
Automorphism Groups of Graphical Models and Lifted Variational Inference

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Abstract

Using the theory of group action, we first introduce the concept of the *automorphism group* of an exponential family or a graphical model, thus formalizing the general notion of symmetry of a probabilistic model. This automorphism group provides a precise mathematical framework for lifted inference in the general exponential family. Its group action partitions the set of random variables and feature functions into equivalent classes (called orbits) having identical marginals and expectations. Then the inference problem is effectively reduced to that of computing marginals or expectations for each class, thus avoiding the need to deal with each individual variable or feature. We demonstrate the usefulness of this general framework in lifting two classes of variational approximation for MAP inference: local LP relaxation and local LP relaxation with cycle constraints; the latter yields the first lifted inference that operate on a bound tighter than local constraints. Initial experimental results demonstrate that lifted MAP inference with cycle constraints achieved the state of the art performance, obtaining much better objective function values than local approximation while remaining relatively efficient.

1 Introduction

Classical approaches to probabilistic inference – an area now reasonably well understood – have traditionally exploited low tree-width and sparsity of the graphical model for efficient exact and approximate inference. A more recent approach known as *lifted inference* [3, 13, 7, 8] has demonstrated the possibility to perform very efficient inference in highly-connected, but *symmetric* models such as those arising in the context of relational (or first-order) probabilistic models. While it is clear that symmetry is the essential element in lifted inference, there is currently no formally defined notion of symmetry of a probabilis-

tic model, and thus no formal account of what “exploiting symmetry” means in lifted inference.

The mathematical formulation of symmetry of an object is typically defined via a set of transformations that preserve the object of interest. Since this set forms a mathematical group (so-called the *automorphism group* of that object), the theory of groups and group action are essential in the study of symmetry.

In this paper, we first introduce the concept of the *automorphism group* of an exponential family or a graphical model, thus formalizing the notion of symmetry of a general graphical model. This automorphism group provides a precise mathematical framework for lifted inference in graphical models. Its group action partitions the set of random variables and feature functions into equivalent classes (a.k.a. orbits) having identical marginals and expectations. The inference problem is effectively reduced to that of computing marginals or expectations for each class, thus avoiding the need to deal with each individual variable or feature. We demonstrate the usefulness of this general framework in lifting two classes of variational approximation for MAP inference: local LP relaxation and local LP relaxation with cycle constraints; the latter yields the first lifted inference that operates on a bound tighter than local constraints. Initial experimental results demonstrate that lifted MAP inference with cycle constraints achieved the state of the art performance, obtaining much better objective function values than local approximation while remaining relatively efficient.

For brevity, we omit the proofs of all theorems in this paper. All the proofs can be found in the extended version [2].

2 Background on Groups and Graph Automorphisms

A *partition* $\Delta = \{\Delta_1 \dots \Delta_k\}$ of a set V is a set of disjoint nonempty subsets of V whose union is V . Each element Δ_i is called a *cell*. A partition Δ defines an equivalence relation on V , denoted as $\overset{\Delta}{\sim}$, by letting $u \overset{\Delta}{\sim} v$ iff u and v are in the same cell. A partition Λ is finer than Δ if every

cell of Λ is a subset of some cell of Δ .

We now briefly review some important concepts in group theory and graph automorphisms [6].

A *group* (\mathbb{G}, \cdot) is a non-empty set \mathbb{G} with a binary operation \cdot such that it is associative, closed in \mathbb{G} ; \mathbb{G} contains an identity element, denoted as $\mathbf{1}$, such that $\forall g \in \mathbb{G}, \mathbf{1} \cdot g = g \cdot \mathbf{1} = g$ and there exists an element g^{-1} such that $g \cdot g^{-1} = g^{-1} \cdot g = \mathbf{1}$. A group containing $\mathbf{1}$ as its only element is called a *trivial group*. A *subgroup* of \mathbb{G} is a subset of \mathbb{G} that forms a group with the same binary operation as \mathbb{G} . We write $\mathbb{G}_1 \leq \mathbb{G}_2$ when \mathbb{G}_1 is a subgroup¹ of \mathbb{G}_2 .

A permutation on a set V is a bijective mapping from V to itself. The set of all permutations of V together with the mapping-composition operator forms a group named the *symmetric group* $\mathbb{S}(V)$. A symmetric group that plays a central role in this paper is the symmetric group \mathbb{S}_n , the set of all permutations of $\{1, 2, \dots, n\}$. For a permutation $\pi \in \mathbb{S}_n$, $\pi(i)$ is the image of i under π . For each vector $x \in \mathcal{X}^n$, the vector x permuted by π , denoted by x^π , is $(x_{\pi(1)} \dots x_{\pi(n)})$; for a set $A \subset \mathcal{X}^n$, the set A permuted by π , denoted by A^π is $\{x^\pi | x \in A\}$.

The *action* of a group \mathbb{G} on a set V is a mapping that assigns every $g \in \mathbb{G}$ to a permutation on V , denoted as $g(\cdot) : V \rightarrow V$ such that the identity element $\mathbf{1}$ is assigned to the identity permutation, and the group product of two elements $g_1 \cdot g_2$ is assigned to the composition $g_1(\cdot) \circ g_2(\cdot)$. The action of a group \mathbb{G} on V induces an equivalence relation on V defined as $v \sim v'$ iff there exists $g \in \mathbb{G}$ such that $g(v) = v'$ (the fact that \sim is an equivalence relation follows from the definition of group). The group action therefore induces a partition on V called the *orbit partition*, denoted as $\text{Orb}_{\mathbb{G}}(V)$. The *orbit* of an element $v \in V$ under the action of \mathbb{G} is the set of elements in V equivalent to v : $\text{orb}_{\mathbb{G}}(v) = \{v' \in V | v' \sim v\}$. Any subgroup $\mathbb{G}_1 \leq \mathbb{G}$ will also act on V and induces a finer equivalence relation (and hence a more refined orbit partition). Given $v \in V$, if under the group action, every element $g \in \mathbb{G}$ preserves v , that is $\forall g \in \mathbb{G}, g(v)=v$, then the group \mathbb{G} is said to stabilize v .

Next, we consider the action of a permutation group on the vertex set of graph, which leads to the concept of graph automorphisms.

An *automorphism* of a graph \mathfrak{G} on a set of vertices V is a permutation $\pi \in \mathbb{S}(V)$ that permutes the vertices of \mathfrak{G} but preserves the structure (e.g., adjacency, direction, color) of \mathfrak{G} . The set of all automorphisms of \mathfrak{G} forms a group named the *automorphism group* of \mathfrak{G} , denoted as $\mathbb{A}(\mathfrak{G})$. It is clear that $\mathbb{A}(\mathfrak{G})$ is a subgroup of $\mathbb{S}(V)$. The cardinality of $\mathbb{A}(\mathfrak{G})$ indicates the level of symmetry in \mathfrak{G} ; if $\mathbb{A}(\mathfrak{G})$ is the trivial group then \mathfrak{G} is asymmetric.

The action of $\mathbb{A}(\mathfrak{G})$ on the vertex set V partitions V into the node-orbits $\text{Orb}_{\mathbb{A}(\mathfrak{G})}(V)$ where each node orbit is a set of vertices equivalent to one another up to some node rela-

beling. Furthermore, $\mathbb{A}(\mathfrak{G})$ also acts on the set of graph edges E by letting $\pi(\{u, v\}) = \{\pi(u), \pi(v)\}$ and this action partitions E into a set of edge-orbits $\text{Orb}_{\mathbb{A}(\mathfrak{G})}(E)$.

Similarly, we also obtain the set of arc-orbits $\text{Orb}_{\mathbb{A}(\mathfrak{G})}(\vec{E})$.

Computing the automorphism group of a graph is as difficult as determining whether two graphs are isomorphic, a problem that is known to be in NP, but for which it is unknown whether it has a polynomial time algorithm or is NP-complete. In practice, there exists efficient computer programs such as *nauty*² [9] for computing automorphism groups of graphs.

3 Symmetry of the Exponential Family

3.1 Exponential Family and Graphical Model

Consider an exponential family over n random variables $(x_i)_{i \in \mathcal{V}}$ where $\mathcal{V} = \{1 \dots n\}$, $x_i \in \mathcal{X}$ with density function

$$\mathcal{F}(x | \theta) = h(x) \exp(\langle \Phi(x), \theta \rangle - A(\theta))$$

where h is the base density, $\Phi(x) = (\phi_j(x))_{j \in \mathcal{I}}$, $\mathcal{I} = \{1, 2, \dots, m\}$ is an m -dimensional feature vector, $\theta \in \mathbb{R}^m$ is the natural parameter, and $A(\theta)$ the log-partition function. Let $\Theta = \{\theta | A(\theta) < \infty\}$ be the set of natural parameters, $\mathcal{M} = \{\mu \in \mathbb{R}^m | \exists p, \mu = E_p \Phi(x)\}$ the set of realizable mean parameters, $A^* : \mathcal{M} \rightarrow \mathbb{R}$ the convex dual of A , and $\mathbf{m} : \Theta \rightarrow \mathcal{M}$ the mean parameter mapping that maps $\theta \mapsto \mathbf{m}(\theta) = E_\theta \Phi(x)$. Note that $\mathbf{m}(\Theta) = \text{ri } \mathcal{M}$ is the relative interior of \mathcal{M} . For more details, see [16].

Often, a feature function ϕ_i depends only on a subset of the variables in \mathcal{V} . In this case we will write ϕ_i more compactly in factorized form as $\phi_i(x) = f_i(x_{i_1} \dots x_{i_K})$ where the indices i_j are distinct, $i_1 < i_2 \dots < i_K$, and f_i cannot be reduced further, i.e., it must depend on all of its arguments. To keep track of variable indices of arguments of f_i , we let $\text{scope}(f_i)$ denote its set of arguments, $\eta_i(k) = i_k$ the k -th argument and $|\eta_i|$ its number of arguments. Factored forms of features can be encoded as a hypergraph $\mathcal{G}[\mathcal{F}]$ of \mathcal{F} (called the graph structure or graphical model of \mathcal{F}) with nodes \mathcal{V} , and hyperedges (clusters) $\{C | \exists i, \text{scope}(f_i) = C\}$. For models with pairwise features, \mathcal{G} is a standard graph.

For discrete random variables (i.e., \mathcal{X} is finite), we often want to work with the overcomplete family \mathcal{F}^o that we now describe for the case with pairwise features. The set of overcomplete features \mathcal{I}^o are indicator functions on the nodes and edges of the graphical model \mathcal{G} of \mathcal{F} : $\phi_{u:t}^o(x) = \mathbb{I}\{x_u = t\}$, $t \in \mathcal{X}$ for each node $u \in V(\mathcal{G})$; and $\phi_{\{u:t, v:t'\}}^o(x) = \mathbb{I}\{x_u = t, x_v = t'\}$, $t, t' \in \mathcal{X}$ for each edge $\{u, v\} \in E(\mathcal{G})$. The set of overcomplete realizable mean parameters \mathcal{M}^o is also called the *marginal polytope* since the overcomplete mean parameter corresponds to node and edge marginal probabilities. Given a parameter θ , the transformation of $\mathcal{F}(x|\theta)$ to

¹We use the notation $\mathbb{G}_1 \preceq \mathbb{G}_2$ to mean \mathbb{G}_1 is isomorphic to a subgroup of \mathbb{G}_2 .

²<http://cs.anu.edu.au/people/bdm/nauty/>

its overcomplete representation is done by letting θ^o be the corresponding parameter in the overcomplete family: $\theta_{u:t}^o = \sum_{i \text{ s.t. } \text{scope}(f_i)=\{u\}} f_i(t)\theta_i$ and (assuming $u < v$) $\theta_{\{u:t,v:t'\}}^o = \sum_{i \text{ s.t. } \text{scope}(f_i)=\{u,v\}} f_i(t,t')\theta_i$. It is straightforward to verify that $\mathcal{F}^o(x|\theta^o) = \mathcal{F}(x|\theta)$.

3.2 Automorphism Group of an Exponential Family

We define the symmetry of an exponential family \mathcal{F} as the group of transformations that preserve \mathcal{F} (hence preserve h and Φ). The kind of transformation used will be a pair of permutations (π, γ) where π permutes the set of variables and γ permutes the feature vector.

Definition 3.1. An automorphism of the exponential family \mathcal{F} is a pair of permutations (π, γ) where $\pi \in \mathbb{S}_n$, $\gamma \in \mathbb{S}_m$ such that for all vectors x : $h(x^\pi) = h(x)$ and $\Phi^{\gamma^{-1}}(x^\pi) = \Phi(x)$ (or equivalently, $\Phi(x^\pi) = \Phi^\gamma(x)$).

It is straightforward to show that the set of all automorphisms of \mathcal{F} , denoted by $\mathbb{A}[\mathcal{F}]$, forms a subgroup of $\mathbb{S}_n \times \mathbb{S}_m$. This group acts on \mathcal{I} by the permuting action of γ , and on \mathcal{V} by the permuting action of π . In the remainder of this paper, h is always a symmetric function (e.g., $h \equiv 1$); therefore, the condition $h(x^\pi) = h(x)$ automatically holds.

Example. Let $\mathcal{V} = \{1, 2, 3\}$ and $\Phi = \{f_1, f_2, f_3\}$ where $f_1(x_1, x_2) = x_1(1 - x_2)$, $f_2(x_1, x_3) = x_1(1 - x_3)$, and $f_3(x_2, x_3) = x_2x_3$. The pair of permutations (π, γ) where $\pi = (1 \mapsto 1, 2 \mapsto 3, 3 \mapsto 2)$ and $\gamma = (1 \mapsto 2, 2 \mapsto 1, 3 \mapsto 3)$ is an automorphism of \mathcal{F} , since $\Phi^{\gamma^{-1}}(x^\pi) = (\phi_2(x_1, x_3, x_2), \phi_1(x_1, x_3, x_2), \phi_3(x_1, x_3, x_2)) = (f_2(x_1, x_2), f_1(x_1, x_3), f_3(x_3, x_2)) = (x_1(1 - x_2), x_1(1 - x_3), x_3x_2) = \Phi(x_1, x_2, x_3)$.

An automorphism (π, γ) can be characterized in terms of the factorized features f_i as follows.

Proposition 3.1. (π, γ) is an automorphism of \mathcal{F} if and only if the following conditions are true for all $i \in \mathcal{I}$: (1) $|\eta_i| = |\eta_{\gamma(i)}|$; (2) π is a bijective mapping from $\text{scope}(f_i)$ to $\text{scope}(f_{\gamma(i)})$; (3) let $\alpha = \eta_{\gamma(i)}^{-1} \circ \pi \circ \eta_i$ then $\alpha \in \mathbb{S}_{|\eta_i|}$ and $f_i(t^\alpha) = f_{\gamma(i)}(t)$ for all $t \in \mathcal{X}^{|\eta_i|}$.

Remark. Consider automorphisms of the type $(1, \gamma)$: γ must permute between the features having the same scope: $\text{scope}(f_i) = \text{scope}(f_{\gamma(i)})$. Thus if the features do not have redundant scopes (i.e., $\text{scope}(f_i) \neq \text{scope}(f_j)$ when $i \neq j$) then γ must be $\mathbf{1}$. More generally when features do not have redundant scopes, π uniquely determines γ . Next, consider automorphisms of the type $(\pi, \mathbf{1})$: π must permute among variables in a way that preserve all the features f_i . Thus if all features are asymmetric functions then π must be $\mathbf{1}$; more generally, γ uniquely determines π . As a consequence, if the features do not have redundant scopes and are asymmetric functions then there exists a one-to-one correspondence between π and γ that form an automorphism in $\mathbb{A}[\mathcal{F}]$.

An automorphism defined above preserves a number of key characteristics of the exponential family \mathcal{F} (such as its

natural parameter space, its mean parameter space, its log-partition function), as shown in the following theorem.

Theorem 3.1. If $(\pi, \gamma) \in \mathbb{A}[\mathcal{F}]$ then

1. $\pi \in \mathbb{A}(\mathcal{G}[\mathcal{F}])$, i.e. π is an automorphism of the graphical model graph $\mathcal{G}[\mathcal{F}]$.
2. $\Theta^\gamma = \Theta$ and $A(\theta^\gamma) = A(\theta)$ for all $\theta \in \Theta$.
3. $\mathcal{F}(x^\pi|\theta^\gamma) = \mathcal{F}(x|\theta)$ for all $x \in \mathcal{X}^n$, $\theta \in \Theta$.
4. $\mathbf{m}^\gamma(\theta) = \mathbf{m}(\theta)$ for all $\theta \in \Theta$.
5. $\mathcal{M}^\gamma = \mathcal{M}$ and $A^*(\mu^\gamma) = A^*(\mu)$ for all $\mu \in \mathcal{M}$.

4 Lifted Variational Inference Framework

We now discuss the principle of how to exploit the symmetry of the exponential family graphical model for lifted variational inference. In the general variational inference framework [16], marginal inference is viewed as to compute the mean parameter $\mu = \mathbf{m}(\theta)$ given a natural parameter θ by solving the optimization problem

$$\sup_{\mu \in \mathcal{M}} \langle \theta, \mu \rangle - A^*(\mu). \quad (4.1)$$

For discrete models, the variational problem is more conveniently posed using the overcomplete parameterization, for marginal inference

$$\sup_{\mu^o \in \mathcal{M}^o} \langle \mu^o, \theta^o \rangle - A^{*o}(\mu^o) \quad (4.2)$$

and for MAP inference

$$\max_{x \in \mathcal{X}^n} \ln \mathcal{F}(x|\theta) = \sup_{\mu^o \in \mathcal{M}^o} \langle \mu^o, \theta^o \rangle + \text{const}. \quad (4.3)$$

We first focus on lifting the main variational problem in (4.1) and leave discussions of the other problems to subsection 4.3.

4.1 Parameter Tying and Lifting Partition

Lifted inference in essence assumes a parameter-tying setting where some components of θ are the same. More precisely, we assume a partition Δ of \mathcal{I} (called the *parameter-tying partition*) such that $j \overset{\Delta}{\sim} j' \Rightarrow \theta_j = \theta_{j'}$. Our goal is to study how parameter-tying, coupled with the symmetry of the family \mathcal{F} , can lead to more efficient variational inference.

Let \mathbb{R}_Δ^m denote the subspace $\{r \in \mathbb{R}^m \mid r_j = r_{j'} \text{ if } j \overset{\Delta}{\sim} j'\}$. For any set $S \subset \mathbb{R}^m$, let $S_\Delta = S \cap \mathbb{R}_\Delta^m$. Restricting the natural parameter to Θ_Δ is equivalent to parameter tying, and hence, equivalent to working with a different exponential family with $|\Delta|$ aggregating features $(\sum_{j \in \Delta_i} \phi_j)_i$. While this family has fewer parameters, it is not obvious how it would help inference; moreover, in working directly with the

aggregation features, the structure of the original family is lost.

To investigate the effect parameter tying has on the complexity of inference, we turn to the question of how to characterize the image of Θ_Δ under the mean mapping \mathbf{m} . At first, note that in general $\mathbf{m}(\Theta_\Delta) \neq \mathcal{M}_\Delta$: taking Δ to be the singleton partition $\{\mathcal{I}\}$ will enforce all natural parameters to be the same, but clearly this does not guarantee that all mean parameters are the same. However, one can hope that perhaps some mean parameters are forced to be the same due to the symmetry of the graphical model. More precisely, we ask the following question: is there a partition φ of \mathcal{I} such that for all $\theta \in \Theta_\Delta$ the mean parameter is guaranteed to lie inside \mathcal{M}_φ , and therefore the domain of the variational problem (4.1) can be restricted accordingly to \mathcal{M}_φ ? Such partitions are defined for general convex optimization problems below.

Definition 4.1. (Lifting partition) Consider the convex optimization $\inf_{x \in S} J(x)$ where $S \subset \mathbb{R}^m$ is a convex set and J is a convex function. A partition φ of $\{1 \dots m\}$ is a *lifting partition* for the aforementioned problem iff $\inf_{x \in S} J(x) = \inf_{x \in S_\varphi} J(x)$, i.e., the constraint set S can be restricted to S_φ .

Theorem 4.1. Let \mathbb{G} act on $I = \{1 \dots m\}$, so that every $g \in \mathbb{G}$ corresponds to some permutation on $\{1 \dots m\}$. If $S^g = S$ and $J(x^g) = J(x)$ for every $g \in \mathbb{G}$ (i.e., \mathbb{G} stabilizes both S and J) then the induced orbit partition $\text{Orb}_\mathbb{G}(I)$ is a lifting partition for $\inf_{x \in S} J(x)$.

From theorem 3.1, we know that $\mathbb{A}[\mathcal{F}]$ stabilizes \mathcal{M} and A^* ; however, this group does not take the parameter θ into account. Given a partition Δ , a permutation λ on \mathcal{I} is consistent with Δ iff λ permutes only among elements of the same cell of Δ . Such permutations are of special interest since for every $\theta \in \Theta_\Delta$, $\theta^\lambda = \theta$. If \mathbb{G} is a group acting on \mathcal{I} , we denote \mathbb{G}_Δ the set of group elements whose actions are consistent with Δ , that is $\mathbb{G}_\Delta = \{g \in \mathbb{G} \mid \forall u \in \mathcal{I}, g(u) \overset{\Delta}{\sim} u\}$. It is straightforward to verify that \mathbb{G}_Δ is a subgroup of \mathbb{G} . With this notation, $\mathbb{A}_\Delta(\mathcal{F})$ is the subgroup of $\mathbb{A}[\mathcal{F}]$ whose member's action is consistent with Δ . The group $\mathbb{A}_\Delta(\mathcal{F})$ thus stabilizes not just the family \mathcal{F} , but also every parameter $\theta \in \Theta_\Delta$. It is straightforward to verify that $\mathbb{A}_\Delta(\mathcal{F})$ stabilizes both the constraint set and the objective function of (4.1). Therefore by the previous theorem, its induced orbit yields a lifting partition.

Corollary 4.1. Let $\varphi = \varphi(\Delta) = \text{Orb}_{\mathbb{A}_\Delta(\mathcal{F})}(\mathcal{I})$. Then for all $\theta \in \Theta_\Delta$, φ is a lifting partition for the variational problem (4.1), that is

$$\sup_{\mu \in \mathcal{M}} \langle \theta, \mu \rangle - A^*(\mu) = \sup_{\mu \in \mathcal{M}_\varphi} \langle \theta, \mu \rangle - A^*(\mu) \quad (4.4)$$

In (4.4), we call the LHS the *ground* formulation of the variational problem, and the RHS the *lifted* formulation. Let $\ell = |\varphi|$ be the number of cells of φ , the *lifted* constraint set \mathcal{M}_φ then effectively lies inside an ℓ -dimensional

subspace where $\ell \leq m$. This forms the core idea of the principle of lifted variational inference: to perform optimization over the lower dimensional (and hopefully easier) constraint set \mathcal{M}_φ instead of \mathcal{M} .

Remark. The above result also holds for *any subgroup* \mathbb{G} of $\mathbb{A}_\Delta(\mathcal{F})$ since $\varphi_\mathbb{G} = \text{Orb}_\mathbb{G}(\mathcal{I})$ is finer than φ . Thus, it is obvious that $\varphi_\mathbb{G}$ is also a lifting partition. However, the smaller is the group \mathbb{G} , the finer is the lifting partition $\varphi_\mathbb{G}$, and the less symmetry can be exploited. In the extreme, \mathbb{G} can be the trivial group, $\varphi_\mathbb{G}$ is the discrete partition on \mathcal{I} putting each element in its own cell, and $\mathcal{M}_{\varphi_\mathbb{G}} = \mathcal{M}$, which corresponds to no lifting.

4.2 Characterization of \mathcal{M}_φ

We now give a characterization of \mathcal{M}_φ in the case of discrete random variables. Note that \mathcal{M} is the convex hull $\mathcal{M} = \text{conv} \{\Phi(x) \mid x \in \mathcal{X}^n\}$ which is a polytope in \mathbb{R}^m , and $\mathbb{A}[\mathcal{F}]$ acts on the set of configurations \mathcal{X}^n by the permuting action of π which maps $x \mapsto x^\pi$.

Theorem 4.2. Let $\mathcal{O} = \text{Orb}_{\mathbb{A}_\Delta(\mathcal{F})}(\mathcal{X}^n)$ be the set of \mathcal{X} -configuration orbits. For each orbit $\mathcal{C} \in \mathcal{O}$, let $\bar{\Phi}(\mathcal{C}) = \frac{1}{|\mathcal{C}|} \sum_{x \in \mathcal{C}} \Phi(x)$ be the feature-centroid of all the configurations x in \mathcal{C} . Then $\mathcal{M}_{\varphi(\Delta)} = \text{conv} \{\bar{\Phi}(\mathcal{C}) \mid \mathcal{C} \in \mathcal{O}\}$.

As a consequence, the *lifted polytope* \mathcal{M}_φ can have at most $|\mathcal{O}|$ extreme points. The number of configuration orbits $|\mathcal{O}|$ can be much smaller than the total number of configurations $|\mathcal{X}|^n$ when the model is highly symmetric. For example, for a fully connected graphical model with identical pairwise and unary potentials and $\mathcal{X} = \{0, 1\}$ then every permutation $\pi \in \mathbb{S}_n$ is part of an automorphism; thus, every configuration with the same number of 1's belongs to the same orbit, and hence $|\mathcal{O}| = n+1$. In general, however, $|\mathcal{O}|$ often is still exponential in n . We discuss approximations of \mathcal{M}_φ in Section 5.

A representation of the lifted polytope \mathcal{M}_φ by a set of constraints in $\mathbb{R}^{|\varphi|}$ can be directly obtained from the constraints of the polytope \mathcal{M} . For each cell φ_j ($j = 1, \dots, |\varphi|$) of φ , let $\bar{\mu}_j$ be the common value of the variables μ_i , $i \in \varphi_j$. Let ρ be the *orbit mapping function* that maps each element $i \in \mathcal{I}$ to the corresponding cell $\rho(i) = j$ that contains i . Substituting μ_i by $\bar{\mu}_{\rho(i)}$ in the constraints of \mathcal{M} , we obtain a set of constraints in $\bar{\mu}$ (in vector form, we substitute μ by $D\bar{\mu}$ where $D_{ij} = 1$ if $i \in \varphi_j$ and 0 otherwise). In doing this, some constraints will become identical and thus redundant. In general, the number of non-redundant constraints can still be exponential.

4.3 Overcomplete Variational Problems

We now state analogous results in lifting the overcomplete variational problems (4.2) and (4.3) when \mathcal{X} is finite. To simplify notation, we will consider only the case where features are unary or pairwise. As before, the group $\mathbb{A}_\Delta(\mathcal{F})$ will be used to induce a lifting partition. However, we need to define the action of this group on the set of overcomplete

features \mathcal{I}° .

Recall that if $(\pi, \gamma) \in \mathbb{A}[\mathcal{F}]$ then π is an automorphism of the graphical model graph \mathcal{G} . Since overcomplete features naturally correspond to nodes and edges of \mathcal{G} , π has a natural action on \mathcal{I}° that maps $v:t \mapsto \pi(v):t$ and $\{u:t, v:t'\} \mapsto \{\pi(u):t, \pi(v):t'\}$. Define $\varphi^\circ = \varphi^\circ(\Delta) = \text{Orb}_{\mathbb{A}[\mathcal{F}]}(\mathcal{I}^\circ)$ to be the induced orbits of $\mathbb{A}[\mathcal{F}]$ on the set of overcomplete features.

Corollary 4.2. *For all $\theta \in \Theta_\Delta$, φ° is a lifting partition for the variational problems (4.2) and (4.3).*

Thus, the optimization domain can be restricted to $\mathcal{M}_{\varphi^\circ}^\circ$ which we term the *lifted marginal polytope*. The cells of φ° are intimately connected to the node, edge and arc orbits of the graph \mathcal{G} induced by $\mathbb{A}[\mathcal{F}]$. We now list all the cells of φ° in the case where $\mathcal{X} = \{0, 1\}$: each node orbit \bar{v} corresponds to 2 cells $\{v : t | v \in \bar{v}\}, t \in \{0, 1\}$; each edge orbit \bar{e} corresponds to 2 cells $\{\{u : t, v : t\} | \{u, v\} \in \bar{e}\}, t \in \{0, 1\}$; and each arc orbit \bar{a} corresponds to the cell $\{\{u : 0, v : 1\} | (u, v) \in \bar{a}\}$. The orbit mapping function ρ maps each element of \mathcal{I}° to its orbit as follows: $\rho(v:t) = \bar{v}:t$, $\rho(\{u:t, v:t\}) = \{\bar{u}, \bar{v}\}:t$, $\rho(\{u:0, v:1\}) = (\bar{u}, \bar{v}):01$.

The total number of cells of φ° is $O(|\bar{V}| + |\bar{E}|)$ where $|\bar{V}|$ and $|\bar{E}|$ are the number of node and edge orbits of \mathcal{G} (each edge orbit corresponds to at most 2 arc orbits). Thus, in working with $\mathcal{M}_{\varphi^\circ}^\circ$, the big- O order of the number of variables is reduced from the number of nodes and edges in \mathcal{G} to the number of node and edge orbits.

5 Lifted Approximate MAP Inference

Approximate variational inference typically works with a tractable approximation of \mathcal{M} and a tractable approximation of A^* . In this paper, we focus only on lifted outer bounds of \mathcal{M}° (and thus restrict ourselves to the discrete case). We leave the problem of handling approximations of A^* to future work. Thus, our focus will be on the LP relaxation of the MAP inference problem (4.3).

By corollary 4.2, (4.3) is equivalent to the lifted problem $\sup_{\mu^\circ \in \mathcal{M}_{\varphi^\circ}^\circ} \langle \theta^\circ, \mu^\circ \rangle$. Since any outer bound $\text{OUTER} \supset \mathcal{M}^\circ$ yields an outer bound $\text{OUTER}_{\varphi^\circ}$ of $\mathcal{M}_{\varphi^\circ}^\circ$, we can always relax the lifted problem and replace $\mathcal{M}_{\varphi^\circ}^\circ$ by $\text{OUTER}_{\varphi^\circ}$. But is the relaxed lifted problem on $\text{OUTER}_{\varphi^\circ}$ equivalent to the relaxed ground problem on OUTER ? This depends on whether φ° is a lifting partition for the relaxed ground problem.

Theorem 5.1. *If the set $\text{OUTER} = \text{OUTER}(\mathcal{G})$ depends only on the graphical model structure \mathcal{G} of \mathcal{F} , then for all $\theta \in \Theta_\Delta$, φ° is a lifting partition for the relaxed MAP problem*

$$\sup_{\mu^\circ \in \text{OUTER}} \langle \theta^\circ, \mu^\circ \rangle = \sup_{\mu^\circ \in \text{OUTER}_{\varphi^\circ}} \langle \theta^\circ, \mu^\circ \rangle$$

The most often used outer bound of \mathcal{M}° is the local marginal polytope $\text{LOCAL}(\mathcal{G})$ [16], which enforces consistency for marginals on nodes and between nodes and edges of \mathcal{G} . [14, 15] used $\text{CYCLE}(\mathcal{G})$, which is a tighter bound that also enforces consistency of edge marginals

on the same cycle of \mathcal{G} . The Sherali-Adams hierarchy³ [12] provides a sequence of outer bounds of \mathcal{M}° , starting from $\text{LOCAL}(\mathcal{G})$ and progressively tightening it to the exact marginal polytope \mathcal{M}° . All of these outer bounds depend only on the structure of the graphical model \mathcal{G} , and thus the corresponding relaxed MAP problems admit φ° as a lifting partition. Note that with the exception when $\text{OUTER} = \text{LOCAL}$, equitable partitions [6] of \mathcal{G} such as those used in [10] are not lifting partitions for the approximate variational problem in theorem 5.1.⁴

6 Lifted MAP Inference on the Local Polytope

We now focus on lifted approximate MAP inference using the local marginal polytope LOCAL . From this point on, we also restrict ourselves to models where the features are pairwise or unary, and variables are binary ($\mathcal{X} = \{0, 1\}$).

We first aim to give an explicit characterization of the constraints of the lifted local polytope $\text{LOCAL}_{\varphi^\circ}$. The local polytope $\text{LOCAL}(\mathcal{G})$ is defined as the set of locally consistent pseudo-marginals.

$$\left\{ \tau \geq 0 \left| \begin{array}{ll} \tau_{v:0} + \tau_{v:1} = 1 & \forall v \in \mathcal{V}(\mathcal{G}) \\ \tau_{\{u:0, v:0\}} + \tau_{\{u:0, v:1\}} = \tau_{u:0} & \\ \tau_{\{u:0, v:0\}} + \tau_{\{v:0, u:1\}} = \tau_{v:0} & \forall \{u, v\} \in E(\mathcal{G}) \\ \tau_{\{u:1, v:1\}} + \tau_{\{u:0, v:1\}} = \tau_{v:1} & \\ \tau_{\{u:1, v:1\}} + \tau_{\{v:0, u:1\}} = \tau_{u:1} & \end{array} \right. \right\}$$

Substituting τ_i by the corresponding $\bar{\tau}_{\rho(i)}$ where $\rho()$ is given in subsection 4.3, and by noting that constraints generated by $\{u, v\}$ in the same edge orbits are redundant, we obtain the constraints for the *lifted local polytope* $\text{LOCAL}_{\varphi^\circ}$ as follows.

$$\left\{ \bar{\tau} \geq 0 \left| \begin{array}{ll} \bar{\tau}_{\bar{v}:0} + \bar{\tau}_{\bar{v}:1} = 1 & \forall \text{ node orbit } \bar{v} \\ \bar{\tau}_{\bar{e}:00} + \bar{\tau}_{(\bar{u}, \bar{v}):01} = \bar{\tau}_{\bar{u}:0} & \\ \bar{\tau}_{\bar{e}:00} + \bar{\tau}_{(\bar{v}, \bar{u}):01} = \bar{\tau}_{\bar{v}:0} & \forall \text{ edge orbit } \bar{e} \\ \bar{\tau}_{\bar{e}:11} + \bar{\tau}_{(\bar{u}, \bar{v}):01} = \bar{\tau}_{\bar{v}:1} & (\bar{u}, \bar{v}), (\bar{v}, \bar{u}) : \text{arc} \\ \bar{\tau}_{\bar{e}:11} + \bar{\tau}_{(\bar{v}, \bar{u}):01} = \bar{\tau}_{\bar{u}:1} & \text{orbits of } \bar{e} \end{array} \right. \right\}$$

Thus, the number of constraints needed to describe the lifted local polytope $\text{LOCAL}_{\varphi^\circ}$ is $O(|\bar{V}| + |\bar{E}|)$. Similar to the ground problem, these constraints can be derived from a graph representation of the node and edge orbits. Define the *lifted graph* $\bar{\mathcal{G}}$ be a graph whose nodes are the set of

³A note about terminology: Following the tradition in lifted inference, this paper uses the term *lift* to refer to the exploitation of symmetry for avoiding doing inference on the *ground* model. It is unfortunate that the term *lift* has also been used in the context of coming up with better bounds for the marginal polytopes. There, *lift* (as in lift-and-project) means to move to a higher dimensional space where constraints can be more easily expressed with auxiliary variables.

⁴As a counter example, consider a graphical model whose structure is the Frucht graph (http://en.wikipedia.org/wiki/Frucht_graph). Since this is a regular graph, LOCAL approximation yields identical constraints for every node. However, the nodes on this graph participate in cycles of different length, hence are subject to different cycle constraints.

node orbits \bar{V} of \mathcal{G} . For each edge orbit \bar{e} with a representative $\{u, v\} \in \bar{e}$, there is a corresponding edge on $\bar{\mathcal{G}}$ that connects the two node orbits \bar{u} and \bar{v} . Note that unlike \mathcal{G} , the lifted graph $\bar{\mathcal{G}}$ in general is not a simple graph and can contain self-loops and multi-edges between two nodes. Figure 6.1 shows the ground graph \mathcal{G} and the lifted graph $\bar{\mathcal{G}}$ for the example described in subsection 3.2.

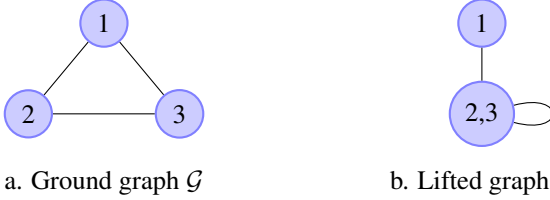


Figure 6.1: \mathcal{G} and $\bar{\mathcal{G}}$ of the example described in section 3.2

We now consider the linear objective function $\langle \theta^o, \tau \rangle$. Substituting τ_i by the corresponding $\bar{\tau}_{\rho(i)}$, we can rewrite the objective function in terms of $\bar{\tau}$ as $\langle \bar{\theta}, \bar{\tau} \rangle$ where the coefficients $\bar{\theta}$ are defined on nodes and edges of the lifted graph $\bar{\mathcal{G}}$ as follows. For each node orbit \bar{v} , $\bar{\theta}_{\bar{v}:t} = \sum_{v' \in \bar{v}} \theta_{v':t}^o = |\bar{v}| \theta_{v:t}^o$ where $t \in \{0, 1\}$ and v is any representative of \bar{v} . For each edge orbit \bar{e} with a representative $\{u, v\} \in \bar{e}$, $\bar{\theta}_{\bar{e}:tt} = \sum_{\{u', v'\} \in \bar{e}} \theta_{\{u':t, v':t\}}^o = |\bar{e}| \theta_{\{u:t, v:t\}}^o$ where $t \in \{0, 1\}$, $\bar{\theta}_{(\bar{u}, \bar{v}):01} = \sum_{(u', v') \in (\bar{u}, \bar{v})} \theta_{\{u':0, v':1\}}^o = |(\bar{u}, \bar{v})| \theta_{\{u:0, v:1\}}^o$. Note that typically the two arc-orbits (\bar{u}, \bar{v}) and (\bar{v}, \bar{u}) are not the same, in which case $|(\bar{u}, \bar{v})| = |(\bar{v}, \bar{u})| = |\bar{e}|$. However, in case $(\bar{u}, \bar{v}) = (\bar{v}, \bar{u})$ then $|(\bar{u}, \bar{v})| = |(\bar{v}, \bar{u})| = 2|\bar{e}|$.

So, we have shown that the lifted formulation for MAP inference on the local polytope can be described in terms of the lifted variables $\bar{\tau}$ and the lifted parameters $\bar{\theta}$. These lifted variables and parameters are associated with the orbits of the ground graphical model. Thus, the derived lifted formulation can also be read out directly from the lifted graph $\bar{\mathcal{G}}$. In fact, the derived lifted formulation is the local relaxed MAP problem of the lifted graphical model $\bar{\mathcal{G}}$. Therefore, any algorithm for solving the local relaxed MAP problem on \mathcal{G} can also be used to solve the derived lifted formulation on $\bar{\mathcal{G}}$. From lifted inference point of view, we can lift any algorithm for solving the local relaxed MAP problem on \mathcal{G} by constructing $\bar{\mathcal{G}}$ and run the same algorithm on $\bar{\mathcal{G}}$. This allows us to lift even asynchronous message passing algorithms such as the max-product linear programming (MPLP) algorithm [5], which cannot be lifted using existing lifting techniques.

7 Beyond Local Polytope: Lifted MAP Inference with Cycle Inequalities

We now discuss lifting the MAP relaxation on $\text{CYCLE}(\mathcal{G})$, a bound obtained by tightening $\text{LOCAL}(\mathcal{G})$ with an additional set of linear constraints that hold on cycles of the graphical model structure \mathcal{G} , called cycle constraints [14]. These constraints arise from the fact that the number of cuts (transitions from 0 to 1 or vice versa) in any configuration

on a cycle of \mathcal{G} must be even. Cycle constraints can be framed as linear constraints on the mean vector μ^o as follows. For every cycle C (set of edges that form a cycle in \mathcal{G}) and every odd-sized subset $F \subseteq C$

$$\sum_{\{u, v\} \in F} \text{nocut}(\{u, v\}, \tau) + \sum_{\{u, v\} \in C \setminus F} \text{cut}(\{u, v\}, \tau) \geq 1 \quad (7.1)$$

where $\text{nocut}(\{u, v\}, \tau) = \tau_{\{u:0, v:0\}} + \tau_{\{u:1, v:1\}}$ and $\text{cut}(\{u, v\}, \tau) = \tau_{\{u:0, v:1\}} + \tau_{\{v:0, u:1\}}$.

Theorem 5.1 guarantees that MAP inference on CYCLE can be lifted by restricted the feasible domain to CYCLE_{φ^o} , which we term the *lifted cycle polytope*. Substituting the original variables τ by the lifted variables $\bar{\tau}$, we obtain the *lifted cycle constraints* in terms of $\bar{\tau}$

$$\sum_{\{u, v\} \in F} \text{nocut}(\{\bar{u}, \bar{v}\}, \bar{\tau}) + \sum_{\{u, v\} \in C \setminus F} \text{cut}(\{\bar{u}, \bar{v}\}, \bar{\tau}) \geq 1 \quad (7.2)$$

where $\text{nocut}(\{\bar{u}, \bar{v}\}, \bar{\tau}) = \bar{\tau}_{\{\bar{u}, \bar{v}\}:00} + \bar{\tau}_{\{\bar{u}, \bar{v}\}:11}$ and $\text{cut}(\{\bar{u}, \bar{v}\}, \bar{\tau}) = \bar{\tau}_{(\bar{u}, \bar{v}):01} + \bar{\tau}_{(\bar{v}, \bar{u}):01}$ where (\bar{u}, \bar{v}) and (\bar{v}, \bar{u}) are the arc-orbits corresponding to the node-orbit $\{u, v\}$.

7.1 Lifted Cycle Constraints on All Cycles Passing Through a Fixed Node

Fix a node i in \mathcal{G} , and let $\text{Cyc}[i]$ be the set of cycle constraints generated from all cycles passing through i . A cycle is simple if it does not intersect with itself or contain repeated edges; [14] considers only simple cycles, but we will also consider any cycle, including non-simple cycles in $\text{Cyc}[i]$. Adding non-simple cycles to the mix does not change the story since constraints on non-simple cycles of \mathcal{G} are redundant. We now give a precise characterization of $\overline{\text{Cyc}}[i]$, the set of lifted cycle constraints obtained by lifting all cycle constraints in $\text{Cyc}[i]$ via the transformation from (7.1) to (7.2).

The lifted graph fixing i , $\bar{\mathcal{G}}[i]$ is defined as follows. Let $\mathbb{A}_{\Delta}[\mathcal{F}, i]$ be the subgroup of $\mathbb{A}_{\Delta}[\mathcal{F}]$ that fixes i , that is $\pi(i) = i$. The set of nodes of $\bar{\mathcal{G}}[i]$ is the set of node orbits $\bar{V}[i]$ of \mathcal{G} induced by $\mathbb{A}_{\Delta}[\mathcal{F}, i]$, and the set of edges is the set of edge orbits $\bar{E}[i]$ of \mathcal{G} . Each edge orbit connects to the orbits of the two adjacent nodes (which could form just one node orbit). Since i is fixed, $\{i\}$ is a node orbit, and hence is a node on $\bar{\mathcal{G}}[i]$. Note that $\bar{\mathcal{G}}[i]$ in general is not a simple graph: it can have multi-edges and loops.

Theorem 7.1. *Let \bar{C} be a cycle (not necessarily simple) in $\bar{\mathcal{G}}[i]$ that passes through the node $\{i\}$. For any odd-sized $\bar{F} \subset \bar{C}$*

$$\sum_{\mathbf{e} \in \bar{F}} \text{nocut}(\mathbf{e}, \bar{\tau}) + \sum_{\mathbf{e} \in \bar{C} \setminus \bar{F}} \text{cut}(\mathbf{e}, \bar{\tau}) \geq 1 \quad (7.3)$$

is a constraint in $\overline{\text{Cyc}}[i]$. Furthermore, all constraints in $\overline{\text{Cyc}}[i]$ can be expressed this way.

7.2 Separation of Lifted Cycle Constraints

While the number of cycle constraints may be reduced significantly in the lifted space, it may still be computationally expensive to list all of them. To address this issue, we follow [14] and employ a cutting plane approach in which we find and add only the most violated lifted cycle constraint in each iteration (separation operation).

For finding the most violated lifted cycle constraint, we propose a lifted version of the method presented by [14], which performs the separation by iterating over the nodes of the graph \mathcal{G} and for each node i finds the most violated cycle constraint from all cycles passing through i . Theorem 7.1 suggests that all lifted cycle constraints in $\overline{\text{Cyc}}[i]$ can be separated by mirroring $\overline{\mathcal{G}}[i]$ and performing a shortest path search from $\{i\}$ to its mirrored node, similar to the way separation is performed on ground cycle constraints [14].

To find the most violated lifted cycle constraint, we could first find the most violated lifted cycle constraint C_i in $\overline{\text{Cyc}}[i]$ for each node i , and then take the most violated constraints over all C_i . However, note that if i and i' are in the same node orbit, then $\overline{\text{Cyc}}[i] = \overline{\text{Cyc}}[i']$. Hence, we can perform separation using the following algorithm:

1. For each node orbit $\bar{v} \in \bar{V}$, choose a representative $i \in \bar{v}$ and find its most violated lifted cycle constraint $C_{\bar{v}} \in \overline{\text{Cyc}}[i]$ using a shortest path algorithm on the mirror graph of $\overline{\mathcal{G}}[i]$.
2. Return the most violated constraint over all $C_{\bar{v}}$.

Notice that both $\overline{\mathcal{G}}[i]$ and its mirror graph have to be calculated only once per graph. In each separation iteration we can reuse these structures, provided that we adapt the edge weights in the mirror graph according to the current marginals.

8 Detecting Symmetries in Exponential Families

8.1 Detecting Symmetries via Graph Automorphisms

We now discuss the computation of a subgroup of the automorphism group $\mathbb{A}_\Delta(\mathcal{F})$. Our approach is to construct a suitable graph whose automorphism group is guaranteed to be a subgroup of $\mathbb{A}_\Delta(\mathcal{F})$, and thus any tool and algorithm for computing graph automorphism can be applied. The constructed graph resembles a factor graph representation of \mathcal{F} . However, we also use colors of factor nodes to mark feature functions that are identical and in the same cell of Δ , and colors of edges to encode symmetry of the feature functions themselves.

Definition 8.1. The colored factor graph induced by \mathcal{F} and Δ , denoted by $\mathfrak{G}_\Delta[\mathcal{F}]$ is a bipartite graph with nodes $V(\mathfrak{G}) = \{x_1 \dots x_n\} \cup \{f_1 \dots f_m\}$ and edges $E(\mathfrak{G}) = \{\{x_{\eta_i(k)}, f_i\} \mid i \in \mathcal{I}, k = 1 \dots |\eta_i|\}$. Variable nodes are assigned the same color which is different from the colors of factor nodes. Factor nodes f_i and f_j have the same

color iff $f_i \equiv f_j$ and $i \overset{\Delta}{\sim} j$. If the function f_i is symmetric, then all edges adjacent to f_i have the same color; otherwise, they are colored according to the argument number of f_i , i.e., $\{x_{\eta_i(k)}, f_i\}$ is assigned the k -th color.

Theorem 8.1. The automorphism group $\mathbb{A}[\mathfrak{G}_\Delta]$ of $\mathfrak{G}_\Delta[\mathcal{F}]$ is a subgroup of $\mathbb{A}_\Delta(\mathcal{F})$, i.e., $\mathbb{A}[\mathfrak{G}_\Delta] \leq \mathbb{A}_\Delta[\mathcal{F}]$.

Finding the automorphism group $\mathbb{A}[\mathfrak{G}_\Delta]$ of the graph $\mathfrak{G}_\Delta[\mathcal{F}]$ therefore yields a procedure to compute a subgroup of $\mathbb{A}_\Delta[\mathcal{F}]$. Thus, according to corollary 4.1, the induced orbit partition on the factor node of $\mathfrak{G}_\Delta[\mathcal{F}]$ is a lifting partition for the variational problems discussed earlier. *Nauty*, for example, directly supports the operation of computing the automorphism group of a graph and extracting the induced node orbits.

8.2 Symmetries of Markov Logic Networks

A Markov Logic Network (MLN) [11] is prescribed by a list of weighted formulas $F_1 \dots F_K$ (consisting of a set of predicates, logical variables, constants, and a weight vector \mathbf{w}) and a logical domain $\mathcal{D} = \{a_1 \dots a_{|\mathcal{D}|}\}$. Let \mathcal{D}_0 be the set of objects appearing as constants in these formulas, then $\mathcal{D}_* = \mathcal{D} \setminus \mathcal{D}_0$ is the set of objects in \mathcal{D} that do not appear in these formulas. Let Gr be the set of all ground predicates $p(a_1 \dots a_\ell)$'s. If s is a substitution, $F_i[s]$ denotes the result of applying the substitution s to F_i and is a grounding of F_i if it does not contain any logical free variables. The set of all groundings of F_i is $\text{Gr}F_i$, and let $\text{GrF} = \text{Gr}F_1 \cup \dots \cup \text{Gr}F_K$. The MLN corresponds to an exponential family \mathcal{F}_{MLN} where Gr is the variable index set and each grounding $F_i[s] \in \text{Gr}F_i$ is a feature function $\phi_{F_i[s]}(\omega) = \mathbb{I}(\omega \models F_i[s])$ with the associated parameter $\theta_{F_i[s]} = w_i$ where ω is a truth assignment to all the ground predicates in Gr and w_i is the weight of the formula F_i . Since all the ground features of the formula F_i have the same parameter w_i , the MLN also induces the parameter-tying partition $\Delta_{MLN} = \{\{\phi_{F_1[s]}(\omega)\} \dots \{\phi_{F_K[s]}(\omega)\}\}$.

Let a renaming permutation r be a permutation over \mathcal{D} that fixes every object in \mathcal{D}_0 , i.e., r only permutes objects in \mathcal{D}_* . Thus, the set of all such renaming permutations is a group \mathbb{G}^{re} that is isomorphic to the symmetric group $\mathbb{S}(\mathcal{D}_*)$. Consider the following actions of \mathbb{G}^{re} on Gr and GrF : $\pi_r : p(a_1 \dots a_\ell) \mapsto p(r(a_1) \dots r(a_\ell))$ and $\gamma_r : F_i[s] \mapsto F_i[r(s)]$ where $r(s) = (x_1/r(a_1), \dots, x_k/r(a_k)) = (x_1/r(a_1), \dots, x_k/r(a_k))$. Basically, π_r and γ_r rename the constants in each ground predicate $p(a_1 \dots a_\ell)$ and ground formula $F_i[s]$ according to the renaming permutation r . The following theorem (a consequence of Lemma 1 from Bui et al. [1]) shows that \mathbb{G}^{re} is isomorphic to a subgroup of $\mathbb{A}[\mathcal{F}_{MLN}]$, the automorphism group of the exponential family \mathcal{F}_{MLN} .

Theorem 8.2. For every renaming permutation r , $(\pi_r, \gamma_r) \in \mathbb{A}[\mathcal{F}_{MLN}]$. Thus, $\mathbb{G}^{re} \preceq \mathbb{A}[\mathcal{F}_{MLN}]$.

Furthermore, observe that γ_r only maps between groundings of a formula F_i , thus the action of \mathbb{G}^{re} on GrF is consistent with the parameter-tying partition

$\Delta_{MLN} = \{\{\phi_{F_1[s]}(\omega)\} \dots \{\phi_{F_K[s]}(\omega)\}\}$. Thus, $\mathbb{G}^{re} \preceq \mathbb{A}_{\Delta_{MLN}}[\mathcal{F}_{MLN}]$. According to corollary 4.1, the orbit partition induced by the action of \mathbb{G}^{re} on GrF is a lifting partition for the variational inference problems associated with the exponential family \mathcal{F}_{MLN} . In addition, this orbit partition can be quickly derived from the first-order representation of an MLN; the size of this orbit partition depends only on the number of observed constants $|\mathcal{D}_o|$, and does not depend on actual domain size $|\mathcal{D}|$.

9 Experiments

We experiment with several propositional and lifted methods for variational MAP inference by varying the domain size of the following MLN:

$$\begin{aligned} w_1 \quad & x \neq y \wedge x \neq z \wedge y \neq z \Rightarrow \text{pred}(x, y) \Leftrightarrow \text{pred}(y, z) \\ w_2 \quad & x \neq y \wedge \text{obs}(x, y) \Rightarrow \text{pred}(x, y) \\ & \text{obs}(A, B) \end{aligned}$$

This MLN is designed to be a simplified version of models that enforce transitivity for the predicate `pred`, and will be called the *semi-transitive* model.⁵ We set the weights as $w_1 = -100$ and $w_2 = 0.1$. The negative w_1 yields a repulsive model with relatively strong interaction, while the shared predicate and variables in the first formula are known to be a difficult case for lifted inference. The third formula is an observation with two constants A and B .

The ground Markov network of the above MLN is corresponding to an exponential family \mathcal{F}_{MLN} , and we use the two methods described in Sections 8.1 and 8.2 to derive lifting partitions. The first method (*nauty*) fully grounds the MLN, then finds a lifting partition using *nauty*. The second (*renaming*) works directly with the MLN, and uses the renaming group to find a lifting partition. We use two outer bounds to the marginal polytope: LOCAL and CYCLE. There are three variants of each method: propositional, lifting using *nauty* orbit partition, and lifting using renaming orbit partition. This yields a total of six methods to compare. For reference, we also calculate the exact solution to the MAP problem using ILP.

Figure 9.1a shows the runtime (in milliseconds) until convergence for different domain sizes of the logical variables in our MLN. We can make a few observations. First, in most cases lifting dramatically reduces runtime for larger domains. Second, *nauty*-based methods suffer from larger domain sizes. This is expected, as we perform automorphism finding on propositional graphs with increasing size. Third, the renaming partition outperforms *nauty* partitions, by virtue of working directly with the first-order representation. Notice in particular for lifted-via-renaming methods, we can still observe a dependency on domain size, but

⁵If $\text{pred}(x, y) = 1$ is interpreted as having a (directed) edge from x to y , then this model represents a random graph whose nodes are elements of the domain of the MLN. More specifically, the model can be thought of as a 2-star Markov graph [4].

this is an artifact of our current implementation—in the future these curves will be constant. Finally, all but the propositional cycle method are faster than ILP.

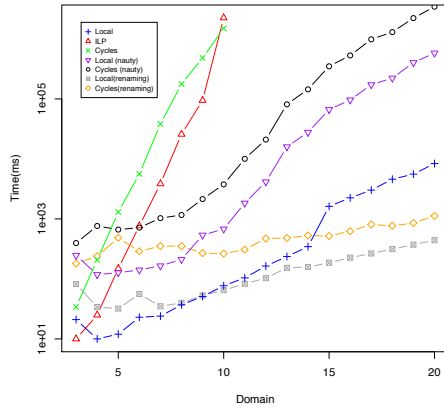
Figure 9.1b illustrates how the objective changes over cutting plane iterations (and hence time), all for the case of domain size 10. Both the local polytope and ILP approaches have no cutting plane iterations, and hence are represented as single points. Given that ILP is exact, the ILP point gives the optimal solution. Notice how all methods are based on outer/upper bounds on the variational objective, and hence are decreasing over time. First, we can observe that the CYCLE methods converge to the (almost) optimal solution, substantially better than the LOCAL methods. However, in the propositional case the CYCLE algorithm converges very slowly, and is only barely faster than ILP.

Lifted CYCLE methods are the clear winners for this problem. We can also see how the different lifting partitions affect CYCLE performance. The renaming partition performs its first iteration much quicker than the *nauty*-based partition, since *nauty* needs to work on the full grounded network. Consequently, it converges much earlier, too. However, we can also observe that the renaming partition is more fine-grained than the *nauty* partition, leading to larger orbit graphs and hence slower iterations. Notably, working with lifted cycle constraints gives us substantial runtime improvements, and effectively optimal solutions.

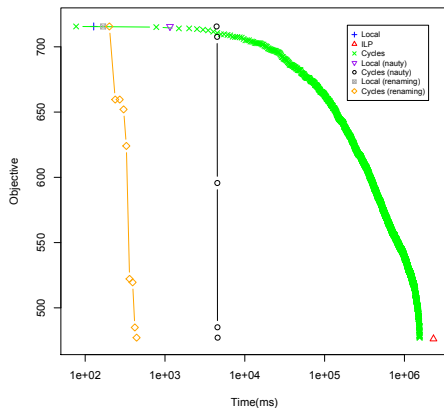
10 Conclusion

We presented a new general framework for lifted variational inference. In doing this, we introduce and study a precise mathematical definition of symmetry of graphical models via the construction of their automorphism groups. Using the device of automorphism groups, orbits of random variables are obtained, and lifted variational inference is materialized as performing the corresponding convex variational optimization problem in the space of per-orbit random variables. Our framework enables lifting a large class of approximate variational MAP inference algorithms, including the first lifted algorithm for MAP inference with cycle constraints. We presented experimental results demonstrating that lifted MAP inference with cycle constraints achieved the state of the art performance, obtaining much better objective function values than LOCAL approximation while remaining relatively efficient. Our future work includes extending this approach to handle approximations of convex upper-bounds of A^* , which would enable lifting the full class of approximate convex variational marginal inference.

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(a) Runtime vs. domain size.



(b) Objective over time for domain size 10.

Figure 9.1: Experiments with a semi-transitive model with one observed variable. Due to large differences between runtimes, time is always presented in logarithmic scale.

FA8750-09-C-0181. Any opinions, findings, and conclusions or recommendations expressed in this material are those of the author(s) and do not necessarily reflect the view of DARPA, AFRL, or the U.S. government.

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Dedicated to the late Prof. Hai Bui of Hanoi University of Technology who passed away the day before the submission deadline.

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