Fast Sampling Constraint Satisfaction Solutions via the Lovász Local Lemma

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**Constraint Satisfaction Problem**

\[ \Phi = (V, Q, C) \]

- **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 \( \text{vbl}(c) \) of variables
    \[
    c : \bigotimes_{i \in \text{vbl}(c)} Q_i \rightarrow \{\text{True, False}\}
    \]

- **CSP formula**: \( \forall x \in Q_1 \times Q_2 \times \cdots \times Q_n \)
  \[
  \Phi(x) = \bigwedge_{c \in C} \left( x_{\text{vbl}(c)} \right)
  \]

- **Example (k-SAT)**: Boolean variables \( V = \{x_1, x_2, x_3, x_4, x_5\} \)
  \[
  k\text{-CNF } \Phi = (x_1 \lor \neg x_2 \lor x_3) \land (x_1 \lor x_2 \lor x_4) \land (x_3 \lor \neg x_4 \lor \neg x_5) \]
  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. $\leq p$
- **Dependency Degree**: each $c \in C$ shares variables with $\leq D$ other constraints $c' \in C$, i.e. $\text{vbl}(c) \cap \text{vbl}(c') \neq \emptyset$
- LLL [Erdős, Lovász, 1975]:
  \[ epD \leq 1 \implies \text{solution exists} \]
- **Constructive LLL** [Moser, Tardos, 2010]:
  \[ epD \leq 1 \implies \text{solution can be found very efficiently} \]
Lovász Local Lemma (LLL)

- \((k, d)\)-CNF: \(\Phi = (x_1 \lor \neg x_2 \lor x_3) \land (x_1 \lor x_2 \lor x_4) \land (x_3 \lor \neg x_4 \lor \neg x_5)\)

- Uniform random \(X_1, X_2, \ldots, X_n \in \{\text{True}, \text{False}\}\)

- Violation probability: \(p = 2^{-k}\)

- Dependency degree: \(D \leq dk\)

- LLL: \(k \geq \log d \ (k \geq \log_2 d + \log_2 k + O(1))\)

\[ epD \leq edk2^{-k} \leq 1 \]

LLL

Moser-Tados

a SAT solution exists and can be found in \(O(dkn)\) time
**Sampling & Counting**

**Input:** a CSP formula $\Phi = (V, Q, C)$

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

- $\mu$: uniform distribution over all satisfying solutions of $\Phi$

---

**Rejection Sampling**

generate a uniform random $\forall x \in Q_1 \times Q_2 \times \cdots \times Q_m$:

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

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

**SAT solutions may be exponentially rare!**
Sampling & Counting

**Input:** a CSP formula $\Phi = (V, Q, C)$

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

- exact counting is $\#\text{P}$-hard
- **Almost Uniform Sampling**
  - self-reduction [Jerrum, Valiant, Vazirani 1986]
  - adaptive simulated annealing [Stefankovič, Vempala, Vigoda 2009]
- **Approximate Counting**

- Application: inference in probabilistic graphical models

Gibbs distribution

$\mu(x) \propto \Phi(x) = \prod_{c \in C} c \left( x_{vbl(c)} \right)$

where each $c : \bigotimes_{i \in vbl(c)} Q_i \rightarrow \mathbb{R}_{\geq 0}$

Inference:

$\Pr_{X \sim \mu} [X_i \cdot | X_S = x_S]$
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):

Rapid Mixing

Slow (Torpid) Mixing

Not Mixing
Sampling $k$-SAT Solutions

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

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Moitra
STOC’17 JACM’19

| $k \geq 60 \log d$ | $n^{O(d^2 k^2)}$ | Coupling + LP |

Feng, Guo, Y., Zhang ’20

| $k \geq 20 \log d$ | $\tilde{O}(d^2 k^3 n^{1.000001})$ | **Projected MCMC** |

$^1$ Monotone CNF: all variables appear **positively**, e.g. $\Phi = (x_1 \lor x_2 \lor x_3) \land (x_1 \lor x_2 \lor x_4) \land (x_3 \lor x_4 \lor x_5)$

$^2$ $s$: two dependent clauses share at least $s$ variables.
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 $\tilde{O}(d^2k^3n^{1+\zeta})$

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

Start from an arbitrary satisfying \( x \in \{ \text{T}, \text{F} \}^V \)

At each step:

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

- \( \mu \): uniform distribution over all SAT solutions \( x \in \{ \text{T}, \text{F} \}^V \)
- \( \mu_i(\cdot \mid x_{V \setminus \{i\}}) \): marginal distribution of \( x_i \) cond. on current values of all other variables
Markov Chain for $k$-SAT

Glauber Dynamics

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

At each step:

- pick $i \in V$ uniformly at random
- resample $x_i \sim \mu_i(\cdot | x_{V \setminus \{i\}})$

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

$$(x_1 \lor \neg x_2 \lor x_3) \land (x_2 \lor x_7 \lor x_5) \land (x_4 \lor \neg x_3 \lor x_6)$$
Markov Chain for $k$-SAT

Glauber Dynamics

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

At each step:

• pick $i \in V$ uniformly at random

• resample $x_i \sim \mu_i(\cdot | x_{V \setminus \{i\}})$

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$(x_1 \lor \neg x_2 \lor x_3) \land (x_2 \lor x_7 \lor x_5) \land (x_4 \lor \neg x_5 \lor x_6)$
Markov Chain for $k$-SAT

Glauber Dynamics

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

At each step:

- pick $i \in V$ uniformly at random
- resample $x_i \sim \mu_i(\cdot | x_{V\setminus\{i\}})$

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

- The Markov chain has stationary distribution $\mu$

- If rapidly mixing: $\tau_{\text{mix}}(\epsilon) = \max_{X_0} \min_t \{ t \mid d_{TV}(X_t, \mu) \leq \epsilon \} = \text{poly}(n, 1/\epsilon)$

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

- $\mu$: uniform distribution over SAT solutions of $\Phi$

- A set $M \subseteq V$ of marked variables

- $\mu_M$: distribution of $X_M$ where $X \sim \mu$

- $\mu_M$ 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

\[
\begin{align*}
\text{Sampling} \quad x_M &\sim \mu_M \\
\text{Start from a uniform random } x &\in \{\text{T, F}\}^M \\
\text{Repeat for sufficiently many steps:} \\
&\quad \text{pick } i \in V \text{ uniformly at random} \\
&\quad \text{resample } x_i \sim \mu_i(\cdot | x_{M\setminus\{i\}})
\end{align*}
\]

Draw $x_{V\setminus M}$ according to $\mu$ conditional on $x_M$

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

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

- Constructive LLL (Moser-Tardos):

\[
0.11k \leq \sum_{i \in \text{vbl}(c)} x_i \leq 0.49k, \quad \forall c \in C
\]

\[
x_i \in \{0,1\}, \quad \forall i \in V
\]

\(k \geq 20 \log d\)  

A good \(M\) can be constructed in time \(\tilde{O}(dkn)\) w.h.p.
Our Algorithm (Projected MCMC)

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

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

Repeat for sufficiently many steps:
- pick $i \in V$ uniformly at random
- resample $x_i \sim \mu_i(\cdot | x_{M\setminus \{i\}})$

Draw $x_{V\setminus M}$ according to $\mu$ conditional on $x_M$

There exists an efficiently constructible subset $M \subseteq V$ of variables s.t.:
- The idealized Glauber dynamics for $\mu_M$ is rapidly mixing
- It is efficient to draw from $\mu_i(\cdot | x_{M\setminus \{i\}})$ (to implement the idealized Glauber dynamics)
- It is efficient to extend $x_M \sim \mu_M$ to an $x \sim \mu$
Inference in the Solution Space

Sample variable(s) conditional on a partial assignment:

- 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 $M \subseteq V$)

- Clauses satisfied by the partial assignment deconstructs $\Phi$ into connected components

- For good $M \subseteq V$, w.h.p. all components are of sizes $O(dk \log n)$

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

Rejection sampling succeeds w.p. $n^{-\zeta}$
Our Algorithm (Projected MCMC)

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

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

Repeat for sufficiently many steps:

- pick $i \in V$ uniformly at random
- resample $x_i \sim \mu_{i}(\cdot | x_{M \setminus \{i\}})$

Draw $x_{V \setminus M}$ according to $\mu$ conditional on $x_M$

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

- The idealized Glauber dynamics for $\mu_M$ is rapidly mixing
  - It is efficient to draw from $\mu_i(\cdot | x_{M \setminus \{i\}})$ (to implement the idealized Glauber dynamics)
  - It is efficient to extend $x_M \sim \mu_M$ to an $x \sim \mu$
Rapid Mixing of Projected Chain

The idealized Glauber dynamics for the projected measure $\mu_M$:

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

Repeat for sufficiently many steps:
- pick $i \in V$ uniformly at random
- resample $x_i \sim \mu_i(\cdot | x_{M\setminus\{i\}})$

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 $\mu_M$ rapidly mixes in $O(n \log n)$ steps
Our Algorithm (Projected MCMC)

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

\[
\begin{align*}
\text{Sampling} \quad & x_{M} \sim \mu_{M} \\
\text{Start from a uniform random} \quad & x \in \{T, F\}^{M} \\
\text{Repeat for sufficiently many steps:} & \\
& \quad \bullet \text{pick } i \in V \text{ uniformly at random} \\
& \quad \bullet \text{resample } x_{i} \sim \mu_{i}(\cdot | x_{M\setminus\{i\}}) \\
\text{Draw } x_{V \setminus M} \text{ according to } \mu \text{ conditional on } x_{M}
\end{align*}
\]

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

\[
\begin{align*}
& \checkmark \quad \text{The idealized Glauber dynamics for } \mu_{M} \text{ is rapidly mixing} \\
& \checkmark \quad \text{It is efficient to draw from } \mu_{i}(\cdot | x_{M\setminus\{i\}}) \text{ (to implement the idealized Glauber dynamics)} \\
& \checkmark \quad \text{It is efficient to extend } x_{M} \sim \mu_{M} \text{ to an } x \sim \mu
\end{align*}
\]
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 $\tilde{O}(d^2k^3n^{1+\zeta})$

- **Simulated Annealing** [Štefankovič, Vempala, Vigoda ’09]

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

\[ \Phi = (V, Q, C) \]

- **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 \( \text{vbl}(c) \) of variables

\[ c : \bigotimes_{i \in \text{vbl}(c)} Q_i \rightarrow \{\text{True}, \text{False}\} \]

- **CSP formula:** \( \forall x \in Q_1 \times Q_2 \times \cdots \times Q_n \)

\[ \Phi(x) = \bigwedge_{c \in C} \left( x_{vbl(c)} \right) \]

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

\[ \Phi = (x_1 \lor \neg x_2 \lor x_3) \land (x_1 \lor x_2 \lor x_4) \land \fbox{(x_3 \lor \neg x_4 \lor \neg x_5)} \]

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 \( \text{vbl}(c) \) of variables

  \[
  c(x_{\text{vbl}(c)}) = \begin{cases} 
  \text{False} & \text{if } x_{\text{vbl}(c)} = \text{a forbidden pattern } \sigma^c \in \bigotimes_{i \in \text{vbl}(c)} Q_i \\
  \text{True} & \text{otherwise}
  \end{cases}
  \]

- **CSP formula:** \( \forall x \in Q_1 \times Q_2 \times \cdots \times Q_n, \quad \Phi(x) = \bigwedge_{c \in C} c(x_{\text{vbl}(c)}) \)

- **Sampling:** draw almost uniform SAT solution \( x \)
The Connectivity Barrier

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

  Rapid Mixing
  Slow (Torpid) Mixing
  Not Mixing

• In general, there is no good $M \subseteq V$ such that $\mu_M$ 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**: $h_i : Q_i \rightarrow \Sigma_i$ for every variable $x_i$ with $|Q_i| \geq |\Sigma_i|$

- For Boolean variables $Q_i = \{T, F\}$,
  - marked variable: $h_i : Q_i \rightarrow \Sigma_i$ with $|\Sigma_i| = 2$ and $h_i$ is identity mapping
  - unmarked variable: $h_i : Q_i \rightarrow \Sigma_i$ with $|\Sigma_i| = 1$

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

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

$H(\cdot)$: Shannon entropy
State Compression

[Feng, He, Y. ’20]

• Variables: $V = \{x_1, x_2, \ldots, x_n\}$ with domains $Q_1, \ldots, Q_n$

• Compression: $h_i : Q_i \rightarrow \Sigma_i$ for every variable $x_i$ with $|\Sigma_i| \leq |Q_i|$

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

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

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- **Variables**: $V = \{x_1, x_2, \ldots, x_n\}$ with domains $Q_1, \ldots, Q_n$

- **Compression**: $h_i : Q_i \rightarrow \Sigma_i$ for every variable $x_i$ with $|\Sigma_i| \leq |Q_i|$

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

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State Compression

[Feng, He, Y. ’20]

• **Variables:** $V = \{x_1, x_2, \ldots, x_n\}$ with domains $Q_1, \ldots, Q_n$

• **Compression:** $h_i : Q_i \rightarrow \Sigma_i$ for every variable $x_i$ with $|\Sigma_i| \leq |Q_i|$

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

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

Easy to recover $x \sim \mu$ given $h(x) = y$
Our Algorithm (State Compression)

Construct a good compression $h$ (using Moser-Tados)

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

Repeat for sufficiently many steps:

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

Draw $x$ according to $\mu$ conditional on $h(x) = y$

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

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

- Dependency Degree: each $c \in C$ shares variables with $\leq D$ other constraints

- LLL: $epD \leq 1 \implies$ solution exists

- Sampling lower bound [Bezáková et al ’16]:
  \[ pD^2 \lesssim 1 \] is necessary for sampling
Main Theorem (for Atomic CSP)

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

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

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

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

[Feng, He, Y. ’20]
Follow-Ups and Related Works

- Fast sampling: $O(n^{1.000001})$ time
  - [Jain, Pham, Vuong ’21]: use information percolation to bound mixing,
    $$pD^{7.043} \lesssim 1 \text{ for atomic CSP}$$
  - [He, Sun, Wu ’21]: use CFTP to get perfect sampler, unified analysis,
    $$pD^{5.714} \lesssim 1 \text{ for atomic CSP}$$

- Deterministic approximate counting: $n^{O(poly(D))}$ time
  - [Guo, Liao, Lu, Zhang ’18]: adaptive marking/unmarking,
    $$pD^{16} \lesssim 1 \text{ for hypergraph coloring}$$
  - [Jain, Pham, Vuong ’20]: adaptive marking/unmarking, refine Moitra,
    $$pD^{7} \lesssim 1 \text{ for general CSP}$$
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 $\Omega$
  • 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.
- [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.