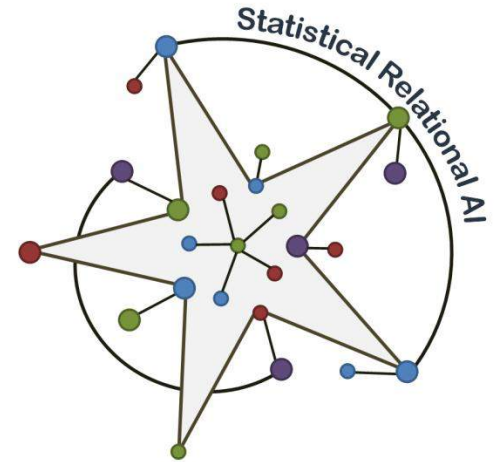


# StarAI 2015



- Fifth International Workshop on Statistical Relational AI
- At the 31st Conference on Uncertainty in Artificial Intelligence (**UAI**) (right after ICML)
- In **Amsterdam**, The Netherlands, on **July 16**.
- Paper Submission: **May 15**
  - Full, 6+1 pages
  - Short, 2 page position paper or abstract

What we can't do (yet, well)?

# Approximate Symmetries in Lifted Inference

Guy Van den Broeck

(on joint work with Mathias Niepert and Adnan Darwiche)

KU Leuven

# Overview


- Lifted inference in 2 slides
- Complexity of evidence
- Over-symmetric approximations
- Approximate symmetries
- Conclusions

# Overview

- **Lifted inference in 2 slides**
- Complexity of evidence
- Over-symmetric approximations
- Approximate symmetries
- Conclusions

# Lifted Inference

- In AI: exploiting symmetries/exchangeability
- Example: WebKB

Domain:   
url  $\in$  { "google.com", "ibm.com", "aaai.org", ... }

Weighted clauses:

0.049 CoursePage(x)  $\wedge$  Linked(x,y)  $\Rightarrow$  CoursePage(y)

-0.031 FacultyPage(x)  $\wedge$  Linked(x,y)  $\Rightarrow$  FacultyPage(y)

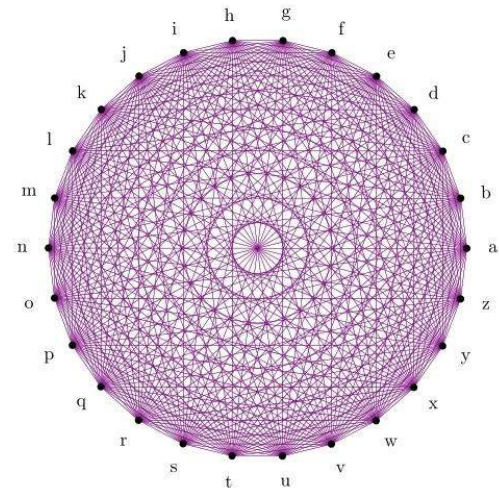
...

0.235 HasWord("Lecture",x)  $\Rightarrow$  CoursePage(x)

0.048 HasWord("Office",x)  $\Rightarrow$  FacultyPage(x)

...

5000 more first-order sentences



# The State of Lifted Inference

- UCQ database queries: **solved**  
PTIME in database size (when possible)
- MLNs and related
  - Two logical variables: **solved**  
Partition function PTIME in domain size (always)
  - Three logical variables: **#P<sub>1</sub>-hard**
- Bunch of great approximation algorithms
- Theoretical connections to **exchangeability**

# Overview

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- **Complexity of evidence**
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# Problem: Prediction with Evidence

- Add evidence on links:

Linked("google.com", "gmail.com")

Linked("google.com", "aai.org")



Symmetry google.com – ibm.com? **No!**

Linked("ibm.com", "watson.com")

Linked("ibm.com", "ibm.ca")

- Add evidence on words

HasWord("Android", "google.com")

HasWord("G+", "google.com")



Symmetry google.com – ibm.com? **No!**

HasWord("Blue", "ibm.com")

HasWord("Computing", "ibm.com")



# Complexity in Size of “Evidence”

- Consider a model liftable for model counting:

3.14  $\text{FacultyPage}(x) \wedge \text{Linked}(x,y) \Rightarrow \text{CoursePage}(y)$

- Given database DB, compute  $P(Q|DB)$ . Complexity in DB size?
  - Evidence on unary relations: **Efficient**

$\text{FacultyPage}(\text{"google.com"})=0$ ,  $\text{CoursePage}(\text{"coursera.org"})=1$ , ...

- Evidence on binary relations: **#P-hard**

$\text{Linked}(\text{"google.com"},\text{"gmail.com"})=1$ ,  $\text{Linked}(\text{"google.com"},\text{"aai.org"})=0$

*Intuition: Binary evidence breaks symmetries*

*Consequence: Lifted algorithms reduce to ground (also approx)*

# Approach

- Conditioning on **binary** evidence is **hard**
- Conditioning on **unary** evidence is **efficient**
- Solution: Represent binary evidence as unary
- Matrix notation:

$$e = p(a, a) \wedge p(a, b) \wedge \neg p(a, c) \wedge \cdots \wedge \neg p(d, c) \wedge p(d, d)$$

$$\mathbf{P} = \begin{array}{l} p(X, Y) \\ X = a \\ X = b \\ X = c \\ X = d \end{array} \begin{array}{ccccc} Y = a & Y = b & Y = c & Y = d & \\ \left[ \begin{array}{ccccc} 1 & 1 & 0 & 0 & \\ 1 & 1 & 0 & 1 & \\ 0 & 0 & 1 & 0 & \\ 1 & 0 & 0 & 1 & \end{array} \right] \end{array}$$

# Vector Product

- Solution: Represent binary evidence as unary
- Case 1:  $\forall X, \forall Y, p(X, Y) \Leftrightarrow q(X) \wedge r(Y)$

$$\mathbf{P} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix}$$

$$e = \neg p(a, a) \wedge \neg p(a, b) \wedge \cdots \wedge \neg p(d, c) \wedge p(d, d)$$

# Vector Product

- Solution: Represent binary evidence as unary
- Case 1:  $\forall X, \forall Y, p(X, Y) \Leftrightarrow q(X) \wedge r(Y)$

$$\mathbf{P} = \begin{matrix} & \begin{matrix} 0 & 1 & 0 & 1 \end{matrix} \\ \begin{matrix} 0 \\ 1 \\ 0 \\ 1 \end{matrix} & \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix} \end{matrix}$$

$\begin{matrix} 1 & 0 & 0 & 1 \end{matrix}$

$$e = \neg p(a, a) \wedge \neg p(a, b) \wedge \cdots \wedge \neg p(d, c) \wedge p(d, d)$$

# Vector Product

- Solution: Represent binary evidence as unary
- Case 1:  $\forall X, \forall Y, p(X, Y) \Leftrightarrow q(X) \wedge r(Y)$

$$\mathbf{P} = \begin{matrix} & \begin{matrix} 0 & 1 & 0 & 1 \end{matrix} \\ \begin{matrix} 0 \\ 1 \\ 0 \\ 1 \end{matrix} & \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix} \end{matrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix}^T = \mathbf{q} \mathbf{r}^T$$

1
0
0
1

$$e = \neg p(a, a) \wedge \neg p(a, b) \wedge \dots \wedge \neg p(d, c) \wedge p(d, d)$$

# Vector Product

- Solution: Represent binary evidence as unary
- Case 1:  $\forall X, \forall Y, p(X, Y) \Leftrightarrow q(X) \wedge r(Y)$

$$\mathbf{P} = \begin{bmatrix} 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \\ 0 & 0 & 0 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix}^T = \mathbf{q} \mathbf{r}^T$$

$$e = \neg p(a, a) \wedge \neg p(a, b) \wedge \cdots \wedge \neg p(d, c) \wedge p(d, d)$$

$$e = \neg q(a) \wedge q(b) \wedge \neg q(c) \wedge q(d) \quad 0101$$

$$\wedge r(a) \wedge \neg r(b) \wedge \neg r(c) \wedge r(d) \quad 1001$$

# Matrix Product

- Solution: Represent binary evidence as unary
- Case 2:  $\forall X, \forall Y, p(X, Y) \Leftrightarrow (q_1(X) \wedge r_1(Y))$   
 $\vee (q_2(X) \wedge r_2(Y))$   
 $\vee \dots$   
 $\vee (q_n(X) \wedge r_n(Y))$

# Matrix Product

- Solution: Represent binary evidence as unary
- Case 2:  $\forall X, \forall Y, p(X, Y) \Leftrightarrow (q_1(X) \wedge r_1(Y)) \vee (q_2(X) \wedge r_2(Y)) \vee \dots \vee (q_n(X) \wedge r_n(Y))$

$$\mathbf{P} = \mathbf{q}_1 \mathbf{r}_1^\top \vee \mathbf{q}_2 \mathbf{r}_2^\top \vee \dots \vee \mathbf{q}_n \mathbf{r}_n^\top = \mathbf{Q} \mathbf{R}^\top$$

$$\text{where } (\mathbf{Q} \mathbf{R}^\top)_{i,j} = \bigvee_r \mathbf{Q}_{i,r} \wedge \mathbf{R}_{j,r}$$



# Boolean Matrix Factorization

- Decompose

$$\mathbf{P} = \mathbf{q}_1 \mathbf{r}_1^\top \vee \mathbf{q}_2 \mathbf{r}_2^\top \vee \cdots \vee \mathbf{q}_n \mathbf{r}_n^\top = \mathbf{Q} \mathbf{R}^\top$$

- In Boolean algebra, where  $1+1=1$
- Minimum  $n$  is the Boolean rank
- Always possible

# Matrix Product

- Solution: Represent binary evidence as unary
- Example:  $\mathbf{P} = \mathbf{q}_1 \mathbf{r}_1^\top \vee \mathbf{q}_2 \mathbf{r}_2^\top \vee \dots \vee \mathbf{q}_n \mathbf{r}_n^\top = \mathbf{Q} \mathbf{R}^\top$

$$\mathbf{P} = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix}^\top \vee \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix}^\top \vee \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}^\top$$

# Matrix Product

- Solution: Represent binary evidence as unary
- Example:  $\mathbf{P} = \mathbf{q}_1 \mathbf{r}_1^T \vee \mathbf{q}_2 \mathbf{r}_2^T \vee \dots \vee \mathbf{q}_n \mathbf{r}_n^T = \mathbf{Q} \mathbf{R}^T$

$$\mathbf{P} = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 1 \end{bmatrix} \begin{bmatrix} 1 & 0 & 0 & 1 \end{bmatrix}^T \vee \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix} \begin{bmatrix} 1 & 1 & 0 & 0 \end{bmatrix}^T \vee \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \begin{bmatrix} 0 & 0 & 1 & 0 \end{bmatrix}^T$$

# Matrix Product

- Solution: Represent binary evidence as unary
- Example:  $\mathbf{P} = \mathbf{q}_1 \mathbf{r}_1^T \vee \mathbf{q}_2 \mathbf{r}_2^T \vee \dots \vee \mathbf{q}_n \mathbf{r}_n^T = \mathbf{Q} \mathbf{R}^T$

$$\mathbf{P} = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix}^T \vee \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix}^T \vee \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}^T$$

$$= \begin{bmatrix} 0 \\ 1 \\ 0 \\ 1 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}^T$$

# Matrix Product

- Solution: Represent binary evidence as unary
- Example:  $\mathbf{P} = \mathbf{q}_1 \mathbf{r}_1^T \vee \mathbf{q}_2 \mathbf{r}_2^T \vee \dots \vee \mathbf{q}_n \mathbf{r}_n^T = \mathbf{Q} \mathbf{R}^T$

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Boolean rank n=3

$$= \begin{bmatrix} 0 & 1 & 0 \\ 1 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix} \begin{bmatrix} 1 & 1 & 0 \\ 0 & 1 & 0 \\ 0 & 0 & 1 \\ 1 & 0 & 0 \end{bmatrix}^T$$

# Theoretical Consequences

- Theorem:

Complexity of computing  $\Pr(q | e)$  in SRL is **polynomial in  $|e|$** , when  $e$  has bounded Boolean rank.

- Boolean rank

- key parameter in the complexity of conditioning
- says how much lifting is possible

# Analogy with Treewidth in Probabilistic Graphical Models

Probabilistic graphical models:

1. Find tree decomposition

1. Perform inference

- **Exponential** in **(tree)width** of decomposition
- **Polynomial** in **size** of Bayesian network



SRL Models:

1. Find Boolean matrix factorization of evidence

2. Perform inference

- **Exponential** in **Boolean rank** of evidence
- **Polynomial** in **size** of evidence database
- **Polynomial** in **domain size**

# Overview

- Lifted inference in 2 slides
- Complexity of evidence
- **Over-symmetric approximations**
- Approximate symmetries
- Conclusions



# Over-Symmetric Approximation

- Approximate  $\Pr(q|e)$  by  $\Pr(q|e')$   
 $\Pr(q|e')$  has more symmetries, is more liftable
- E.g.: Low-rank Boolean matrix factorization

$$\mathbf{P} = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 \\ 0 & 0 & 1 & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 1 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \\ 0 \\ 1 \end{bmatrix}^{\top} \vee \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix} \begin{bmatrix} 1 \\ 1 \\ 0 \\ 0 \end{bmatrix}^{\top} \vee \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix} \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}^{\top}$$

Boolean rank 3

# Over-Symmetric Approximation

- Approximate  $\Pr(q|e)$  by  $\Pr(q|e')$   
 $\Pr(q|e')$  has more symmetries, is more liftable
- E.g.: Low-rank Boolean matrix factorization

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Boolean rank 2 approximation  $\approx$

$$\begin{bmatrix} 0 & 1 \\ 1 & 1 \\ 0 & 0 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 & 1 \\ 0 & 1 \\ 0 & 0 \\ 1 & 0 \end{bmatrix}^T = \begin{bmatrix} 1 & 1 & 0 & 0 \\ 1 & 1 & 0 & 1 \\ 0 & 0 & \mathbf{0} & 0 \\ 1 & 0 & 0 & 1 \end{bmatrix}$$

# Over-Symmetric Approximations

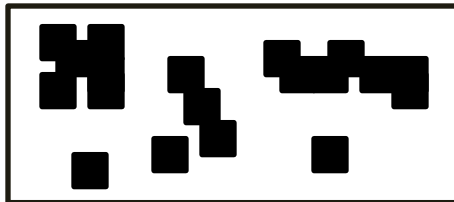
- OSA makes model more symmetric
- E.g., low-rank Boolean matrix factorization

Link ("aai.org", "google.com")  
Link ("google.com", "aai.org")  
Link ("google.com", "gmail.com")  
Link ("ibm.com", "aai.org")



Link ("aai.org", "google.com")  
Link ("google.com", "aai.org")  
~~- Link ("google.com", "gmail.com")~~  
+ Link ("aai.org", "ibm.com")  
Link ("ibm.com", "aai.org")

google.com and ibm.com become symmetric!

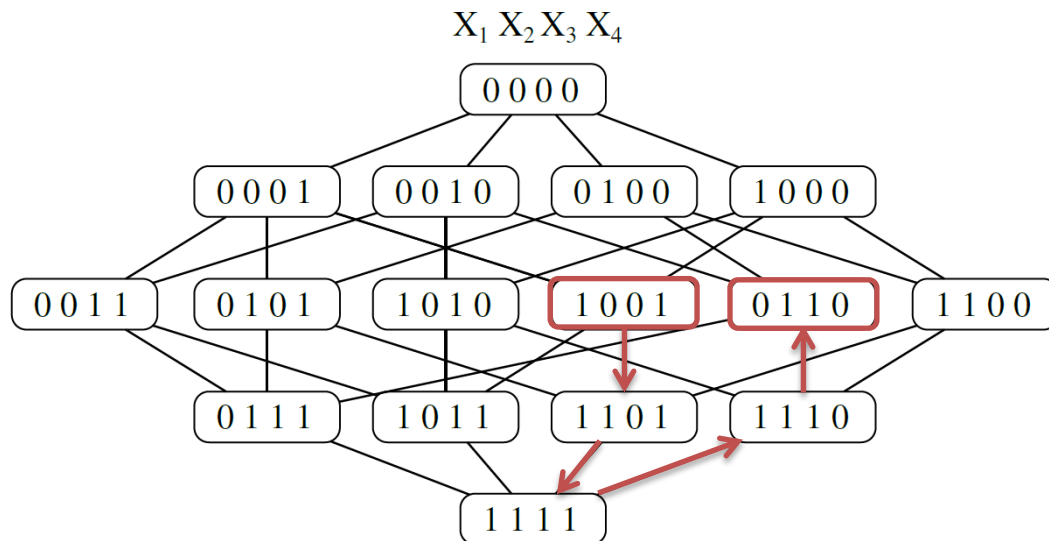


# Markov Chain Monte-Carlo

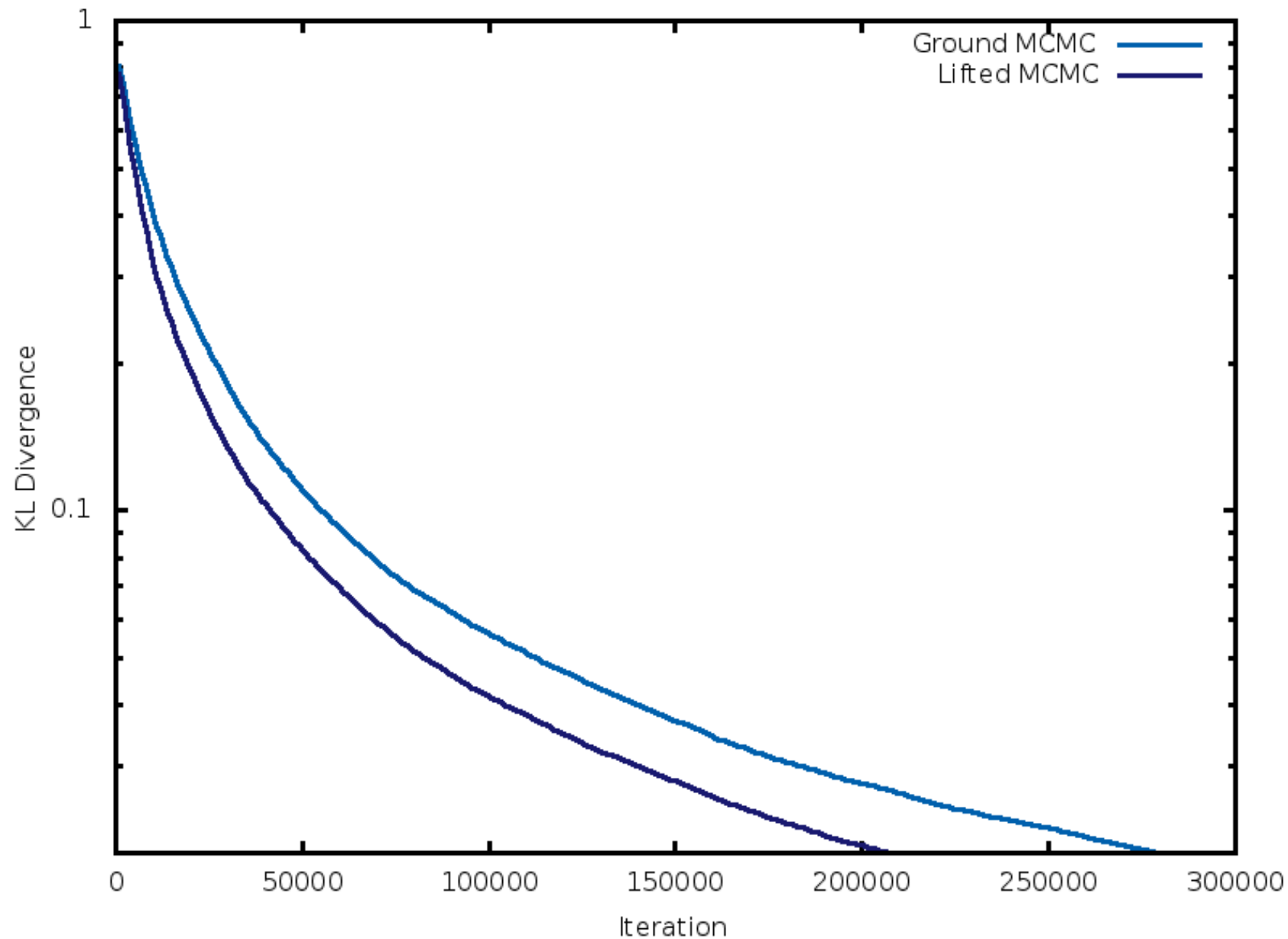
## Gibbs sampling or MC-SAT

- Problem: slow convergence, one variable changed
- One million random variables: need at least one million iteration to move between two states

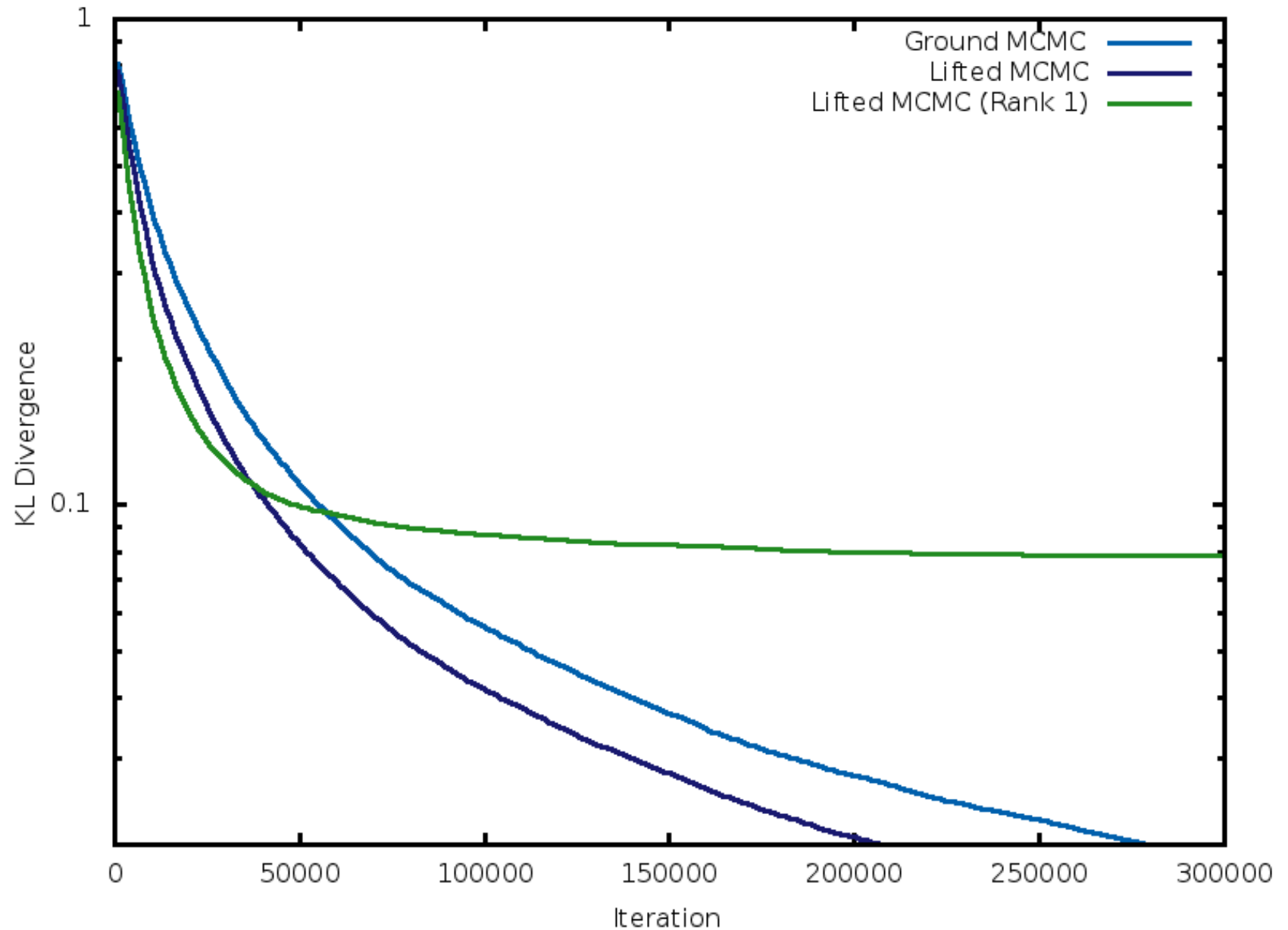
Lifted MCMC: move between symmetric states



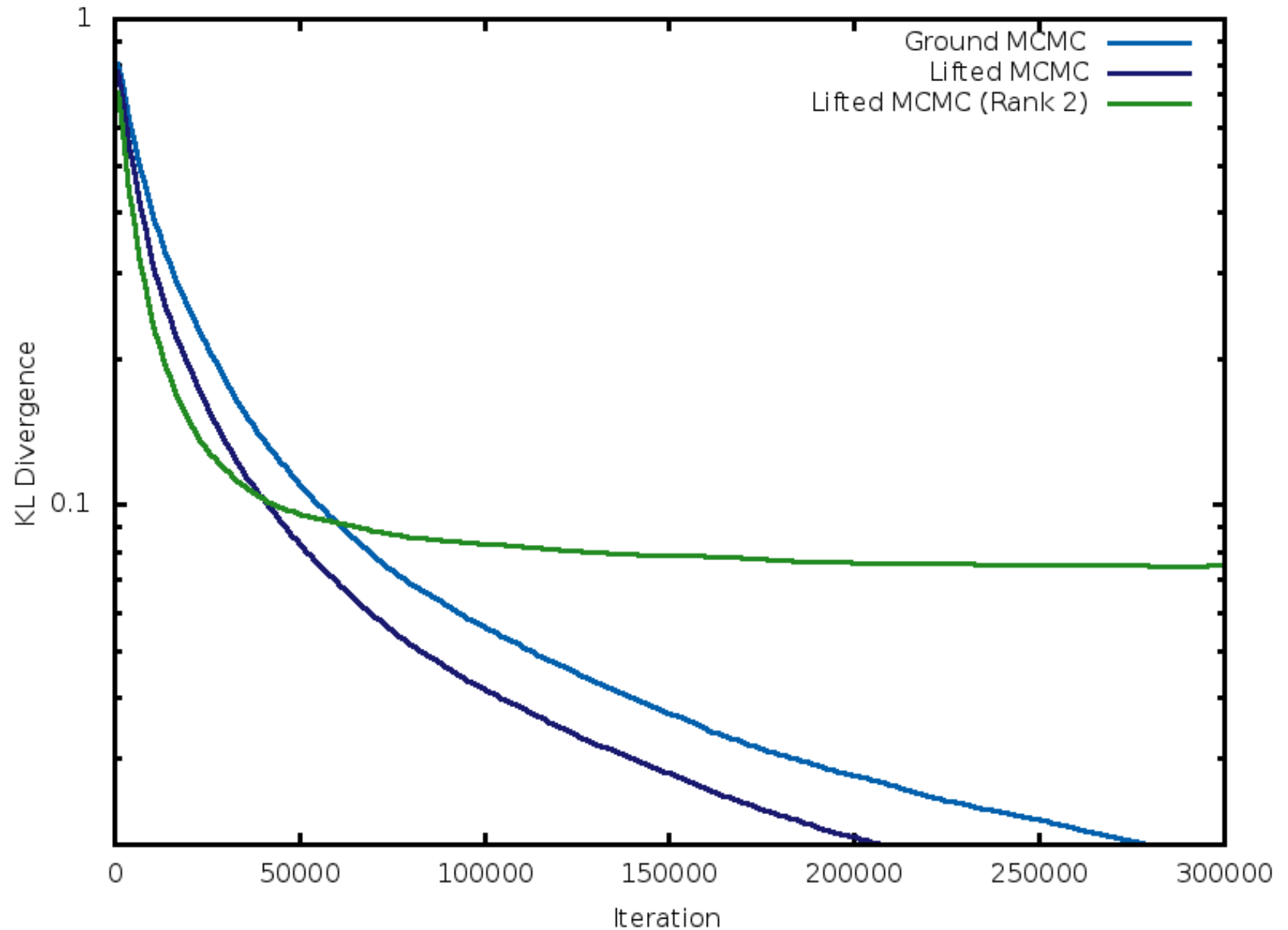
# Lifted MCMC on WebKB



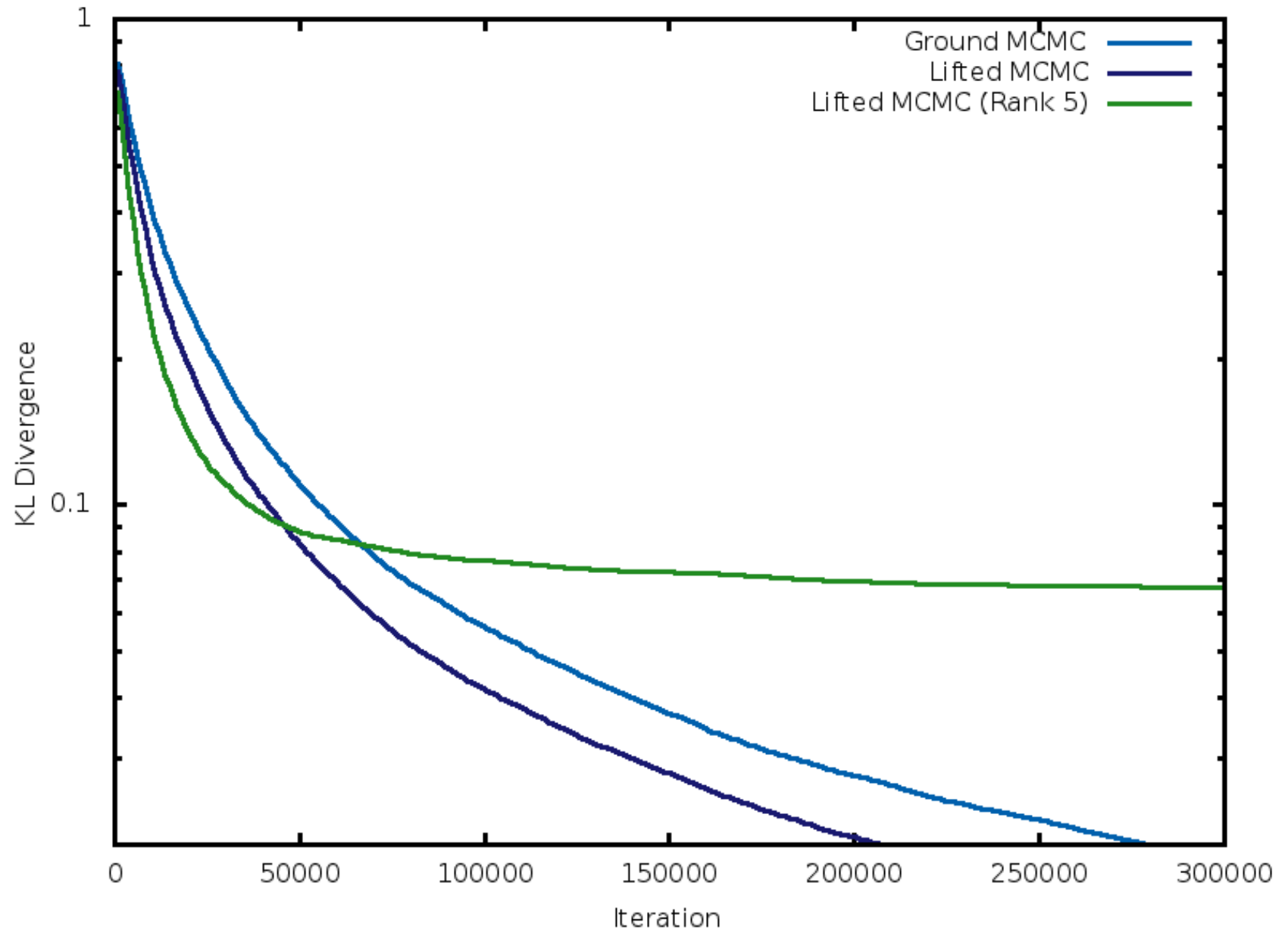
# Rank 1 Approximation



# Rank 2 Approximation

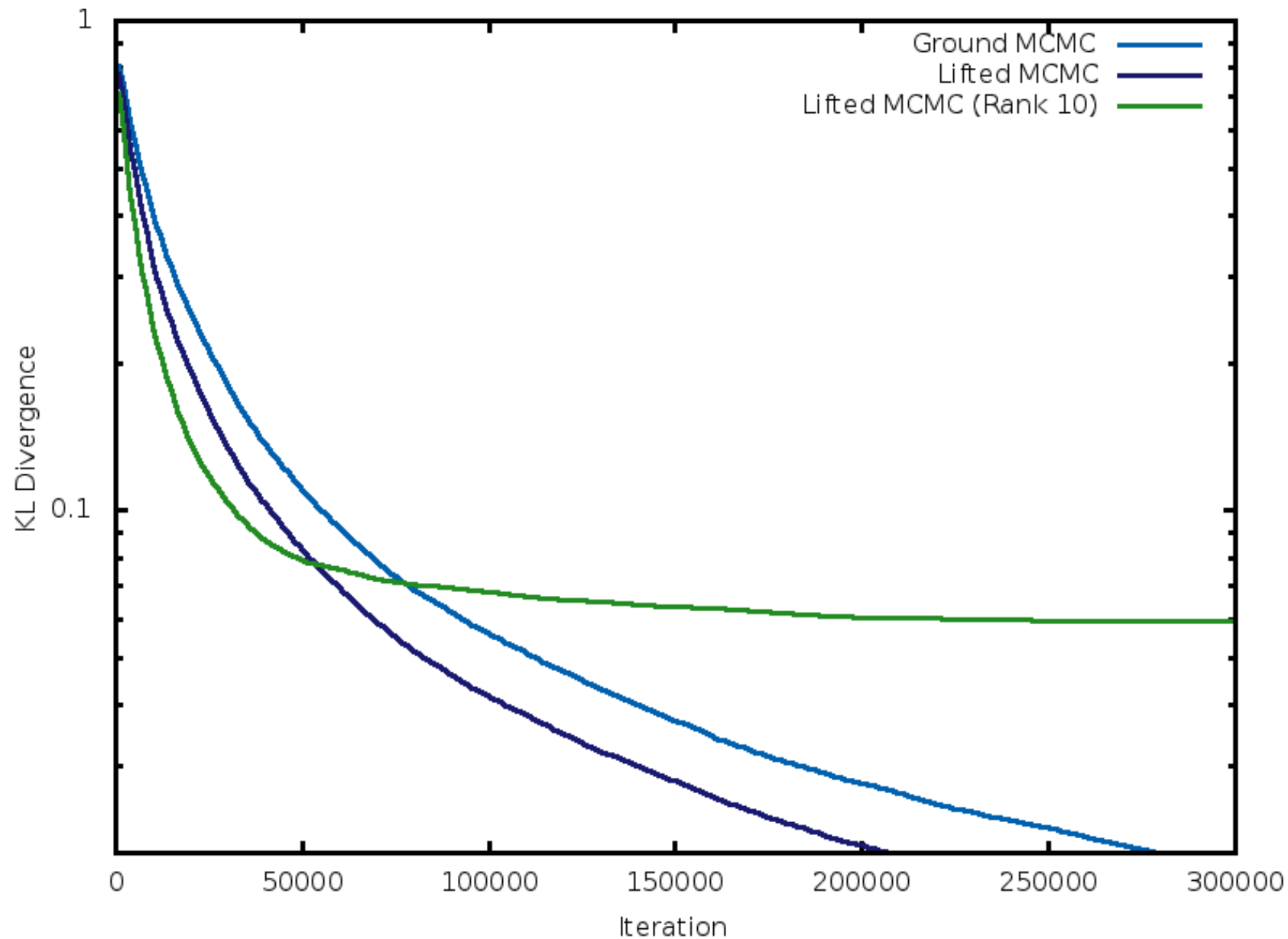


# Rank 5 Approximation

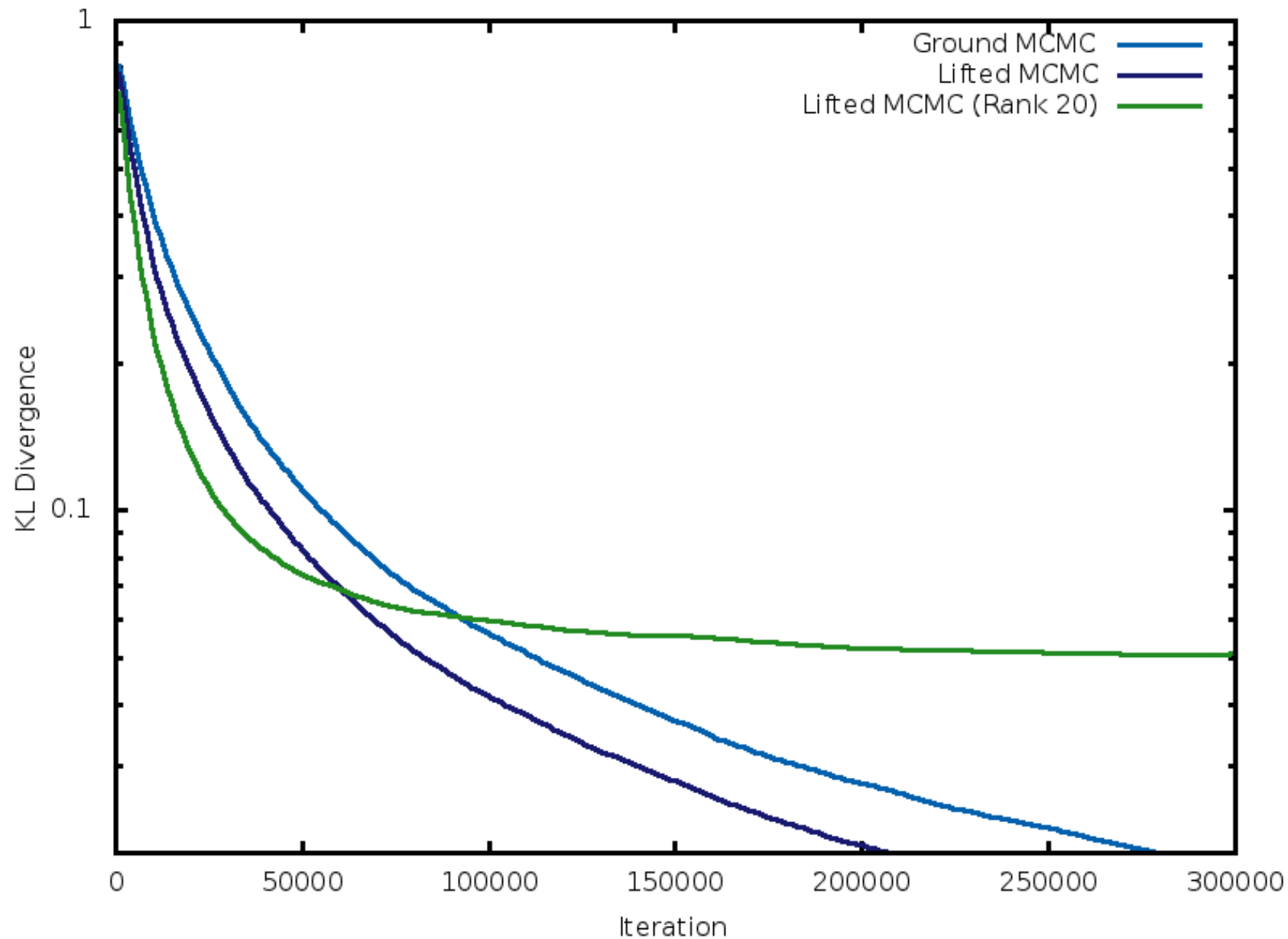




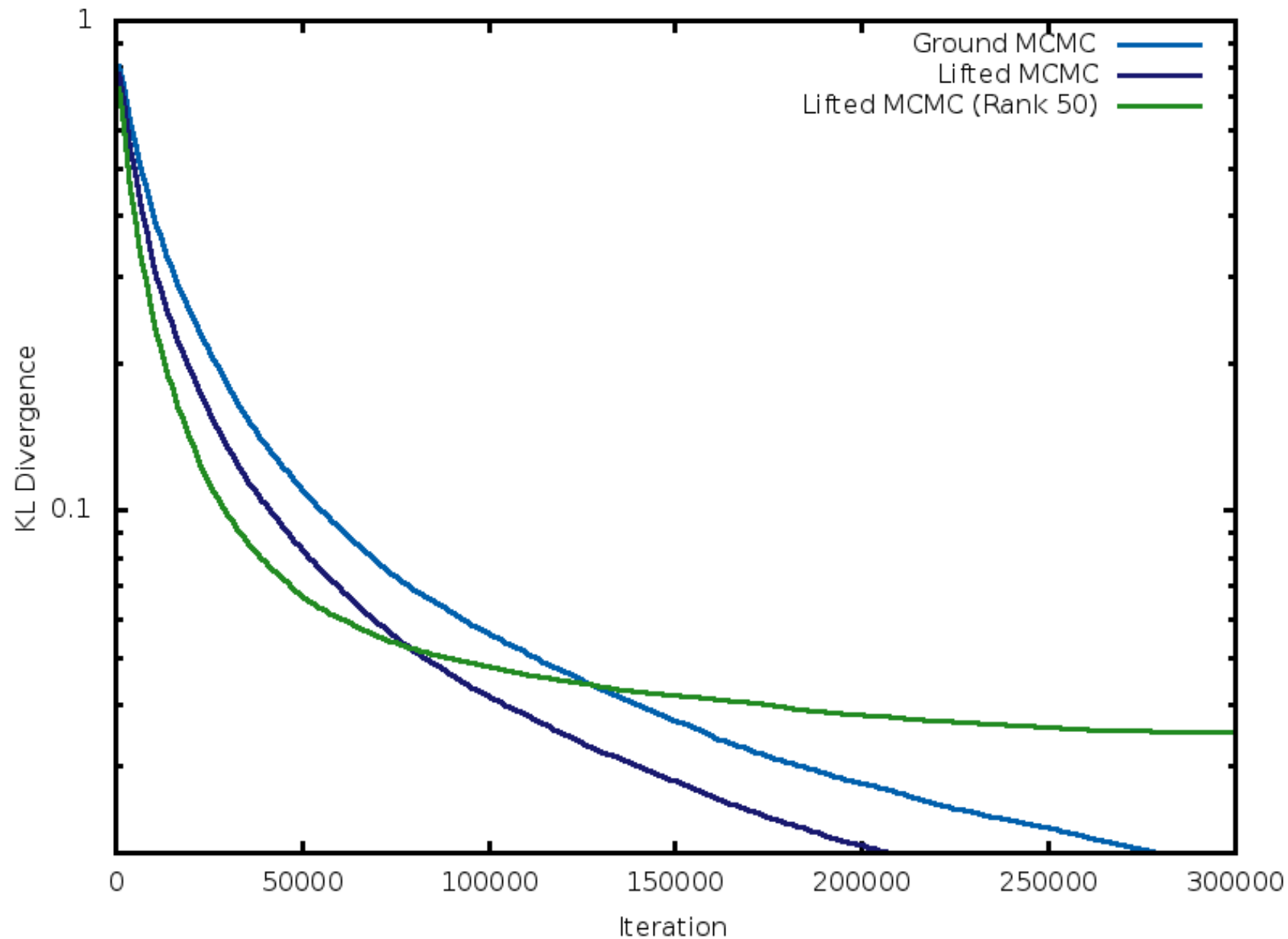
# Rank 10 Approximation



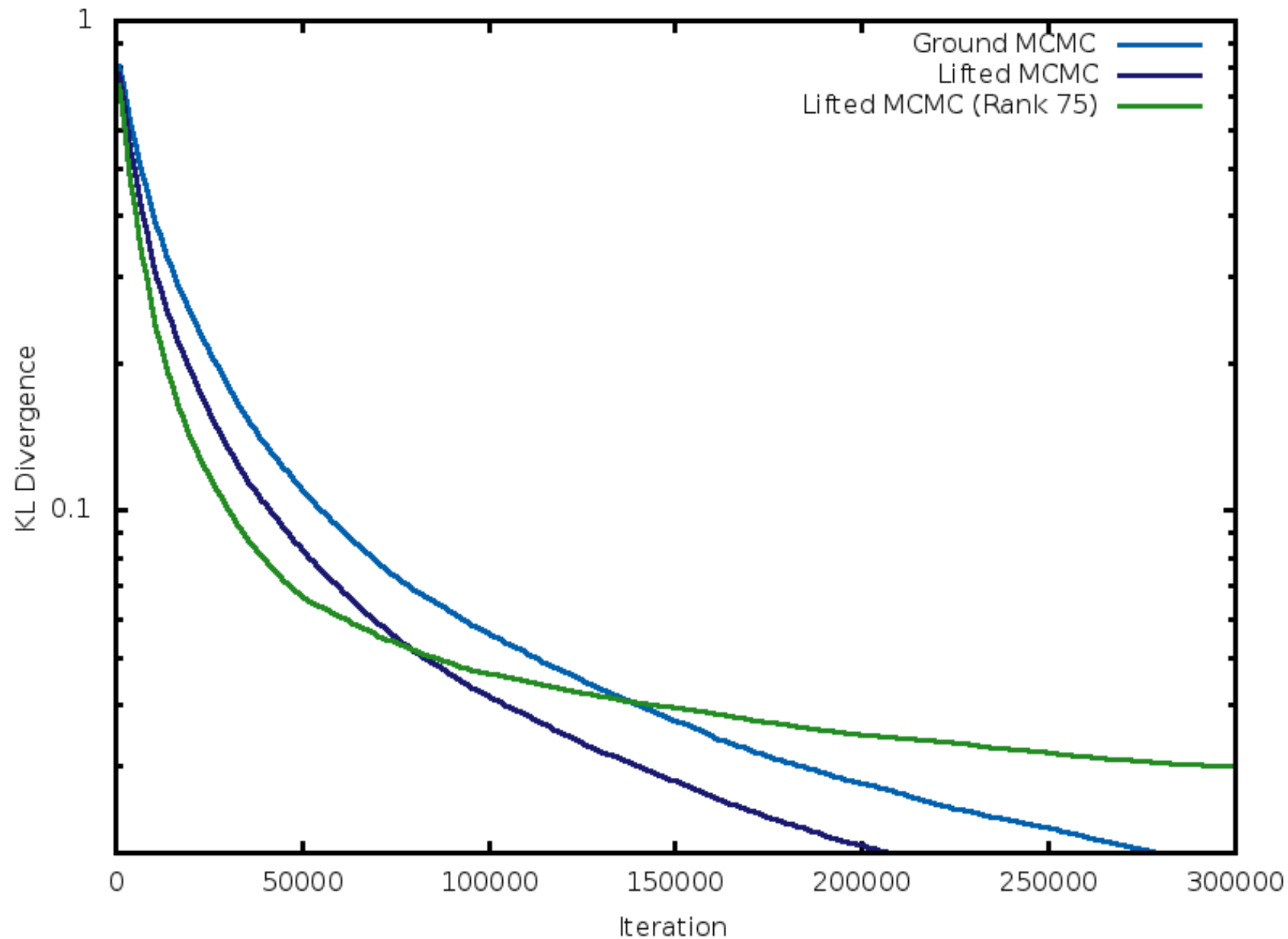
# Rank 20 Approximation



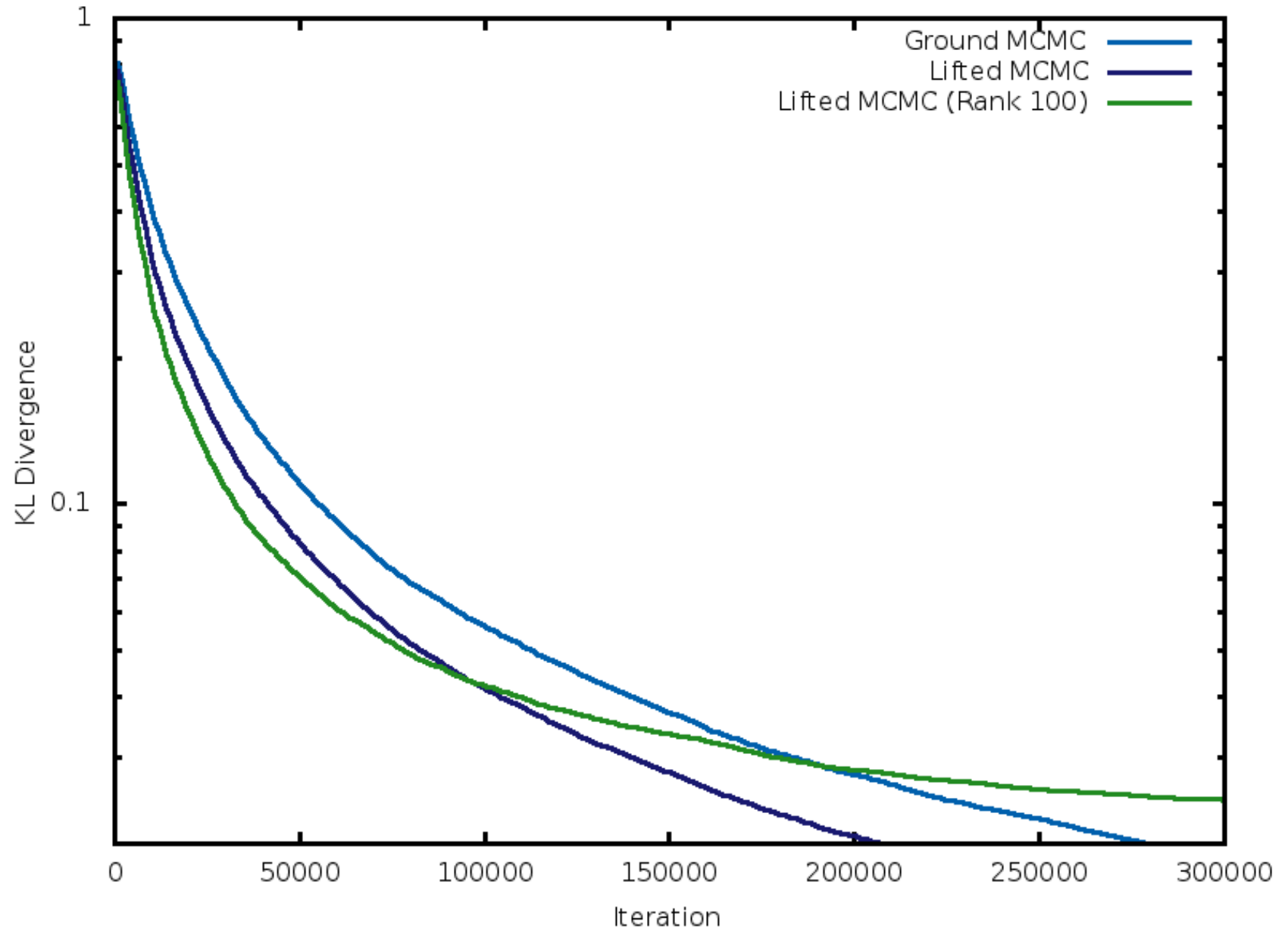
# Rank 50 Approximation



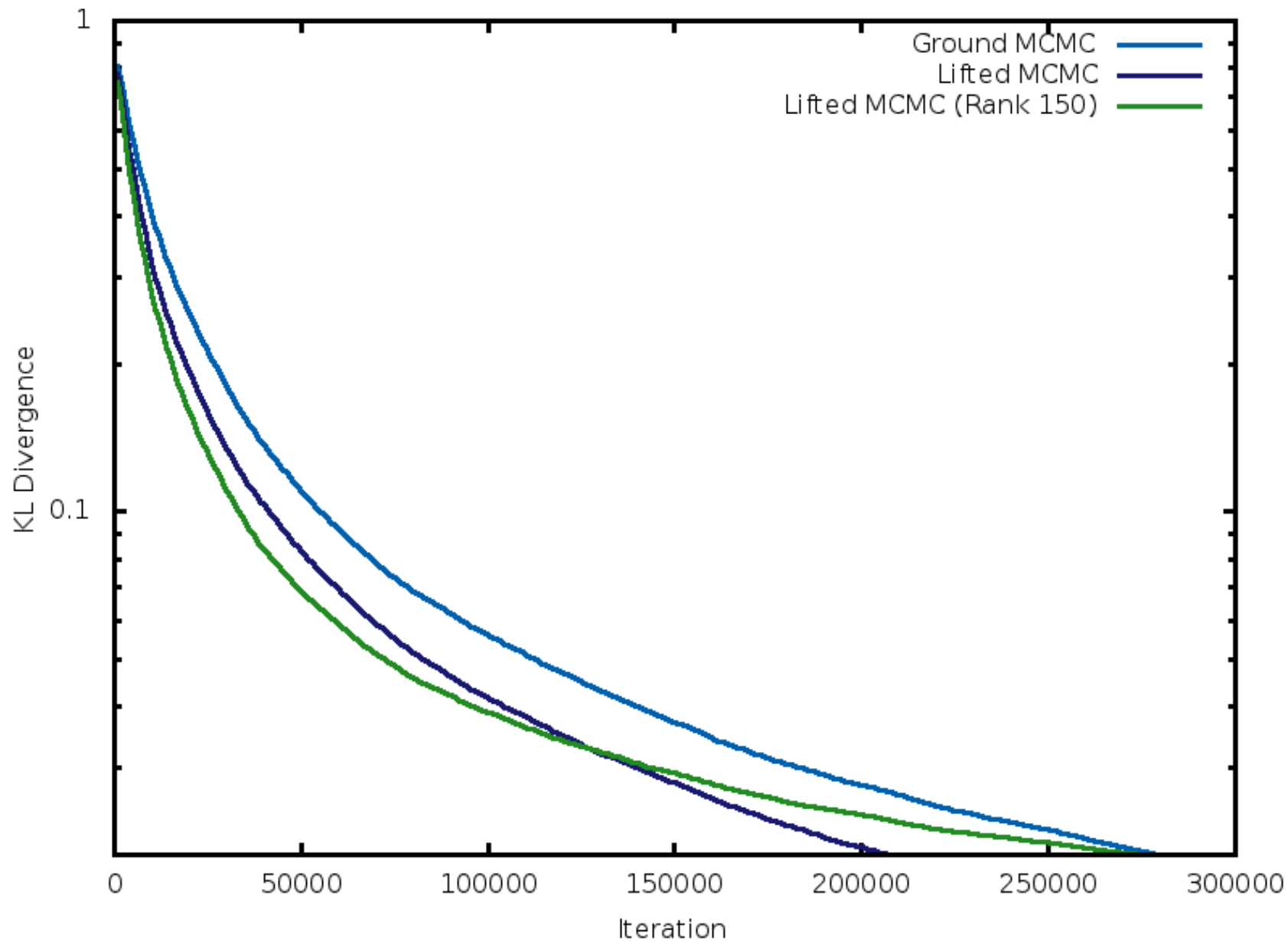
# Rank 75 Approximation



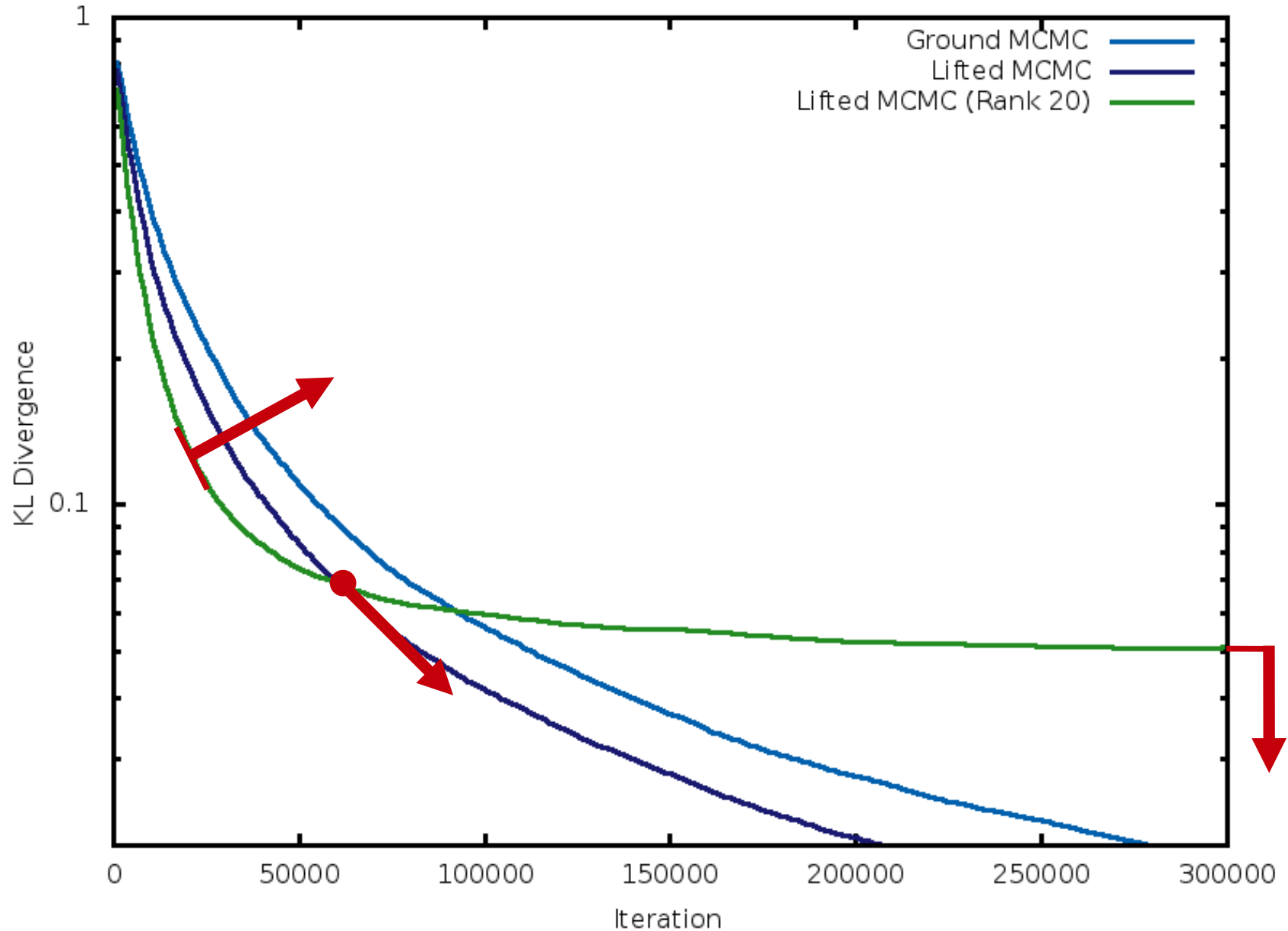
# Rank 100 Approximation



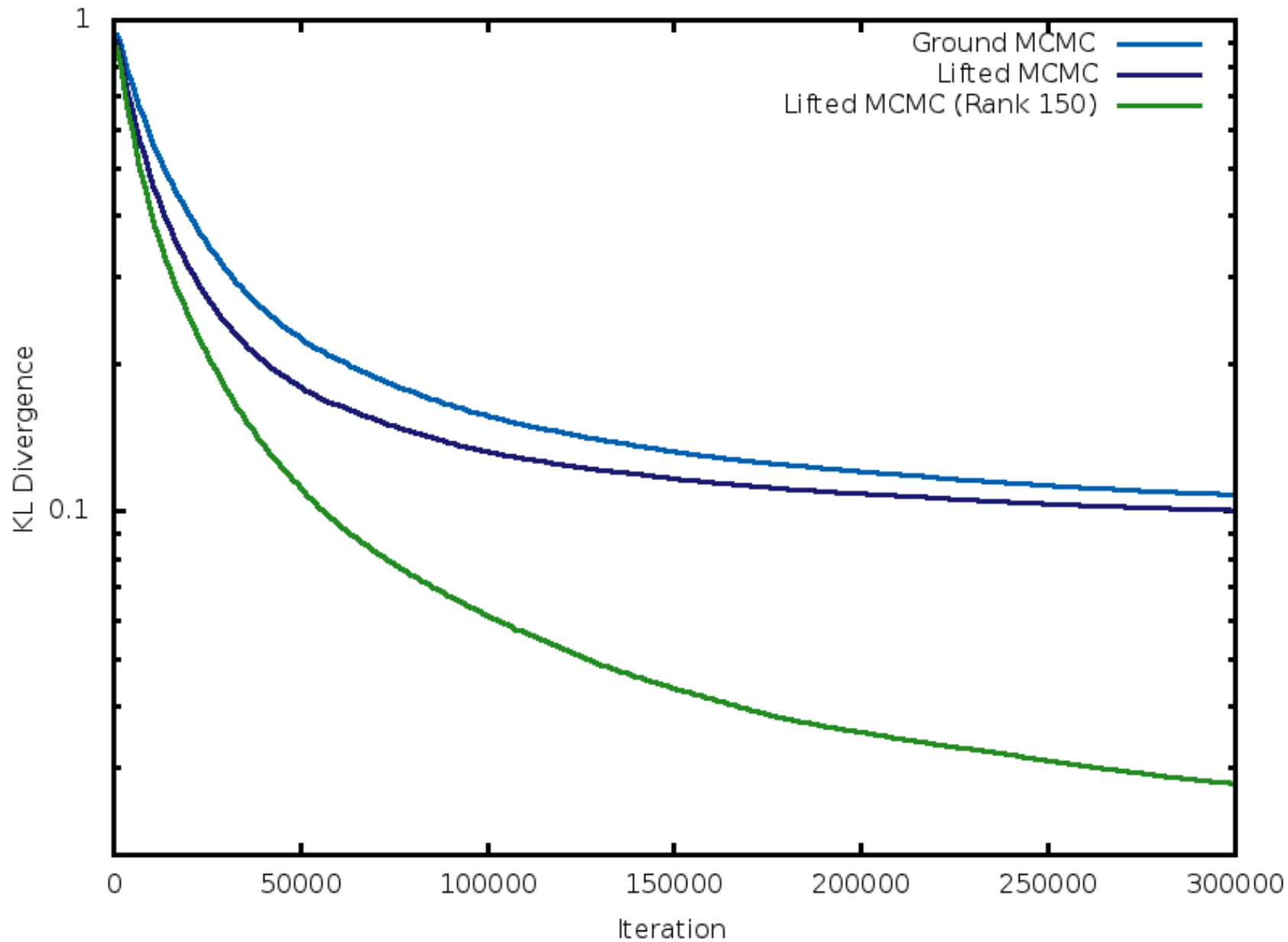
# Rank 150 Approximation



# Trend for Increasing Boolean Rank



# Best Case





# Overview

- Lifted inference in 2 slides
- Complexity of evidence
- Over-symmetric approximations
- **Approximate symmetries**
- Conclusions

# Problem with OSAs

- Approximation can be crude
- Cannot converge to true distribution
- Lose information about subtle differences
  - Real distribution

$$\Pr(\text{PageClass}(\text{"Faculty"}, \text{"http://.../~pedro/"})) = 0.47$$

$$\Pr(\text{PageClass}(\text{"Faculty"}, \text{"http://.../~luc/"})) = 0.53$$

- OSA distribution

$$\Pr(\text{PageClass}(\text{"Faculty"}, \text{"http://.../~pedro/"})) = 0.50$$

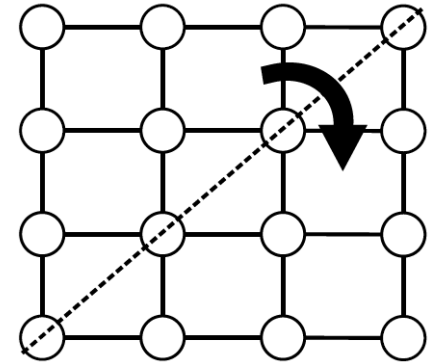
$$\Pr(\text{PageClass}(\text{"Faculty"}, \text{"http://.../~luc/"})) = 0.50$$

# Approximate Symmetries

- Exploit approximate symmetries:

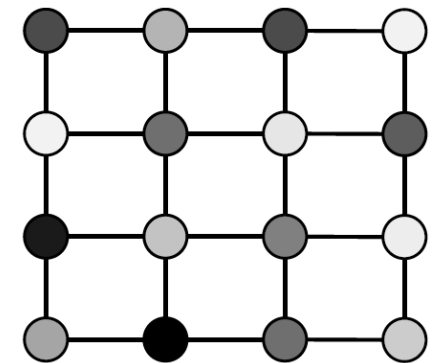
- Exact symmetry  $g$ :  $\Pr(\mathbf{x}) = \Pr(\mathbf{x}^g)$

- E.g. Ising model  
without external field



- Approximate symmetry  $g$ :  $\Pr(\mathbf{x}) \approx \Pr(\mathbf{x}^g)$

- E.g. Ising model with external field



$$P \left[ \begin{array}{c} \text{Image of a woman's face} \end{array} \right] \approx P \left[ \begin{array}{c} \text{Image of a woman's face} \end{array} \right]$$

# Orbital Metropolis Chain: Algorithm

- Given symmetry group  $G$  (approx. symmetries)
- Orbit  $\mathbf{x}^G$  contains all states approx. symm. to  $\mathbf{x}$
- In state  $\mathbf{x}$ :
  1. Select  $\mathbf{y}$  uniformly at random from  $\mathbf{x}^G$
  2. Move from  $\mathbf{x}$  to  $\mathbf{y}$  with probability  $\min\left(\frac{\Pr(\mathbf{y})}{\Pr(\mathbf{x})}, 1\right)$
  3. Otherwise: stay in  $\mathbf{x}$  (reject)
  4. Repeat

# Orbital Metropolis Chain: Analysis

- ✓ Pr(.) is stationary distribution
- ✓ Many variables change (fast mixing)
- ✓ Few rejected samples:

$$\Pr(\mathbf{y}) \approx \Pr(\mathbf{x}) \Rightarrow \min\left(\frac{\Pr(\mathbf{y})}{\Pr(\mathbf{x})}, 1\right) \approx 1$$

Is this the perfect proposal distribution?

# Orbital Metropolis Chain: Analysis

- ✓ Pr(.) is stationary distribution
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$$\Pr(\mathbf{y}) \approx \Pr(\mathbf{x}) \Rightarrow \min\left(\frac{\Pr(\mathbf{y})}{\Pr(\mathbf{x})}, 1\right) \approx 1$$

Is this the perfect proposal distribution?

✗ Not irreducible...

Can never reach 0100 from 1101.

# Lifted Metropolis-Hastings: Algorithm

- Given an **orbital Metropolis chain**  $M_S$  for  $\text{Pr}(\cdot)$
- Given a **base Markov chain**  $M_B$  that
  - is irreducible and aperiodic
  - has stationary distribution  $\text{Pr}(\cdot)$
  - (e.g., Gibbs chain or MC-SAT chain)
- In state  $\mathbf{x}$ :
  1. With probability  $\alpha$ , apply the kernel of  $M_B$
  2. Otherwise apply the kernel of  $M_S$

# Lifted Metropolis-Hastings: Analysis

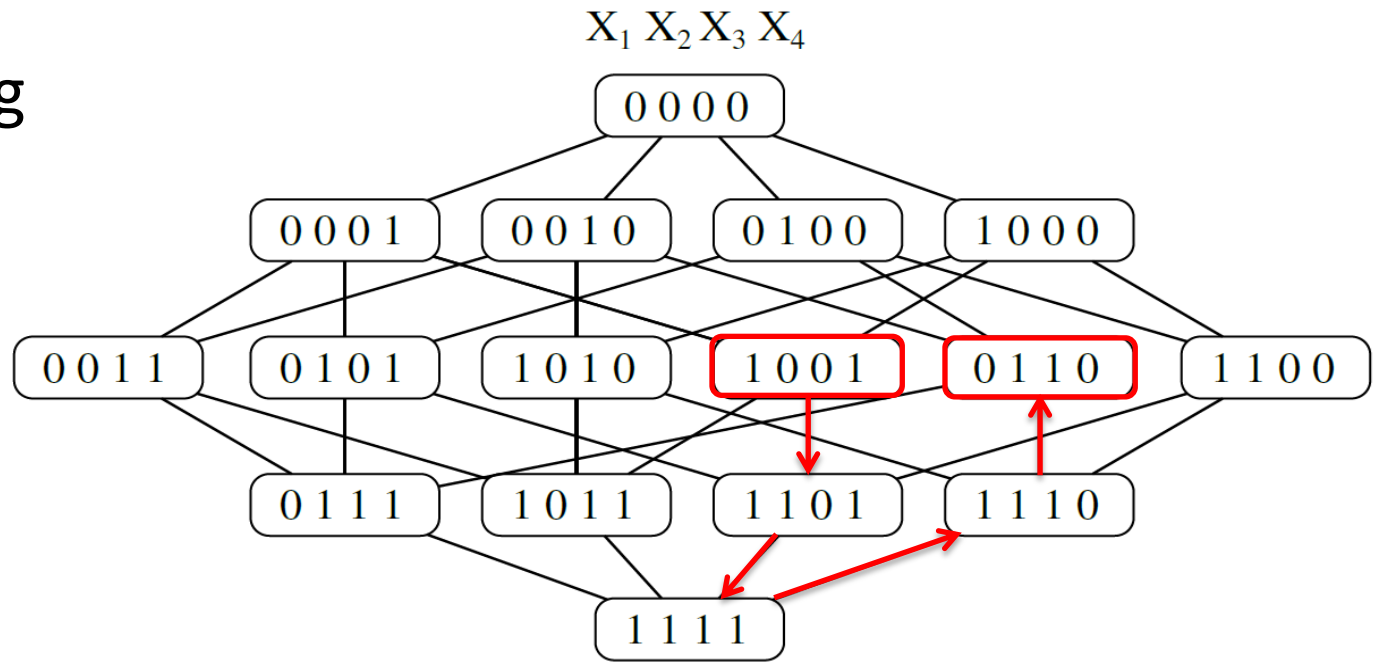
Theorem [Tierney 1994]:

*A mixture of Markov chains is irreducible and aperiodic if at least one of the chains is irreducible and aperiodic .*

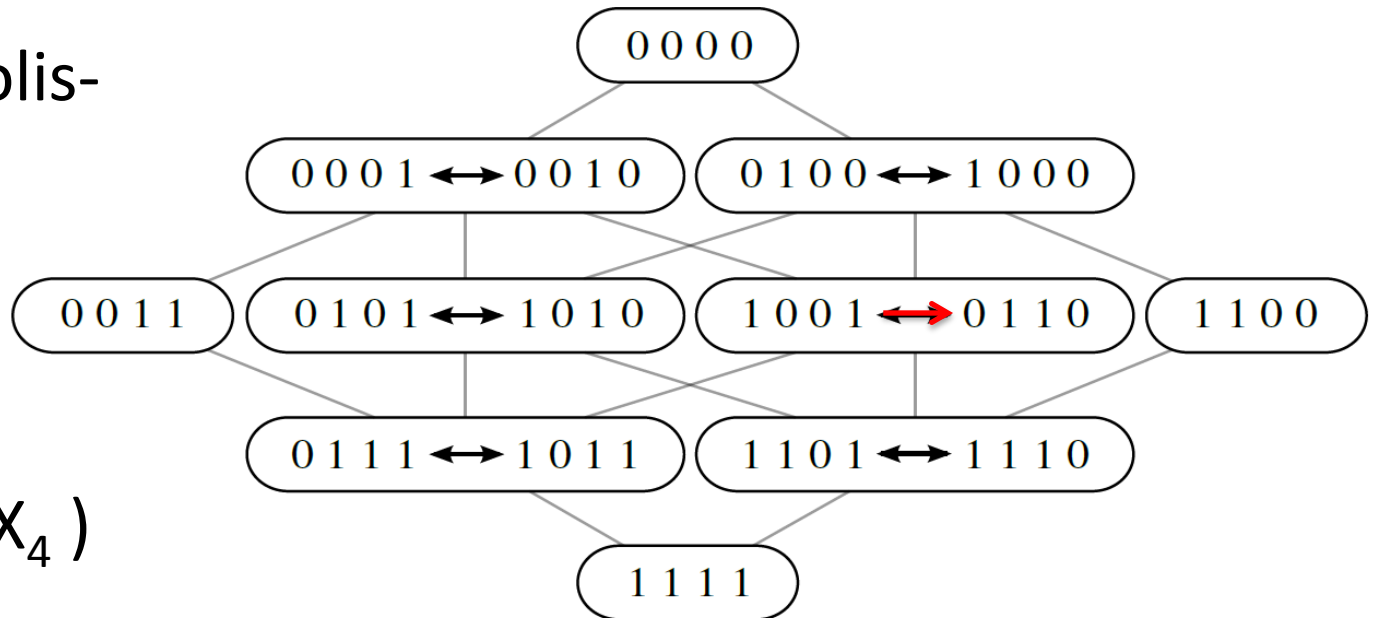
- ✓ Pr(.) is stationary distribution
- ✓ Many variables change (fast mixing)
- ✓ Few rejected samples
- ✓ Irreducible
- ✓ Aperiodic



# Gibbs Sampling

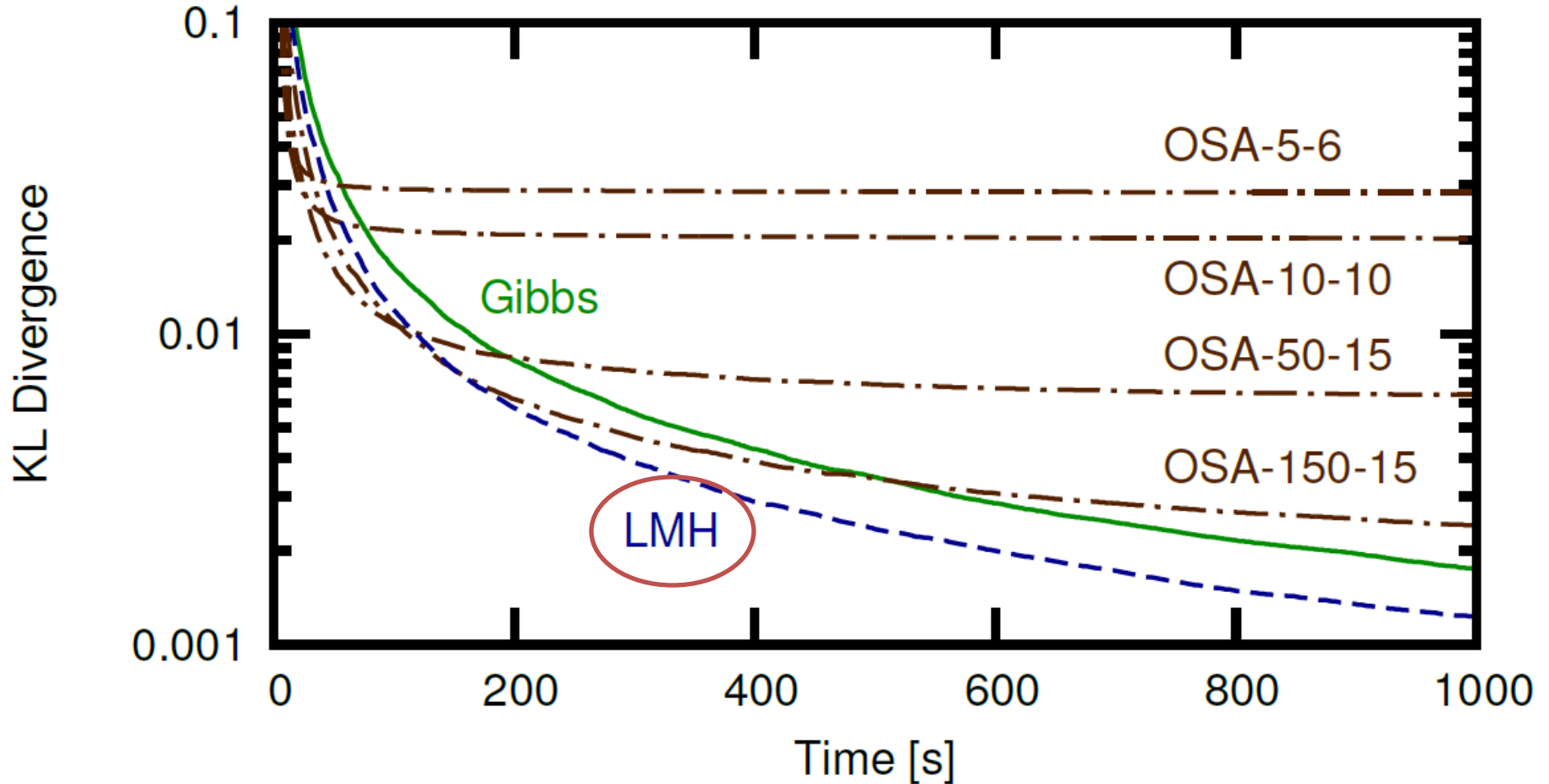


# Lifted Metropolis-Hastings

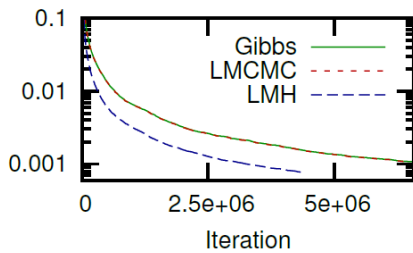


$$G = (X_1 X_2)(X_3 X_4)$$

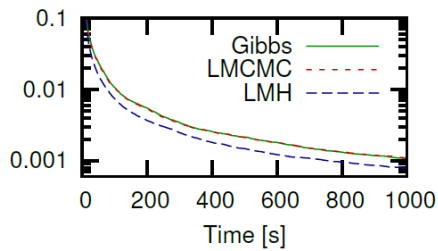
# Experiments: WebKB



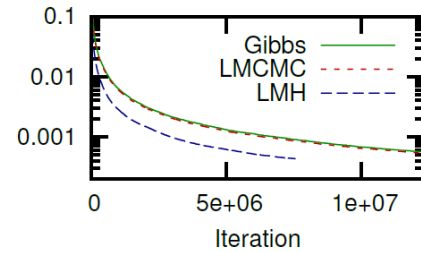
# Experiments: WebKB



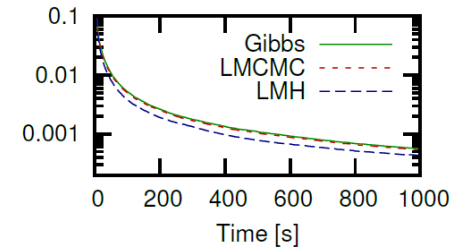
(a) Texas - Iterations



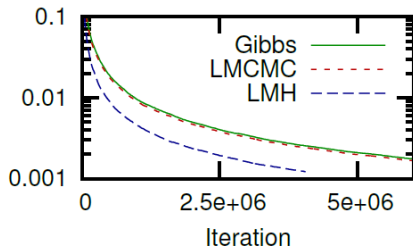
(b) Texas - Time



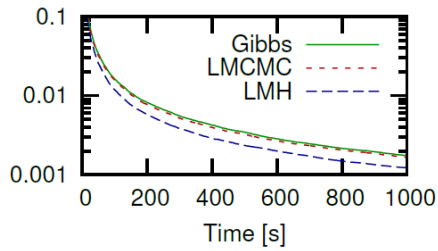
(a) Cornell - Iterations



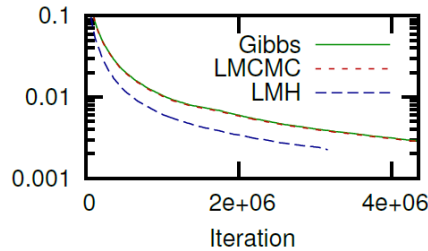
(b) Cornell - Time



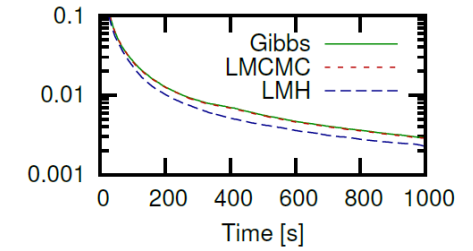
(c) Washington - Iterations



(d) Washington - Time



(c) Wisconsin - Iterations



(d) Wisconsin - Time

# Overview

- Lifted inference in 2 slides
- Complexity of evidence
- Over-symmetric approximations
- Approximate symmetries
- **Conclusions**

# Take-Away Message

Two problems:

1. Lifted inference gives **exponential speedups** in **symmetric** graphical models.  
But what about real-world **asymmetric** problems?
2. When there are **many variables**, MCMC is **slow**.  
How to sample quickly in large graphical models?

One solution: Exploit **approximate symmetries!**

# Open Problems

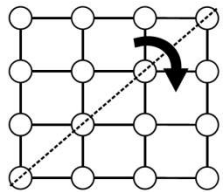
- Find approximate symmetries
  - Principled (theory)
  - Is a type of machine learning?
  - During inference, not preprocessing?
- Give guarantees on approximation quality/convergence speed
- Plug in lifted inference from prob. databases

# Lots of Recent Activity

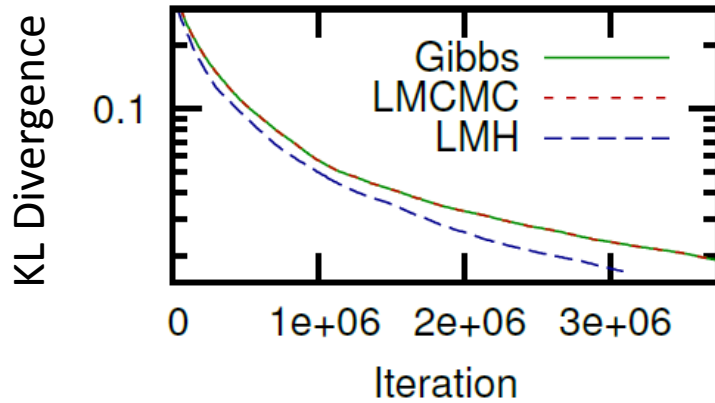
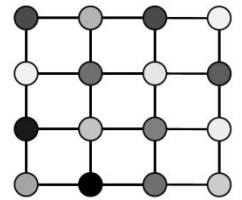
- Singla, Nath, and Domingos (2014)
- Venugopal and Gogate (2014)
- Kersting et al. (2014)

Thanks

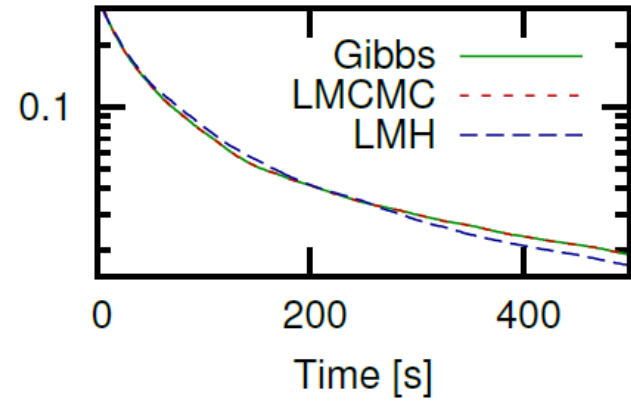




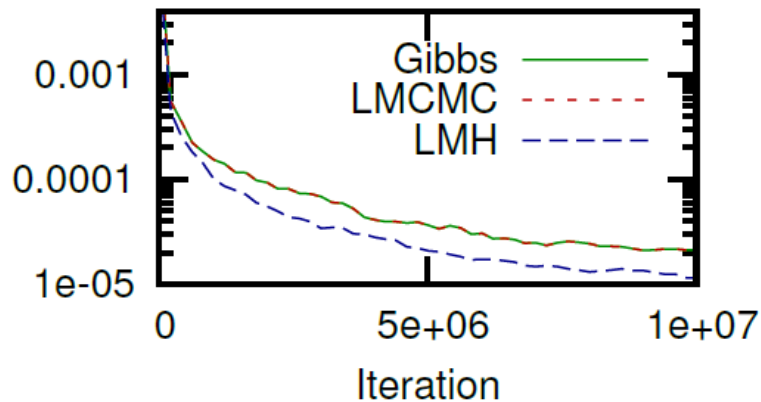
# Example: Grid Models



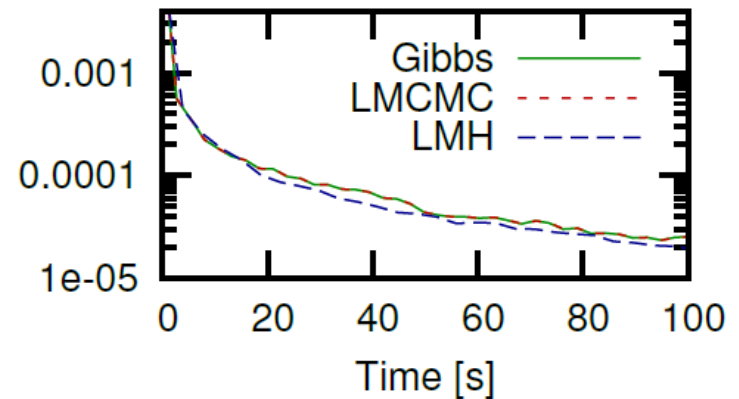
(a) Ising - Iterations



(b) Ising - Time



(c) Chimera - Iterations



(d) Chimera - Time