Pi \in G \), if all the edges in the path belong to \( G \), that is, \( ij, j = 0, \ldots, t \). The set of \( ij \)-paths that belong to \( G \) is denoted as \( \mathcal{P}^{ij}(G) \). With some abuse of notation, we let \( \mathcal{P}^{ij} = \mathcal{P}^{ij}([d]) \) denote the set of all \( ij \)-path on \([d]\) (corresponding to the complete graph). The set of all \( ij \)-paths of \( G \) of length \( t + 1 \) is denoted as \( \mathcal{P}^{ij}_t(G) \), that is

\[
\mathcal{P}^{ij}_t(G) := \{\Pi \in \mathcal{P}^{ij} : \Pi \in G, |\Pi| = t + 1\}.
\]

We let \( \mathcal{P}_t(G) := \bigcup_{ij \in [d]} \mathcal{P}^{ij}_t(G) \), the set of all paths of length \( t + 1 \) in \( G \). The parallel notations for \( i \)-cycles, namely

\[
\mathcal{C}^i(G), \quad \mathcal{C}^i = \mathcal{C}^i([d]), \quad \mathcal{C}^i_t(G), \quad \text{and} \quad \mathcal{C}_t(G)
\]

are defined similarly (by setting \( i = j \) in the corresponding definitions for paths).

For an \( ij \)-path \( \Pi = \{i_0 = i, i_1, \ldots, i_t, j = i_{t+1}\} \in \mathcal{P}^{ij} \) and a matrix \( B = (b_{ij}) \in \mathbb{R}^{d \times d} \), let

\[
b_{\Pi} = \prod_{j=0}^{t} b_{i_j,i_{j+1}}. \tag{27}
\]

Note that if, instead, \( b \in \mathbb{R}^G \) and \( \Pi \) is a path that belongs to \( G \), then \( b_{\Pi} \) as above is still well-defined (i.e., we do not need \( b \) to be defined outside \( G \)). A similar notation, namely \( b_C \), is well-defined when \( C \) is an \( i_0 \)-cycle. (In this case, \( i_{t+1} = i_0 \) in (27).)

The proof of Theorem 5 relies on the following key technical lemma, which is as an extension of Lemma 4 in [LM07] and is proven in Appendix A.1. Here, we treat node 1 specially, hence the emphasis on the collection of 1-cycles (cycles which begin and end on node 1) of a given length \( t \), namely \( \mathcal{C}^1_t(G) \). The special role given to 1 becomes clear in the proof of Theorem 6 below, where in dealing with an \( ij \)-path of \( G \), we identify the endpoints with node 1 of a new graph \( H \), hence obtaining a 1-cycle of \( H \). Let \( \mathbb{C}[x] \) be the set of polynomials in indeterminate variable \( x \), with complex coefficients. For \( p \in \mathbb{C}[x] \), we say that \( p = 0 \in \mathbb{C}[x] \), or \( p(x) = 0 \) in \( \mathbb{C}[x] \), if \( p \) is the zero polynomial (i.e., all its coefficients are zero). For a square matrix \( B, |B| \) denotes its determinant.

**Lemma 14.** Consider a graph \( H \) on \([r]\) with no self-loops on any node except possibly node 1. Let \( \delta_{ij} \neq 0 \), for \( ij \in H \) with \( i \neq j \), and \( \delta_{11} \neq 0 \). Define a matrix \( B(x) = (b_{ij}(x)) \in \mathbb{R}^{r \times r} \) by

\[
b_{ii} = 1, \quad \forall i > 1, \quad \text{and} \quad b_{ij}(x) = \delta_{ij} x 1\{ij \in H\}, \quad \text{for } i \neq j \text{ and } i = j = 1,
\]

treating \( b_{ij}(x) \) as a polynomial in \( \mathbb{C}[x] \). Assume that \( |B(x)| = 0 \) in \( \mathbb{C}[x] \), that is, \( |B(x)| \) is the zero polynomial. Then, either \( \mathcal{C}^1_t(H) = \emptyset \) for all \( t \geq 0 \) or

\[
\exists t \in [d] \text{ such that } \mathcal{C}^1_t(H) \neq \emptyset, \quad \sum_{C \in \mathcal{C}^1_t(H)} \delta_C = 0. \tag{28}
\]
Note that in the case \( t = 0 \), \( C_1^t(H) \) is nonempty only if \( H \) has a self-loop on node 1. Following [LM07], let \( \mathcal{N} = [d] \) and \( \mathcal{R}(\mathcal{N}) \) the set of all couples \((ij|K)\) such that \( i \) and \( j \) are distinct singletons of \( \mathcal{N} \) and \( K \subset \mathcal{N} \setminus ij \). Subsets of \( \mathcal{R}(\mathcal{N}) \) are called relations. To simplify notation, unless otherwise stated, couples of the form \((ij|K)\) are always assumed to belong to \( \mathcal{R}(\mathcal{N}) \). The dual couple of \((ij|K)\) is \((ij|N \setminus ijK)\). For a relation \( \mathcal{L} \subset \mathcal{R}(\mathcal{N}) \), the dual relation \( \mathcal{L}^\dagger \) is defined as the relation containing all the dual couples of the elements of \( \mathcal{L} \). For any matrix \( A \in \mathbb{R}^{d \times d} \), let

\[
\langle A \rangle := \{(ij|K) : |A_{iK,jK}| = 0\}.
\]

By Lemma 1 in [LM07], for an invertible matrix \( A \), we have \( \langle A \rangle^\dagger = \langle A^{-1} \rangle \). For a simple undirected graph \( G \) with vertex set \( \mathcal{N} \), let

\[
\langle \rangle := \{(ij|K) : \text{\( K \) separates \( i \) and \( j \) in } G \}\}.
\]

Recalling the notation \( \mathcal{P}^ij_t(G) \), let us write \( \mathcal{P}^ij_t(G;K) := \{\Pi \in \mathcal{P}^ij_t(G) : \Pi \subset ijK\} \) to denote the set of \( ij \)-paths in \( G \) of length \( t + 1 \) that pass entirely through \( K \). Also recall that for \( \delta \in \mathbb{R}^G \) and any path \( \Pi \in \mathcal{P}_t(G) \) (of length \( t \)) in \( G \), the quantity \( \delta_{\Pi} \) is well-defined using (27). We define:

\[
\mathcal{D} = \mathcal{D}_G := \left\{ \delta \in [-1,1]^\mathbb{N}_d : \sum_{\Pi \in \mathcal{P}} \delta_{\Pi} \neq 0, \text{ for all nonempty } \mathcal{P} \subset \mathcal{P}_t(G), t \in [d] \right\}.
\]

\[
\text{Theorem 6. Let } G \text{ be a simple graph with vertex set } \mathcal{N}. \text{ Then, for any } \delta \in \mathcal{D}, \text{ there are finitely many } \varepsilon \in \mathbb{C} \text{ for which } \langle \rangle^\dagger = \langle (\mathcal{G},\delta,\varepsilon) \rangle \text{ fails, where } \mathcal{G},\delta,\varepsilon \text{ is defined in (22).}
\]

\[
\text{Proof. Let } A^{\mathcal{G},\delta,\varepsilon} \text{ be the matrix with elements in } \mathbb{C}[x] \text{ obtained by replacing } \varepsilon \text{ in } A^{\mathcal{G},\delta,\varepsilon} \text{ by indeterminate } x. \text{ Consider }
\]

\[
\langle (\mathcal{G},\delta,\varepsilon) \rangle \subseteq \mathbb{C}[x] := \{(ij|K) : |A_{iK,jK}^{\mathcal{G},\delta,\varepsilon}| = 0 \text{ in } \mathbb{C}[x]\}.
\]

\[
\text{Step 1. Fix } \delta \in \mathcal{D}. \text{ We show that } \langle \rangle^\dagger = \langle (\mathcal{G},\delta,\varepsilon) \rangle \subseteq \mathbb{C}[x]. \text{ Consider } A_{iK,jK}^{\mathcal{G},\delta,\varepsilon} \text{ and transpose rows } 1 \text{ and } i, \text{ and columns } 1 \text{ and } j. \text{ This operation does not change the determinant, and from now on, we can identify } (i,j) \text{ with element } (1,1) \text{ in Lemma 14. In particular, let } H \text{ be the subgraph of } G \text{ induced on nodes } ijK, \text{ with nodes } i \text{ and } j \text{ identified together and renamed node } 1. \text{ Thus, a path from } i \text{ to } j \text{ in } G \text{ that lies entirely in } ijK \text{ corresponds to a cycle in } H \text{ starting at node } 1. \text{ In other words, we can identify } \mathcal{P}_t^ij(G;K) \text{ with } C_1^t(H). \text{ Also note that a possible edge between } i \text{ and } j \text{ in } G \text{ will be a self-loop on node } 1 \text{ in } H, \text{i.e., } \delta_{ij}x \text{ plays the role of } \delta_{11}x \text{ in Lemma 14. Assumption (29) then implies that (28) of Lemma 14 cannot hold for } H \text{ derived from any } (ij|K) \in \mathcal{R}(\mathcal{N}). \text{ It follows from Lemma 14 that } |A_{iK,jK}^{\mathcal{G},\delta,\varepsilon}| = 0 \text{ iff } C_1^t(H) \text{ or equivalently } \mathcal{P}_t^ij(G;K) \text{ is empty for all } t \geq 0. \text{ That is, there is no } ij \text{-path in } G \text{ of any length that passes entirely through } K. \text{ In other words, every } ij \text{ path in } G \text{ should intersect } \mathcal{N} \setminus ijK, \text{i.e., } i \text{ and } j \text{ are separated in } G \text{ by } \mathcal{N} \setminus ijK, \text{ or in symbols } (ij|K) \in \langle \rangle^\dagger.
\]

\[
\text{Step 2. Fix } \delta \in \mathbb{R}^G. \text{ For any } \varepsilon \in \mathbb{C}, \text{ } |A_{iK,jK}^{\mathcal{G},\delta,\varepsilon}| = 0 \text{ in } \mathbb{C}[x] \text{ implies } |A_{iK,jK}^{\mathcal{G},\delta,\varepsilon}| = 0. \text{ (A zero polynomial evaluates to zero at every point.) That is, }
\]

\[
\langle (\mathcal{G},\delta,\varepsilon) \rangle \subset \langle (\mathcal{G},\delta,\varepsilon) \rangle, \text{ } \forall \varepsilon \in \mathbb{C}.
\]
The inclusion is strict iff there is \((ij|K)\) such that \(p_{ijK}(x, \delta) := |A_{jk}^{G,\delta}(x)|\) is a nonzero polynomial (in \(\mathbb{C}[x]\)) with root \(\varepsilon\). Since any such polynomial has a finite number of roots, we have \(\langle A_{jk}^{G,\delta}\rangle_{\mathbb{C}[x]} = \langle A_{jk}^{G,\delta}\rangle\), for all but finitely many \(\varepsilon \in \mathbb{C}\). Combined with Step 1, the assertion follows. \(\square\)

**Lemma 15.** Let \(\Sigma\) be a covariance matrix such that \(\langle G \rangle = \langle \Sigma^{-1} \rangle\). Then, \(\Sigma\) is \(L^2\) Markov perfect w.r.t. \(G\).

**Proof.** First we note that by Lemma 1 in [LM07], \(\langle G \rangle = \langle G \rangle = \langle \Sigma^{-1} \rangle = \langle \Sigma \rangle\). Recall \(\mathcal{N} := [d]\). Assume that \(\Sigma\) is not perfect. Then, there exist nonempty disjoint sets \(A, B \subset \mathcal{N}\) and \(K \subset \mathcal{N} \setminus AB\) such that \(P_AP_BK = 0\) and \(K\) does not separate \(A\) and \(B\). Then, \(\exists i \in A, j \in B\) such that \(\neg(i - K - j)\) and clearly \(K \subset \mathcal{N} \setminus ij\). That is, \((ij|K) \in \mathcal{R}N\). We also have \(P_AP_BK = P_AP_BK = 0\) since \(P_i \leq P_A\) and \(P_j \leq P_B\), hence \(|\Sigma_{ijij}| = 0\) by Lemma 3. That is, \((ij|K) \in \langle \Sigma \rangle\), hence we should have \((ij|K) \in \langle G \rangle\), contradicting \(\neg(i - K - j)\). The proof is complete. \(\square\)

**Proof of Theorem 5.** Part (c) of Theorem 5, with \(\mathcal{D}\) given by (29), follows from Theorem 6 and Lemma 15 and the relation \(\Sigma^{-1} = A_{jk}^{G,\delta,\varepsilon}\). For part (a), we note that \(\mathcal{D}^c := \{\delta \in [-1, 1]^G : \delta \notin \mathcal{D}\}\) is the unique union of the zero sets of nontrivial polynomials, hence of \(L^2\)-measure zero in \([-1, 1]^G\) (as a subset of \(\mathbb{R}^G \simeq \mathbb{R}^g\)). For part (b), let \(S^c_G = \bigcup_{ij} (F^+_ij \cup F^-ij)\) be the decomposition of \(S^c_G\) into its \((g - 1)\)-dimensional faces: \(F^+ij = \{\delta : \delta_{ij} = \pm 1\}\). It is enough to show, for example, that \(F^+ij \cap \mathcal{D}^c\) has \(\mathcal{H}^{g-1}\)-measure zero. Let \(G'\) be \(G\) with edge \(ij\) removed. By fixing \(\delta_{ij} = 1\), we can view \(F^+ij \cap \mathcal{D}^c\) as a subset of \(F^+ij \subset \mathbb{R}^{g'} \simeq \mathbb{R}^{g-1}\). Recalling the definition of \(\mathcal{D}\), (29), we observe, as before, that \(F^+ij \cap \mathcal{D}^c\) as a subset of \(\mathbb{R}^{g-1}\) has \(L^{g-1}\)-measure zero as a finite union of the zero sets of nontrivial polynomials in \(g - 1\) variables \(\delta_{ij} = (\delta_{rs}, rs \in G')\). Since \(L^{g-1} = \mathcal{H}^{g-1}\) on \(\mathbb{R}^{g-1}\), the assertion follows.

For part (d), both \(L^{g+1}(N^G) = 0\) and \(\mathcal{H}^g(\mathcal{N}^G) = 0\) follow from the Fubini theorem for the Lebesgue measure. For example, consider the latter assertion. It is enough to show \(\mathcal{H}^g(\mathcal{N}^G \cap (F^+ij \times \mathbb{R})) = 0\). Viewing \(\mathcal{N}^G \cap (F^+ij \times \mathbb{R})\) as a subset of \(\mathbb{R}^{g-1} \times \mathbb{R}\), as above, and using the decomposition of the Lebesgue measure \(L^g = L^{g-1} \times L^1\), Fubini theorem gives

\[
\mathcal{H}^g(\mathcal{N}^G \cap (F^+ij \times \mathbb{R})) = \int_{F^+ij} L^1(B_\delta) d\mathcal{H}^{g-1}(\delta) = \int_{F^+ij \cap \mathcal{D}^c} L^1(B_\delta) d\mathcal{H}^{g-1}(\delta) + \int_{F^+ij \cap \mathcal{D}} L^1(B_\delta) d\mathcal{H}^{g-1}(\delta).
\]

Both integrals are zero, the first since \(\mathcal{H}^{g-1}(F^+ij \cap \mathcal{D}^c) = 0\) by part (b), and the second since \(B_\delta\) has finitely many elements hence \(L^1(B_\delta) = 0\), by part (c). The proof is complete. \(\square\)

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A Proofs of auxiliary results

We recall the following notational conventions: For a matrix \( \Sigma \in \mathbb{R}^{d \times d} \), and subsets \( A, B \subset [d] \), we use \( \Sigma_{A,B} \) for the submatrix on rows and columns indexed by \( A \) and \( B \), respectively. Single index notation is used for principal submatrices, so that \( \Sigma_A = \Sigma_{A,A} \). For example, \( \Sigma_{i,j} \) is the \((i,j)\)th element of \( \Sigma \) (using the singleton notation), whereas \( \Sigma_{ij} = \Sigma_{ij,ij} \) is the \(2 \times 2\) submatrix on \( \{i,j\} \) and \( \{i,j\} \).

A.1 Proof of Lemma 14

Recall the definition of the \( i_0 \)-cycle (of \([d]\) or a graph \( G \)) from Section 8.5. In proving Lemma 14, we will use the term cycle to also refer to cycles of a permutation. The necessary background
on cycle decomposition is briefly reviewed below. The two notions of cycle (graph versus permutation) are related in our arguments, and the distinction in each occurrence should be clear from the context.

Recall that every permutation \( \pi \) on \([d]\), that is, a bijective map \( \pi : [d] \to [d] \), has a unique cycle decomposition, once we agree on a particular order within cycles and among them [Sta97, Section 1.3]. For example, representing \( \pi = (142)(3)(5) \) means that \( \pi \) has two cycles \( C_1 = \{1, 4, 2\} \) and \( C_2 = \{3, 5\} \). \( C_1 \) being a cycle means that \( \pi \) maps 1 to 4, 4 to 2, and 2 back to 1, and similarly for \( C_2 \). We treat the cycles of \( \pi \) as ordered sets with the smallest element written first, and the rest of the order determined by the action of \( \pi \). (That is, if \( C = \{i_0, i_1, \ldots, i_t\} \) is a cycle of \( \pi \), we have \( i_0 < i_j \) and \( \pi(i_{j-1}) = i_j \) for \( j = 1, \ldots, t \).) Thus, permutation cycles are also graph cycles in the sense of Section 8.5. The (unordered) collection of cycles of \( \pi \) will be denoted as \( S_\pi \), in this case, \( S_\pi = \{C_1, C_2\} \). The ordering among the cycles is unimportant. We also follow the convention of disregarding trivial cycles, that is, those containing a single element. In this sense, the identity permutation has no cycles. We often talk about “single cycle” permutations: for example, \( \pi' = (142)(3)(5) \) has a single cycle \( C_1 = \{1, 4, 2\} \) in our convention.

For matrix \( B = (b_{i,j}) \in \mathbb{R}^{d \times d} \) and permutation \( \pi \) on \([d]\), we write

\[
b_\pi := \prod_{i \in [d]} b_{i,\pi(i)} = \prod_{C \in S_\pi} b_C,
\]

where \( b_C \) is as defined\(^3\) in (27). For the example above the two expressions are

\[
b_\pi = b_{1,4}b_{2,1}b_{3,5}b_{4,2}b_{5,3} = (b_{1,4}b_{4,2}b_{2,1})(b_{3,5}b_{5,3}).
\]

For any permutation, \( \pi \), let \( C_\pi \) be its 1-cycle, i.e., its cycle that contains 1 and let \( t_\pi = |C_\pi \setminus \{1\}| = |C_\pi| - 1 \). We will call \( C_\pi \) the first cycle of \( \pi \). Note that \( b_{C_\pi} = \prod_{i \in C_\pi} b_{i,\pi(i)} \) is a factor of \( b_\pi \). Note that for every permutation \( \pi \), there is a “single cycle” permutation \( \pi' \) (as in the example above) such that \( C_\pi = C_{\pi'} \), hence \( b_{C_\pi} = b_{C_{\pi'}} \).

**Proof of Lemma 14.** For simplicity, we will drop the explicit dependence on \( x \) and write \( B = (b_{i,j}) \). By assumption, we have \( 0 = |B| = \sum_\pi \text{sign}(\pi)b_\pi \). Note that \( b_\pi \) has \( b_{C_\pi} \) as a factor. We will show that \( b_{C_\pi} = 0 \) for all \( \pi \), form which the claim follows. (See the last paragraph of the proof.) We proceed by induction on \( t_\pi = |C_\pi| - 1 \in \{0, \ldots, r\} \), proving the induction step and the case \( t_\pi = 0 \) simultaneously. Assume that \( 0 \leq t \leq r \) and that \( b_{C_\pi} = 0 \) for all \( \pi \) with \( t_\pi < t \). We would like to show that \( b_{C_\pi} = 0 \) for all \( \pi \) with \( t_\pi = t \). It is enough to restrict to single 1-cycle permutations, that is, permutations with a single cycle \( C \), containing 1 (\( C \in C^1 \)). In fact, it is enough to show

\[
b_C = 0, \quad \forall C \in C^1 : |C| = t + 1.
\]

We note that for any cycle \( C \),

\[
b_C = \delta_{C^1}1\{C \in H\},
\]

that is, \( b_C \) is equal to 0 or \( \delta_{C^1}1\{|C| \}, \) the latter iff \( C \in H \). Here, \( \delta_C \) is defined similar to \( b_C \). (\( \delta_C \) is well-defined when \( C \in H \), otherwise define it arbitrarily.)

---

\(^3\) The notation \( b_{C_\pi} \) is also consistent with the definition of \( b_C \) in Section 8.5 due to the following connection: Every (graph) cycle \( C \) can be viewed as a permutation that leaves elements outside \( C \) intact.
By the induction assumption, $b_\pi = 0$ when $t_\pi < t$, hence $0 = |B| = \sum_{\pi; |t_\pi| \geq t} \text{sign}(\pi)b_\pi$. There are three categories of terms in this expansion: ($S_\pi$ is the cycle decomposition of $\pi$.)

- $|S_\pi| = 1, t_\pi = t$: These are the single 1-cycle permutations of cycle length $t + 1$. All of these permutations have the same sign, and we have
  
  $b_\pi = b_{C_\pi} = \delta_{C_\pi}x^{t+1}1\{C_\pi \in H\}$

  The first equality is since $b_{\pi i} = 1$ for all $i \neq 1$. Recall that $|C_\pi| = t_\pi + 1 = t + 1$. Thus, the overall contribution of these terms to $|B|$ is $\pm \left(\sum_{C \in \mathcal{C}_1(H)} \delta_C\right)x^{t+1}$, with the convention that the sum is zero if $\mathcal{C}_1(H) = \emptyset$.

- $|S_\pi| \geq 2, t_\pi = t$: Any such permutation has at least a cycle $C$ of size $r \geq 1$ in $[r] \setminus C_\pi$. Hence, $b_\pi$ has a factor of the form
  
  $b_{C_\pi}b_C = \delta_{C_\pi}\delta_Cx^{t+r+1}1\{C_\pi, C \in G\}$

  Thus, any such $b_\pi$ if nonzero contributes a polynomial of degree at least $t + 2$.

- $t_\pi \geq t + 1$: In this case, $b_\pi$ has a factor of $b_{C_\pi} = \delta_{C_\pi}x^{t_\pi+1}1\{C_\pi \in G\}$ and as the previous case contributes a polynomial of degree at least $t + 2$, if nonzero.

  Thus, setting the coefficient of the $x^{t+1}$ in the expansion of $|B|$ equal to zero, we conclude that $\sum_{C \in \mathcal{C}_1(H)} \delta_C = 0$. which proves the desired claim. (Note in addition that this implies (31) in view of (32). In particular, with $t = 0$, it means that $H$ cannot have a self-loop on node 1 if $|B| = 0$.)

\[\Box\]

### A.2 Proof of Lemma 3

Let $\mathcal{H}$ be the underlying Hilbert space and $x_i \in \mathcal{H}$ such that $\Sigma = (\langle x_i, x_j \rangle) > 0$. Define the operator $\mathcal{L}_S : \mathbb{R}^{|S|} \rightarrow \mathcal{H}$ by $\mathcal{L}_S a = \sum_{i \in S} a_i x_i$. The adjoint operator $\mathcal{L}_S^* : \mathcal{H} \rightarrow \mathbb{R}^{|S|}$ is given by $\mathcal{L}_S^* y = (\langle y, x_j \rangle)_{i \in S}$. Since $\Sigma > 0$, we have $\Sigma_S = (\langle x_i, x_j \rangle)_{i, j \in S} > 0$ for all $S \subset [d]$. By considering $\Sigma_S : \mathbb{R}^{|S|} \rightarrow \mathbb{R}^{|S|}$ as an operator, we have the identification $\Sigma_S = \mathcal{L}_S^* \mathcal{L}_S$. To simplify notation, let $\mathcal{L}_i = \mathcal{L}_{\{i\}}$, so that $\mathcal{L}_i a = ax_i$ for any $a \in \mathbb{R}$ and $\mathcal{L}_i^* y = \langle y, x_i \rangle$ for any $y \in \mathcal{H}$. Then,

$$P_S = \mathcal{L}_S (\mathcal{L}_S^* \mathcal{L}_S)^{-1} \mathcal{L}_S^* = \mathcal{L}_S \Sigma_S^{-1} \mathcal{L}_S^*. \tag{33}$$

(To see (33), note that the projection $P_S$ is characterized by the residual $x - P_S x$, for any $x \in \mathcal{H}$, being orthogonal to ran($P_S$) = ran($\mathcal{L}_S$), that is, $x - P_S x \in [\text{ran}(\mathcal{L}_S)]^\perp = \ker(\mathcal{L}_S^*)$. Thus, $P_S$ is characterized by $\mathcal{L}_S^*(I - P_S) = 0$ which is satisfied by (33). Alternatively, write $P_S x = \mathcal{L}_S a$ so that $\mathcal{L}_S^*(x - \mathcal{L}_S a) = 0$ and solve for $a$.)

It follows that $P_i P_j^* P_j = 0$ is equivalent to $\mathcal{L}_i \Sigma_i^{-1} \mathcal{L}_i^* P_i^\perp \mathcal{L}_j \Sigma_j^{-1} \mathcal{L}_j^* = 0$. Note that $\Sigma_i$ and $\Sigma_j$ are both positive scalars ($i$th and $j$th diagonal entries of $\Sigma$). Hence we can take them out and get the equivalent statement $\mathcal{L}_i \mathcal{L}_i^* P_i^\perp \mathcal{L}_j^* \mathcal{L}_j = 0$. We also note that $\mathcal{L}_i (\mathcal{L}_i^* P_i^\perp \mathcal{L}_j) \mathcal{L}_j^* = (\mathcal{L}_i^* P_i^\perp \mathcal{L}_j) \mathcal{L}_i \mathcal{L}_j^*$ since the expression in parentheses is a scalar. $\mathcal{L}_i \mathcal{L}_j^*$ is not the identically zero operator, hence we get the equivalent statement

$$0 = \mathcal{L}_i^* P_i^\perp \mathcal{L}_j = \mathcal{L}_i^* (I - P_S) \mathcal{L}_j = \mathcal{L}_i^* \mathcal{L}_j - \mathcal{L}_i^* \mathcal{L}_S \Sigma_S^{-1} \mathcal{L}_S^* \mathcal{L}_j = \Sigma_{ij} - \Sigma_{Sij} \Sigma_S^{-1} \Sigma_{Sj} \tag{34}$$

34
where \( \Sigma_{S,i} \in \mathbb{R}^{\vert S \vert} \) is the vector obtained from rows indexed by \( S \) in column \( i \) of \( \Sigma \). By a Schur complement argument, (34) in turn is equivalent to the determinant of \( (\Sigma_{ij} \Sigma_{S,j}^{-1}) = \Sigma_{S,i} \Sigma_{S,j} \) being zero, as desired.

### A.3 Proof of Proposition 1

Let us start by computing \( A \).

#### A.3.1 Proof of Proposition 1

Let us fix \( i \in S \) and \( j \in A \). Applying (33) we have \( [\beta_j(S)]_i = \sum_{k \in A} [\beta_j(A)]_k x_k \) for all \( i \in S \). Hence, (b) is equivalent to

\[
[\beta_j(S)]_i = \sum_{k \in A} [\beta_j(A)]_k x_k \quad \text{for all} \quad i \in S.
\]

Using \( P_A x_j = \sum_{k \in A} [\beta_j(A)]_k x_k \) and equating the coefficients of \( x_k \), we obtain the system of equations given in (b).

To see the equivalence of (b) and (c), let \( I_{S,i} \) be the subvector of the identity matrix \( I \in \mathbb{R}^{d \times d} \) on \( S \times \{i\} \). Note that we have \( [\beta_j(S)]_i = \sum_{k \in A} [\beta_j(A)]_k x_k \), and rearranging we have (\( \Sigma_{j,S} \Sigma_{S,j}^{-1} \))

\[
\Sigma_{j,S} \Sigma_{S,j}^{-1} \Sigma_{S,A} \Sigma_{A}^{-1} I_{A,k} = \Sigma_{j,S} \Sigma_{S,j}^{-1} \sum_{i \in S} (I_{S,i} \Sigma_{i,A}) \Sigma_{A}^{-1} I_{A,k}.
\]

The RHS of (b) is equal to

\[
\sum_{i \in S} (\Sigma_{j,S} \Sigma_{S,j}^{-1} I_{S,i})(\Sigma_{i,A} \Sigma_{A}^{-1} I_{A,k}) = \sum_{i \in S} (I_{S,i} \Sigma_{i,A}) \Sigma_{A}^{-1} I_{A,k}.
\]

the latter summation being equal to \( I_{S,S} \Sigma_{S,A} = \Sigma_{S,A} \). Similarly, the LHS of (b) is equal to \( \Sigma_{j,A} \Sigma_{A}^{-1} I_{A,k} \). Hence, (b) is equivalent to

\[
\Sigma_{j,A} \Sigma_{A}^{-1} I_{A,k} = \Sigma_{j,S} \Sigma_{S,j}^{-1} \Sigma_{S,A} \Sigma_{A}^{-1} I_{A,k}, \quad \forall k \in A, \ j \in B,
\]

or in matrix form \( \Sigma_{B,A} \Sigma_{A}^{-1} I_{A,A} = \Sigma_{B,S} \Sigma_{S,j}^{-1} \Sigma_{S,A} \Sigma_{A}^{-1} I_{A,A} \). Dropping the identity \( I_{A,A} \) and rearranging we have \( (\Sigma_{B,A} - \Sigma_{B,S} \Sigma_{S,j}^{-1} \Sigma_{S,A}) \Sigma_{A}^{-1} = 0 \) which is equivalent to (c).

Let us now show the equivalence of (a) and (d). First we note that (a) is equivalent to \( P_i P_S^\perp P_j = 0 \) for all \( i \in A \) and \( j \in B \). Alternatively, it is equivalent to \( \langle x_i, P_S^\perp x_j \rangle_H = 0 \) for all \( i \in A \) and \( j \in B \). Let us fix \( i \in A \) and \( j \in B \), and show that

\[
\langle x_i, P_S^\perp x_j \rangle_H = 0 \iff [\beta_j(S)]_i = 0
\]

which establishes (a) \( \iff \) (d). By definition of SEM coefficients in (3), we have \( P_{S,i} x_j = \sum_{k \in S_i} [\beta_j(S)]_k x_k \). To simplify notation, let us write \( u = \beta_j(S) \) and \( u = P_{S,i} x_j \). We have

\[
u = \sum_{k \in S_i} \alpha_k x_k, \quad x_j = P_{S,i} x_j + u.
\]

Applying \( P_S^\perp \) to both sides of the first equation, we get \( P_S^\perp u = \alpha_i P_S^\perp x_i \). (Since, \( P_S^\perp x_k =\)
0, ∀k ∈ S.) Taking the inner product with xi (dropping H subscript for simplicity), we obtain
\[ \alpha_i(x_i, P_S^i x_i) = \langle x_i, P_S^i u \rangle \]
\[ = \langle x_i, P_S^i (x_j - P_S^i x_j) \rangle \]
\[ = \langle x_i, P_S^i x_j \rangle - \langle x_i, P_S^i x_j \rangle \quad \text{(Since } P_S^i \leq P_S, \text{ i.e. } P_S^i P_S^i = P_S^i) \]
\[ = \langle x_i, P_S^i x_j \rangle - \langle P_S^i x_i, x_j \rangle \quad \text{(Projections are self-adjoint.)} \]
\[ = \langle x_i, P_S^i x_j \rangle \quad \text{(Since } P_S^i x_i = 0 \text{.)} \]

Note that \( P_S^i \leq P_S \) is equivalent to \( P_S \leq P_S \) which is perhaps easier to see. Since assumption \( \Sigma > 0 \) implies \( \langle x_i, P_S^i x_i \rangle > 0 \), we have the equivalence of \( \alpha_i = 0 \) and \( \langle x_i, P_S^i x_j \rangle = 0 \) which is the desired result. Note that we have also established (7). The proof is complete.

A.4 Auxiliary lemmas

The following lemma is used in the proof of Theorem 2. The notation \( \xi_*\mu \) denotes the push-forward of measure \( \mu \) by map \( \xi \).

Lemma 16. With \( \xi : \mathbb{R}^d_+ \times \mathbb{R}^g \rightarrow \mathbb{R}^g \) defined as in (25), we have \( \xi_*\mathcal{L}^{d+g} \ll \mathcal{L}^g \), that is, \( \mathcal{L}^g(A) = 0 \) implies \( \mathcal{L}^{d+g}(\xi^{-1}(A)) = 0 \).

Proof. Let \( \Omega := \mathbb{R}^d_+ \times \mathbb{R}^g \) be a subset of \( \mathbb{R}^{d+g} \). Let \( x = (x_k, k \in [d]) \) and \( y = (y_{ij}, ij \in G) \). Consider the function \( F_1 : \Omega \rightarrow \Omega \) defined by
\[ F_1(x, y) = \left( x, \frac{y_{ij}}{\sqrt{x_i x_j}}, ij \in G \right) \]

\( F_1 \) is a \( C^\infty \) diffeomorphism of \( \Omega \) onto itself, that is, \( F_1 : \Omega \rightarrow \Omega \) is a bijection and both \( F_1 \) and its inverse \( F_2 := F_1^{-1} \) belong to class \( C^\infty \). This implies that \( F_1 \) and \( F_2 \) are locally Lipschitz (i.e., Lipschitz when restricted to any compact subset of \( \Omega \)), hence they both preserve \( \mathcal{L}^{g+d} \)-null sets (i.e., map null sets to null sets).

Let \( \pi : \mathbb{R}^{d+g} \rightarrow \mathbb{R}^g \) be the projection \( \pi(x, y) = y \). We can write \( \xi = \pi \circ F_1 \). Below we will show that \( \pi_*\mathcal{L}^{d+g} \ll \mathcal{L}^g \). Assuming that \( \mathcal{L}^g(A) = 0 \), we thus have \( \mathcal{L}^{d+g}(\pi^{-1}(A)) = 0 \). But then \( \mathcal{L}^{d+g}(F_2 \circ \pi^{-1}(A)) = 0 \), due to the diffeomorphic nature of \( F_2 \). Noting that \( \pi^{-1} = (\pi \circ F_1)^{-1} = F_1^{-1} \circ \pi^{-1} = F_2 \circ \pi^{-1} \), we have the desired result.

It remains to prove the claim about the projection \( \pi \). But this follows from Fubini theorem: Let \( A \subset \mathbb{R}^g \) be such that \( \mathcal{L}^g(A) = 0 \). We have \( \pi^{-1}(A) = \mathbb{R}^d \times A \). Hence, \( \mathcal{L}^{d+g}(\pi^{-1}(A)) = \mathcal{L}^d(\mathbb{R}^d) \cdot \mathcal{L}^g(A) = 0 \) since Lebesgue measure is \( \sigma \)-finite. The proof is complete.

A.5 Proof of Lemma 5

The idea is to reduce the general case to the case where the underlying random variables are Gaussian, in which case PCG is the same as CIG. The result the follows that for CIGs.

The first step is to show that PCGs are preserved under isometries between Hilbert spaces. Let us recall some facts about isometries: An operator \( L \in B(\mathcal{H}_1, \mathcal{H}_2) \) between two Hilbert spaces is called an isometry if \( \|L\xi\|_{\mathcal{H}_2} = \|\xi\|_{\mathcal{H}_1} \) for all \( \xi \in \mathcal{H}_1 \), i.e. it preserves norms. Equivalently (using polarization identity), it is an isometry if \( \langle L\xi, L\eta \rangle_{\mathcal{H}_2} = \langle \xi, \eta \rangle_{\mathcal{H}_1} \), \( \forall \xi, \eta \in \mathcal{H}_1 \), i.e., it preserves inner products. One has that \( L \) is an isometry iff \( L^*L = I_{\mathcal{H}_1} \).
Step 1 (PCGs are preserved by isometries): Let $\mathcal{H}_0 := \text{span}\{x_1, \ldots, x_d\} \subset L^2(\mathbb{P})$. Let $\mathcal{K}$ be a d-dimensional Hilbert space and let us define the linear operator $V : \mathcal{K} \to \mathcal{H}_0$ by taking a linearly independent set $\{y_1, \ldots, y_d\} \subset \mathcal{K}$ with and letting $V y_i = x_i, \forall i \in [d]$. We can further assume that $\{y_i\}$ are chosen such that $\langle y_i, y_j \rangle_{\mathcal{K}} = \Sigma_{ij} = \langle x_i, x_j \rangle_{\mathcal{H}}$. It then follows that $V$ is an isometry, hence $V^* V = I_{\mathcal{K}}$. On the other hand, $V$ is also surjective, hence a unitary operator, hence $V V^* = I_{\mathcal{H}_0}$.

Let $Q_A = V^* P_A V$. We claim that this is the (orthogonal) projection operator onto the span of $y_A := \{y_i : i \in A\}$. We have, for $i \in A$, $Q_A y_i = V^* P_A x_i = V^* x_i = V^* V y_i = y_i$. On the other hand, assume $z \perp_{\mathcal{K}} y_i, \forall i \in A$. Then, for all $i \in A$, $0 = \langle z, y_i \rangle_{\mathcal{K}} = \langle V z, V y_i \rangle_{\mathcal{H}_0} = \langle V z, x_i \rangle_{\mathcal{H}_0}$. It follows that $P_A V z = 0$, hence $Q_A z = 0$.

This shows that any of the pairwise or global $L^2$ Markov properties are preserved under isometries: Note that $Q_A^\perp := I_{\mathcal{K}} - Q_A = V^* (I_{\mathcal{H}_0} - P_A) V = V^* P_A^\perp V$. We conclude that $Q_A Q_A^\perp Q_B = V^* (P_A P_A^\perp P_B) V$ and $P_A P_A^\perp P_B = V (Q_A Q_A^\perp Q_B) V^*$. Hence,

$$P_A P_A^\perp P_B = 0 \iff Q_A Q_A^\perp Q_B = 0. \quad (36)$$

Step 2 (Reduction to Gaussian case): Now take $y = (y_1, \ldots, y_d) \sim N(0, \Sigma)$, say on the same probability space, and let $\mathcal{K} = \text{span}\{y_1, \ldots, y_d\}$. By (36), and using the assumption that $x$ satisfies pairwise $L^2$ property w.r.t. some $G$, we conclude that $y$ also satisfies pairwise $L^2$ property w.r.t. $G$. Then, due to the equivalence of orthogonality and independence for Gaussian random variables, $y$ satisfies usual pairwise Markov property (defined via conditional independence) w.r.t. $G$. That is, $G$ is a CIG for $y$.

Invoking (36) again, it is enough to show that if $A$ and $B$ are separated by $S$, then $Q_A Q_S^\perp Q_B = 0$, which is equivalent to $\langle u, Q_S^\perp v \rangle_{\mathcal{K}} = 0, \forall u \in \text{span}\{y_A\}, v \in \text{span}\{y_B\}$. Since $S$ separates $A$ and $B$, we know that $u$ and $v$ are independent given $y_S$. This follows from [Lau96, Thm. 3.9, p. 35] for CIGs, since $N(0, \Sigma)$ has a.e. positive density w.r.t. Lebesgue measure, assuming $\Sigma > 0$. In particular,

$$\mathbb{E}[uv | y_S] = \mathbb{E}[u | y_S] \mathbb{E}[v | y_S] = (Q_S u)(Q_S v) \quad (37)$$

where the second equality uses Gaussianity again to write $\mathbb{E}[u | y_S]$ as the $L^2$ projection to the linear span of $y_S$. Taking expectation on both sides of (37), we have $\langle u, v \rangle_{\mathcal{K}} = (Q_S u, Q_S v)_{\mathcal{K}}$ from which it follows that $\langle Q_S^\perp u, Q_S^\perp v \rangle_{\mathcal{K}} = 0$, which in turn is equivalent to $\langle u, Q_S^\perp v \rangle_{\mathcal{K}} = 0$ since $Q_S^\perp$ is self-adjoint and idempotent.

A.6 Equivalence of the two directed PCG definitions

In this appendix, we show that the two definitions of a directed PCG given in (12) and (13) are equivalent (under the acyclicity assumption). Recall that $\Pi_j$ and $N_j$ denote, respectively, the sets of parents and non-descendants of node $j$ in the underlying graph $G$.

Assume first that (12) holds and take $i, j \in [d]$. Since $G$ is a DAG, one of $i$ and $j$ is a non-descendant of the other, say $i \in N_j$. (If $i$ and $j$ are adjacent, this means that $i$ is a parent of $j$.) Then, any parent of $i$ will be a non-descendant of $j$, that is, $\Pi_i \subset N_j$. It follows that $P_k P_{\Pi_j}^\perp P_j = 0$ for $k \in \{i\} \cup \Pi_i$. In particular, $P_{\Pi_i} P_{\Pi_j}^\perp P_j = 0$ since $P_{\Pi_i} = \bigvee_{k \in \Pi_i} P_k$ (see
Lemma 9), and \( P_i P_{i,j}^\perp P_j = 0 \). Since we have

\[
P_i P_{i,j}^\perp P_j = P_i (P_{i} + P_{i,j}^\perp) P_{i,j}^\perp P_j \\
= P_i P_{i} P_{i,j}^\perp P_j + P_i P_{i,j}^\perp P_{i,j}^\perp P_j \\
\leq P_i P_{i} P_{i,j}^\perp P_j,
\]

we obtain \( P_i P_{i,j}^\perp P_{i,j}^\perp P_j = 0 \), that is (13) holds for \( i \) and \( j \).

Now assume that (13) holds and take \( j \in [d] \) and \( i \in N_j \). Note that it is enough to establish identity (38). An ancestor of \( i \) is any node that has a directed path to \( i \); let us call such a path, a path from the top to \( i \). Let the depth of a node \( i \) be the length of the longest path from the top to it. We proceed by the induction on the depth of node \( i \). For depth zero, we have \( \Pi_i = \emptyset \), hence \( P_{\Pi_i} = 0 \) and (38) holds trivially. Now assume that we have the result for all non-descendants of \( j \) at depth at most \( r - 1 \), and let \( i \in N_j \) have depth \( r \). Any \( k \in \Pi_i \) is at depth at most \( r - 1 \) and belongs to \( N_j \), hence by the induction hypothesis \( P_k P_{i,j}^\perp P_j = 0 \) for \( k \in \Pi_j \). It follows that \( P_{\Pi_i} P_{i,j}^\perp P_j = 0 \), hence (38)(c) holds which then means that (38) holds as a whole. The proof is complete.

**B Abstract lattice theorem**

In this appendix, we present an interesting generalization of the lattice Theorem 1. The result and its argument are due to Tristan Bice [Bic]. Let \( A \) be a von Neumann algebra and \( P \) be its projection lattice, ordered by \( p \leq q \iff p = pq = qp \), the latter equivalence being a result of the self-adjointness of \( p \) and \( q \). The convention is to use lower case letters for elements of \( A \) and \( P \). Note that a general element \( b \in A \) is a bounded operator on the underlying Hilbert space, i.e., \( b \in B(\mathcal{H}) \). Similarly \( p \in P \) is a projection operator in \( B(\mathcal{H}) \).

**Theorem 7.** \( Q = \{ q \in P : pa = qa \} \) is a complete sublattice of \( P \), \( \forall a \in A \) and \( p \in P \).

**Proof.** Let \( [b] \) be the range projection of any \( b \in A \), i.e., projection onto the closure of the range of \( b \). For any \( q \in P \) and \( a \in A \), we have \( [qa] \leq q \) (since the range of \( qa \) is included in the range of \( q \)). Also note the identity (2) \( b = [b]b \), \( \forall b \in A \).

If \( R \subseteq Q \), then for all \( q \in R \), we have (1) \( [pa] = [qa] \leq q \), hence \( [pa] \) is lower bound on \( R \). Letting \( r := \bigwedge R \), by definition of infimum, \( [pa] \leq r \leq q \), \( \forall q \in R \), hence \( [qa] \leq r \leq q, \forall q \in R \) by (1). Hence,

\[
ra = rqa \\
\quad = r[qa]qa \\
\quad = [qa]qa \\
\quad = qa \\
\quad = pa,
\]

showing that \( r \in Q \). So, \( Q \) is closed under infima.

Since \( pa = qa \iff p^\perp a = q^\perp a \) (recall \( p^\perp = 1 - p \)), it follows that \( Q^\perp := \{ q^\perp : q \in Q \} \) is also closed under infima. But since \( q^\perp \leq p^\perp \iff p \leq q \), it follows that \( Q \) is closed under suprema, finishing the proof. \( \square \)