Towards derandomising Markov chain Monte Carlo

Heng Guo (University of Edinburgh)

Based on joint works with Weiming Feng, Jiaheng Wang (Edinburgh), Chunyang Wang, Yitong Yin (Nanjing)

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Deterministic vs randomised counting

Estimating the volume of a convex body:

- No polynomial-time *deterministic* approximation algorithm using membership queries only; (Elekes 1986, Bárány and Füredi 1987)
- Efficient *randomised* approximation algorithm does exist! (Dyer, Frieze, and Kannan 1991)

However, Weitz (2006) gave an FPTAS for the hardcore model up to the tree uniqueness threshold, whose randomised counterparts are not known until very recently (Anari, Liu, and Oveis Gharan, 2020).

Since then, deterministic counting algorithms are catching up in many fronts.
The Gibbs distribution for the hardcore model:

for an independent set $I$, $\mu(I) = \frac{\lambda^{|I|}}{Z}$, where $Z = \sum_{I \in J} \lambda^{|I|}$

We often want to approximate $Z$, or equivalently, sample from $\mu$.

Standard Glauber dynamics converges to $\mu$. 
Systematic scan Glauber dynamics:

Pick the next vertex $v$, resample its state conditioned on its neighbours.

For the resampling step, draw uniform $r \sim [0, 1]$:

- if one of its neighbour is occupied, make $v$ unoccupied regardless of $r$;
- if none of its neighbour is occupied, make $v$ unoccupied if $r \leq \frac{1}{1+\lambda}$; occupied otherwise.

In either case, $v$ is unoccupied if $r \leq \frac{1}{1+\lambda}$. 
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Counting to sampling reduction (Jerrum, Valiant, and Vazirani, 1986)

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\frac{1}{Z} = \frac{Z(\sigma_{v_1} = 0)}{Z} \cdot \frac{Z(\sigma_{v_1} = 0, \sigma_{v_2} = 0)}{Z(\sigma_{v_1} = 0)} \cdot \ldots \cdot \frac{Z(\land_{i=1}^{n} \sigma_{v_i} = 0)}{Z(\land_{i=1}^{n-1} \sigma_{v_i} = 0)}
\]

Each term \(\frac{Z(\land_{i=1}^{j} \sigma_{v_i} = 0)}{Z(\land_{i=1}^{j-1} \sigma_{v_i} = 0)}\) is the marginal probability of \(v_j\) where \(\forall i < j, v_i\) is pinned to 0. Equivalently, we can remove \(v_i\) for all \(i < j\) from \(G\) and consider the marginal of \(v_j\).

It suffices to approximate these marginals within \(\frac{\epsilon}{n}\) to get an \(\epsilon\)-approximation to \(Z\).
Counting to sampling reduction

Standard self-reduction (Jerrum, Valiant, and Vazirani, 1986)

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While the whole Glauber dynamics requires a lot of time / randomness to simulate, can we draw from for the marginal distribution more efficiently?

For example, instead of \( O(n \log n) \), can we use \( O(\log n) \) time / random variables for each vertex?
An alternative sampling algorithm

Target distribution: $\mu(I) \propto \lambda^{|I|}$
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Draw a uniform $r_0 \sim [0, 1]$ first, then

- if $r_0 \leq \frac{1}{1+\lambda}$, $v$ is unoccupied;
- otherwise, $r_0 > \frac{1}{1+\lambda}$, we need its neighbours’ states.
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- If all neighbours are not occupied, $v$ must be occupied as $r_0 > \frac{1}{1+\lambda}$.
- Otherwise, say some neighbour $u$ is $\bot$, we recursively resolve $u$. 

At $t = 0$
An alternative sampling algorithm

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- Otherwise, say some neighbour $u$ is $\perp$, we recursively resolve $u$.

Suppose all neighbours of $u$ at $t_{u}$ are all unoccupied. Then as $r_{t_{u}} > \frac{1}{1+\lambda}$, $u$ was occupied.
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Back to time 0, we deduce that $v$ has to be unoccupied.
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When resolving \((v, t)\), first check if \(X_t(v)\) is known, or if \(r_t\) has been drawn before.

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\begin{align*}
\text{Resolve}(v, t) & \\
\text{if } & \\
\text{and } & \\
X_t(v) & = 0
\end{align*}
\]

\[
\begin{align*}
\mathcal{R} & = \{r_t \mid t \leq 1\} \\
\mathcal{U} & = \{u \mid u \geq 1\}
\end{align*}
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\text{Resolve}(v, t) \quad \text{if } r_t > \frac{1}{1+\lambda} \quad \forall (u, v) \in E, \text{Resolve}(u, \text{upd}_t(u))
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\[X_v = 0\]

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\[
\exists u, X_u = 1
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This can be viewed as either

- a coupling with the stationary process, or
- a grand coupling (using the same \(\tau_t\)) for all possible starting \(X_0\).

This grand coupling is very similar to Coupling From The Past by \textit{Wilson and Propp} (1996).
Truncation

Running CTTP till it terminates yields a perfect sample.

Truncate it if $\geq T$ random variables are revealed.

$$d_{TV}(\mu_{V}, \mu_{alg}) \leq \text{Pr}[\text{Truncation}]$$

In a typical application (such as $\lambda < \frac{1}{\Delta - 1}$ for hardcore),

$$\text{Pr}[t_{run} \geq T] \leq \exp(-O(T))$$

Thus, taking $T = O(\log \frac{n}{\epsilon})$ yields $\frac{\epsilon}{n}$ error.
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By enumerating all possible \( \exp(T) = \left( \frac{n}{\epsilon} \right)^C \) random choices, we can deterministically estimate the marginal probability with \( \frac{\epsilon}{n} \) error.
Our algorithm is inspired by the algorithm of Anand and Jerrum (2022):

- recursive marginal sampler
- designed for spin systems on infinite graphs
- constant expected running time with exponential tail bounds
- uses strong spatial mixing

The main difference is that in Anand–Jerrum, once a vertex is fixed, it has to stay fixed in all future recursive calls.
**What are these algorithms good for?**

**Pros**

- Approximate samples from the marginal distribution in $O(\log n)$ time
- Can be used to perfectly sample a full configuration in linear expected running time
- Deterministic approximation algorithm

**Cons**

- Weaker bounds for spin systems
  
  For hardcore models in bounded degree graphs, CTTP works if $\lambda \leq \frac{1}{\Delta-1}$, smaller than the critical $\lambda_{c}(\Delta) \approx \frac{c}{\Delta}$ (Weitz, 2006).
APPLICATIONS
Let $H = (V, E)$ be a hypergraph. $S \subseteq V$ is **independent** if there is no $e \in E$ such that $e \subseteq S$. 
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Running CTTP for HIS is almost the same as for the hard-core model.

To update $v$, we need to find a “boundary” of $v$, conditioned on which the value of $v$ is independent from the rest.

There is a $1/2$ lower bound for “unoccupy”.

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Hypergraph independent sets

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Theorem

Let $k \geq 2$ and $\Delta \geq 2$ be two integers such that $\Delta \leq \frac{1}{\sqrt{8ek^2}} \cdot 2^{\frac{k}{2}}$. There is an FPTAS for the number of independent sets in $k$-uniform hypergraphs with maximum degree $\Delta$.

Bezáková, Galanis, Goldberg, G., and Štefankovič (2019): $\Delta \geq 5 \cdot 2^{\frac{k}{2}}$, NP-hard

Hermon, Sly, and Zhang (2019): $\Delta \leq c2^{\frac{k}{2}}$, randomised algorithm

Qiu, Wang, and Zhang (2022): $\Delta \leq \frac{c}{k} \cdot 2^{\frac{k}{2}}$, perfect sampler

He, Wang, and Yin (2023): $\Delta \lesssim 2^{\frac{k}{3}}$, deterministic algorithm

Other previous work:

Bordewich, Dyer, and Karpinski (2008, 2006); Jain, Pham, and Vuong (2021)
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The local lemma ensures that with suitable parameters, every vertex’s marginal distribution, under an arbitrary conditioning, is close to uniform.
The original local lemma (Erdős and Lovász 1975) was introduced to show the existence of 3-colourings in hypergraphs.

Let $H = (V, E)$ be the hypergraph, and $\Gamma(e)$ be the set of hyperedges intersecting $e \in E$. Then $|\Gamma(e)| \leq (\Delta - 1)k$.

**Theorem (Lovász 1977)**

If there exists an assignment $x : E \to \{0, 1\}$ such that for every $e \in E$ we have

$$\Pr(\text{e is monochromatic}) \leq x(e) \prod_{e' \in \Gamma(e)} (1 - x(e')) \quad (1)$$

then a proper colouring exists.

Typically we set $x(e) = \frac{1}{k\Delta}$. It gives

$$x(e) \prod_{e' \in \Gamma(e)} (1 - x(e')) \geq \frac{1}{k\Delta} \left(1 - \frac{1}{k\Delta}\right)^{k(\Delta - 1)} \geq \frac{1}{ek\Delta} \quad (2)$$

Notice that $\Pr(\text{e is monochromatic}) = \frac{q}{q^k} = \frac{1}{q^{k-1}}$. Thus $\Delta \leq \frac{q^{k-1}}{ek}$ suffices.
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The original local lemma (Erdős and Lovász 1975) was introduced to show the existence of 3-colourings in hypergraphs.

Let $H = (V, E)$ be the hypergraph, and $\Gamma(e)$ be the set of hyperedges intersecting $e \in E$. Then $|\Gamma(e)| \leq (\Delta - 1)k$.

**Theorem (Lovász 1977)**

If there exists an assignment $\alpha : E \rightarrow \{0, 1\}$ such that for every $e \in E$ we have

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The local lemma also gives an upper bound for any event under $\mu(\cdot)$.

**Theorem (Haeupler, Saha, and Srinivasan 2011)**

If the local lemma holds for every $e \in \mathcal{E}$, then for any event $B$, $\mu(B) \leq \Pr(B) \prod_{e \in \Gamma(B)} (1 - \chi(e))^{-1}$.

This implies that buckets are almost uniform, even with arbitrary conditioning. (Recall that $s = q^{2/3}$.)

**Lemma (local uniformity)**

If $\lfloor q/s \rfloor^k \geq 4es\Delta k$, then for any $v \in V$, any subset $\Lambda \subseteq V \setminus \{v\}$ and partial configuration $\sigma_{\Lambda} \in [s]^{\Lambda}$, it follows that

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There are a few issues with CTTP for hypergraph colourings.

1. We run Glauber dynamics in the projected state space, meaning that the “boundary” of a vertex $v$ needs to adapt to the current configuration. We find a boundary such that all crossing hyperedges are non-monochromatic.

2. We cannot do the telescoping product reduction for the marginals. Instead, we consider a sequence of hypergraphs by removing hyperedges one by one. Thus we need to sample the marginal distribution of $k$ vertices, instead of one. Some extra care for consistency is required.

3. The above only samples buckets. To get the colours, we condition on the buckets of all vertices within the boundary of the last update, and use brute force to get the colours.
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To bound the truncation probability, we consider the extended hypergraph, introduced by He, Sun, and Wu (2021). It creates a copy of each variable every time it is updated.

If truncation happens, then there must be a large connected component in the extended hypergraph, inside which there are a linear fraction of variables getting $\perp$ when they are first resolved. The last event is very unlikely because of local uniformity from the local lemma.

This analysis requires $\Delta \lesssim s^{k/2}$. Recall that local uniformity requires $\Delta \lesssim (q/s)^k$.

Thus, the best we can do is $\Delta \lesssim q^{k/3}$ by choosing $s \approx q^{2/3}$.

This highlights a major difference between CTTP and Anand–Jerrum: in AJ, once a variable is pinned, it will stay pinned for all future recursive calls. Thus, in the analysis above, it only contributes once.
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Linear hypergraphs

Linear: $\forall e_1, e_2 \in E, |e_1 \cap e_2| \leq 1$

**Theorem**

For any real $\delta > 0$, let $k \geq \frac{25(1+\delta)^2}{\delta^2}$ and $\Delta \geq 2$ be two integers such that $\Delta \leq \frac{1}{100k^3}2^{k/(1+\delta)}$. There is an FPTAS for the number of independent sets in $k$-uniform linear hypergraphs with maximum degree $\Delta$.

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These match various bounds for randomised algorithms in the leading order by Hermon, Sly, and Zhang (2019); Qiu, Wang, and Zhang (2022); Feng, G., and Wang (2022).

For linear hypergraph independent sets, no hardness result is known.

For colouring linear hypergraphs, Galanis, G., and Wang (2022+) showed that it is $\text{NP}$-hard to find a colouring if $\Delta \geq 2kq^k \log q + 2q$. 
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Spin systems

With little additional effort, one can show that the algorithm by Anand and Jerrum (2022) obtains approximate marginal samples within $O(\log n)$ time for spin systems with strong spatial mixing in subexponential neighbourhood growth graphs.

This implies various new FPTASes, most notably, for lattices, such as 6-colourings on $\mathbb{Z}^2$.

The main challenge remains:

find a $O(\log n)$-time marginal sampler for the hardcore model or graph colourings under conditions where other methods work.

For $q$-colouring graphs with degree $\leq \Delta$, our method works when $q = O(\Delta^2)$, and yet many rapid mixing or perfect sampling results are known when $q > C\Delta$ for various constant $C$. 
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Open problems

• Hypergraph colourings: $\Delta \lesssim q^{k/2}$?

• Running time:
  we take $T = \text{poly}(\Delta, k, \log q) \log \frac{n}{\varepsilon}$, which leads to $\left(\frac{n}{\varepsilon}\right)^{\text{poly}(\Delta, k, \log q)}$ for FPTAS.

  Does $f(\Delta, k, q) \left(\frac{n}{\varepsilon}\right)^c$ -time FPTAS exist for a constant $c$?

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Thank you!

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