# Dynamic Sampling from Graphical Models

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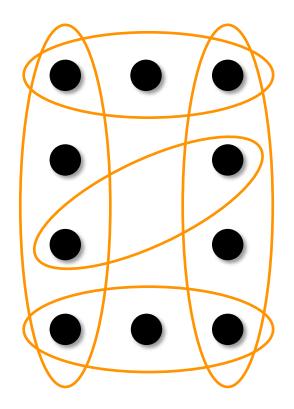
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# Graphical Model

- Hyper graph H = (V, E)
  - V: vertices
  - $E \subseteq 2^V$ : hyper edges.
- Vertex: variable with domain Q.
- Hyper edge: constraint on its variables.
- Weight functions(factors):  $\Phi = (\phi_v)_{v \in V} \cup (\phi_e)_{e \in E}$ 
  - each variable  $\phi_v:Q \to \mathbb{R}_{\geq 0}$ ;
  - each constraint  $\phi_e: Q^e \to \mathbb{R}_{\geq 0}$ .
- Each configuration  $\sigma \in Q^V$ : its weight

$$w(\sigma) = \prod_{v \in V} \phi_v(\sigma_v) \prod_{e \in E} \phi_e(\sigma_e).$$



hyper graph 
$$H = (V, E)$$

# Graphical Model

Instance 
$$\mathcal{I} = (V, E, Q, \Phi)$$

- V: variables
- E: constraints
- Q: domain
- $\Phi = (\phi_v)_{v \in V} \cup (\phi_e)_{e \in E}$ : weight functions (factors)

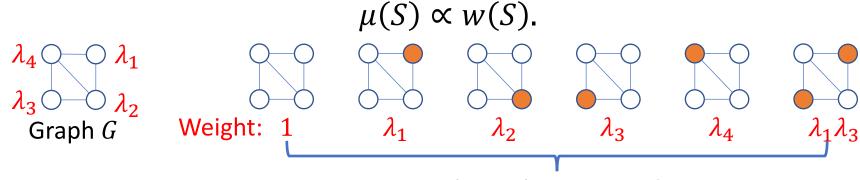
## Gibbs distribution $\mu$ over $Q^V$ :

$$\forall \sigma \in Q^V : \ \mu(\sigma) \propto w(\sigma) = \prod_{v \in V} \phi_v(\sigma_v) \prod_{e \in E} \phi_e(\sigma_e)$$

## Hardcore Model

- Graph G = (V, E)
- $I(G) = \{ \text{independent sets in } G \}.$
- Fugacity of vertex  $v \in V$ :  $\lambda_v \in \mathbb{R}_{\geq 0}$ .
- Weight of independent set  $S \in I(G)$ :

• Hardcore model: distribution  $\mu$  over I(G), each  $S \in I(G)$ :



independent sets in G

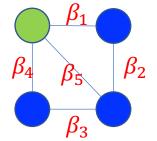
# Ising Model

- Graph G = (V, E).
- Inverse temperature of edge  $e \in E$ :  $\beta_e \in \mathbb{R}_{\geq 0}$ .
- Spin state of vertex  $v \in V: \{-1, +1\}$ .
- Weight of configuration  $\sigma \in \{-1, +1\}^V$

$$w(\sigma) = \prod_{e=\{u,v\}\in E} \exp(\beta_e \sigma_u \sigma_v)$$
. product of pairwise interactions

• Ising model: distribution  $\mu$  over  $\{-1, +1\}^V$ :

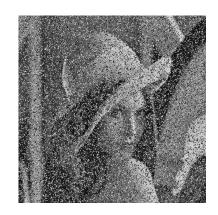
$$\mu(\sigma) \propto w(\sigma)$$
.



Weight= $\exp(-\beta_1) \exp(\beta_2) \exp(\beta_3) \exp(-\beta_4) \exp(-\beta_5)$ .

# Graphical Model

- Machine Learning representation, inference, learning;
- Statistical Physics
  Ising model, hardcore model;
- Theoretical Computer Science sampling, counting.





application: image denoising

## **Sampling from Graphical Model**

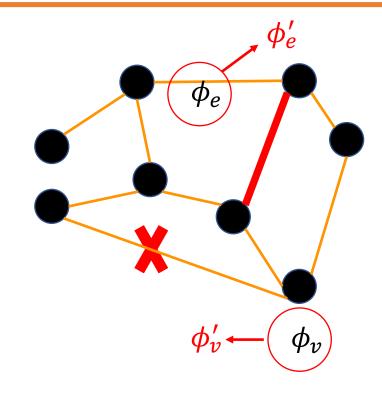
- Input: a graphical model  $\mathcal{I}$ ;
- Output: a sample  $X \sim \mu_{7}$ .

# Dynamic Sampling Problem

• Graphical model  $\mathcal{I} = (V, E, Q, \Phi)$ 

$$\mu_{\mathcal{I}}(\sigma) \propto \prod_{v \in V} \phi_v(\sigma_v) \prod_{e \in E} \phi_e(\sigma_e).$$

- Random sample:  $X \sim \mu_{\mathcal{I}}$ .
- Updates of graphical model  $\mathcal{I} \to \mathcal{I}'$ 
  - add/delete constraints;
  - change weight functions.



Question: Can we modify X to  $X' \sim \mu_{J'}$  with a *small incremental cost*?

random sample for updated graphical model

#### Update is **represented** by a pair $(D, \Phi_D)$

- $D \subseteq V \cup 2^V$ : updated variables & updated constraints;
- $\Phi_D = (\phi_a)_{a \in D}$ : new weight functions.

#### input graphical model

$$\mathcal{I} = (V, E, Q, \Phi)$$



#### updated graphical model

$$\mathcal{I}' = (V, E', Q, \Phi')$$

updated constraints updated weight functions

## **Dynamic Sampling from Graphical Model**

- a graphical model  $\mathcal{I}$ ; a sample  $X \sim \mu_{\mathcal{I}}$ • Input: an update  $(D, \Phi_D)$  that modifies  $\mathcal{I}$  to  $\mathcal{I}'$ ;
- **Output**: a sample  $X' \sim \mu_{\tau'}$ .

**Offline adversary**: update is **independent** with the input sample X.

## Motivations

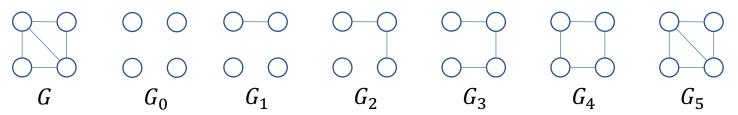
- Online learning with dynamic or streaming data
- Dynamic graphical models
  - Video: a sequence of closely related images.







- Approximate counting [Jerrum, Valiant, Vazirani, 1986]
  - Graph G = (V, E), count #{independent sets of G}.
  - Self reduction: a sequence of graphs  $G_0, G_1, \dots, G_{|E|}$ :



#### **Static Sampling**

- Input: a graphical model  $\mathcal{I}$ ;
- Output: a sample  $X \sim \mu_{\mathcal{I}}$ .

#### Well studied

#### **Dynamic Sampling**

- Input: a graphical model  $\mathcal{I}$ ; a sample  $\pmb{X} \sim \mu_{\mathcal{I}}$  a update  $(D, \Phi_D)$
- Output: a sample  $X' \sim \mu_{\mathcal{I}'}$ .

**Lacking** studies

#### Algorithms for static sampling

- Markov chain Monte Carlo (MCMC)
  - Metropolis Hastings [Metropolis 1953]
  - Glauber Dynamics [Glauber 1963]
- Coupling from the past (CFTP) [Propp and Wilson 1996]

#### Not suitable for dynamic sampling, per se.

- can not use the input sample X;
- rerunning sampling algorithm on  $\mathcal{I}'$  is wasteful.

## Our Contribution

# New **Algorithm**



#### **Dynamic Sampling Problem**

- **Input**: a graphical model  $\mathcal{I}$ ; a sample  $X \sim \mu_{\mathcal{I}}$ a update  $(D, \Phi_D)$
- **Output**: a sample  $X' \sim \mu_{I'}$ .

- Fast
  - a broad class of graphical models  $\Longrightarrow \mathbb{E}[\text{running time}] = O(|D|)$



- Exact Sampling
  - **X** follows precisely distribution  $\mu_{I'}$
- Las Vegas algorithm knows when to stop
- Distributed / Parallel each step uses only local information

# Graphical Model

Instance 
$$\mathcal{I} = (V, E, Q, \Phi)$$

- V: variables
- E: constraints
- Q: domain
- $\Phi = (\phi_v)_{v \in V} \cup (\phi_e)_{e \in E}$ : weight functions (factors)

## Gibbs distribution $\mu$ over $Q^V$ :

$$\forall \sigma \in Q^V : \ \mu(\sigma) \propto w(\sigma) = \prod_{v \in V} \phi_v(\sigma_v) \prod_{e \in E} \phi_e(\sigma_e)$$

# Rejection Sampling

Graphical model  $\mathcal{I} = (V, E, Q, \Phi)$  with Gibbs distribution

$$\mu_{\mathcal{I}}(\sigma) \propto \prod_{v \in V} \phi_v(\sigma_v) \prod_{e \in E} \phi_e(\sigma_e).$$

#### **Assumption: normalized weighted functions**

- each  $\phi_v: Q \to [0,1]$  is a **distribution** over  $Q: \sum_{c \in Q} \phi_v(c) = 1$ ;
- each  $\phi_e: Q^e \to [0,1]$ .

#### **Rejection Sampling**

- Each  $v \in V$  samples  $X_v \sim \phi_v$  ind.;
- Each  $e \in E$  becomes accepted ind. w.p.  $\phi_e(X_e)$ ; o.w. e becomes rejected
- Accept  $X = (X_v)_{v \in V}$  if all  $e \in E$  are accepted;
- **Reject** *X* if otherwise.

$$\Pr[X = \sigma \land X \text{ is accepted}] = \prod_{v \in V} \phi_v(\sigma_v) \prod_{e \in E} \phi_e(\sigma_e).$$

$$\text{generate } X = \sigma \text{ all } e \in E \text{ are accepted}$$

$$\Pr[\text{all } e \in E \text{ are accepted}] = \exp(-\Omega(|E|)).$$

Rejection Sampling is Correct but Slow.

#### Question

Can we obtain an **efficient** rejection sampling algorithm?

- Fast
- Dynamic
- Distributed / Parallel

This problem was **partially solved** by Partial Rejection Sampling (PRS) [Guo, Jerrum, Liu, 2017].

- Boolean weight function  $\phi_e \to \{0,1\}$
- Not known to be dynamic
- Not distributed / parallel

## Our Contribution

New Algorithm





#### **Dynamic Sampling Problem**

• Input: a graphical model  $\mathcal{I}$ ;

a sample  $X \sim \mu_{\mathcal{I}}$ 

a update  $(D, \Phi_D)$ 

• Output: a sample  $X' \sim \mu_{I'}$ .

#### **Efficient Rejection Sampling**

- Fast
- Dynamic
- Distributed/Parallel

#### **Rejection Sampling**

- Each  $v \in V$  samples  $X_v \sim \phi_v$  ind.;
- Each  $e \in E$  becomes accepted ind. w.p.  $\phi_e(X_e)$ ; o.w. e becomes rejected
- Accept  $X = (X_v)_{v \in V}$  if all  $e \in E$  are accepted;
- Reject X if otherwise.

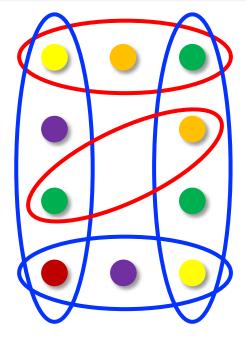
#### The sample X is rejected



Set of **Bad Variables** 

$$\mathcal{R} = \bigcup_{\substack{e \in E:\\ e \text{ is rejected}}} e,$$

 $\mathcal{R}$ : variables in rejected constraints

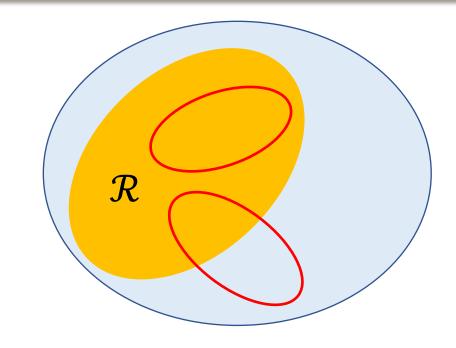




- each  $v \in \mathcal{R}$  resamples  $X_v \sim \phi_v$  ind.; o.w. e becomes rejected
- each  $e \in ICD(\mathcal{R})$  becomes accepted ind. w.p.  $\phi_e(X_e)$ ;
- construct new  $\mathcal{R} \leftarrow \bigcup_{e \in E:e \text{ is rejected } e}$ .

 $ICD(\mathcal{R})$ : constraints **incident** to  $\mathcal{R}$ 

$$ICD(\mathcal{R}) = \{ e \in E \mid e \cap \mathcal{R} \neq \emptyset \}.$$



- each  $v \in \mathcal{R}$  resamples  $X_v \sim \phi_v$  ind.; o.w. e becomes rejected
- each  $e \in ICD(\mathcal{R})$  becomes accepted ind. w.p.  $\phi_e(X_e)$ ;
- construct new  $\mathcal{R} \leftarrow \bigcup_{e \in E:e \text{ is rejected }} e$ .

While  $(\mathcal{R} \neq \emptyset)$ Update  $(X, \mathcal{R})$  by "Natural" Resampling Algorithm Output X.



- Similar to Morse-Tardos for LLL. [Morse, Tardos, 2009]
- The output X does **NOT** follow the Gibbs distribution  $\mu$ . [Harris, Srinivasan, 2016], [Guo, Jerrum, Liu, 2017]

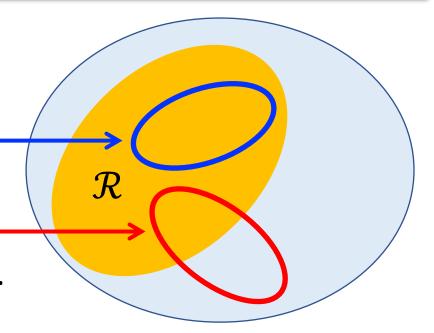
- each  $v \in \mathcal{R}$  resamples  $X_v \sim \phi_v$  ind.;
- each  $e \in ICD(\mathcal{R})$  becomes accepted ind. w.p.  $\phi_e(X_e)$ ;
- construct new  $\mathcal{R} \leftarrow \bigcup_{e \in E:e \text{ is rejected } e}$ .

 $ICD(\mathcal{R})$ : constraints incident to set  $\mathcal{R}$ 

internal constraints

$$E(\mathcal{R}) = \{ e \in E \mid e \subseteq \mathcal{R} \};$$

ICD(
$$\mathcal{R}$$
) = {  $e \in E \mid e \subseteq \mathcal{R}$  };  
• boundary constraints  $\delta(\mathcal{R}) = \{ e \in E \setminus E(\mathcal{R}) \mid e \cap \mathcal{R} \neq \emptyset \}.$ 



- each  $v \in \mathcal{R}$  resamples  $X_v \sim \phi_v$  ind.;
- each  $e \in ICD(\mathcal{R})$  becomes accepted ind. w.p.  $\phi_e(X_e)$ ;
- construct new  $\mathcal{R} \leftarrow \bigcup_{e \in E:e \text{ is rejected } e}$ .

#### Our Algorithm: Local-Resample(X, $\mathcal{R}$ )

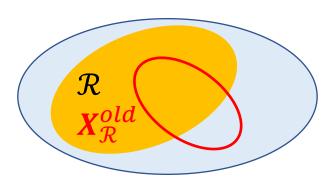
- each  $v \in \mathcal{R}$  resamples  $X_v \sim \phi_v$  ind.;
- each  $e \in E(\mathcal{R})$  becomes accepted ind. w.p.  $\phi_e(X_e)$ ;
- each  $e \in \delta(\mathcal{R})$  becomes accepted ind. with a modified probability;
- construct new  $\mathcal{R} \leftarrow \bigcup_{e \in E:e}$  is rejecte e.
- return  $(X, \mathcal{R})$ ;

#### Our Algorithm: Local-Resample( $X, \mathcal{R}$ )

- each  $v \in \mathcal{R}$  resamples  $X_v \sim \phi_v$  ind.;
- 2 each  $e \in E(\mathcal{R})$  becomes accepted ind. w.p.  $\phi_e(X_e)$ ;
- ③ each  $e \in \delta(\mathcal{R})$  becomes accepted ind. w.p.  $C_e \cdot \frac{\phi_e(X_e)}{\phi_e(X_e^{old})} \le 1$ ;
- 4 construct new  $\mathcal{R} \leftarrow \bigcup_{e \in E:e \text{ is rejected } e} e$ . normalization factor
- (5) return  $(X, \mathcal{R})$ ;

 $X^{old} \in Q^V$  is the old X before the resampling in step 1

Normalization Factor 
$$C_e = C_e(X_{\mathcal{R}}^{old})$$
:
$$C_e = \min_{y \in Q^e: y_{e \cap \mathcal{R}} = X_{e \cap \mathcal{R}}^{old}} \phi_e(y).$$



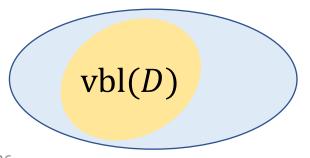
While(
$$\mathcal{R} \neq \emptyset$$
)  
 $(X, \mathcal{R}) \leftarrow \text{Local-Resample}(X, \mathcal{R})$   
Output  $X$ .

Correct **Distribution** 

# Dynamic Sampler

#### **Dynamic Sampling from Graphical Model**

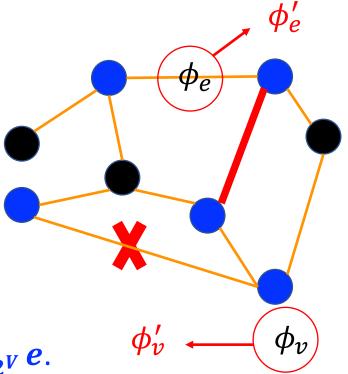
- Input: a graphical model  $\mathcal{I}$ ; a sample  $X \sim \mu_{\mathcal{I}}$  a update  $(D, \Phi_D)$  that modifies  $\mathcal{I}$  to  $\mathcal{I}'$ ;
- Output: a sample  $X' \sim \mu_{\gamma'}$ .
- D: updated variables & updated constraints;
- vbl(D): variables **involved** by the update:
  - updated variables:  $D \cap V$ ;
  - variables incident to updated constraints:  $\bigcup_{e \in D \cap 2^V} e$ .



Graphical models  $\mathcal{I}$  and  $\mathcal{I}'$  differ only on  $\mathrm{vbl}(D)$ .



The initial bad set  $\mathcal{R} = \text{vbl}(D)$ .



#### **Dynamic Sampler**

- Apply changes  $(D, \Phi_D)$  to current graphical model  $\mathcal{I}$ .
- $\mathcal{R} \leftarrow \text{vbl}(D)$ ;
- While( $\mathcal{R} \neq \emptyset$ )
  - $(X, \mathcal{R}) \leftarrow \text{Local-Resample}(X, \mathcal{R});$
- Return *X*;

#### **Theorem: Correctness [This Work]**

Upon termination, the dynamic sampler outputs  $X \sim \mu_{J'}$ .

#### A dynamic sampler for general graphical model:

- Exact sampling
- Las Vegas
- Distributed / Parallel

## **Proof of Correctness**

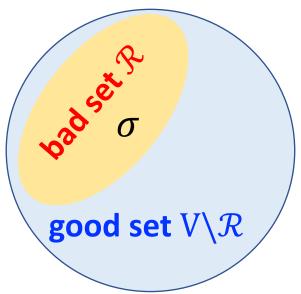
#### **Dynamic Sampler**

- Apply changes  $(D, \Phi_D)$  to current graphical model  $\mathcal{I}$ .
- $\mathcal{R} \leftarrow \text{vbl}(D)$ ;
- While( $\mathcal{R} \neq \emptyset$ )
  - $(X, \mathcal{R}) \leftarrow \text{Local-Resample}(X, \mathcal{R});$
- Return X;

The algorithm maintains  $(X, \mathcal{R}) \in Q^V \times 2^V$ 

- $\mathcal{R}$ : bad set;
- $V \setminus \mathcal{R}$ : good set

 $X_{V \setminus \mathcal{R}}$  follows "correct" distribution.



#### Conditional Gibbs property w.r.t. $\mu$

Conditioning on any  $\mathcal{R} \subseteq V$  and any assignment  $\sigma \in Q^{\mathcal{R}}$  of  $X_{\mathcal{R}}$ , the distribution of  $X_{V \setminus \mathcal{R}}$  is  $\mu_{V \setminus \mathcal{R}}^{\sigma}$ .

 $\mu_{V\setminus\mathcal{R}}^{\sigma}$ : marginal distribution of  $\mu$  on  $V\setminus\mathcal{R}$  conditioning on  $\sigma$ .

#### Local-Resample(X, $\mathcal{R}$ )



#### **Resampling chain**

- Markov chain on  $\Omega = Q^V \times 2^V$
- Transition Matrix  $P \in \mathbb{R}^{\Omega \times \Omega}$

 $P \colon (X, \mathcal{R}) \to (X', \mathcal{R}')$ 

#### **Equilibrium Condition**

If  $(X, \mathcal{R})$  satisfies the conditionally Gibbs property w.r.t.  $\mu$ , then so does  $(X', \mathcal{R}')$ .



#### **Equation System for Equilibrium Condition**

$$\forall \ S,T\subseteq V,\sigma\in Q^{V\backslash S} \ \text{and} \ \tau\in Q^{V\backslash T},$$
 
$$\forall y\in Q^V,y_{V\backslash T}=\tau:\sum_{\substack{x\in Q^V\\x_{V\backslash S}=\sigma}}\mu_S^\sigma(x_S)\cdot P\big((x,S),(y,T)\big)=C(S,\sigma,T,\tau)\cdot \mu_T^\tau(y_T).$$

Our algorithm is a solution to this equation system.

### **Theorem: Fast Convergence [This Work]**

The updated graphical model satisfies d = O(1),  $\max_{e \in E'} |e| = O(1)$ , and

$$\forall e \in E': \min_{x} \phi'_{e}(x) > \sqrt{1 - \frac{1}{d+1}}$$

where d is the maximum degree of the dependency graph.

The cost of the dynamic sampler is

- $O(\log |D|)$  iterations in expectation;
- O(|D|) resamplings in expectation.

$$\mathcal{J}$$
 Update ( $D, \Phi_D$ )  $\mathcal{J}'$ 

Ising Model:  $\forall e \in E$ :

Uniqueness Regime:  $\forall e \in E$ :

$$1 - \exp(-2|\beta_e|) < \frac{2}{\Delta}$$

#### Theorem: Fast Convergence [This Work]

Hardcore model and Ising model on bounded degree graph s.t.

- Hardcore model:  $\forall v \in V$ :  $\lambda_v \leq \frac{1}{\sqrt{2}\Delta 1}$ .
- Ising model:  $\forall e \in E$ :  $1 \exp(-2|\beta_e|) \le \frac{1}{2.2214+1}$ ,

where  $\Delta$  is the maximum degree.

#### The **cost** of the dynamic sampler is

- $O(\log |D|)$  iterations in expectation;
- O(|D|) resamplings in expectation;

#### **Uniqueness Regime:**

- Hardcore model:  $\forall v \in V$ :  $\lambda_v < \frac{(\Delta 1)^{\Delta 1}}{(\Delta 2)^{\Delta}} \approx \frac{e}{\Delta 2}$ .  $\lambda_v = O\left(\frac{1}{\Delta}\right)$  Ising model:  $\forall e \in E$ :  $1 \exp(-2|\beta_e|) < \frac{2}{\Delta}$ .  $1 \exp(-2|\beta_e|) = O\left(\frac{1}{\Delta}\right)$

$$\lambda_{v} = O\left(\frac{1}{\Delta}\right)$$

$$1 - \exp(-2|\beta_e|) = O\left(\frac{1}{\Delta}\right)$$

# Proof of the Fast Convergence

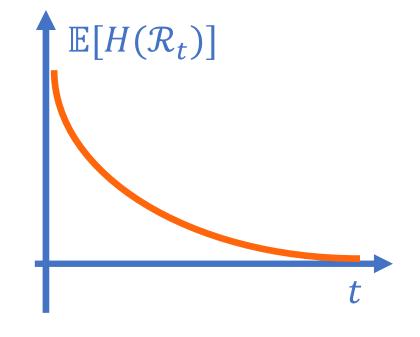
$$\mathcal{R}_0 = \mathrm{vbl}(D)$$
  $\longrightarrow$   $\mathcal{R}_1$   $\longrightarrow$   $\mathcal{R}_2$   $\longrightarrow$   $\circ$   $\circ$   $\longrightarrow$   $\mathcal{R}_T = \emptyset$ 

#### Potential function on bad set $\mathcal{R}_t$

$$H: 2^V \to \mathbb{Z}_{\geq 0}$$

Step-wise decay on expectation of  $H(\mathcal{R}_t)$ 

$$\mathbb{E}[H(\mathcal{R}_t)] \le (1 - \delta)\mathbb{E}[H(\mathcal{R}_{t-1})].$$



## Summary

- Dynamic sampling problem.
- Dynamic sampler for general graphical models
   Exact Sampling & Las Vegas & Distributed/Parallel.
- Equilibrium conditions for resampling.

#### **Future Work**

- Dynamic MCMC sampling [Feng, He, Yin, Sun, arXiv:1904.11807]
- Improve the regimes for efficient dynamic sampling correlation decay  $\Rightarrow$ ? efficient dynamic sampling algorithm.
- Extend to continuous distributions & global constraints.

# **Thank You**

# See you at the poster session #131

