

Perfect sampling from spatial mixing

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Joint work with

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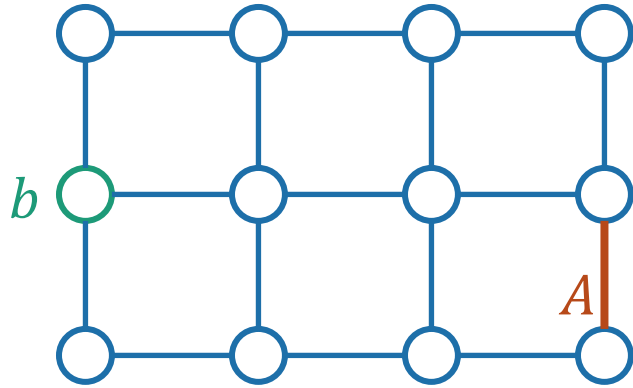
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Spin systems and Gibbs distributions

finite graph $G = (V, E)$



Parameters

vertex: random variable in $[q] = \{0, 1, \dots, q - 1\}$

external field: vector $b \in \mathbb{R}_{\geq 0}^q$ in each vertex

interaction: symmetric matrix $A \in \mathbb{R}_{\geq 0}^{q \times q}$ on each edge

$$\forall \sigma \in [q]^V,$$



configuration

$$\mu(\sigma) \propto \prod_{v \in V} b(\sigma_v) \prod_{e = \{u, v\} \in E} A(\sigma_u, \sigma_v)$$

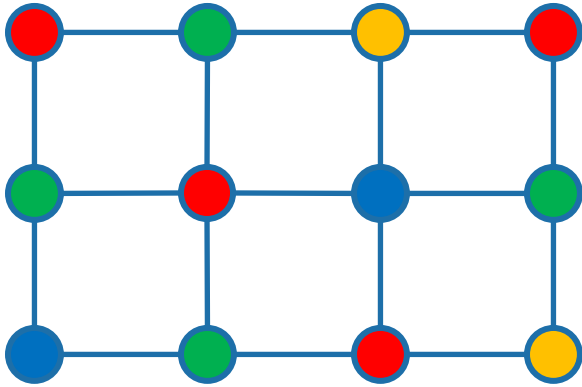


Gibbs distribution



weight $w(\sigma)$

Example: graph coloring



proper q -colouring in graph $G = (V, E)$

- Each vertex $v \in V$ take a colour $\sigma_v \in [q]$
- Each edge $\{u, v\} \in E$ is **not monochromatic**
 $\sigma_u \neq \sigma_v$

$$b = \begin{bmatrix} 1 \\ \vdots \\ 1 \end{bmatrix}$$

$$A = \begin{bmatrix} 0 & \cdots & 1 \\ \vdots & 0 & \vdots \\ 1 & \cdots & 0 \end{bmatrix}$$

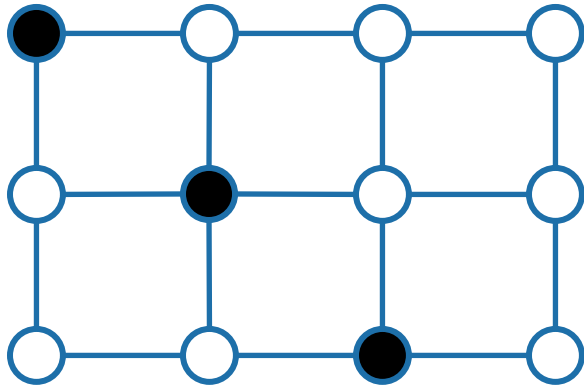
$$\mu(\sigma) \propto \begin{cases} 1 & \text{if } \sigma \text{ is a proper colouring} \\ 0 & \text{otherwise} \end{cases}$$

constant
vector

$$A(i, i) = 0 \\ A(i, j) = 1$$

uniform distribution over
all proper q -colourings in G

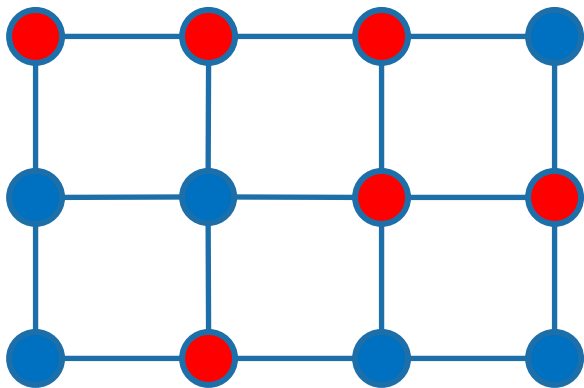
Examples: hardcore model and Ising model



Hardcore model in G with parameter $\lambda > 0$

$\forall \sigma \in \{0,1\}^V$ s.t. $S_\sigma = \{v \in V \mid \sigma_v = 1\}$ is an **independent set**

$$\mu(\sigma) \propto \lambda^{|S_\sigma|}$$



Ising model in G with parameter $\beta > 0$

$$\forall \sigma \in \{0,1\}^V, \mu(\sigma) \propto \beta^{m(\sigma)}$$

$m(\sigma) = |\{\{u, v\} \in E \mid \sigma_u = \sigma_v\}|$ is **#monochromatic edges**

Sampling problem for spin systems

Input: ① a graph $G = (V, E)$, vector $b \in \mathbb{R}_{\geq 0}^q$, symmetric matrix $A \in \mathbb{R}_{\geq 0}^{q \times q}$

specify **Gibbs distribution** $\mu(\sigma) \propto \prod_{v \in V} b(\sigma_v) \prod_{e = \{u, v\} \in E} A(\sigma_u, \sigma_v)$

② an error bound $\epsilon \geq 0$

Output: a **random sample** $X \in [q]^V$ such that

$$d_{TV}(X, \mu) = \frac{1}{2} \sum_{\sigma \in [q]^V} |\Pr[X = \sigma] - \mu(\sigma)| \leq \epsilon$$

- **Approximate** sampling problem: return random samples with **bounded error** $\epsilon > 0$ ($\epsilon = \frac{1}{\text{poly}(n)}$)
- **Perfect** sampling problem: return random samples **without error** $\epsilon = 0$

Sampling problem for spin systems

Input: ① a *sub-exp growth graph* $G = (V, E)$, vector $b \in \mathbb{R}_{\geq 0}^q$, symmetric matrix $A \in \mathbb{R}_{\geq 0}^{q \times q}$

specify **Gibbs distribution** $\mu(\sigma) \propto \prod_{v \in V} b(\sigma_v) \prod_{e = \{u, v\} \in E} A(\sigma_u, \sigma_v)$

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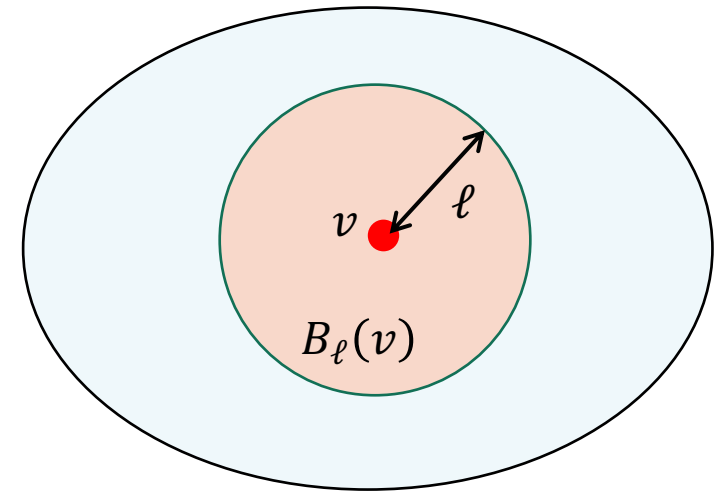
Sub-exp growth graph

A family of graphs \mathcal{G} has sub-exp growth if

\exists a **sub-exp** function $s: \mathbb{N} \rightarrow \mathbb{N}$ s.t. $\forall G = (V, E) \in \mathcal{G}$,

$$\forall v \in V, \ell \in \mathbb{N}, |B_\ell(v)| \leq \mathbf{s}(\ell) = \mathbf{exp}(\mathbf{o}(\ell))$$

$B_\ell(v) = \{u \in V \mid \text{dist}_G(v, u) \leq \ell\}$ **ball** of radius ℓ centred at v



Sampling problem for spin systems

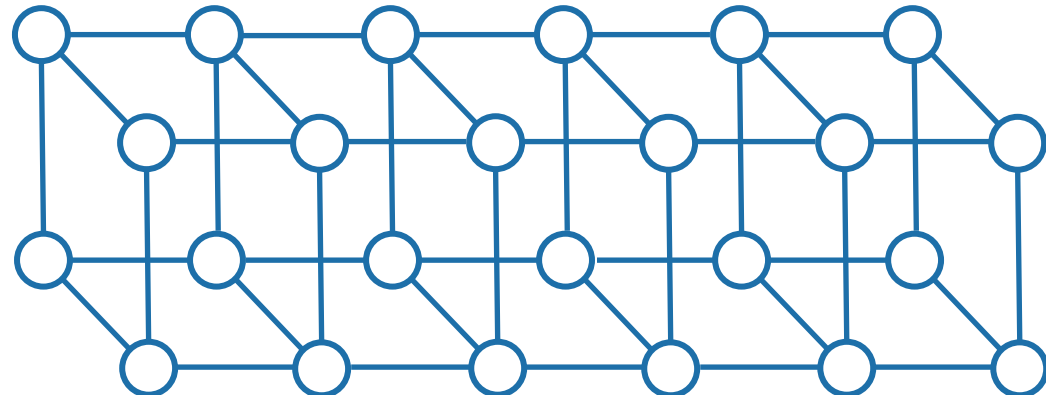
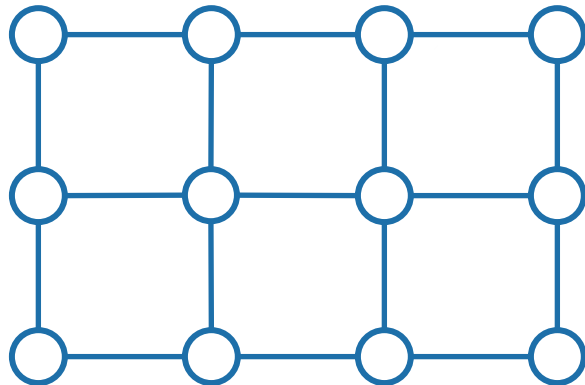
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Example: let $d \in \mathbb{N}$, any **finite sub-graph** $G = (V, E)$ of \mathbb{Z}^d has sub-exp growth

$$\forall v \in V, \ell \in \mathbb{N}, \quad |B_\ell(v)| \leq (2\ell + 1)^d = \text{poly}(\ell) = \exp(o(\ell))$$



Sampling problem for spin systems

Input: ① a *sub-exp growth* graph $G = (V, E)$, vector $b \in \mathbb{R}_{\geq 0}^q$, symmetric matrix $A \in \mathbb{R}_{\geq 0}^{q \times q}$

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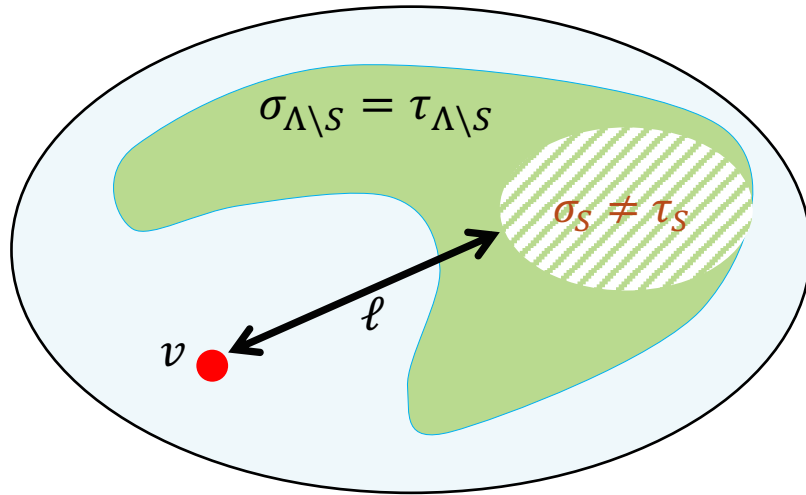
Question:

μ satisfies
??? condition



poly-time sampling
algorithm exists

Previous work: Strong spatial mixing v.s. approximate sampling



- Partial configurations $\sigma, \tau \in [q]^\Lambda$ on $\Lambda \subseteq V$
 $S = \{w \in \Lambda \mid \sigma_w \neq \tau_w\}$
- Vertex $v \in V$ with distance to **disagreement**
 $\ell = \min\{\text{dist}_G(v, w) \mid w \in S\}$
- Strong Spatial Mixing (**SSM**)

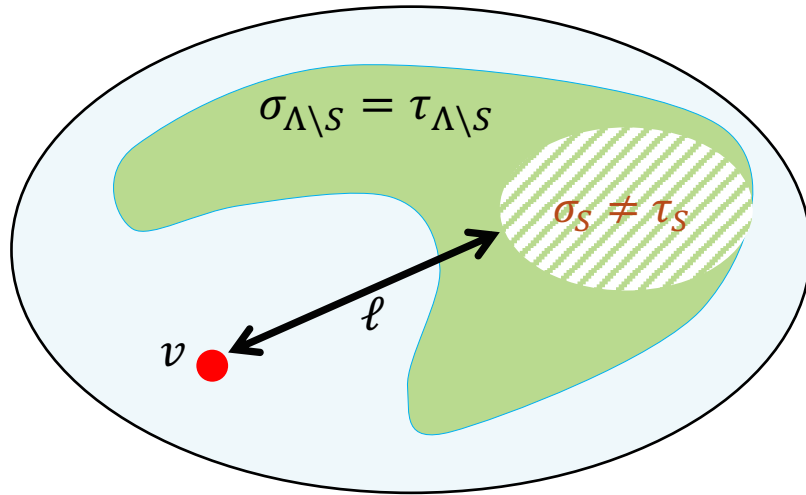
$$d_{TV}(\mu_v^\sigma, \mu_v^\tau) \leq \alpha \exp(-\beta \ell)$$

TV distance
 Influence on v

marginals on v
 conditional on σ or τ

exponential decay
 $\alpha, \beta = \Theta(1)$

Previous work: Strong spatial mixing v.s. approximate sampling

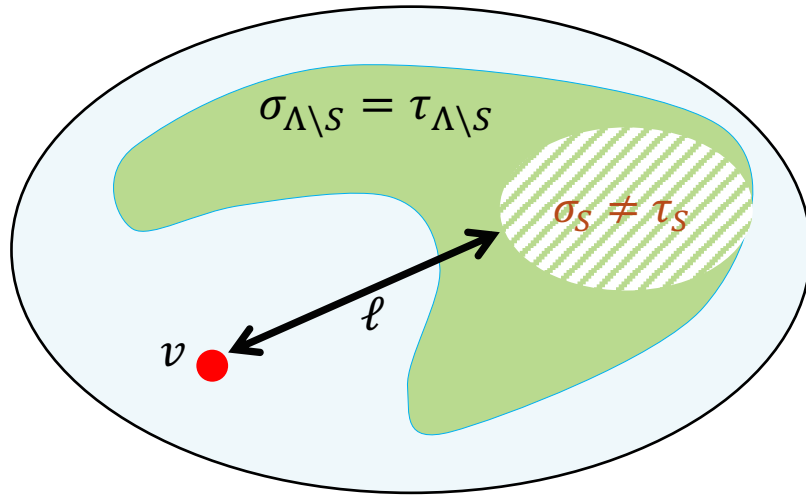


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Some sufficient conditions for SSM on graph G with max degree Δ

- q -colouring: ($q > 2\Delta$) or (triangle-free and $q > 1.763\Delta$)
- hardcore: $\lambda < \lambda_c(\Delta) = \frac{(\Delta-1)^{(\Delta-1)}}{(\Delta-2)^\Delta} \approx \frac{e}{\Delta}$
- Ising model: $\frac{\Delta-2}{\Delta} < \beta < \frac{\Delta}{\Delta-2}$

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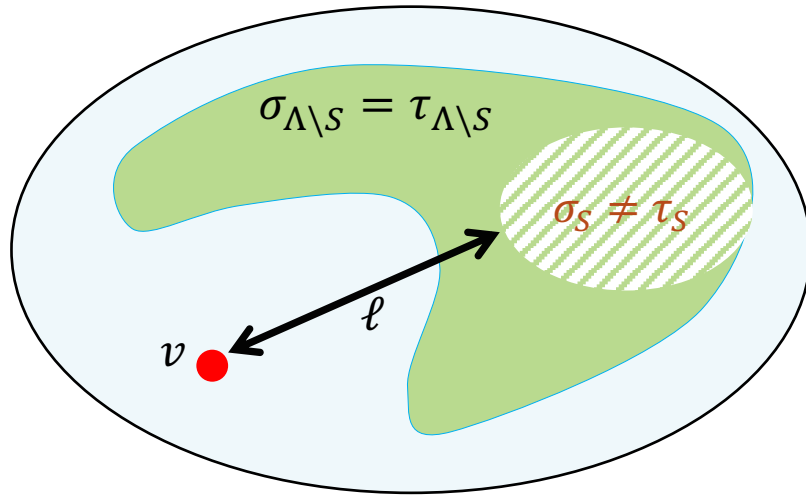
Theorem [Dyer, Sinclair, Vigoda and Weitz 2004]

SSM

sub-exp growth

near-linear time
approximate sampler

Previous work: Strong spatial mixing v.s. approximate sampling



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Theorem [Dyer, Sinclair, Vigoda and Weitz 2004]

SSM

sub-exp growth

Markov chain
optimal mixing

Our results



Main result [This work]

Constants $q \in \mathbb{N}$, $b \in \mathbb{R}_{\geq 0}^q$ and $A \in \mathbb{R}_{\geq 0}^{q \times q}$. There exists an algorithm such that

- given any graph $G = (V, E)$ with **sub-exp growth**
- output a **perfect sample** from Gibbs distribution μ in time $O(n)$, $n = |V|$

Remark: the linear running time $C \cdot n$ of the algorithm

the **constant** $C = C(q, b, A, s)$ depends on

- number of spins q , external vector b and interaction matrix A
- parameters in sub-exp function $s: \mathbb{N} \rightarrow \mathbb{N}$ (recall $|B_\ell(v)| \leq s(\ell) = \exp(o(\ell))$)

C does **not** depend on n

Our results



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- given any graph $G = (V, E)$ with **sub-exp growth**
- output a **perfect sample** from Gibbs distribution μ in time $O(n)$, $n = |V|$

Remark: the linear running time $C \cdot n$ of the algorithm

Example: if $G = (V, E)$ is a **finite subgraph of \mathbb{Z}^d** , then the constant

$$C = C(q, A, b, d)$$

Applications for spin systems

Model	Graph	Parameters
q -colouring	sub-exp growth	$q > 2\Delta$
q -colouring	sub-exp growth triangle-free	$q > 1.763\Delta$
hardcore	sub-exp growth	$\lambda < \lambda_c(\Delta) \approx \frac{e}{\Delta}$
Ising	sub-exp growth	$1 - \frac{2}{\Delta} < \beta < 1 + \frac{2}{\Delta}$

Our algorithm also works for **general graphs**, but with a **stronger SSM condition**

Example: q -colouring on general graphs

- our condition: $q \geq \Delta^2 - \Delta + 2$
- state-of-the-art: $q = \Omega(\Delta)$ [Jain, Sah, Sawhney, 2021] [Liu, Sinclair, Srivastava, 2019]

Other techniques & our technical contribution

Techniques	Graph	#Colours	Running time
Reduction to deterministic approximate counting [JVV86,LSS19]	general	$q > 2\Delta$	$n^{\text{poly}(\Delta)}$

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The Depth-First-Sampling algorithm could recover our main result



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same principle

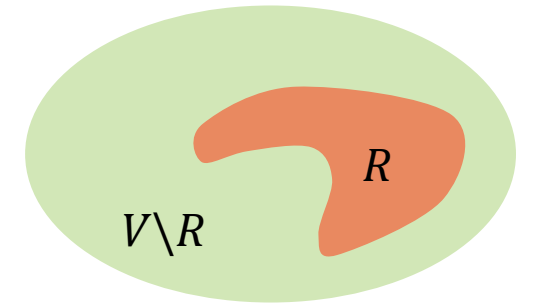
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MCMC approximate sampler [Chen, Delcourt, Moitra, Perarnau, 2019]	general	$q \geq \left(\frac{11}{6} - \epsilon_0\right)\Delta, \epsilon_0 \geq 10^{-5}$	$\tilde{O}_{q,\Delta}(n)$

Open problem: close the *gap* between perfect sampling and approximate sampling

The perfect sampling algorithm

Maintains a random pair (X, R) , where $X \in [q]^V$ and $R \subseteq V$ s.t.
 (X, R) satisfies the **conditional Gibbs property**



Conditional Gibbs property [Huber, Fill, 2000; Guo, Jerrum, Liu, 2017; Feng, Vishnoi, Yin 2019]

For any $\Lambda \subseteq V$, any $\sigma \in [q]^\Lambda$, conditional on $R = \Lambda$ and $X_R = \sigma$, $X_{V \setminus R} \sim \mu_{V \setminus R}^\sigma$:

$$\forall \tau \in [q]^{V \setminus R}, \Pr_{(X,R)} [X_{V \setminus R} = \tau \mid R = \Lambda \wedge X_R = \sigma] = \mu_{V \setminus R}^\sigma(\tau)$$

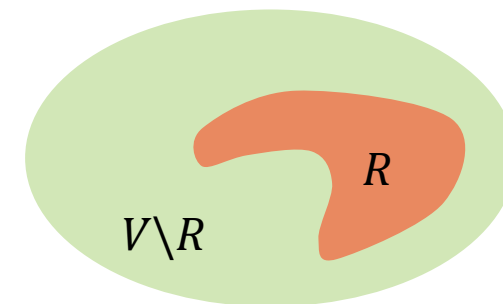
Remarks about Conditional Gibbs property

The distribution of (X_R, R) can be **arbitrary**, but $X_{V \setminus R}$ must follow $\mu_{V \setminus R}^{X_R}$ if (X_R, R) is given.

- R is the set of “**bad variables**” and $V \setminus R$ is the set of “**good variables**”
- In general, the distribution of (X, R) is **not unique**
- If $R = V$, then X is arbitrary; if $R = \emptyset$, then $X \sim \mu$

The perfect sampling algorithm

Maintains a random pair (X, R) , where $X \in [q]^V$ and $R \subseteq V$ s.t.
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$R = V$
arbitrary $X \in [q]^V$

modify the pair (X, R)
maintain *conditional Gibbs*
algorithm

$R = \emptyset$
 $X \sim \mu$

Warm-up: A simple case

Input: Gibbs distribution μ in $G = (V, E)$ (e.g., uniform distribution over q -colourings)
random pair (X, R) such that

- $R = \{u\}$ and $X_u = \text{Red}$
- $X_{V \setminus \{u\}} \sim \mu_{V \setminus \{u\}}(\cdot | u \text{ is Red})$

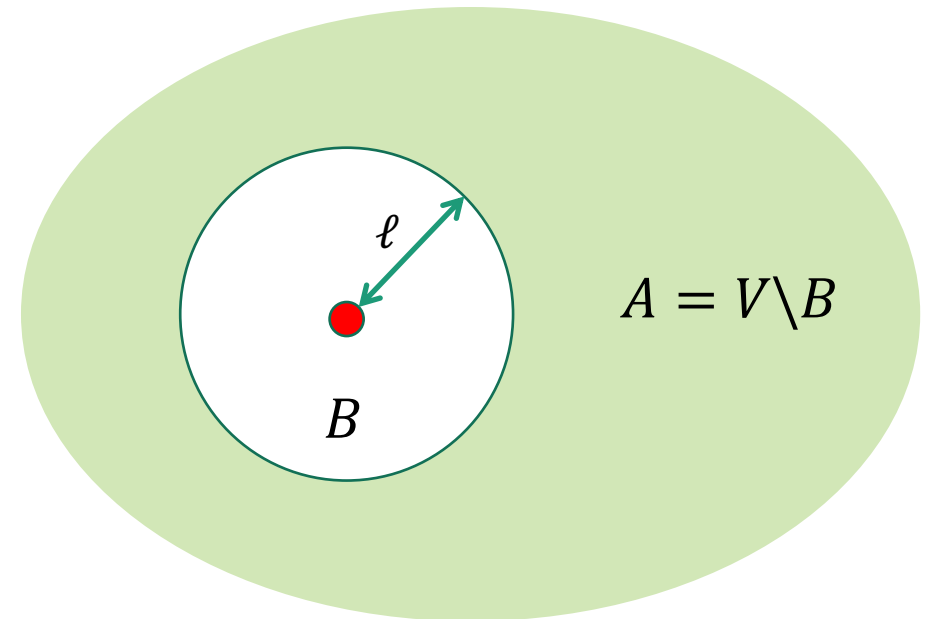
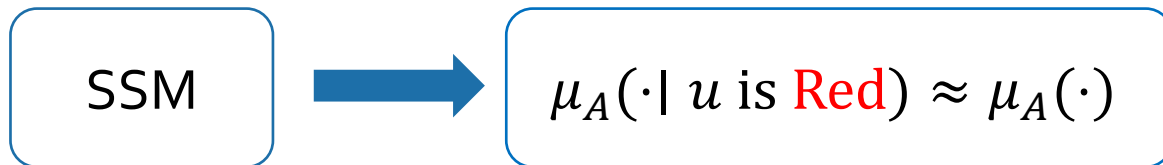
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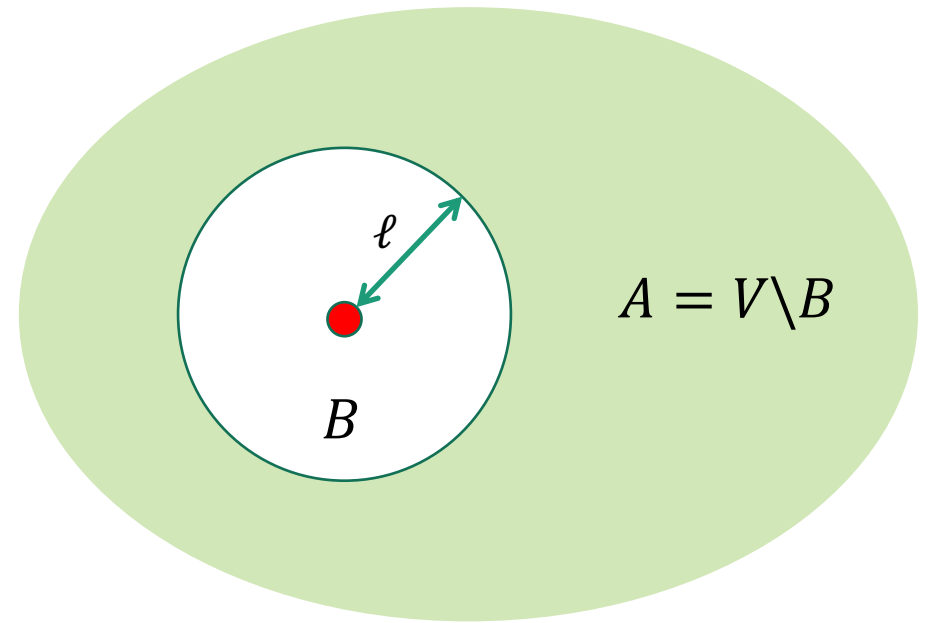
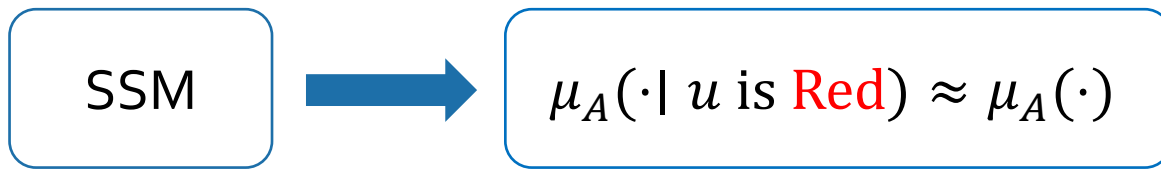
Idealised goal: modify such $(X, R = \{u\})$ so that $R = \emptyset$ and $X \sim \mu$

B : ℓ -ball centred at u , $\ell = O(1)$; $A = V \setminus B$

Input: $X_A \sim \mu_A(\cdot | u \text{ is Red})$

Idealised goal: $X_A \sim \mu_A(\cdot) = \sum_{c \in [q]} \mu_u(c) \mu_A(\cdot | u \text{ is } c)$





Idea: use a *filter* to transform the distribution

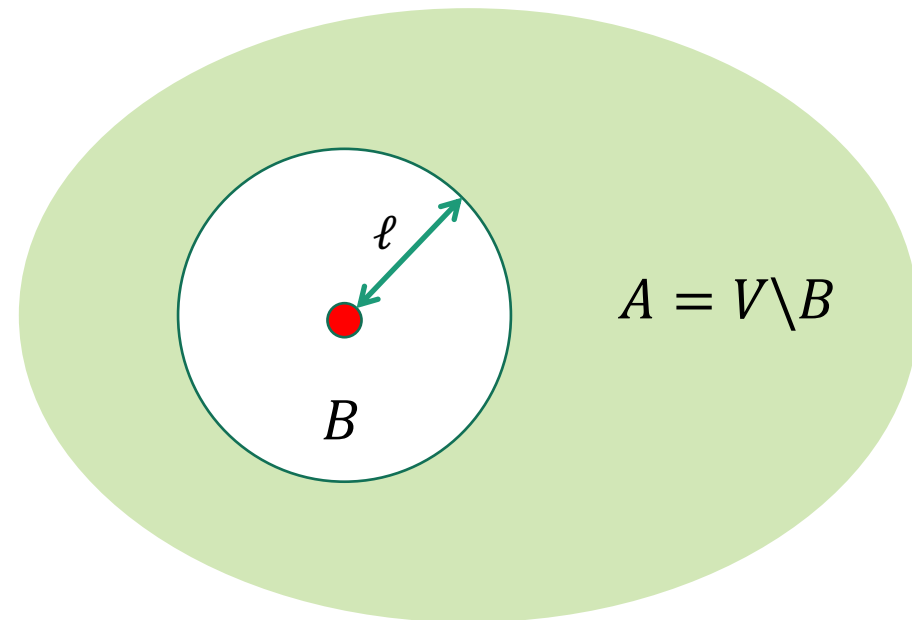
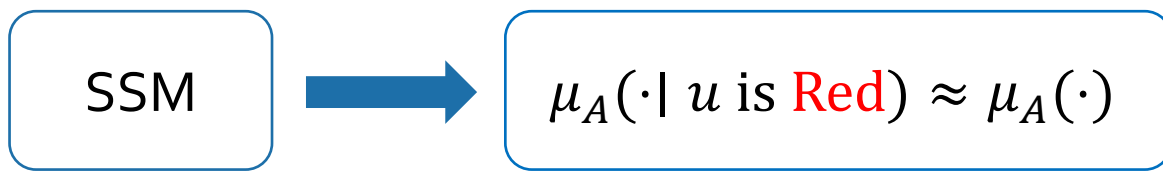
$$\forall \sigma \in [q]^A, \quad \Pr[X_A \text{ passes filter} \mid X_A = \sigma] \propto \frac{\mu_A(\sigma)}{\mu_A(\sigma \mid u \text{ is Red})}$$

\longleftarrow target distribution
 \longleftarrow input distribution

$$\Pr[X_A = \sigma \wedge X_A \text{ passes filter}] \propto \mu_A(\sigma \mid u \text{ is Red}) \cdot \frac{\mu_A(\sigma)}{\mu_A(\sigma \mid u \text{ is Red})} = \mu_A(\sigma)$$

\longrightarrow $\Pr[X_A = \sigma \mid X_A \text{ passes filter}] = \mu_A(\sigma)$

If X_A passes the filter, then $X_A \sim \mu_A$



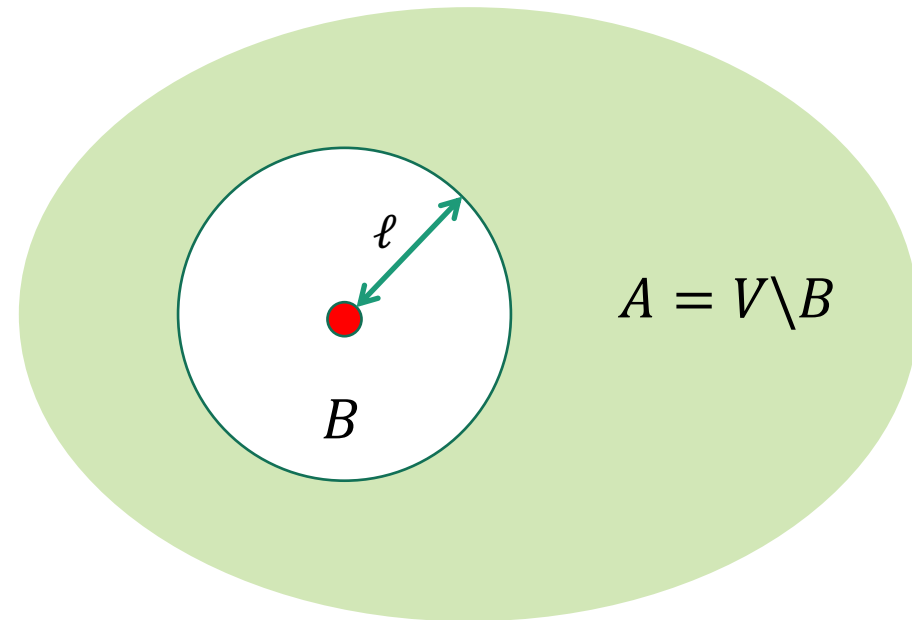
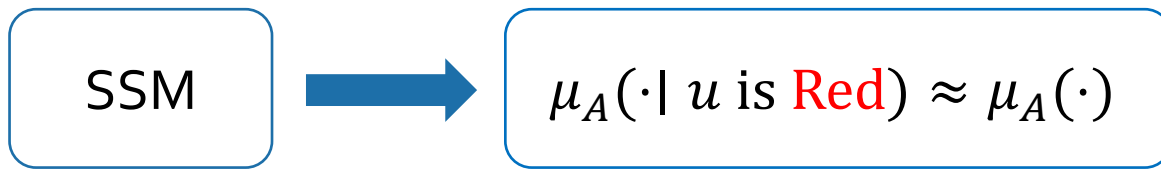
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\longleftarrow target distribution
 \longleftarrow input distribution

(by Bayes' Law) $\mu_A(\sigma \mid u \text{ is Red}) = \frac{\mu_A(u \text{ is Red} \mid A \leftarrow \sigma) \mu_A(\sigma)}{\mu_u(\text{Red})}$

the event $A \leftarrow \sigma$:
vertices in A are coloured as σ



Idea: use a *filter* to transform the distribution

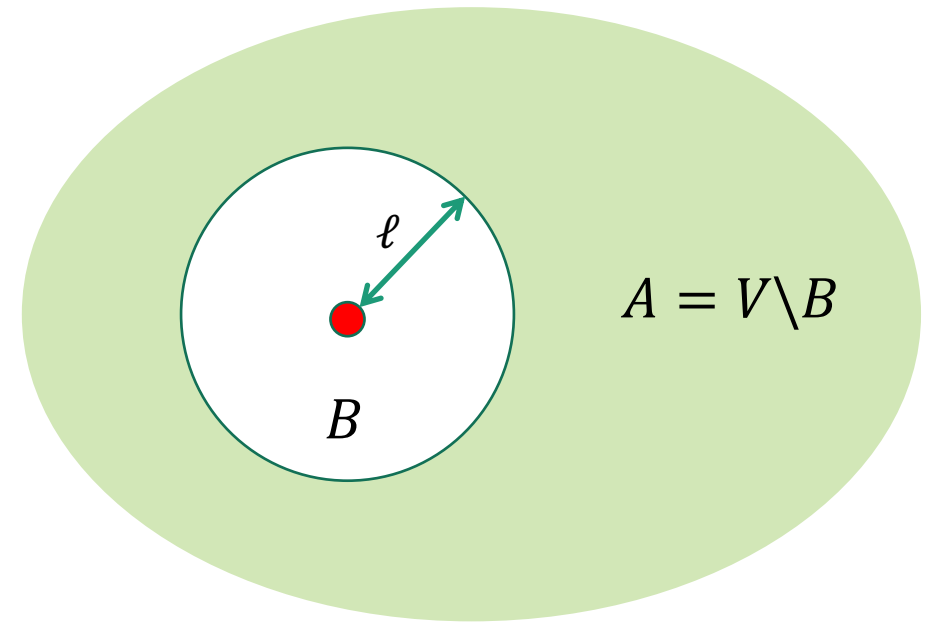
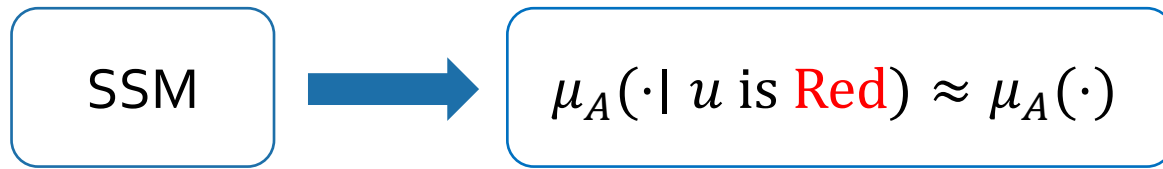
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(by Bayes' Law)

$$= \frac{\mu_A(\sigma) \mu_u(\text{Red})}{\mu_u(\text{Red} \mid A \leftarrow \sigma) \mu_A(\sigma)}$$

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Idea: use a *filter* to transform the distribution

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(by Bayes' Law)

$$= \frac{\mu_A(\sigma) \mu_u(\text{Red})}{\mu_u(\text{Red} \mid A \leftarrow \sigma) \mu_A(\sigma)} \quad \begin{array}{l} \text{the event } A \leftarrow \sigma: \\ \text{vertices in } A \text{ are coloured as } \sigma \end{array}$$

(cancel $\mu_A(\sigma)$)

$$= \frac{\mu_u(\text{Red})}{\mu_u(\text{Red} \mid A \leftarrow \sigma)} \propto \frac{1}{\mu_u(\text{Red} \mid A \leftarrow \sigma)}$$

($\mu_u(\text{Red})$ is independent with σ)

$$\forall \sigma \in [q]^A, \quad \Pr[X_A \text{ passes filter} \mid X_A = \sigma] \propto \frac{1}{\mu_u(\text{Red} \mid A \leftarrow \sigma)} = \frac{1}{\mu_u(\text{Red} \mid \partial B \leftarrow \sigma_{\partial B})}$$

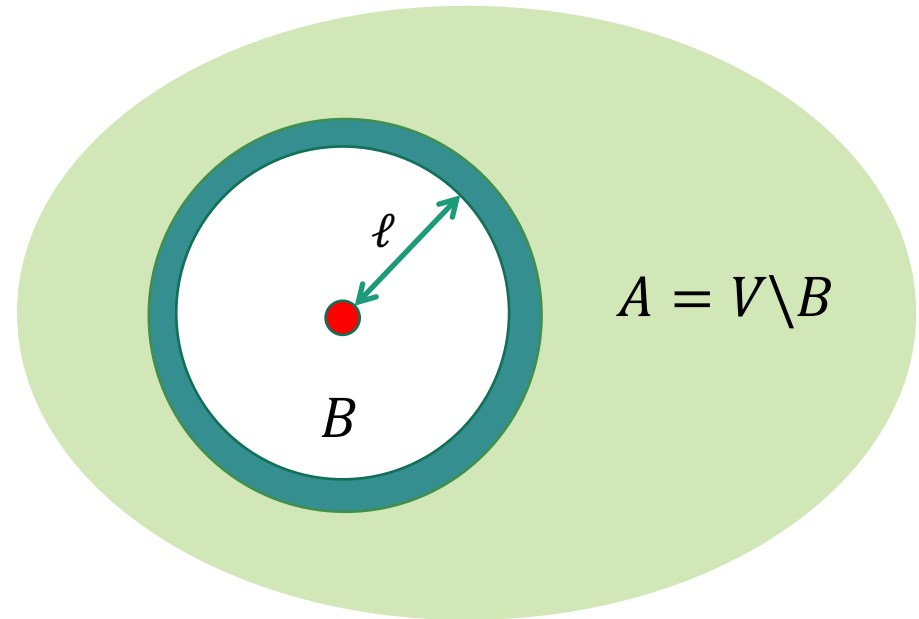
(by conditional independence)

$\partial B \subseteq A$ is the *outside boundary* of B

$$\partial B = \{w \notin B \mid \exists w' \in B \text{ st } \{w, w'\} \in E\}$$

∂B *separates* B and $A \setminus \partial B$ in graph G

 conditional independence



$$\forall \sigma \in [q]^A, \quad \Pr[X_A \text{ passes filter} \mid X_A = \sigma] \propto \frac{1}{\mu_u(\text{Red} \mid A \leftarrow \sigma)} = \frac{1}{\mu_u(\text{Red} \mid \partial B \leftarrow \sigma_{\partial B})}$$

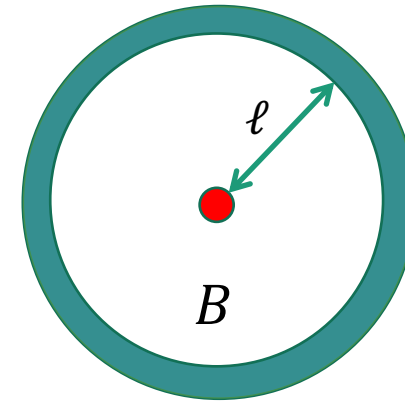
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∂B *separates* B and $A \setminus \partial B$ in graph G

 conditional independence



$$\ell = O(1)$$

$$|B| = O(1)$$

$$\forall \sigma \in [q]^A, \quad \Pr[X_A \text{ passes filter} \mid X_A = \sigma] = \frac{\min_{\tau \in [q]^{\partial B}} \mu_u(\text{Red} \mid \partial B \leftarrow \tau)}{\mu_u(\text{Red} \mid \partial B \leftarrow \sigma_{\partial B})} \leq 1$$

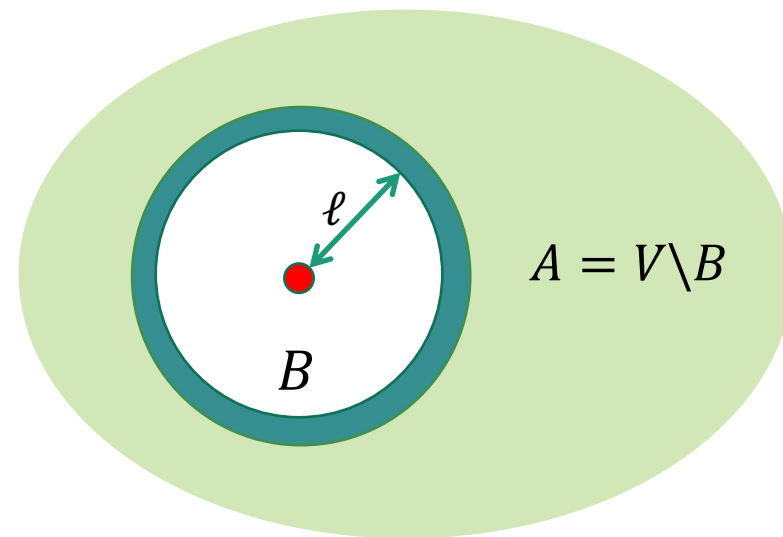
Bayes filter: simple case

- Reveal the configuration $X_{\partial B}$
- flip a coin such that

$$\Pr[\text{HEADS}] = \frac{\min_{\tau \in [q]^{\partial B}} \mu_u(\text{Red} \mid \partial B \leftarrow \tau)}{\mu_u(\text{Red} \mid \partial B \leftarrow X_{\partial B})}$$

- **If** the outcome is HEADS, **then**
 - resample $X_B \sim \mu_B(\cdot \mid X_{\partial B})$
 - **Return** the pair (X, \emptyset)
- **If** the outcome is not HEAD, **then**
 - **Return** the pair $(X, \underbrace{\{u\} \cup \partial B}_R)$

(Bayes filter)



(pass the Bayes filter, then $X_A \sim \mu_A$)

($X_B \sim \mu_B^{X_A} = \mu_B^{X_{\partial B}}$, then $X \sim \mu$)

(not pass the Bayes filter)

(Bayes filter only reveal $X_{\partial B}$, $R = \{u\} \cup \partial B$)

General case

arbitrary (X, R)
(conditional Gibbs)

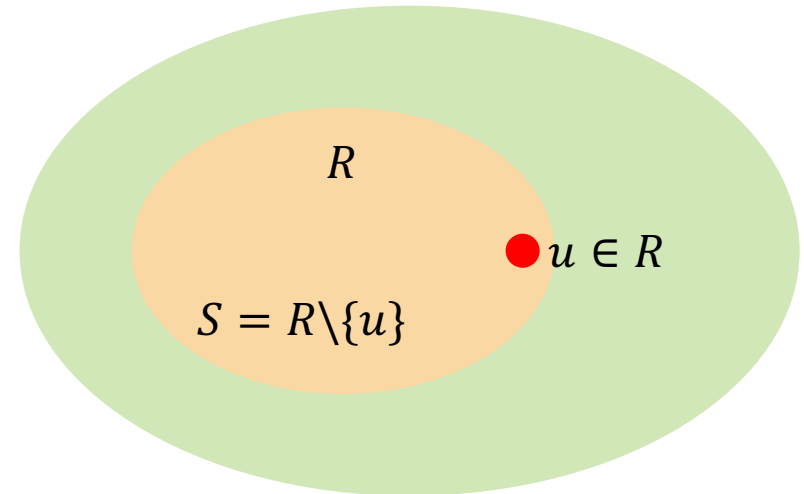
algorithm



new (X, R)
(conditional Gibbs)

size of R decreases in expectation $V \setminus R$

- Reveal X on R , say $X_R = \sigma$;
- Pick the vertex $u \in R$ with the lowest index
- Define set $S = R \setminus \{u\}$



General case

arbitrary (X, R)
(conditional Gibbs)

algorithm



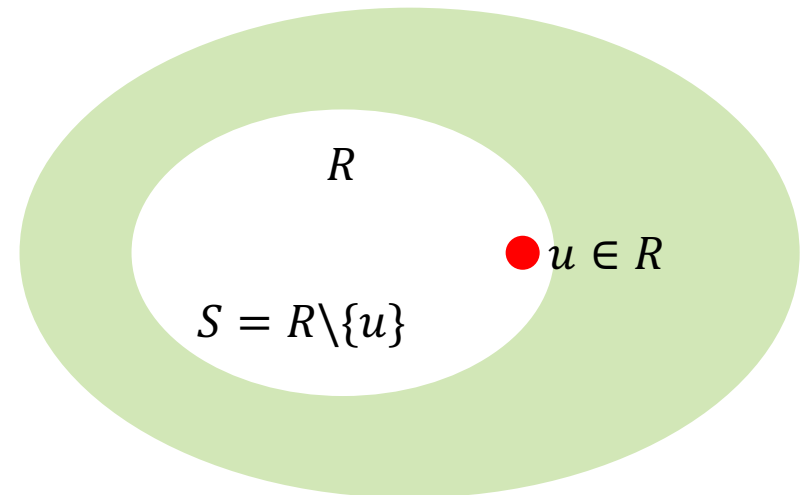
new (X, R)
(conditional Gibbs)

size of R decreases in expectation $V \setminus R$

- Reveal X on R , say $X_R = \sigma$;
- Pick the vertex $u \in R$ with the lowest index
- Define set $S = R \setminus \{u\}$
- Consider the Gibbs distribution

$$\pi = \mu_{V \setminus S}(\cdot \mid S \leftarrow \sigma_S)$$

- $(X_{V \setminus S}, \{u\})$ satisfies conditional Gibbs w.r.t. π
 $(\{u\} = R \setminus S) \quad X_{V \setminus \{u\}} \sim \pi_{V \setminus \{u\}}(\cdot \mid u \leftarrow \sigma_u)$
- Back to the **simple case** that R only contains 1 vertex

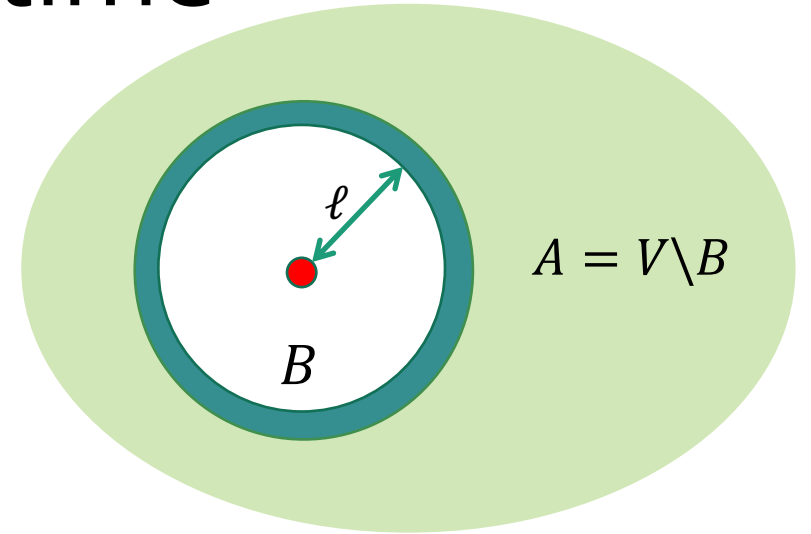


Analysis of running time

Bayes Filter

$$\Pr[\text{HEADS}] = \frac{\mu_{\min}}{\mu_u(X_u | X_{\partial B})} = \frac{\mu_u(X_u | \partial B \leftarrow \tau^*)}{\mu_u(X_u | \partial B \leftarrow X_{\partial B})}$$

$\mu_{\min} = \min\{\mu_u(X_u | \tau) \mid \tau \in [q]^{\partial B}\}$ is achieved by τ^*



SSM

[Spinka 2020]



$\Pr[\text{HEADS}] = 1 - \exp(-\Omega(\ell))$

Pass the Bayes filter

Not pass the Bayes filter



Eliminate vertex u from R

Add ∂B into R , where $|\partial B| = \exp(o(\ell))$

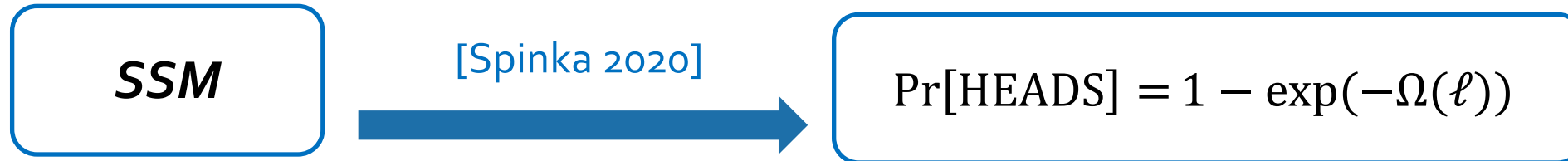
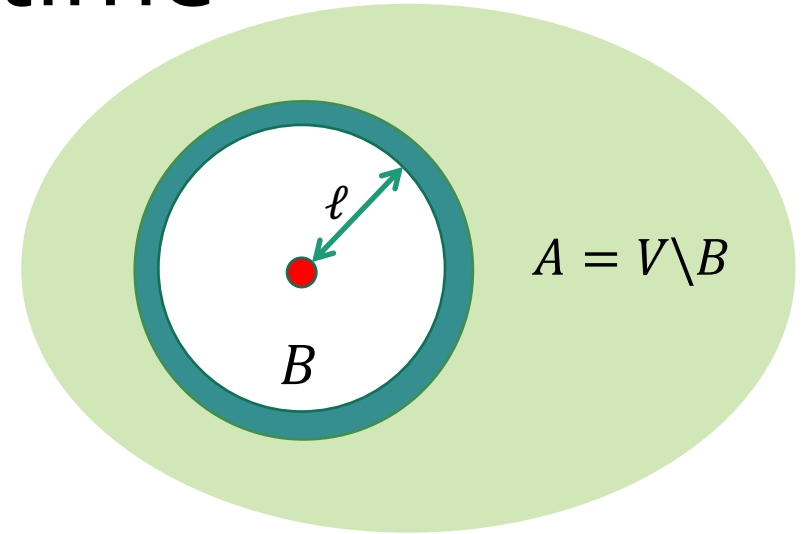
Choose $\ell = O(1)$ such that the **size of R decays in expectation** in every step

Analysis of running time

Bayes Filter

$$\Pr[\text{HEADS}] = \frac{\mu_{\min}}{\mu_u(X_u | X_{\partial B})} = \frac{\mu_u(X_u | \partial B \leftarrow \tau^*)}{\mu_u(X_u | \partial B \leftarrow X_{\partial B})}$$

$\mu_{\min} = \min\{\mu_u(X_u | \tau) \mid \tau \in [q]^{\partial B}\}$ is achieved by τ^*



Pass the Bayes filter

Not pass the Bayes filter

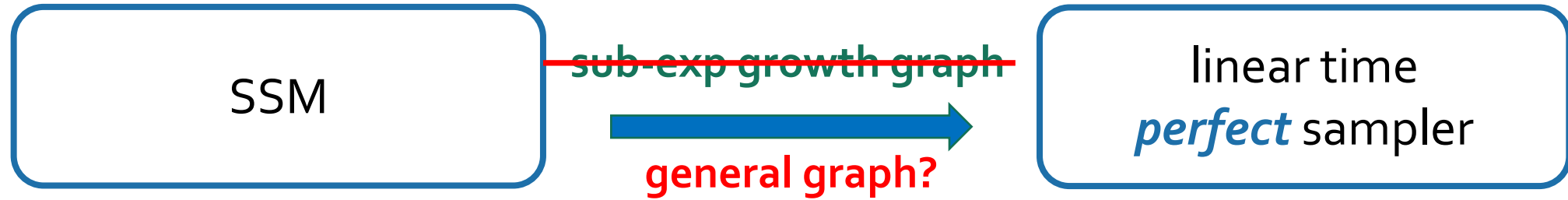
Eliminate vertex u from R

Add ∂B into R , where $|\partial B| = \exp(o(\ell))$

Q: Is the **Weak Spatial Mixing (WSM)** enough for this analysis?

A: **No**, in the general case, we do analysis on **conditional distributions**.

Open Problems



Uniform q -colourings on graph $G = (V, E)$ with max degree Δ

- Perfect sampler when $q > 2\Delta$ with running time $\tilde{O}_{q,\Delta}(n)$??

Hardcore model on graph $G = (V, E)$ with parameter $\lambda > 0$ and max degree Δ

- perfect sampler when $\lambda_c < \lambda_c(\Delta)$ with running time $\tilde{O}_{\lambda,\Delta}(n)$??

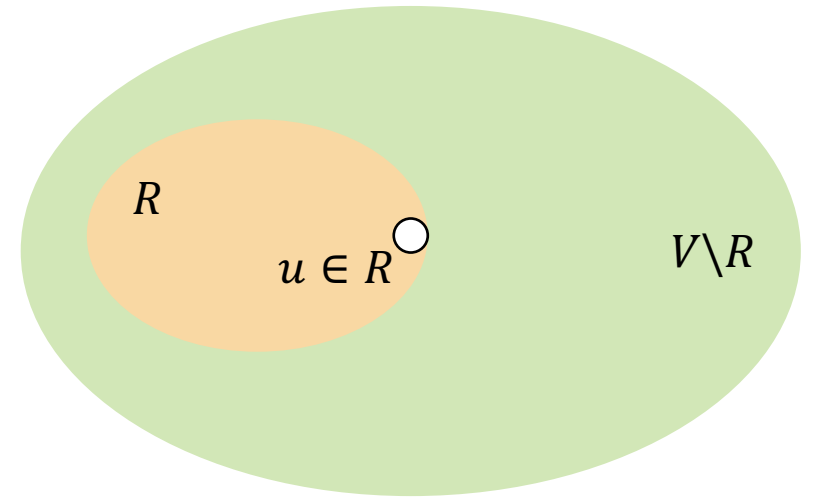
Thank you!

Q&A

Appendix

Unified Bayes filter

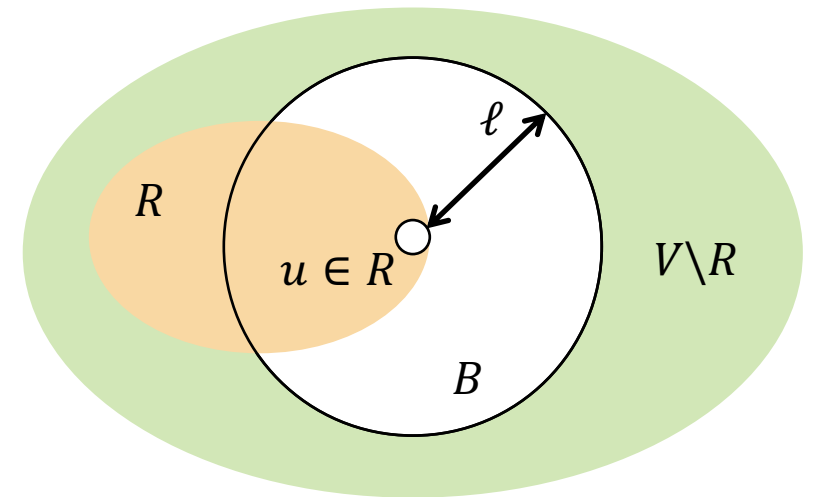
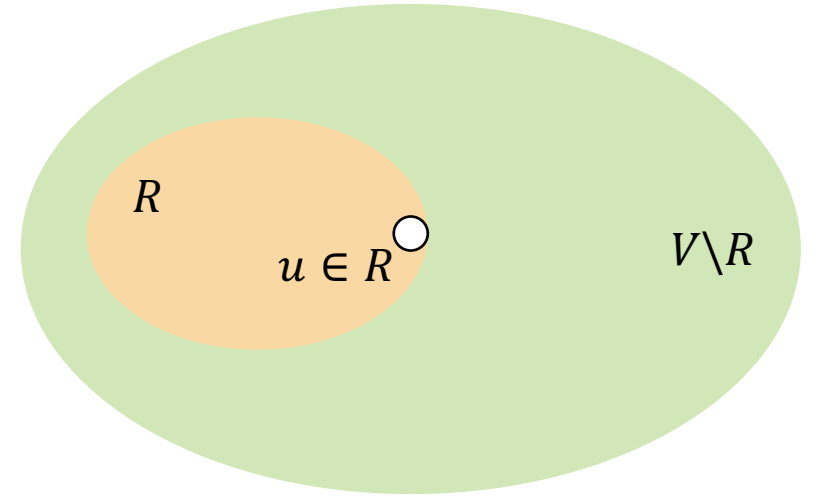
- Pick the vertex $u \in R$ with the lowest index



Unified Bayes filter

- Pick the vertex $u \in R$ with the lowest index
- Define the regime

$$B = B_\ell(u) \setminus R \cup \{u\}$$



Unified Bayes filter

- Pick the vertex $u \in R$ with the lowest index
- Define the regime

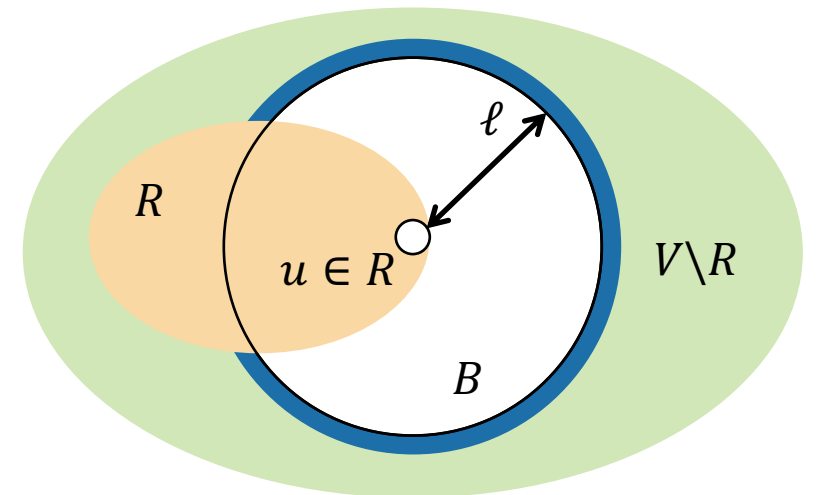
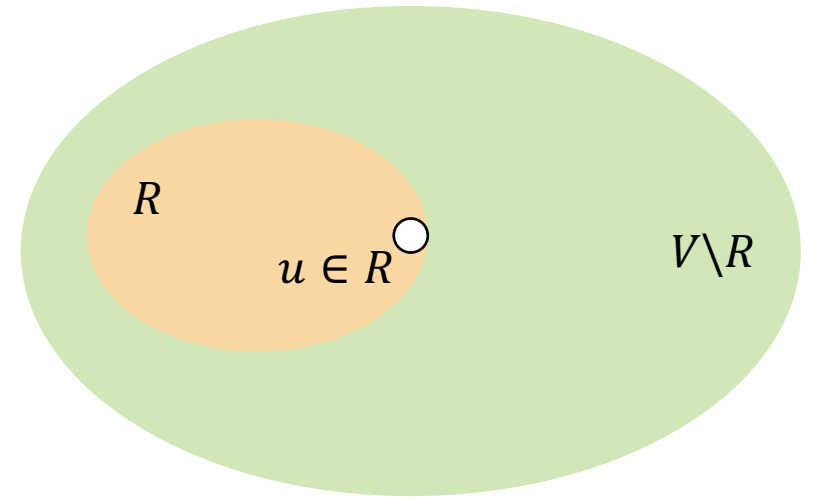
$$B = B_\ell(u) \setminus R \cup \{u\}$$

- Compute the minimum probability

$$\mu_{\min} = \min\{ \mu_u(X_u \mid \tau) \mid \tau \in [q]^{\partial B} : \tau_{\partial B \cap R} = X_{\partial B \cap R} \}$$

- Flip a coin such that **Bayes Filter**

$$\Pr[\text{HEADS}] = \frac{\mu_{\min}}{\mu_u(X_u \mid \partial B \leftarrow X_{\partial B})}$$



Unified Bayes filter

- Pick the vertex $u \in R$ with the lowest index
- Define the regime

$$B = B_\ell(u) \setminus R \cup \{u\}$$

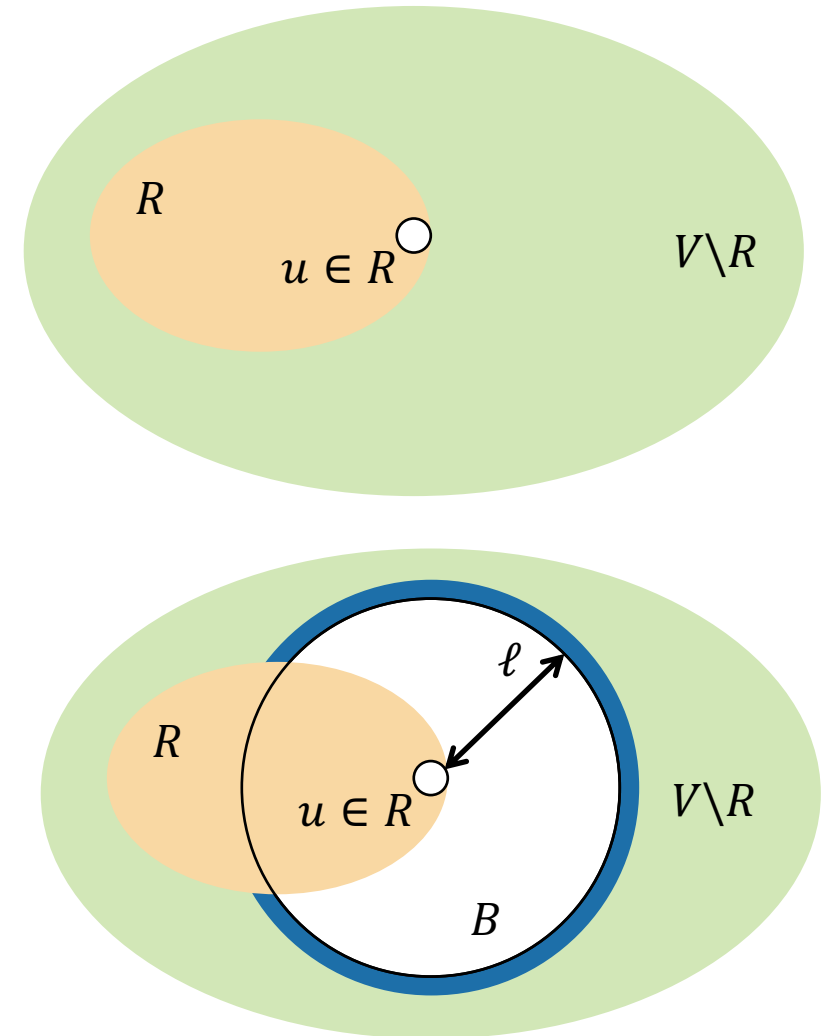
- Compute the minimum probability

$$\mu_{\min} = \min\{ \mu_u(X_u \mid \tau) \mid \tau \in [q]^{\partial B} : \tau_{\partial B \cap R} = X_{\partial B \cap R} \}$$

- Flip a coin such that **(Bayes Filter)**

$$\Pr[\text{HEADS}] = \frac{\mu_{\min}}{\mu_u(X_u \mid \partial B \leftarrow X_{\partial B})}$$

- **If** the outcome is HEADS, **then**
 Resample $X_B \sim \mu_B(\cdot \mid \partial B \leftarrow X_{\partial B})$
Return $(X, R \setminus \{u\})$
- **If** the outcome is not HEADS, **then**
Return $(X, R \cup \partial B)$

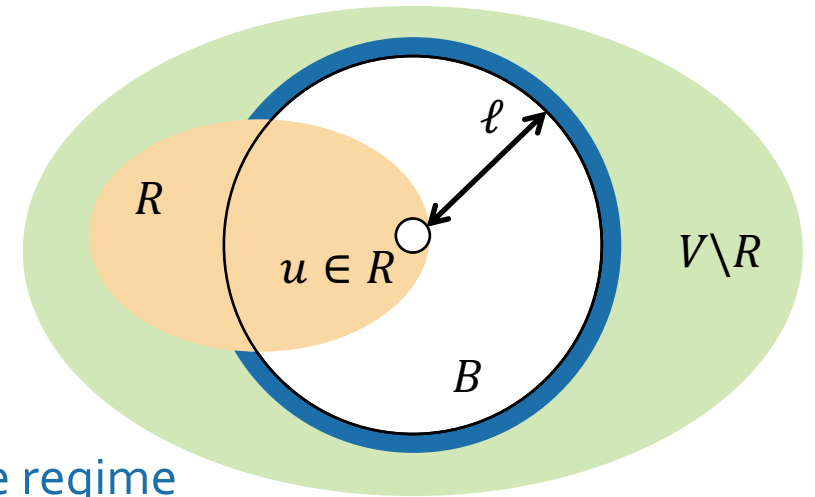


Bayes Filter

$$\Pr[\text{HEADS}] = \frac{\mu_{\min}}{\mu_u(X_u | X_{\partial B})} = \frac{\mu_u(X_u | \partial B \leftarrow \tau^*)}{\mu_u(X_u | \partial B \leftarrow X_{\partial B})}$$

$$\mu_{\min} = \min\{ \mu_u(X_u | \tau) \mid \tau \in [q]^{\partial B} : \tau_{\partial B \cap R} = X_{\partial B \cap R} \}$$

τ^* and $X_{\partial B}$ disagree only at blue regime



SSM

$$\Pr[\text{HEADS}] = \frac{\mu_u(X_u | \partial B \leftarrow \tau^*)}{\mu_u(X_u | \partial B \leftarrow X_{\partial B})} = 1 - \exp(-\Omega(\ell))$$

Pass the Bayes filter

Eliminate vertex u from R

Not pass the Bayes filter

Add ∂B into R , where $|\partial B| \leq |S_\ell(v)| = \exp(o(\ell))$

$$\begin{aligned} \mathbb{E}[|\text{new } R| - |R| \mid R] &= -\Pr[\text{HEADS}] + (1 - \Pr[\text{HEADS}]) \cdot |\partial B| \\ &= -1 + \exp(-\Omega(\ell)) + \exp(-\Omega(\ell) + o(\ell)) \end{aligned}$$

$$(\ell = \Theta(1)) \quad < 0$$