# Mismatched Monte Carlo for the Planted clique problem 

Maria Chiara Angelini

Sapienza, Università di Roma

Rigorous Evidence for Information-Computation Trade-offs Workshop Simons Institute - EPFL

15092021

## The Random Clique Problem

## Max-Clique Problem <br> Given $G \in \mathcal{G}(N, 1 / 2)$, find the largest random clique

Clique $\mathcal{C}$ : fully-connected subgraph of $G$

## The Random Clique Problem

## Max-Clique Problem

Given $G \in \mathcal{G}(N, 1 / 2)$, find the largest random clique
Clique $\mathcal{C}$ : fully-connected subgraph of $G$

$$
\begin{gathered}
\bar{Y}_{K}=\text { Average number of cliques } \mathcal{C} \text { of size } K=\binom{n}{K} \frac{1}{2}\binom{K}{2} \\
\bar{Y}_{K} \rightarrow 0 \text { if } K>K_{S}(N)=2 \log _{2}(N)-O(\log \log (N))
\end{gathered}
$$

## The Random Clique Problem

## Max-Clique Problem

Given $G \in \mathcal{G}(N, 1 / 2)$, find the largest random clique
Clique $\mathcal{C}$ : fully-connected subgraph of $G$
$\bar{Y}_{K}=$ Average number of cliques $\mathcal{C}$ of size $K=\binom{n}{K} \frac{1}{2}\binom{K}{2}$ $\bar{Y}_{K} \rightarrow 0$ if $K>K_{S}(N)=2 \log _{2}(N)-O(\log \log (N))$

Probability that a $K$-clique is contained in a $K+1$-clique:

$$
\mathcal{P}_{\text {grow }}(K \rightarrow K+1)=\frac{(K+1) \bar{Y}_{K+1}}{\bar{Y}_{K}}
$$

## The Random Clique Problem

## Max-Clique Problem

Given $G \in \mathcal{G}(N, 1 / 2)$, find the largest random clique
Clique $\mathcal{C}$ : fully-connected subgraph of $G$
$\bar{Y}_{K}=$ Average number of cliques $\mathcal{C}$ of size $K=\binom{n}{K} \frac{1}{2}\binom{K}{2}$ $\bar{Y}_{K} \rightarrow 0$ if $K>K_{S}(N)=2 \log _{2}(N)-O(\log \log (N))$

Probability that a $K$-clique is contained in a $K+1$-clique: $\mathcal{P}_{\text {grow }}(K \rightarrow K+1)=\frac{(K+1) \bar{Y}_{K+1}}{\bar{Y}_{K}} \rightarrow 0$ if $K=(1+\epsilon) \log _{2}(N)$

Any polinomial algorithm stops at $K=\log _{2}(N)$

## The Jerrum Metropolis MC

- Start from $x_{i}=0 \quad \forall i$
- At each time $n$ choose $i$ u.a.r. and flip $x_{i}$ with probabilities:

$$
\begin{gathered}
P_{\text {Jerrum }}\left(x_{i}^{n}=0 \rightarrow x_{i}^{n+1}=1\right)= \begin{cases}0 & \text { if } \exists j: x_{j}^{n}=1 \text { and } A_{i j}=0 \\
1 & \text { otherwise }\end{cases} \\
P_{\text {Jerrum }}\left(x_{i}^{n}=1 \rightarrow x_{i}^{n+1}=0\right)=\lambda^{-1}, \quad \lambda \geq 1
\end{gathered}
$$

## The Jerrum Metropolis MC

- Start from $x_{i}=0 \quad \forall i$
- At each time $n$ choose $i$ u.a.r. and flip $x_{i}$ with probabilities:

$$
\begin{gathered}
P_{\text {Jerrum }}\left(x_{i}^{n}=0 \rightarrow x_{i}^{n+1}=1\right)= \begin{cases}0 & \text { if } \exists j: x_{j}^{n}=1 \text { and } A_{i j}=0 \\
1 & \text { otherwise }\end{cases} \\
P_{\text {Jerrum }}\left(x_{i}^{n}=1 \rightarrow x_{i}^{n+1}=0\right)=\lambda^{-1}, \quad \lambda \geq 1
\end{gathered}
$$

State space: collection $\Omega$ of cliques $\mathcal{C}$ of any size in $G$. Stationary distribution on $\Omega$ : $\pi(\mathcal{C})=\frac{w(\mathcal{C})}{\sum_{\mathcal{C} \in \Omega} w(\mathcal{C})}$ $w(\mathcal{C})=\lambda^{|\mathcal{C}|}$ : weight asssigned to each clique $\mathcal{C} \in \Omega$

## The Jerrum Metropolis MC

- Start from $x_{i}=0 \quad \forall i$
- At each time $n$ choose $i$ u.a.r. and flip $x_{i}$ with probabilities:

$$
\begin{gathered}
P_{\text {Jerrum }}\left(x_{i}^{n}=0 \rightarrow x_{i}^{n+1}=1\right)= \begin{cases}0 & \text { if } \exists j: x_{j}^{n}=1 \text { and } A_{i j}=0 \\
1 & \text { otherwise }\end{cases} \\
P_{\text {Jerrum }}\left(x_{i}^{n}=1 \rightarrow x_{i}^{n+1}=0\right)=\lambda^{-1}, \quad \lambda \geq 1
\end{gathered}
$$

State space: collection $\Omega$ of cliques $\mathcal{C}$ of any size in $G$.
Stationary distribution on $\Omega: \pi(\mathcal{C})=\frac{w(\mathcal{C})}{\sum_{\mathcal{C} \in \Omega} w(\mathcal{C})}$ $w(\mathcal{C})=\lambda^{|\mathcal{C}|}$ : weight asssigned to each clique $\mathcal{C} \in \Omega$

## Theorem (Jerrum '92)

Suppose $\epsilon>0$. For a.e. $G \in \mathcal{G}\left(N, \frac{1}{2}\right)$ and every $\lambda \geq 1$, the expected time for MC to reach a clique of size at least $(1+\epsilon) \log N$ exceeds $N^{\Omega(\log N)}$

## The Planted Clique Problem

## Max-Clique Problem

Given $G \in \mathcal{G}(N, 1 / 2)$, select u.a.r. a subset $\mathcal{C}$ of size $|\mathcal{C}| \equiv K$.
Add to $G$ all the edges between two nodes in $\mathcal{C}$.
(These operations define the new ensemble $\mathcal{G}(N, 1 / 2, K)$ )
Try to find $\mathcal{C}$.

## The Planted Clique Problem

## Max-Clique Problem

Given $G \in \mathcal{G}(N, 1 / 2)$, select u.a.r. a subset $\mathcal{C}$ of size $|\mathcal{C}| \equiv K$. Add to $G$ all the edges between two nodes in $\mathcal{C}$. (These operations define the new ensemble $\mathcal{G}(N, 1 / 2, K)$ ) Try to find $\mathcal{C}$.

## Possible for $K>2 \log _{2} N$

BUT many known algorithms are proved to fail in the regime

$$
K / \sqrt{N} \rightarrow 0:
$$

- Spectral algorithms Alon et al., Random Structures \& Algorithms (1998)
- Message Passing Deshpande, Montanari, Found. of Comp. Math. (2015)
- Sum of Squares Barak, SIAM Journal on Computing (2019)



## The Jerrum MC for the planted clique problem

Same algorithm as in the random case

## Theorem (Jerrum '92)

Suppose $\epsilon>0$ and $0<\beta<\frac{1}{2}$. For a.e. $G \in \mathcal{G}\left(N, \frac{1}{2},\left\lceil N^{\beta}\right\rceil\right)$ and every $\lambda \geq 1$ the expected time for the MC process to reach a clique of size at least $(1+\epsilon) \log N$ exceeds $N^{\Omega(\log N)}$

But is the MC linear (polynomial) for $\beta \geq \frac{1}{2}$ ?

## A different Metropolis MC for the planted clique

Gamarnik, Zadik, arXiv:1904.07174 (2019)
$x_{i}=\{0,1\}$, Fixed global magnetization $m=\sum_{i=1}^{N} x_{i} \equiv K$.

## A different Metropolis MC for the planted clique

Gamarnik, Zadik, arXiv:1904.07174 (2019)
$x_{i}=\{0,1\}$, Fixed global magnetization $m=\sum_{i=1}^{N} x_{i} \equiv K$.

- Choose $K$ nodes $x_{k_{i}}, i \in[1, K]$ u.a.r. and set $x_{k_{i}}^{0}=1, x_{j \neq k_{i}}^{0}=0$


## A different Metropolis MC for the planted clique

Gamarnik, Zadik, arXiv:1904.07174 (2019)
$x_{i}=\{0,1\}$, Fixed global magnetization $m=\sum_{i=1}^{N} x_{i} \equiv K$.

- Choose $K$ nodes $x_{k_{i}}, i \in[1, K]$ u.a.r. and set $x_{k_{j}}^{0}=1, x_{j \neq k_{i}}^{0}=0$
- Assign unitary cost for couples of unconnected nodes in the putative clique: $E=\sum_{i j}\left(1-A_{i j}\right) x_{i} x_{j}$


## A different Metropolis MC for the planted clique

Gamarnik, Zadik, arXiv:1904.07174 (2019)
$x_{i}=\{0,1\}$, Fixed global magnetization $m=\sum_{i=1}^{N} x_{i} \equiv K$.

- Choose $K$ nodes $x_{k_{i}}, i \in[1, K]$ u.a.r. and set $x_{k_{j}}^{0}=1, x_{j \neq k_{i}}^{0}=0$
- Assign unitary cost for couples of unconnected nodes in the putative clique: $E=\sum_{i j}\left(1-A_{i j}\right) x_{i} x_{j}$
- Update nodes with Metropolis probabilities:

$$
P\left(\left(x_{a}^{n}, x_{b}^{n}\right)=(1,0) \rightarrow\left(x_{a}^{n+1}, x_{b}^{n+1}\right)=(0,1)\right)=\min \left(1, e^{-\beta \Delta E}\right)
$$

## A different Metropolis MC for the planted clique

Gamarnik, Zadik, arXiv:1904.07174 (2019)
$x_{i}=\{0,1\}$, Fixed global magnetization $m=\sum_{i=1}^{N} x_{i} \equiv K$.

- Choose $K$ nodes $x_{k_{i}}, i \in[1, K]$ u.a.r. and set $x_{k_{j}}^{0}=1, x_{j \neq k_{i}}^{0}=0$
- Assign unitary cost for couples of unconnected nodes in the putative clique: $E=\sum_{i j}\left(1-A_{i j}\right) x_{i} x_{j}$
- Update nodes with Metropolis probabilities:

$$
P\left(\left(x_{a}^{n}, x_{b}^{n}\right)=(1,0) \rightarrow\left(x_{a}^{n+1}, x_{b}^{n+1}\right)=(0,1)\right)=\min \left(1, e^{-\beta \Delta E}\right)
$$

Exponential-in- $K$ time for $K \leq N^{2 / 3}$

## A different Metropolis MC for the planted clique

Gamarnik, Zadik, arXiv:1904.07174 (2019)
$x_{i}=\{0,1\}$, Fixed global magnetization $m=\sum_{i=1}^{N} x_{i} \equiv K$.

- Choose $K$ nodes $x_{k_{i}}, i \in[1, K]$ u.a.r. and set $x_{k_{j}}^{0}=1, x_{j \neq k_{i}}^{0}=0$
- Assign unitary cost for couples of unconnected nodes in the putative clique: $E=\sum_{i j}\left(1-A_{i j}\right) x_{i} x_{j}$
- Update nodes with Metropolis probabilities:

$$
P\left(\left(x_{a}^{n}, x_{b}^{n}\right)=(1,0) \rightarrow\left(x_{a}^{n+1}, x_{b}^{n+1}\right)=(0,1)\right)=\min \left(1, e^{-\beta \Delta E}\right)
$$

Exponential-in- $K$ time for $K \leq N^{2 / 3}$


It becomes polynomial down to
$K=\sqrt{N}$, working with a
mismatched fixed magnetization
$\bar{K}>K$.

## Two questions:

MCA, deFeo, Fachin, arXiv:2106.05720

- Is the Jerrum algorithm suboptimal? (super-polynomial for $K \leq N^{\beta}$ with $\left.\beta>1 / 2\right)$
- If yes, can we introduce a mismatched parameter to enhance its performances?


## Numerical simulation of Jerrum algorithm



$$
t_{50}(K)=\frac{a_{N}}{\left(K-K_{\min }\right)^{\nu}}
$$

## Numerical simulation of Jerrum algorithm



$$
t_{50}(K)=\frac{a_{N}}{\left(K-K_{\text {min }}\right)^{\nu}}
$$



$$
\begin{gathered}
K_{\min }(N)=b N^{\alpha} \\
\alpha=0.91
\end{gathered}
$$

## Two questions:

- Is the Jerrum algorithm suboptimal? (super-polynomial for $K \leq N^{\alpha}$ with $\left.\alpha>1 / 2\right)$

Yes, it seems to be suboptimal, $\alpha \simeq 0.91$

## Two questions:

- Is the Jerrum algorithm suboptimal? (super-polynomial for $K \leq N^{\alpha}$ with $\left.\alpha>1 / 2\right)$

Yes, it seems to be suboptimal, $\alpha \simeq 0.91$

- If yes, can we introduce a mismatched parameter to enhance its performances?

To answer this question we introduce a slightly different MC

## BayesMC

$$
\text { Posterior: } P(x \mid A)=\frac{P(A \mid x) P(x)}{P(A)}
$$

## BayesMC

$$
\text { Posterior: } P(x \mid A)=\frac{P(A \mid x) P(x)}{P(A)}
$$

Likelihood: $p\left(A_{i j}=1 \mid\{x\}\right)=\left\{\begin{array}{ll}1 & \text { if } x_{i} x_{j}=1 \\ \frac{1}{2} & \text { otherwise }\end{array}\right.$.
Prior: $P(x)=\left(\frac{K}{N}\right)^{x}\left(1-\frac{K}{N}\right)^{1-x}$ (local instead of global constraint)

## BayesMC

$$
\text { Posterior: } P(x \mid A)=\frac{P(A \mid x) P(x)}{P(A)}
$$

$$
\text { Likelihood: } p\left(A_{i j}=1 \mid\{x\}\right)= \begin{cases}1 & \text { if } x_{i} x_{j}=1 \\ \frac{1}{2} & \text { otherwise }\end{cases}
$$

Prior: $P(x)=\left(\frac{K}{N}\right)^{x}\left(1-\frac{K}{N}\right)^{1-x}$ (local instead of global constraint)
As statistical physicists, we love Gibbs-Boltzmann weights:

$$
P_{\beta}(\{x\} \mid\{A\}) \equiv P^{\beta}(\{x\} \mid\{A\}) \equiv \frac{1}{\mathcal{N}} e^{-\beta H(\{x\})}, \quad \beta_{\text {Bayes }}=1
$$

introducing the Hamiltonian:

$$
H(\{x\})=-\sum_{i} \log \left(P\left(x_{i}\right)\right)+-\sum_{i j}\left[\left(1-A_{i j}\right) \log \frac{\left(1-x_{i} x_{j}\right)}{2}+A_{i j} \log \frac{\left(1+x_{i} x_{j}\right)}{2}\right] .
$$

## BayesMC

## Metropolis algorithm:

$$
\begin{aligned}
& P\left(x_{i}^{n}=0 \rightarrow x_{i}^{n+1}=1\right)=\left\{\begin{array}{l}
0 \quad \text { if } \exists j: x_{j}^{n}=1 \text { and } A_{i j}=0 \\
\min \left(e^{-\beta \Delta E}, 1\right)=\min \left(e^{-\beta\left[\log \left(1-\frac{K}{N}\right)-\log \left(\frac{K}{N}\right)+m \log \left(\frac{1}{2}\right)\right]}, 1\right) \text { o.w. }
\end{array}\right. \\
& P\left(x_{i}^{n}=1 \rightarrow x_{i}^{n+1}=0\right)=\min \left(e^{\beta \Delta E}, 1\right)
\end{aligned}
$$

## BayesMC

Metropolis algorithm:
$P\left(x_{i}^{n}=0 \rightarrow x_{i}^{n+1}=1\right)=\left\{\begin{array}{l}0 \quad \text { if } \exists j: x_{j}^{n}=1 \text { and } A_{i j}=0 \\ \min \left(e^{-\beta \Delta E}, 1\right)=\min \left(e^{-\beta\left[\log \left(1-\frac{K}{N}\right)-\log \left(\frac{K}{N}\right)+m \log \left(\frac{1}{2}\right)\right]}, 1\right) \text { o.w. }\end{array}\right.$
$P\left(x_{i}^{n}=1 \rightarrow x_{i}^{n+1}=0\right)=\min \left(e^{\beta \Delta E}, 1\right)$
Same class as Jerrum algorithm
Working only on perfect-clique configurations of different sizes $m$.

## BayesMC

## Metropolis algorithm:

$P\left(x_{i}^{n}=0 \rightarrow x_{i}^{n+1}=1\right)=\left\{\begin{array}{l}0 \quad \text { if } \exists j: x_{j}^{n}=1 \text { and } A_{i j}=0 \\ \min \left(e^{-\beta \Delta E}, 1\right)=\min \left(e^{-\beta\left[\log \left(1-\frac{K}{N}\right)-\log \left(\frac{K}{N}\right)+m \log \left(\frac{1}{2}\right)\right]}, 1\right) \text { o.w. }\end{array}\right.$
$P\left(x_{i}^{n}=1 \rightarrow x_{i}^{n+1}=0\right)=\min \left(e^{\beta \Delta E}, 1\right)$
Same class as Jerrum algorithm
Working only on perfect-clique configurations of different sizes $m$.


$-\beta=1 \mathrm{~K}=30$
$-\beta=1 \mathrm{~K}=50$
$-\beta=0.5 \mathrm{~K}=30$

- Jerrum
$P\left(x_{i}^{n}=0 \rightarrow x_{i}^{n+1}=1\right)$
$P\left(x_{i}^{n}=1 \rightarrow x_{i}^{n+1}=0\right)$
$N=2000$


## Finding the optimal $\beta$


$N=2000$
( $\beta=1$ : the planted clique is not recovered in $t \leq 10^{7}$ )

## Finding the optimal $\beta$


$N=2000, K=50$

## Finding the MC threshold



## Finding the MC threshold



## Answers to the two questions:

MCA, deFeo, Fachin, arXiv:2106.05720

- Is the Jerrum algorithm suboptimal? (super-polynomial for $K \leq N^{\alpha}$ with $\alpha>1 / 2$ )

Yes, it seems to be suboptimal, $\alpha \simeq 0.91$

## Answers to the two questions:

MCA, deFeo, Fachin, arXiv:2106.05720

- Is the Jerrum algorithm suboptimal? (super-polynomial for $K \leq N^{\alpha}$ with $\left.\alpha>1 / 2\right)$

Yes, it seems to be suboptimal, $\alpha \simeq 0.91$

- If yes, can we introduce a mismatched parameter to enhance its performances?

Yes, we introduce a "temperature". MC seems to reach the threshold for linear algorithms $K=\sqrt{\frac{N}{e}}$ at "mismatched" temperature $T>1$.

## Conclusions, comments, perspectives

- We look forward for mathematical proofs of our numerical findings


## Conclusions, comments, perspectives

- We look forward for mathematical proofs of our numerical findings
- What is the reason for the failure of standard MC? Glassy states/RSB?


## Conclusions, comments, perspectives

- We look forward for mathematical proofs of our numerical findings
- What is the reason for the failure of standard MC? Glassy states/RSB?
- Parallel Tempering ( $n$ exchangeable replicas at different temperatures) works extremingly well for Planted Clique, why?



## Conclusions, comments, perspectives

- We look forward for mathematical proofs of our numerical findings
- What is the reason for the failure of standard MC? Glassy states/RSB?
- Parallel Tempering ( $n$ exchangeable replicas at different temperatures) works extremingly well for Planted Clique, why?

- Overparametrization is essential in Deep NN. Simple cases can be useful in understanding complex ones.

