

SUPPLEMENTARY MATERIAL

A PROOFS

Proof of Theorem 1. First assume $\Sigma \in \mathcal{M}(G)$, and consider the equations

$$[(I - \Lambda)^T \Sigma (I - \Lambda)]_{vw} = 0 \quad \text{for all } \{v, w\} \notin B \quad (4)$$

(this is equation (9.2) in Foygel et al. (2012)). Treating the entries of Λ and Σ as variables λ and σ , define the rational function $\delta := \det(I - \Lambda)^{-1}$. Then the left-hand sides of (4) are polynomials in $\mathbb{R}[\lambda, \sigma, \delta]$ generating an ideal \mathcal{I} . This ideal consists of all polynomials that are zero everywhere on the set of all (λ, σ) with δ well-defined and $\Sigma = \phi_G(\Lambda, \Omega)$ for some $\Omega \in \text{PD}(B)$ (Foygel et al., 2012, Section 8 of the supplement). In addition to the left-hand sides of (4), (using that G is rationally identifiable) the ideal \mathcal{I} contains for each directed edge $(u, v) \in D$ an element $a(\sigma)\lambda_{uv} - b(\sigma)$ for some nonzero polynomials $a, b \in \mathbb{R}[\sigma]$. By multiplying a left-hand side of (4) by some polynomial and adding polynomial multiples of the ideal elements mentioned above, we can eliminate λ and find an element in $\mathcal{I} \cap \mathbb{R}[\sigma]$. This represents a polynomial constraint that *all* $\Sigma \in \mathcal{M}(G)$ must satisfy, and we see that the polynomial constraints described in the main text can be obtained in this way. This implies that also the rational constraints (2) are satisfied for any Σ that is additionally in the domain of $\Lambda_{\mathcal{Y}}$.

If $\Sigma \in \mathcal{M}(G)$, then there exist $\Lambda \in \mathbb{R}_{\text{reg}}^D$ and $\Omega \in \text{PD}(B)$ for which $\Sigma = \phi_G(\Lambda, \Omega)$. In the generic case, $\Lambda_{\mathcal{Y}}$ will recover the parameter matrix Λ ; in particular, $\Lambda_{\mathcal{Y}}(\Sigma) \in \mathbb{R}_{\text{reg}}^D$.

Conversely, suppose Σ is in the domain of $\Lambda_{\mathcal{Y}}$, $\Lambda_{\mathcal{Y}}(\Sigma) \in \mathbb{R}_{\text{reg}}^D$, and Σ satisfies (2). Let $\Lambda = \Lambda_{\mathcal{Y}}(\Sigma)$ and $\Omega = (I - \Lambda)^T \Sigma (I - \Lambda)$. Σ and Λ again satisfy (4):

For $\{v, w\}$ with $v \notin Y_w$ and $w \notin Y_v$: by (2);

For $\{v, w\}$ with $w = y_i \in Y_v \cap \text{htr}(v)$:

$$\begin{aligned} [(I - \Lambda)^T \Sigma \Lambda]_{vw} &= (\mathbf{A} \cdot \Lambda_{\text{pa}(v), v})_i = \mathbf{b}_i \\ &= [(I - \Lambda)^T \Sigma]_{vw} \end{aligned}$$

(with \mathbf{A} and \mathbf{b} as in Foygel et al. (2012) / in Section 2.1), which implies (4) for $\{v, w\}$;

For $\{v, w\}$ with $w \in Y_v \setminus \text{htr}(v)$: Fix any node v , and let $W = Y_v \setminus \text{htr}(v)$ and $I = \{i \mid y_i \in W\}$. Then

$$[\Sigma \Lambda]_{Wv} = (\mathbf{A} \cdot \Lambda_{\text{pa}(v), v})_I = \mathbf{b}_I = \Sigma_{Wv},$$

from which follows

$$\begin{aligned} \mathbf{0} &= [\Sigma(I - \Lambda)]_{Wv} \\ &= [(I - \Lambda)^{-T} (I - \Lambda)^T \Sigma (I - \Lambda)]_{Wv} \\ &= [(I - \Lambda)^{-T} \Omega]_{Wv} = \sum_{x \in V} [(I - \Lambda)^{-T}]_{Wx} \Omega_{xv}. \end{aligned}$$

In the case distinction that follows, we use that for all $x \neq v$ with $x \notin \text{sib}(v)$, we have $x \in Y_v$, $v \in Y_x$, or neither. For x in one of the sets $Y_v \cap \text{htr}(v)$, $\{x \mid v \in Y_x \cap \text{htr}(x)\}$, or $\{x \mid x \neq v, x \notin \text{sib}(v), x \notin Y_v, v \notin Y_x\}$, we know from the previous two cases that $\Omega_{xv} = \Omega_{vx} = 0$. For $x = v$ or $x \in \text{sib}(v)$, $[(I - \Lambda)^{-T}]_{wx} = 0$ for any $w \in W$, because such a directed path from such x to w would form a half-trek from v to w . Similarly, for x such that $v \in Y_x \setminus \text{htr}(x)$, also $[(I - \Lambda)^{-T}]_{wx} = 0$, or there would again be a half-trek from v to w . The above covers all cases except $x \in W$. So all terms in the previous sum with $x \notin W$ are zero, and we get

$$\mathbf{0} = [(I - \Lambda)^{-T}]_{WW} \Omega_{Wv}.$$

The entries of $[(I - \Lambda)^{-T}]_{WW}$ are polynomials in the variables Λ_{ij} and $\delta := \det(I - \Lambda)^{-1}$. The matrix $(I - \Lambda)^{-1}$ equals δ times the adjugate matrix of $(I - \Lambda)$; this adjugate matrix includes the constant term 1 in each diagonal entry, and no constant terms in any other entries. We see that the determinant of $[(I - \Lambda)^{-T}]_{WW}$ contains the term $\delta^{|W|}$ so it is not the zero polynomial. It follows that $[(I - \Lambda)^{-T}]_{WW}$ is generically invertible, so the only solution to the above equation is $\Omega_{wv} = 0$ for all $w \in W$. This again implies (4).

Then $\Omega = (I - \Lambda)^T \Sigma (I - \Lambda)$ is positive definite (using that Σ is positive definite and $I - \Lambda$ is invertible) and obeys $\Omega_{vw} = 0$ for $\{v, w\} \notin B$. For these parameters, $\Sigma = \phi_G(\Lambda, \Omega)$, showing that $\Sigma \in \mathcal{M}(G)$.

For generic $\Sigma \in \mathcal{M}(G)$, the matrices \mathbf{A} that occur in the HTC-identifiability algorithm are invertible by (Foygel et al., 2012, Lemma 2), so the assumption above that Σ is in the domain of $\Lambda_{\mathcal{Y}}$ holds in the generic case. \square

Example of a constraint that is not HT-overidentifying.

Figure 9 gives an example graph which imposes one equality constraint, namely a vanishing tetrad constraint, which is not reported by Algorithm 2 of Chen et al. (2014). The graph is HTC-identifiable, so Theorem 1 will report the constraint. \square

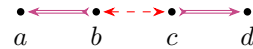


Figure 9: Graph imposing an equality constraint that is not HT-overidentifying.

Proof of Theorem 2. Define the *rank deficiency* of a graph as the difference between the number of columns and the generic rank of the Jacobian in (Foygel et al., 2012, proof of Theorem 2). The rank deficiency of a graph is zero iff that graph is finite-to-one, so the rank deficiency of G' is zero. Removing a directed edge from a graph removes a column from the Jacobian, which will not increase the rank, so this reduces the rank deficiency by at most one; removing a bidirected edge adds a row, which will increase the largest order of a non-vanishing minor (this order equals the rank) by at most one. It follows that the rank deficiency of G is at most k . In fact, it must be equal to k : suppose the rank deficiency of G is $k' < k$. Then by deleting k' columns from the Jacobian, a matrix of full column rank can be obtained. By deleting the corresponding k' directed edges from G , a graph with rank deficiency 0 is obtained; however, this is a contradiction with the conditions of the theorem, which imply that all such graphs are infinite-to-one.

By the statements in the beginning and end of the proof of Lemma 2 in the supplement of (Foygel et al., 2012), the dimensions of the images of ϕ_G and $\phi_{G'}$ (i.e. of $\mathcal{M}(G)$ and $\mathcal{M}(G')$) equal the ranks of the respective Jacobians as considered above plus the respective numbers of (co)variance parameters in Ω . It follows that the models' dimensions are equal. Because the models are defined by rational parameterizations, their Zariski closures are irreducible affine varieties (Cox et al., 2015, Proposition 4.5.6). For two such varieties, $W \subsetneq V$ would imply that the dimension of W is smaller than that of V . Because $\mathcal{M}(G') \subseteq \mathcal{M}(G)$, the models' Zariski closures must be equal; in other words, the models are algebraically equivalent.

If additionally G' imposes no inequality constraints, then $\mathcal{M}(G')$ is equal to its Zariski closure up to a measure zero subset. Using again that $\mathcal{M}(G') \subseteq \mathcal{M}(G)$ and that $\mathcal{M}(G)$ is contained in the models' common Zariski closure, we find that $\mathcal{M}(G')$ and $\mathcal{M}(G)$ are equal up to a measure zero subset. \square

Proof of Proposition 5. First consider the special case of two acyclic bow-free graphs G'_1, G'_2 that differ in only one arrowhead which does not form a collider. Then the graph G containing the union of their edges (so having a bow where G'_1 and G'_2 had a different type of edge) is HTC-nonidentifiable, as the directed edge of the bow cannot be identified. An application of Corollary 4 shows that G'_1 and G'_2 are algebraically equivalent.

The algebraic equivalence of two arbitrary graphs G'_1, G'_2 with the same skeleton and colliders can now be shown using a finite sequence of such steps. Let G_1^Δ be the subgraph consisting of the edges of G'_1 that are not

in G'_2 , and let $W \subseteq V$ be the set of nodes where G'_1 and G'_2 have different incoming arrowheads. In G_1^Δ , at each node $w \in W$, there is at most one arrowhead (otherwise there is a collider in either G'_1 or G'_2 that is not in the other) and at most one arrowtail (two tails would become two colliding heads in G'_2), so each node $w \in W$ has degree at most 2 in G_1^Δ .

Now find the finest partition of the edges in G_1^Δ that groups two edges together if they are incident at a node $w \in W$. The edge sets in this partition form paths that may only meet each other at the endpoints, at nodes not in W . None of these paths can have two directed edges pointing away from each other (with possibly other edges in between), as that would imply G'_2 contains a collider not in G'_1 . So each of these paths is a half-trek. At each step, modify the first edge of such a half-trek by adding an arrowhead that appears in G'_2 or removing one that does not. \square

Proof of Proposition 6. Assume w.l.o.g. that Σ is normalized to a correlation matrix (with ones on the diagonal). Let $W = \{b, c, d\}$. Then for each pair of distinct nodes $x, y \in W$,

$$\begin{aligned}\sigma_{xy} &= \lambda_{ax}\lambda_{ay} + \lambda_{ax}\omega_{ay} + \omega_{ax}\lambda_{ay} \\ &= (\lambda_{ax} + \omega_{ax})(\lambda_{ay} + \omega_{ay}) - \omega_{ax}\omega_{ay} \\ &= \sigma_{ax}\sigma_{ay} - \omega_{ax}\omega_{ay}.\end{aligned}$$

It follows that

$$\omega_{ax}\omega_{ay} = \sigma_{ax}\sigma_{ay} - \sigma_{xy}. \quad (5)$$

We have three of these equations for the three possible pairs in W . If all three ω_{aw} 's have the same sign, all these expressions will be positive; otherwise, two will be negative and one positive. Other combinations of positive and negative cannot be attained by any choice of Ω . Using that (5) has the same sign as $-\rho_{xy.a}$, we can write this as the inequality constraint $\rho_{bc.a} \cdot \rho_{cd.a} \cdot \rho_{bd.a} \leq 0$.

The observed covariance matrix

$$\Sigma = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 1/2 & 1/2 \\ 0 & 1/2 & 1 & 1/2 \\ 0 & 1/2 & 1/2 & 1 \end{bmatrix}$$

is an example of a positive definite matrix (so an element of the saturated model) that does not satisfy this inequality constraint. In fact, it is easy to see that an open ball around Σ has this property, showing that the inequality constraint rules out a part of the saturated model having nonzero measure. \square

B ACYCLIC ALGEBRAIC EQUIVALENCE CLASSES ON FOUR NODES

Before presenting in Section B.2 a full description of the algebraic equivalence classes of four-node acyclic graphs, we first introduce the additional graph notation we will use.

B.1 NOTATION FOR SETS OF GRAPHS, CONTINUED

In Section 2.3, we described how our graph patterns represent directed edges, bidirected edges, and bows. The full list of markings we use in Section B.2 is displayed in Figure 10. To describe these markings, we need to extend the well-known concept of colliders (see e.g. Spirtes et al. (2000)) to graph skeletons. A 2-edge path in the skeleton $S(G)$ of G along three distinct nodes (v_1, v_2, v_3) is called a *collider* if for both edges of the path, a corresponding edge exists in the original graph G with an arrowhead at v_2 . Such an edge could be either bidirected, or directed towards v_2 . We distinguish two cases: if *all* corresponding edges in the original graph G have arrowheads at v_2 (in other words, there are no directed edges in G from v_2 to either v_1 or v_3), we call the path a *full collider*; otherwise we call it a *partial collider*. An example of a partial collider is the path (a, b, c) in the instrumental variable model (Figure 2(a)). When looking at the endpoint at v_2 of an edge in $S(G)$ between v_1 and v_2 , we say that it *forms a (full/partial) collider* if a node v_3 exists for which the path along (v_1, v_2, v_3) is a (full/partial) collider. Note that an endpoint can simultaneously form a full collider and a partial collider, for different choices of v_3 .

In a graph pattern denoting a set of graphs, if all graphs in the set have the same edge(s) between two given nodes, this edge is displayed as for a single graph, as in Section 2.3. If the graphs in the set have different edges between two nodes, these are represented in the graph pattern by a green edge, which may have different endpoint markings. First of all, if all edges to be represented have an arrowhead at an endpoint, then the graph pattern will also show an arrowhead. Otherwise, the following special markings are used (illustrated in Figure 10): a plus sign if the endpoint never forms a collider in any of the graphs; a bracket if it always forms a partial collider; and a star in all other cases. Finally, if two nodes are adjacent in some graphs in the set but not in others, then an edge is shown in dotted grey; other aspects of the edge's appearance are determined using only the graphs in which the nodes are adjacent.

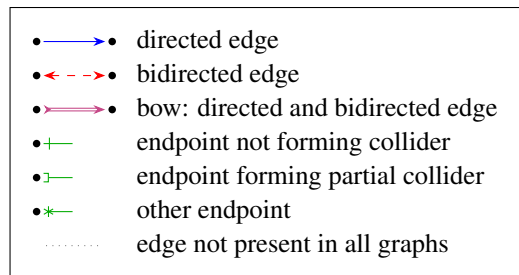


Figure 10: Legend for the edges and endpoints we use to denote (sets of) graphs.

B.2 TABLE OF EQUIVALENCE CLASSES

Each entry in the table below represents one algebraic equivalence class and its isomorphisms (obtained by relabelling the nodes). The leftmost column shows the set of graphs in this equivalence class, using the notation for graph patterns explained in Sections 2.3 and B.1. For each equivalence class, its algebraic constraints (found by Theorem 1 and converted to polynomial form) are also listed.

For many equivalence classes, the set of graphs that fit the pattern in the leftmost column is a superset of the equivalence class: some acyclic graphs that match the pattern do not actually belong in the class, but our notation is not expressive enough to show the precise inclusions in one figure. For each equivalence class where this is the case, a second column of smaller graph patterns appears. The union of the sets of graphs described by these patterns equals the equivalence class exactly. Because many of the graph patterns in the union are graph isomorphisms of each other, we show only one member of each isomorphism class, and indicate how many isomorphisms there are by writing ' $n \times$ '. (Each of these isomorphisms is an automorphism of the leftmost graph pattern, and there are always exactly n such isomorphic patterns, so no information is lost by not listing them explicitly.) For example, the first equivalence class listed in Section B.2.3 consists of all acyclic graphs with at least one edge of any type between each pair of nodes in $\{a, b, c\}$, as well as all graphs in which one of those pairs has no edge between it, but the other two pairs make up a partial collider.

The equivalence classes are split out below according to their dimension. This refers to the dimension of the set of *correlation* rather than covariance matrices, thus normalizing out the variance Σ_{vv} associated with each node. This number has the convenient property that it equals the minimum number of edges among all graphs in an equivalence class.

B.2.0 Dimension 0

$$\begin{array}{cccc} \bullet & \bullet & \bullet & \bullet \\ a & b & c & d \end{array}$$

$$\sigma_{ab} = 0, \sigma_{ac} = 0, \sigma_{ad} = 0,$$

$$\sigma_{bc} = 0, \sigma_{bd} = 0, \sigma_{cd} = 0$$

B.2.1 Dimension 1

$$\begin{array}{cccc} \bullet \text{---} \bullet & \bullet & \bullet & \\ a & b & c & d \end{array}$$

$$\sigma_{ac} = 0, \sigma_{ad} = 0, \sigma_{bc} = 0, \sigma_{bd} = 0, \sigma_{cd} = 0$$

B.2.2 Dimension 2

$$\begin{array}{cccc} \bullet \text{---} \bullet & \bullet \text{---} \bullet & & \\ a & b & c & d \end{array}$$

$$\sigma_{ac} = 0, \sigma_{ad} = 0, \sigma_{bc} = 0, \sigma_{bd} = 0$$

$$\begin{array}{cccc} \bullet \text{---} \bullet \text{---} \bullet & \bullet & & \\ a & b & c & d \end{array}$$

$$\rho_{ac.b} = 0, \sigma_{ad} = 0, \sigma_{bd} = 0, \rho_{cd.b} = 0$$

$$\begin{array}{cccc} \bullet \text{---} \bullet \text{---} \bullet & & \bullet & \\ a & b & c & d \end{array}$$

$$\sigma_{ac} = 0, \sigma_{ad} = 0, \sigma_{bd} = 0, \sigma_{cd} = 0$$

B.2.3 Dimension 3

$1 \times$

$$\sigma_{ad} = 0, \sigma_{bd} = 0,$$

$$\sigma_{cd} = 0$$

$3 \times$

$$\rho_{ac.b} = 0, \rho_{ad.b} = 0, \rho_{bd.c} = 0$$

$$\sigma_{ac} = 0, \sigma_{ad} = 0, \rho_{bd.c} = 0$$

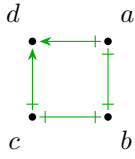
$$\sigma_{ac} = 0, \sigma_{ad} = 0, \sigma_{bd} = 0$$

$$\rho_{bc.a} = 0, \rho_{bd.a} = 0, \rho_{cd.a} = 0$$

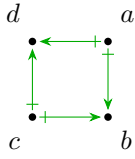
$$\sigma_{bc} = 0, \rho_{bd.a} = 0, \rho_{cd.a} = 0$$

$$\sigma_{bc} = 0, \sigma_{bd} = 0, \sigma_{cd} = 0$$

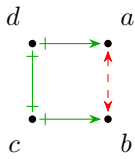
B.2.4 Dimension 4



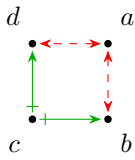
$$\rho_{ac.b} = 0, \rho_{bd.ac} = 0$$



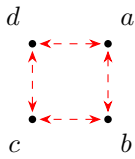
$$\sigma_{ac} = 0, \rho_{bd.ac} = 0$$



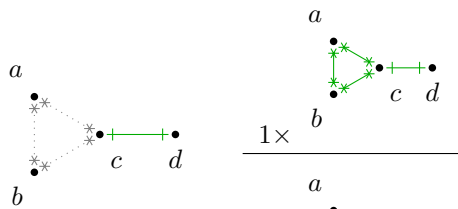
$$\rho_{ac.d} = 0, \rho_{bd.c} = 0$$



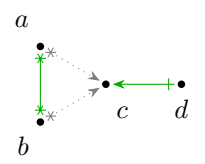
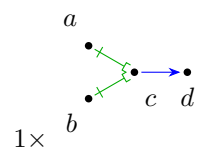
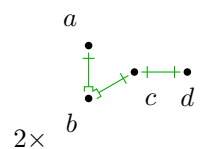
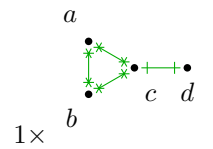
$$\sigma_{ac} = 0, \rho_{bd.c} = 0$$



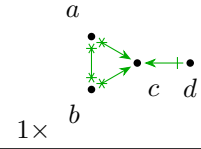
$$\sigma_{ac} = 0, \sigma_{bd} = 0$$



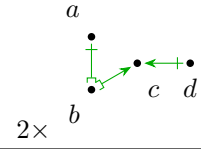
$$\rho_{ad.c} = 0, \rho_{bd.c} = 0$$



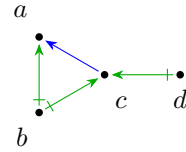
$$\sigma_{ad} = 0, \sigma_{bd} = 0$$



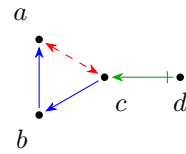
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2×

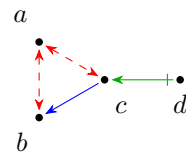


$$\rho_{ad.bc} = 0, \sigma_{bd} = 0$$

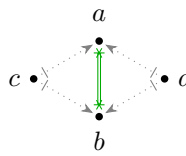


$$\rho_{bd.c} = 0,$$

$$\sigma_{cc}\sigma_{ab}\sigma_{bd} - \sigma_{cc}\sigma_{bb}\sigma_{ad} - \sigma_{bc}\sigma_{ac}\sigma_{bd} + \sigma_{bc}^2\sigma_{ad} = 0$$



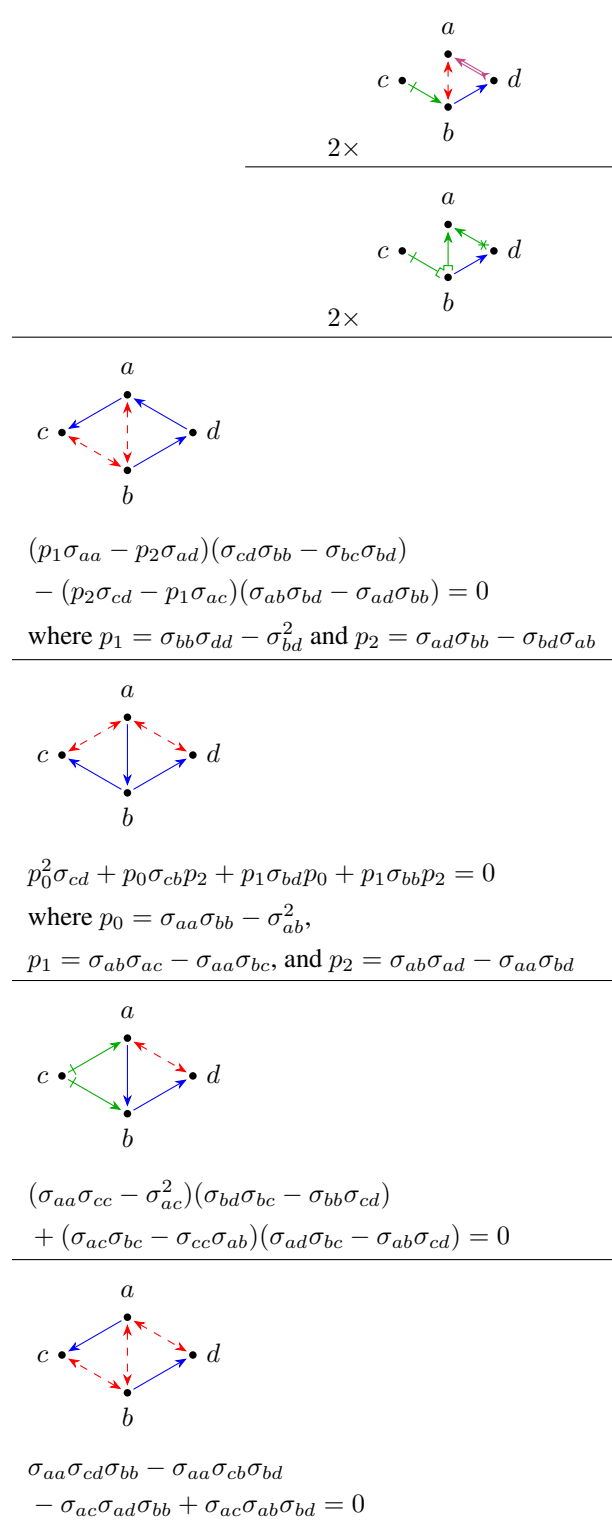
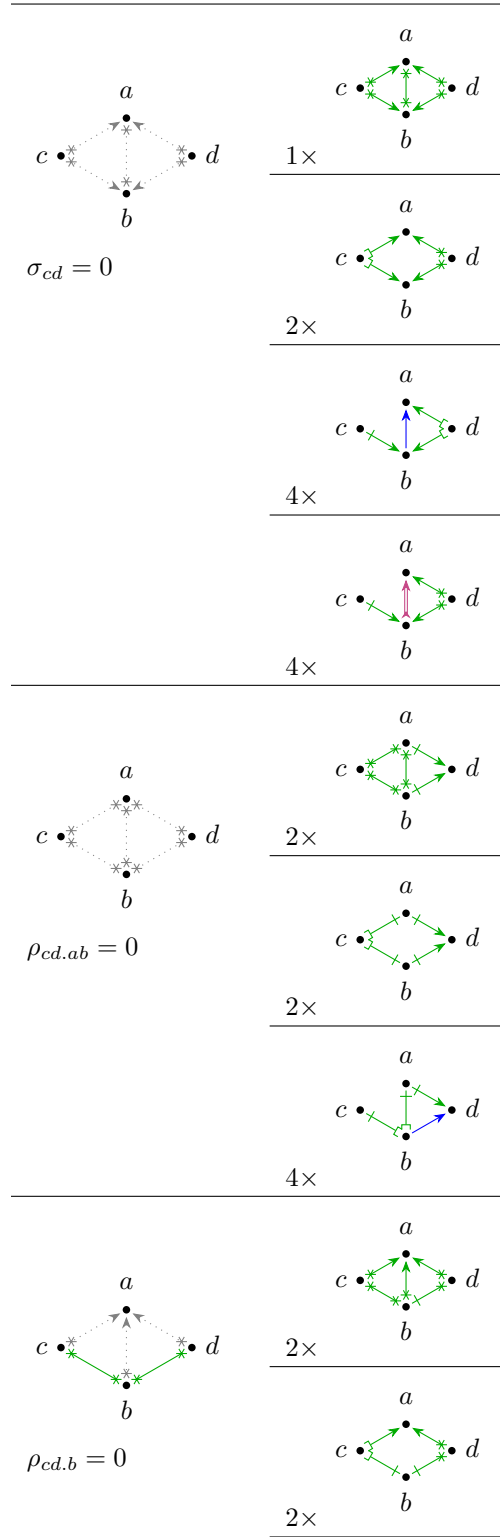
$$\sigma_{ad} = 0, \rho_{bd.c} = 0$$

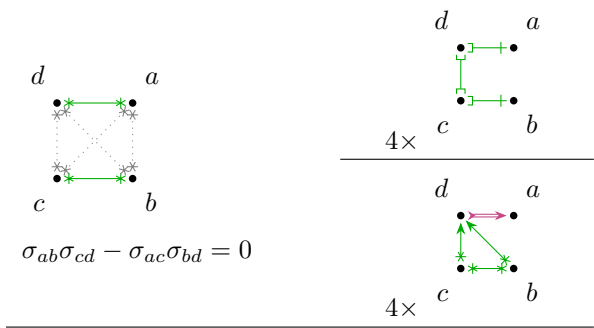
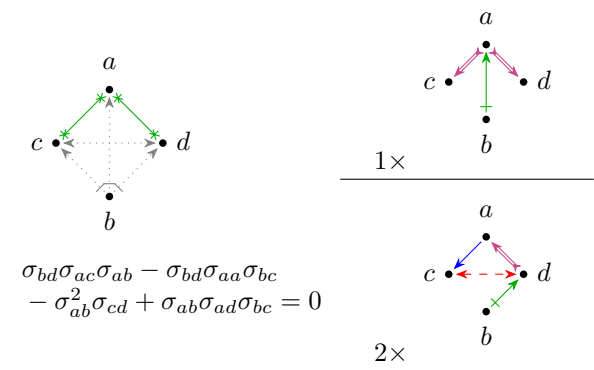
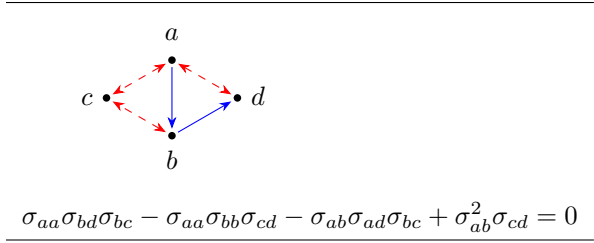


2×

$$\sigma_{cd} = 0, \sigma_{ac}\sigma_{bd} - \sigma_{ad}\sigma_{bc} = 0$$

B.2.5 Dimension 5





B.2.6 Dimension 6

