On Characterizations of Markov Random Fields and Subfields

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Abstract

Let $X_i, i \in V$ form a Markov random field (MRF) represented by an undirected graph $G = (V, E)$, and $V'$ be a subset of $V$. We determine the smallest graph that can always represent the subfield $X_i, i \in V'$ as an MRF. Based on this result, we obtain a necessary and sufficient condition for a subfield of a Markov tree to be also a Markov tree. When $G$ is a path so that $X_i, i \in V$ form a Markov chain, it is known that the I-Measure is always nonnegative [10]. We prove that Markov chain is essentially the only MRF that possesses this property. Our work is built on the set-theoretic characterization of an MRF in [13]. Unlike most works in the literature, we do not make the standard assumption that the underlying probability distribution is factorizable with respect to the graph representing the MRF, which is possible by the Hammersley-Clifford theorem provided that the underlying distribution is strictly positive. As such, our results apply even when such a factorization does not exist.

Key Words: I-Measure, conditional independence, Markov random field, subfield, Markov tree.

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1 Introduction

A Markov random field (MRF) is often regarded as a generalization of a one-dimensional discrete-time Markov chain in the sense that the time index for the latter is replaced by a space index for the former. Historically, the study of MRF stems from statistical physics. The classical Ising model, which is defined on a rectangular lattice, was used to explain certain empirically observed facts about ferromagnetic materials. In statistics, the dependencies between variables in a contingency table may also be modeled as an MRF [7]. In image processing and computer vision, the dependencies between pixels or image features are also commonly modeled by MRFs [18]. MRFs have also been used in wireless and ad hoc networking [14] [17] [16]. In recent years, MRFs have been used as a model for studying social networks [19] [20] and big data [21].

The foundation of the theory of MRFs may be found in [5] or [3] (also see [6] and [11]). It was described in [5] that the theory can be generalized to the context of an arbitrary graph. In this paper, we discuss such MRFs whose random variables are discrete. Before we present their formulation, we first introduce some notations that are used throughout the paper and state the definitions of a few basic notions regarding independence of random variables.

In this paper, all random variables are discrete. Let $X$ be a random variable taking values in an alphabet $X$. The probability distribution for $X$ is denoted as \{$p_X(x), x \in X$\}, with $p_X(x) = \Pr\{X = x\}$. When there is no ambiguity, $p_X$ is abbreviated as $p$. The support of $X$, denoted by $S_X$, is the set of all $x \in X$ such that $p(x) > 0$. If $S_X = X$, we say that $p$ is strictly positive, denoted by $p > 0$. Otherwise, $p$ contains zero probability masses, and we say that $p$ is not strictly positive. Note that probability distributions with zero probability masses are in general very delicate, and they need to be handled very carefully (see Example 1 below). All the above notations naturally extend to two or more random variables.

Throughout this paper, for random variables $X$, $Y$, and $Z$, we write $X \indep Y$ if $X$ and $Y$ are independent, and write $X \indep Z \mid Y$ if $X$ is independent of $Z$ conditioning on $Y$, so on and so forth. The following proposition is a very useful characterization for conditional independence. A careful proof of this proposition can be found in [15, p. 8] (Proposition 2.5).
Proposition 1. For random variables $X, Y,$ and $Z$, $X \independent Z \mid Y$ if and only if

$$p(x, y, z) = a(x, y)b(y, z)$$  \hspace{1cm} (1)

for all $x, y,$ and $z$ such that $p(y) > 0$, where $a$ is some function of $x$ and $y$ and $b$ is some function of $y$ and $z$.

The example below illustrates the subtlety of conditional independence when the probability distribution contains zero probability masses.

Example 1. Let $p$ denote the joint distribution of three random variables $X_1, X_2,$ and $X_3$. In this example, we show that

$$X_1 \independent X_2 \mid X_3 \quad \text{and} \quad X_1 \independent X_3 \mid X_2 \quad \Rightarrow \quad X_1 \independent (X_2, X_3)$$  \hspace{1cm} (2)

holds if $p > 0$, but does not hold in general.

Assume that $p > 0$. Then for all $x_1, x_2,$ and $x_3$, by $X_1 \independent X_2 \mid X_3$, we have

$$p(x_1, x_2, x_3) = \frac{p(x_1, x_3)p(x_2, x_3)}{p(x_3)},$$  \hspace{1cm} (3)

and by $X_1 \independent X_3 \mid X_2$, we have

$$p(x_1, x_2, x_3) = \frac{p(x_1, x_2)p(x_2, x_3)}{p(x_2)}.$$  \hspace{1cm} (4)

Equating [3] and [4], we have

$$p(x_1, x_3) = \frac{p(x_1, x_2)p(x_3)}{p(x_2)}.$$  

Then

$$p(x_1) = \sum_{x_3} \frac{p(x_1, x_2)p(x_3)}{p(x_2)} = \frac{p(x_1, x_2)}{p(x_2)},$$

or

$$p(x_1, x_2) = p(x_1)p(x_2).$$
Substituting this into (4), we have

\[ p(x_1, x_2, x_3) = p(x_1) p(x_2, x_3), \]

i.e., \( X_1 \perp (X_2, X_3) \).

However, (2) does not hold in general, because if \( X_1 = X_2 = X_3 \), we see that \( X_1 \perp X_2 \mid X_3 \) and \( X_1 \perp X_3 \mid X_2 \) but \( X_1 \not\perp (X_2, X_3) \). Note that \( p \) is not strictly positive if \( X_1 = X_2 = X_3 \).

Following the above discussion, we now present the formulation of an MRF defined on an arbitrary graph. Let \( G = (V, E) \) be an undirected graph, where \( V = \{1, 2, \ldots, n\} \) is the set of vertices and \( E \subset V \times V \) is the set of edges. We assume that there is no edge in \( G \) which joins a vertex to itself.

For any (possibly empty) subset \( U \) of \( V \), denote by \( G \setminus U \) the graph obtained from \( G \) by removing all the vertices in \( U \) and all the edges joining a vertex in \( U \). Let \( s(U) \) be the number of components in \( G \setminus U \). Denote the sets of vertices of these components by \( V_1(U), V_2(U), \ldots, V_{s(U)}(U) \). If \( s(U) > 1 \), we say that \( U \) is a cutset in \( G \). Throughout this paper, whenever we remove a subset of vertices \( U \) from \( G \), we always assume that we also remove all the edges joining a vertex in \( U \).

Consider a collection of random variables \( X_i, i \in V \) whose joint distribution is specified by a probability measure \( p \) on \( X_1 \times X_2 \times \cdots \times X_n \), where random variable \( X_i \) is associated with vertex \( i \) in graph \( G \). We now define a few Markov properties for random variables \( X_1, \ldots, X_n \) pertaining to a graph \( G = (V, E) \):

**Definition 1** (Pairwise Markov Property). For all distinct \( i, j \in V \) such that \( \{i, j\} \notin E \), \( X_i \) and \( X_j \) are independent conditioning on \( X_V \setminus \{i, j\} \).

**Definition 2** (Local Markov Property). For all \( i \in V \), \( X_i \) and \( X_{V \setminus N(i)} \) are independent conditioning on \( X_{N(i)} \), where \( N(i) = \{j \in V : \{i, j\} \in E\} \) is the set of neighbors of vertex \( i \) and \( \bar{N}(i) = N(i) \cup \{i\} \).

**Definition 3** (Global Markov Property I). Let \( \{U, V_1, V_2\} \) be a partition of \( V \) such that the sets of vertices \( V_1 \) and \( V_2 \) are disconnected in \( G \setminus U \). Then the sets of random variables \( X_{V_1} \) and \( X_{V_2} \) are independent conditioning on \( X_U \).

**Definition 4** (Global Markov Property II). For all cutsets \( U \) in \( G \), the sets of random variables \( X_{V_1(U)}, \ldots, X_{V_{s(U)}(U)} \) are mutually independent conditioning on \( X_U \).
When $U = \emptyset$, Global Markov Property II states that if the graph $G$ has more than one component, i.e., $s(\emptyset) > 1$, then the sets of random variables $X_{V_1}(\emptyset), \cdots, X_{V_2}(\emptyset), \cdots, X_{V_{s(\emptyset)}}(\emptyset)$ are mutually independent. Here we regard unconditional mutual independence as a special case of conditional mutual independence. It is not difficult to show that Global Markov Property I and Global Markov Property II are equivalent [13], and so we will refer to both of them as the *Global Markov Property*.

Denote the Pairwise Markov Property, the Local Markov Property, and the Global Markov Property by (P), (L), and (G), respectively. It can readily be seen from their definitions that $(G) \Rightarrow (L) \Rightarrow (P)$.

**Definition 5** (Markov Random Field). *The probability measure $p$, or equivalently, the random variables $X_i, i \in V$, are said to form an MRF represented by a graph $G = (V,E)$ if and only if the Global Markov Property is satisfied by $X_i, i \in V$.*

If $X_i, i \in V$ form an MRF represented by a graph $G$, we also say that $X_i, i \in V$ form a Markov graph $G$, $X_i, i \in V$ are represented by $G$, or $G$ is a (graph) representation for $X_i, i \in V$. When $G$ is a path, we say that $X_i, i \in V$ form a Markov chain. When $G$ is a tree, we say that $X_i, i \in V$ form a Markov tree. When $G$ is a cycle graph, we say that $X_i, i \in V$ form a Markov ring.

In general, $X_i, i \in V$ can be represented by more than one graph. In particular, $X_i, i \in V$ are always represented by $K_n$, the complete graph with $n$ vertices. The graph $K_n$ specifies a degenerate MRF, because for every $U \subseteq V$, $U$ is not a cutset in $K_n$. In other words, no Markov constraints are imposed on $X_i, i \in V$ by $K_n$.

Suppose the random variables $X_i, i \in V$ are represented by both $G = (V,E)$ and $G' = (V,E')$, where $E' \subseteq E$, i.e., $G'$ is a proper subgraph of $G$. Then $G'$ imposes a larger set of Markov constraints on $X_i, i \in V$ than $G$, because a cutset in $G$ is also a cutset in $G'$ (but not vice versa). Thus we are naturally interested in the “smallest” graph (to be discussed in Section 2.4) that represents $X_i, i \in V$.

**Definition 6** (Subfield). *A subset of the random variables forming an MRF is called a subfield of the MRF.*

1. A path is a graph whose vertices can be linearly ordered so that every pair of consecutive vertices forms an edge.
2. The term “Markov tree” is also used in the number theory literature in the context of the Markov number, but it is not to be confused with the Markov tree in this paper.
3. A cycle graph is a graph that consists of a single cycle.
Definition 7. A \( n \)-tuple \( \mathbf{x} = (x_1, x_2, \ldots, x_n) \in X_1 \times X_2 \times \cdots \times X_n \) is called a configuration. A probability measure \( p \) on \( X_1 \times X_2 \times \cdots \times X_n \) is strictly positive, denoted by \( p > 0 \), if \( p(\mathbf{x}) > 0 \) for all configurations \( \mathbf{x} \).

If \( p > 0 \), it can be shown that \( (G) = (L) = (P) \) (see for example [11]). In general, however, a probability measure \( P \) may contain zero probability masses, i.e., \( p(\mathbf{x}) = 0 \) for some configuration \( \mathbf{x} \). For example, if some random variables in \( X_1, X_2, \ldots, X_n \) are functions of other random variables, then \( p \) is not strictly positive.

Definition 8 (Factorization). A probability measure \( p \) on \( X_1 \times X_2 \times \cdots \times X_n \) is said to be factorizable with respect to a graph \( G \) if for all configurations \( \mathbf{x} \),

\[
p(\mathbf{x}) = \prod_{C \in \text{cl}(G)} \psi_C(\mathbf{x}_C),
\]

where \( \text{cl}(G) \) is the set of all cliques of \( G \), and \( \psi_C(\mathbf{x}_C) \) is a local function that depends only on \( \mathbf{x}_C = (x_i : i \in C) \). Note that the definition is unchanged if the product in (5) is instead over all the maximal cliques of \( G \).

The factorization form in Definition 8 stems from the Gibbs measure [6], which has an exponential form so that it is always strictly positive. Note that a local function \( \psi_C(\mathbf{x}_C) \) in (5) may vanish for certain \( \mathbf{x}_C \), and so \( p \) is not necessarily strictly positive. Therefore, the factorization form in Definition 8 is somewhat more general than the Gibbs measure.

It is straightforward to prove via an application of Proposition 1 that if \( p \) is factorizable with respect to \( G \), then \( p \) satisfies the Global Markov Property. However, the converse is true only with the additional assumption that \( p > 0 \).

Theorem 1 (Hammersley-Clifford [2]). Let \( p \) be a probability measure on \( X_1 \times X_2 \times \cdots \times X_n \) that can be represented by a graph \( G \). If \( p > 0 \), then \( p \) can be factorized with respect to \( G \).

Though unnatural, the assumption \( p > 0 \) in the above theorem cannot be relaxed. It was shown in [4] by a counterexample that involves only four random variables that the assumption \( p > 0 \) is necessary.
When a probability measure $p$ is represented by a graph $G$, if $p > 0$, the Hammersley-Clifford theorem establishes a factorization form for $p$. Based on this form, many properties pertaining to the Markov random field can be established. However, if $p$ is not strictly positive, due to lack of a general form for $p$, very little is known for such MRFs.

In information theory, conditional independence of random variables is characterized by the following fundamental property of mutual information.

**Proposition 2.** Random variables $X$ and $Z$ are independent conditioning on $Y$ if and only if $I(X; Z|Y) = 0$.

Note that in the above, each of $X$, $Y$, and $Z$, instead of being a single random variable, may as well be a finite collection of random variables, and the underlying probability measure does not have to be strictly positive. Unlike Proposition 1, the characterization in the above proposition is not in terms of the underlying probability measure (although it does depend on the underlying probability measure).

In this paper, we study the structure of MRFs by means of an information-theoretic approach. Specifically, structural properties of MRFs are obtained through the investigation of the set-theoretic structure of Shannon’s information measures under the constraints imposed by the MRF. With this approach, we do not have to manipulate the underlying probability measure directly. As such, we can establish our results without making the assumption that the underlying probability measure takes any particular form.

An identity involving only Shannon’s information measures (i.e., entropy, mutual information, and their conditional versions) is referred to as an information identity. The set-theoretic structure of Shannon’s information measures was first studied in [1], where it was proved that for every information identity, there is a corresponding set identity. This was further developed into the theory of $I$-Measure in [9]. Under this framework, every Shannon’s information measure can formally be regarded as the value of a unique signed measure called the $I$-Measure, denoted by $\mu^*$, on a set corresponding to that Shannon’s information measure. This establishes a complete set-theoretic interpretation of Shannon’s information measures.

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See [15, Ch. 2] for a careful treatment.
Subsequent to \[9\], the structure of the \(I\)-Measure for a Markov chain and more generally an MRF was investigated in \[10\] and \[13\], respectively. In particular, it was proved in \[10\] that the \(I\)-Measure for a Markov chain is always nonnegative. The current work, consisting of the following two main results, is built on \[1, 9, 10, 13\]:

1. Let \(X_i, i \in V\) be any set of random variables that form an MRF represented by a graph \(G\), and let \(X_i, i \in V'\), where \(V' \subset V\), be any subfield of the MRF. We determine the smallest graph \(G'(V')\) that can always represent \(X_i, i \in V'\).

2. The \(I\)-Measure of an MRF is always nonnegative if and only if the MRF is represented by either a path or a forest of paths.\(^5\)

The rest of the paper is organized as follows. Section 2 contains an overview of the concepts and tools to be used in this paper. In Section 3, we define the graph \(G'(V')\) and establish the first main result, namely that \(G'(V')\) is the smallest graph that can always represent the subfield \(X_i, i \in V'\). Applying this result to Markov tree, we obtain in Section 4 a necessary and sufficient condition for a subfield of a Markov tree to form a Markov subtree. In Section 5, we establish the second main result, namely that the Markov chain is essentially the only MRF for which the \(I\)-Measure is always nonnegative. The paper is concluded in Section 6.

2 Preliminaries

In this section, we introduce the notations and present the preliminaries for the rest of the paper. For a detailed discussion, we refer the readers to \[15\] Chapters 3 and 12.

2.1 \(I\)-Measure

We first give an overview of the basics of the \(I\)-Measure. Let \(X_i, i \in V = \{1, 2, \cdots, n\}\) be jointly distributed discrete random variables, and \(\tilde{X}\) be a set variable corresponding to a random variable \(X\). We note that the \(I\)-Measure does not have to be defined in the context of an MRF, but here we use

\(^5\)A forest of paths is a graph with at least two components such that each component is a path.
V (the vertex set of a graph) as the index set of the random variables for the sake of convenience. Here we assume that \( H(X_i) < \infty \) for \( 1 \leq i \leq n \), so that the I-Measure \([9]\) for \( p \) is well-defined.

Define the universal set \( \Omega_V \) to be \( \bigcup_{i \in V} \tilde{X}_i \) and let \( F_V \) be the \( \sigma \)-field generated by \{\( \tilde{X}_i, i \in V \}\). The atoms of \( F_V \) have the form \( \bigcap_{i \in V} Y_i \), where \( Y_i \) is either \( \tilde{X}_i \) or \( \tilde{X}^c_i \). Let \( A_V \subset F_V \) be the set of all the atoms of \( F_V \) except for \( \bigcap_{i \in V} \tilde{X}^c_i \), which is equal to the empty set because

\[
\bigcap_{i \in V} \tilde{X}^c_i = \left( \bigcup_{i \in V} \tilde{X}_i \right)^c = (\Omega_V)^c = \emptyset.
\]

Note that \( |A_V| = 2^n - 1 \). In the rest of the paper, when we refer to an atom of \( F_V \), we always mean an atom in \( A_V \) unless otherwise specified.

To simplify notation, we will use \( X_U \) to denote \( (X_i, i \in U) \) and \( \tilde{X}_U \) to denote \( \bigcup_{i \in U} \tilde{X}_i \) for any \( U \subset V \). We will not distinguish between \( i \) and the singleton containing \( i \). It was shown in \([9]\) that there exists a unique \textit{signed} measure \( \mu^* \) on \( F_V \) which is consistent with all Shannon’s information measures via the following substitution of symbols:

\[
\begin{align*}
H/I & \to \mu^* \\
, & \to \cup \\
; & \to \cap \\
| & \to -
\end{align*}
\]

where “−” denotes the set difference. For example,

\[
\mu^*((\tilde{X}_1 \cup \tilde{X}_2) \cap \tilde{X}_3 - \tilde{X}_4) = I(X_1, X_2; X_3|X_4).
\]

Note that \( \mu^* \) in general is not nonnegative. However, if \( X_i, i \in V \) form a Markov chain, then \( \mu^* \) is always nonnegative \([10]\).

### 2.2 Full Conditional Mutual Independency

**Definition 9.** Let \( \{T, Q_1, Q_2, \ldots, Q_k\} \) be a partition of \( V' \), where \( k \geq 2 \) and \( V' \subset V \). The tuple \( K = (T; Q_i, 1 \leq i \leq k) \) defines the following conditional mutual independency (CMI) on \( X_i, i \in V \):

\( X_{Q_1}, X_{Q_2}, \ldots, X_{Q_k} \) are mutually independent conditioning on \( X_T \).
If $V' = V$, $K$ is called a full conditional mutual independency (FCMI).

**Example 2.** For $n = 6$, $K = (\{4\}; \{1, 3\}, \{2, 5\}, \{6\})$ defines the FCMI

$$(X_1, X_3), (X_2, X_5), X_6$$

are mutually independent conditioning on $X_4$.

However, for $n = 7$, $K$ is not an FCMI because $\{\{4\}, \{1, 3\}, \{2, 5\}, \{6\}\}$ is not a partition of $\{1, 2, \ldots, 7\}$.

**Definition 10.** Let $K = (T; Q_i, 1 \leq i \leq k)$ be an FCMI on $X_i, i \in V$. The image of $K$, denoted by $\text{Im}(K)$, is the set of atoms of $F_V$ of the form

$$\left(\bigcap_{i=1}^{k} \bigcap_{j \in W_i} \tilde{X}_j \right) - \tilde{X}_{T \cup \cup_{i=1}^{k} (Q_i - W_i)}$$

where $W_i \subset Q_i$, $1 \leq i \leq k$, and there exist at least two $i$ such that $W_i \neq \emptyset$.

The following proposition gives a more explicit expression for $\text{Im}(K)$. The proof is elementary and so is omitted.

**Proposition 3.** Let $K = (T; Q_i, 1 \leq i \leq k)$ be an FCMI on $X_i, i \in V$. Then

$$\text{Im}(K) = \left\{ A \in \mathcal{A}_n : A \subset \bigcup_{1 \leq i < j \leq k} (\tilde{X}_{Q_i} \cap \tilde{X}_{Q_j} - \tilde{X}_T) \right\}.$$

In the rest of the paper, we denote the atom $\tilde{X}_1 \cap \tilde{X}_2 \cap \tilde{X}_3$ of $F_{\{1, 2, 3\}}$ by $123$, etc.

**Example 3.** Let $n = 3$ and consider the FCMI $K = (\emptyset; \{1\}, \{2\}, \{3\})$. Then $\text{Im}(K)$ is the set containing all the atoms in $(\tilde{X}_1 \cap \tilde{X}_2) \cup (\tilde{X}_1 \cap \tilde{X}_3) \cup (\tilde{X}_2 \cap \tilde{X}_3)$, as given by Proposition 3. This is illustrated in Fig. 1. Equivalently, the atoms in $\text{Im}(K)$ are $12\bar{3}$, $1\bar{2}3$, $\bar{1}23$, and $123$, as given by Definition 10.

For example, for the atom $12\bar{3}$, we have $W_1 = \{1\}$, $W_2 = \{2\}$, and $W_3 = \emptyset$, so there are at least two $i$ such that $W_i \neq \emptyset$.

The following theorem from [15] will be useful for proving some of the results in this work.

**Theorem 2.** Let $K$ be an FCMI on $X_i, i \in V$. Then $K$ holds if and only if $\mu^*(A) = 0$ for all $A \in \text{Im}(K)$. 

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We remark that if \( \{T, Q_1, Q_2, \cdots, Q_k\} \) is a partition of \( V' \) where \( V' \subseteq V \), then \( K = (T; Q_1, Q_2, \cdots, Q_k) \) holds if and only if \( \mu^* \) vanishes on all the sets prescribed in (6), although these sets are no longer atoms of \( \mathcal{F}_V \).

**Example 4.** Following Example 3, the random variables \( X_1, X_2, \) and \( X_3 \) are mutually independent if and only if \( \mu^* \) vanishes on the atoms \( 1 \bar{2} \bar{3}, \bar{1} 2 \bar{3}, \bar{1} \bar{2} 3, \) and \( \bar{1} 2 3 \).

Let \( A = \bigcap_{i \in V} \tilde{Y}_i \) be a nonempty atom of \( \mathcal{F}_V \). Define the set
\[
U_A = \{ i \in V : \tilde{Y}_i = \tilde{X}_i \}.
\]
(7)

Note that \( A \) is uniquely specified by \( U_A \) because
\[
A = \left( \bigcap_{i \in V-U_A} \tilde{X}_i \right) \cap \left( \bigcap_{i \in U_A} \tilde{X}_i \right) = \left( \bigcap_{i \in V-U_A} \tilde{X}_i \right) \cap \left( \bigcup_{i \in U_A} \tilde{X}_i \right) = \left( \bigcap_{i \in V-U_A} \tilde{X}_i \right) - \tilde{X}_{U_A}.
\]

Define \( w(A) = n - |U_A| \) as the weight of the atom \( A \), the number of \( \bar{X}_i \) in \( A \) which are not complemented. We now show that an FCMI \( K = (T; Q_i, 1 \leq i \leq k) \) is uniquely specified by \( \text{Im}(K) \). First, by letting \( W_i = Q_i \) for \( 1 \leq i \leq k \) in (6), we see that the atom
\[
\left( \bigcap_{j \in \bigcup_{i=1}^k Q_i} \tilde{X}_j \right) - \tilde{X}_T
\]
is in \( \text{Im}(K) \), and it is the unique atom in \( \text{Im}(K) \) with the largest weight. From this atom, \( T \) can be determined. To determine \( Q_i, 1 \leq i \leq k \), we define a relation \( q \) on \( T^c = V - T \) as follows. For \( l, l' \in T^c, (l, l') \) is in \( q \) if and only if one of the following is satisfied:

i) \( l = l' \);

ii) \( l \neq l' \) and the atom
\[
\tilde{X}_l \cap \tilde{X}_{l'} \cap \left( \bigcap_{j \in V-\{l,l'\}} \tilde{X}_j^c \right)
\]
is not in \( \text{Im}(K) \).

The idea of ii) is that \( (l, l') \) is in \( q \) if and only if \( l, l' \in Q_i \) for some \( 1 \leq i \leq k \), which can be seen as follows. If \( l, l' \in Q_i \) for some \( i \), then the atom in (8) is not in \( \text{Im}(K) \) by Definition 10 because
\{l, l'\} \subset W_i$ and so $W_j = \emptyset$ for all $j \neq i$ (an atom in $Im(K)$ has at least two $i$ such that $W_i \neq \emptyset$). On the other hand, if $l \in Q_i$ and $l' \in Q_{i'}$ where $i \neq i'$, then by letting $W_i = \{l\}$ and $W_{i'} = \{l'\}$, we see that the atom in (8) is in $Im(K)$.

Then $q$ is reflexive by i), and is symmetric because the definition of $q$ is symmetrical in $l$ and $l'$. Moreover, $q$ is transitive from the discussion above because if $l, l' \in Q_i$ for some $1 \leq i \leq k$ and $l', l'' \in Q_{i'}$ for some $1 \leq i' \leq k$, then $i = i'$ and $l, l'' \in Q_i$. In other words, $q$ is an equivalence relation that partitions $T_c$ into $\{Q_i, 1 \leq i \leq k\}$. Therefore, $K$ can be recovered from $Im(K)$, and so it is uniquely specified by $Im(K)$.

Let $\Pi = \{K_l, 1 \leq l \leq m\}$ be a collection of FCMIs on $X_i, i \in V$, and define

$$Im(\Pi) = \bigcup_{l=1}^{k} Im(K_l).$$

Since $\Pi$ holds if and only if $K_l$ holds for all $l$, it follows from Theorem 2 that $\Pi$ holds if and only if $\mu^r(A) = 0$ for all $A \in Im(\Pi)$. However, the following example shows that unlike an FCMI, a collection of FCMIs is in general not uniquely specified by its image.

**Example 5.** Let $n = 3$. Let $\Pi_1 = \{K_1\}$ and $\Pi_2 = \{K_2, K_3\}$, where

\[
\begin{align*}
K_1 &= (\emptyset; \{1\}, \{2\}, \{3\}) \\
K_2 &= (\emptyset; \{1\}, \{2\}, \{3\}) \\
K_3 &= (\{3\}; \{1\}, \{2\}).
\end{align*}
\]

Then $\Pi_1 \neq \Pi_2$ but $Im(\Pi_1) = Im(\Pi_2)$.

### 2.3 Markov Random Field

In the definition of an MRF, each cutset $U$ in $G$ specifies an FCMI on $X_1, X_2, \cdots, X_n$, denoted by $[U]$. Formally,

$$[U] : X_{V(U)}, \cdots, X_{V_{n(U)}}(U) \text{ are mutually independent conditioning on } X_U.$$ 

For a collection of cutsets $U_1, U_2, \cdots, U_k$ in $G$, we introduce the notation

$$[U_1, U_2, \cdots, U_k] = [U_1] \land [U_2] \land \cdots \land [U_k]$$

(9)
where ‘∧’ denotes ‘logical AND.’ Using this notation, $X_1, X_2, \cdots, X_n$ form a Markov graph $G$ if and only if

$$[U \subset V : U \neq V \text{ and } s(U) > 1]$$

holds. In light of (7), the above can be written as

$$[U_A : A \in \mathcal{A}_n \text{ and } s(U_A) > 1].$$

(11)

Denote this collection of FCMIs induced by graph $G$ by $[U_G]$.

**Definition 11.** Let $G = (V, E)$ be a graph. For an atom $A$ of $\mathcal{F}_V$, if $s(U_A) = 1$, i.e., $G\backslash U_A$ is connected, then $A$ is a Type I atom of $G$, otherwise, i.e., $s(U_A) > 1$, $A$ is a Type II atom of $G$. The sets of all Type I and Type II atoms of $G$ are denoted by $\mathcal{T}_I(G)$ and $\mathcal{T}_{II}(G)$, respectively.

**Definition 12.** For a graph $G = (V, E)$, the image of $G$ is defined by

$$\text{Im}(G) = \text{Im}([U_G]).$$

**Theorem 3.** (cf. [15, Theorem 12.25]) $\text{Im}(G) = \mathcal{T}_{II}(G)$.

The above theorem gives a precise characterization of $\text{Im}(G)$. It follows from the discussion in Section 2.2 that $X_1, X_2, \cdots, X_n$ form a Markov graph $G$ if and only if $\mu^*(A) = 0$ for all $A \in \mathcal{T}_{II}(G)$, i.e., $\mu^*$ vanishes on all the Type II atoms of $G$.

**Example 6.** For the cycle graph $G$ in Fig. 2, $\mathcal{T}_{II}(G) = \{1\bar{2}3\bar{4}, \bar{1}2\bar{3}4\}$. Random variables $X_1, X_2, X_3$ and $X_4$ are represented by $G$ if and only if $\mu^*(1\bar{2}3\bar{4}) = \mu^*(\bar{1}2\bar{3}4) = 0$.

A graph $G = (V, E)$ and the collection $[U_G]$ of FCMIs it induces uniquely specify each other, because for distinct $u, v \in V$, $\{u, v\} \in E$ if and only if the FCMI $(V - \{u, v\}; \{u\}, \{v\})$ is not in $[U_G]$. This can be seen as follows. If $\{u, v\} \in E$, then $V - \{u, v\}$ is not a cutset in $G$, and so $(V - \{u, v\}; \{u\}, \{v\}) \notin [U_G]$. On the other hand, if $(V - \{u, v\}; \{u\}, \{v\}) \notin [U_G]$, then $V - \{u, v\}$ is not a cutset in $G$, which implies $\{u, v\} \in E$.

Although a collection of FCMIs is in general not uniquely determined by its image (cf. Example 5), the following proposition asserts that a graph $G$ (and hence $[U_G]$) is uniquely determined by its image $\text{Im}(G)$.
**Proposition 4.** For a graph $G = (V, E)$, $\{u, v\} \in E$ if and only if the atom

$$\bar{X}_u \cap \bar{X}_v - \bar{X}_{V - \{u, v\}}$$

(12)
is not in $\text{Im}(G)$.

**Proof** Denote the atom in (12) by $A$. If $\{u, v\} \not\subset E$, then $G$ induces the FCMI $K = (V - \{u, v\}; \{u\}, \{v\})$. Obviously, $\text{Im}(K) = \{A\}$, and hence $A \in \text{Im}(K) \subset \text{Im}(G)$.

To prove the converse, assume that atom $A$ is in $\text{Im}(G)$, and specifically in some $\text{Im}(\{U_A'\})$ such that $s(U_{A'}) > 1$. It follows from Definition 10 that in order for $A$ to be in $\text{Im}(\{U_A'\})$, it is necessary for $u$ and $v$ to be in different sets in $V_1(U_A'), V_2(U_A'), \ldots, V_{s(U_{A'})}(U_A')$. This implies that $V - \{u, v\}$ is a cutset in $G$, and hence $\{u, v\} \not\subset E$. □

With this proposition, a graph $G$ can be recovered from $\text{Im}(G)$ as follows. Start with the complete graph $K_n$. If there exists an atom in $\text{Im}(G)$ as prescribed by (12) for some distinct $u, v \in V$, then remove edge $\{u, v\}$ from the graph. Repeat this step until no more edges can be removed. Note that this algorithm produces a unique graph, i.e., $G$. As a corollary, the uniqueness of the Markov graph induced by $G$ is proved, i.e., for two graphs $G = (V, E)$ and $G' = (V, E')$ where $E \neq E'$, $[U_G] \neq [U_{G'}]$.

### 2.4 Smallest Graph Representation

As discussed in Section 1, we are interested in the “smallest” graph that can represent a given set of random variables $X_i, i \in V$. To fix ideas, we first give a formal definition of this notion.

**Definition 13.** A graph $G = (V, E)$ is the smallest graph representation for a set of random variables $X_i, i \in V$ if $G$ is a representation for $X_i, i \in V$ and is a subgraph of any representation $G'$ for $X_i, i \in V$.

We know from Section 2.3 that a graph $G = (V, E)$ can represent $X_i, i \in V$ if and only if $\mu^*$ vanishes on all the atoms in $\text{Im}(G)$. Note that if $G$ is a subgraph of $G'$, then a cutset in $G'$ is also a cutset in $G$. It follows that $[U_{G'}]$ is a “subset” of $[U_G]$, and hence $\text{Im}(G') \subset \text{Im}(G)$.

For the given set of random variables $X_i, i \in V$, let $\mathcal{A}_H$ be the set of nonempty atoms of $\mathcal{F}_V$ on which $\mu^*$ vanishes. Following the last paragraph, if $G$ is the smallest representation for $X_i, i \in V$,
then $\text{Im}(G) \subset \mathcal{A}_I$ and $\text{Im}(G') \subset \text{Im}(G)$ for any representation $G'$ for $X_i, i \in V$. The next theorem gives a characterization of such a graph if it exists.

**Theorem 4.** For a given set of random variables $X_i, i \in V$, let $\mathcal{A}_I$ be the set of nonempty atoms of $\mathcal{F}_V$ on which $\mu^*$ vanishes. Let $\hat{G} = (V, \hat{E})$ be such that $\{u, v\} \in \hat{E}$ if and only if the atom in (12) is not in $\mathcal{A}_I$. Then if the smallest graph representation for $X_i, i \in V$ exists, it is equal to $\hat{G}$.

We first prove the following two lemmas.

**Lemma 1.** Every graph that can represent $X_i, i \in V$ contains $\hat{G}$ as a subgraph.

**Proof** Let $G' = (V, E')$ be any graph that can represent $X_i, i \in V$. Consider any edge $\{u, v\}$ in $\hat{G}$, i.e., $\{u, v\} \in \hat{E}$. By construction, the atom in (12) is not in $\mathcal{A}_I$. Then $\{u, v\} \in E'$, otherwise the FCMI $(V - \{u, v\}; \{u\}, \{v\})$ holds, i.e.,

$$I(X_u; X_v | X_{V - \{u, v\}}) = \mu^*(\tilde{X}_u \cap \tilde{X}_v - \tilde{X}_{V - \{u, v\}}) = 0,$$

which is a contradiction because the atom in (12) is not in $\mathcal{A}_I$. Thus if $G'$ can represent $X_i, i \in V$, then $G'$ contains $\hat{G}$ as a subgraph. □

**Lemma 2.** If $\{u, v\}$ is an edge in every graph that can represent $X_i, i \in V$, then $\{u, v\}$ is an edge in $\hat{G}$.

**Proof** Let $\{u, v\}$ be an edge in every graph that can represent $X_i, i \in V$. If a graph does not contain $\{u, v\}$, then it cannot represent $X_i, i \in V$. In particular, the graph $K_n \setminus \{u, v\}$ obtained by removing $\{u, v\}$ from the complete graph $K_n$ cannot represent $X_i, i \in V$. Since the only FCMI imposed by $K_n \setminus \{u, v\}$ is $[\{u, v\}]$ (i.e., $X_u$ and $X_v$ are independent conditioning on $X_{V - \{u, v\}}$), this means that $X_u$ and $X_v$ are not independent conditioning on $X_{V - \{u, v\}}$, or $\mu^*(\tilde{X}_u \cap \tilde{X}_v - \tilde{X}_{V - \{u, v\}}) > 0$. In other words, the atom $\tilde{X}_u \cap \tilde{X}_v - \tilde{X}_{V - \{u, v\}}$ is not in $\mathcal{A}_I$, which implies that $\{u, v\}$ is an edge in $\hat{G}$. □

**Proof of Theorem 4** Assume the smallest graph representation for $X_i, i \in V$ exists and let it be $\hat{G}$. By Lemma 1, $\hat{G}$ is a subgraph of $\tilde{G}$. On the other hand, since $\tilde{G}$ is a subgraph of every graph that can represent $X_i, i \in V$, Lemma 2 implies that $\tilde{G}$ is a subgraph of $\hat{G}$. Hence, $\tilde{G} = \hat{G}$. □
**Corollary 1.** The smallest graph representation for $X_i, i \in V$ exists if and only if $\hat{G}$ is a representation for $X_i, i \in V$.

**Proof** Assume that the smallest graph representation for $X_i, i \in V$ exists. By Theorem 4, it is equal to $\hat{G}$, and so $\hat{G}$ is a representation for $X_i, i \in V$. Conversely, if $\hat{G}$ is a representation for $X_i, i \in V$, then by Lemma 1, it is the smallest representation for $X_i, i \in V$. □

**Example 7.** Let $n = 3$ and consider $\mu^*$ such that

$$\mathcal{A}_{II} = \{12\bar{3}, 1\bar{2}3\}. \quad (13)$$

Accordingly, the graph $\hat{G}$ defined in Proposition 4 is illustrated in Fig. 3. However,

$$\text{Im}(\hat{G}) = \{12\bar{3}, 1\bar{2}3, 123\} \notin \mathcal{A}_{II},$$

i.e., $\hat{G}$ cannot represent $X_1, X_2,$ and $X_3$. Then by Corollary 1, there does not exist a smallest graph representation of $X_1, X_2,$ and $X_3$.

The above example shows that the smallest graph representation may not exist for a given set of random variables. However, if $\mathcal{A}_{II} = \text{Im}(G)$ for some graph $G$, then $G$ is in fact the smallest graph representation for $X_i, i \in V$. This is proved in the next proposition.

**Proposition 5.** If $\mathcal{A}_{II} = \text{Im}(G)$ for some graph $G$, then $G$ is the smallest graph representation for $X_i, i \in V$.

**Proof** We see that a graph $G$ can be recovered from its image $\text{Im}(G)$ using the algorithm described at the end of Section 2.3, and in fact $G = \hat{G}$. Therefore, $\text{Im}(\hat{G}) = \text{Im}(G) = \mathcal{A}_{II}$, which implies that $\text{Im}(\hat{G}) \subset \mathcal{A}_{II}$. Hence, $\hat{G}$ is a graph representation for $X_i, i \in V$. It then follows from Theorem 4 that $\hat{G}$, i.e., $G$, is the smallest graph representation for $X_i, i \in V$. □

To our knowledge, Corollary 1 is new. A related result can be found in [8], where it was proved that if the underlying probability measure $p$ is strictly positive, then the smallest graph representation for $X_i, i \in V$ always exists and is equal to $\hat{G}$.
Example 8. In Example 7 the constraint (13) is equivalent to $X_1 \perp X_2 | X_3$ and $X_1 \perp X_3 | X_2$, while $[U_G] = [U_0, U_{\{2\}}, U_{\{3\}}]$ consists of the FCMIs

$$X_1 \perp (X_2, X_3), \ X_1 \perp X_3 | X_2, \ X_1 \perp X_2 | X_3.$$ 

We have shown in Example 7 that

$$\begin{align*}
X_1 \perp X_2 | X_3 \quad \Rightarrow \\
X_1 \perp (X_2, X_3),
\end{align*}$$

holds if the underlying probability distribution $p$ is strictly positive, or $p > 0$, but does not hold in general. This means that if $p > 0$, then $\hat{G}$ represents $X_1, X_2,$ and $X_3$, but in general it does not. These conclusions are consistent with the result in [8] and the discussion in Example 7 respectively.

3 Subfield of a Markov Random Field

Let $X_i, i \in V$ form an MRF represented by some graph $G = (V, E)$. Note that such a graph $G$ can always be found, because $K_n$ is always a representation of $X_i, i \in V$. Let $V'$ be a subset of $V$. In this section, we seek the smallest graph that can always represent the subfield $X_i, i \in V'$.

Definition 14. Let $G = (V, E)$ and $G' = (V', E')$ where $V' \subset V$. If $[U_G] \Rightarrow [U_{G'}]$, we write $G \Rightarrow G'$.

Let $X_i, i \in V$ form an MRF represented by a graph $G$. Following the definition above, if $G \Rightarrow G'$, then $X_i, i \in V'$ form an MRF represented by $G'$.

Definition 15. Let $G = (V, E)$, and let $V' \subset V$. Let $G^*(V') = (V', E')$ be such that for distinct $u, v \in V'$, $\{u, v\} \in E'$ if and only if there exists a path between $u$ and $v$ in $G$ on which all the vertices except for $u$ and $v$ are in $V \setminus V'$.

Obviously, $G^*(V) = G$. We will prove in Theorem 9 the main theorem of this section, that $G^*(V')$ is the smallest $G'$ such that $G \Rightarrow G'$.

Example 9. Consider an MRF represented by the graph $G$ in Fig. 4, which indeed is a Markov chain. Let $V' = \{1, 3, 5, 6\}$. Then $G^*(V')$ is illustrated as the overlay graph in grey.
Example 10. Consider an MRF represented by the more elaborate graph $G$ in Fig. 5. Let $V' = \{1, 2, 5, 6, 8, 9\}$. Then $G^*(V')$ is illustrated as the overlay graph in grey.

Consider $G'(V - V') = (V', E'')$, where

$$E'' = \{(v, w) : v, w \in V' \text{ and } \{v, w\} \in E\}.$$  

For distinct $v, w \in V'$, if $\{v, w\} \in E''$, then $\{v, w\} \in E'$ by the definition of $G^*(V')$. In other words, $G^*(V')$ always contains $G'(V - V')$ as a subgraph. However, $G^*(V') \neq G'(V - V')$ in general. In other words, $G^*(V')$ is not necessarily a subgraph of $G$. The following proposition gives the condition for $G^*(V')$ to be exactly equal to $G'(V - V')$.

Proposition 6. Let $G = (V, E)$, and let $V' \subset V$. Let $\rho(V')$ be the set of elements of $V'$ such that some of their neighbors are in $V - V'$, i.e.,

$$\rho(V') = \{v \in V' : \{u, v\} \in E \text{ for some } u \in V - V'\}. \quad (14)$$

Then $G^*(V') = G'(V - V')$ if and only if for distinct $v, w \in \rho(V')$, if $\{v, w\}$ is not an edge in $G'(V - V')$, then there exists no path between $v$ and $w$ in $G$ on which all the vertices other than $v$ and $w$ are in $V - V'$.

Proof. Note that $G^*(V') = G'(V - V')$ is equivalent to $E' = E''$. We already have proved that $E'' \subset E'$ always holds, so we only need to prove that the condition in the proposition for $G^*(V') = G'(V - V')$ is necessary and sufficient for $E' \subset E''$.

For any distinct $v, w \in V'$, consider two cases. If either $v$ or $w$ is not in $\rho(V')$, then $\{v, w\} \in E'$ implies $\{v, w\} \in E''$. If both $v$ and $w$ are in $\rho(V')$, then the condition in the proposition for $G^*(V') = G'(V - V')$ is necessary and sufficient for $\{v, w\} \in E'$ to imply $\{v, w\} \in E''$. The proposition is proved.  

Example 11. Consider the graph $G$ in Fig. 5 and let $V' = \{2, 3, 4\}$. Here $\rho(V') = V'$ because each vertex in $V'$ is connected to some vertex in $V - V'$. Now $\{2, 4\}$ is the only pair of vertices that is not an edge in $G'(V - V')$. Since there exists no path between vertices 2 and 4 on which all the vertices other than 2 and 4 are in $V - V' = \{1, 5\}$, by Proposition 3, $G^*(V') = G'(V - V')$, which is illustrated as the overlay graph in grey.
Corollary 2. Let \( V = \{1, 2, \cdots , n\} \) and \( V' = V \setminus \{n\} \), where \( n \geq 2 \). Let \( X_i, i \in V \) be represented by a graph \( G = (V, E) \) such that \( \{n-1,n\} \in E \) and \( n-1 \) is the only neighbor of \( n \). Then \( X_i, i \in V' \) is represented by \( G \setminus \{n\} \).

**Proof**  This is a special case of Proposition 6 with \( \rho(V') = \{n-1\} \).

As discussed above, \( G^*(V') \) always contains \( G \setminus (V - V') \) as a subgraph. The next theorem gives an alternative characterization of \( G^*(V') \) that describes the relation between \( G^*(V') \) and \( G \setminus (V - V') \) more explicitly. For \( U \subseteq V \), let

\[
\phi(U) = \{v \in V - U : \{v, w\} \in E \text{ for some } w \in U\}
\]

be the set of neighbors of \( U \) in graph \( G \) and

\[
\kappa(U) = \{\{u, v\} : u, v \in U\}
\]

be the clique formed by the vertices in \( U \).

**Theorem 5.** Let \( G = (V, E) \). For \( V' \subset V \), let \( G^*(V') = (V', E') \) and \( G \setminus (V - V') = (V', E'') \). Then

\[
E' = E'' \cup \bigcup_{i=1}^{s(V')} \kappa(\phi(V_i(V'))), \tag{15}
\]

where \( V_1(V'), V_2(V'), \cdots , V_{s(V')}(V') \) are the components of \( G \setminus V' \).

**Proof**  To facilitate our discussion, let \( \tilde{E} \) denote the set on the right hand side of (15). We first prove that \( E' \subset \tilde{E} \). By Definition 15 if \( \{u, v\} \in E' \), then there exists a path between \( u \) and \( v \) in \( G \) on which all the vertices except for \( u \) and \( v \) are in \( V - V' \). Denote this set of vertices in \( V - V' \) by \( S' \). If \( S' = \emptyset \), then we have \( \{u, v\} \in E'' \). Otherwise, since the vertices in \( S' \) are connected in \( G \setminus V' \), \( S' \) is a subset of \( V_i(V') \) for some \( 1 \leq i \leq s(V') \). As such, \( u, v \in \phi(V_i(V')) \) and hence \( \{u, v\} \in \kappa(\phi(V_i(V'))) \). This completes the proof for \( E' \subset \tilde{E} \).

It remains to prove that \( \tilde{E} \subset E' \). Let \( \{u, v\} \in \tilde{E} \). If \( \{u, v\} \in E'' \), then \( \{u, v\} \in E' \) because \( E'' \subset E' \) as discussed. If \( \{u, v\} \in \kappa(\phi(V_i(V'))) \) for some \( 1 \leq i \leq s(V') \), then \( u, v \in \phi(V_i(V')) \), i.e., there

\[6\text{Note that } \phi(U) = \rho(V - U), \text{ where } \rho \text{ is defined in (14).} \]
exists \(u', v' \in V_i(V')\) (\(u'\) and \(v'\) are not necessarily distinct) such that \(\{u, u'\}, \{v, v'\} \in E\). Since \(u'\) and \(v'\) are in the same component of \(G\setminus V'\), namely \(V_i(V')\), they are connected and it follows that there exists a path between \(u\) and \(v\) in \(G\) on which all the vertices except for \(u\) and \(v\) are in \(V - V'\). Therefore, \(\{u, v\} \in E'\) and we conclude that \(\tilde{E} \subset E'\). The theorem is proved. \(\Box\)

**Example 12.** Refer to Example 10 and Fig. 5. Here \(V - V' = \{3, 4, 7\}\). The components of \(G\setminus V'\) are \(\{3, 4\}\) and \(\{7\}\), and \(\phi(\{3, 4\}) = \{1, 2, 5, 6\}\) and \(\phi(\{7\}) = \{2, 5, 8, 9\}\). Then

\[
E' = E'' \cup \kappa(\{1, 2, 5, 6\}) \cup \kappa(\{2, 5, 8, 9\}).
\]

**Theorem 6.** If \(G \Rightarrow G' = (V', E')\), then \(\{u, v\} \in E'\) if there exists a path between \(u\) and \(v\) in \(G\) on which all the vertices except for \(u\) and \(v\) are in \(V - V'\).

**Proof** Consider distinct \(u, v \in V'\) such that there exists a path between \(u\) and \(v\) in \(G\) on which all the vertices except for \(u\) and \(v\) are in \(V - V'\). Denote this set of vertices in \(V - V'\) by \(S'\). Consider

\[
\tilde{X}_u \cap \tilde{X}_v - \tilde{X}_{V' - \{u, v\}} = \bigcup_{S \subseteq V - V'} \left(\tilde{X}_u \cap \tilde{X}_v \cap \left(\bigcap_{t \in S} \tilde{X}_t\right) - \tilde{X}_{V - S' - \{u, v\}}\right).
\]  

(16)

Since \(S' \subset V - V'\), we see that

\[
A' = \tilde{X}_u \cap \tilde{X}_v \cap \left(\bigcap_{t \in S'} \tilde{X}_t\right) - \tilde{X}_{V - S' - \{u, v\}}
\]

is one of the atoms in the union in (16). Note that \(s(U_{A'}) = 1\) because \(u, v\), and the vertices in \(S'\) form a path in \(G\). Thus \(A'\) is a Type I atom for \(G\).

Now construct \(X_i, i \in V\) by

\[
X_i = \begin{cases} 
Z & \text{if } i \in S' \cup \{u, v\} \\
\text{constant} & \text{otherwise},
\end{cases}
\]

where \(Z\) is a random variable such that \(0 < H(Z) < \infty\). Then by the proof of Theorem 3.11 in [13], for all nonempty atom \(A\),

\[
\mu^\star(A) = \begin{cases} 
H(Z) & \text{if } A = A' \\
0 & \text{otherwise}.
\end{cases}
\]
Now for $X_i, i \in V$ so constructed, $\mu^*$ vanishes on all the Type II atoms of $G$ because $A'$, the only atom on which $\mu^*$ does not vanish, is a Type I atom. Then from the discussion following Theorem 3, we see that $X_i, i \in V$ satisfy $[U_G]$. On the other hand, in light of (16), we have

$$
\mu^*(\tilde{X}_u \cap \tilde{X}_v - \tilde{X}_{V'-(u,v)}) = \sum_{S \subseteq V' - V} \mu^*(\tilde{X}_u \cap \tilde{X}_v \cap \left(\bigcap_{t \in S} \tilde{X}_t\right) - \tilde{X}_{V'-(u,v)}) = H(Z) > 0,
$$

i.e., $X_u$ and $X_v$ are not independent conditioning on $X_{V'-(u,v)}$. Hence, for any $G' = (V', E')$, if $G \Rightarrow G'$, then $V' - \{u, v\}$ is not a cutset in $G'$, which implies that $\{u, v\} \in E'$. The theorem is proved.

□

The next theorem is a rephrase of Theorem 6 in light of the definition of $G^*(V')$ (Definition 15).

**Theorem 7.** If $G \Rightarrow G'$, then $G'$ contains $G^*(V')$ as a subgraph.

**Theorem 8.** $G \Rightarrow G^*(V')$.

**Proof** Let $X_i, i \in V$ be any set of random variables which satisfy $[U_G]$. We need to prove that $X_i, i \in V$ satisfy $[U_{G^*(V')}].$ For a fixed cutset $T \subseteq V'$ in $G^*(V')$, let $k$ be the number of components in $G^*(V'\setminus T)$ and denote these components by $Q_1, Q_2, \ldots, Q_k$. To prove that $X_i, i \in V$ satisfy $[U_{G^*(V')}],$ it suffices to prove that for every cutset $T$ in $G^*(V')$, $X_{Q_1}, X_{Q_2}, \ldots, X_{Q_k}$ are mutually independent conditioning on $X_T$.

Note that $\{T, Q_1, Q_2, \ldots, Q_k\}$ is a partition of $(T \cup (\bigcup_i Q_i)) \subseteq V$. Following the discussion immediately after Theorem 2, we see that it suffices to prove that $\mu^*$ vanishes on the sets prescribed in (6). The atoms of $\mathcal{F}_V$ contained in a set prescribed in (6) have the form

$$
\left(\bigcap_{i=1}^k \tilde{X}_j\right) \cap \left(\bigcap_{t \in S} \tilde{X}_t\right) - \tilde{X}_{T \cup (\bigcup_{i=1}^k (Q_i - W_i)) \cup (V' - S)},
$$

where $S \subseteq V - V'$, $W_i \subseteq Q_i, 1 \leq i \leq k$, and there exist at least two $i$ such that $W_i \neq \emptyset$.

We will prove that every atom prescribed in (17) is a Type II atom of $G$. Since $X_i, i \in V$ satisfy
[\{U_G\}, \mu^*] vanishes on these atoms. It then follows that
\[
\mu^*\left(\bigcap_{i=1}^{k} \bigcap_{j \in W_i} \tilde{X}_j \right) - \tilde{X}_{T \cup (\bigcup_{i=1}^{j} (Q_i - W_i))}
\]
\[
= \sum_{S \subseteq V - V'} \mu^*\left(\left(\bigcap_{i=1}^{k} \bigcap_{j \in W_i} \tilde{X}_j \right) \cap \left(\bigcap_{i \in S} \tilde{X}_i \right) - \tilde{X}_{T \cup (\bigcup_{i=1}^{j} (Q_i - W_i)) \cup (V - V' - S)}\right)
\]
\[
= \sum_{S \subseteq V - V'} 0
\]
i.e., \(\mu^*\) vanishes on the sets prescribed in \(G\), as is to be proved.

To prove that the atom in \([17]\) is a Type II atom of \(G\), we need to show that \((T \cup (\bigcup_{i=1}^{k} (Q_i - W_i)) \cup (V - V' - S))\) is a cutset in \(G\). Now in \([17]\), let \(u \in W_{i'} \subset Q_{i'}\) and \(v \in W_{i''} \subset Q_{i''}\) where \(i' \neq i''\) and \(W_{i'}\) and \(W_{i''}\) are nonempty. We claim that \(u\) and \(v\) are disconnected in \(G\). Assume the contrary is true, i.e., there exists a path between \(u\) and \(v\) in \(G\). First of all, both \(u\) and \(v\) are in \(V' - T\) and they belong to different components in \(G^*(V')\). Since \(T \subset V' \subset V\), the vertices between \(u\) and \(v\) on this path are either in \(V' - T\) or \(V - V'\). Then on this path (including \(u\) and \(v\)) there exists two distinct vertices \(w\) and \(z\) in \(V' - T\) such that

1) \(w\) and \(z\) are in different components in \(G^*(V')\);

2) all the vertices between \(w\) and \(z\) on the path are in \(V - V'\)

(it is possible that \(w = u\) and \(z = v\)). Then 2) above implies that \(\{w, z\}\) is an edge in \(G^*(V')\) (cf. Definition \([15]\), which is a contradiction to 1). Therefore, we conclude that \(u\) and \(v\) are disconnected in \(G\). Hence \(G\) has at least two components and \((T \cup (\bigcup_{i=1}^{k} (Q_i - W_i)) \cup (V - V' - S))\) is a cutset in \(G\). This completes the proof of the theorem.

The following corollary gives a structural property of \(G^*(V')\).

**Corollary 3.** If \(T\) is a cutset in \(G^*(V')\), then \(T\) is also a cutset in \(G\).
Proof In the proof of Theorem 8 we have proved that if $T$ is a cutset in $G^*(V')$, then $(T \cup ( \bigcup_{i=1}^{k} (Q_i - W_i))) \cup (V - V' - S)$ is a cutset in $G$. By setting $S = V - V'$ and $W_i = Q_i$ for all $i$, this cutset becomes $T$. This proves the corollary. □

Combining Theorem 7 and Theorem 8 we have proved the main result of this section.

Theorem 9. Let $G = (V, E)$, and let $V' \subset V$. Then $G^*(V')$ is the smallest $G'$ such that $G \Rightarrow G'$.

Remark If we assume that the underlying probability measure $p$ is factorizable with respect to $G$ as in Definition 8, then Theorem 9 can be proved in a straightforward manner by summing over all $x_i \in X_i$ for $i \in V - V'$. However, without this assumption, Theorem 9 is nontrivial.

4 Markov Tree

Suppose $X_i, i \in V$ are represented by a graph $G$. If $G$ is a tree, then $X_i, i \in V$ form a Markov tree. If $G^*(V')$ is also a tree, we say that $X_i, i \in V'$ form a Markov subtree. For the special case when $G$ is a path, it is easy to see that $G^*(V')$ is always a path (see Example 9 for instance). In other words, if $X_i, i \in V$ form a Markov chain, then for any $V' \subset V$, $X_i, i \in V'$ always form a Markov subchain.

However, if $X_i, i \in V$ form a Markov tree, for an arbitrary subset $V'$ of $V$, $X_i, i \in V'$ may or may not form a Markov subtree. The following theorem, which is an application of Theorem 9, gives a necessary and sufficient condition for $X_i, i \in V'$ to form a Markov subtree.

Theorem 10. Let $X_i, i \in V$ form an MRF represented by a tree $G = (V, E)$. For $V' \subset V$, $G^*(V')$ is a tree if and only if there do not exist $u \in V - V'$ and $v_1, v_2, v_3 \in V'$ such that for $i = 1, 2, 3$, all the vertices on the path between $u$ and $v_i$ except for $v_i$ are in $V - V'$.

Proof We first prove the “only if” part. Assume that $G^*(V') = (V', E')$ is a tree and there exist $u \in V - V'$ and $v_1, v_2, v_3 \in V'$ and such that for $i = 1, 2, 3$, all the vertices on the path between $u$ and $v_i$ except for $v_i$ are in $V - V'$. By Definition 15 the edges $(v_1, v_2), (v_2, v_3), \text{and } (v_1, v_3)$ are in $E'$. Hence $v_1, v_2, v_3$ form a cycle in $G^*(V')$, a contradiction to the assumption that $G^*(V')$ is a tree.

We now prove the “if” part. Assume that $G^*(V') = (V', E')$ is not a tree. Then there exists a cycle $w_0, w_1, \cdots, w_{m-1}, w_0$ in $G^*(V')$, where $m \geq 3$ and $w_0, w_1, \cdots, w_{m-1} \in V'$ are distinct. By
Definition [15] for each \( 0 \leq i \leq m - 1 \), there exists a path between \( w_i \) and \( w_{i+1} \) in \( T \) on which all the vertices except for \( w_i \) and \( w_{i+1} \) are in \( V - V' \), where ‘+’ in the subscript denotes modulo \( m \) addition. This path is in fact unique because \( G \) is a tree, so we denote it by \( \text{Path}(w_i, w_{i+1}) \).

If all the vertices on the collection of paths \( \text{Path}(w_i, w_{i+1}) \), \( 0 \leq i \leq m - 1 \), except for the endpoints, are distinct, since \( w_0, w_1, \cdots, w_{m-1} \) are distinct, these paths together form a cycle in \( T \) which is a contradiction because \( T \) is a tree. Otherwise, there exists a vertex \( u \in V - V' \) which is on both \( \text{Path}(w_i, w_{i+1}) \) and \( \text{Path}(w_j, w_{j+1}) \) for some \( 0 \leq i < j \leq m - 1 \). Note that \( |\{w_i, w_{i+1}\} \cup \{w_j, w_{j+1}\}| \geq 3 \), with equality if and only if \( j = i+1 \mod m \). Then there exist \( v_1, v_2, v_3 \in \{w_i, w_{i+1}\} \cup \{w_j, w_{j+1}\} \subset V' \) such that for \( i = 1, 2, 3 \), all the vertices on the path between \( u \) and \( v_i \) except for \( v_i \) are in \( V - V' \). The theorem is proved.

Example 13. Consider a Markov tree represented by the tree \( G \) in Fig. 7 and let \( V' = \{1, 4, 8, 9, 12\} \). The graph \( G^*(V') \), illustrated as the overlay graph in grey, is evidently a tree. We call \( G^*(V') \) a Markov subtree. It can be checked that the condition in Theorem 10 is satisfied.

However, if \( V' \) also includes vertex 7, then \( G^*(V') \) as shown in Fig. 8 is not a tree. By letting \( u = 6, v_1 = 4, v_2 = 7, \) and \( v_3 = 8 \), we see that the condition in Theorem 10 is violated because \( u \) is connected to each of \( v_1, v_2, \) and \( v_3 \) by an edge in \( V - V' \).

5 Markov Chain

A Markov chain is a special case of a Markov tree. However, there are certain properties that are possessed by a Markov chain but not by a Markov tree in general. Consider the graph \( G = (V, E) \), where \( V = \{1, 2, \cdots, n\} \) and the edges in \( E \) are \( \{i, i + 1\} \) for \( i = 1, 2, \cdots, n - 1 \). Evidently, \( G \) is a path. If \( X_i, i \in V \) is represented by \( G \), then \( X_i, i \in V \) form the Markov chain \( X_1 \to X_2 \to \cdots \to X_n \).

The following properties of a (finite-length) Markov chain were proved in [10]:

(C1) An atom \( A \) of \( F_V \) is a Type I atom if and only if

\[
U_A = V - \{l, l + 1, \cdots, u\}
\]

where \( 1 \leq l \leq u \leq n \), i.e., the indices of the set variables in \( A \) that are not complemented are consecutive.

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(C2) The values of $\mu^*$ on all the Type I atoms are nonnegative.

(C3) $\mu^*$ vanishes on all the Type II atoms.

Since $\mu^*$ vanishes on all the Type II atoms and is nonnegative on all the Type I atoms, it is a measure on $\mathcal{F}_V$. Also, the I-Measure $\mu^*$ of a finite-length Markov chain can be represented by a 2-dimensional information diagram as in Fig. [9] in which all the Type II atoms are suppressed.

Subsequently, (C3) was generalized for arbitrary finite undirected graphs [13]. However, the nonnegativity of the I-Measure does not hold even for the simplest Markov tree that is not a Markov chain [13].

**Example 14.** Let $Z_1$ and $Z_2$ be i.i.d. random variables each distributing uniformly on $\{0, 1\}$. Let $X_1 = Z_1$, $X_2 = Z_2$, $X_3 = Z_1 + Z_2 \mod 2$, and $X_4 = (Z_1, Z_2)$. Since $X_1$, $X_2$, and $X_3$ are functions of $X_4$, they are mutually independent conditioning on $X_4$. Thus $X_1, X_2, X_3,$ and $X_4$ form a Markov tree represented by the “star” in Figure [10]. It is not difficult to show that (see [13, Example 3.10])

$$\mu^*(\tilde{X}_1 \cap \tilde{X}_2 \cap \tilde{X}_3) = -1,$$

and hence $\mu^*$ is not nonnegative.

Fix a graph $G$ and let $\mathcal{P}_G$ be the class of probability measures $P$ on $X_1 \times X_2 \times \cdots \times X_n$ such that $P$ forms an MRF represented by $G$. In this section, we prove that the I-Measure $\mu^*$ of every $P \in \mathcal{P}_G$ is nonnegative if and only if $G$ is either a path or a forest of paths. In other words, the MRF represented by such a graph $G$ is either a Markov chain or a collection of mutually independent Markov chains. In this sense we say that the Markov chain is the only MRF for which the I-Measure is always nonnegative. Toward establishing this result, we first review the following result in [10] which is instrumental in proving the nonnegativity of $\mu^*$ for a Markov chain.

**Lemma 3.** If $X_1 \rightarrow X_2 \rightarrow \cdots \rightarrow X_n$ form a Markov chain, then for a Type I atom with $U_A$ defined in (18),

$$\mu^*(A) = \mu^*(\tilde{X}_1 \cap \tilde{X}_n \cap \cdots \cap \tilde{X}_n - \tilde{X}_{U_A}) = \mu^*(\tilde{X}_1 \cap \tilde{X}_n - \tilde{X}_{U_A}).$$  

(19)
Note that the first equality above follows directly from the definition of $U_A$, and the quantity on the right hand side is equal to $I(X_l; X_u | X_{U_A})$ which is always nonnegative. In other words, Lemma 3 asserts that the values of $\mu^*$ on all the Type I atoms are nonnegative. Therefore, $\mu^*$ is a measure.

Previously, the same result (and also the converse) was proved in [1] for the special case $U_A = \emptyset$. In the following, we present a theorem which is a generalization of Lemma 3. Unlike Lemma 3 that applies only to Markov chains, this theorem applies to all MRFs.

**Theorem 11.** Let $X_1, X_2, \cdots, X_n$ form a Markov graph $G = (V, E)$. For a Type I atom $A$ of $G$ with $|U_A| \leq n - 2$,

$$\mu^*(A) = \mu^*\left(\bigcap_{k \in V_2 - U_A} \tilde{X}_k - \tilde{X}_{U_A}\right) = \mu^*\left(\bigcap_{k \in B} \tilde{X}_k - \tilde{X}_{U_A}\right),$$

(20)

where $B \subset V - U_A$ and $k \in B$ if and only if $s(U_A \cup \{k\}) = 1$, i.e., upon removing the vertices in $U_A$ and vertex $k$, the graph remains connected.

**Example 15.** Consider an MRF represented by the graph in Fig. 11. For the Type I atom $\bar{12}\bar{3}\bar{4}56\bar{7}8$, using Theorem 11, $B = \{2, 7, 8\}$, and so

$$\mu^*\left(\tilde{X}_2 \cap \tilde{X}_4 \cap \tilde{X}_5 \cap \tilde{X}_6 \cap \tilde{X}_7 \cap \tilde{X}_8 - \tilde{X}_{\{1,3\}}\right) = \mu^*\left(\tilde{X}_2 \cap \tilde{X}_7 \cap \tilde{X}_8 - \tilde{X}_{\{1,3\}}\right).$$

For the Type I atom $\bar{1}\bar{2}\bar{3}\bar{4}54\bar{6}\bar{7}8$, $B = \{3, 4, 6, 7\}$, and so

$$\mu^*\left(\tilde{X}_3 \cap \tilde{X}_4 \cap \tilde{X}_5 \cap \tilde{X}_6 \cap \tilde{X}_7 - \tilde{X}_{\{1,2,8\}}\right) = \mu^*\left(\tilde{X}_3 \cap \tilde{X}_4 \cap \tilde{X}_6 \cap \tilde{X}_7 - \tilde{X}_{\{1,2,8\}}\right).$$

To gain insight into Theorem 11, we first state the next lemma. This lemma and the technical lemma that follows will be proved in Appendix B.

**Lemma 4.** In Theorem 11 $|B| \geq 2$.

**Remark** When $|B| = 2$, the term on the right hand side of (20) becomes a (conditional) mutual information, which is always nonnegative.

The following lemma will be used in the proof of Theorem 11.

**Lemma 5.** In Theorem 11 let $W = V - U_A - B$. For any $S \subseteq W$, $s(U_A \cup (W - S)) > 1$. 

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Proof of Theorem 11 Let $A$ be a Type I atom of $G$ with $|U_A| \leq n - 2$. Let $W = V - U_A - B$ and consider
\[
\begin{align*}
\mu^* \left( \bigcap_{k \in B} \tilde{X}_k - \bigcap_{j \in U_A} \tilde{X}_j \right) \\
= \mu^* \left( \bigcup_{S \subseteq W} \left( \bigcap_{k \in B} \tilde{X}_k \right) \cap \left( \bigcap_{t \in S} \tilde{X}_t \right) - \tilde{X}_{U_A \cup (W - S)} \right) \\
= \sum_{S \subseteq W} \mu^* \left( \left( \bigcap_{k \in B} \tilde{X}_k \right) \cap \left( \bigcap_{t \in S} \tilde{X}_t \right) - \tilde{X}_{U_A \cup (W - S)} \right).
\end{align*}
\]
In the above summation, for $S \subseteq W$, $s(U_A \cup (W - S)) > 1$ by Lemma 5. Therefore, except for the atom corresponding to $S = W$, i.e., $A$, all the atoms are Type II atoms of $G$. It then follows that
\[
\begin{align*}
\mu^* \left( \bigcap_{k \in B} \tilde{X}_k - \bigcap_{j \in U_A} \tilde{X}_j \right) \\
= \mu^* \left( \left( \bigcap_{k \in B} \tilde{X}_k \right) \cap \left( \bigcap_{t \in W - U_A} \tilde{X}_t \right) - \tilde{X}_{U_A} \right) \\
= \mu^* \left( \left( \bigcap_{k \in V - U_A} \tilde{X}_k \right) - \tilde{X}_{U_A} \right).
\end{align*}
\]
The theorem is proved. \[\square\]

Theorem 11 can be applied to identify atoms on which the value of $\mu^*$ is always nonnegative, because when $|B| = 2$, the term on the right hand side of (20) corresponds to a (conditional) mutual information.

Consider the graph $G = (V, E)$, where $V = \{1, 2, \cdots, n\}$ and the edges in $E$ are $\{i, i + 1\}$ for $i = 1, 2, \cdots, n - 1$ and $\{1, n\}$. Evidently, $G$ is a cycle graph, and if random variables $X_i, i \in V$ are represented by $G$, they form a Markov ring. Then $A$ is a Type I atom of $G$ if and only if $U_A = \emptyset$ or $U_A$ is a consecutive subset of $V$ in the cyclic sense (e.g., $\{1, n\}$ is regarded as a consecutive subset of $V$). An application of Theorem 11 reveals that $\tilde{X}_n \cap \tilde{X}_2 \cap \cdots \cap \tilde{X}_n$ (i.e., $U_A = \emptyset$) is the only atom on which $\mu^*$ may take a negative value, because the value of $\mu^*$ on any other Type I atom is a conditional mutual information. This observation is instrumental in the proof of the next theorem, the main result in this section.
Theorem 12. Let $G$ be a connected graph. Then $\mu^*$ is nonnegative for every $P \in \mathcal{P}_G$ if and only if $G$ is a path.

The ‘if’ part of Theorem 12 is immediate because the $I$-Measure for a Markov chain is always nonnegative. Toward proving the ‘only if’ part, we first classify all connected graphs into the following two classes:

$K1$: there exists a vertex whose degree is at least 3;

$K2$: all the vertices have degree less than or equal to 2.

We further classify the graphs in $K2$ into two subclasses:

$K2-a$: all the vertices have degree 2;

$K2-b$: some vertices have degree 1.

It is easy to see that a graph belonging to subclass $K2-a$ is a cycle graph, and a graph belonging to subclass $K2-b$ is a path. Thus in order to establish Theorem 12 it suffices to prove Theorem 13 and Theorem 14 below which assert that $\mu^*$ is not always nonnegative if $X_i, i \in V$ are represented by a graph belonging to $K1$ and $K2-a$, respectively.

Theorem 13. The $I$-Measure $\mu^*$ for an MRF represented by a graph $G$ belonging to $K1$ is not always nonnegative.

Proof Consider a graph $G = (V, E)$ in $K1$. Let $u \in V$ be a vertex whose degree is at least 3, and let $\{u, v_l\} \in E$, where $l = 1, 2, 3$ and $v_1, v_2$, and $v_3$ are distinct. Let $Z$ and $T$ be independent fair bits. Define random variables $X_i, i \in V$ as follows:

$$X_i = \begin{cases} 
Z & i = v_1 \\
T & i = v_2 \\
Z + T \mod 2 & i = v_3 \\
(Z, T) & i = u \\
\text{constant} & \text{otherwise}
\end{cases}$$

Consider any cutset $U$ of $G$:
Thus in either case \( \mu \) where the first equality can be seen by expanding [15, Theorem 3.19] into a linear combination of \( \mu \) being a function of \( (\mu) \). Hence, \( \mu \) are pairwise independent but not mutually independent, and that for any distinct \( \alpha \) where \( \mu \) is not always nonnegative. Let \( \alpha \), \( i \), \( i = 1, 2, 3 \) are functions of \( X_\alpha \) and \( X_i \) = constant for all \( i \neq u, v_1, v_2, v_3 \), it is readily seen that \( X_{v_1(U)}, X_{v_2(U)}, \cdots, X_{v_3(U)} \) are mutually independent conditioning on \( X_U \).

Thus in either case \( X_i, i \in V \) are represented by \( G \). Then

\[
\mu^* \left( \tilde{X}_u \cap \tilde{X}_{v_1} \cap \tilde{X}_{v_2} \cap \tilde{X}_{v_3} - \bigcup_{i \neq u, v_1, v_2, v_3} \tilde{X}_i \right) = \mu^* (\tilde{X}_u \cap \tilde{X}_{v_1} \cap \tilde{X}_{v_2} \cap \tilde{X}_{v_3}) = -1,
\]

where the first equality can be seen by expanding \( \mu^* (\tilde{X}_u \cap \tilde{X}_{v_1} \cap \tilde{X}_{v_2} \cap \tilde{X}_{v_3} - \bigcup_{i \neq u, v_1, v_2, v_3} \tilde{X}_i) \) using [15] Theorem 3.19] into a linear combination of \( H(\cdot | \tilde{X}_i, i \neq u, v_1, v_2, v_3) = H(\cdot) \), and the second equality can easily be verified (cf. Problem 5, Ch. 12 in [15]). Hence, \( \mu^* \) for \( X_i, i \in V \) represented by a graph \( G \) belonging to K1 is not always nonnegative.

**Theorem 14.** The I-Measure \( \mu^* \) for an MRF represented by a graph \( G \) belonging to K2-a is not always nonnegative.

**Proof** Consider a graph \( G = (V, E) \) in K2-a, i.e., \( G \) is a cycle graph. For convenience, let \( V = \{0, 1, \cdots, n-1\} \). The edge set \( E \) is specified by \( |u, v| \in E \) if and only if \( |u - v| = 1 \), where “-” denotes modulo \( n \) subtraction. Let \( F \) denote a finite field containing at least \( n - 1 \) elements. Let \( Z \) and \( T \) be independent random variable, each taking values in \( F \) according to the uniform distribution. Now define random variables \( X_i, i \in V \) as follows:

\[
X_i = \begin{cases} 
Z & i = 0 \\
T & i = 1 \\
Z + \alpha_i T & i = 2, 3, \cdots, n-1
\end{cases}
\]

where \( \alpha_i, i = 2, 3, \cdots, n-1 \) are distinct nonzero elements of \( F \). It is evident that \( X_i, i = 0, 1, \cdots, n-1 \) are pairwise independent but not mutually independent, and that for any distinct \( i, i', i'' \), we have \( X_{i''} \) being a function of \( (X_i, X_{i'}) \).
We now show that $X_i, i \in V$ is represented by $G$. Since $G$ is a cycle graph, for any $U \subset V$, if the vertices in $U$ are connected in $G$, the vertices in $V - U$ are also connected in $G$. Therefore, if $U$ is a cutest in $G$, the vertices in $U$ are not connected in $G$. This implies that $|U| \geq 2$. From the foregoing, $X_{V - U}$ is a function of $X_U$. Then we see that $X_{V(U)}, X_{V_2(U)}, \ldots , X_{V_{n(U)}(U)}$ are mutually independent conditioning on $X_U$. Therefore, $X_i, i \in V$ is represented by $G$.

It remains to show that $\mu^*$ is not nonnegative. For the sake of convenience, assume the logarithms defining entropy are in the base $|F|$. Then for $B \subset V$ where $B \neq \emptyset$,

$$H(X_B) = \begin{cases} 
1 & \text{if } |B| = 1 \\
2 & \text{if } 2 \leq |B| \leq n.
\end{cases} \tag{21}$$

We will show that $\mu^*$ is given by

$$\mu^*\left(\bigcap_{i \in W} \tilde{X}_i - \bigcup_{j \in V - W} \tilde{X}_j \right) = \begin{cases} 
0 & \text{if } 1 \leq |W| \leq n - 2 \\
1 & \text{if } |W| = n - 1 \\
-(n - 2) & \text{if } |W| = n
\end{cases} \tag{22}$$

for $W \subset V$. Toward this end, owing to the uniqueness of $\mu^*$, we only need to verify that $\mu^*$ as prescribed by (22) satisfies (21). The details are given in Appendix A. Then the theorem is proved because $\mu^*$ is not nonnegative. \hfill \Box

**Theorem 15.** Let $G$ be a graph with at least two components. Then $\mu^*$ is nonnegative for every $P \in \mathcal{P}_G$ if and only if $G$ is a forest of paths.

**Proof** We first prove the ‘only if’ part. Assume that $G$ is not a forest of paths, i.e., there exists a component of $G$ which is not a path. Denote the vertices of this component by $V'$ and let $X_i, i \in V \setminus V'$ be constant. Then by Theorem 12 we can construct $X_i, i \in V$ such that $\mu^*(S) < 0$ for some $S \subset \mathcal{F}_V \subset \mathcal{F}_V$, where $\mathcal{F}_V'$ is the $\sigma$-field generated by $\{\tilde{X}_i, i \in V'\}$. Hence $\mu^*$ is not nonnegative, and the ‘only if’ part is proved.

To prove the ‘if’ part, we need to prove that if an MRF is represented by a graph $G$ which is a forest of paths, then $\mu^*$ is always nonnegative. Let $m$ be the number of components of $G$, where $m \geq 2$, and denote the sets of vertices of these components by $V_1, V_2, \ldots , V_m$. Without loss of generality, assume that the indices in each $V_i$ are consecutive.
Now observe that a nonempty atom $A$ of $\mathcal{F}_V$ is a Type I atom of $\mathcal{F}_V$ if and only if $U_A$ has the form (18) and $\{l, l + 1, \cdots, u\} \subset V_i$ for some $1 \leq i \leq m$. If $l = u$, then

$$\mu^*(A) = H(\tilde{X}_l | \tilde{X}_{V-\{l\}}) \geq 0.$$ 

If $l < u$, then by Theorem[11]

$$\mu^*(A) = \mu^*\left(\bigcap_{l \leq k \leq u} \tilde{X}_k - \tilde{X}_{U_A}\right) = \mu^*(\tilde{X}_l \cap \tilde{X}_k - \tilde{X}_{U_A}) \geq 0.$$ 

Hence $\mu^*$ is nonnegative, and the theorem is proved.

\[\square\]

6 Concluding Remarks

The theory of $I$-Measure proves to be a very useful tool for characterizing full conditional independence structures and MRFs[13], because with $I$-Measure, the fundamental set-theoretic structure of the problem is exposed. In this paper, we apply this tool to obtain two main results related to MRFs.

For an MRF represented by an undirected graph, a subfield is a subset of the random variables forming the MRF. We have determined the smallest undirected graph that can always represent a subfield as an MRF. This is our first main result. Based on this result, we have obtained a necessary and sufficient condition for a subfield of a Markov tree to be also a Markov tree.

A Markov chain can be regarded a special case of an MRF. It was previously known that the $I$-Measure of a Markov chain is always nonnegative[10]. Here, we have proved that the $I$-Measure is nonnegative for every MRF represented by a given undirected graph if and only if the graph is a forest of paths, i.e., the Markov random field is a collection of independent Markov chains. This means that Markov chain is essentially the only MRF such that the $I$-Measure is always nonnegative. This is our second main result. In the course of proving this result, we have obtained some interesting properties of the $I$-Measure pertaining to an MRF.

By virtue of the $I$-Measure characterization of MRFs, the proofs in this paper involve nothing but elementary set manipulations. The advantage of this approach is two-fold. First, by employing the rich set of tools in set theory, the proofs can be made very compact. Second, since we do not need to work on the underlying probability measure directly, our proofs do not rely on the probability
measure taking a particular factorization form or any form. The subtleties of non-strictly-positive probability measures are encapsulated in pure set-theoretic terms. As such, unlike most other works in the literature, our results apply to general instead of a restricted class of MRFs.

A Verification of $\mu^*$ in the Proof of Theorem 14

In this appendix, we verify that $\mu^*$ as prescribed by (22) satisfies (21). First, for $i \in V$, consider

$$\mu^*(\tilde{X}_i) = \mu^* \left( \bigcup_{S \subset V - \{i\}} (\tilde{X}_i \cap \tilde{X}_S - \tilde{X}_{V - S - \{i\}}) \right) = \sum_{S \subset V} \mu^* (\tilde{X}_i \cap \tilde{X}_S - \tilde{X}_{V - S - \{i\}}).$$

From (22), we see that $\mu^*(\cdot)$ in the above summation vanishes if $|S| \leq n - 3$, and so

$$\mu^*(\tilde{X}_i) = \sum_{j \neq i} \mu^* \left( \bigcap_{k \neq j} \tilde{X}_k - \tilde{X}_j \cup \tilde{X}_0 \cap \tilde{X}_1 \cap \cdots \cap \tilde{X}_{n-1} \right) = (n - 1) \cdot 1 = 1. \quad (23)$$

This verifies (21) for the case $|B| = 1$. Next, for $0 \leq i < j \leq n - 1$, consider

$$\mu^*(\tilde{X}_i \cap \tilde{X}_j) = \sum_{S \subset V - \{i,j\}} \mu^* \left( \tilde{X}_i \cap \tilde{X}_j \cap \left( \bigcap_{k \in S} \tilde{X}_k \right) - \left( \bigcup_{l \in V - \{i,j\} - S} \tilde{X}_l \right) \right)$$

$$= \sum_{S : |S| = 3} \mu^* \left( \tilde{X}_i \cap \tilde{X}_j \cap \left( \bigcap_{k \in S} \tilde{X}_k \right) - \left( \bigcup_{l \in V - \{i,j\} - S} \tilde{X}_l \right) \right)$$

$$= \sum_{m \neq i,j} \mu^* \left( \bigcap_{r \in V - \{m\}} \tilde{X}_r - \tilde{X}_m \right) + \mu^* \left( \bigcap_{s=1}^n \tilde{X}_s \right) = (n - 2) \cdot 1 - (n - 2) = 0. \quad (24)$$

It follows from (23) and (24) that

$$\mu^*(\tilde{X}_i \cup \tilde{X}_j) = \mu^*(\tilde{X}_i) + \mu^*(\tilde{X}_j) - \mu^*(\tilde{X}_i \cap \tilde{X}_j) = 1 + 1 - 0 = 2. \quad (25)$$

(27)
This verifies (21) for the case $|B| = 2$. Now for $1 \leq i < j < k \leq n$, consider

$$\mu^*(\tilde{X}_k - (\tilde{X}_i \cup \tilde{X}_j)) = \sum_{S \subseteq V \setminus \{i, j, k\}} \mu^*\left(\tilde{X}_k \cap \left(\bigcap_{l \in S} \tilde{X}_l\right) - \left(\tilde{X}_i \cup \tilde{X}_j \cup \bigcup_{m \in V \setminus \{i, j, k\} \setminus S} \tilde{X}_m\right)\right).$$

In the above, since $|k \cup S| \leq n - 2$, we see from (22) that every term in the above summation vanishes, and so

$$\mu^*(\tilde{X}_k - (\tilde{X}_i \cup \tilde{X}_j)) = 0. \tag{28}$$

Finally, consider $B \subseteq V$ such that $3 \leq |B| \leq n$ and let $i, j$ be two arbitrary elements of $B$. Then in light of (27) and (28), we have

$$\mu^*(\tilde{X}_B) = \mu^*(\tilde{X}_i \cup \tilde{X}_j) + \mu^*(\tilde{X}_{B \setminus \{i, j\}} - (\tilde{X}_i \cup \tilde{X}_j)) \leq \mu^*(\tilde{X}_i \cup \tilde{X}_j) + \sum_{k \in B \setminus \{i, j\}} \mu^*(\tilde{X}_k - (\tilde{X}_i \cup \tilde{X}_j)) = 2 + 0 = 2,$$

where the inequality above is justified by the union bound because $\mu^*$ is nonnegative on all the atoms in $\tilde{X}_{B \setminus \{i, j\}} - (\tilde{X}_i \cup \tilde{X}_j)$ (cf. (22)). On the other hand, we have

$$\mu^*(\tilde{X}_B) = \mu^*(\tilde{X}_i \cup \tilde{X}_j) + \mu^*(\tilde{X}_{B \setminus \{i, j\}} - (\tilde{X}_i \cup \tilde{X}_j)) \geq \mu^*(\tilde{X}_i \cup \tilde{X}_j) = 2,$$

again because $\mu^*$ is nonnegative on all the atoms in $\tilde{X}_{B \setminus \{i, j\}} - (\tilde{X}_i \cup \tilde{X}_j)$. Therefore, $\mu^*(\tilde{X}_B) = 2$, verifying (21) for the case $3 \leq |B| \leq n$.

**B Proof of Lemmas 4 and 5**

In this appendix, we prove Lemmas 4 and 5 via the following lemma.

**Lemma 6.** Let $G = (V, E)$ be a connected undirected graph and $B = \{v \in V : s(\{v\}) = 1\}$. Then
a) for any \( k \in V - B \), we have \( B \cap J_i \neq \emptyset \) for all \( 1 \leq i \leq s_k \), where \( J_1, J_2, \ldots, J_{s_k} \) \((s_k \geq 2)\) are the components of \( G \setminus \{k\} \);

b) \( s(R) > 1 \) for all nonempty subset \( R \) of \( V - B \).

**Proof** We assume that \( B \neq V \), since otherwise \( V - B = \emptyset \) and the lemma has no assertion.

We first prove a). Let \( k \in V - B \), and by the definition of \( B \), we have \( s_k \geq 2 \). Consider any spanning tree \( T \) of \( G \). Note that \( T \) must contain at least one edge connecting \( k \) and each \( J_i \) \((1 \leq i \leq s_k)\) because \( G \) is connected. For any fixed \( i \), consider such an edge and call it \( e \). Upon removing \( e \), \( T \) is disconnected with one component being a subtree containing \( k \) and the other component a subtree not containing \( k \). For the latter subtree, all the vertices are in \( J_i \), otherwise there exists an edge connecting \( J_i \) and \( J_{i'} \) \((i' \neq i)\), which is a contradiction because \( J_1, J_2, \ldots, J_{s_k} \) are the components of \( G \setminus \{k\} \). Then this subtree must have at least one leaf in \( J_i \), say \( l \). Note that \( \{l\} \) is not a cutset in \( T \) and hence not a cutset in \( G \). Therefore \( B \cap J_i \neq \emptyset \), proving a).

We now prove b). Consider any nonempty subset \( R \) of \( V - B \) and fix \( k \in R \). By a), \( B \cap J_i \neq \emptyset \) for all \( 1 \leq i \leq s_k \), with \( s_k \geq 2 \). Then the vertices in \( B \) are not connected in \( G \setminus \{k\} \), and hence not connected in \( G \setminus R \) because \( k \in R \). Since \( R \subset V - B \) is equivalent to \( B \subset V - R \), this implies that \( G \setminus R \) is not connected, or \( s(R) > 1 \). The lemma is proved. \( \square \)

Lemmas 4 and 5 can now be obtained as corollaries of Lemma 6 as follows. First, note that in Theorem 11, \( U_A \) is a Type I atom, and so \( G \setminus U_A \) is connected. The same holds for Lemmas 4 and 5. By applying Part a) of Lemma 6 to \( G \setminus U_A \), we obtain Lemma 4. By applying Part b) of Lemma 6 to \( G \setminus U_A \) with \( R = W - S \), we obtain Lemma 5.

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Figure 1: The information diagram for Example 3.
Figure 2: The graph $G$ in Example 6.
Figure 3: The graph $\hat{G}$ corresponding to the set $\mathcal{A}_H$ in Example 7.
Figure 4: The graphs $G$ (black) and $G^*(V')$ (grey) in Example [9] with $V'\{1, 3, 5, 6\}$.
Figure 5: The graphs $G$ (black) and $G'(V')$ (grey) in Example 10 with $V' = \{1, 2, 5, 6, 8, 9\}$. 
Figure 6: The graphs $G$ (black) and $G'(V')$ (grey) in Example [11] with $V' = \{2, 3, 4\}$. 
Figure 7: The trees $G$ (black) and $G^*(V')$ (grey) in Example 13 with $V' = \{1, 4, 8, 9, 12\}$. 
Figure 8: The tree $G$ (black) and the graph $G'(V')$ (grey) in Example [13] with $V' = \{1, 4, 7, 8, 9, 12\}$. 
Figure 9: The information diagram for the Markov chain $X_1 \rightarrow X_2 \rightarrow \cdots \rightarrow X_n$. 
Figure 10: The “star” representing the Markov tree in Example [14]
Figure 11: The graph in Example 15.