

SUPPORT SETS OF DISTRIBUTIONS WITH GIVEN INTERACTION STRUCTURE

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Abstract

We study closures of hierarchical models which are exponential families associated with hypergraphs by decomposing the corresponding interaction spaces in a natural and transparent way. Here, we apply general results on closures of exponential families.

1 Introduction

The set of probability measures on a Cartesian product of finite state sets of nodes allows for the analysis of interaction structures among the nodes [DS]. An important class of such structures, the so-called *graphical models*, is induced by graphical representations of the interactions [Lau, St]. Given an undirected graph G , the set of strictly positive probability measures that satisfy corresponding Markov properties forms an exponential family [BN, Am]. Dealing with probability distributions associated with G that are not necessarily strictly positive requires the study of the closure of that exponential family. In this note, we apply general results from [BN, CMb] on closures of exponential families for the explicit (but not constructive) description of the closure of an *hierarchical model* associated with hypergraphs [Lau] which generalize the class of graphical models. By decomposing corresponding interaction spaces in terms of linear algebra we hope to approach a constructive method that specifies the closure of a hierarchical model.

2 Preliminaries

Given a non-empty finite set \mathcal{X} , we denote the set of probability distributions on \mathcal{X} by $\bar{\mathcal{P}}(\mathcal{X})$. The *support* of $P \in \bar{\mathcal{P}}(\mathcal{X})$ is defined as $\text{supp}(P) := \{x \in \mathcal{X} : P(x) > 0\}$. For a subset $\mathcal{Y} \subseteq \mathcal{X}$ we consider the set $\mathcal{P}(\mathcal{Y})$ of probability vectors

with support equal to \mathcal{Y} , and one obviously has

$$\bar{\mathcal{P}}(\mathcal{X}) = \bigcup_{\emptyset \neq \mathcal{Y} \subseteq \mathcal{X}} \mathcal{P}(\mathcal{Y}).$$

With the map

$$\exp : \mathbb{R}^{\mathcal{X}} \rightarrow \mathcal{P}(\mathcal{X}), \quad f \mapsto \frac{\exp(f)}{\sum_{x \in \mathcal{X}} \exp(f(x))},$$

an *exponential family* (in $\mathcal{P}(\mathcal{X})$) is defined as the image $\exp(\mathcal{V})$ of a linear subspace \mathcal{V} of $\mathbb{R}^{\mathcal{X}}$.

Now we assume a compositional structure of \mathcal{X} induced by a set V of $1 \leq N < \infty$ nodes with state sets \mathcal{X}_v , $v \in V$. Here, we will only treat the binary case, i.e. $\mathcal{X}_v = \{0, 1\}$ for all $v \in V$. Given a finite subset $A \subseteq V$, we write \mathcal{X}_A instead of $\times_{v \in A} \mathcal{X}_v$, and we have the natural projections

$$X_A : \mathcal{X}_V \rightarrow \mathcal{X}_A, \quad (x_v)_{v \in V} \mapsto (x_v)_{v \in A}.$$

With a probability vector P on \mathcal{X}_V , the X_A become random variables.

We use the compositional structure of \mathcal{X}_V in order to define exponential families in $\mathcal{P}(\mathcal{X}_V)$ given by interaction spaces. We decompose $x \in \mathcal{X}_V$ in the form $x = (x_A, x_{V \setminus A})$ with $x_A \in \mathcal{X}_A$, $x_{V \setminus A} \in \mathcal{X}_{V \setminus A}$, and define \mathcal{I}_A to be the subspace of functions that do not depend on the configurations $x_{V \setminus A}$:

$$\mathcal{I}_A := \left\{ f \in \mathbb{R}^{\mathcal{X}} : f(x_A, x_{V \setminus A}) = f(x_A, x'_{V \setminus A}) \right. \\ \left. \text{for all } x_A \in \mathcal{X}_A, \text{ and all } x_{V \setminus A}, x'_{V \setminus A} \in \mathcal{X}_{V \setminus A} \right\}.$$

In the following, we apply these interaction spaces as building blocks for more general interaction spaces and associated exponential families [DS]. The most general construction is based on a set of subsets of V , a so-called *hypergraph* [Lau]. Given such a set $\mathcal{A} \subseteq 2^V$, we define the corresponding interaction space by

$$\mathcal{I}_{\mathcal{A}} := \sum_{A \in \mathcal{A}} \mathcal{I}_A$$

and consider the corresponding exponential family $\mathcal{E}_{\mathcal{A}} := \exp(\mathcal{I}_{\mathcal{A}})$.

Example 1.

(1) **Graphical models:** Let $G = (V, E)$ be an undirected graph, and define

$$\mathcal{A}_G := \{C \subseteq V : C \text{ is a clique with respect to } G\}.$$

Here, a *clique* is a set C that satisfies the following property:

$$a, b \in C, \quad a \neq b \quad \Rightarrow \quad \text{there is an edge between } a \text{ and } b.$$

The exponential family $\mathcal{E}_{\mathcal{A}_G}$ is characterized by Markov properties with respect to G (see [Lau]).

(2) Interaction order: The hypergraph associated with a given interaction order $k \in \{0, 1, 2, \dots, N\}$ is defined as

$$\mathcal{A}_k := \{A \subseteq V : |A| \leq k\} .$$

This gives us a corresponding hierarchy of exponential families studied in [Am, AK]:

$$\mathcal{E}_{\mathcal{A}_0} \subseteq \mathcal{E}_{\mathcal{A}_1} \subseteq \mathcal{E}_{\mathcal{A}_2} \subseteq \dots \subseteq \mathcal{E}_{\mathcal{A}_N} = \mathcal{P}(\mathcal{X}_V) .$$

In Example (3), we will discuss \mathcal{A}_i and $\mathcal{E}_{\mathcal{A}_i}$, $i = 1, 2$, in the case of two units.

3 Problem Statement and the Main Result

Given a complete hypergraph \mathcal{A} (i.e. $A \in \mathcal{A}, B \subseteq A \Rightarrow B \in \mathcal{A}$), we consider the closure $\text{cl } \mathcal{E}_{\mathcal{A}}$ of the exponential family $\mathcal{E}_{\mathcal{A}}$, and the map

$$\text{supp} : \text{cl } \mathcal{E}_{\mathcal{A}} \rightarrow 2^{\mathcal{X}_V}, \quad P \mapsto \text{supp}(P),$$

that assigns to each $P \in \text{cl } \mathcal{E}_{\mathcal{A}}$ the support $\text{supp}(P)$. In our main result (Theorem 2) we characterize the image of this map. To this end, we define the following family of functions:

$$e_A : \mathcal{X}_V \rightarrow \mathbb{R}, \quad x \mapsto (-1)^{E(A,x)}, \quad (A \in \mathcal{A}) \quad (1)$$

where $E(A, x)$ denotes the number of entries of x in A that are equal to one. More formally,

$$E(A, x) := |\{v \in A : X_v(x) = 1\}| . \quad (2)$$

Obviously, the functions $e_A \in \mathbb{R}^{\mathcal{X}_V}$ can be represented by the canonical basis e_x , $x \in \mathcal{X}_V$, as follows:

$$e_A = \sum_{x \in \mathcal{X}_V} (-1)^{E(A,x)} e_x .$$

Now fix an arbitrary numbering of $\mathcal{A} \setminus \{\emptyset\}$, set $s := |\mathcal{A}| - 1$, and consider the following composed map:

$$e_{\mathcal{A}} : \mathcal{X}_V \rightarrow \mathbb{R}^s, \quad x \mapsto (e_{A_1}(x), \dots, e_{A_s}(x)) .$$

The image of this map is a subset of the extreme points $\{-1, 1\}^s$ of the hypercube in \mathbb{R}^s . Note that for \mathcal{A}_1 (see Example 1), the image of $e_{\mathcal{A}_1}$ coincides with $\{-1, 1\}^s$. In general this is not the case, and Example 3 will illustrate this.

Let $\mathcal{F}_{\mathcal{A}}$ denote the set of (non-empty) faces of the polytope in \mathbb{R}^s spanned by the image of $e_{\mathcal{A}}$. Our main result characterizes the support sets of the closure of $\mathcal{E}_{\mathcal{A}}$ in terms of $\mathcal{F}_{\mathcal{A}}$:

Theorem 2. *A subset \mathcal{Y} of \mathcal{X}_V is the support set of an element of $\text{cl } \mathcal{E}_{\mathcal{A}}$ if and only if it is the preimage of a face $F \in \mathcal{F}_{\mathcal{A}}$ with respect to the map $e_{\mathcal{A}}$.*

The proof of the theorem will follow in Section 4.4. To illustrate the statement we consider the following instructive example:

Example 3. Consider the case of two binary units. We have $V = \{1, 2\}$, $\mathcal{X}_1 = \mathcal{X}_2 = \{0, 1\}$, and therefore $\mathcal{X}_V = \{(0, 0), (0, 1), (1, 0), (1, 1)\}$. The set of probability distributions is the three-dimensional simplex whose extreme points are the Dirac measures $\delta_{(x_1, x_2)}$, $x_1, x_2 \in \{0, 1\}$ (see Figure 1). As mentioned in Example 1 (2), we are going to discuss interactions of order one and two:

(1) For interactions of order one we have

$$\mathcal{A}_1 = \{\emptyset, \{1\}, \{2\}\}.$$

The exponential family $\mathcal{E}_1 := \mathcal{E}_{\mathcal{A}_1}$ coincides with the set of probability measures that factor over the two units. (It can be seen that $P(x_1, x_2) = P_1(x_1)P_2(x_2) \Leftrightarrow P \in \mathcal{E}_1$).

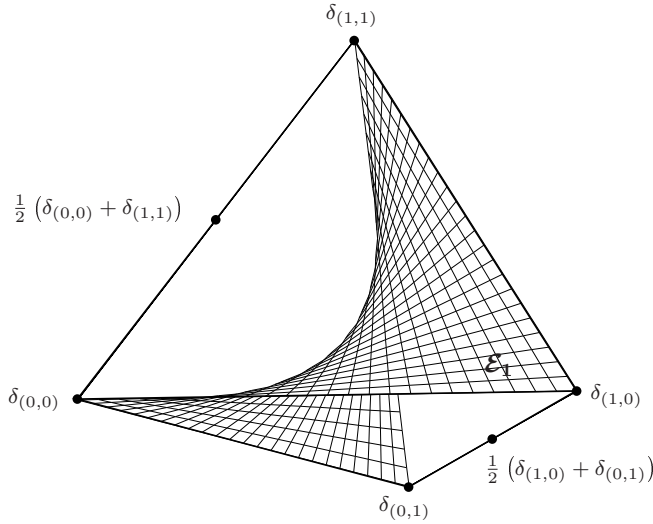


Figure 1: The exponential family \mathcal{E}_1 in the simplex of probability distributions.

The interaction space $\mathcal{I}_{\mathcal{A}_1}$ has dimension three, and one natural orthonormal basis (see Section 4.3) is the following:

$$\begin{aligned} e_{\emptyset} &= (1, 1, 1, 1) \\ e_{\{1\}} &= (1, 1, -1, -1) \\ e_{\{2\}} &= (1, -1, 1, -1). \end{aligned} \tag{3}$$

Here, the components are chosen with respect to the ordering $(e_{00}, e_{01}, e_{10}, e_{11})$ of the canonical basis of $\mathbb{R}^{\{0,1\}^2}$. The composed map is given as

$$e_{\mathcal{A}_1} : \mathcal{X}_V \rightarrow \mathbb{R}^2, \quad x \mapsto (e_{\{1\}}(x), e_{\{2\}}(x)).$$

The image of that map consists of the four points $(-1, -1), (1, -1), (-1, 1), (1, 1)$ which have the square in \mathbb{R}^2 as their convex hull. Denoting the convex hull of points p_1, \dots, p_k by $[p_1, \dots, p_k]$, we have the following (non-empty) faces in $\mathcal{F}_{\mathcal{A}_1}$:

$$\begin{aligned} F_1 &= [(-1, -1), (-1, 1), (1, -1), (1, 1)] \\ F_2 &= [(-1, -1), (-1, 1)] & F_3 &= [(-1, -1), (1, -1)] \\ F_4 &= [(-1, 1), (1, 1)] & F_5 &= [(1, -1), (1, 1)] \\ F_6 &= \{(-1, -1)\} & F_7 &= \{(-1, 1)\} & F_8 &= \{(1, -1)\} & F_9 &= \{(1, 1)\} \end{aligned}$$

The face F_1 is the square itself, F_2 to F_5 are the four edges, and F_6 to F_9 are the extreme points of the square. By Theorem 2, $\mathcal{Y}_i := e_{\mathcal{A}_1}^{-1}(F_i)$ are all support sets of probability measures in $\text{cl } \mathcal{E}_1$ (compare with Figure 1):

$$\begin{aligned} \mathcal{Y}_1 &= \{0, 1\}^2 \\ \mathcal{Y}_2 &= \{(1, 0), (1, 1)\} & \mathcal{Y}_3 &= \{(0, 1), (1, 1)\} \\ \mathcal{Y}_4 &= \{(0, 0), (1, 0)\} & \mathcal{Y}_5 &= \{(0, 0), (0, 1)\} \\ \mathcal{Y}_6 &= \{(1, 1)\} & \mathcal{Y}_7 &= \{(1, 0)\} & \mathcal{Y}_8 &= \{(0, 1)\} & \mathcal{Y}_9 &= \{(0, 0)\}. \end{aligned}$$

(2) Now we consider the hypergraph of interactions of order two, i.e.

$$\mathcal{A}_2 = \{\emptyset, \{1\}, \{2\}, \{1, 2\}\}.$$

The exponential family $\mathcal{E}_2 := \mathcal{E}_{\mathcal{A}_2}$ coincides with the whole simplex shown in Figure 1. The interaction space has dimension four, and the vector $e_{\{1,2\}} = (1, -1, -1, 1)$ completes the basis (3) to an orthonormal basis of the space $\mathcal{I}_{\mathcal{A}_2}$. The image of $e_{\mathcal{A}_2}$ is given by $\{(-1, -1, 1), (-1, 1, -1), (1, -1, -1), (1, 1, 1)\}$ which is a subset of the extreme points of the cube in \mathbb{R}^3 . It defines a simplex which is the image of the simplex in Figure 1 under the map $P \mapsto \mathbb{E}_P(e_{\mathcal{A}_2})$ (see Figure 2).

The faces in $\mathcal{F}_{\mathcal{A}_2}$ are given by

$$\begin{aligned} F_1 &= [(-1, -1, 1), (-1, 1, -1), (1, -1, -1), (1, 1, 1)] \\ F_2 &= [(-1, -1, 1), (-1, 1, -1), (1, 1, 1)] & F_3 &= [(-1, -1, 1), (-1, 1, -1), (1, 1, 1)] \\ F_4 &= [(-1, -1, 1), (1, -1, -1), (1, 1, 1)] & F_5 &= [(-1, 1, -1), (1, -1, -1), (1, 1, 1)] \\ F_6 &= [(-1, 1, -1), (1, -1, -1)] & F_7 &= [(1, 1, 1), (1, -1, -1)] \\ F_8 &= [(1, 1, 1), (-1, 1, -1)] & F_9 &= [(1, 1, 1), (-1, -1, 1)] \\ F_{10} &= [(-1, 1, -1), (1, -1, -1)] & F_{11} &= [(-1, -1, 1), (1, -1, -1)] \\ F_{12} &= \{(-1, 1, -1)\} & F_{13} &= \{(-1, -1, 1)\} \\ F_{14} &= \{(1, -1, -1)\} & F_{15} &= \{(1, 1, 1)\}. \end{aligned}$$

The face F_1 is the nothing but the simplex in Figure 2, F_2 to F_5 are its four triangles, F_6 to F_{11} are the six edges, and the remaining faces are the extreme points. The preimages of these faces with respect to the map $e_{\mathcal{A}_2}$ are exactly the 15 non-empty subsets of $\{0, 1\}^2$.

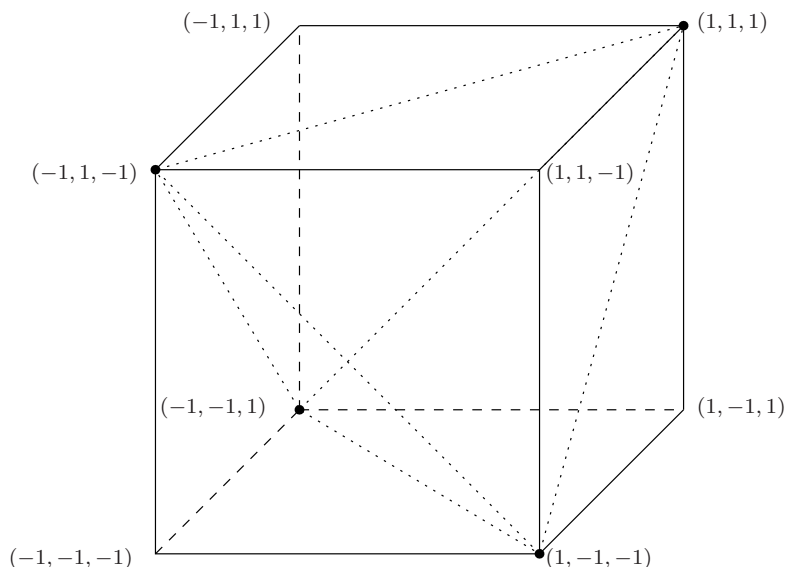


Figure 2: The convex hull of $\text{im } e_{\mathcal{A}_2} = \text{im}(e_{\{1\}}, e_{\{2\}}, e_{\{1,2\}})$ inside the cube in \mathbb{R}^3 .

4 Proof of the Main Result

In this section, we are going to prove our main result in several steps. In the first step, we review a classical result of [BN, CMb] on closures of exponential families. The second step deals with the decomposition of the interaction spaces $\mathcal{I}_{\mathcal{A}}$ into orthogonal components, and a natural basis is constructed. Based on these two steps, finally, the proof of Theorem 2 is a straightforward implication.

4.1 Closures of exponential families

In a recent paper [CMb] the different closures and extensions of exponential families were studied. As a special case of this considerations, namely the case of finite configuration spaces, a classical result of [BN, pp. 154-155] appears. It is shown that $\text{cl } \mathcal{E}$ can be written as a union of certain exponential families. To explain this we have to introduce some further notation. Let

$$P_{\theta, f}(x) := \frac{1}{Z} \exp(\langle \theta, f(x) \rangle)$$

be a Gibbs measure, where $Z = \sum_{x \in \mathcal{X}} \exp(\langle \theta, f(x) \rangle)$ is a normalization, $f : \mathcal{X} \rightarrow \mathbb{R}^d$ is a statistic, and $\theta \in \mathbb{R}^d$ is a vector of coefficients. As θ ranges over \mathbb{R}^d the P_{θ} form an exponential family which we denote by

$$\mathcal{E}_f := \{P_{\theta, f} : \theta \in \mathbb{R}^d\}.$$

Since \mathcal{X} is finite, the image of f is a finite subset of \mathbb{R}^d , and its convex hull \mathcal{F} is a polytope. For every non-empty face F of \mathcal{F} define

$$\mathcal{Y}^F := \{x \in \mathcal{X} : f(x) \in F\} = f^{-1}(F). \quad (4)$$

Finally, for every \mathcal{Y}^F consider the restriction

$$\mathcal{E}_{\mathcal{Y}^F, f} := \begin{cases} \frac{1}{Z^F} \exp(\langle \theta, f \rangle(x)), & \text{if } x \in \mathcal{Y}^F \\ 0, & \text{otherwise} \end{cases}, \quad Z^F := \sum_{x' \in \mathcal{Y}^F} \exp(\langle \theta, f \rangle(x'))$$

The following statement is a special case of a more general result of [CMb]:

Theorem 4.

$$\text{cl}(\mathcal{E}_f) = \bigcup_F \mathcal{E}_{\mathcal{Y}^F, f}$$

Remark. The formulation given here is a special case of the considerations in [CMa, CMb] where more general sets \mathcal{X} and corresponding reference measures are studied in detail within the context of various notions of closure. In our case of finite \mathcal{X} all notions coincide with the natural topological closure.

4.2 Orthogonal decomposition of the interaction space

In this section, we decompose the interaction space $\mathcal{I}_{\mathcal{A}}$ into orthogonal components by means of the construction of a basis. We then have an explicit description of the statistic that generates $\mathcal{E}_{\mathcal{A}}$ and can apply Theorem 4 to examine the closure $\text{cl } \mathcal{E}_{\mathcal{A}}$. In what follows, all concepts of projections and orthogonality are meant with respect to the scalar product

$$\langle f, g \rangle := \frac{1}{2^N} \sum_{x \in \mathcal{X}_V} f(x)g(x).$$

In previous work [DS, Lau, AK], the spaces of *pure interactions among elements of* $A \subseteq V$ were defined as follows:

$$\tilde{\mathcal{I}}_A := \mathcal{I}_A \cap \left(\bigcap_{B \subsetneq A} \mathcal{I}_B^\perp \right). \quad (5)$$

This implies an orthogonal decomposition

$$\mathcal{I}_A = \bigoplus_{B \subseteq A} \tilde{\mathcal{I}}_B, \quad (6)$$

where $\dim \tilde{\mathcal{I}}_A = 1$ (see [AK]). In particular, $\mathbb{R}^{\mathcal{X}_V} = \bigoplus_{A \subseteq V} \tilde{\mathcal{I}}_A$.

4.3 A basis of the pure interaction spaces

In Proposition 6, we prove that the functions e_A , $A \subseteq V$, which are defined according to (1) form an orthonormal basis of the interaction space $\mathcal{I}_{\mathcal{A}}$. To this end we need the following lemma:

Lemma 5. *Let $\emptyset \neq A \subseteq V$, then*

$$\sum_{x \in \mathcal{X}_V} (-1)^{E(A,x)} = 0.$$

Proof. Let i be an element of A , and define

$$\mathcal{X}_- := \{x \in \mathcal{X}_V : X_i(x) = 1\}, \quad \mathcal{X}_+ := \{x \in \mathcal{X}_V : X_i(x) = 0\}$$

Obviously, $E(A,x) = E(A \setminus \{i\}, x) + 1$ if $x \in \mathcal{X}_-$, and $E(A,x) = E(A \setminus \{i\}, x)$ if $x \in \mathcal{X}_+$. This implies

$$\sum_{x \in \mathcal{X}_V} (-1)^{E(A,x)} = \sum_{x \in \mathcal{X}_+} (-1)^{E(A \setminus \{i\}, x)} - \sum_{x \in \mathcal{X}_-} (-1)^{E(A \setminus \{i\}, x)} = 0$$

□

Proposition 6. *The vectors $(e_A)_{A \in \mathcal{A}}$ form an orthonormal basis of $\mathcal{I}_{\mathcal{A}}$.*

Proof. The e_A are normalized with respect to our scalar product. Since \mathcal{A} is assumed to be complete, we have the decomposition

$$\mathcal{I}_{\mathcal{A}} = \bigoplus_{A \in \mathcal{A}} \tilde{\mathcal{I}}_A,$$

where $\dim \tilde{\mathcal{I}}_A = 1$, and it is sufficient to show that $e_A \in \tilde{\mathcal{I}}_A$. The case of e_\emptyset is clear since $e_\emptyset = \sum_{x \in \mathcal{X}_V} e_x$ and $\tilde{\mathcal{I}}_\emptyset = \mathcal{I}_\emptyset$ is the space of constants. Now let A be non-empty and observe that, denoting by Π_B the projection onto \mathcal{I}_B , the definition (5) of the pure interaction spaces can be reformulated as

$$f \in \tilde{\mathcal{I}}_A \iff f \in \mathcal{I}_A \text{ and } \Pi_B f = 0 \text{ for all } B \subsetneq A. \quad (7)$$

The projection onto the space \mathcal{I}_A is given by

$$\Pi_A(f)(x_A, x_{V \setminus A}) = \frac{1}{2^{|V \setminus A|}} \sum_{x'_{V \setminus A} \in \mathcal{X}_{V \setminus A}} f(x_A, x'_{V \setminus A}).$$

We now check property (7):

$$\Pi_A(e_A)(x_A, x_{V \setminus A}) = \frac{1}{2^{|V \setminus A|}} \sum_{x'_{V \setminus A} \in \mathcal{X}_{V \setminus A}} e_A(x_A, x'_{V \setminus A}) = e_A.$$

This follows from the fact that changing x outside A does not alter the values in (1). On the other hand, for a given subset $B \subsetneq A$ we have

$$\begin{aligned} \Pi_B(e_A)(x_B, x_{V \setminus B}) &= \frac{1}{2^{|V \setminus B|}} \sum_{x'_{V \setminus B} \in \mathcal{X}_{V \setminus B}} e_A(x_B, x'_{V \setminus B}) \\ &= \frac{1}{2^{|V \setminus B|}} \sum_{x'_{V \setminus B} \in \mathcal{X}_{V \setminus B}} (-1)^{E(A, (x_B, x'_{V \setminus B}))} \\ &= \frac{1}{2^{|V \setminus B|}} \sum_{x'_{V \setminus B} \in \mathcal{X}_{V \setminus B}} (-1)^{(E(B, (x_B, x_{V \setminus B})) + E(A \setminus B, (x_B, x'_{V \setminus B})))} \\ &= 0 \end{aligned}$$

This equation is true since $(-1)^{E(B, (x_B, x'_{V \setminus B}))}$ does not depend on $x'_{V \setminus B}$, and, since $A \setminus B \neq \emptyset$, Lemma 5 implies

$$\sum_{x' \in \mathcal{X}_{V \setminus B}} (-1)^{E(A \setminus B, x')} = 0.$$

□

Remark (Orthonormal Basis). Since the e_A form an orthonormal basis, one can invert the transformation to find

$$e_x = \frac{1}{2^N} \sum_{A \in 2^V} (-1)^{E(A, x)} e_A,$$

and obviously none of the coefficients is zero.

Combining the results of the previous sections we can now proceed with proving Theorem 2.

4.4 Proof

Proof of Theorem 2. From the above discussion it is clear that the exponential family under consideration can be written as

$$\mathcal{E}_{\mathcal{A}} = \left\{ \frac{1}{Z} \exp \left\{ \sum_{i=1}^s \theta^{A_i} e_{A_i}(x) \right\} : \theta = (\theta^{A_i})_{i=1, \dots, s} \in \mathbb{R}^s \right\}$$

Thus, the exponential family has the form of Theorem 4

$$\mathcal{E}_{\mathcal{A}} = \bigcup_{F \in \mathcal{F}_{\mathcal{A}}} \mathcal{E}_{\mathcal{Y}^F, e_{\mathcal{A}}}$$

with the definition (4) of \mathcal{Y}^F now becoming

$$\mathcal{Y}^F = e_{\mathcal{A}}^{-1}(F).$$

□

5 Conclusions

Applying general results on closures of exponential families from [BN, CMb] we studied the closure of hierarchical models including graphical models. Using a natural orthonormal basis of the corresponding interaction space allows for an explicit description of this closure. We hope that this description in terms of linear algebra will lead to a constructive method for specifying closures of hierarchical models.

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