# On Functions of Markov Random Fields

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Abstract—We derive two sufficient conditions for a function of a Markov random field (MRF) on a given graph to be a MRF on the same graph. The first condition is information-theoretic and parallels a recent information-theoretic characterization of lumpability of Markov chains. The second condition, which is easier to check, is based on the potential functions of the corresponding Gibbs field. We illustrate our sufficient conditions at the hand of several examples and discuss implications for practical applications of MRFs. As a side result, we give a partial characterization of functions of MRFs that are information-preserving.

Index Terms—Markov random field, Gibbs field, lumpability, hidden Markov random field

#### I. INTRODUCTION

Since the late 1950s, researchers have actively investigated properties of functions of Markov chains. In particular, considerable effort has been devoted to obtain sufficient and necessary conditions for *lumpability*, the rare scenario in which a function of a Markov chain has the Markov property [1]–[3].

In this work, we extend the concept of lumpability and its investigation to Markov random fields (MRFs). Specifically, given a MRF  $X:=(X_1,\ldots,X_N)$  on a graph  $\mathcal G$ , we determine conditions for a set of functions  $\{g_1,\ldots,g_N\}$  such that the transformation  $Y:=(g_1(X_1),\ldots,g_N(X_N))$  is a MRF on  $\mathcal G$ . In other words, the problem we investigate asks the question under which functions an independence structure (i.e., a collections of independence statements) remains valid.

Aside from being an interesting problem in its own right, it is also practically motivated from an inference perspective. Namely, multidimensional data X is often modeled as a hidden MRF, i.e., the data X is hidden and can be inferred from some observed random variable  $Z := (Z_1, \ldots, Z_N)$ , where each  $Z_i$  is conditionally independent of X given  $X_i$ . In some scenarios, however, not X is of interest but its transformation Y. For example, in image processing, in which  $\mathcal{G}$  is a graph on a lattice with a distance-based neighborhood structure and in which X and Z denote the true and observed pixel values, respectively, one may be interested in subsampling the image, clustering regions of the image, or quantizing pixel values for the sake of identifying regions with similar intensities. Transforming X to Y potentially creates additional or breaks existing dependencies, i.e., the graph  $\mathcal{G}_Y$  w.r.t. which Y is a MRF is generally different from G. Rather than inferring X from the observed Z and subsequently computing Y via the known transformations, in this work, we are interested in scenarios where Y is directly inferred from Z. This is computationally tractable if (Y, Z) turns out to be a hidden MRF itself. Among other things, this requires determining the graph  $\mathcal{G}_Y$  w.r.t. which Y is a MRF.

The remainder of this paper can be summarized as follows. Section II introduces notation and basic definitions, and Section III formulates the problem and provides some examples. Section IV places the current work in context with previous results on stochastic transformations of MRFs [4, Sec. IV] and subfields of MRFs [4]–[6]. Section V gives two sufficient conditions for Y to be a MRF on the same graph as X, i.e., for  $\mathcal{G}_Y = \mathcal{G}$ . The first condition is based on the characterization of MRFs via clique potentials, while the second is information-theoretic and resembles the information-theoretic characterization of Markov chain lumpability [3, Th. 2]. As a side result, Section VI presents necessary and sufficient conditions for the transformation Y to have the same information content as X. For the sake of readability, all proofs are in Section VII.

#### II. NOTATION AND PRELIMINARIES

Let  $\mathcal{G} := (\mathcal{V}, E)$  be an undirected graph with vertices  $\mathcal{V} := \{1, \ldots, N\}$  and edges  $E \subseteq [\mathcal{V}]^2$ , where  $[A]^2$  is the set of two-element subsets of A. We call  $\mathcal{G}$  complete if  $E = [\mathcal{V}]^2$ , chordal if every induced cycle of  $\mathcal{G}$  has length three, a tree if  $\mathcal{G}$  is connected and acyclic, and a path if there is a permutation  $v_1, \ldots, v_N$  of the vertices such that  $E = \{\{v_i, v_{i+1}\}, i = 1, \ldots, N-1\}$ . If  $\{i, j\} \in E$ , then the vertices i and j are neighbors, and we use  $\mathcal{N}_i$  to denote the neighbors of i, i.e.,

$$\mathcal{N}_i := \{ j \in \mathcal{V} \setminus \{i\} \colon \{i, j\} \in E \}. \tag{1}$$

A set  $C \subseteq \mathcal{V}$  is called a clique if it is a singleton or if  $[C]^2 \subseteq E$ . We use  $\mathcal{C}$  to denote the set of cliques of  $\mathcal{G}$ .

We denote random variables (RVs) by upper case letters, e.g., X, alphabets by calligraphic letters, e.g.,  $\mathcal{X}$ , and realizations by lower case letters, e.g., x. We assume that all our RVs are defined on a common probability space  $(\Omega, \mathcal{T}, \mathbb{P})$ . Specifically, let  $X_i$  be a discrete RV with alphabet  $\mathcal{X}_i$  that is associated with vertex  $i \in \mathcal{V}$ . For a set  $A \subseteq \mathcal{V}$ , we write  $X_A := (X_i, i \in A)$  and  $\mathcal{X}_A := \prod_{i \in A} \mathcal{X}_i$ . We furthermore use the abbreviations  $X := X_{\mathcal{V}}$  and  $X_{\dot{\mathcal{V}}} := X_{\mathcal{V} \setminus \{i\}}$ , and similarly for the alphabets of these RVs. The RV  $X_A$  is characterized by its probability mass function (PMF)

$$p_{X_A}(x_A) := \mathbb{P}(\{\omega \in \Omega : X_A(\omega) = x_A\}), \forall x_A \in \mathcal{X}_A.$$
 (2)

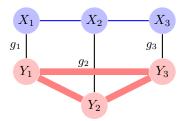


Fig. 1. The problem of lumpability. The blue vertices and edges correspond to the original  $(\mathcal{G}, p_X)$ -MRF X, the black labeled edges correspond to functions through which the RVs in the MRF are observed, thus defining  $Y:=(g_1(X_1),g_2(X_2),g_3(X_3))$ . In general, the minimal graph w.r.t. which Y is a MRF is complete (see red vertices and edges): By observing a Markov path  $X_1-X_2-X_3$  through a non-injective function, the Markov property is lost in general. The lumpability problem seeks conditions on  $p_X$  and  $\{g_i\}$  such that the minimal graph for Y is equivalent to the original graph  $\mathcal G$  or a subgraph of  $\mathcal G$ .

**Definition 1.** Let  $\mathcal{G} = (\mathcal{V}, E)$  be a graph and  $X = (X_i, i \in \mathcal{V})$  be a RV with PMF  $p_X$ , then X is a *Markov random field* (MRF) on  $\mathcal{G}$ , abbreviated X is a  $(\mathcal{G}, p_X)$ -MRF, if

$$\forall i \in \mathcal{V}: \quad p_{X_i|X_{i'}} = p_{X_i|X_{\mathcal{N}_i}}, \tag{3}$$

i.e., if the distribution of  $X_i$  depends on the remaining RVs only via the RVs neighboring i. If  $p_X$  is unspecified, but known to belong to a family of distributions for which (3) holds for every member, then we say that X is a  $\mathcal{G}$ -MRF.

For any  $A, B \subseteq \mathcal{V}$ , the entropy of  $X_A$  is defined as

$$H(X_A) := -\sum_{x_A \in \mathcal{X}_A} p_{X_A}(x_A) \log p_{X_A}(x_A)$$
 (4)

and the conditional entropy of  $X_A$  given  $X_B$  as  $H(X_A|X_B) := H(X_{A \cup B}) - H(X_B)$ . With this notation, the lemma below follows immediately from Definition 1.

**Lemma 1.** X is a  $\mathcal{G}$ -MRF if and only if (iff), for every  $i \in \mathcal{V}$ ,  $H(X_i|X_{i}) = H(X_i|X_{\mathcal{N}_i})$ .

Note that if X is a  $\mathcal{G}$ -MRF, then it is a MRF on every graph with vertices  $\mathcal{V}$  whose edge set is a superset of E. Trivially, every X is a MRF on the complete graph. Of particular interest is thus the *minimal* graph w.r.t. which X is a MRF. We will assume throughout this paper that the graph  $\mathcal{G}$  w.r.t. which X is a MRF is minimal.

#### III. PROBLEM STATEMENT AND MOTIVATING EXAMPLES

In this work, we consider functions of MRFs. Specifically, let  $\{g_i, i \in \mathcal{V}\}$  (subsequently abbreviated as  $\{g_i\}$  to simplify notation) be a set of functions  $g_i \colon \mathcal{X}_i \to \mathcal{Y}_i$  indexed by the vertices  $i \in \mathcal{V}$ , and let  $Y_i := g_i(X_i)$ . For  $A \subseteq \mathcal{V}$ , we define the function  $g_A \colon \mathcal{X}_A \to \mathcal{Y}_A$  as the functions  $g_i, i \in A$ , applied to  $X_A$  coordinate-wise, i.e.,  $g_A(X_A) := (g_i(X_i), i \in A) = Y_A$ , and, as before, use the abbreviation  $g(X) := g_{\mathcal{V}}(X) = Y_A$ . We call a set of functions  $\{g_i\}$  non-trivial if at least one function  $g_i$  is non-injective. Given a  $(\mathcal{G}, p_X)$ -MRF X and a set of functions  $\{g_i\}$ , we call the tuple  $(\mathcal{G}, p_X, \{g_i\})$  the lumping of X. We will focus on the following two problems:

**Problem 1** (Lumpability). Determine conditions on the lumping  $(\mathcal{G}, p_X, \{g_i\})$  so that Y is a MRF w.r.t.  $\mathcal{G}$ , where in this case we say  $(\mathcal{G}, p_X, \{g_i\})$  is lumpable, see Fig. 1. By the remark below Lemma 1,  $(\mathcal{G}, p_X, \{g_i\})$  is lumpable whenever it does not introduce new edges, i.e., whenever Y is a  $(\mathcal{G}', p_Y)$ -MRF with  $\mathcal{G}' = (\mathcal{V}, E')$  and  $E' \subseteq E$ 

**Problem 2** (Information Preservation). Determine conditions on the lumping  $(\mathcal{G}, p_X, \{g_i\})$  so that H(Y) = H(X), where in this case we say  $(\mathcal{G}, p_X, \{g_i\})$  is information-preserving.

Throughout this work we assume the set of functions  $\{g_i\}$  is non-trivial. Otherwise, if all the functions  $g_i$  are injective, then X and Y would have the same distribution since  $\{g_i\}$  is simply a relabeling of the distribution's domain, and so the lumping would be trivially lumpable and information preserving. We also assume that  $\mathcal{G}$  is connected, which is w.l.o.g. since the RVs of different components of the graph are independent, and this independence is retained for any set of functions  $\{g_i\}$ .

To get some intuition on why a function of a MRF may not be a MRF on the same graph, note that  $X_i$  and  $X_{i'}$  are conditionally independent given  $X_{\mathcal{N}_i}$  only when  $X_{\mathcal{N}_i}$  contains all the information about  $X_i$  that is available in  $X_{i'}$  Taking a function of  $X_{\mathcal{N}_i}$  may reduce this information to a point where  $Y_{\mathcal{N}_i}$  no longer contains all the information about  $Y_i$ that is available in  $Y_{i/i}$  which effectively introduces edges in the minimal graph for Y that have not been present in  $\mathcal{G}$ . This parallels the fact that a function of a Markov chain rarely results in a Markov chain [1, Th. 31]. (A Markov chain is a G-MRF where  $\mathcal{G}$  is the infinite path graph, i.e., with the natural numbers  $\mathbb{N}$  as the set of vertices and  $\{\{i, i+1\} : i \in \mathbb{N}\}$ as the set of edges.) Regarding information-preservation, a lumping is information-preserving iff  $\{q_i\}$  maps the support of  $p_X$  injectively. Thus, both lumpability and informationpreservation appear to be the exception rather than the rule. The following examples demonstrate different lumpability and information-preservation scenarios and give some intuition on the corresponding lumpings  $(\mathcal{G}, p_X, \{g_i\})$ .

**Example 1** (Neither Information-Preserving nor Lumpable). Let  $X_1$ — $X_2$ — $X_3$  be a Markov path, i.e., a  $\mathcal{G}$ -MRF on the path graph  $\mathcal{G} = (\{1, 2, 3\}, \{\{1, 2\}, \{2, 3\}\})$ , where each RV  $X_i$  takes values from  $\{0,1,2\}$ . Suppose that  $p_{X_1|X_2}(1|0) =$  $p_{X_3|X_2}(1|2) = 0, \ p_{X_1|X_2}(1|2) = p_{X_3|X_2}(1|0) = p > 0,$ and  $p_{X_2}(0) = p_{X_2}(2) \in (0,0.5)$ . For all other configurations, assume  $p_{X_1|X_2}$  and  $p_{X_3|X_2}$  are positive. Let  $g_i(x_i)$  $\operatorname{mod}(x_i, 2)$  for every i, then one can verify that  $p_{Y_1|Y_2}(1|0) =$  $p/2 = p_{Y_3|Y_2}(1|0)$ , while  $p_{Y_1,Y_3|Y_2}(1,1|0) = 0$ . Thus,  $Y_1$ and  $Y_3$  are not conditionally independent given  $Y_2$ , and so the minimal graph for Y contains the new edge  $\{1,3\}$ , i.e., the lumping  $(\mathcal{G}, p_X, \{g_i\})$  is not lumpable. (In this example the minimal graph for Y is the complete graph, see Fig. 1.) Furthermore, since, e.g., x = (0,0,0) and x' = (0,0,2)both have positive probabilities, but are mapped to the same y = (0, 0, 0), the lumping is not information-preserving.

**Example 2** (Information-Preserving but not Lumpable). Let  $X_1 := X_2 + Z_1$  and  $X_3 := X_2 + Z_3$ , where  $Z_1 \in \{0, 1\}, X_2 \in \{0, 1\}$ 

 $\{-1,1\}$ , and  $Z_3 \in \{-1,0\}$  are mutually independent RVs. It follows that  $X_1 - X_2 - X_3$  is a Markov path as in the previous example with edges  $E = \{\{1,2\},\{2,3\}\}$ . Assume  $g_1$  and  $g_3$  are the identity functions and  $g_2 \equiv 0$ . Since  $Y_2$  is constant,  $Y_1$  and  $Y_3$  are conditionally independent given  $Y_2$  iff  $Y_1$  and  $Y_3$  are independent, which is not true due to the coupling through  $X_2$ . (Assuming  $p_{X_2}$  is strictly positive.) Hence, the lumping  $(\mathcal{G}, p_X, \{g_i\})$  is not lumpable since the minimal graph for Y must contain the edge  $\{1,3\}$ , which is not in E. (Indeed, Y is a MRF w.r.t. the graph  $(\{1,2,3\}, \{\{1,3\}\})$ .) Furthermore, one can show that  $X_2 = 1$  iff  $X_1 > 0$  and that  $X_2 = -1$  iff  $X_3 < 0$ , hence  $Y = (X_1, 0, X_3)$  contains the same information as X, i.e., the lumping is information-preserving.

**Example 3** (Lumpable and Information-Preserving). Let  $X_2 := (X_1, Z_2, X_3)$ , where  $X_1, Z_2$ , and  $X_3$  are mutually independent. Then, we have the Markov path  $X_1$ — $X_2$ — $X_3$  again, where the PMF  $p_X$  satisfies

$$p_X(x_1, (z_1, z_2, z_3), x_3) = \begin{cases} p_{X_1}(x_1)p_{Z_2}(z_2)p_{X_3}(x_3), & x_1 = z_1, x_3 = z_3 \\ 0, & \text{else.} \end{cases}$$
 (5)

Now suppose that  $g_1$  and  $g_3$  are the identity mappings and that  $g_2$  is such that  $g_2(z_1, z_2, z_3) = z_2$ . Obviously, the thus defined RVs  $Y_1$ ,  $Y_2$ , and  $Y_3$  are independent, i.e., Y is a MRF on the empty graph, and so  $(\mathcal{G}, p_X, \{g_i\})$  is lumpable. Furthermore, it is clear that H(g(X)) = H(X), and so the lumping is information-preserving.

#### IV. PREVIOUS WORK ON MRFS

Yeung et al. characterized MRFs using the *I*-measure [5], [6]. Specifically, if X is a G-MRF and  $A \subseteq \mathcal{V}$ , they investigated the minimal graph  $\mathcal{G}_A = (A, E_A)$  on which  $X_A$ is a MRF. They showed that  $E_A$  contains  $\{i, j\} \in [A]^2$  if either  $\{i, j\} \in E$  or if there is a path between i and j in  $\mathcal{G}$  of which all intermediate vertices lie in  $\mathcal{V} \setminus A$ , see [5, Th. 5] or [6, Th. 8]. More generally, Sadeghi [7] characterized probabilistic graphical models, admitting mixed graphs  $\mathcal{G}$  with directed, doubly-directed, and undirected edges, and presented an algorithm that generates a corresponding graph for a subset  $A \subseteq \mathcal{V}$  of the vertices of  $\mathcal{G}$ , cf. [7, Algorithm 1]. With the restriction to undirected graphs, this algorithm terminates with  $\mathcal{G}_A$  as discussed in [6]. Much earlier, Pérez and Heitz investigated this problem from a Gibbs field perspective, i.e., using potential functions, where they showed that  $X_A$  is a  $(\mathcal{G}_A, p_{X_A})$ -MRF [4, Th. 2], but that  $\mathcal{G}_A$  is only minimal if additional conditions are fulfilled [4, Th. 3].

Below we clarify some connections between previous works and the current one. Given a MRF X w.r.t. a graph  $\mathcal{G}_X$  and a transformation  $p_{Y|X}$  of X to Y, assume the joint RV (X,Y) is a MRF on a graph  $\mathcal{G}_{X,Y}$ . (According to the problem formulation in Problem 1, such a graph is not needed in the current paper and only assumed in this paragraph to facilitate discussions relative to previous works.) The vertex set of this graph is the disjoint union of the vertices of  $\mathcal{G}_X$  and a set of

vertices associated with Y, and the edge set is obtained from the edges of  $\mathcal{G}_X$  and the transformation  $p_{Y|X}$ . Determining on which graph  $\mathcal{G}_Y$  the RV Y is a MRF can then be done by applying [5, Th. 5] or [4, Th. 2 & 3] to  $\mathcal{G}_{X,Y}$  for the subset of vertices that are associated with Y. With this setup, the primary distinctions between previous works and the current one are the following: [5], [6] make no assumptions on  $p_{Y|X}$ , [4] assumes  $p_{Y|X}$  is strictly positive, and this work assumes

$$p_{Y|X}(y|x) = \prod_{i \in \mathcal{V}} \mathbb{I}[g_i(x_i) = y_i], \tag{6}$$

where  $\mathbb{I}[\cdot]$  is the indicator function, i.e.,  $p_{Y|X}$  factors as the product of degenerate distributions  $p_{Y_i|X_i}$  that account to the fact that  $Y_i$  is a deterministic function of  $X_i$ .

Unfortunately, Problem 1 cannot be solved with the framework in [4] since the conditional distribution (6) is not strictly positive, nor can it be solved using [5], [6] since the framework therein finds a graph  $\mathcal{G}_Y$  that is minimal for any  $\{g_i\}$  (in fact for any  $p_{Y_i|X_i}$ ) and any  $p_X$  in the family of distributions specified by  $\mathcal{G}_X$ . In contrast, here we are given a fixed set of transformations  $\{g_i\}$  and (often) a fixed distribution  $p_X$ . Indeed, if  $\mathcal{G}_X$  is connected, then [5, Th. 5] leads to  $\mathcal{G}_Y$  being complete. In other words, for any MRF X on a connected graph, [5, Th. 5] states that one can find a PMF  $p_X$  and a set of functions  $\{g_i\}$  (more precisely  $p_{Y_i|X_i}$ ,  $i=1,\ldots,N$ , as the theorem does not assume deterministic mappings) such that Y does not satisfy any conditional independence statements. (See Example 1 for an explicit choice of  $p_X$  and  $\{g_i\}$  that results in the complete graph in the case of the Markov path.)

Little work has been done regarding information-preserving lumpings of a MRF, see Problem 2. A work in a related direction is [8], which shows that under certain conditions the entropy  $H(X_A)$ , for  $A \subseteq \mathcal{V}$ , can be bounded from above by the entropy of a MRF w.r.t. the subgraph of  $\mathcal{G}$  induced by A.

#### V. SUFFICIENT CONDITIONS FOR MRF LUMPABILITY

Below we investigate Problem 1, namely, we determine sufficient conditions for the lumping  $(\mathcal{G}, p_X, \{g_i\})$  to be lumpable. Note that according to Problem 1,  $(\mathcal{G}, p_X, \{g_i\})$  is lumpable if Y is a  $(\mathcal{G}, p_Y)$ -MRF, even if  $\mathcal{G}$  is not minimal for Y. We further assume within this section that  $p_X(x) > 0$  for every  $x \in \mathcal{X}$ , and that g is surjective, i.e.,  $\mathcal{Y}$  is the image of  $\mathcal{X}$  under g. This allows the characterization of a MRF via its connection to Gibbs fields. (Despite this assumption, the joint distribution  $p_{XY}$  is not strictly positive, see (6).) Specifically, let  $\psi_A \colon \mathcal{X}_A \to \mathbb{R}$  be a potential function. We abuse notation and extend the domain of  $\psi_A$  to  $\mathcal{X}$ , i.e., for  $x = (x_1, \dots, x_N) \in \mathcal{X}$  we write  $\psi_A(x) := \psi_A(x_A)$ , where  $x_A := (x_i, i \in A)$ . The following lemma gives the characterization required in this section.

**Lemma 2** (Hammersley-Clifford [9]). X is a  $(\mathcal{G}, p_X)$ -MRF satisfying  $p_X(x) > 0$  for every  $x \in \mathcal{X}$  iff there exists a family of potential functions  $\{\psi_C, C \in \mathcal{C}\}$  such that

$$\forall x \in \mathcal{X}: \quad p_X(x) = \frac{1}{Z} \prod_{C \in \mathcal{C}} \psi_C(x),$$
 (7a)

where C is the set of cliques of G and

$$Z := \sum_{x \in \mathcal{X}} \prod_{C \in \mathcal{C}} \psi_C(x). \tag{7b}$$

Since the potential functions in the family  $\{\psi_C, C \in \mathcal{C}\}$  are defined on cliques, we call  $\psi_C$  a *clique potential*. Note that the choice of  $\{\psi_C, C \in \mathcal{C}\}$  is not unique. Indeed, Lemma 2 may be satisfied with a subset of potential functions being identically one.

For a non-trivial set of functions  $\{g_i\}$ , Y is a  $(\mathcal{G}, p_Y)$ -MRF iff we can find a family of potential functions  $\{U_C, C \in \mathcal{C}\}$  such that, for every  $y \in \mathcal{Y}$ 

$$Z \cdot p_Y(y) = Z \cdot \sum_{x \in g^{-1}(y)} p_X(x)$$

$$= \sum_{x \in g^{-1}(y)} \prod_{C \in \mathcal{C}} \psi_C(x) = \prod_{C \in \mathcal{C}} U_C(y) \quad (8)$$

where Z is the partition function from (7b). Such a family can obviously be found if, for all  $y \in \mathcal{Y}$ , the family  $\{\psi_C, C \in \mathcal{C}\}$  is constant on the preimage  $g^{-1}(y) := \{x \in \mathcal{X} : g(x) = y\}$ . Specifically, if for every  $C \in \mathcal{C}$  and for every  $y \in \mathcal{Y}$  we have

$$\psi_C(x) = \psi_C(x'), \ \forall x, x' \in g^{-1}(y),$$
 (9)

then we can choose  $U_C(y)$  as this common value multiplied by the cardinality of the preimage  $g^{-1}(y)$  to satisfy (8). The remainder of this section will give milder conditions than (9) that guarantee lumpability.

For any clique C that contains vertex i, we say  $\psi_C$  depends on  $x_i$  only via  $y_i$  if for all  $y_i \in \mathcal{Y}_i$  and  $x_i, x_i' \in g_i^{-1}(y_i)$ 

$$\psi_C(x_{i}, x_i) = \psi_C(x_{i}, x_i'), \forall x_{i} \in \mathcal{X}_{i}, \tag{10}$$

otherwise, we say  $\psi_C$  strictly depends on  $x_i$ . The following result will assume that for every vertex i there is at most one clique potential that is allowed to strictly depend on  $x_i$ . For all i, let C'(i) denote the corresponding clique. (If no potential function strictly depends on  $x_i$  then C'(i) is chosen as any clique involving i.) We can view this as a mapping  $C' \colon \mathcal{V} \to \mathcal{C}$  that assigns to each vertex i the unique clique that may strictly depend on  $x_i$ , which in effect partitions  $\mathcal{V}$  into equivalence classes  $\mathcal{V}_\ell$ ,  $\ell=1,\ldots,L$ , such that all the vertices  $i\in\mathcal{V}_\ell$  are assigned the same clique C'(i). For convenience, the clique C'(i), common to all  $i\in\mathcal{V}_\ell$ , will be denoted  $C'(\mathcal{V}_\ell)$ .

**Proposition 1.** Assume X is a  $(\mathcal{G}, p_X)$ -MRF characterized by a family  $\{\psi_C, C \in \mathcal{C}\}$  of potential functions such that, for all  $i \in \mathcal{V}$ , there is at most one clique whose potential may strictly depend on  $x_i$ , then Y is a  $(\mathcal{G}, p_Y)$ -MRF.

Moreover, with C' and  $V_1, \ldots, V_L$  as above, the  $(\mathcal{G}, p_Y)$ -MRF is characterized by the family  $\{U_C, C \in \mathcal{C}\}$  of potential functions, where

$$U_{C'(\mathcal{V}_{\ell})}(g(x)) = \sum_{x'_{\mathcal{V}_{\ell}} \in g_{\mathcal{V}_{\ell}}^{-1}(g_{\mathcal{V}_{\ell}}(x_{\mathcal{V}_{\ell}}))} \psi_{C'(\mathcal{V}_{\ell})}(x'_{\mathcal{V}_{\ell}}, x_{\mathcal{V} \setminus \mathcal{V}_{\ell}}) \quad (11a)$$

for  $\ell = 1, \ldots, L$ , and

$$U_C(q(x)) = \psi_C(x), \forall C \in \mathcal{C} \setminus \bigcup_{i \in \mathcal{V}} C'(i).$$
 (11b)

**Corollary 1.** If (9) holds, then Proposition 1 is trivially fulfilled. In this case, C'(i) is any clique of which i is a member and (11a) simplifies to

$$U_{C'(\mathcal{V}_{\ell})}(g(x)) = |g_{\mathcal{V}_{\ell}}^{-1}(g_{\mathcal{V}_{\ell}}(x_{\mathcal{V}_{\ell}}))| \cdot \psi_{C'(\mathcal{V}_{\ell})}(x). \tag{12}$$

Since, even for a fixed joint PMF  $p_X$ , the family of potential functions is not unique, Y is a  $(\mathcal{G}, p_Y)$ -MRF if we can find at least one family of potential functions that characterizes  $p_X$  and for which Proposition 1 holds.

**Example 4.** Let  $X_1 \! - \! X_2 \! - \! X_3$  be a Markov path and fix a set of functions  $\{g_1,g_2,g_3\}$ . Suppose that  $\psi_{\{i\}}$ , for i=1,2,3, are arbitrary, and  $\psi_{\{1,2\}}(x_1,x_2) = U_{\{1,2\}}(g_1(x_1),g_2(x_2))$  and  $\psi_{\{2,3\}}(x_2,x_3) = U_{\{2,3\}}(g_2(x_2),g_3(x_3))$  for some  $U_{\{1,2\}}$  and  $U_{\{2,3\}}$ . Thus, only  $\psi_{\{i\}}$  may strictly depend on  $x_i$ , and so Proposition 1 applies. Now, the same PMF  $p_X$  can be characterized using the potentials  $\psi'_{\{1,2\}} = \psi_{\{1,2\}} \cdot \sqrt{\psi_{\{2\}}},$   $\psi'_{\{2,3\}} = \psi_{\{2,3\}} \cdot \sqrt{\psi_{\{2\}}},$   $\psi'_{\{1\}} = \psi_{\{1\}},$   $\psi'_{\{2\}} = 1$ , and  $\psi_{\{3\}} = \psi_{\{3\}}$ . Assuming  $\psi_2$  strictly depends on  $x_2$ , then both  $\psi_{\{1,2\}}$  and  $\psi'_{\{2,3\}}$  strictly depend on  $x_2$ , and so the condition in Proposition 1 is violated.

We now complement Proposition 1, which is based on clique potentials, by a sufficient condition for lumpability based on conditional entropies. This condition follows from Lemma 1, the data processing inequality, and the fact that conditioning reduces entropy.

**Proposition 2.** Let X be a G-MRF. If, for every  $i \in V$ ,

$$H(Y_i|Y_{\mathcal{N}_i}) = H(Y_i|X_{\mathcal{N}_i}) \tag{13}$$

then Y is a G-MRF.

Equation (13) gives an intuitive interpretation for lumpability of MRFs: If (but not only if, see Example 5 below) the neighbors of  $X_i$  are not more informative about the outcome of  $Y_i$  than the function of these neighbors, then Y is a  $\mathcal{G}$ -MRF. In other words, Y is a  $\mathcal{G}$ -MRF if the lumping is such that  $Y_{\mathcal{N}_i}$  captures all information in  $X_{\mathcal{N}_i}$  that is relevant to  $Y_i$ .

**Example 5.** Let  $X=(X_1,X_2)$  be a Markov path, i.e.,  $\mathcal{V}=\{1,2\}$  and  $E=\{1,2\}$ . Trivially, since  $\mathcal{G}$  is the complete graph, Y is a  $\mathcal{G}$ -MRF for every set of functions  $\{g_1,g_2\}$ . However, one can construct examples for  $p_X$  and  $\{g_1,g_2\}$  such that there exists  $y\in\mathcal{Y}$  and a pair  $x_1,x_1'\in g_1^{-1}(y_1)$  such that

$$p_{Y_2|X_1}(y_2|x_1) \neq p_{Y_2|X_1}(y_2|x_1').$$
 (14)

Thus, the condition of Proposition 2 does not hold, showing that it is only sufficient but not necessary.

There is some similarity between (13) and an information-theoretic sufficient condition for the lumpability of an irreducible and aperiodic Markov chain  $X_1 - X_2 - X_3 - \cdots$  (see [2] for terminology). Suppose that X is stationary, i.e., the alphabets of  $X_i$  are all the same,  $p_{X_{i+1}|X_i} = p_{X_{j+1}|X_j}$  for every  $i,j \in \mathbb{N}$ , and the initial distribution  $p_{X_1}$  coincides with the unique distribution invariant under the one-step conditional distribution  $p_{X_{i+1}|X_i}$ . If further all the functions  $g_i$  are

identical, i.e.,  $g_i = g_0$ ,  $i \in \mathcal{V}$ , for some function  $g_0$ , then one can show that the tuple  $(\mathcal{G}, p_X, g_0)$  is lumpable if [3, Th. 2]

$$H(Y_i|X_{i-1}) = H(Y_i|Y_{i-1}). (15)$$

(By stationarity, it suffices that (15) holds for any i.) The main difference between (13) and (15) is that the latter is conditioned on only a subset of the neighbors, which corresponds to the case in which  $\mathcal G$  is directed, i.e., for  $X_1 \to X_2 \to \cdots$ . Proposition 2 shows that, for undirected graphs, (13) takes the place of (15) in a sufficient condition for lumpability.

We end this section with a sufficient condition for (13) to hold for a MRF with a strictly positive  $p_X$ . Namely, while Proposition 1 restricts the number of cliques whose potential functions strictly depend on  $x_i$ ; it does not restrict the number of components of x on which the potential function of a given clique may strictly depend on. The following proposition limits the number of components (of x) a clique potential may strictly depend on to one.

**Proposition 3.** Let X be a  $(\mathcal{G}, p_X)$ -MRF as in Proposition 1 with  $C'(i) \neq C'(j)$  for every pair of distinct vertices  $i, j \in \mathcal{V}$ , then

$$H(Y_i|Y_{\mathcal{N}_i}) = H(Y_i|X_{\mathcal{N}_i}), \ \forall i \in \mathcal{V}.$$
 (16)

### VI. INFORMATION-PRESERVING MRF LUMPINGS

We next briefly talk about information-preserving lumpings of MRFs, see Problem 2. A lumping can only be information-preserving if g maps the support of  $p_X$  injectively. If the support of  $p_X$  coincides with  $\mathcal{X}$ , then only trivial sets of functions  $\{g_i\}$ , in which every  $g_i$  is injective, can be information-preserving. In this section, we therefore drop the assumption that  $p_X$  is positive on  $\mathcal{X}$ . However, while it is clear that H(X) = H(Y) iff g is injective on the support of  $p_X$ , this does not imply that every  $g_i$  is injective on the support of  $p_{X_i}$ . In other words, a lumping  $(\mathcal{G}, p_X, \{g_i\})$  can be information-preserving even if some or all of the functions  $g_i$  are non-injective, i.e., even if  $H(X_i) > H(Y_i)$  for some  $i \in \mathcal{V}$ .

## **Proposition 4.** Let X be a $(\mathcal{G}, p_X)$ -MRF.

• For any graph  $\mathcal{G}$ , if the lumping  $(\mathcal{G}, p_X, \{g_i\})$  is information-preserving, then

$$\forall i \in \mathcal{V}: \quad H(X_i|Y_i, X_{\mathcal{N}_i}) = 0. \tag{17a}$$

• For any chordal graph  $\mathcal{G}$ , the lumping  $(\mathcal{G}, p_X, \{g_i\})$  is information-preserving if there exist a vertex permutation  $v_1, \ldots, v_N$  and sets  $A_{v_i} = \mathcal{N}_{v_i} \cap \{v_1, \ldots, v_{i-1}\}$  such that

$$\forall i \in \mathcal{V}: \quad H(X_{v_i}|Y_{v_i}, X_{A_{v_i}}) = 0. \tag{17b}$$

**Example 6.** Let  $X_1 = X_2$ , i.e., X is a MRF on a path, which is a chordal graph. Assume that  $g_1 \equiv g_2$  and that  $g = (g_1, g_2)$  is non-injective on the support of  $p_X$ . Thus, H(g(X)) < H(X).

Since  $H(X_1|X_2)=0$  and  $H(X_2|X_1)=0$ , we have  $H(X_1|g_1(X_1),X_2)=0$  and  $H(X_2|g_2(X_2),X_1)=0$ , i.e., the necessary condition for information preservation (17a) holds. However, we have that  $H(X_1|Y_1)>0$  due to the noninjectivity of  $g_1$ , and so (17b) does not hold for the permutation

 $(v_1, v_2) = (1, 2)$ . A similar argument holds for the permutation  $(v_1, v_2) = (2, 1)$ . Thus, the sufficient condition for chordal graphs (17b) is violated.

**Remark 1.** Let  $X_1$ — $X_2$ — $X_3$ — $\cdots$  be an irreducible, aperiodic, and stationary Markov chain. The graph w.r.t. which X is a MRF is an (infinite) path, which is chordal. Since  $A_i = \{i-1\}$  (under the choice  $v_i = i$  for all i) and due to stationarity, the sufficient condition in (17b) simplifies to  $H(X_2|Y_2,X_1)=0$ . We thus recover [3, Prop. 4].

While the condition that g maps the support of  $p_X$  injectively is an equivalent characterization of information-preservation, the conditions in Proposition 4 (that are only necessary or sufficient) have practical justification. Indeed, for alphabets  $\mathcal{X}_i$  with fixed cardinality, the support of  $p_X$  grows exponentially in the number N of vertices. In contrast, (17a) requires checking whether  $g_i$  maps the support of  $p_{X_i|X_{N_i}}$  injectively for every i; the number of parameters characterizing this conditional PMF is exponential only in the size of the neighborhood of i, which is much smaller than N for sparse graphs. Thus, rather than checking g globally, which is exponential in N, it suffices to check a computationally less expensive local condition for each  $g_i$ .

We finally remark that Proposition 4 holds regardless whether Y is a  $\mathcal{G}$ -MRF or not, i.e., whether  $(\mathcal{G}, p_X, \{g_i\})$  is lumpable or not. A better understanding of the interactions between lumpability and information-preservation, i.e., between Problems 1 and 2, seems to be of practical and theoretical interest. Thus, a closer investigation of these interactions shall be the subject of future work.

#### VII. PROOFS

#### A. Proof of Proposition 1

First, note that if for  $C \in \mathcal{C}$  and  $i, j \in \mathcal{V}$  the clique potential  $\psi_C$  is constant on the preimages under  $g_i$  and  $g_j$ , then  $\psi_C$  is also constant on the Cartesian product of these preimages. Indeed, if this is the case, then for all  $x_{\mathcal{V} \setminus \{i,j\}} \in \mathcal{X}_{\mathcal{V} \setminus \{i,j\}}$ , for all  $y_i \in \mathcal{Y}_i$ ,  $y_j \in \mathcal{Y}_j$ , and all  $x_i, x_i' \in g_i^{-1}(y_i)$ ,  $x_j, x_j' \in g_i^{-1}(y_j)$  we have

$$\psi_C(x_{\mathcal{V}}) = \psi_C(x_i', x_{\mathcal{V}\setminus\{i\}}) = \psi_C(x_i', x_j', x_{\mathcal{V}\setminus\{i,j\}}), \quad (18)$$

where the first and second equalitys follow from the assumption that  $\psi_C$  is constant on the preimages under  $g_i$  and  $g_j$ , respectively. Thus, if  $\psi_C$  depends on  $x_i$  only via  $y_i$  and on  $x_j$  only via  $y_j$ , then it also depends on  $x_{\{i,j\}}$  only via  $y_{\{i,j\}}$ .

We write

$$Z \cdot p_Y(y) = \sum_{x \in g^{-1}(y)} \prod_{C'(i): i \in \mathcal{V}} \psi_{C'(i)}(x) \prod_{C \in \mathcal{C} \setminus \bigcup_{j \in \mathcal{V}} C'(j)} \psi_C(x) \quad (19)$$

where the second product is a product over cliques whose potentials are constant on the preimages under g. In other words, each potential in the second product depends on x only

via y, and so we can define a potential function  $U_C: \mathcal{Y} \to \mathbb{R}$  by setting  $U_C(g(x)) := \psi_C(x)$ . From this, we have

$$Z \cdot p_{Y}(y) = \prod_{C \in \mathcal{C} \setminus \bigcup_{j \in \mathcal{V}} C'(j)} U_{C}(y) \times \sum_{x \in g^{-1}(y)} \prod_{C'(i):i \in \mathcal{V}} \psi_{C'(i)}(x)$$

$$= \prod_{C \in \mathcal{C} \setminus \bigcup_{j \in \mathcal{V}} C'(j)} U_{C}(y) \times \sum_{x v_{1} \in g_{\mathcal{V}_{1}}^{-1}(yv_{1})} \cdots \sum_{x v_{L} \in g_{\mathcal{V}_{L}}^{-1}(yv_{\ell})} \prod_{C'(i):i \in \mathcal{V}} \psi_{C'(i)}(x)$$

$$= \prod_{C \in \mathcal{C} \setminus \bigcup_{j \in \mathcal{V}} C'(j)} U_{C}(y) \times \prod_{\ell=1}^{L} \sum_{x v_{\ell} \in g_{\mathcal{V}_{\ell}}^{-1}(yv_{\ell})} \psi_{C'(\mathcal{V}_{\ell})}(xv_{\ell}, x'_{\mathcal{V} \setminus \mathcal{V}_{\ell}}),$$

where  $x'_{\mathcal{V}\setminus\mathcal{V}_{\ell}}$  is such that  $g_{\mathcal{V}\setminus\mathcal{V}_{\ell}}(x'_{\mathcal{V}\setminus\mathcal{V}_{\ell}})=y_{\mathcal{V}\setminus\mathcal{V}_{\ell}}$ , and the last equality follows from (18) since  $\psi_{C'(\mathcal{V}_{\ell})}$  depends on  $x_i$  only via  $y_i$  for all  $i\in\mathcal{V}\setminus\mathcal{V}_{\ell}$ . Define clique potentials  $U_{C'(\mathcal{V}_{\ell})}\colon\mathcal{Y}\to\mathbb{R}$  by setting

$$U_{C'(\mathcal{V}_{\ell})}(g(x)) := \sum_{x'_{\mathcal{V}_{\ell}} \in g_{\mathcal{V}_{\ell}}^{-1}(g_{\mathcal{V}_{\ell}}(x_{\mathcal{V}_{\ell}}))} \psi_{C'(\mathcal{V}_{\ell})}(x'_{\mathcal{V}_{\ell}}, x_{\mathcal{V} \setminus \mathcal{V}_{\ell}}),$$

$$(20)$$

then we have

$$Z \cdot p_Y(y) = \prod_{C \in \mathcal{C} \setminus \bigcup_{i \in \mathcal{V}} C'(i)} U_C(y) \times \prod_{\ell=1}^L U_{C'(\mathcal{V}_\ell)}(y) = \prod_{C \in \mathcal{C}} U_C(y),$$

which completes the proof.

#### B. Proof of Proposition 2

Since X is a  $\mathcal{G}$ -MRF and  $Y_i$  is a function of  $X_i$ , we have  $H(Y_i|X_{\mathcal{N}_i})=H(Y_i|X_{ij})\leq H(Y_i|Y_{ij})\leq H(Y_i|Y_{\mathcal{N}_i})$ , where the first and second inequalities are due to the data processing inequality and the fact that conditioning reduces the entropy, respectively. Thus, given (13), the above inequalitis hold with equality, i.e., we have  $H(Y_i|Y_{ij})=H(Y_i|Y_{\mathcal{N}_i})$ . Lemma 1 completes the proof.

### C. Proof of Proposition 3

We have, for all  $x \in \mathcal{X}$ ,

$$p_{X_i|X_{ij}}(x_i|x_{ij}) = \frac{\prod_{C \in \mathcal{A}} \psi_C(x)}{\sum_{x_i' \in \mathcal{X}_i} \prod_{C \in \mathcal{A}} \psi_C(x_i', x_{ij})}$$
$$= p_{X_i|X_{\mathcal{N}_i}}(x_i|x_{\mathcal{N}_i}), \tag{21}$$

where  $A \subseteq C$  is the set of cliques containing vertex i. The first equality is by (7a) and the definition of the conditional

distribution, and the second equality is by the definition of a MRF (3). Fix  $y \in \mathcal{Y}$  and  $x \in g^{-1}(y)$ , then we have

$$\begin{split} & p_{Y_i|X_{\mathcal{N}_i}}(y_i|x_{\mathcal{N}_i}) \\ & \stackrel{(\underline{a})}{=} \frac{\sum\limits_{\substack{x_i' \in g_i^{-1}(y_i) \\ \sum\limits_{i' \in \mathcal{Y}_i} \sum\limits_{\substack{x_i'' \in g_i^{-1}(y_i') \\ i'' \in \mathcal{A}}} \prod\limits_{\substack{V_C(x_i'', x_i') \\ V_C(y_i', y_i')}} \psi_{C'(i)}(x_i', x_i') \\ & \stackrel{(\underline{b})}{=} \frac{\prod\limits_{\substack{C \in \mathcal{A} \backslash \{C'(i)\} \\ y_i' \in \mathcal{Y}_i}} \prod\limits_{\substack{C \in \mathcal{A} \backslash \{C'(i)\} \\ V_C(y_i', y_i')}} U_{C}(y_i', y_i') \times \sum\limits_{\substack{x_i'' \in g_i^{-1}(y_i') \\ x_i'' \in g_i^{-1}(y_i')}} \psi_{C'(i)}(x_i'', x_i') \\ & \stackrel{(\underline{c})}{=} \frac{\prod\limits_{\substack{C \in \mathcal{A} \backslash \{C'(i)\} \\ \sum\limits_{\substack{C \in \mathcal{A} \backslash \{C'(i)\} \\ V_i' \in \mathcal{Y}_i}}} U_{C}(y_i', y_i')} \\ & = p_{Y_i|Y_{\mathcal{N}_i}}(y_i|y_{\mathcal{N}_i}), \end{split}$$

as desired. In the above, (a) follows from (21) using  $p_{Y_i|X_{\mathcal{N}_i}}(y_i|x_{\mathcal{N}_i}) = \sum_{x_i' \in g_i^{-1}(y_i)} p_{X_i|X_{\mathcal{N}_i}}(x_i'|x_{\mathcal{N}_i})$  and the fact that the set of preimages  $g^{-1}(y_i)$ , for  $y_i \in \mathcal{Y}_i$ , is a partition of  $\mathcal{X}_i$ ; (b) follows since at most one clique C'(i) may strictly depend on  $x_i$  where we define  $U_C(g(x)) := \psi_C(x)$  for  $C \in \mathcal{A} \setminus \{C'(i)\}$ ; and (c) follows since the potential function of C'(i) depends on  $x_{i'}$  only via  $y_{i'}$  where we define  $U_{C'(i)}(y) := \sum_{x_i' \in g_i^{-1}(y_i)} \psi_{C'(i)}(x_i', x_{i'})$ , see (18) (or (20)).

## D. Proof of Proposition 4

Note that a lumping is information-preserving iff H(X|Y)=0, then we have

$$0 = H(X|Y) \stackrel{\text{(a)}}{=} \sum_{i=1}^{|\mathcal{V}|} H(X_i|X_1^{i-1}, Y)$$

$$\stackrel{\text{(b)}}{\geq} \sum_{i=1}^{|\mathcal{V}|} H(X_i|X_{i'}, Y)$$

$$\stackrel{\text{(c)}}{=} \sum_{i=1}^{|\mathcal{V}|} H(X_i|X_{i'}, Y_i)$$

$$\stackrel{\text{(d)}}{=} \sum_{i=1}^{|\mathcal{V}|} H(X_i|X_{\mathcal{N}_i}, Y_i),$$

where (a) is by the chain rule of entropy, (b) by the fact that conditioning reduces entropy, (c) by  $Y_j = g_j(X_j)$  for  $j \neq i$ , and (d) by the fact that X is a  $\mathcal{G}$ -MRF.

The proof of the sufficient condition for chordal graphs makes use of the following lemma stating that for a MRF on a chordal graph the entropy can be decomposed in a particular form.

**Lemma 3.** If  $\mathcal{G}$  is chordal, then there exists a permutation  $v_1, \ldots, v_N$  of the vertex indices such that

$$H(X) = \sum_{i=1}^{N} H(X_{v_i}|X_{A_{v_i}})$$
 (22)

for  $A_{v_i} = \mathcal{N}_{v_i} \cap \{v_1, \dots, v_{i-1}\}.$ 

To prove the sufficient condition, we have

$$\begin{split} H(X) &\stackrel{\text{(a)}}{=} \sum_{i=1}^{N} H(X_{v_{i}}|X_{A_{v_{i}}}) \\ &\stackrel{\text{(b)}}{=} \sum_{i=1}^{N} H(X_{v_{i}},Y_{v_{i}}|X_{A_{v_{i}}}) \\ &= \sum_{i=1}^{N} \left( H(Y_{v_{i}}|X_{A_{v_{i}}}) + H(X_{v_{i}}|X_{A_{v_{i}}},Y_{v_{i}}) \right) \\ &\stackrel{\text{(c)}}{=} \sum_{i=1}^{N} \left( H(X_{v_{i}}|X_{A_{v_{i}}},Y_{v_{i}}) + H(Y_{v_{i}}|X_{A_{v_{i}}},Y_{v_{1},...,v_{i-1}}) \right) \\ &\stackrel{\text{(d)}}{\leq} \sum_{i=1}^{N} \left( H(X_{v_{i}}|X_{A_{v_{i}}},Y_{v_{i}}) + H(Y_{v_{i}}|Y_{v_{1},...,v_{i-1}}) \right) \\ &\stackrel{\text{(e)}}{=} \sum_{i=1}^{N} H(X_{v_{i}}|X_{A_{v_{i}}},Y_{v_{i}}) + H(Y), \end{split}$$

where (a) is by Lemma 3, (b) is because  $Y_{v_i}$  is a function of  $X_{v_i}$ , (c) is because  $Y_{v_i}$  and  $Y_{\{v_1,\ldots,v_{i-1}\}}$  are independent conditioned on  $X_{A_{v_i}}$ , (d) is because conditioning reduces the entropy, and (e) is by the entropy chain rule. Now the claim follows from H(X|Y) = H(X) - H(Y), which is true since Y is a function of X.

Proof of Lemma 3: A maximum cardinality search [10, Section 3.2.4] provides the desired permutation, where the permutation can also be viewed as an orientation of the graph into a directed acyclic graph (DAG). Since the original graph is chordal, the resulting DAG is such that the tails of any two converging arrows are adjacent, and so d-separation (on the DAG) and vertex cuts (on the original graph) are equivalent. That is, they describe the same independence structure, i.e., the same family of distributions. Now the factorization form (22) is easy to obtain from the DAG.

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