

Smoothness of Gaussian Conditional Independence Models

Mathias Drton and Han Xiao

Department of Statistics
The University of Chicago

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- 1 **Introduction**
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Gaussian CI Models

Roughly speaking, a Gaussian CI Model is the family of all gaussian random vectors satisfying a certain set of CI statements.

$[m] = \{1, 2, \dots, m\}$	a finite set
$X = (X_i)_{i \in [m]}$	a random vector
X_A	the sub-vector $(X_i)_{i \in A}$, where $A \subset [m]$
$A \perp\!\!\!\perp B C$	X_A and X_B are conditionally independent given X_C
$ij C$	X_i and X_j are conditionally independent given X_C , where $i \neq j$ and $C \subset [m] \setminus ij$
$\mathcal{R}([m])$	the set of all couples $(ij C)$ such that $i \neq j$ and $C \subset [m] \setminus ij$

A **conditional independence relation** \mathcal{L} is a set of CI couples, *i.e.* \mathcal{L} is a subset of $\mathcal{R}([m])$.

Proposition 1.1

Let $X \sim \mathcal{N}(\mu, \Sigma)$ be a regular Gaussian random vector, for pairwise disjoint $A, B, C \subset [m]$,

$$A \perp\!\!\!\perp B | C \iff \text{rank}(\Sigma_{AC, BC}) = \#C. \quad (1.1)$$

Moreover, $A \perp\!\!\!\perp B | C$ if and only if $i \perp\!\!\!\perp j | C$ for all $i \in A$ and $j \in B$.

A CI relation $\mathcal{L} \subseteq \mathcal{R}(m)$ determines a **Gaussian conditional independence model**, namely, the family of all multivariate normal distributions for which $i \perp\!\!\!\perp j | C$ whenever $ij | C \in \mathcal{L}$. The Gaussian model given by \mathcal{L} corresponds to the algebraic subset

$$V_{pd}(\mathcal{L}) = \{ \Sigma \in \text{PD}_m : \det(\Sigma_{iC, jC}) = 0 \text{ for all } ij | C \in \mathcal{L} \}$$

of the cone of positive definite $m \times m$ -matrices, denoted by PD_m .

Main Question

Drton (2009)

Chernoff's regularity condition holds for semi-algebraic sets such that the asymptotics of the likelihood ratio tests are determined by the tangent cone at the true parameter point. At boundary points or singularities, the tangent cone need not be a linear space and limiting distributions other than χ^2 distributions may arise.

Questions

For which conditional independence relations $\mathcal{L} \subseteq \mathcal{R}(m)$ is the associated set $V_{pd}(\mathcal{L})$ a smooth manifold?

Representable and Complete Relations

Given a set of covariance matrices $W \subset \text{PD}_m$, we can define a relation as

$$\mathcal{L}(W) = \{ ij|C \in \mathcal{R}(m) : \det(\Sigma_{iC,jC}) = 0 \text{ for all } \Sigma \in W \}.$$

Definition 1.2 (Complete Relation)

A relation \mathcal{L} is *complete* if $\mathcal{L} = \mathcal{L}(V_{pd}(\mathcal{L}))$, that is, if for every couple $ij|C \notin \mathcal{L}$ there exists a covariance matrix $\Sigma \in V_{pd}(\mathcal{L})$ with $\det(\Sigma_{iC,jC}) \neq 0$.

Definition 1.3 (Representable Relation, Lněnička 2007)

A relation \mathcal{L} is *representable* if there exists a covariance matrix $\Sigma \in \text{PD}_m$ for which $\det(\Sigma_{iC,jC}) = 0$ if and only if $ij|C \in \mathcal{L}$.

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Representable Decomposition

Theorem 2.1

Every conditional independence model $V_{pd}(\mathcal{L})$ has a representable decomposition, that is, it can be decomposed as

$$V_{pd}(\mathcal{L}) = V_{pd}(\mathcal{L}_1) \cup \dots \cup V_{pd}(\mathcal{L}_k),$$

where $\mathcal{L}_1, \dots, \mathcal{L}_k$ are representable relations. The decomposition can be chosen minimal (i.e., $\mathcal{L}_i \not\subseteq \mathcal{L}_j$ for all $i \neq j$), in which case the relations $\mathcal{L}_1, \dots, \mathcal{L}_k$ are unique up to reordering.

Corollary 2.2

A relation \mathcal{L} is complete if and only if it is an intersection of representable relations. The representable relations can be chosen to yield a representable decomposition of the model $V_{pd}(\mathcal{L})$.

Definition 2.3 (CI Implication)

A (Gaussian) conditional independence implication is an ordered pair of disjoint CI relations $(\mathcal{L}_1, \mathcal{L}_2)$ such that $V_{pd}(\mathcal{L}_1) = V_{pd}(\mathcal{L}_1 \cup \mathcal{L}_2)$. We denote the implication as $\mathcal{L}_1 \Rightarrow \mathcal{L}_2$ and say that a relation \mathcal{L} satisfies $\mathcal{L}_1 \Rightarrow \mathcal{L}_2$, if $\mathcal{L}_1 \subseteq \mathcal{L}$ implies that $\mathcal{L}_2 \subseteq \mathcal{L}$.

Definition 2.4 (Semigaussoid)

A relation $\mathcal{L} \subset \mathcal{R}([m])$ is called a **semigaussoid** if it satisfies

$$\{(ij|C), (ik|jC)\} \subset \mathcal{L} \Rightarrow \{(ik|C), (ij|kC)\} \subset \mathcal{L} \quad (2.1)$$

$$\{(ij|kC), (ik|jC)\} \subset \mathcal{L} \Rightarrow \{(ij|C), (ik|C)\} \subset \mathcal{L} \quad (2.2)$$

$$\{(ij|C), (ik|C)\} \subset \mathcal{L} \Rightarrow \{(ij|kC), (ik|jC)\} \subset \mathcal{L} \quad (2.3)$$

whenever $i, j, k \in [m]$ are distinct and $C \subset [m] \setminus ijk$.

Dual Relation

The **dual** of a couple $ij|C \in \mathcal{R}(m)$ is the couple $ij|\bar{C}$ where $\bar{C} = [m] \setminus ijC$. The **dual** of a relation \mathcal{L} on $[m]$ is the relation

$$\mathcal{L}^d = \{ij|\bar{C} : ij|C \in \mathcal{L}\}$$

made up of the dual couples of the elements of \mathcal{L} .

Lemma 2.5 (Lněnička 2007)

For a positive definite matrix Σ and two relations \mathcal{L} and \mathcal{K} :

- (i) $\mathcal{L}(\{\Sigma\})^d = \mathcal{L}(\{\Sigma^{-1}\})$;
- (ii) $\mathcal{L} \Rightarrow \mathcal{K}$ if and only if $\mathcal{L}^d \Rightarrow \mathcal{K}^d$;
- (iii) \mathcal{L} is complete if and only if \mathcal{L}^d has this property.

Lemma 2.6

The duals of semigaussoids are semigaussoids.

Undirected Graphical Model

For a simple undirected graph G with the vertex set $[m]$, let

$$\langle\langle G \rangle\rangle = \{(ij|C) \in \mathcal{R}([m]) : 'C \text{ separates } i \text{ and } j \text{ in } G'\}.$$

The relation $\langle\langle G \rangle\rangle$ is called **separation graphoid**. It is a semigaussoid since it is **ascending** and **transitive**

$$(ij|L) \in \mathcal{L} \Rightarrow (ij|kL) \in \mathcal{L} \quad (2.4)$$

$$(ij|L) \in \mathcal{L} \Rightarrow (ik|L) \in \mathcal{L} \vee (jk|L) \in \mathcal{L} \quad (2.5)$$

for any i, j, k distinct and $L \subset [m] \setminus ijk$.

Let $\mathcal{R}_*([m])$ denote the set of couples $(ij|C)$ with $C = [m] \setminus ij$.

Lemma 2.7

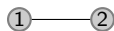
If $\mathcal{M} \subset \mathcal{R}_([m])$ and G is a graph with the vertex set $[m]$ having i and j adjacent if and only if $(ij|[m] \setminus ij) \notin \mathcal{M}$, then every semigaussoid \mathcal{L} containing \mathcal{M} also contains $\langle\langle G \rangle\rangle$.*

Find the Semigaussoids

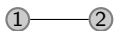
An element $(ij|C)$ is called a t -couple if $|C| = t$. It suffices to consider semigaussoids who have more 2-couples than 0-couples.

- Step 1.** Starting from each of the 11 separation graphoids, add all the possible 0-couples and 1-couples while keeping the number of 0-couples smaller than the number of 2-couples.
- Step 2.** For each relation obtained in this way check whether it is a semigaussoid, and whether it is equivalent to a previously discovered semigaussoid.
- Step 3.** Find the duals of the semigaussoids discovered in Steps 1 and 2. Check which new semigaussoids are equivalent to earlier found semigaussoids.

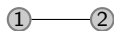
Find the Semigaussoids



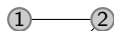
$\mathcal{L}_2 : 1$



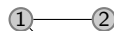
$\mathcal{L}_3 : 2$



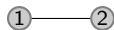
$\mathcal{L}_4 : 1$



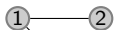
$\mathcal{L}_5 : 1$



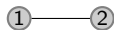
$\mathcal{L}_6 : 6$



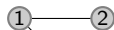
$\mathcal{L}_7 : 4$



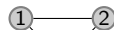
$\mathcal{L}_8 : 11$



$\mathcal{L}_{12} : 25$



$\mathcal{L}_{16} : 47$



$\mathcal{L}_{53} : 10$

Steps 1 and 2 produce 109 semigaussoids. In step 3 of our search we obtain an additional 48 semigaussoids. Hence, there are $109 + 48 = 157$ equivalence classes of semigaussoids.

More Implications

Among the 157 semigaussoids found above are the 53 representable relations determined in Lněnička (2007), but not all the remaining 104 semigaussoids are complete. For instance, 10 semigaussoids fail to satisfy the following CI implications:

Lemma 2.8 (Lněnička 2007)

Any Gaussian CI model over $[m]$ satisfies

$$\{(ij|L), (kl|L), (ik|jL), (jl|ikL)\} \subset \mathcal{L} \Rightarrow (ik|L) \in \mathcal{L},$$

$$\{(ij|L), (kl|iL), (kl|jL), (ij|klL)\} \subset \mathcal{L} \Rightarrow (kl|L) \in \mathcal{L},$$

$$\{(ij|L), (jl|kL), (kl|iL), (ik|jL)\} \subset \mathcal{L} \Rightarrow (ik|L) \in \mathcal{L},$$

$$\{(ij|kL), (ik|lL), (il|jL)\} \subset \mathcal{L} \Rightarrow (ij|L) \in \mathcal{L},$$

$$\{(ij|kL), (jk|lL), (kl|iL), (il|jL)\} \subset \mathcal{L} \Rightarrow (ij|L) \in \mathcal{L}$$

for all distinct i, j, k, l and $L \subset [m] \setminus ijkl$.

Theorem 2.9

There are 101 equivalence classes of complete relations on the set $[m] = [4]$.

There are 629 representable relations on $[m] = [4]$, when treating equivalent but unequal relations as different. For each relation \mathcal{L} among the remaining 94 non-representable semigaussoids find all of the 629 representable relations that contain it. By Theorem 2.2, \mathcal{L} is complete if and only if it is equal to the intersection of these representable relations. We obtain 48 complete relations in addition to the representable ones. This yields the claimed 101 Gaussian CI models (counting up to equivalence).

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CI Ideals

Correlation matrices can also be used to address the smoothness problem. Let $\text{PD}_{m,1} \subset \text{PD}_m$ be the set of positive definite matrices with ones along the diagonal. Given a relation \mathcal{L} , we can define the set

$$V_{cor}(\mathcal{L}) = \{ R \in \text{PD}_{m,1} : \det(R_{iC,jC}) = 0 \text{ for all } ij|C \in \mathcal{L} \}.$$

Let $\mathbb{R}[\mathbf{r}] = \mathbb{R}[r_{ij} : 1 \leq i < j \leq m]$ be the real polynomial ring associated with the entries r_{ij} of a correlation matrix R . The algebraic geometry of the set $V_{cor}(\mathcal{L})$ is captured by

$$\mathcal{I}(V_{cor}(\mathcal{L})) = \{ f \in \mathbb{R}[\mathbf{r}] : f(R) = 0 \text{ for all } R \in V_{cor}(\mathcal{L}) \}.$$

However, it is generally difficult to compute this ideal. Instead we start algebraic computations with the **(pairwise) conditional independence ideal**

$$I_{\mathcal{L}} = \langle \det(R_{iC,jC}) : ij|C \in \mathcal{L} \rangle \subseteq \mathcal{I}(V_{cor}(\mathcal{L})).$$

Proposition 3.1

Let \mathcal{L} be a relation on $[m] = [4]$. If \mathcal{L} is representable, then $I_{\mathcal{L}}$ is a radical ideal. The ideal $I_{\mathcal{L}}$ need not be radical even if \mathcal{L} is complete.

Algebraic calculations with an ideal $I \subset \mathbb{R}[\mathbf{r}]$ directly reveal geometric structure of the associated complex algebraic variety

$$V_{\mathbb{C}}(I) = \{ R \in \mathbb{S}_{m,1}(\mathbb{C}) : f(R) = 0 \text{ for all } f \in I \}.$$

Here, $\mathbb{S}_{m,1}(\mathbb{C})$ is the space of complex symmetric $m \times m$ matrices with ones on the diagonal. Studying the complex variety will provide insight into the geometry of the corresponding set of correlation matrices $V_{cor}(I)$ but, as we will see later, care must be taken when making this transfer.

Proposition 3.2

If \mathcal{L} is a representable relation on $[m] = [4]$, then the conditional independence ideal $I_{\mathcal{L}}$ is a prime ideal except when \mathcal{L} is equivalent to one of the relations \mathcal{L}_{15} , \mathcal{L}_{24} , \mathcal{L}_{28} and \mathcal{L}_{37} .

For the representable relation $\mathcal{L}_{15} = \{14, 14|23, 23, 23|14\}$, the ideal $I_{\mathcal{L}_{15}}$ has 4 prime components:

$$\begin{aligned} Q_1 &= \langle r_{12}, r_{14}, r_{23}, r_{34} \rangle, & Q_2 &= \langle r_{13}, r_{14}, r_{23}, r_{24} \rangle, \\ Q_3 &= \langle r_{14}, r_{23}, r_{12} + r_{34}, r_{13} - r_{24} \rangle, & Q_4 &= \langle r_{14}, r_{23}, r_{12} - r_{34}, r_{13} + r_{24} \rangle \end{aligned}$$

For $\mathcal{L}_{24} = \{12, 23|14, 24|3\}$, the ideal $I_{\mathcal{L}_{24}}$ has two prime components:

$$Q_1 = \langle r_{12}, r_{23}r_{34} - r_{24}, r_{13}r_{14}r_{34} - r_{14}^2 - r_{34}^2 + 1 \rangle, \quad Q_2 = \langle r_{12}, r_{23}, r_{24} \rangle.$$

Irreducible Decomposition

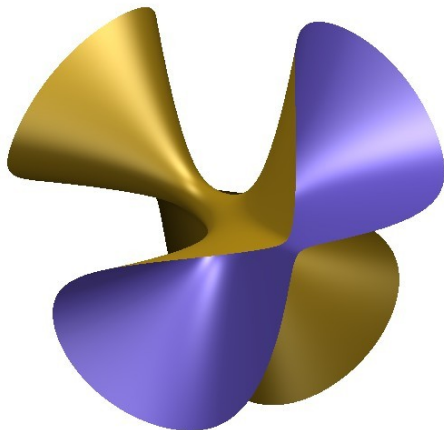


Figure: Surface defined by $r_{13}r_{14}r_{34} - r_{14}^2 - r_{34}^2 + 1 = 0$. It arises for a component of $V_{cor}(\mathcal{L}_{24}) = V_{cor}(\{12, 23|14, 24|3\})$.

Singular Point

Suppose V is an algebraic variety in the space $\mathbb{S}_{m,1}(\mathbb{C})$ of. Let $\mathcal{I}(V)$ be the ideal of polynomials vanishing on V . Choose $\{f_1, f_2, \dots, f_\ell\} \subset \mathbb{R}[\mathbf{r}]$ to be a finite generating set of $\mathcal{I}(V)$, and define $J(\mathbf{r})$ to be the $\ell \times \binom{m}{2}$ Jacobian matrix with (k, ij) entry equal to $\partial f_k(\mathbf{r}) / \partial r_{ij}$. It can be shown that the maximum rank the Jacobian matrix achieves over V is equal to $\text{codim}(V) = \binom{m}{2} - \dim(V)$ and, in particular, independent of the choice of the generating set $\{f_1, f_2, \dots, f_\ell\}$.

Definition 3.3

If the variety $V \subseteq \mathbb{S}_{m,1}(\mathbb{C})$ is irreducible then a matrix $R = (r_{ij}) \in V$ is a *singular point* if the rank of $J(R)$ is smaller than $\text{codim}(V)$. If V is not irreducible, then the singular points are the singular points of the irreducible components of V together with the points in the intersection of any two irreducible components.

Lemma 3.4 (Bochnak et al 1998)

The set of all points in $V_{cor}(\mathcal{L})$ that are non-singular points of $V_{\mathbb{C}}(I_{\mathcal{L}})$ is a smooth manifold.

- Calculate the locus of singular points of $V_{\mathbb{C}}(I_{\mathcal{L}})$.
- Saturate the ideal $S_{\mathcal{L}}$ describing this singular locus on the product of principal minors D and then compute a primary decomposition of $(S_{\mathcal{L}} : D^{\infty})$.
- If the singular locus is seen not to intersect $\text{PD}_{m,1}$ then the computation proves that $V_{cor}(\mathcal{L})$ is a smooth manifold.
- If, however, there are correlation matrices that are singular points of $V_{\mathbb{C}}(I_{\mathcal{L}})$, then we may not yet conclude that $V_{cor}(\mathcal{L})$ is non-smooth around these points.

An algebraic obstacle is the fact that $I_{\mathcal{L}}$ might differ from the vanishing ideal $\mathcal{I}(V_{cor}(\mathcal{L}))$.

Proposition 3.5

Let $f_1 = \det(R_{iC_1, jC_1})$, $f_2 = \det(R_{iC_2, jC_2}) \in \mathbb{R}[\mathbf{r}]$ be the two determinants encoding the relation $\mathcal{L} = \{ij|C_1, ij|C_2\}$ on $[m]$. Let $J(R)$ be the $2 \times \binom{m}{2}$ Jacobian matrix for f_1, f_2 evaluated at a correlation matrix R . Then the maximal rank of $J(R)$ over $V_{\text{cor}}(\mathcal{L})$ is two but this rank drops to one exactly when R satisfies the two conditional independence constraints

$$i \perp\!\!\!\perp j(C_1 \Delta C_2) | (C_1 \cap C_2) \quad \text{and} \quad j \perp\!\!\!\perp i(C_1 \Delta C_2) | (C_1 \cap C_2).$$

Here, $C_1 \Delta C_2 = (C_1 \setminus C_2) \cup (C_2 \setminus C_1)$ is the symmetric difference.

Theorem 3.6

If \mathcal{L} is a representable relation on $[m] = [4]$, then $V_{cor}(\mathcal{L})$ is a smooth manifold unless \mathcal{L} is equivalent to one of 12 relations \mathcal{L}_i with index $i \in \{14, 15, 20, 24, 28, 29, 30, 32, 36, 37, 46, 51\}$.

(a) *Union of smooth components:* If $i \in \{24, 28\}$ then $V_{cor}(\mathcal{L}_i)$ is the union of two components that are both smooth manifolds. If $i \in \{15, 37\}$ then $V_{cor}(\mathcal{L}_i)$ is the union of four smooth components. The singular loci are obtained by forming intersections of components.

(b) *Singular at identity matrix:* Six models have the identity matrix as their only singular point.

(c) *Singular at almost diagonal matrices:* For two models, the correlation matrices that are singularities have at most one nonzero above diagonal entry.

Tangent Direction and Tangent Cone

Definition 3.7

A *tangent direction* of $V_{cor}(\mathcal{L})$ at the correlation matrix $R_0 \in \text{PD}_{m,1}$ is a matrix in $\mathbb{R}^{m \times m}$ that is the limit of a sequence $\alpha_n(R_n - R_0)$, where the α_n are positive reals and the $R_n \in V_{cor}(\mathcal{L})$ converge to R_0 . The *tangent cone* $TC_{\mathcal{L}}(R_0)$ is the closed cone made up of all these tangent directions.

Let the correlation matrix $R_0 \in \text{PD}_{m,1}$ correspond to a root of the polynomial $f \in \mathbb{R}[\mathbf{r}]$. Write

$$f(R) = \sum_{h=l}^L f_h(R - R_0)$$

as a sum of homogeneous polynomials f_h in $R - R_0$, where $f_h(t)$ has degree h and $f_l \neq 0$. Since $f(R_0) = 0$, the minimal degree l is at least one, and we define $f_{R_0, \min} = f_l$.

Tangent Direction and Tangent Cone

Consider the cone $AC_{\mathcal{L}}(R_0)$ given by the real algebraic variety of the ideal

$$C_{\mathcal{L}}(R_0) = \{f_{R_0, \min} : f \in I_{\mathcal{L}}\} \subset \mathbb{R}[\mathbf{r}].$$

We have the inclusion $TC_{\mathcal{L}}(R_0) \subseteq AC_{\mathcal{L}}(R_0)$.

Theorem 3.8

If \mathcal{L}_i is one of the 8 representable relations on $[m] = [4]$ with index $i \in \{14, 20, 29, 30, 32, 36, 46, 51\}$, then at all singularities R_0 of $V_{\text{cor}}(\mathcal{L}_i)$ the tangent cone $TC_{\mathcal{L}}(R_0)$ is equal to the algebraically defined cone $AC_{\mathcal{L}}(R_0)$. In particular, the models $V_{\text{cor}}(\mathcal{L}_i)$ are indeed non-smooth.

An Example

For $\mathcal{L}_{29} = \{23, 23|14\}$, the singular points $R_0 = (\rho_{ij})$ have all off-diagonal entries zero except for possibly ρ_{14} . The cone ideal varies continuously with ρ_{14} :

$$C_{\mathcal{L}_{29}}(R_0) = \langle r_{23}, r_{13}(r_{12} - \rho_{14}r_{24}) + r_{34}(r_{24} - \rho_{14}r_{12}) \rangle.$$

Consider a generic direction $\mathbf{t} = (t_{12}, t_{13}, t_{14}, t_{23}, t_{24}, t_{34})$ in the cone $AC_{\mathcal{L}_{29}}(R_0)$. We may assume $\rho t_{12} - t_{24} \neq 0$, and obtain

$$\mathbf{t} = \left(t_{12}, t_{13}, t_{14}, 0, t_{24}, \frac{t_{13}(t_{12} - \rho t_{24})}{\rho t_{12} - t_{24}} \right).$$

Let

$$\mathbf{r}_n = \left(\frac{t_{12}}{n}, \frac{t_{13}}{n}, \rho + \frac{t_{14}}{n}, 0, \frac{t_{24}}{n}, \frac{nt_{13}(t_{12} - \rho t_{24}) - t_{13}t_{14}t_{24}}{n^2(\rho t_{12} - t_{24}) + nt_{12}t_{14}} \right).$$

It is easy to show that $\mathbf{r}_n \in V_{cor}(\mathcal{L}_{29})$ for large n ; and $\mathbf{r}_n \rightarrow \mathbf{r}_0$ and $n(\mathbf{r}_n - \mathbf{r}_0) \rightarrow \mathbf{t}$ as $n \rightarrow \infty$. Thus, $\mathbf{t} \in TC_{\mathcal{L}_{29}}(R_0)$, and it follows that $TC_{\mathcal{L}_{29}}(R_0) = AC_{\mathcal{L}_{29}}(R_0)$.

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Conclusion

- The model associated with a representable relation need not correspond to an irreducible variety.
- We provide a negative answer (\mathcal{L}_{24} and \mathcal{L}_{28}) to Question 7.11 in Drton et al (2009), which asked whether Gaussian conditional independence models that are smooth locally at the identity matrix are smooth manifolds.

$$\mathcal{L}_{24} = \{12, 23|14, 24|3\} \quad \langle r_{12}, r_{23}, r_{24}, r_{13}r_{14}r_{34} - r_{14}^2 - r_{34}^2 + 1 \rangle$$

$$\mathcal{L}_{28} = \{13|2, 14, 23|14, 24|3\} \quad \langle r_{13}, r_{14}, r_{23}, r_{24}, r_{12}^2 + r_{34}^2 - 1 \rangle.$$

- Gaussian conditional independence models for $m = 3$ variables are smooth except for the model given by ij and $ij|k$, and that singular models can arise more generally when combining two CI couples $ij|C$ and $ij|D$ (recall Proposition 3.5). This observation may lead one to guess that if a complete relation \mathcal{L} does not contain two CI couples $ij|C$ and $ij|D$ that repeat the pair ij , then the model $V_{pd}(\mathcal{L})$ is smooth. Unfortunately, this is false, again because of \mathcal{L}_{24} and \mathcal{L}_{28} .

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Thank You!