

10

Lifted Markov Chain Monte Carlo

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Abstract.

This chapter presents an approach to utilize exact and approximate symmetries in probabilistic graphical models during Markov chain Monte Carlo (MCMC) inference. We discuss permutation groups representing the symmetries of graphical models and how to compute them. Next, we introduce orbital Markov chains, a family of lifted Markov chains leveraging model symmetries to reduce mixing times. Unfortunately, the majority of real-world graphical models is asymmetric. This is even the case for relational representations when evidence is given. Therefore, we extend lifted MCMC to instead utilize approximate symmetries. Lifted MCMC leads to improved probability estimates while remaining unbiased. Experiments demonstrate that the approach outperforms existing MCMC algorithms.

10.1 Introduction

This chapter describes the use of group theoretical concepts and algorithms to perform Markov chain Monte Carlo sampling in probabilistic models. Since relational models often exhibit strong topological symmetries, permutation groups offer a compact and well-understood representation. Moreover, numerous efficient group theoretical algorithms are implemented in comprehensive open-source group algebra frameworks such as GAP (GAP).

Symmetries on different syntactical levels of statistical relational formalism ultimately lead to symmetries in the space of joint variable assignments. This space of possible assignments corresponds to the state space of Monte Carlo Markov chains such as the Gibbs sampler that are often used for approximate probabilistic inference. Since the permutation group modeling the symmetries induces a partition (the so-called orbit partition) on the state space of these Markov chains, we investigate whether this can be exploited for more efficient MCMC approaches to probabilistic inference. The basic idea is that *lifted* Markov chains implicitly or explicitly operate on the partition of the state space instead of the space of individual assignments. We describe orbital Markov chains, which are derived from an existing Markov chain so as to leverage the symmetries in the underlying model. Under mild conditions, orbital Markov chains have the same convergence properties as chains operating on the state space partition without the need to explicitly compute this partition.

While lifted inference algorithms perform well for highly symmetric graphical models, they depend heavily on the presence of symmetries and perform worse for asymmetric models due to their computational overhead. This is especially unfortunate as numerous real-world graphical models are not symmetric. To bring the achievements of the lifted inference community to the mainstream of machine learning and uncertain reasoning it is crucial to explore ways to apply ideas from the lifted inference literature to inference problems in asymmetric graphical models. This chapter further describes a lifted inference algorithm for asymmetric graphical models. It uses a symmetric approximation of the original model to compute a proposal distribution for a Metropolis-Hastings chain. The approach combines a base MCMC algorithm such as the Gibbs sampler with the Metropolis chain that performs jumps in the approximate symmetric model, while producing unbiased probability estimates.

We conducted several experiments verifying that orbital Markov chains converge faster to the true distribution than state of the art Markov chains. We also conduct experiments where lifted inference is applied to graphical models with no exact symmetries and no color-passing symmetries, and where every random variable has distinct soft evidence. Yet, we are able to show improved probability estimates while remaining unbiased.

10.2 Background

We first recall basic concepts of group theory and finite Markov chains both of which are crucial for understanding this chapter.

10.2.1 Group Theory

A **symmetry** of a discrete object is a structure-preserving bijection on its components. A natural way to represent symmetries are **permutation groups**. A group is an algebraic structure (\mathcal{G}, \circ) , where \mathcal{G} is a set closed under a binary associative operation \circ with an identity element and a unique inverse for each element. We often write \mathcal{G} rather than (\mathcal{G}, \circ) .

A permutation group \mathcal{G} *acting on* a finite set Ω is a finite set of bijections $g : \Omega \rightarrow \Omega$ that form a group. Let Ω be a finite set and let \mathcal{G} be a permutation group acting on Ω . If $\alpha \in \Omega$ and $g \in \mathcal{G}$ we write α^g to denote the image of α under g . A cycle $(\alpha_1 \alpha_2 \dots \alpha_n)$ represents the permutation that maps α_1 to α_2 , α_2 to α_3, \dots , and α_n to α_1 . Every permutation can be written as a product of disjoint cycles where each element that does not occur in a cycle is understood as being mapped to itself. A generating set R of a group is a subset of the group's elements such that every element of the group can be written as a product of finitely many elements of R and their inverses.

We define a relation \sim on Ω with $\alpha \sim \beta$ if and only if there is a permutation $g \in \mathcal{G}$ such that $\alpha^g = \beta$. The relation partitions Ω into equivalence classes which we call **orbits**. We call this partition of Ω the orbit partition induced by \mathcal{G} . We use the notation $\alpha^{\mathcal{G}}$ to

denote the orbit $\{\alpha^g \mid g \in \mathbb{G}\}$ containing α . Let $f : \Omega \rightarrow \mathbb{R}$ be a function from Ω into the real numbers and let \mathbb{G} be a permutation group acting on Ω . We say that \mathbb{G} is an **automorphism group** for (Ω, f) if and only if for all $\omega \in \Omega$ and all $g \in \mathbb{G}$, $f(\omega) = f(\omega^g)$.

10.2.2 Finite Markov Chains

Given a finite set Ω a **Markov chain** defines a random walk $(\mathbf{x}_0, \mathbf{x}_1, \dots)$ on elements of Ω with the property that the conditional distribution of \mathbf{x}_{n+1} given $(\mathbf{x}_0, \mathbf{x}_1, \dots, \mathbf{x}_n)$ depends only on \mathbf{x}_n . For all $\mathbf{x}, \mathbf{y} \in \Omega$, $P(\mathbf{x} \rightarrow \mathbf{y})$ is the chain's probability to transition from \mathbf{x} to \mathbf{y} , and $P^t(\mathbf{x} \rightarrow \mathbf{y}) = P_{\mathbf{x}}^t(\mathbf{y})$ the probability of being in state \mathbf{y} after t steps if the chain starts at state \mathbf{x} . We often refer to the conditional probability matrix P as the *kernel* of the Markov chain. A Markov chain is *irreducible* if for all $\mathbf{x}, \mathbf{y} \in \Omega$ there exists a t such that $P^t(\mathbf{x} \rightarrow \mathbf{y}) > 0$ and *aperiodic* if for all $\mathbf{x} \in \Omega$, $\gcd\{t \geq 1 \mid P^t(\mathbf{x} \rightarrow \mathbf{x}) > 0\} = 1$.

Theorem 10.1 *Any irreducible and aperiodic Markov chain has exactly one stationary distribution.*

A distribution π on Ω is reversible for a Markov chain with state space Ω and transition probabilities P , if for every $\mathbf{x}, \mathbf{y} \in \Omega$

$$\pi(\mathbf{x})P(\mathbf{x} \rightarrow \mathbf{y}) = \pi(\mathbf{y})P(\mathbf{y} \rightarrow \mathbf{x}).$$

We say that a Markov chain is reversible if there exists a reversible distribution for it. The AI literature often refers to reversible Markov chains as Markov chains satisfying the detailed balance property.

Theorem 10.2 *Every reversible distribution for a Markov chain is also a stationary distribution for the chain.*

10.2.3 Markov Chain Monte Carlo

Numerous approximate inference algorithms for probabilistic graphical models draw sample points from a Markov chain whose stationary distribution is that of the probabilistic model, and use the sample points to estimate marginal probabilities. Sampling approaches of this kind are referred to as **Markov chain Monte Carlo** methods. We discuss the **Gibbs sampler**, a sampling algorithm often used in practice.

Let \mathbf{X} be a finite set of random variables with probability distribution π . The Markov chain for the *Gibbs sampler* is a Markov chain $\mathcal{M} = (\mathbf{x}_0, \mathbf{x}_1, \dots)$ which, being in state \mathbf{x}_t , performs the following steps at time $t + 1$:

1. Select a variable $X \in \mathbf{X}$ uniformly at random;
2. Sample $\mathbf{x}'_{t+1}(X)$, the value of X in the state \mathbf{x}'_{t+1} , according to the conditional π -distribution of X given that all other variables take their values according to \mathbf{x}_t ; and
3. Let $\mathbf{x}'_{t+1}(Y) = \mathbf{x}_t(Y)$ for all variables $Y \in \mathbf{X} \setminus \{X\}$.

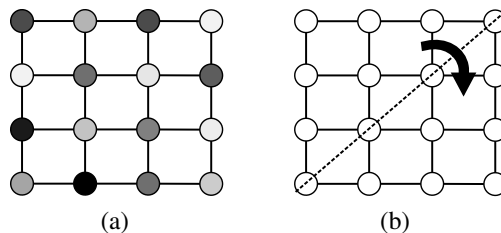


Figure 10.1: A ferromagnetic Ising model with constant interaction strength. In the presence of an external field, that is, when the variables have different unary potentials, the probabilistic model is asymmetric (a). However, the model is rendered symmetric by assuming a constant external field (b). In this case, the symmetries of the model are generated by the reflection and rotation automorphisms.

The Gibbs chain is aperiodic and has π as a stationary distribution. If the chain is irreducible, then the marginal estimates based on sample points drawn from the chain are unbiased once the chain reaches the stationary distribution.

10.3 Symmetries of Probabilistic Models

This section describes notions of symmetry in the context of probabilistic graphical models, as well as their relational extensions.

10.3.1 Graphical Model Symmetries

Symmetries of a set of random variables and graphical models have been formally defined in the lifted and symmetry-aware probabilistic inference literature with concepts from group theory (Niepert, 2013; Bui et al., 2012).

Definition 10.1 Let \mathbf{X} be a set of discrete random variables with distribution π and let Ω be the set of states (configurations) of \mathbf{X} . We say that a permutation group \mathcal{G} acting on Ω is an automorphism group for \mathbf{X} if and only if for all $\mathbf{x} \in \Omega$ and all $g \in \mathcal{G}$ we have that $\pi(\mathbf{x}) = \pi(\mathbf{x}^g)$.

Note that the definition of an automorphism group is independent of the particular representation of the probabilistic model. For particular representations, there are efficient algorithms for computing the automorphism group. Typically, one computes the generators of the automorphism group with algorithms that derive permutation groups for colored undirected graphs such as SAUCY and NAUTY (Niepert, 2012b). Note that we do not require the automorphism group to be maximal, that is, it can be a subgroup of a different automorphism group for the same set of random variables.

Most probabilistic models are asymmetric. For instance, the Ising model which is used in numerous applications, is asymmetric if we assume an external field as it leads to different

unary potentials. However, we can make the model symmetric simply by assuming a constant external field. Figure 10.1 depicts this situation. This is an example of an over-symmetric approximation of the model, which we will use later in this chapter to do lifted MCMC without biasing the probability estimates.

10.3.2 Relational Model Symmetries

Naturally, there is a close connection between the concept of symmetry and lifted inference. There are deep connections between automorphisms and the statistical notion of exchangeability (Niepert, 2012b, 2013; Bui et al., 2012), which has been used to explain the tractability of exact lifted inference algorithms (Niepert and Van den Broeck, 2014). Moreover, the (fractional) automorphisms of the graphical model representation have been related to lifted inference and exploited for more efficient inference (Niepert, 2012b; Bui et al., 2012; Noessner et al., 2013; Mladenov and Kersting, 2013). For instance, lifted belief propagation identifies and clusters indistinguishable ground atoms and features by keeping track of the messages sent and received by each of the corresponding nodes in a factor graph (Singla and Domingos, 2008; Kersting et al., 2009). Bi-simulation type procedures group indistinguishable elements and, therefore, exploit symmetry in the model as well (Sen et al., 2009b). There are a number of sampling algorithms that take advantage of symmetries (Venugopal and Gogate, 2012; Gogate et al., 2012).

The algorithms in this chapter use group theory and, in particular, permutation groups to compactly represent (exact and approximate) symmetries in graphical models (Niepert, 2012b). There are several reasons to consider group theory and permutation groups a natural representation of symmetries in graphical models. First, an irredundant set of generators of a permutation group ensures exponential compression. For instance, for a set of n exchangeable binary random variables, the permutation group acting on the variables is the symmetric group on n which has $n!$ permutations. However, we only need at most $n - 1$ irredundant generators to represent this permutation group. In addition to the compact representation, group theory also provides numerous remarkably efficient algorithms for manipulating and sampling from groups. The product replacement algorithm (Celler et al., 1995), for instance, samples group elements uniformly at random with impressive performance.

Symmetry in statistical relational languages manifests itself at various syntactic levels ranging from the set of constants to the assignment space. There is often symmetry at the level of constants. In the well-known social network model (Singla and Domingos, 2008) without evidence, for example, we have that the constants are indistinguishable meaning that swapping two constants leads to an isomorphic statistical relational model. Now, the permutations on the constant level induce permutations on the level of ground atoms and formulas. From the irredundant generators of the permutation group modeling the symmetries on the constant level we can directly compute the irredundant generators of the permutation group modeling the corresponding symmetries on the ground level. Indeed,

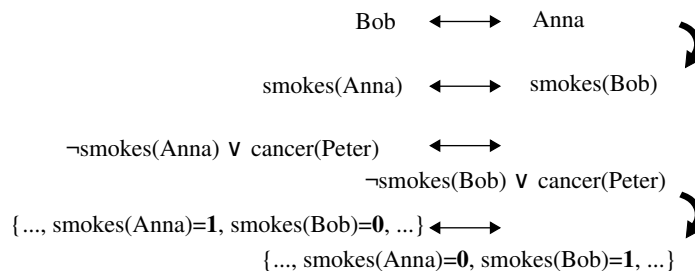


Figure 10.2: Symmetry in the model is observable on different syntactical levels of the relational model. The level of constants, the level of ground atoms (variables), the level of clauses (features) and the level of possible worlds (assignments). Each permutation group acting on the set of constants induces a permutation group acting on the set of ground atoms. The latter induces a permutation group acting on the set of features. This permutation partitions (a) the variables and feature and (b) the assignment space.

it is well-known that isomorphisms between permutation groups always map irredundant generators in one group to irredundant generators in the other. However, symmetry on the ground level does not necessarily lead to symmetry on the constant level. Similarly, while symmetry on the ground level induces symmetry on the space of assignments to the random variables this is not true for the other direction. Figure 10.2 depicts the different syntactical levels on which symmetries can arise.

Niepert (2012b) describes an approach that maps weighted formulas to colored undirected graphs and applies graph automorphism algorithms to compute the symmetries of the log-linear models defined over the weighted formulas (Niepert, 2012b). The resulting permutation groups partition the (exponential) space of variable assignments when acting on it. Since the state space of MCMC approaches is identical to the assignment space of the probabilistic graphical models, we will investigate whether and to what extent the partition induced by the models' symmetries can be leveraged for more efficient MCMC algorithms.

10.4 Lifted MCMC for Symmetric Models

We have seen that symmetries on different syntactical levels of statistical relational formalism ultimately lead to symmetries in the space of joint variable assignments. Now, the space of possible variable assignments is the state space of Monte Carlo Markov chains such as the Gibbs sampler that are often used for approximate probabilistic inference. Since the permutation group modeling the symmetries induces a partition (the so-called orbit partition) on the state space of these Markov chains, we will investigate whether this can be exploited for more efficient MCMC approaches to probabilistic inference. The ba-

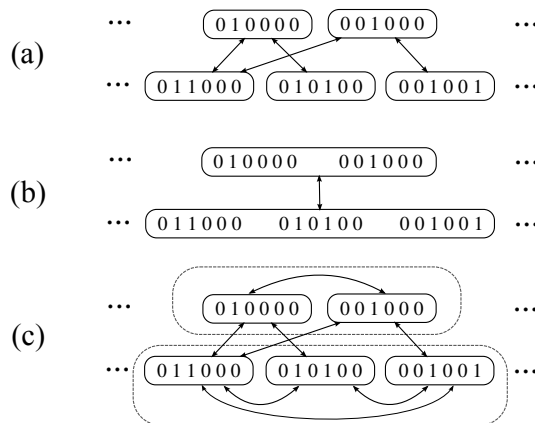


Figure 10.3: (a) A fragment of a finite state space of a Markov chain with non-zero transition probabilities indicated by directed arcs. (b) A lumping of the state space. Instead of moving between individual states, the lumped chain moves between classes of states of the original chain. (c) The benefits of lumping are also achievable by sampling uniformly at random from the implicit equivalence classes (orbits) in each step.

sic idea is that *lifted* MCMC algorithms implicitly or explicitly operate on the partition of the state space instead of the original state space.

10.4.1 Lumping

A *lumping* (also: collapsing, projection) of a Markov chains is a compression of its state space which is possible under certain conditions on the transition probabilities of the original Markov chain (Buchholz, 1994; Derisavi et al., 2003). The following definition formalizes the notion.

Definition 10.2 Let \mathcal{M} be a Markov chain with transition matrix P and state space Ω , and let $\mathcal{C} = \{C_1, \dots, C_n\}$ be a partition of the state space. If for all $C_i, C_j \in \mathcal{C}$ and all $j', j'' \in C_j$

$$\sum_{i' \in C_i} P(i', j') = \sum_{i' \in C_i} P(i', j'')$$

then \mathcal{M} is ordinary lumpable. If, in addition, the stationary distribution has $\pi(j') = \pi(j'')$ for all $j', j'' \in C_j$ and all $C_j \in \mathcal{C}$ then \mathcal{M} is exactly lumpable.

Let $\hat{\pi}$ be the stationary distribution of the *quotient Markov chain*, that is, the exactly lumped Markov chain whose state space consists of partitions \mathcal{C} . Then, the probability $\pi(i)$ of a state $i \in C_i \subseteq \Omega$ of the original chain can be computed as $\pi(i) = \hat{\pi}(i)/|C_i|$.

The benefit of lumping a Markov chain is the potentially much smaller state space and ultimately more rapid mixing. For instance, consider the case of n binary random vari-

ables that are exchangeable. Here, the natural choice of a partition of the state space is $\{C_0, C_1, \dots, C_n\}$ where each C_i contains the states with Hamming weight i , that is, the states with i non-zeros. Please note that the C_i 's are the orbits (equivalence classes) of the orbit partition of the permutation group acting on the set of states (variable assignments). Instead of 2^n states the resulting lumped Markov chain has only $n + 1$ states and mixes more rapidly than the original one. Figure 10.3 depicts (a) a fragment of a finite Markov chain with non-zero probability transitions indicated by arrows and (b) a lumped Markov chain that bundles several states of the original chain into a single one of the lumped chain.

The crucial question is whether the explicit construction of the lumped chain is computationally feasible. After all, if the computation of lumped Markov chains was intractable we would not have gained much. Unfortunately, it turns out that the explicit construction of the lumped state space is indeed intractable. Computing the coarsest lumping quotient of a Markov chain with a bi-simulation procedure is linear in the *number of non-zero probability transitions* of the chain (Derisavi et al., 2003) and, hence, in most cases exponential in the number of random variables. Moreover, other theoretical results show that special cases of the lumping problem are also intractable. The results are negative even for the important special case of partitions resulting from permutation groups acting on the state space of the Markov chains. It is known that, given a permutation group acting on the state space, merely computing the number of equivalence classes of the resulting orbit partition of the state space is a #P-complete problem (Goldberg, 2001).

We hypothesize that the intractability of the explicit construction of the lumped chain's state space is the main reason that the technique of lumping, while well-understood on a theoretical level, has not been seriously considered by communities that apply Markov chain Monte Carlo methods to large-scale applications requiring probabilistic inference. We are not aware of MCMC approaches to probabilistic reasoning that leverage the theory of lumping.

10.4.2 Orbital Markov Chains

Under certain circumstances, the *explicit* computation of the partition of the state space is not necessary to achieve the same computational gains as the lumped chain (Niepert, 2012b). The basic idea is that we only need, for each $\omega \in \Omega$, an efficient way to sample uniformly at random from $[\omega]$ the equivalence class containing ω . The product replacement algorithm (Celler et al., 1995) provides such an efficient method of sampling uniformly from the equivalence classes induced by a permutation group. This novel family of Markov chains is referred to as **orbital Markov chains** (Niepert, 2012b). An orbital Markov chain is always derived from an existing Markov chain so as to leverage the symmetries in the underlying model. In the presence of symmetries orbital Markov chains are able to perform wide-ranging transitions reducing the time until convergence. In the absence of symmetries they are equivalent to the original Markov chains. Orbital Markov chains only require a generating set of a permutation group \mathcal{G} acting on the chain's state

space as additional input. These generators can be computed on a colored graph representation of the distribution at hand, or directly on the relational representation, as described in the previous section.

Let Ω be a finite set, let $\mathcal{M}' = (X'_0, X'_1, \dots)$ be a Markov chain with state space Ω , let π be a stationary distribution of \mathcal{M}' , and let \mathfrak{G} be an automorphism group for (Ω, π) . The *orbital Markov chain* $\mathcal{M} = (X_0, X_1, \dots)$ for \mathcal{M}' is a Markov chain which at each integer time $t + 1$ performs the following steps:

1. Let X'_{t+1} be the state of the *original* Markov chain \mathcal{M}' at time $t + 1$;
2. Sample X_{t+1} , the state of the orbital Markov chain \mathcal{M} at time $t + 1$, uniformly at random from $X'_{t+1}{}^{\mathfrak{G}}$, the orbit of X'_{t+1} .

The orbital Markov chain \mathcal{M} , therefore, runs at every time step $t \geq 1$ the original chain \mathcal{M}' first and samples the state of \mathcal{M} at time t uniformly at random from the orbit of the state of the original chain \mathcal{M}' at time t . Figure 10.3 (c) depicts a fragment of the orbital Markov chain for the original Markov chain (a). Instead of computing the equivalence of the state space explicitly (b) novel transitions are introduced that make the chain behave *as if it was lumped*.

Given a state X_t and a permutation group \mathfrak{G} orbital Markov chains sample an element from $X_t{}^{\mathfrak{G}}$, the orbit of X_t , uniformly at random. By the orbit-stabilizer theorem this is equivalent to sampling an element $g \in \mathfrak{G}$ uniformly at random and computing $X_t{}^g$. Sampling group elements uniformly at random is a well-researched problem (Celler et al., 1995) and computable in polynomial time in the size of the generating sets with product replacement algorithms (Pak, 2000). These algorithms are implemented in several group algebra systems such as GAP (GAP) and exhibit remarkable performance. Once initialized, product replacement algorithms can generate pseudo-random elements by performing, depending on the variant, 1 to 3 group multiplications. We could verify that the overhead of step 2 during the sampling process is indeed negligible.

The following theorem relates properties of the orbital Markov chain to those of the Markov chain it is derived from. A detailed proof can be found in the appendix.

Theorem 10.3 (Niepert (2012b)) *Let Ω be a finite set and let \mathcal{M}' be a Markov chain with state space Ω and transition matrix P' . Moreover, let π be a probability distribution on Ω , let \mathfrak{G} be an automorphism group for (Ω, π) , and let \mathcal{M} be the orbital Markov chain for \mathcal{M}' . Then,*

- (a) *if \mathcal{M}' is aperiodic then \mathcal{M} is also aperiodic;*
- (b) *if \mathcal{M}' is irreducible then \mathcal{M} is also irreducible;*
- (c) *if π is a reversible distribution for \mathcal{M}' and, for all $g \in \mathfrak{G}$ and all $x, y \in \Omega$ we have that $P'(x, y) = P'(x^g, y^g)$, then π is also a reversible and, hence, a stationary distribution for \mathcal{M} .*

The condition in statement (c) requiring for all $g \in \mathcal{G}$ and all $x, y \in \Omega$ that $P'(x, y) = P'(x^g, y^g)$ expresses that the original Markov chain is compatible with the symmetries captured by the permutation group \mathcal{G} . This weak assumption is met by all of the practical Markov chains we are aware of and, in particular, Metropolis chains and Gibbs sampler.

10.5 Lifted MCMC for Asymmetric Models

This section extends the lifted MCMC framework to construct mixtures of Markov chains where one of the chains operates on the **approximate symmetries** of the probabilistic model. The framework assumes a base Markov chain $\mathcal{M}_{\mathcal{B}}$ such as the Gibbs chain, the MC-SAT chain (Poon and Domingos, 2006), or any other MCMC algorithm. We then construct a mixture of the base chain and an Orbital Metropolis chain which exploits approximate symmetries for its proposal distribution.

10.5.1 Mixing

Two or more Markov chains can be combined by constructing mixtures and compositions of the kernels (Tierney, 1994). Let P_1 and P_2 be the kernels for two Markov chains \mathcal{M}_1 and \mathcal{M}_2 both with stationary distribution π . Given a positive probability $0 < \alpha < 1$, a *mixture* of the Markov chains is a Markov chain where, in each iteration, kernel P_1 is applied with probability α and kernel P_2 with probability $1 - \alpha$. The resulting Markov chain has π as a stationary distribution. The following result relates properties of the individual chains to properties of their mixture.

Theorem 10.4 (Tierney (1994)) *A mixture of two Markov chains \mathcal{M}_1 and \mathcal{M}_2 is irreducible and aperiodic if at least one of the chains is irreducible and aperiodic.*

For a more in-depth discussion of combining Markov chains and the application to machine learning, we refer the interested reader to an overview paper (Andrieu et al., 2003).

10.5.2 Metropolis-Hastings Chains

Before we describe the approach in more detail, let us first review Metropolis samplers. The construction of a **Metropolis-Hastings Markov chain** is a popular general procedure for designing reversible Markov chains for MCMC-based estimation of marginal probabilities. Metropolis-Hastings chains are associated with a **proposal distribution** $Q(\cdot | \mathbf{x})$ that is utilized to *propose* a move to the next state given the current state \mathbf{x} . The closer the proposal distribution to the distribution π to be estimated, that is, the closer $Q(\mathbf{x} | \mathbf{x}_t)$ to $\pi(\mathbf{x})$ for large t , the better the convergence properties of the Metropolis-Hastings chain.

We first describe the Metropolis algorithm, a special case of the Metropolis-Hastings algorithm (Häggström, 2002). Let \mathbf{X} be a finite set of random variables with probability distribution π and let Ω be the set of states of the random variables. The Metropolis chain is governed by a transition graph $G = (\Omega, \mathbf{E})$ whose nodes correspond to states of the random variables. Let $\mathbf{n}(\mathbf{x})$ be the set of neighbors of state \mathbf{x} in G , that is, all states reachable

from \mathbf{x} with a single transition. The Metropolis chain with graph G and distribution π has transition probabilities

$$P(\mathbf{x} \rightarrow \mathbf{y}) = \begin{cases} \frac{1}{|\mathbf{n}(\mathbf{x})|} \min \left\{ \frac{\pi(\mathbf{y})|\mathbf{n}(\mathbf{x})|}{\pi(\mathbf{x})|\mathbf{n}(\mathbf{y})|}, 1 \right\} & \text{if } x \text{ and } y \text{ are neighbors,} \\ 1 - \sum_{\mathbf{y}' \in \mathbf{n}(\mathbf{x})} \frac{1}{|\mathbf{n}(\mathbf{x})|} \min \left\{ \frac{\pi(\mathbf{y}')|\mathbf{n}(\mathbf{x})|}{\pi(\mathbf{x})|\mathbf{n}(\mathbf{y}')|}, 1 \right\} & \text{if } x = y, \\ 0, & \text{otherwise.} \end{cases}$$

Being in state \mathbf{x}_t of the Markov chain $\mathcal{M} = (\mathbf{x}_0, \mathbf{x}_1, \dots)$, the Metropolis sampler therefore performs the following steps at time $t + 1$:

1. Select a state \mathbf{y} from $\mathbf{n}(\mathbf{x}_t)$, the neighbors of \mathbf{x}_t , uniformly at random;
2. Let $\mathbf{x}_{t+1} = \mathbf{y}$ with probability $\min \left\{ \frac{\pi(\mathbf{y})|\mathbf{n}(\mathbf{x})|}{\pi(\mathbf{x})|\mathbf{n}(\mathbf{y})|}, 1 \right\}$;
3. Otherwise, let $\mathbf{x}_{t+1} = \mathbf{x}_t$.

Note that the proposal distribution $Q(\cdot|\mathbf{x})$ is simply the uniform distribution on the set of \mathbf{x} 's neighbors. It is straight-forward to show that π is a stationary distribution for the Metropolis chain by showing that π is a reversible distribution for it (Häggström, 2002).

Now, the performance of the Metropolis chain hinges on the structure of the graph G . We would like the graph structure to facilitate global moves between high probability modes, as opposed to the local moves typically performed by MCMC chains. To design such a graph structure, we take advantage of approximate symmetries in the model.

10.5.3 Orbital Metropolis Chains

This section describes a class of **orbital Metropolis chains** that move between approximate symmetries of a distribution. The approximate symmetries form an automorphism group \mathfrak{G} . We will discuss approaches to obtain such an automorphism group in Section 10.6. Here, we introduce a Markov chain that takes advantage of the approximate symmetries.

Given a distribution π over random variables \mathbf{X} with state space Ω , and a permutation group \mathfrak{G} acting on Ω , the orbital Metropolis chain $\mathcal{M}_{\mathfrak{G}}$ for \mathfrak{G} performs the following steps:

1. Select a state \mathbf{y} from $\mathbf{x}_t^{\mathfrak{G}}$, the orbit of \mathbf{x}_t , uniformly at random;
2. Let $\mathbf{x}_{t+1} = \mathbf{y}$ with probability $\min \left\{ \frac{\pi(\mathbf{y})}{\pi(\mathbf{x})}, 1 \right\}$;
3. Otherwise, let $\mathbf{x}_{t+1} = \mathbf{x}_t$.

Note that a permutation group acting on Ω partitions the states into disjoint orbits. The orbital Metropolis chain simply moves between states in the same orbit. Hence, two states in the same orbit have the same number of neighbors and, thus, the expressions cancel out in line 2 above. It is straight-forward to show that the chain $\mathcal{M}_{\mathfrak{G}}$ is reversible and, hence, that it has π as a stationary distribution. However, the chain is *not* irreducible as it never moves between states that are not symmetric with respect to the permutation group \mathfrak{G} . In

the binary case, for example, it cannot reach states with a different Hamming weight from the initial state.

10.5.4 Lifted Metropolis-Hastings

To obtain an irreducible Markov chain that exploits approximate symmetries, we construct a mixture of (a) some base chain \mathcal{M}_B with stationary distribution π for which we know that it is irreducible and aperiodic; and (b) an orbital Metropolis chain \mathcal{M}_S . We can prove the following theorem.

Theorem 10.5 *Let \mathbf{X} be a set of random variables with distribution π and approximate automorphisms \mathcal{G} . Moreover, let \mathcal{M}_B be an aperiodic and irreducible Markov chain with stationary distribution π , and let \mathcal{M}_S be the orbital Metropolis chain for \mathbf{X} and \mathcal{G} . The mixture of \mathcal{M}_B and \mathcal{M}_S is aperiodic, irreducible, and has π as its unique stationary distribution.*

The mixture of the base chain and the orbital Metropolis chain has several advantages. First, it exploits the approximate symmetries of the model which was shown to be advantageous for marginal probability estimation (Van den Broeck and Darwiche, 2013). Second, the mixture of Markov chains performs wide ranging moves via the orbital Metropolis chain, exploring the state space more efficiently and, therefore, improving the quality of the probability estimates. Figure 10.4 depicts the state space and the transition graph of (a) the Gibbs chain and (b) the mixture of the Gibbs chain and an orbital Metropolis chain. It illustrates that the mixture is able to more freely move about the state space by jumping between orbit states. For instance, moving from state 0110 to 1001 would require 4 steps of the Gibbs chain but is possible in one step with the mixture of chains. The larger the size of the automorphism groups, the more densely connected is the transition graph. Since the moves of the orbital Metropolis chain are between approximately symmetric states of the random variables, it does not suffer from the problem of most proposals being rejected. We will be able to verify this hypothesis empirically.

The general Lifted Metropolis-Hastings framework can be summarized as follows.

1. Obtain an approximate automorphism group \mathcal{G} ;
2. Run the following mixture of Markov chains:
 - (a) With probability $0 < \alpha < 1$, apply the kernel of the base chain \mathcal{M}_B ;
 - (b) Otherwise, apply the kernel of the orbital Metropolis chain \mathcal{M}_S for \mathcal{G} .

Note that the proposed approach is a generalization of lifted MCMC for symmetric models, as described in the previous section, essentially using it as a subroutine, and that all MH proposals are accepted if \mathcal{G} is an exact automorphism group of the original model. Moreover, note that the framework allows one to combine multiple orbital Metropolis chains with a base chain.

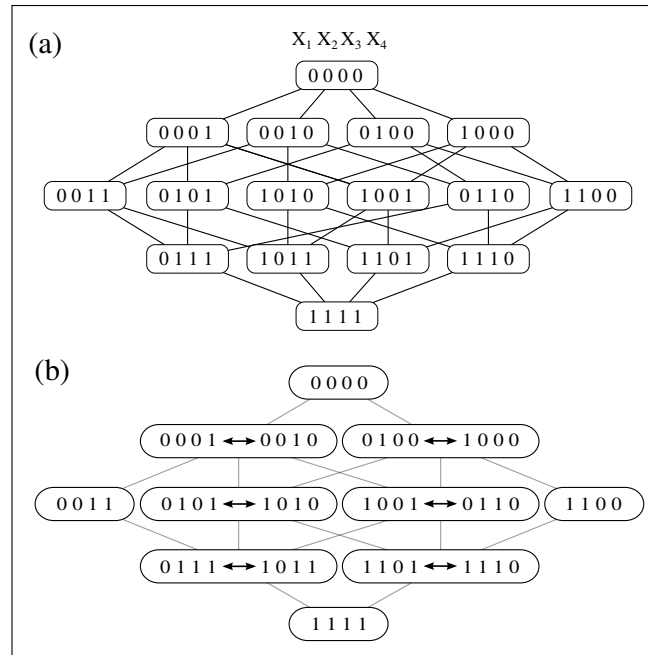


Figure 10.4: The state space (self-arcs are omitted) of (a) the Gibbs chain for four binary random variables and (b) the orbit partition of its state space induced by the permutation group generated by the permutation $(X_1 X_2)(X_3 X_4)$. The permutations are approximate symmetries, derived from an over-symmetric approximation of the original model. The Gibbs chain proposes moves to states whose Hamming distance to the current state is at most 1. The orbital Metropolis chain, on the other hand, proposes moves between orbit elements which have a Hamming distance of up to 4. The mixture of the two chains leads to faster convergence while maintaining an unbiased stationary distribution.

10.6 Approximate Symmetries

The Lifted Metropolis-Hastings algorithm assumes that a permutation group \mathcal{G} is given, representing the approximate symmetries. We now discuss several approaches to the computation of such an automorphism group. While it is not possible to go into technical detail here, we will provide pointers to the relevant literature.

There exist several techniques to compute the *exact symmetries* of a graphical model and construct \mathcal{G} ; see (Niepert, 2012b; Bui et al., 2012). The color refinement algorithm is also well-studied in lifted inference (Kersting et al., 2014). It can find (exact) orbits of random variables for a slightly weaker notion of symmetry, called fractional automorphism. These techniques all require some form of exact symmetry to be present in the model.

Detecting *approximate symmetries* is a problem that is largely open. One key idea is that of an *over-symmetric approximations* (OSAs) (Van den Broeck and Darwiche, 2013). Such approximations are derived from the original model by rendering the model more symmetric. After the computation of an over-symmetric model, we can apply existing tools for exact symmetry detection. Indeed, the exact symmetries of an approximate model are approximate symmetries of the exact model. These symmetrization techniques are indispensable to our algorithm.

10.6.1 Relational Symmetrization

Existing symmetrization techniques operate on relational representations, such as Markov logic networks (MLNs). Relational models have numerous symmetries. For example, swapping the web pages **A** and **B** in a web page classification model does not change the MLN. This permutation of constants induces a permutations of random variables (e.g., between $\text{Page}(\mathbf{A}, \text{Faculty})$ and $\text{Page}(\mathbf{B}, \text{Faculty})$). Unfortunately, hard and soft evidence breaks symmetries, even in highly symmetric relational models (Van den Broeck and Darwiche, 2013). When the variables $\text{Page}(\mathbf{A}, \text{Faculty})$ and $\text{Page}(\mathbf{B}, \text{Faculty})$ get assigned distinct soft evidence, the symmetry between **A** and **B** is removed, and lifted inference breaks down.²⁰ Similarly, when the **Link** relation is given, its graph is unlikely to be symmetric (Erdős and Rényi, 1963), which in turn breaks the symmetries in the MLN. These observations motivated research on OSAs. Van den Broeck and Darwiche (2013) propose to approximate binary relations, such as **Link**, by a low-rank Boolean matrix factorization. Venugopal and Gogate (2014a) cluster the constants in the domain of the MLN. Singla et al. (2014) present a message-passing approach to clustering similar constants.

10.6.2 Propositional Symmetrization

A key property of our LMH algorithm is that it operates at the propositional level, regardless of how the graphical model was generated. It also means that the relational symmetrization approaches outlined above are inadequate in the general case. Unfortunately, we are not aware of any work on OSAs of propositional graphical models. However, some existing techniques provide a promising direction. First, basic clustering can group together similar potentials. Second, the low-rank Boolean matrix factorization used for relational approximations can be applied to any graph structure, including graphical models. Third, color passing techniques for exact symmetries operate on propositional models (Kersting et al., 2009, 2014). Combined with early stopping, they can output approximate variable orbits.

²⁰ Solutions to this problem exist if the soft evidence is on a single unary relation (Bui et al., 2012)

10.6.3 From OSAs to Automorphisms

Given an OSA of our model, we need to compute an automorphism group \mathcal{G} from it. The obvious choice is to compute the exact automorphisms from the OSA. While this works in principle, it may not be optimal. Let us first consider the following two concepts. When a group \mathcal{G} operates on a set Ω , only a subset of the elements in Ω can actually be mapped to an element other than itself. When Ω is the set of random variables, we call these elements the *moved variables*. When Ω is the set of potentials in a probabilistic graphical model, we call these the *moved potentials*. It is clear that we want \mathcal{G} to move many random variables, as this will create the largest jumps and improve the mixing behavior. However, each LMH step comes at a cost: in the second step of the algorithm, the probability of the proposed approximately-symmetric state $\pi(\mathbf{y})$ is estimated. This requires the re-evaluation of all potentials that are moved by \mathcal{G} . Thus, the time complexity of an orbital Metropolis step is linear in the number of moved potentials. It will therefore be beneficial to construct *subgroups* of the automorphism group of the OSA and, in particular, ones that move many variables and few potentials.

10.7 Empirical Evaluation

This section empirically evaluates lifted MCMC, both on symmetric models where we use orbital Markov chains, and on asymmetric models with approximate symmetries, where we use then lifted Metropolis-Hastings algorithm.

10.7.1 Symmetric Model Experiments

We conduct experiments with the well-established social network Markov logic network (the smokes-cancer MLN) exactly as specified in (Singla and Domingos, 2008). Here we created two ground MLNs with 50 and 100, respectively, people in the domain, leading to Markov networks with 2600 and 10200 variables, respectively. Building the ground models took only a fraction of a second. We proceeded to apply the symmetry detection algorithm (Niepert, 2012b) taking 24 and 136 ms, respectively, to compute the irredundant generators of the automorphism group of the models. For n people in the domain, there are $n - 1$ irredundant generators of the automorphism group and the group has size $n!$ which is exactly the size of the symmetric group on n . Please note that, based on our observation of indistinguishability of objects on different syntactical levels of the model, it is actually not necessary to use symmetry detection algorithms in this case. The irredundant generators of the symmetric group representing the symmetries on the level of constants can be directly used to compute the irredundant generators for the permutation group representing the symmetries on the level of ground atoms and formulas.

We compared the standard Gibbs sampler, Alchemy's MC-SAT algorithm (Poon and Domingos, 2006), and the orbital Gibbs sampler on the models. The overhead of the product replacement algorithm was again negligible and far outweighed by the faster con-

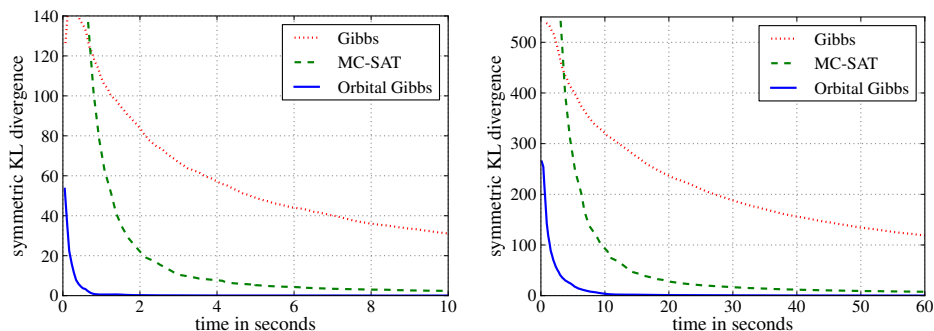


Figure 10.5: The results of the standard Gibbs sampler, Alchemy’s MC-SAT algorithm, and the orbital Gibbs sampler for the social network MLN with 50 (top) and 100 (bottom) people in the domain.

vergence of the orbital chain. Figure 10.5 plots the symmetric Kullback-Leibler divergence for the single variable marginals.

Finally, Niepert (2012b) reports additional experiments on using orbital Markov chains to sample independent sets, building on *insert/delete* Markov chains (Luby and Vigoda, 1999; Dyer and Greenhill, 2000).

10.8 Asymmetric Model Experiments

The LMH algorithm is implemented in the GAP algebra system which provides basic algorithms for automorphism groups such as the product replacement algorithm that allows one to sample uniformly from orbits of states (Niepert, 2012b).

For our first experiments, we use the standard WebKB data set, consisting of web pages from four computer science departments (Craven and Slattery, 2001). The data has information about approximately 800 words that appear on 1000 pages, 7 page labels and links between web pages. There are 4 folds, one for each university. We use the standard MLN structure for the WebKB domain, which has MLN formulas of the form shown above, but for all combinations of labels and words, adding up to around 5500 first-order MLN formulas. We learn the MLN parameters using Alchemy.

We consider a collective classification setting, where we are given the link structure and the word content of each web page, and want to predict the page labels. We run Gibbs sampling and the Lifted MCMC algorithm (Niepert, 2012b), and show the average KL divergence between the estimated and true marginals in Figure 10.6. When true marginals are not computable, we used a very long run of a Gibbs sampler for the gold standard marginals. Since every web page contains a unique set of words, the evidence on the word content creates distinct soft evidence on the page labels. Moreover, the link structure is largely asymmetric and, therefore, there are no exploitable exact symmetries and Lifted

MCMC coincides with Gibbs sampling. Next we construct an OSA using a rank-5 approximation of the link structure (Van den Broeck and Darwiche, 2013) and group the potential weights into 6 clusters.

From this OSA we construct a set of automorphisms that is efficient for LMH as follows. First, we compute the exact automorphisms \mathfrak{G}_1 of the OSA. Second, we compute the variable orbits of \mathfrak{G}_1 , grouping together all variables that can be mapped into each other. Then, for every orbit O , we construct a set of automorphisms as follows. We greedily search for a $O' \subseteq O$ such that the symmetric group $\mathfrak{G}_{O'}$ on O' maximizes the ratio between the number of moved variables (i.e., $|O'|$) and the number of moved potentials, while keeping the number of moved potentials bounded by a constant K . This guarantees that $\mathfrak{G}_{O'}$ yields an efficient orbital Metropolis chain. Finally, we remove O' from O and recurse until O is empty. From this set of symmetric groups $\mathfrak{G}_{O'}$, we construct a set of orbital Metropolis chains, each with its own set of moved potentials.

Figure 10.6 shows that the LMH chain, with mixing parameter $\alpha = 4/5$, has a lower KL divergence than Gibbs and Lifted MCMC vs. the number of iterations. Note that there is a slight overhead to LMH because the orbital Metropolis chain is run between base chain steps. Despite this overhead, LMH outperforms the baselines as a function of time. The orbital Metropolis chain accepts approximately 70% of its proposals.

Figure 10.7 illustrates the effect of running Lifted MCMC on OSA, which is the current state-of-the-art approach for asymmetric models. As expected, the drawn sample points produce biased estimates. As the quality of the approximation increases, the bias reduces, but so do the speedups. LMH does not suffer from a bias. Moreover, we observe that its performance is stable across different OSAs (not depicted).

We also ran experiments for two propositional models that are frequently used in real world applications. The first model is a 100x100 ferromagnetic Ising model with constant interaction strength and external field (see Figure 10.1(a) for a 4x4 version). Due to the different potentials induced by the external field, the model has no symmetries. We use the model without external field to compute the approximate symmetries. The automorphism group representing these symmetries is generated by the rotational and reflectional symmetries of the grid model (see Figure 10.1(b)). As in the experiments with the relational models, we used the mixing parameter $\alpha = 4/5$ for the LMH algorithm. Figure 10.8(c) and (d) depicts the plots of the experimental results. The LMH algorithm performs better with respect to the number of iterations and, to a lesser extent, with respect to time.

We also ran experiments on the Chimera model which has recently received some attention as it was used to assess the performance of quantum annealing (Boixo et al., 2013). We used exactly the model as described in Boixo et al. (2013). This model is also asymmetric but can be made symmetric by assuming that all pairwise interactions are identical. The KL divergence vs. number of iterations and vs. time in seconds is plotted in Figure 10.8(a) and (b), respectively. Similar to the results for the Ising model, LMH outperforms Gibbs and

LMCMC both with respect to the number of iterations and wall clock time. In summary, the LMH algorithm outperforms standard sampling algorithms on these propositional models in the absence of any symmetries. We used very simple symmetrization strategies for the experiments. This demonstrates that the LMH framework is powerful and allows one to design state-of-the-art sampling algorithms.

10.9 Conclusions

We have presented a perspective on lifted inference, where instead of directly operating on the space of joint variable assignments, *orbital* Markov chains operate on a symmetry-induced partition of this space. We related lifted MCMC to the notion of lumping of Markov chains. Instead of computing the partition of the state space explicitly which is usually intractable, orbital Markov chains operate on the original state space while having convergence properties identical to the corresponding lumped Markov chain. We want to point out that in the MCMC literature a lifting of a Markov chain (Chen et al., 1999) is *not* the same as what has been coined lifted inference by the statistical relational AI community. Quite the opposite, instead of operating on a more compact state space, lifting in the classical sense introduces additional states. Nevertheless, there might be interesting relationships between lumping, lifting and lifted inference.

We have also presented a Lifted Metropolis-Hastings algorithms capable of mixing two types of Markov chains. The first is a non-lifted base chain, and the second is an orbital Metropolis chain that moves between approximately symmetric states. This allows lifted inference techniques to be applied to asymmetric graphical models.

Numerous extensions to the lifted MCMC framework have been developed in recent years, for example towards exploiting contextual and block-valued symmetries (Anand et al., 2016; Madan et al., 2018), and continuous symmetries (Shariff et al., 2015). Holtzen et al. (2019a) showed how to build an exact lifted inference algorithm that enumerates and counts orbits, and how to sample orbits directly, without the need for Gibbs sampling to move between orbits.

10.10 Acknowledgments

Lifted MCMC for symmetric models first appeared as Niepert (2012b) and Niepert (2012a). Lifted MCMC for asymmetric models first appeared as Van den Broeck and Niepert (2015).

10.11 Appendix: Proof of Theorem 10.3

We first prove (a). Since \mathcal{M} is aperiodic we have, for each state $x \in \Omega$ and every time step $t \geq 0$, a non-zero probability for the Markov chain \mathcal{M} to remain in state x at time $t + 1$. At each time $t + 1$, the orbital Markov chain transitions uniformly at random to one of the states in the orbit of the original chain's state at time $t + 1$. Since every state is an element of its own orbit, we have, for every state $x \in \Omega$ and every time step $t \geq 0$,

a non-zero probability for the Markov chain \mathcal{M} to remain in state x at time $t + 1$. Hence, \mathcal{M} is aperiodic. The proof of statement (b) is accomplished in an analogous fashion and omitted.

Let $P(x, y)$ and $P'(x, y)$ be the probabilities of \mathcal{M} and \mathcal{M}' , respectively, to transition from state x to state y . Since π is a reversible distribution for \mathcal{M}' we have that $\pi(x)P'(x, y) = \pi(y)P'(y, x)$ for all states $x, y \in \Omega$. For every state $x \in \Omega$ let $x^{\mathfrak{G}}$ be the orbit of x . Let $\mathfrak{G}_x := \{g \in \mathfrak{G} \mid x^g = x\}$ be the stabilizer subgroup of x with respect to \mathfrak{G} . We have that

$$\begin{aligned} \sum_{g \in \mathfrak{G}} P'(x, y^g) &= \sum_{y' \in y^{\mathfrak{G}}} |\mathfrak{G}_{y'}| P'(x, y') \\ &= |\mathfrak{G}_y| \sum_{y' \in y^{\mathfrak{G}}} P'(x, y') \\ &= (|\mathfrak{G}|/|y^{\mathfrak{G}}|) \sum_{y' \in y^{\mathfrak{G}}} P'(x, y') \end{aligned} \tag{10.1}$$

where the last two equalities follow from the orbit-stabilizer theorem. We will now prove that $\pi(x)P(x, y) = \pi(y)P(y, x)$ for all states $x, y \in \Omega$. By definition of the orbital Markov chain we have that $\pi(x)P(x, y) = \pi(x)(1/|y^{\mathfrak{G}}|) \sum_{y' \in y^{\mathfrak{G}}} P'(x, y')$ and, by equation (1), we have

$$\begin{aligned} &= \pi(x)(1/|y^{\mathfrak{G}}|)(|y^{\mathfrak{G}}|/|\mathfrak{G}|) \sum_{g \in \mathfrak{G}} P'(x, y^g) \\ &= \pi(x)(1/|\mathfrak{G}|) \sum_{g \in \mathfrak{G}} P'(x, y^g) \\ &= (1/|\mathfrak{G}|) \sum_{g \in \mathfrak{G}} \pi(x)P'(x, y^g). \end{aligned}$$

Since P' is reversible and $\pi(x) = \pi(x^g)$ for all $g \in \mathfrak{G}$ we have $(1/|\mathfrak{G}|) \sum_{g \in \mathfrak{G}} \pi(x)P'(x, y^g) = (1/|\mathfrak{G}|) \sum_{g \in \mathfrak{G}} \pi(y^g)P'(y^g, x) = \pi(y)(1/|\mathfrak{G}|) \sum_{g \in \mathfrak{G}} P'(y^g, x)$. Now, since $P'(x, y) = P'(x^g, y^g)$ for all $x, y \in \Omega$ and all $g \in \mathfrak{G}$ by assumption, we have that $\pi(y)(1/|\mathfrak{G}|) \sum_{g \in \mathfrak{G}} P'(y^g, x) = \pi(y)(1/|\mathfrak{G}|) \sum_{g \in \mathfrak{G}} P'(y, x^{-g}) = \pi(y)(1/|\mathfrak{G}|) \sum_{g \in \mathfrak{G}} P'(y, x^g)$ and, again by equation (1), we have

$$\begin{aligned} &= \pi(y)(1/|\mathfrak{G}|)(|\mathfrak{G}|/|x^{\mathfrak{G}}|) \sum_{x' \in x^{\mathfrak{G}}} P'(y, x') \\ &= \pi(y)(1/|x^{\mathfrak{G}}|) \sum_{x' \in x^{\mathfrak{G}}} P'(y, x') = \pi(y)P(y, x). \quad \square \end{aligned}$$

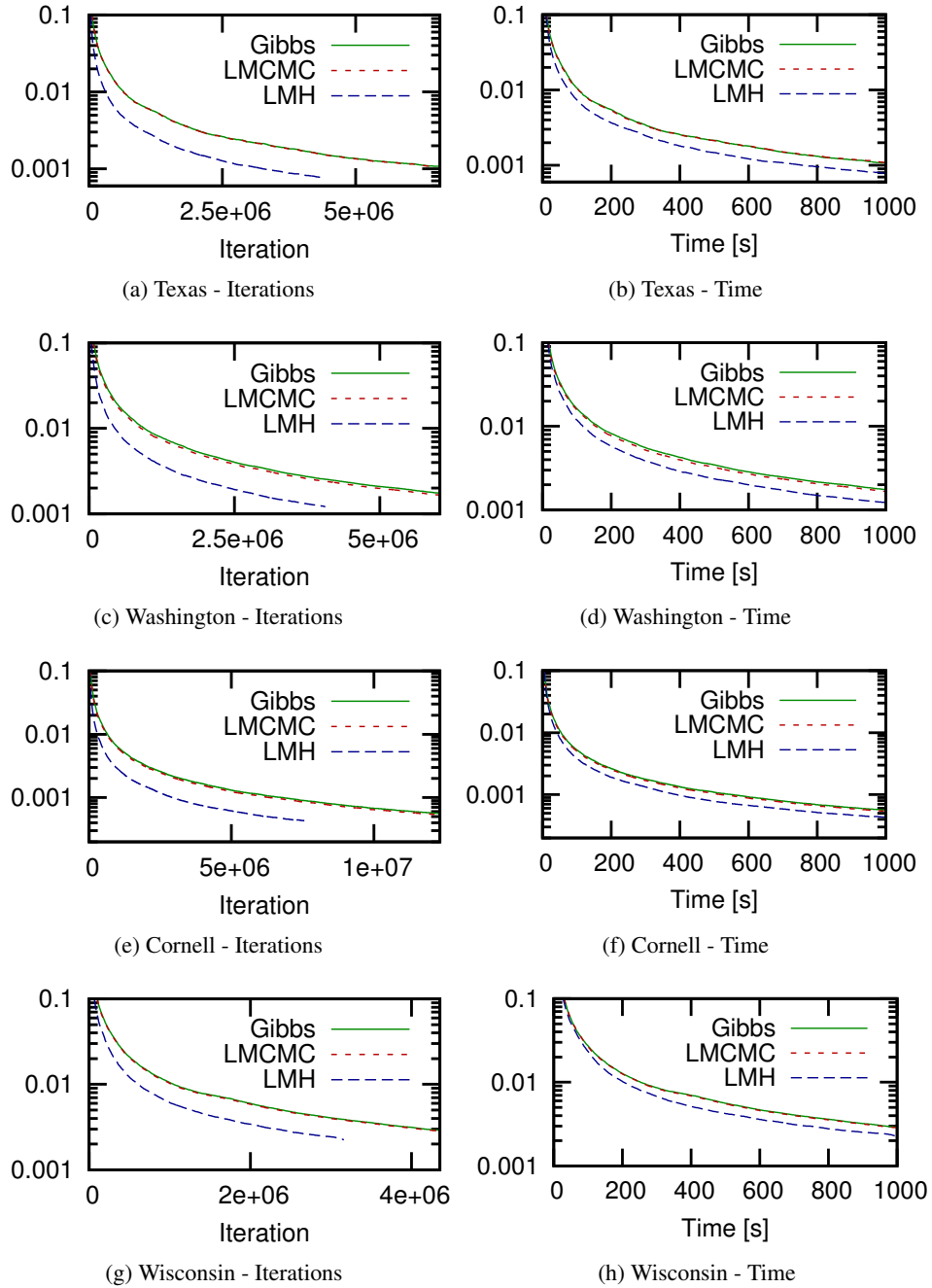


Figure 10.6: WebKB - KL Divergences

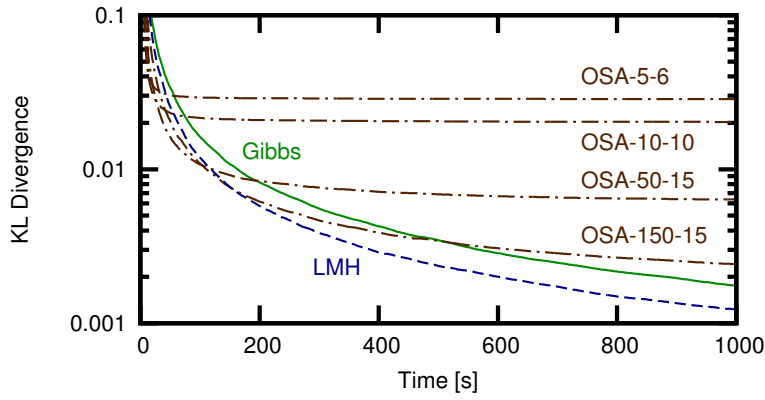


Figure 10.7: LMH vs. over-symmetric approximations (OSA) on WebKB Washington. OSA- r - c denotes binary evidence of Boolean rank r and c clusters of formula weights.

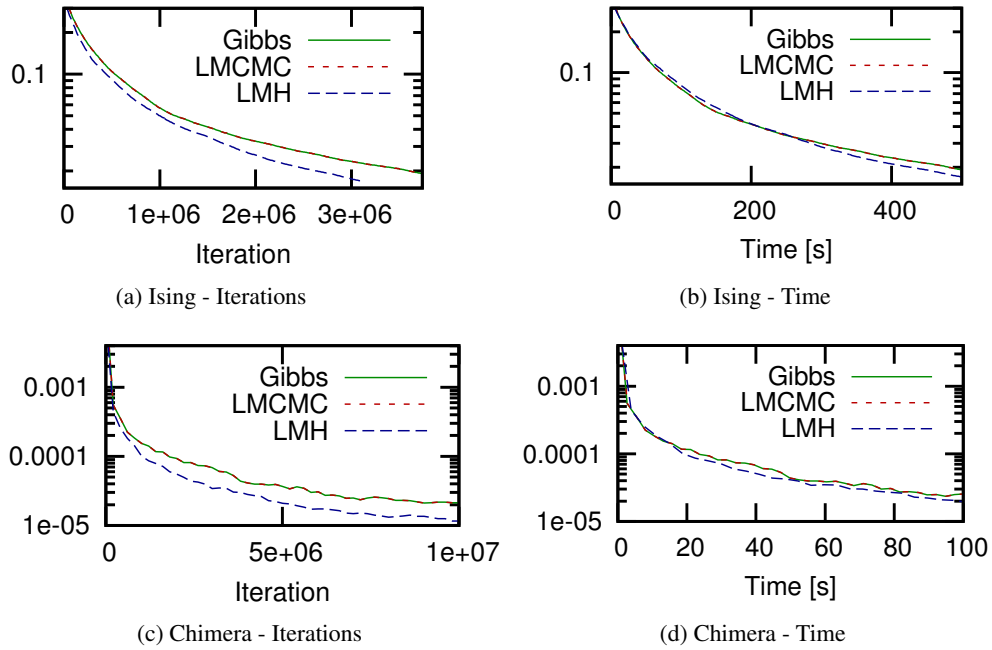


Figure 10.8: KL Divergences for the propositional models.

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