

On conditional independence and log-convexity¹

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Abstract. If conditional independence constraints define a family of positive distributions that is log-convex then this family turns out to be a Markov model over an undirected graph. This is proved for the distributions on products of finite sets and for the regular Gaussian ones. As a consequence, the assertion known as Brook factorization theorem, Hammersley–Clifford theorem or Gibbs–Markov equivalence is obtained.

Résumé. Si des contraintes d'indépendance conditionnelle définissent une famille de distributions positives qui est log-convexe, alors cette famille doit être un modèle de Markov sur un graphe non-dirigé. Ceci est démontré pour les distributions sur les produits d'ensembles finis et pour les distributions gaussiennes régulières. Par conséquent, l'assertion connue comme le théorème de factorisation de Brook, le théorème de Hammersley–Clifford ou l'équivalence de Gibbs–Markov est obtenue.

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1. Main result

Let N be a finite set, X_i , $i \in N$, finite nonempty state spaces, X_I the product of X_i over $i \in I$, and π_I the coordinate projection of X_N to X_I , $I \subseteq N$. The marginal of a probability measure (p.m.) P on X_N to I is the p.m. $\pi_I P$ on X_I given by

$$\pi_I P(\pi_I x) = \sum_{y \in X} P(y) \delta_{x,y}^I, \quad x \in X_N,$$

where $\delta_{x,y}^I$ equals one if $\pi_I x = \pi_I y$ and zero otherwise.

A p.m. P on X_N satisfies a *conditional independence (CI-)* constraint if

$$\pi_{i j K} P(\pi_{i j K} x) \cdot \pi_K P(\pi_K x) = \pi_{i K} P(\pi_{i K} x) \cdot \pi_{j K} P(\pi_{j K} x), \quad x \in X_N, \quad (1)$$

where $i, j \in N$ are different and $K \subseteq N \setminus ij$. By convention, an element $i \in N$ is not distinguished from the singleton $\{i\}$ and the sign \cup for unions of subsets of N is omitted.

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The family of all ordered couples $(ij|K)$ with i, j and K as above is denoted by \mathcal{R} . For $\mathcal{L} \subseteq \mathcal{R}$ let $\mathcal{P}_{\mathcal{L}}$ denote the family of p.m.'s on X_N that satisfy the CI-constraint given by each $(ij|K) \in \mathcal{L}$ and $\mathcal{P}_{\mathcal{L}}^+ = \mathcal{P}_{\mathcal{L}} \cap \mathcal{P}^+$. Here, \mathcal{P}^+ is the family of p.m.'s on X_N that are positive in the sense $P(x) > 0$ for all $x \in X_N$. Given a p.m. P , the projections π_i , $i \in N$, can be interpreted as the random variables jointly distributed according to P . Their distribution belongs to $\mathcal{P}_{\mathcal{L}}$ if and only if π_i and π_j are stochastically independent given $(\pi_k)_{k \in K}$ for all $(ij|K) \in \mathcal{L}$.

A nonempty subfamily of \mathcal{P}^+ is *log-convex* if it contains together with p.m.'s P and Q also the p.m. proportional to $x \mapsto P^t(x)Q^{1-t}(x)$, $x \in X_N$, for all $0 < t < 1$. The general definition of log-convexity is recalled and discussed in Section 5.3.

A hypergraph (N, \mathcal{A}) consists of the vertex set N and a nonempty family \mathcal{A} of subsets of N , called hyperedges. A p.m. P on X_N is *factorizable* w.r.t. the hypergraph if for each $I \in \mathcal{A}$ there exists a real-valued function ψ_I on X_I such that

$$P(x) = \prod_{I \in \mathcal{A}} \psi_I(\pi_I x), \quad x \in X_N. \tag{2}$$

The family of all p.m.'s on X_N that factorize w.r.t. the hypergraph is denoted by $\mathcal{F}_{\mathcal{A}}$ and $\mathcal{F}_{\mathcal{A}}^+ = \mathcal{F}_{\mathcal{A}} \cap \mathcal{P}^+$. An undirected graph $G = (N, E)$ has a vertex set N and an edge set E , contained in the family $\binom{N}{2}$ of all two-element subsets of N . A set L of vertices is a clique of G if $\binom{L}{2} \subseteq E$. If \mathcal{A} is the family of cliques of G , the notation \mathcal{F}_G^+ is preferred to $\mathcal{F}_{\mathcal{A}}^+$ and one speaks about the factorization w.r.t. G .

Theorem 1. *If $\mathcal{L} \subseteq \mathcal{R}$ and $\mathcal{P}_{\mathcal{L}}^+$ is log-convex then this family coincides with \mathcal{F}_G^+ where $G = (N, E)$ is the graph with $ij \in E$ if and only if $(ij|K) \notin \mathcal{L}$ for all $K \subseteq N \setminus ij$.*

In other words, given a family \mathcal{L} the graph G is constructed on N by removing from $\binom{N}{2}$ all ij such that $(ij|K) \in \mathcal{L}$ for some $K \subseteq N \setminus ij$; Theorem 1 asserts that the log-convexity of $\mathcal{P}_{\mathcal{L}}^+$ implies $\mathcal{P}_{\mathcal{L}}^+ = \mathcal{F}_G^+$.

If \mathcal{L} consists exclusively of the couples $(ij|K)$ having $K = N \setminus ij$ then it is log-convex. This follows easily from a well-known equivalent definition of CI-constraints, see (6) below. In this special case Theorem 1 implies what is called by statisticians Brook factorization theorem [5,16] or Hammersley–Clifford theorem [3,7] and by physicists Gibbs–Markov equivalence [19,26].

Corollary 1. *If $G = (N, E)$ is an undirected graph and \mathcal{L} consists of all couples $(ij|N \setminus ij)$ such that ij is not an edge of G then $\mathcal{P}_{\mathcal{L}}^+ = \mathcal{F}_G^+$.*

A proof of Theorem 1 is deferred to Section 4. It is based on properties of interaction spaces, summarized in Section 2, and new observations on the behaviour of the family $\mathcal{P}_{\mathcal{L}}$ around the uniform p.m., presented in Section 3. Discussion and remarks are collected in Section 5 that contains also a short independent proof of Corollary 1 of geometric flavor. Section 6 is devoted to a version of Theorem 1 involving regular multidimensional Gaussian p.m.'s, formulated as Theorem 2.

2. Interaction spaces and factorizability

The factorization (2) of positive p.m.'s w.r.t. a hypergraph can be equivalently described on the exponential scale by a linear space. The space decomposes orthogonally to interaction spaces. The material of this section is standard, see [10] and [20], Appendix B.2. The aim is to prepare arguments used in Sections 3 and 4, and supply self-contained proofs.

For $I \subseteq N$ let \mathcal{V}_I denote the linear space of those functions v of $x \in X_N$ that depend on x only through $\pi_I x$, thus $v(x) = v(y)$ once $\pi_I x = \pi_I y$, $x, y \in X_N$. For $v \in \mathcal{V}_I$

$$\pi_I v(\pi_I x) = |X_{N \setminus I}| v(x), \quad x \in X_N, \tag{3}$$

where the marginalization of functions on X_N is defined analogously to that of p.m.'s, thus $\pi_I v(\pi_I x)$ is the sum of $v(y)$ over $y \in X_N$ satisfying $\pi_I x = \pi_I y$.

Lemma 1. A function u on X_N is orthogonal to \mathcal{V}_J , $J \subseteq N$, if and only if $\pi_J u = 0$.

Proof. A function v belongs to \mathcal{V}_J if and only if it can be written as the composition $v = v_J \pi_J$ where $v_J : X_J \rightarrow \mathbb{R}$. Since

$$\langle u, v \rangle = \sum_{x \in X_N} u(x) \cdot v(x) = \sum_{x_J \in X_J} \pi_J u(x_J) \cdot v_J(x_J) = \langle \pi_J u, v_J \rangle$$

and v_J is arbitrary the assertion follows. \square

For $I \subseteq N$ let \mathcal{U}_I denote the orthogonal complement in \mathcal{V}_I to the sum of \mathcal{V}_J over $J \subsetneq I$, and be referred to as an *interaction space*.

Lemma 2. If $J \subseteq N$ does not contain $I \subseteq N$ and $u \in \mathcal{U}_I$, then $\pi_J u = 0$.

Proof. Since $\mathcal{U}_I \subseteq \mathcal{V}_I$ the marginal $\pi_J u$ of $u \in \mathcal{U}_I$ to J depends on $x_J \in X_J$ only through $\pi_{I \cap J}^J x_J$ where $\pi_{I \cap J}^J$ denotes the coordinate projection of X_J to $X_{I \cap J}$. It follows from (3), applied to $\pi_J u$ and $I \cap J$ in the roles of v and I , that $\pi_{I \cap J}^J \pi_J u(\pi_{I \cap J}^J x_J)$ equals $|\pi_J u(x_J)|$ for $x_J \in X_J$. Therefore, it suffices to prove that the marginal $\pi_{I \cap J}^J \pi_J u = \pi_{I \cap J} u$ of $u \in \mathcal{U}_I$ vanishes. By Lemma 1, this is equivalent to the orthogonality of u and $\mathcal{V}_{I \cap J}$ which holds by the definition of \mathcal{U}_I and $I \cap J \neq I$. \square

Lemma 3. The spaces \mathcal{U}_I , $I \subseteq N$, are pairwise orthogonal.

Proof. If $I, J \subseteq N$ are different then, up to symmetry, J does not contain I . By Lemma 2, if $u \in \mathcal{U}_I$ then $\pi_J u = 0$. Lemma 1 implies that u is orthogonal to \mathcal{V}_J . Thus, \mathcal{U}_I and \mathcal{U}_J are orthogonal. \square

For a hypergraph (N, \mathcal{A}) , let $\mathcal{W}_{\mathcal{A}}$ denote the sum of \mathcal{V}_I over $I \in \mathcal{A}$.

Lemma 4. For a hypergraph (N, \mathcal{A}) the space $\mathcal{W}_{\mathcal{A}}$ equals the orthogonal sum of \mathcal{U}_I over all $I \subseteq N$ that are covered by some hyperedge from \mathcal{A} .

Proof. By Lemma 3, the assertion follows from its special instance disregarding orthogonality. On account of the definition of $\mathcal{W}_{\mathcal{A}}$, it suffices to restrict to the hypergraphs with $\mathcal{A} = \{I\}$, $I \subseteq N$, in which case $\mathcal{W}_{\mathcal{A}} = \mathcal{V}_I$. Induction on the cardinality of I is employed to prove that \mathcal{V}_I is the sum of \mathcal{U}_J over $J \subseteq I$. If $I = \emptyset$ then \mathcal{V}_{\emptyset} and \mathcal{U}_{\emptyset} coincide with the space of constant functions on X_N and the assertion is trivial. Otherwise, \mathcal{V}_I decomposes orthogonally into \mathcal{U}_I and the sum of \mathcal{V}_J over $J \subsetneq I$. By the induction assumption, this sum equals the sum of \mathcal{U}_J over $J \subsetneq I$ whence the induction step is completed. \square

Corollary 2. The Euclidean space $\mathcal{V}_N = \mathbb{R}^{X_N}$ decomposes orthogonally to \mathcal{U}_I , $I \subseteq N$.

Lemma 5. For every hypergraph (N, \mathcal{A}) the family $\mathcal{F}_{\mathcal{A}}^+$ consists of the p.m.'s that are proportional to e^w where w belongs to the orthogonal sum of \mathcal{U}_I over all $I \subseteq N$ that are covered by some hyperedge from \mathcal{A} .

Proof. If w belongs to the above sum of \mathcal{U}_I then it is in the sum of \mathcal{V}_I over $I \in \mathcal{A}$. Writing w as the sum of functions $v_I \pi_I$ where $v_I : X_I \rightarrow \mathbb{R}$, a p.m. proportional to e^w is given by $x \mapsto t \exp[\sum_{I \in \mathcal{A}} v_I(\pi_I x)]$, $x \in X_N$, with some constant $t > 0$. Such a p.m. belongs to $\mathcal{F}_{\mathcal{A}}^+$, choosing ψ_I in (2) proportional to e^{v_I} .

If $P \in \mathcal{F}_{\mathcal{A}}^+$ then, by (2), positive functions ψ_I exist such that $P(x) = e^{w(x)}$, $x \in X_N$, where w is the sum over $I \in \mathcal{A}$ of the functions $x \mapsto \ln \psi_I(\pi_I x)$. Thus, P is proportional to e^w , with the proportionality constant equal to 1. By definition, w belongs to $\mathcal{W}_{\mathcal{A}}$, equal to the above sum of \mathcal{U}_I by Lemma 4. \square

Corresponding to the interaction spaces \mathcal{U}_I , a special base α_y , $y \in X_N$, of the space \mathbb{R}^{X_N} is constructed. To this end, it is assumed that each X_i has a distinguished element denoted by 0_i and $0 = (0_i)_{i \in N}$. The function α_y is defined at $x \in X_N$ by

$$\alpha_y(x) = \begin{cases} (-1)^{|s(y) \cap s(x)|}, & x \sim y, \\ 0, & \text{otherwise,} \end{cases}$$

where $s(y)$ denotes the support $\{i \in N: y_i \neq 0_i\}$ of y and $x \sim y$ abbreviates the equality of projections of x and y onto $s(x) \cap s(y)$.

Lemma 6. *If $I \subseteq N$ then $\{\alpha_y: s(y) \subseteq I\}$ is a base of \mathcal{V}_I and $\{\alpha_y: s(y) = I\}$ a base of \mathcal{U}_I .*

Proof. For $y, z \in X_N$ the scalar product of α_y and α_z equals the sum of $(-1)^{|s(y) \Delta s(z) \cap s(x)|}$ over $x \in X_N$ such that $x \sim y$ and $x \sim z$. For $i \in s(y) \setminus s(z)$ the range of summation is partitioned into the pairs that differ only in the i th coordinate, belonging to $\{0_i, y_i\}$. By the summations over the pairs, the scalar product vanishes. Therefore, α_y and α_z are orthogonal when $s(y) \neq s(z)$. If y and z have the same support then $\alpha_y(z) = (-1)^{|s(y)|} \delta_{y,z}^N$, and thus the functions α_y with $s(y) = I$ are independent. It follows that $\{\alpha_y: s(y) \subseteq I\}$ is an independent set. This set is a base of \mathcal{V}_I because $\alpha_y \in \mathcal{V}_{s(y)} \subseteq \mathcal{V}_I$ and $\dim \mathcal{V}_I = |X_I|$. Then, $\{\alpha_y: s(y) = I\}$ is a base of \mathcal{U}_I by Lemma 4. \square

In particular, the space \mathcal{U}_I has a positive dimension if and only if $|X_i| > 1$ for all $i \in I$. If $X_i = \{0_i, 1_i\}$, $i \in N$, then each \mathcal{U}_I is spanned by the single function α_y where $y = (y_i)_{i \in N}$ has y_i equal to 1_i for $i \in I$ and 0_i otherwise. These functions form an orthogonal base of \mathbb{R}^{X_N} by Corollary 2.

The following technical lemma is prepared for the discussion in Section 5.2.

Lemma 7. *For any hypergraph (N, \mathcal{A}) the family $\mathcal{W}_{\mathcal{A}}$ is the direct sum of the spaces*

$$\mathcal{V}_{0,I} = \{v \in \mathcal{V}_I: v(x) = 0 \text{ once } x_i = 0_i \text{ for some } i \in I\}$$

over $I \subseteq N$ that can be covered by some $J \in \mathcal{A}$.

The space $\mathcal{V}_{0,I}$ consists of the functions $v_I \pi_I$ where $v_I: X_I \rightarrow \mathbb{R}$ vanishes on each $x_I \in X_I$ having a coordinate $x_i = 0_i$. Such a function v_I is said to be *adapted* to 0 .

Proof of Lemma 7. For $I \subseteq N$ let ρ_I map $x \in X_N$ to $y \in X_N$ given by $\pi_I y = \pi_I x$ and $\pi_{N \setminus I} y = \pi_{N \setminus I} 0$. Let $w \in \mathbb{R}^{X_N}$ be decomposed as the sum of $v_I \pi_I$ over $I \subseteq N$ where every v_I is adapted to 0 . If $x \in X_N$ and $I = s(x)$ then

$$\begin{aligned} \sum_{L \subseteq I} (-1)^{|I \setminus L|} w(\rho_L x) &= \sum_{L \subseteq I} (-1)^{|I \setminus L|} \sum_{K \subseteq L} v_K(\pi_K \rho_L x) \\ &= \sum_{K \subseteq I} v_K(\pi_K x) \sum_{K \subseteq L \subseteq I} (-1)^{|I \setminus L|} = v_I(\pi_I x). \end{aligned} \quad (4)$$

Therefore, the functions v_I are unique and, in turn, the sum of all $\mathcal{V}_{0,I}$, $I \subseteq N$, is direct.

If v is a function on X_N then

$$\sum_{I \subseteq N} (-1)^{|N \setminus I|} v \rho_I \in \mathcal{V}_{0,N}.$$

In fact, if $x \in X_N$ has a coordinate $x_i = 0_i$ then $\rho_I x = \rho_{I \setminus i} x$ for $i \in I \subseteq N$, and grouping the summands into the pairs $I, I \setminus i$ the sum vanishes. Since $v = v \rho_N$ and $v \rho_I \in \mathcal{V}_I$ it follows that $\mathcal{V}_N = \mathbb{R}^{X_N}$ equals $\mathcal{V}_{0,N}$ plus the sum of \mathcal{V}_I over $I \subsetneq N$. By induction on the cardinality of N , \mathcal{V}_N is the sum of $\mathcal{V}_{0,I}$ over $I \subseteq N$, which implies the assertion. \square

3. Conditional independence and interactions

In this section, the *CI*-constraints are related to interaction spaces. This is done via the relation $(ij|K) \diamond L$ between $(ij|K) \in \mathcal{R}$ and $L \subseteq N$ defined by the statement ‘ $i \notin L$ or $j \notin L$ or $L \not\subseteq ijK$.’ In other words, $(ij|K) \diamond L$ if and only if $ij \subseteq L \subseteq ijK$, see Section 5.3. From now on, m_I denotes $|X_I|^{-1}$, $I \subseteq N$.

Lemma 8. *If $(ij|K) \diamond L$ and $u \in \mathcal{U}_L$ then the measure given by $P(x) = m_N[1 + u(x)]$, $x \in X_N$, satisfies the *CI*-constraint given by $(ij|K)$.*

Proof. By Lemma 2, if ijK does not contain L then the marginal of P to ijK is uniform. Thus, the *CI*-constraint (1) reduces to $m_{ijK}m_K = m_{iK}m_{jK}$. Otherwise, $L \subseteq ijK$, and it follows from $(ij|K) \diamond L$ that $i \notin L$ or $j \notin L$. By the symmetry between i and j , it suffices to restrict to the case $i \notin L$. Then, $L \subseteq jK$ which implies that u belongs to $\mathcal{V}_{jK} \subseteq \mathcal{V}_{ijK}$. By the double use of (3) with ijK and jK in the role of I , the constraint (1) rewrites to

$$m_{ijK}[1 + u(x)] \cdot \pi_K P(\pi_K x) = \pi_{iK} P(\pi_{iK} x) \cdot m_{jK}[1 + u(x)], \quad x \in X_N. \quad (5)$$

If $j \in L$ then K and iK do not contain L . By Lemma 2, the marginals of P to K and iK are uniform whence (5) holds. If $j \notin L$ then $L \subseteq K$, and thus $u \in \mathcal{V}_K \subseteq \mathcal{V}_{iK}$. By the double use of (3) with K and iK in the role of I , $\pi_K P(\pi_K x) = m_K[1 + u(x)]$ and $\pi_{iK} P(\pi_{iK} x) = m_{iK}[1 + u(x)]$. Hence, (5) is always satisfied. \square

For $\mathcal{L} \subseteq \mathcal{R}$ let \mathcal{L}^\diamond denote the family of $L \subseteq N$ such that $(ij|K) \diamond L$ for all $(ij|K) \in \mathcal{L}$.

Corollary 3. *If $\mathcal{L} \subseteq \mathcal{R}$ and $L \in \mathcal{L}^\diamond$ then any p.m. on X_N that differs from the uniform one by a vector from \mathcal{U}_L , as in Lemma 8, belongs to $\mathcal{P}_{\mathcal{L}}$.*

An example of the construction $\mathcal{L} \mapsto \mathcal{L}^\diamond$ arises from a graph $G = (N, E)$ and $\mathcal{K}_G = \{(ij|N \setminus ij) : ij \in \binom{N}{2} \setminus E\}$, arriving at the family \mathcal{K}_G^\diamond of cliques of G .

For a later reference the following simple assertion is needed.

Lemma 9. *For any $\mathcal{L} \subseteq \mathcal{R}$, if $M \subseteq N$ and every different $i, j \in M$ can be covered by some $L_{ij} \in \mathcal{L}^\diamond$ contained in M then $M \in \mathcal{L}^\diamond$.*

Proof. If a couple $(ij|K) \in \mathcal{L}$ has $i, j \in M$ then, by the assumption, $ij \subseteq L_{ij} \subseteq M$ for some $L_{ij} \in \mathcal{L}^\diamond$. The definition of \mathcal{L}^\diamond implies that $(ij|K) \diamond L_{ij}$, and thus $L_{ij} \not\subseteq ijK$ because $ij \subseteq L_{ij}$. Hence, $M \not\subseteq ijK$. It follows that $(ij|K) \diamond M$. In turn, $M \in \mathcal{L}^\diamond$. \square

In the remaining part of this section, the *CI*-constraints (1) are analyzed via the mappings $\Psi_{ij|K}$ given by

$$\Psi_{ij|K}(w) = \left(\pi_{ijK} w(\pi_{ijK} x) \cdot \pi_K w(\pi_K x) - \pi_{iK} w(\pi_{iK} x) \cdot \pi_{jK} w(\pi_{jK} x) \right)_{x \in X_N}.$$

Here, $(ij|K) \in \mathcal{R}$ and w is a function on X_N . A p.m. can play the role of w as well.

Lemma 10. *The Jacobian of $\Psi_{ij|K}$ at the uniform p.m. on X_N is equal to*

$$\left(m_K \delta_{x,y}^{ijK} + m_{ijK} \delta_{x,y}^{iK} - m_{jK} \delta_{x,y}^{iK} - m_{iK} \delta_{x,y}^{jK} \right)_{x,y \in X_N}.$$

Proof. The coordinate function of $\Psi_{ij|K}$ indexed by $x \in X_N$ equals

$$\sum_{z \in X_N} \sum_{\underline{z} \in X_N} w(z) w(\underline{z}) \left[\delta_{x,z}^{ijK} \delta_{x,\underline{z}}^{iK} - \delta_{x,z}^{iK} \delta_{x,\underline{z}}^{jK} \right].$$

Differentiating w.r.t. $w(y)$, $y \in X_N$,

$$\sum_{z \in X_N} \sum_{\underline{z} \in X_N} [\delta_{y,z}^N w(\underline{z}) + w(z) \delta_{\underline{z},y}^N] [\delta_{x,z}^{ijK} \delta_{x,\underline{z}}^K - \delta_{x,z}^{iK} \delta_{x,\underline{z}}^{jK}].$$

When $w(z) = m_N$, $z \in X_N$, this equals

$$m_N \sum_{\underline{z} \in X_N} [\delta_{x,y}^{ijK} \delta_{x,\underline{z}}^K - \delta_{x,y}^{iK} \delta_{x,\underline{z}}^{jK}] + m_N \sum_{z \in X_N} [\delta_{x,z}^{ijK} \delta_{x,y}^K - \delta_{x,z}^{iK} \delta_{x,y}^{jK}]$$

and the assertion follows. \square

Let $\text{Ker}_{(ij|K)}$ denote the kernel of the Jacobian of $\Psi_{ij|K}$ at the uniform p.m.

Lemma 11. For $\mathcal{L} \subseteq \mathcal{R}$ the intersection of $\text{Ker}_{(ij|K)}$ over $(ij|K) \in \mathcal{L}$ is equal to the sum of \mathcal{U}_L over $L \in \mathcal{L}^\diamond$.

Proof. If $L \notin \mathcal{L}^\diamond$ then $ij \subseteq L \subseteq ijK$ for some $(ij|K) \in \mathcal{L}$. For $u \in \mathcal{U}_L$ and $v \in \text{Ker}_{(ij|K)}$

$$\sum_{x \in X_N} u(x) \sum_{y \in X_N} [m_K \delta_{x,y}^{ijK} + m_{ijK} \delta_{x,y}^K - m_{jK} \delta_{x,y}^{iK} - m_{iK} \delta_{x,y}^{jK}] v(y) = 0$$

because the inner sums equal zero due to Lemma 10. Since none of the sets K , iK and jK contains L the marginals of u to these sets vanish by Lemma 2 and the above equation rewrites to

$$\sum_{x \in X_N} \sum_{y \in X_N} u(x) v(y) \delta_{x,y}^{ijK} = 0.$$

Since $L \subseteq ijK$ the function u belongs to \mathcal{V}_{ijK} , and thus $u(x) \delta_{x,y}^{ijK} = u(y) \delta_{x,y}^{ijK}$. Therefore, u and v are orthogonal. In turn, $\text{Ker}_{(ij|K)}$ is orthogonal to \mathcal{U}_L .

By Corollary 2, the intersection of $\text{Ker}_{(ij|K)}$ over $(ij|K) \in \mathcal{L}$ is contained in the sum of \mathcal{U}_L over $L \in \mathcal{L}^\diamond$. The opposite inclusion is a consequence of Corollary 3. \square

4. Log-convexity and conditional independence

A nonempty family of positive p.m.'s on X_N is *log-linear* if it contains together with p.m.'s P and Q also the p.m. proportional to $x \mapsto P^t(x) Q^s(x)$, $x \in X_N$, for all real t and s . The family is *log-affine* if this is required only with $s = 1 - t$. The log-convexity assumes the additional restriction $0 < t < 1$. The log-affine families correspond to the full exponential families [20].

In this section, $\mathcal{L} \subseteq \mathcal{R}$.

Lemma 12. If $\mathcal{P}_{\mathcal{L}}^+$ is log-convex then it is log-linear.

Proof. Let $P, Q \in \mathcal{P}_{\mathcal{L}}^+$, $0 < t < 1$ and $R_t(x) = P^t(x) Q^{1-t}(x)$, $x \in X$. By the log-convexity, for $(ij|K) \in \mathcal{L}$ Eqs (1) hold with P replaced by R_t . Thus, the coordinate functions of $t \mapsto \Psi_{ij|K}(R_t)$ vanish when t ranges between 0 and 1. Since they are holomorphic they vanish identically. It follows that $\mathcal{P}_{\mathcal{L}}^+$ is closed to the log-affine combinations. The assertion follows because it is not difficult to see that a log-affine family that contains the uniform p.m. on X_N is log-linear. \square

Lemma 13. If $\mathcal{P}_{\mathcal{L}}^+$ is log-convex and a p.m. P on X_N is proportional to e^w for some $w \in \mathbb{R}^{X_N}$ then $P \in \mathcal{P}_{\mathcal{L}}^+$ if and only if w belongs to the sum of \mathcal{U}_L over $L \in \mathcal{L}^\diamond$.

Proof. The log-convex combinations of P with the uniform p.m.

$$P_t(x) = e^{tw(x)} / \sum_{y \in X_N} e^{tw(y)}, \quad x \in X_N,$$

are viewed as a curve parameterized by t . Its tangent vector at the uniform p.m. P_0 equals

$$m_N w - m_N^2 \sum_{y \in X_N} w(y).$$

If $P \in \mathcal{P}_{\mathcal{L}}^+$ then the log-convexity of $\mathcal{P}_{\mathcal{L}}^+$ implies that the curve ranges in $\mathcal{P}_{\mathcal{L}}^+$. Hence, the tangent belongs to $\text{Ker}_{(ij|K)}$ for $(ij|K) \in \mathcal{L}$. By Lemma 11, the tangent is in the sum of \mathcal{U}_L over $L \in \mathcal{L}^\circ$. Since $\emptyset \in \mathcal{L}^\circ$ and \mathcal{U}_\emptyset consists of the constant functions the sum contains w .

Let w belong to the sum of \mathcal{U}_L over $L \in \mathcal{L}^\circ$. By Lemma 12, $\mathcal{P}_{\mathcal{L}}^+$ is log-linear. Therefore, to prove that $P \in \mathcal{P}_{\mathcal{L}}^+$ it suffices to confine to the case $w \in \mathcal{U}_L$ for some $L \in \mathcal{L}^\circ$. The assertion is trivial if $L = \emptyset$, having w constant and P uniform. Otherwise, $L \neq \emptyset$ and w is orthogonal to \mathcal{U}_\emptyset by Lemma 3. Then, $x \mapsto m_N[1 + \varepsilon w(x)]$ defines a p.m. for ε sufficiently close to 0. By Corollary 3, this p.m. belongs to $\mathcal{P}_{\mathcal{L}}$. It is proportional to $e^{\ln[1 + \varepsilon w]}$. The log-affinity of $\mathcal{P}_{\mathcal{L}}^+$ implies that the p.m. P_ε proportional to e^{w_ε} with $w_\varepsilon = \frac{1}{\varepsilon} \ln[1 + \varepsilon w]$ belongs to $\mathcal{P}_{\mathcal{L}}^+$. Limiting with ε to 0 the functions w_ε converge to w and P_ε converges to $P \in \mathcal{P}^+$. Hence, $P \in \mathcal{P}_{\mathcal{L}}^+$. \square

The CI-constraint (1) given by $(ij|K)$ can be equivalently expressed as

$$Q(x_i x_j x_K) \cdot Q(y_i y_j x_K) = Q(x_i y_j x_K) \cdot Q(y_i x_j x_K), \quad x_i, y_i \in X_i, x_j, y_j \in X_j, x_K \in X_K, \quad (6)$$

where Q denotes the marginal of P to ijK , $x_i x_j x_K$ is the element of X_{ijK} that projects to x_i, x_j and x_K , and $y_i y_j x_K, x_i y_j x_K$ and $y_i x_j x_K$ have analogous meaning. If $K = N \setminus ij$ then $Q = P$ and it is easy to see that if two p.m.'s satisfy the equations in (6) then the equations also hold for the log-linear combinations of the p.m.'s.

Under the additional natural assumption $|X_i| > 1$ for all $i \in N$, the following lemma and the proof of Theorem 1 can be slightly simplified but when not excluding $|X_i| = 1$ only additional minor technicalities are needed.

Lemma 14. *If $\mathcal{P}_{\mathcal{L}}^+$ is log-convex, $L \in \mathcal{L}^\circ$ and $|X_\ell| > 1$ for each $\ell \in L$ then all subsets of L belong to \mathcal{L}° .*

Proof. It suffices to prove that $L \setminus \ell \in \mathcal{L}^\circ$ for all $\ell \in L$. This is accomplished when the violation of $(ij|K) \diamond (L \setminus \ell)$ for some $(ij|K)$ implies that the couple is not in \mathcal{L} . Thus, assume $ij \subseteq L \setminus \ell \subseteq ijK$. By the assumption on cardinalities, there exists $y \in X_N$ with $s(y) = L$. Let $z \in X_N$ have $s(z) = \ell$ and the same ℓ th coordinate as y , $y_\ell \neq 0_\ell$. Since $L, \ell \in \mathcal{L}^\circ$ Lemma 6 implies $\alpha_y \in \mathcal{U}_L$ and $\alpha_z \in \mathcal{U}_\ell$. By the log-convexity and Lemma 13, the p.m. P proportional to $e^{\alpha_y + \alpha_z}$ is in $\mathcal{P}_{\mathcal{L}}^+$.

There exists $t > 0$ such that $t \cdot \pi_{N \setminus \ell} P(x_{N \setminus \ell})$ equals

$$\begin{aligned} & e^{\alpha_y(0_\ell x_{N \setminus \ell}) + \alpha_z(0_\ell x_{N \setminus \ell})} + e^{\alpha_y(y_\ell x_{N \setminus \ell}) + \alpha_z(y_\ell x_{N \setminus \ell})} + \sum_{x_\ell \in X_\ell \setminus \{0, y_\ell\}} e^{\alpha_y(x_\ell x_{N \setminus \ell}) + \alpha_z(x_\ell x_{N \setminus \ell})} \\ & = e^{\alpha_y(0_\ell x_{N \setminus \ell}) + 1} + e^{\alpha_y(y_\ell x_{N \setminus \ell}) - 1} + |X_\ell| - 2, \quad x_{N \setminus \ell} \in X_{N \setminus \ell}, \end{aligned}$$

where α_y and α_z vanish at $x_\ell x_{N \setminus \ell}$. Combining $ij \subseteq L \setminus \ell \subseteq ijK$ and $L \in \mathcal{L}^\circ$, the set ijK cannot contain ℓ . Therefore, $\pi_{ijK} P = Q$ is a marginal of $\pi_{N \setminus \ell} P$. Since $\pi_{N \setminus \ell} P$ depends on $x_{N \setminus \ell}$ only through $\pi_{ijK}^{N \setminus \ell} x_{N \setminus \ell}$ it follows from (3) that $Q(\pi_{ijK}^{N \setminus \ell} x_{N \setminus \ell})$ is equal to $|X_{N \setminus \ell ijK}| \pi_{N \setminus \ell} P(x_{N \setminus \ell})$. Therefore,

$$Q(0_i 0_j 0_K) Q(y_i y_j 0_K) - Q(0_i y_j 0_K) Q(y_i 0_j 0_K)$$

is a positive multiple of $[e^2 + e^{-2} + |X_\ell| - 2]^2 - |X_\ell|^2$. Using (6), this implies $(ij|K) \notin \mathcal{L}$. \square

Proof of Theorem 1. Let $\mathcal{R}_{N, X}$ consist of the couples $(ij|N \setminus ij)$ with $|X_i| = 1$ or $|X_j| = 1$. By (1), $\mathcal{P}_{\mathcal{L}} = \mathcal{P}_{\mathcal{L} \cup \mathcal{R}_{N, X}}$ for all $\mathcal{L} \subseteq \mathcal{R}$. Let $G_{\mathcal{L}} = (N, E)$ be the graph with $ij \notin E$ if and only if $(ij|K) \in \mathcal{L}$ for some $K \subseteq N \setminus ij$. By (2),

a p.m. factorizes w.r.t. $G_{\mathcal{L}}$ if and only if it does w.r.t. $G_{\mathcal{L} \cup \mathcal{R}_{N,X}}$. It follows that it suffices to prove the assertion of Theorem 1 under the additional assumption $\mathcal{R}_{N,X} \subseteq \mathcal{L}$. Hence, any $L \in \mathcal{L}^\diamond$ with at least two elements has $|X_\ell| > 1$ for all $\ell \in L$. By Lemma 14, all subsets of any $L \in \mathcal{L}^\diamond$ belong to \mathcal{L}^\diamond ; thus \mathcal{L}^\diamond is hereditary. Using Lemma 9, a set $L \subseteq N$ with at least two elements belongs to \mathcal{L}^\diamond if and only if $ij \in \mathcal{L}^\diamond$ for every $i, j \in L$; thus \mathcal{L}^\diamond is conformal. It follows that \mathcal{L}^\diamond is the family of cliques of $G_{\mathcal{L}}$. Hence, the assertion of Theorem 1 obtains from Lemmas 5 and 13. \square

5. Discussion and remarks

5.1. The main result and its corollary

For an undirected graph $G = (N, E)$ let \mathcal{K}_G consist of the couples $(ij|N \setminus ij)$ having $ij \notin E$. The p.m.'s from $\mathcal{P}_{\mathcal{K}_G}$ are called *pairwise Markov w.r.t. G* . The families $\mathcal{P}_{\mathcal{K}_G}^+$ parameterized by undirected graphs G have been known in the statistical literature as the *Markov models over undirected graphs* [9,20], over the contingency tables. They are log-convex because each family $\mathcal{P}_{\{(ij|N \setminus ij)\}}^+$ is log-linear by the argument following (6) and intersections of log-linear families are log-linear. Hence, Theorem 1 directly implies the assertion of Corollary 1, $\mathcal{P}_{\mathcal{K}_G}^+ = \mathcal{F}_G^+$. Rephrased verbally, given an undirected graph, a positive p.m. is pairwise Markov if and only if it factorizes. The assumption of positivity matters, see [26], p. 22, and [20], Example 3.10.

Alternatively, $\mathcal{P}_{\mathcal{K}_G}^+ = \mathcal{F}_G^+$ is a simple consequence of the lemmas on the interaction spaces from Section 2. In fact, it is rather straightforward that $P \in \mathcal{P}^+$ satisfies the *CI*-constraint $(ij|N \setminus ij)$ if and only if $\ln P : x \mapsto \ln P(x)$ belongs to the sum of $\mathcal{V}_{N \setminus i}$ and $\mathcal{V}_{N \setminus j}$, see, e.g., [20], (3.6). This is the sum of \mathcal{U}_I where I does not contain ij , on account of Lemma 4. Therefore, by Corollary 2, $P \in \mathcal{P}^+$ is pairwise Markov w.r.t. G if and only if $\ln P$ belongs to the sum of \mathcal{U}_I where I contains no $ij \notin E$, thus I is a clique of G . To conclude $\mathcal{P}_{\mathcal{K}_G}^+ = \mathcal{F}_G^+$ it suffices to evoke Lemma 5. It seems that this short geometric proof of Corollary 1 via the intersections of sums of the interaction spaces is new. The presented argumentation is coordinate-free; no projectors, Moebius transform, algebras, and a special choice of $\theta \in X_N$ are employed. The only comparable proof of Corollary 1 is the inductive one by Brook [5], see also [16], Theorem 7.1, which however has no geometric content.

For $\mathcal{L} \subseteq \mathcal{R}$, Theorem 1 and log-convexity of the Markov models imply that $\mathcal{P}_{\mathcal{L}}^+$ is log-convex if and only if it is Markov over an undirected graph. Thus, the class of these Markov models can be equivalently defined by means of the *CI*-constraints and log-convexity, without any reference to graphs. Here, both the conditional independence [11] and log-convexity [6], including the geometrical viewpoint of [1], have been recognized for decades as basic building stones in statistics. Theorem 1 seems to be a new bridge between them.

5.2. Gibbs probability measures

Given a distinguished element $\theta = (\theta_i)_{i \in N}$ of X_N and a hereditary hypergraph (N, \mathcal{A}) , a p.m. $P \in \mathcal{P}^+$ is *Gibbsian* if there exist real-valued functions v_I on X_I such that

$$\ln P(x) = \sum_{I \in \mathcal{A}, I \subseteq s(x)} v_I(\pi_I x), \quad x \in X. \tag{7}$$

The family of such probability measures is denoted by $\mathcal{G}_{\theta, \mathcal{A}}^+$. If $x_I \in X_I$ and for some $i \in I$ the i th coordinate of x_I equals θ_i then the value $v_I(x_I)$ does not occur in (7). Therefore, it can be equivalently assumed in the above definition that all such values equal zero, thus v_I are adapted to θ . In this situation, the summation in (7) can run equivalently over $I \in \mathcal{A}$. Thus, the Gibbs p.m.'s factorize in a special way, $\mathcal{G}_{\theta, \mathcal{A}}^+ \subseteq \mathcal{F}_{\mathcal{A}}^+$. By Lemmas 5 and 7, if $P \in \mathcal{F}_{\mathcal{A}}^+$ then $P = e^w$ for $w \in \mathcal{W}_{\mathcal{A}}$ in the form $\sum_{I \in \mathcal{A}} v_I \pi_I$ with all v_I adapted to θ . Therefore, $\mathcal{F}_{\mathcal{A}}^+ \subseteq \mathcal{G}_{\theta, \mathcal{A}}^+$. Thus, over a hypergraph, the notion of Gibbs p.m.'s does not depend on the choice of θ and coincides with the factorizability of positive p.m.'s. In literature, e.g., in [7], Theorem 2, [26], Theorem 2, typically (7) is stated to be equivalent to

$$v_K(\pi_K x) = \sum_{I \subseteq K} (-1)^{|K \setminus I|} \ln P(\rho_I x), \quad K \in \mathcal{A}, x \in X_N, s(x) = K,$$

which is a reinterpretation of the computation in (4), based on Moebius transform.

The identity $\mathcal{P}_{\mathcal{K}_G}^+ = \mathcal{F}_G^+$, disguised in Gibbs p.m.'s and potentials, has been revealed and proved independently several times. Over point lattices it goes back to [2,30]. Two early unpublished manuscripts [14,17]² have been frequently cited. Other proofs are in [3], p. 198, [7], p. 22, [15,27,28], and three proofs in [26], Theorem 2. For personal remarks see also Hammersley's discussion in [3], p. 230.

Under topological assumptions on the state spaces, Hammersley–Clifford theorem from [12,20] asserts that over a graph the pairwise Markovness is equivalent to the factorization, for the p.m.'s with continuous and positive densities w.r.t. a product measure.

5.3. Miscellany

When P and Q are p.m.'s on a measurable space that are not mutually singular, p and q are their densities with respect to a dominating measure R and $0 < t < 1$, the log-convex combination of P and Q is defined as the p.m. with the R -density proportional to $p^t q^{1-t}$. The definition is not dependent on the choice of R . A family of p.m.'s is called log-convex if it is closed to the log-convex combinations of pairs of not mutually singular p.m.'s. Log-convex families of mutually absolutely continuous p.m.'s are called 'geodesically convex' in [6]. Examples of log-convex sets comprise the exponential families with convex sets of canonical parameters and their extensions [8].

A crucial role in the proof of Theorem 1 is played by the binary relation \diamond between \mathcal{R} and the power set of N . It appeared previously prior to [23], Theorem 4. In addition to the mapping $\mathcal{L} \mapsto \mathcal{L}^\diamond$, it gives rise to

$$\mathcal{A} \mapsto \mathcal{A}^\diamond = \{(ij|K) \in \mathcal{R}: (ij|K) \diamond L \text{ for all } L \in \mathcal{A}\},$$

where \mathcal{A} is a family of subsets of N . The pair of mappings forms a Galois connection [4], Chapter V, Sections 7 and 8. By the remark preceding [23], Theorem 4, the connection gives rise to an antiisomorphism between DCI -relations and C^w -families, similarly to [23], Theorem 1.

The implication of Lemma 9 is valid for the family of connected sets in any topological space in the role of \mathcal{L}^\diamond ; it goes back at least to [18].

General conditional independence statements can be reduced to families of the CI -constraints (1) by [22], Lemma 3. The families $\mathcal{P}_{\mathcal{L}}$ and $\mathcal{P}_{\mathcal{L}^\diamond}$ have been, in spite of considerable effort, far from being understood in general [12,24,31].

6. Gaussian probability measures

In this section $N = \{1, 2, \dots, n\}$. A p.m. on \mathbb{R}^n is regular Gaussian (rG) if its density with respect to the Lebesgue measure has the form

$$x \mapsto (2\pi)^{-n/2} (\det A)^{-1/2} \exp\left[-\frac{1}{2}(x - \mu)^T A^{-1}(x - \mu)\right], \quad x \in \mathbb{R}^n,$$

where μ is a (column) vector from \mathbb{R}^n and $A = (a_{i,j})_{i,j \in N}$ a real positive definite matrix. The standard notation $\det A$ is used for the determinant of A and T for the transposition.

An rG p.m. satisfies the CI -constraint given by $(ij|K) \in \mathcal{R}$ if and only if $\det A_{iK,jK}$ vanishes where $A_{iK,jK}$ is the submatrix of A whose rows are indexed by iK and columns by jK , see [21]. Hence, the p.m. is pairwise Markov w.r.t. an undirected graph $G = (N, E)$ if and only if $\det A_{N \setminus j, N \setminus i} = 0$ whenever $ij \notin E$; this equality is equivalent to vanishing of the element of A^{-1} indexed by i, j . It follows that the p.m. factorizes w.r.t. the graph [20], Section 5.1.4, which implies Markovness [20], Proposition 3.8. Thus, as well-known, the pairwise Markovness of any rG p.m. is equivalent to a factorization, over an undirected graph. For the general CI -constraints on Gaussian variables see [12, 13,21,25,29].

Log-convex combinations of two rG p.m.'s parameterized by μ, A and ν, B are the rG p.m.'s parameterized by some $\lambda_{\mu,\nu,t} \in \mathbb{R}^n$ and $[tA^{-1} + (1-t)B^{-1}]^{-1}$, $0 < t < 1$.

Theorem 2. *If the set of rG p.m.'s on \mathbb{R}^n that satisfy all CI -constraints from $\mathcal{L} \subseteq \mathcal{R}$ is log-convex then this set coincides with the set of all rG p.m.'s that factorize w.r.t. the graph (N, E) that has $ij \in E$ if and only if $(ij|K) \notin \mathcal{L}$ for all $K \subseteq N \setminus ij$.*

²The former work is not available to the author.

Proof. Two sets of positive definite $n \times n$ matrices A are introduced: the first one $\mathbf{A}_{\mathcal{L}}$ is given by $\det A_{iK,jK} = 0$ for all $(ij|K) \in \mathcal{L}$, and the second one $\mathbf{B}_{\mathcal{L}}$ by $A_{i,j} = 0$ for $ij \notin E$. The set of rG p.m.'s specified by the CI -constraints from \mathcal{L} is parameterized by the pairs μ, A with $A \in \mathbf{A}_{\mathcal{L}}$. The set of rG p.m.'s that factorize w.r.t. the graph is parameterized by the pairs μ, A with $A^{-1} \in \mathbf{B}_{\mathcal{L}}$.

By [21], Lemma 1, $\det A_{iK,jK} = 0$ if and only if $\det(A^{-1})_{N \setminus jK, N \setminus iK} = 0$, for all invertible matrices A . Thus, $A \in \mathbf{A}_{\mathcal{L}}$ is equivalent to $A^{-1} \in \mathbf{A}_{\mathcal{L}^1}$ where \mathcal{L}^1 is the set of $(ij|N \setminus ijK)$ having $(ij|K) \in \mathcal{L}$. Since $\mathbf{B}_{\mathcal{L}} = \mathbf{B}_{\mathcal{L}^1}$ Theorem 2 asserts that $\mathbf{A}_{\mathcal{L}^1} = \mathbf{B}_{\mathcal{L}^1}$. The assumption of log-convexity is equivalent to the convexity of $\{A^{-1}: A \in \mathbf{A}_{\mathcal{L}}\} = \mathbf{A}_{\mathcal{L}^1}$. Therefore, it suffices to prove that if $\mathbf{A}_{\mathcal{L}}$ is convex then $\mathbf{A}_{\mathcal{L}} = \mathbf{B}_{\mathcal{L}}$.

The unit matrix I always belongs to $\mathbf{A}_{\mathcal{L}}$. This set is closed to the positive multiples. These observations and the convexity of $\mathbf{A}_{\mathcal{L}}$ imply that if $A \in \mathbf{A}_{\mathcal{L}}$ then $A + tI$ belongs to $\mathbf{A}_{\mathcal{L}}$ for all $t > 0$. Therefore, $\det(A + tI)_{iK,jK} = 0$ for $(ij|K) \in \mathcal{L}$. The determinant is a polynomial in t with the leading coefficient $A_{i,j}$. Hence, $A_{i,j} = 0$ for $(ij|K) \in \mathcal{L}$ which implies $\mathbf{A}_{\mathcal{L}} \subseteq \mathbf{B}_{\mathcal{L}}$.

For $ij \in E$ let $I^{[ij]}$ be the symmetric matrix with the elements at the positions i, j and j, i equal to 1 and the remaining elements equal to zero. The matrix $I + \epsilon|E|I^{[ij]}$ belongs to $\mathbf{A}_{\mathcal{L}}$ for ϵ is sufficiently close to zero. By convexity, $I(\epsilon) = I + \epsilon \sum_{ij \in E} I^{[ij]}$ is in $\mathbf{A}_{\mathcal{L}}$. Let \mathcal{K} denote the set of $(ij|K) \in \mathcal{R}$ such that $N \setminus ijK$ separates i from j . Then, [21], Theorem 1, implies that up to finitely many ϵ for all $(ij|K) \in \mathcal{R}$ the determinant of $I(\epsilon)_{iK,jK}$ vanishes if and only if $(ij|K) \in \mathcal{K}$. Thus, $\mathbf{A}_{\mathcal{K}} \subseteq \mathbf{A}_{\mathcal{L}}$. It suffices to show that $\mathbf{B}_{\mathcal{L}} \subseteq \mathbf{A}_{\mathcal{K}}$. Under the separation of i and j by $N \setminus ijK$, the set K partitions into K_i and K_j such that there is no edge between iK_i and jK_j . If $A \in \mathbf{B}_{\mathcal{L}}$ then $A_{k_i,k_j} = 0$ for $k_i \in iK_i$ and $k_j \in jK_j$, implying $\det A_{iK,jK} = 0$, and thus $A \in \mathbf{A}_{\mathcal{K}}$. \square

The version of Theorem 2 that features the rG p.m.'s with the means equal to the zero instead of the rG p.m.'s also holds. This follows from $\lambda_{\mu,\nu,t} = 0$ whenever $\mu = 0$ and $\nu = 0$, and minor modifications in the argumentation of the above proof.

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