Fast Sampling Constraint Satisfaction Solutions via the Lovász Local Lemma

Yitong Yin

Nanjing University

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Constraint Satisfaction Problem

$$\Phi = (V, \boldsymbol{Q}, C)$$

- **Variables:** $V = \{x_1, x_2, \ldots, x_n\}$ with finite domains $Q_1, \ldots, Q_n$
- (local) **Constraints:** $C = \{c_1, c_2, \ldots, c_m\}$
  - each $c \in C$ is defined on a subset vbl(c) of variables

$$c : \bigotimes_{i \in \mathsf{vbl}(c)} Q_i \to \{\mathtt{True}, \mathtt{False}\}$$

- **CSP formula:** $\forall \boldsymbol{x} \in Q_1 \times Q_2 \times \cdots \times Q_n$

$$\Phi(\boldsymbol{x}) = \bigwedge_{c \in C} c\left(\boldsymbol{x}_{\mathsf{vbl}(c)}\right)$$

- **Example** (k-SAT): Boolean variables $V = \{x_1, x_2, x_3, x_4, x_5\}$

k-CNF $\Phi = (x_1 \vee \neg x_2 \vee x_3) \wedge (x_1 \vee x_2 \vee x_4) \wedge (x_3 \vee \neg x_4 \vee \neg x_5)$ clause

Lovász Local Lemma (LLL)

- Variables take independent random values $X_1, X_2, \ldots, X_n$
- **Violation Probability**: each $c \in C$ is violated with prob. ≤ p
- **Dependency Degree**: each $c \in C$ shares variables with ≤ D other constraints $c' \in C$, i.e. vbl(c) ∩ vbl$(c') \neq \emptyset$
- **LLL** [Erdős, Lovász, 1975]:

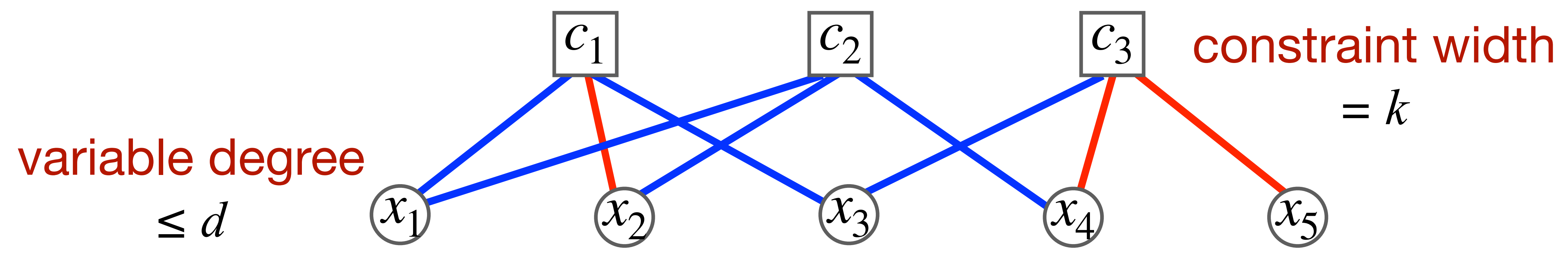
$$\mathrm{e}pD \leq 1 \implies \text{solution exists}$$

- ***Constructive* LLL** [Moser, Tardos, 2010]:

$$\mathrm{e}pD \leq 1 \implies \text{solution can be found very efficiently}$$

Lovász Local Lemma (LLL)

- (k, d)-CNF: $\Phi = (x_1 \vee \neg x_2 \vee x_3) \wedge (x_1 \vee x_2 \vee x_4) \wedge (x_3 \vee \neg x_4 \vee \neg x_5)$



- Uniform random $X_1, X_2, \ldots, X_n \in \{\texttt{True}, \texttt{False}\}$
- Violation probability: $p = 2^{-k}$
- Dependency degree: $D \leq dk$
- **LLL**: $k \gtrsim \log d \ (k \geq \log_2 d + \log_2 k + O(1))$

$e p D \leq e d k 2^{-k} \leq 1$ —*LLL* / Moser-Tados→ a SAT solution exists and can be found in O(dkn) time

Sampling & Counting

Input: a CSP formula $\Phi = (V, \boldsymbol{Q}, C)$

Output :

- (sampling) uniform random satisfying solution
- (counting) # of satisfying solutions

- μ: uniform distribution over all satisfying solutions of Φ

Rejection Sampling

generate a uniform random $\forall \boldsymbol{x} \in Q_1 \times Q_2 \times \cdots \times Q_m$;

if $\Phi(\boldsymbol{x}) = \texttt{True}$ **then** accept else reject;

μ is the distribution of $(\boldsymbol{x} \mid \text{accept})$

SAT solutions may be exponentially rare!

Sampling & Counting

Input: a CSP formula $\Phi = (V, \boldsymbol{Q}, C)$

Output :

- (sampling) almost uniform random satisfying solution
- (counting) an estimation of # of satisfying solutions

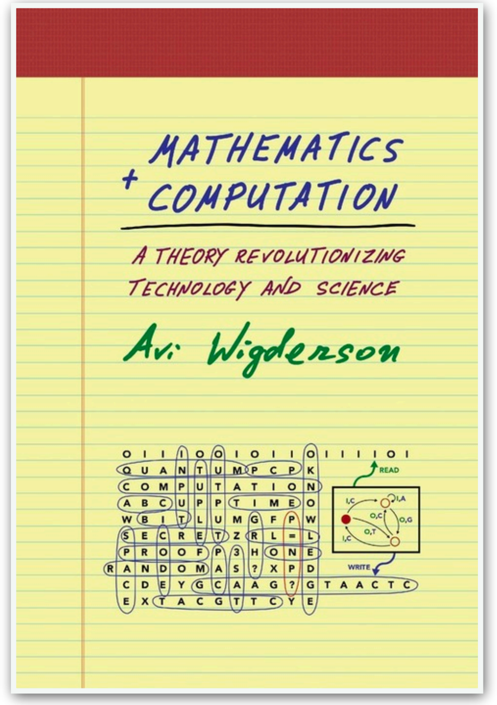
- exact counting is **#P**-hard
- **Almost Uniform Sampling** → **Approximate Counting**
  - self-reduction [Jerrum, Valiant, Vazirani 1986]
  - adaptive simulated annealing [Štefankovič, Vempala, Vigoda 2009]
- Application: inference in probabilistic graphical models

Gibbs distribution $\mu(\boldsymbol{x}) \propto \Phi(\boldsymbol{x}) = \prod_{c \in C} c\left(\boldsymbol{x}_{\mathsf{vbl}(c)}\right)$ where each $c : \bigotimes_{i \in \mathsf{vbl}(c)} Q_i \to \mathbb{R}_{\geq 0}$

Inference: $\Pr_{X \sim \mu}[X_i = \cdot \mid X_S = \boldsymbol{x}_S]$

Sampling *k*-SAT Solutions

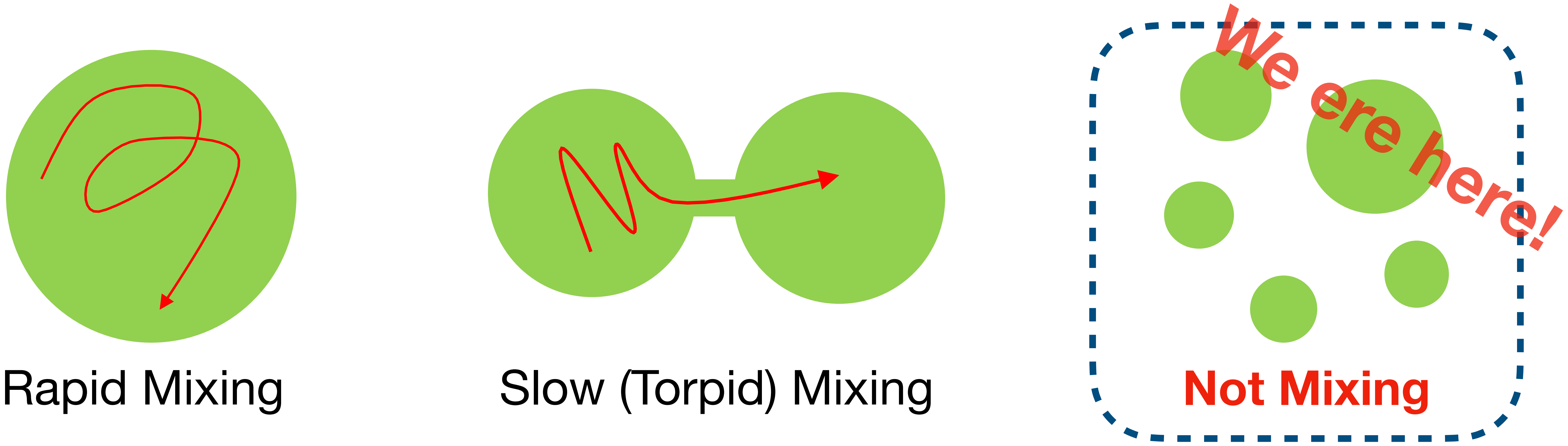
- Sampling almost uniform *k*-SAT solution under *LLL*-like condition?



Mathematics and Computation [Wigderson 2020]:

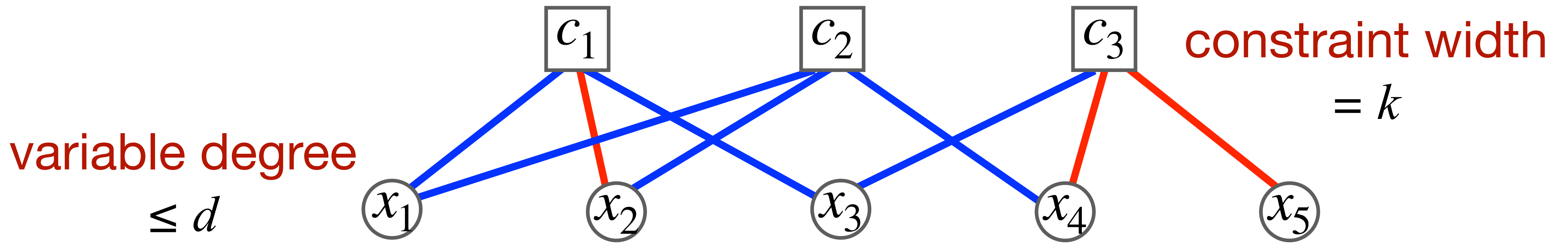
"the solution space (and hence the natural Markov chain) is not connected"

- Random walk in solution space (Markov chain Monte Carlo, **MCMC**):



Sampling k-SAT Solutions

- Sampling almost uniform SAT solution under *LLL*-like condition?



LLL cond.:
$k \gtrsim \log d$

(k,d)-CNF	Condition	Complexity	Technique
Hermon, Sly, Zhang '16	monotone CNF [1] $k \gtrsim 2 \log d$	$(dk)^{O(1)} n \log n$	MCMC
Guo, Jerrum, Liu '17	$s \geq \min(\log dk, k/2)$ [2] $k \gtrsim 2 \log d$	$(dk)^{O(1)} n$	Partial Rejection Sampling
Bezáková *et al* '16	$k \leq 2 \log d - C$	**NP**-hard	lower bound

[1] *Monotone CNF: all variables appear **positively**, e.g.* $\Phi = (x_1 \vee x_2 \vee x_3) \wedge (x_1 \vee x_2 \vee x_4) \wedge (x_3 \vee x_4 \vee x_5)$
[2] s: *two dependent clauses share **at least** s variables.*

Moitra STOC'17 JACM'19	$k \gtrsim 60 \log d$	$n^{O(d^2 k^2)}$	Coupling + LP
Feng, Guo, **Y.**, Zhang '20	$\boldsymbol{k \gtrsim 20 \log d}$	$\boldsymbol{\tilde{O}(d^2 k^3 n^{1.000001})}$	***Projected* MCMC**

Main Theorem (for CNF)

[Feng, Guo, **Y.**, Zhang '20]

For any sufficiently small $\zeta \leq 2^{-20}$, any (k,d)-CNF satisfying

$$k \geq 20 \log d + 20 \log k + 3 \log \frac{1}{\zeta}$$

- **Sampling algorithm**:
  draw almost uniform SAT solution in time $\tilde{O}(d^2 k^3 n^{1+\zeta})$
- **Counting algorithm**:
  count # SAT solutions approximately in time $\tilde{O}(d^2 k^3 n^{2+\zeta})$

Markov Chain for k-SAT

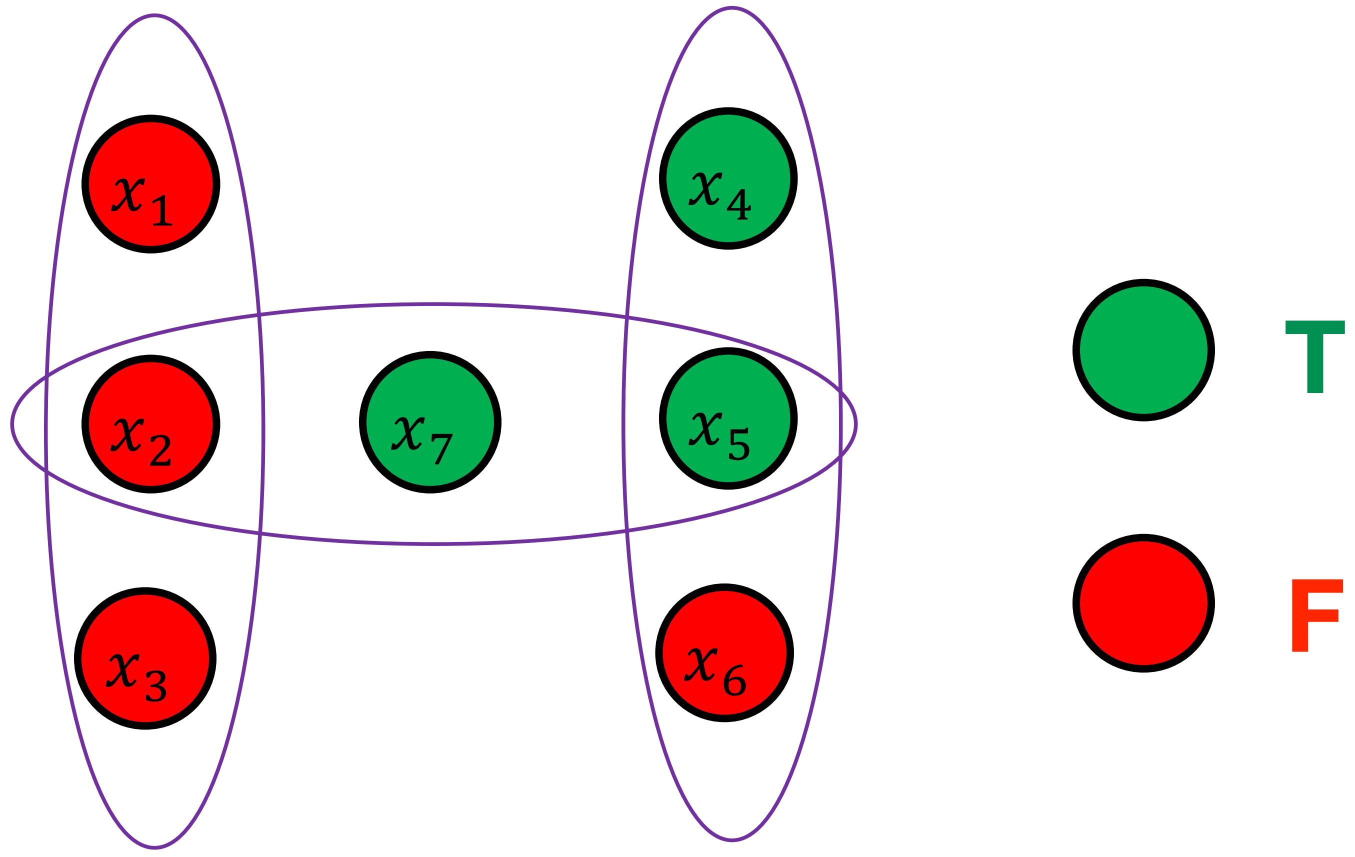
Glauber Dynamics

Start from an arbitrary satisfying $\boldsymbol{x} \in \{\mathtt{T}, \mathtt{F}\}^V$

At each step:

- pick $i \in V$ uniformly at random
- resample $x_i \sim \mu_i(\cdot \mid \boldsymbol{x}_{V\setminus\{i\}})$

$(x_1 \vee \neg x_2 \vee x_3) \wedge (x_2 \vee x_7 \vee x_5) \wedge (x_4 \vee \neg x_5 \vee x_6)$



- μ: uniform distribution over all SAT solutions $\boldsymbol{x} \in \{\mathtt{T}, \mathtt{F}\}^V$
- $\mu_i(\cdot \mid \boldsymbol{x}_{V\setminus\{i\}})$: marginal distribution of x_i cond. on current values of all other variables

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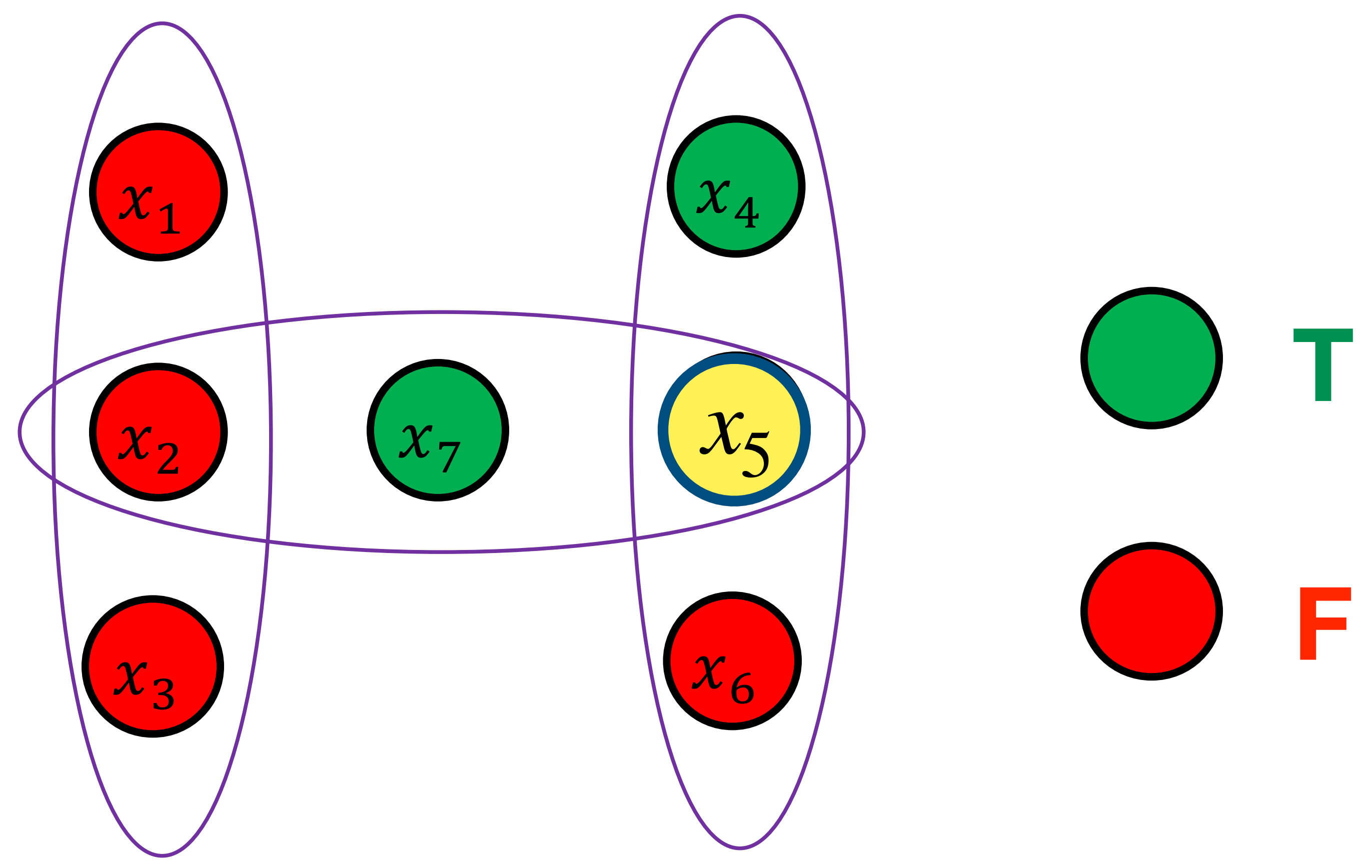

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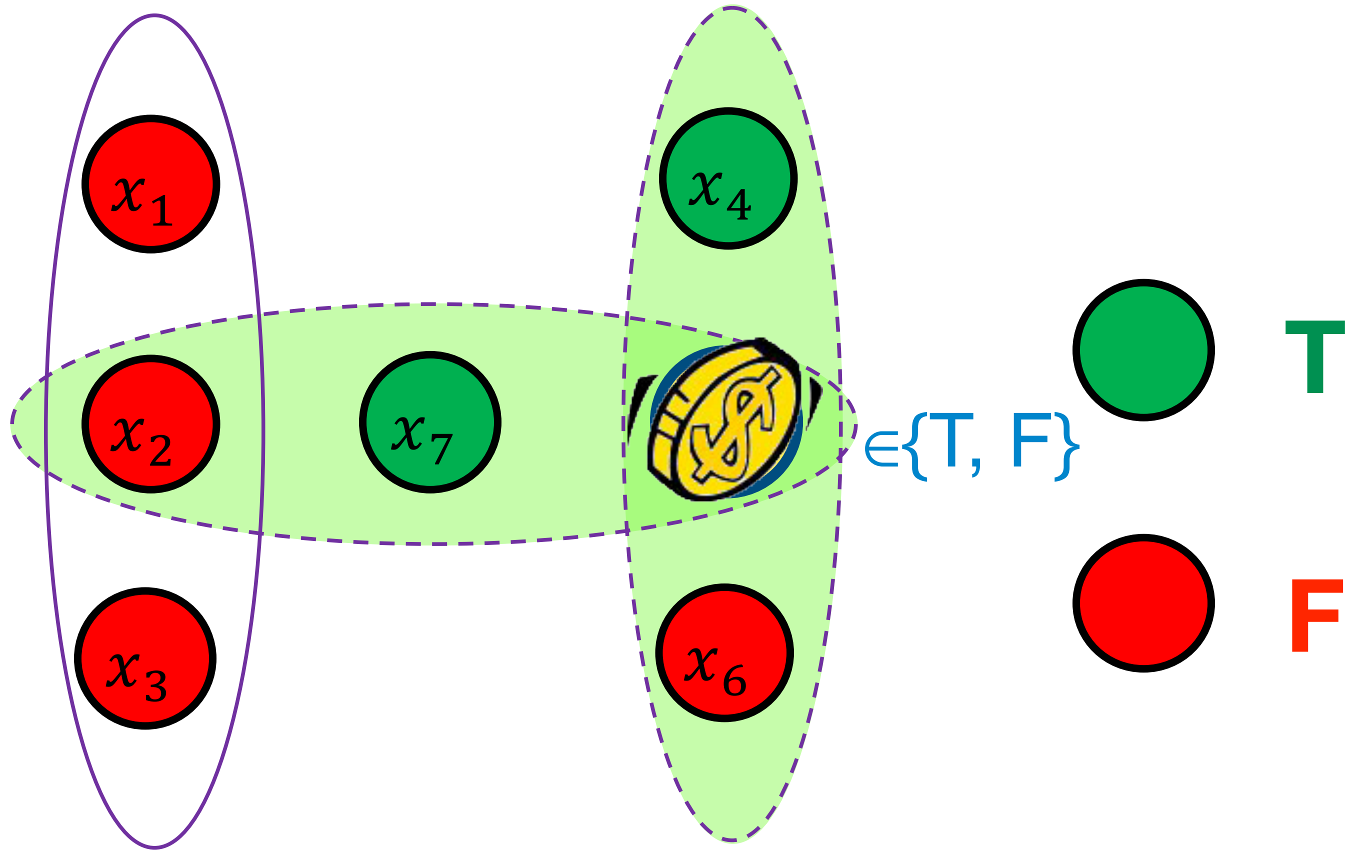

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Markov Chain for *k*-SAT

Glauber Dynamics

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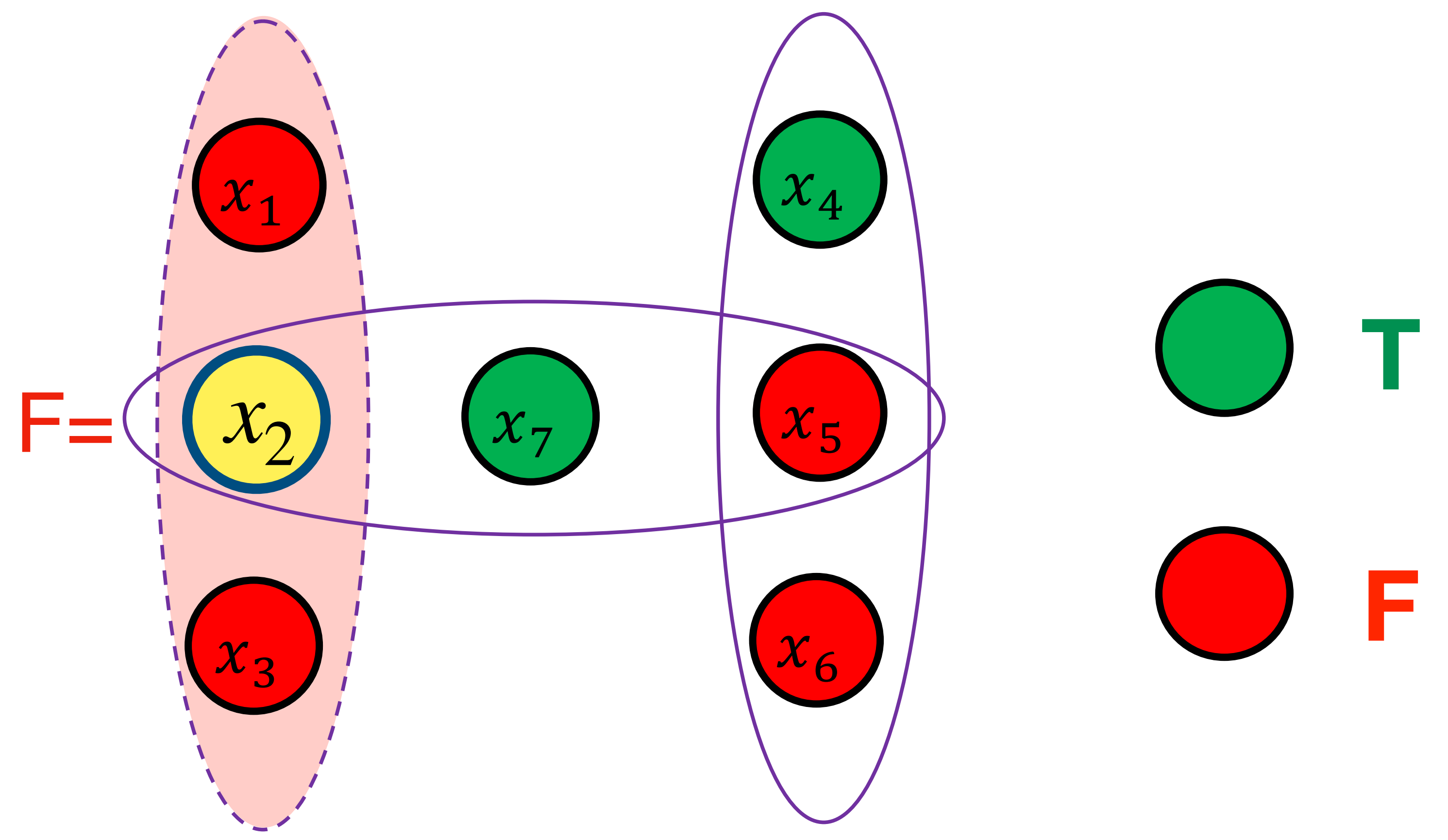


- μ: uniform distribution over all SAT solutions $\boldsymbol{x} \in \{\mathtt{T}, \mathtt{F}\}^V$
- $\mu_i(\cdot \mid \boldsymbol{x}_{V \setminus \{i\}})$: marginal distribution of x_i cond. on current values of all other variables (easy to compute by accessing the adjacent variables)

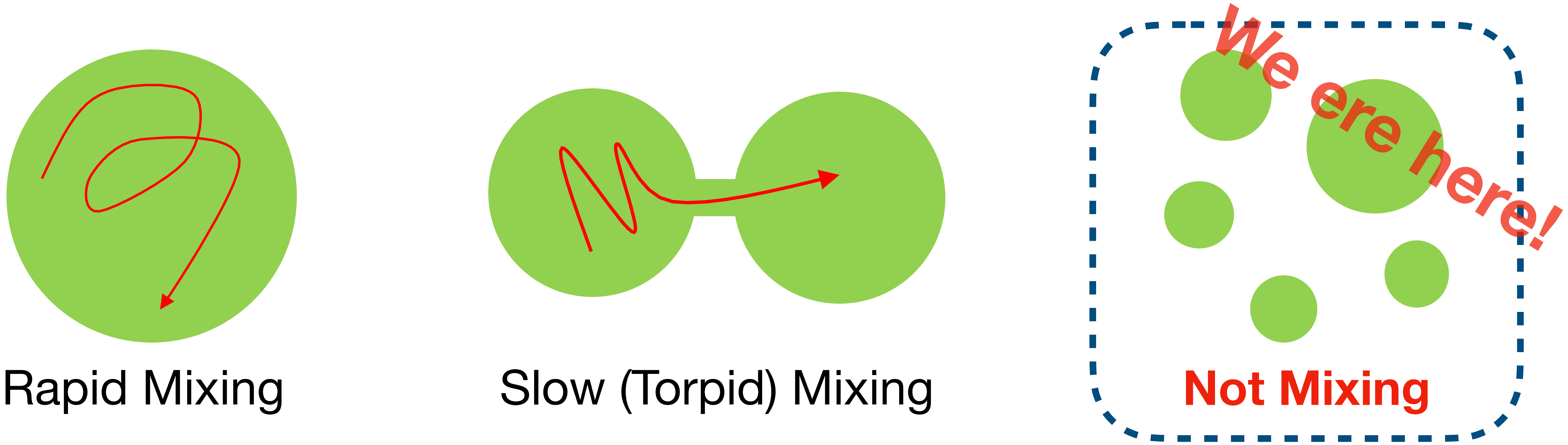
conditional independence (spatial Markovian)

- The Markov chain has stationary distribution μ
- If rapidly mixing: $\tau_{\text{mix}}(\epsilon) = \max_{X_0} \min \left\{ t \mid d_{\text{TV}}(X_t, \mu) \le \epsilon \right\} = \text{poly}\,(n, 1/\epsilon)$

The Solution Space is an Expander!

The Connectivity Barrier

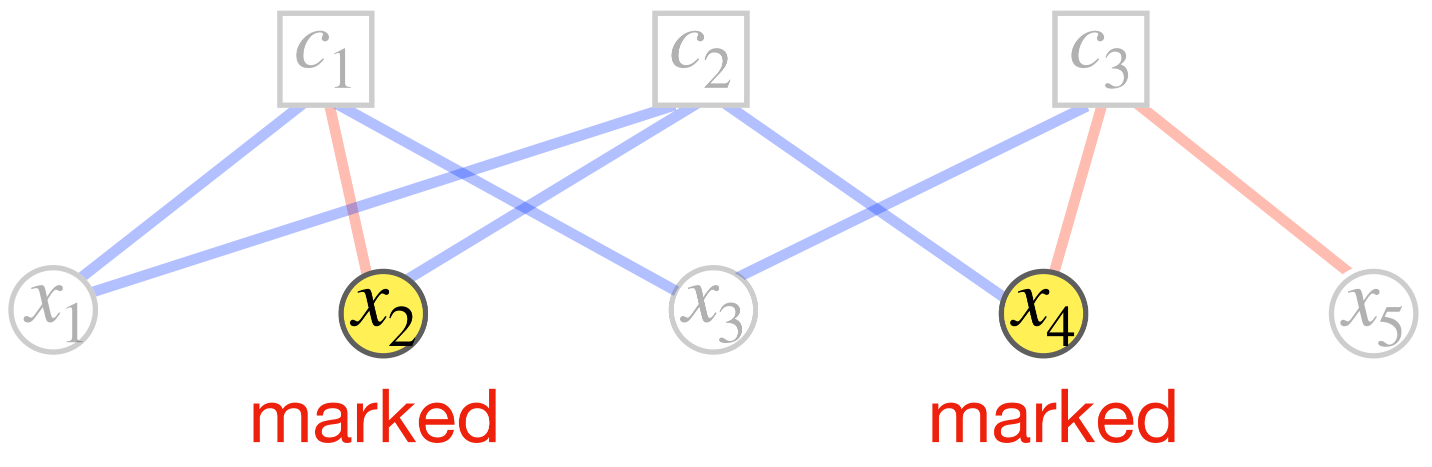
- In the LLL regime (even very far from the critical threshold):



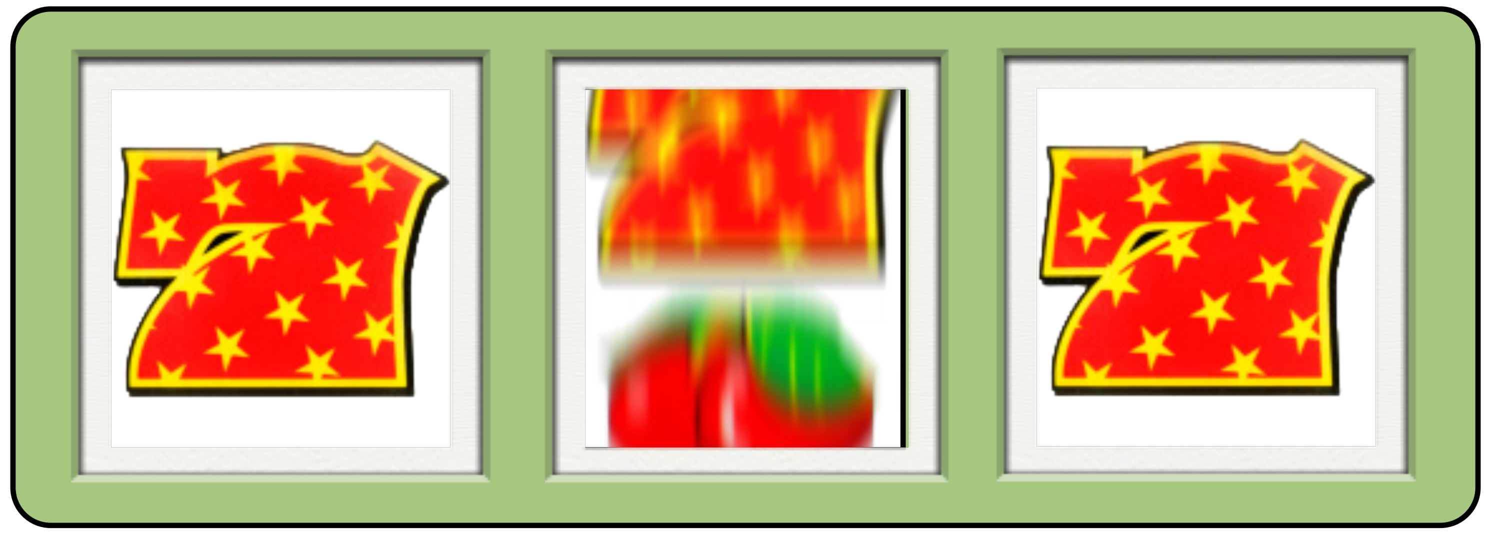
- **Idea**: projecting onto a lower dimension to improve connectivity

Projected Measure

- μ: uniform distribution over SAT solutions of Φ



- A set $M \subseteq V$ of marked variables
- μ_M: distribution of X_M where $X \sim \mu$
- μ_M is a joint distribution: it is no longer a uniform distribution (Gibbs distribution) over solutions of any (weighted) CSP



Our Algorithm (Projected MCMC)

Properly construct a set $M \subseteq V$ of marked variables

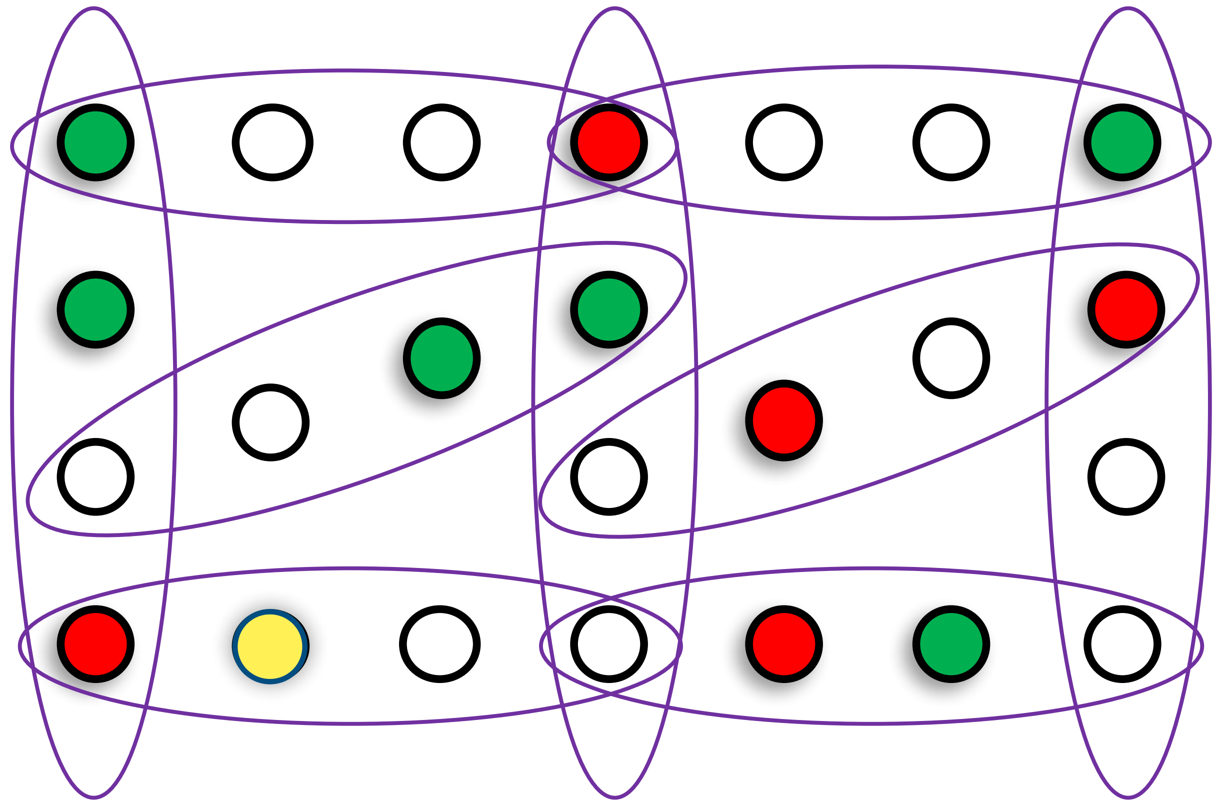
Sampling $\boldsymbol{x}_M \sim \mu_M$

Start from a uniform random $\boldsymbol{x} \in \{\mathrm{T}, \mathrm{F}\}^M$

Repeat for sufficiently many steps:

- pick $i \in V$ uniformly at random
- resample $x_i \sim \mu_i(\cdot \mid \boldsymbol{x}_{M \setminus \{i\}})$

Draw $\boldsymbol{x}_{V \setminus M}$ according to μ conditional on $\boldsymbol{x}_M$



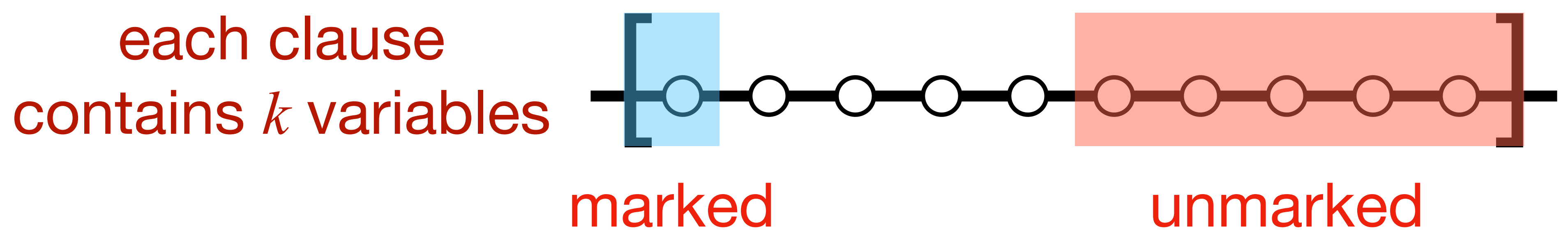
There exists an efficiently constructible subset $M \subseteq V$ of variables s.t.:

- The idealized Glauber dynamics for μ_M is rapidly mixing
- It is efficient to draw from $\mu_i(\cdot \mid \boldsymbol{x}_{M \setminus \{i\}})$ (to implement the idealized Glauber dynamics)
- It is efficient to extend $\boldsymbol{x}_M \sim \mu_M$ to an $\boldsymbol{x} \sim \mu$

Marking/Unmarking Variables

For a (k,d)-formula (corresponds to a k-*uniform hypergraph of max-degree* d):

- Construct a good $M \subseteq V$ of marked variables such that:
  - each clause contains $\geq 0.11k$ marked variables
  - each clause contains $\geq 0.51k$ unmarked variable



$$\begin{aligned} 0.11k \leq \sum_{i \in \mathsf{vbl}(c)} x_i \leq 0.49k, & \qquad \forall c \in C \\ x_i \in \{0,1\}, & \qquad \forall i \in V \end{aligned}$$

- Constructive LLL (Moser-Tardos):

$k \gtrsim 20 \log d$ → A good M can be constructed in time $\tilde{O}(dkn)$ w.h.p.

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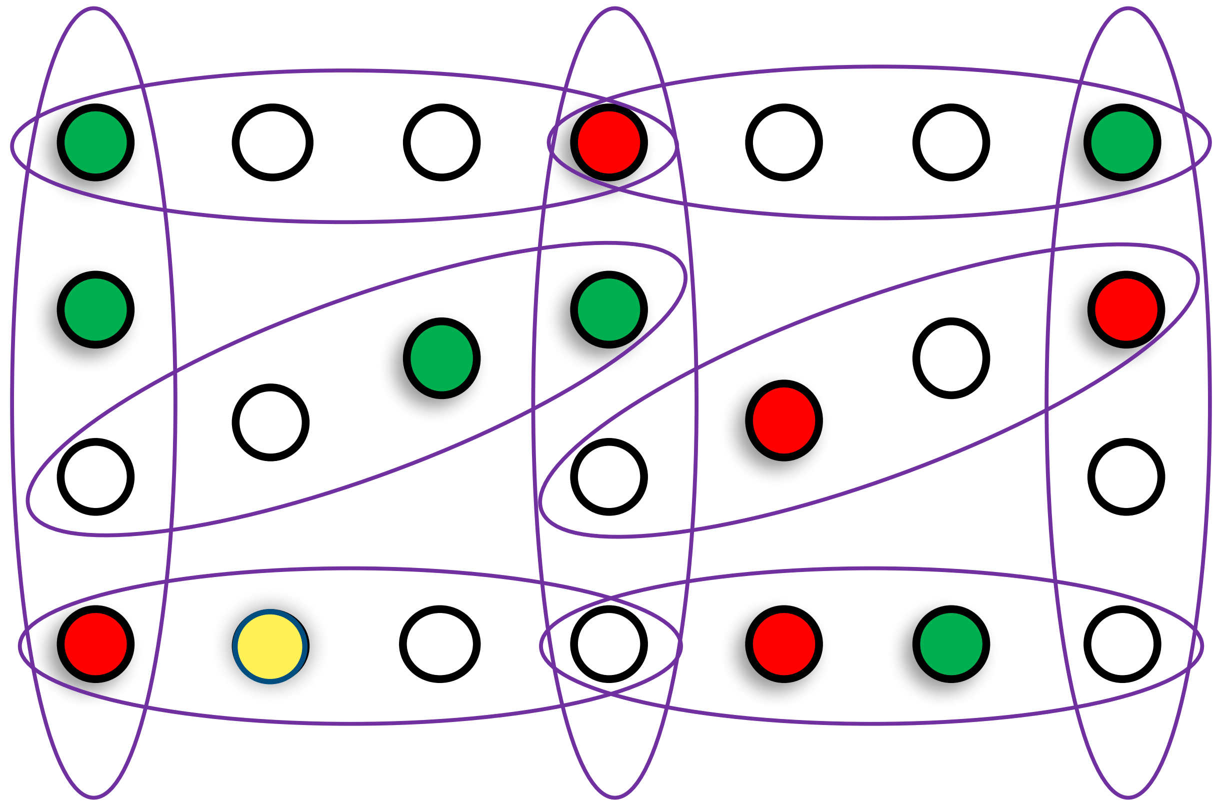
Draw $\boldsymbol{x}_{V \setminus M}$ according to μ conditional on $\boldsymbol{x}_M$



✓

There exists an efficiently constructible subset $M \subseteq V$ of variables s.t.:

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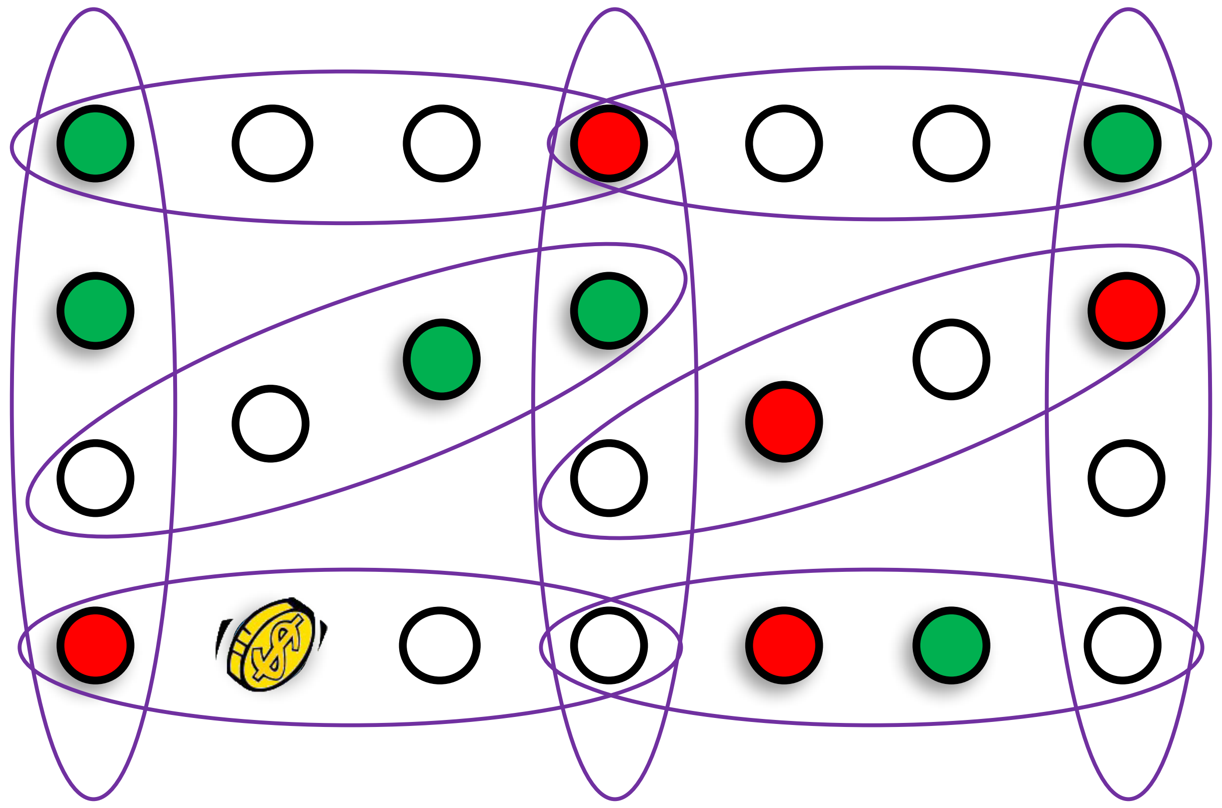
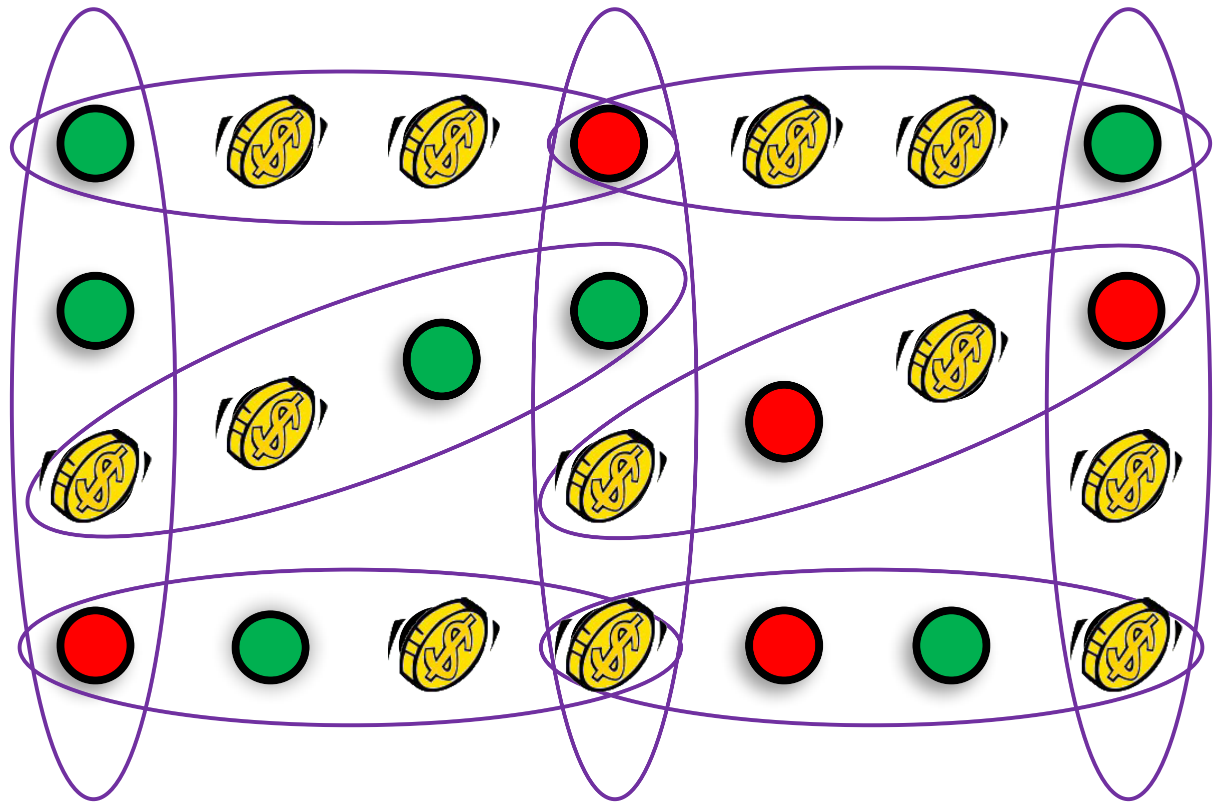
Inference in the Solution Space

Sample variable(s) conditional on a partial assignment:



draw $x_i \sim \mu_i(\cdot \mid \boldsymbol{x}_{M\setminus\{i\}})$



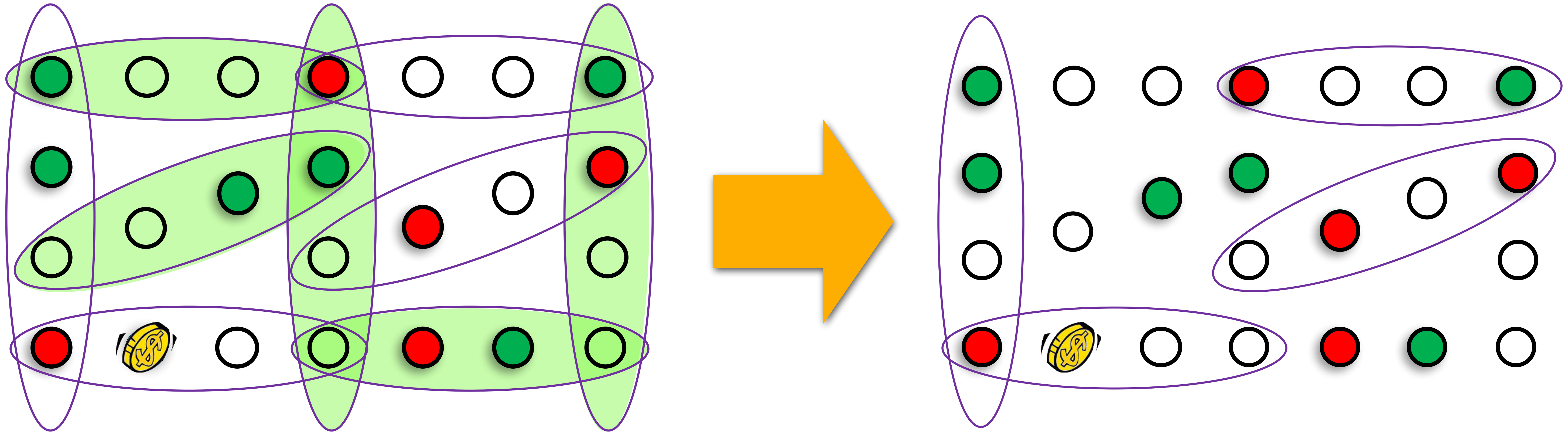
extend $\boldsymbol{x}_M \sim \mu_M$ to $\boldsymbol{x} \sim \mu$

- In general, it is no easier than sampling/counting SAT solutions

Inference in the Solution Space

Sample variable(s) conditioning on a partial assignment:

(on a good $M \subseteq V$)



draw $x_i \sim \mu_i(\cdot \mid \boldsymbol{x}_{M\setminus\{i\}})$

x_i is easy to draw

- Clauses satisfied by the partial assignment deconstructs Φ into connected components
- For good $M \subseteq V$, w.h.p. all components are of sizes $O(dk \log n)$

$$k \geq 20 \log d + 20 \log k + 3 \log \frac{1}{\zeta}$$

in every component →

Rejection sampling succeeds w.p. $n^{-\zeta}$

Our Algorithm (Projected MCMC)

Properly construct a set $M \subseteq V$ of marked variables

Sampling $\boldsymbol{x}_M \sim \mu_M$

Start from a uniform random $\boldsymbol{x} \in \{\mathrm{T}, \mathrm{F}\}^M$

Repeat for sufficiently many steps:

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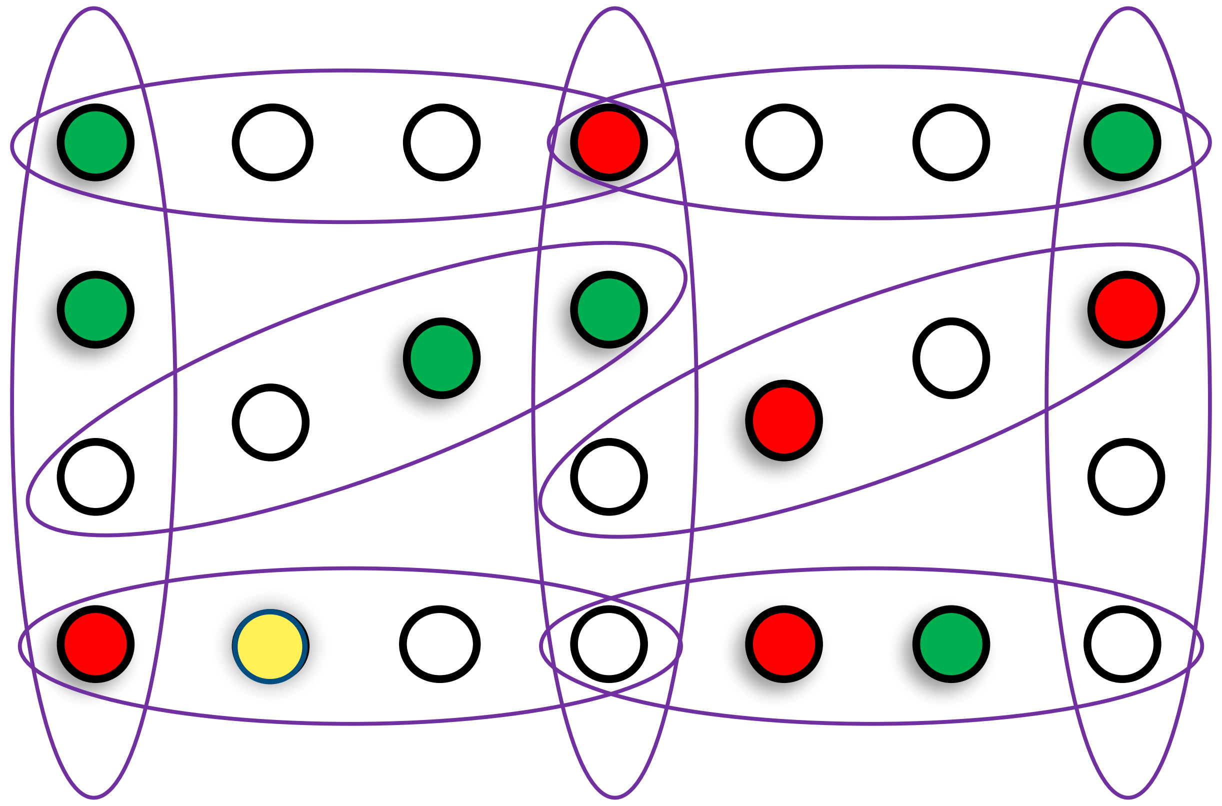
Draw $\boldsymbol{x}_{V \setminus M}$ according to μ conditional on $\boldsymbol{x}_M$



There exists an ✓ efficiently constructible subset $M \subseteq V$ of variables s.t.:

- The idealized Glauber dynamics for μ_M is rapidly mixing
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Rapid Mixing of Projected Chain

The idealized Glauber dynamics for the projected measure μ_M:

Start from a uniform random $\boldsymbol{x} \in \{\mathtt{T}, \mathtt{F}\}^M$

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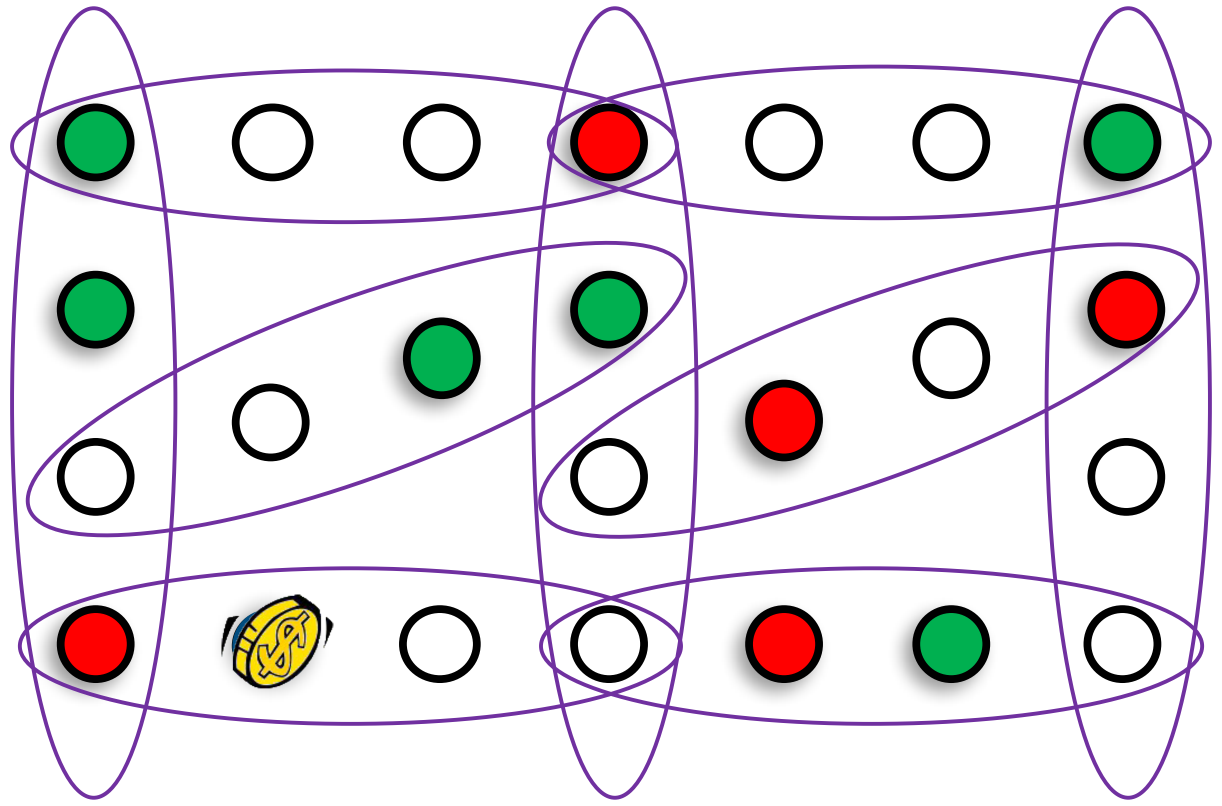

For a good $M \subseteq V$: assuming $k \geq 20 \log d + 20 \log k + 3 \log \frac{1}{\zeta}$

- Use **path coupling** [Bubley, Dyer '97] to bound the mixing time.
- Use **disagreement coupling** [Moitra '17] to bound the discrepancy of path coupling.
- Use **local uniformity** [Haeupler, Saha, Srinivasan '11] to bound the discrepancy of disagreement coupling.

→ The idealized Glauber dynamics for μ_M rapidly mixes in $O(n \log n)$ steps

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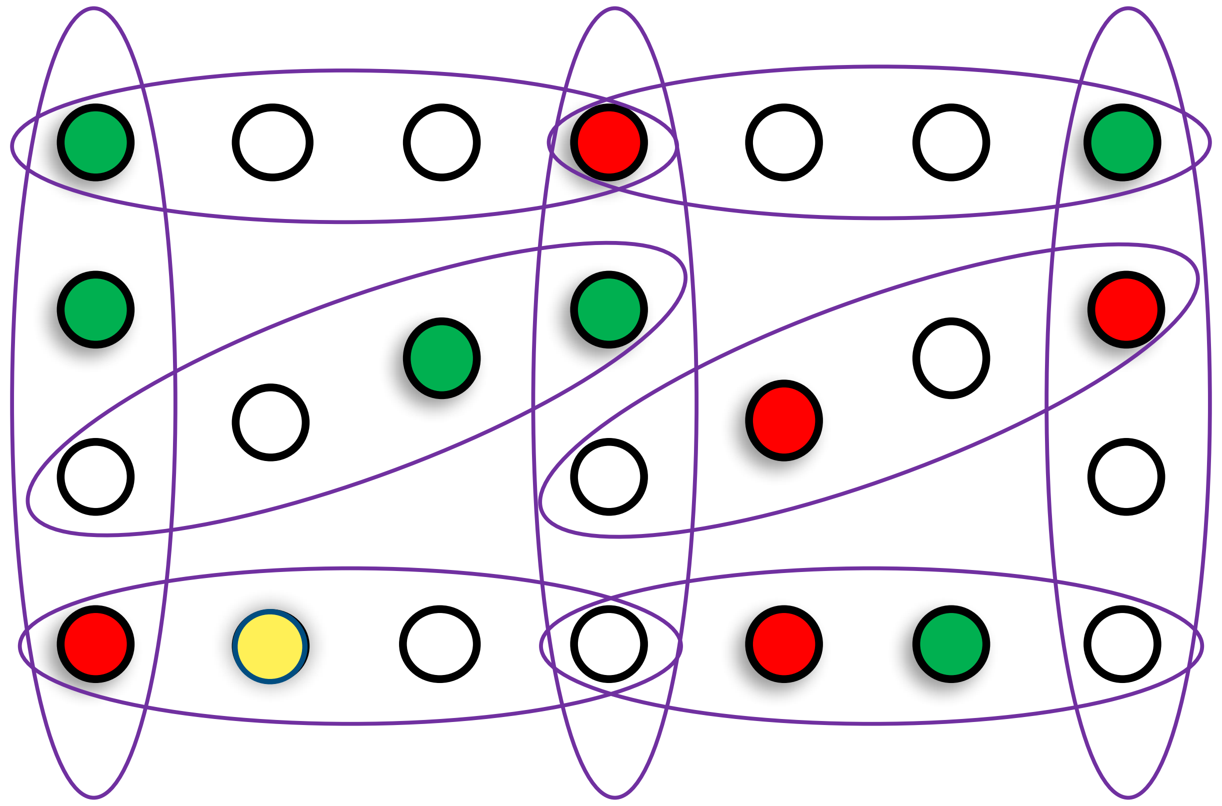

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Main Theorem (for CNF)

[Feng, Guo, **Y.**, Zhang '20]

For any sufficiently small $\zeta \le 2^{-20}$, any (k,d)-CNF satisfying

$$k \ge 20 \log d + 20 \log k + 3 \log \frac{1}{\zeta}$$

- **Sampling algorithm**:
  draw almost uniform SAT solution in time $\tilde{O}(d^2 k^3 n^{1+\zeta})$

Simulated Annealing [Štefankovič, Vempala, Vigoda '09]

- **Counting algorithm**:
  FPRAS for # SAT solutions in time $\tilde{O}(d^2 k^3 n^{2+\zeta})$

Constraint Satisfaction Problem

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- (local) **Constraints:** $C = \{c_1, c_2, \ldots, c_m\}$
  - each $c \in C$ is defined on a subset vbl(c) of variables

$$c : \bigotimes_{i \in \mathsf{vbl}(c)} Q_i \to \{\mathtt{True}, \mathtt{False}\}$$

- **CSP formula:** $\forall \boldsymbol{x} \in Q_1 \times Q_2 \times \cdots \times Q_n$

$$\Phi(\boldsymbol{x}) = \bigwedge_{c \in C} c\left(\boldsymbol{x}_{\mathsf{vbl}(c)}\right)$$

- **Example** (k-SAT): Boolean variables $V = \{x_1, x_2, x_3, x_4, x_5\}$

$$\Phi = (x_1 \vee \neg x_2 \vee x_3) \wedge (x_1 \vee x_2 \vee x_4) \wedge \boxed{(x_3 \vee \neg x_4 \vee \neg x_5)}$$ clause

CSP with Atomic Constraints

(CNF with general domains)

- **Variables:** $V = \{x_1, x_2, \ldots, x_n\}$ with finite domains $Q_1, \ldots, Q_n$
- (*atomic*) **Constraints:** $C = \{c_1, c_2, \ldots, c_m\}$
  - each $c \in C$ forbids an assignment on a subset vbl(c) of variables

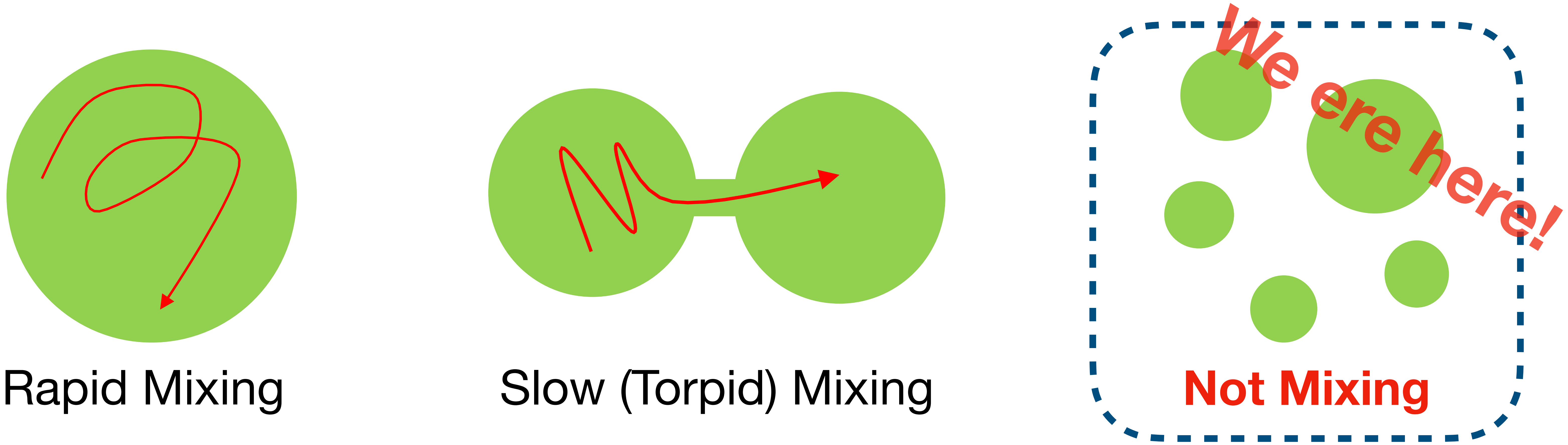
$$c(\boldsymbol{x}_{\mathsf{vbl}(c)}) = \begin{cases} \texttt{False} & \boldsymbol{x}_{\mathsf{vbl}(c)} = \text{a forbidden pattern } \sigma^c \in \bigotimes_{i \in \mathsf{vbl}(c)} Q_i \\ \texttt{True} & \text{otherwise} \end{cases}$$

$$\begin{aligned} \boldsymbol{x}_{\mathsf{vb}(c)} \neq \sigma^c, &\qquad \forall c \in C \\ x_i \in Q_i, &\qquad \forall i \in V \end{aligned}$$

- **CSP formula:** $\forall \boldsymbol{x} \in Q_1 \times Q_2 \times \cdots \times Q_n, \quad \Phi(\boldsymbol{x}) = \bigwedge_{c \in C} c\left(\boldsymbol{x}_{\mathsf{vbl}(c)}\right)$
- **Sampling**: draw almost uniform SAT solution $\boldsymbol{x}$

The Connectivity Barrier

- In the LLL regime (even very far from the critical threshold):



- In general, there is **no** good $M \subseteq V$ such that μ_M is well-connected

State Compression

[Feng, He, **Y.** '20]

- **Variables:** $V = \{x_1, x_2, \ldots, x_n\}$ with domains $Q_1, \ldots, Q_n$
- **Compression:** $h_i : Q_i \to \Sigma_i$ for every variable x_i with $|Q_i| \geq |\Sigma_i|$
- For Boolean variables $Q_i = \{\mathtt{T}, \mathtt{F}\}$,
  - marked variable: $h_i : Q_i \to \Sigma_i$ with $|\Sigma_i| = 2$ and h_i is identity mapping
  - unmarked variable: $h_i : Q_i \to \Sigma_i$ with $|\Sigma_i| = 1$
- **A good compression:** independent random $(X_1, \ldots, X_n) \in Q_1 \times \cdots \times Q_n$

$$\forall c \in C : \quad 0.11 \sum_{i \in \mathsf{vbl}(c)} H(X_i) \leq \sum_{i \in \mathsf{vbl}(c)} H(h_i(X_i)) \leq 0.49 \sum_{i \in \mathsf{vbl}(c)} H(X_i)$$

$H(\cdot)$: Shannon entropy

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[Feng, He, **Y.** '20]

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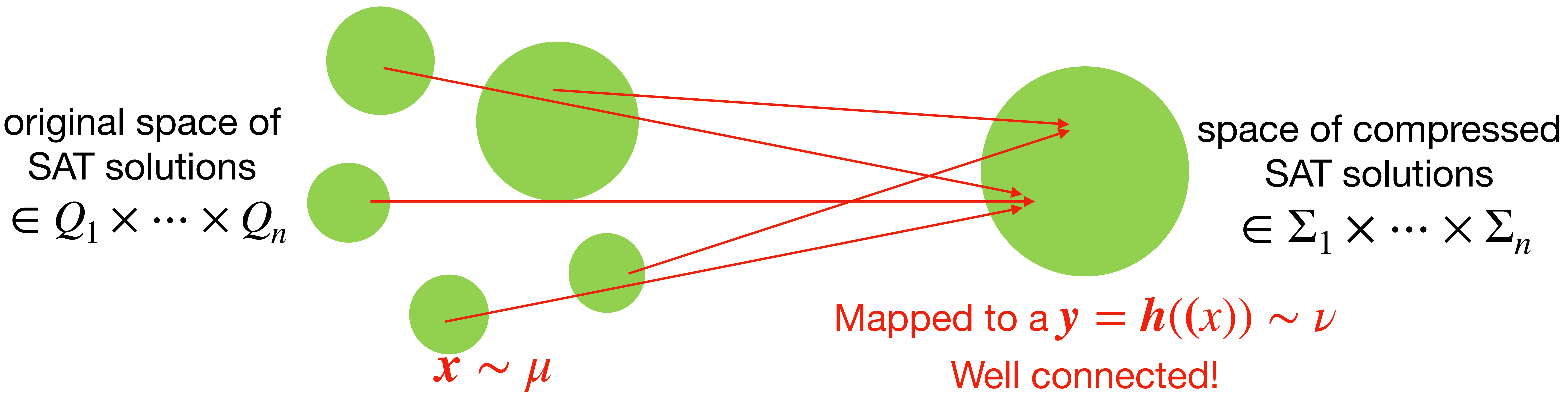
- **Compression:** $h_i : Q_i \to \Sigma_i$ for every variable x_i with $|\Sigma_i| \le |Q_i|$
- **A good compression:** independent random $(X_1, \ldots, X_n) \in Q_1 \times \cdots \times Q_n$

$$\forall c \in C: \quad 0.11 \sum_{i \in \mathsf{vbl}(c)} H(X_i) \le \sum_{i \in \mathsf{vbl}(c)} H(h_i(X_i)) \le 0.49 \sum_{i \in \mathsf{vbl}(c)} H(X_i)$$



State Compression

[Feng, He, **Y.** '20]

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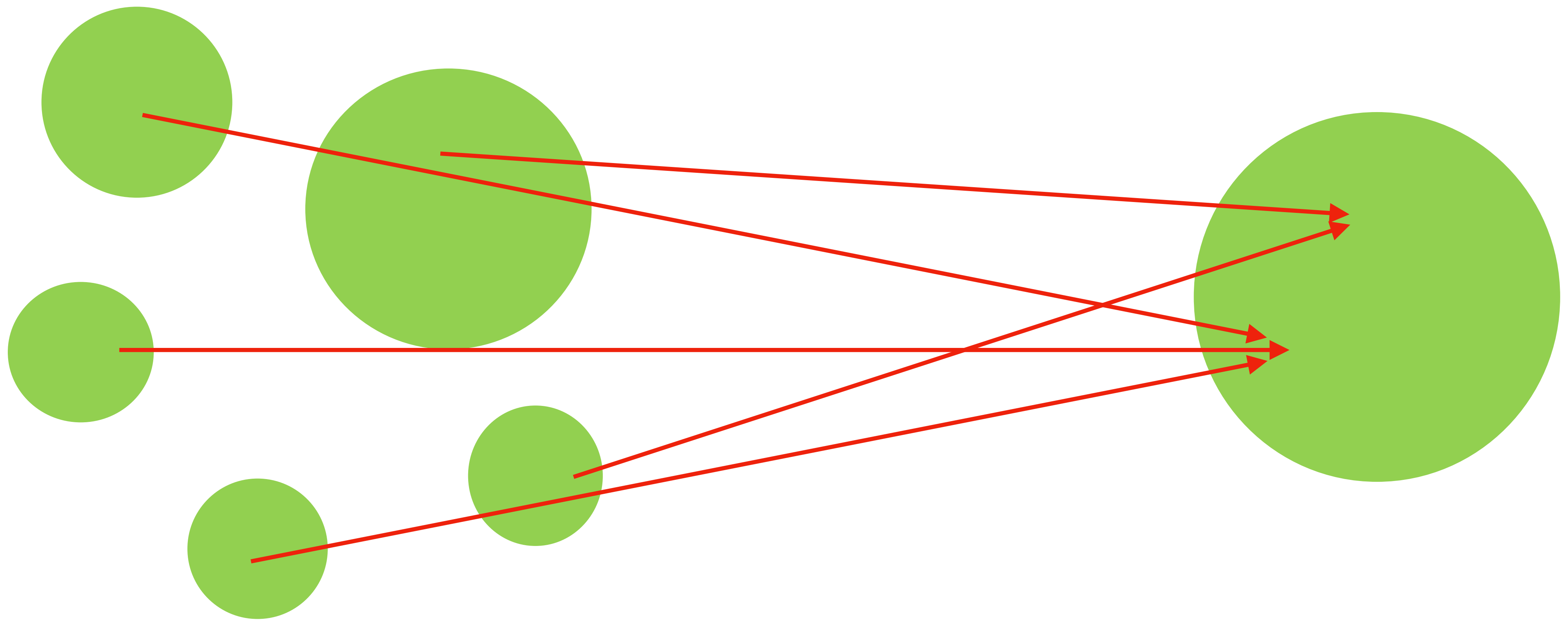

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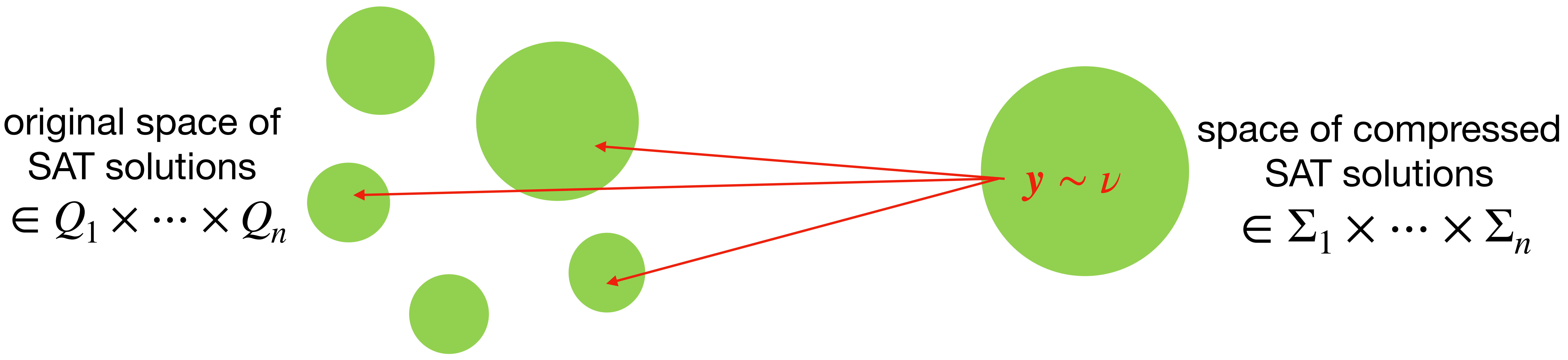

Easy to recover $\boldsymbol{x} \sim \mu$ given $\boldsymbol{h}(x) = \boldsymbol{y}$

Our Algorithm (State Compression)

Construct a good compression $\boldsymbol{h}$ (using Moser-Tados)

Start from a random $\boldsymbol{y}$ in $\Sigma_1 \times \cdots \times \Sigma_n$

Repeat for sufficiently many steps:

- pick $i \in V$ uniformly at random
- resample $y_i \sim \nu_i(\cdot \mid \boldsymbol{y}_{V \setminus \{i\}})$

Draw $\boldsymbol{x}$ according to μ conditional on $\boldsymbol{h}(\boldsymbol{x}) = \boldsymbol{y}$

- **A good compression:** independent random $(X_1, \ldots, X_n) \in Q_1 \times \cdots \times Q_n$

$$\forall c \in C: \quad 0.11 \sum_{i \in \mathsf{vbl}(c)} H(X_i) \le \sum_{i \in \mathsf{vbl}(c)} H(h_i(X_i)) \le 0.49 \sum_{i \in \mathsf{vbl}(c)} H(X_i)$$

Lovász Local Lemma (LLL)

- Variables take independent random values $X_1, X_2, \ldots, X_n$
- **Violation Probability**: each $c \in C$ is violated with prob. ≤ p
- **Dependency Degree**: each $c \in C$ shares variables with ≤ D other constraints
- **LLL**: $\mathrm{e}pD \leq 1 \implies$ solution exists
- **Sampling lower bound** [Bezáková *et al* '16]:

$pD^2 \lesssim 1$ is necessary for sampling

Main Theorem (for Atomic CSP)

[Feng, He, **Y.** ’20]

For atomic CSP with violation prob. p and dependency deg. D

$$pD^{350} \lesssim 1$$

- **Sampling algorithm**:
  draw almost uniform SAT solution in time $\tilde{O}(D^3 n^{1.000001})$
- **Counting algorithm**:
  count # SAT solutions approximately in time $\tilde{O}(D^3 n^{2.000001})$

Follow-Ups and Related Works

- Fast sampling: $O(n^{1.000001})$ time
  - [Jain, Pham, Vuong '21]: use information percolation to bound mixing,

    $pD^{7.043} \lesssim 1$ for atomic CSP

  - [He, Sun, Wu '21]: use CFTP to get perfect sampler, unified analysis,

    $pD^{5.714} \lesssim 1$ for atomic CSP

- Deterministic approximate counting: $n^{O(\mathrm{poly}(D))}$ time
  - [Guo, Liao, Lu, Zhang '18]: adaptive marking/unmarking,

    $pD^{16} \lesssim 1$ for hypergraph coloring

  - [Jain, Pham, Vuong '20]: adaptive marking/unmarking, refine Moitra,

    $pD^{7} \lesssim 1$ for general CSP

Open Problems

- Fast (near-linear time) sampling algorithm for general (non-atomic) CSP solutions.
- Truly polynomial-time (n^c where c is universal constant) deterministic approximate counting for CSP solutions.
- The sharp LLL condition for sampling CSP solutions:
  - $k \gtrsim 2 \log d$ for (k, d)-CNF?
  - For general CSP? $pD^{350} \lesssim 1$
- Sampling LLL in non-variable framework:
  - Bad events $A_1, \ldots, A_m$ in probability space Ω
  - Draw a sample $s \in \Omega$ avoiding all bad events.

Thank you!

- [Moitra '17]: **Approximate counting, the Lovász local lemma, and inference in graphical models.** STOC'17, JACM'19.
- [Guo, Liao, Lu, Zhang '18]: **Counting hypergraph colorings in the local lemma regime.** STOC'18, SICOMP'19.
- [Feng, Guo, Y., Zhang '20]: **Fast sampling and counting k-SAT solutions in the local lemma regime.** STOC'20.
- [Feng, He, Y. '21]: **Sampling constraint satisfaction solutions in the local lemma regime.** STOC'21.
- [Jain, Pham, Vuong '20]: **Towards the sampling Lovász local lemma.** FOCS'21.
- [Jain, Pham, Vuong '21]: **On the sampling Lovász local lemma for atomic constraint satisfaction problems.** arXiv:2102.08342.
- [He, Sun, Wu '21]: **Perfect Sampling for (Atomic) Lovász Local Lemma.** arXiv:2107.03932.