Computational phase transitions and the hard-core model

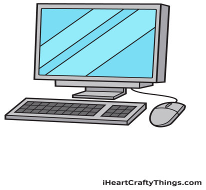
Andreas Göbel

Part I: survey talk

Part II based on joint work with
Tobias Friedrich, Max Katzmann, Martin Krejca and Marcus Pappik

The computational lens (for this talk)

Polynomial-time computation



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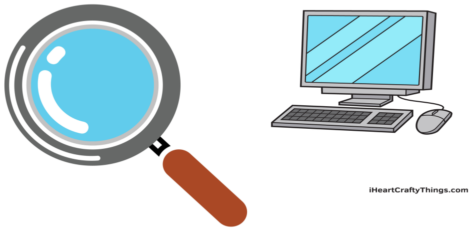

Polynomial-time computation

P vs NP

- P: computational problems for which we can find a solution efficiently (e.g. Sorting integers, MinCut)
- NP: computational problems for which, given a solution, we can verify it efficiently (e.g. Satisfiability, MaxCut)

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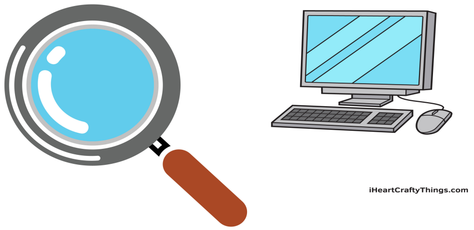

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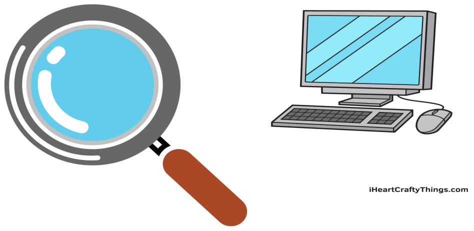

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- Tractable ($C \in$ P): there is an algorithm that solves it in polynomial time
- Intractable (NP-hard): there is a polynomial-time reduction from a known NP-hard problem to C

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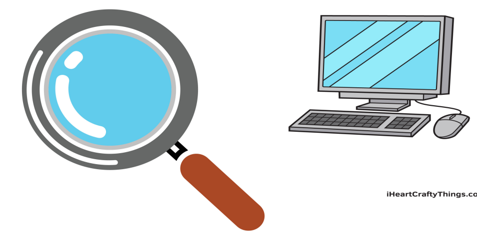

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Spin systems $\to$ computational problems to solve efficiently

The hard-core model as a computational problem

Burley ’60 as a lattice version of the hard-sphere model

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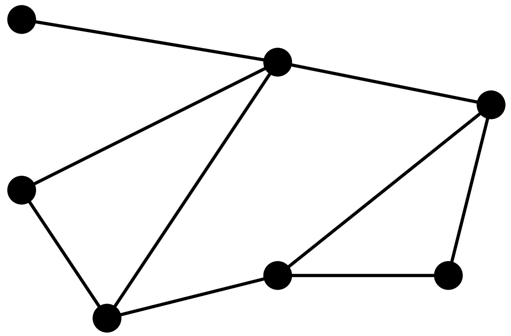
Undirected graph $G = (V, E)$ and parameter $\lambda \in \mathbb{R}_{\geq 0}$



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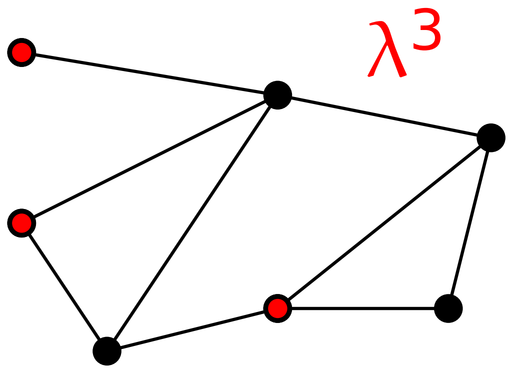

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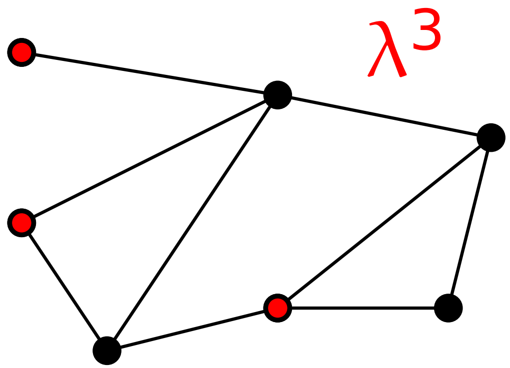

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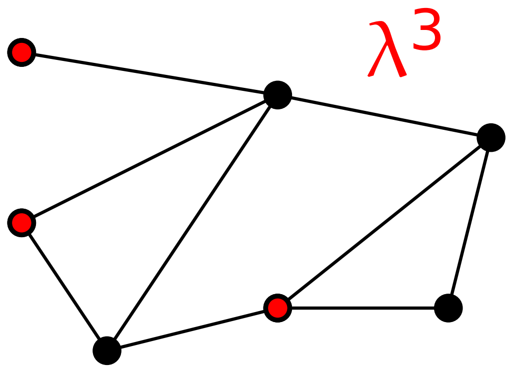

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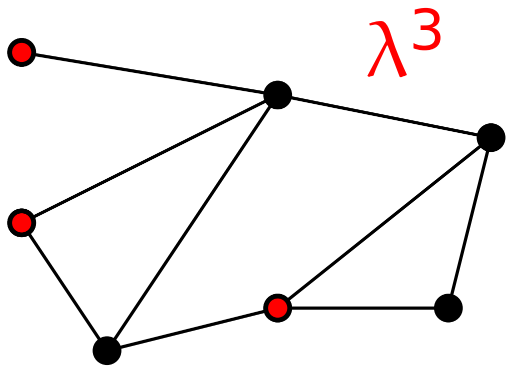

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Sample from the Gibbs distribution

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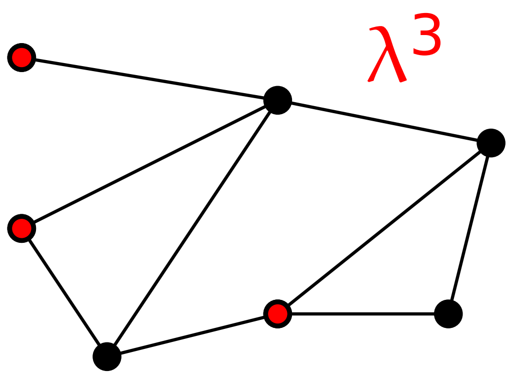

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Sample from the Gibbs distribution

Compute the partition function $Z(G, \lambda)$ Shown to be ($>>$ NP-hard $\forall G, \lambda$)

Roth '96

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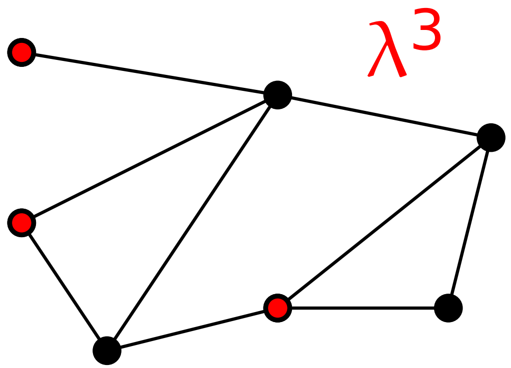

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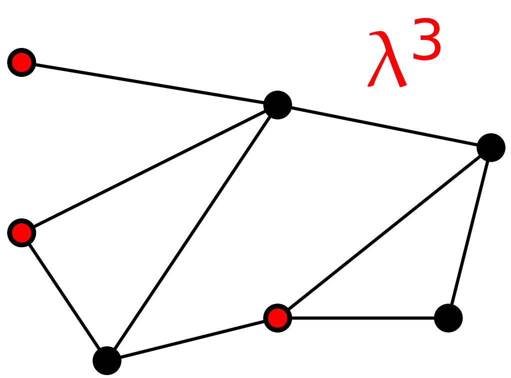

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- Input: G with n vertices and max degree Δ, $\varepsilon \in (0, 1)$. Parameter: λ
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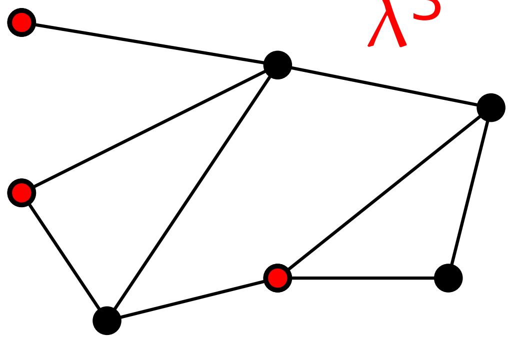

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Sample from the Gibbs distribution (Approximately)

$\Updownarrow$ Sinclair and Jerrum '89

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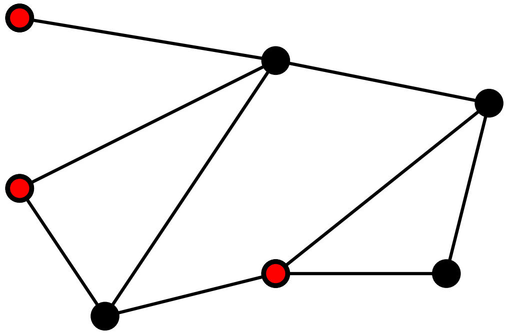

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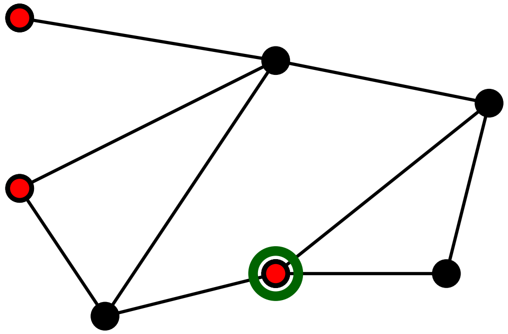

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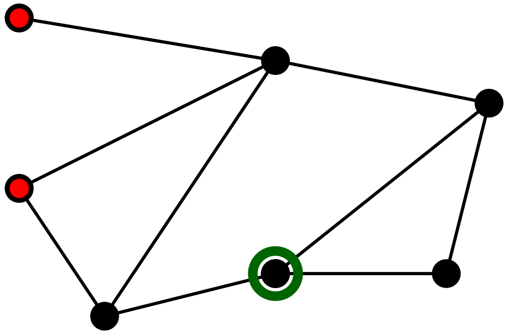

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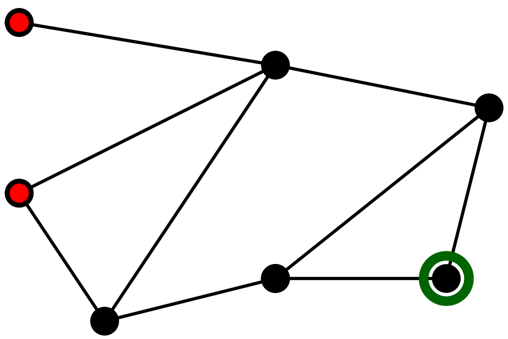

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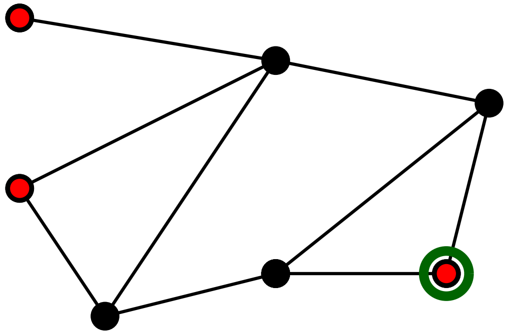

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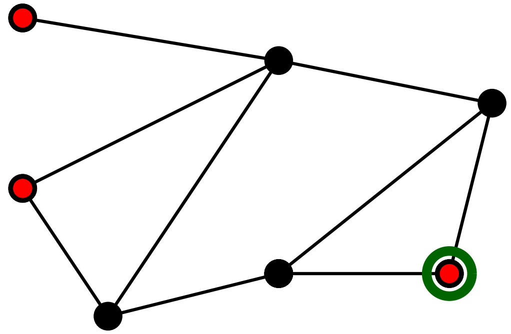

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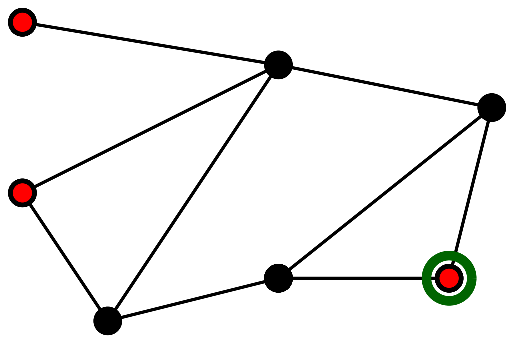

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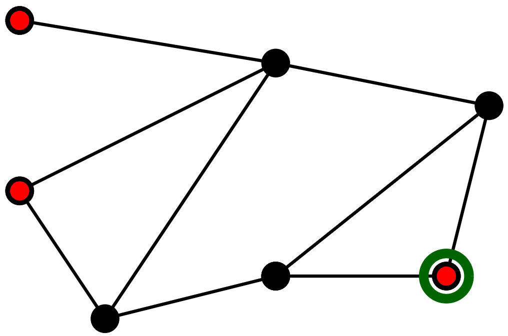

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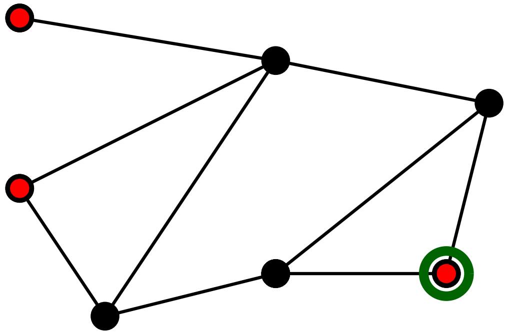

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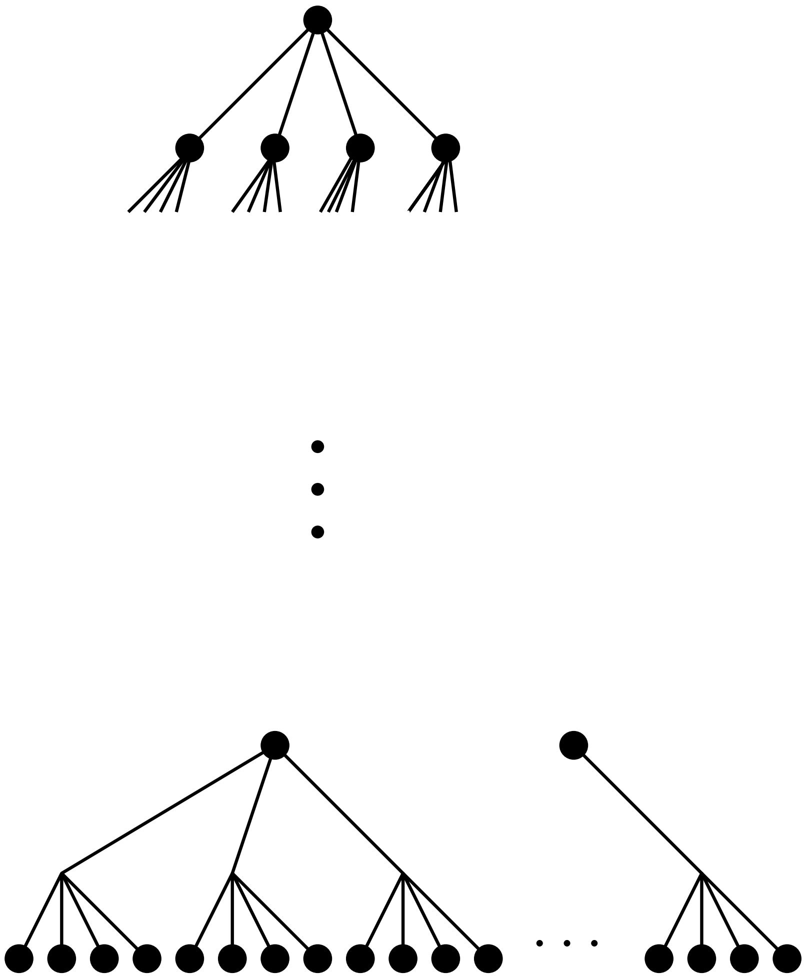
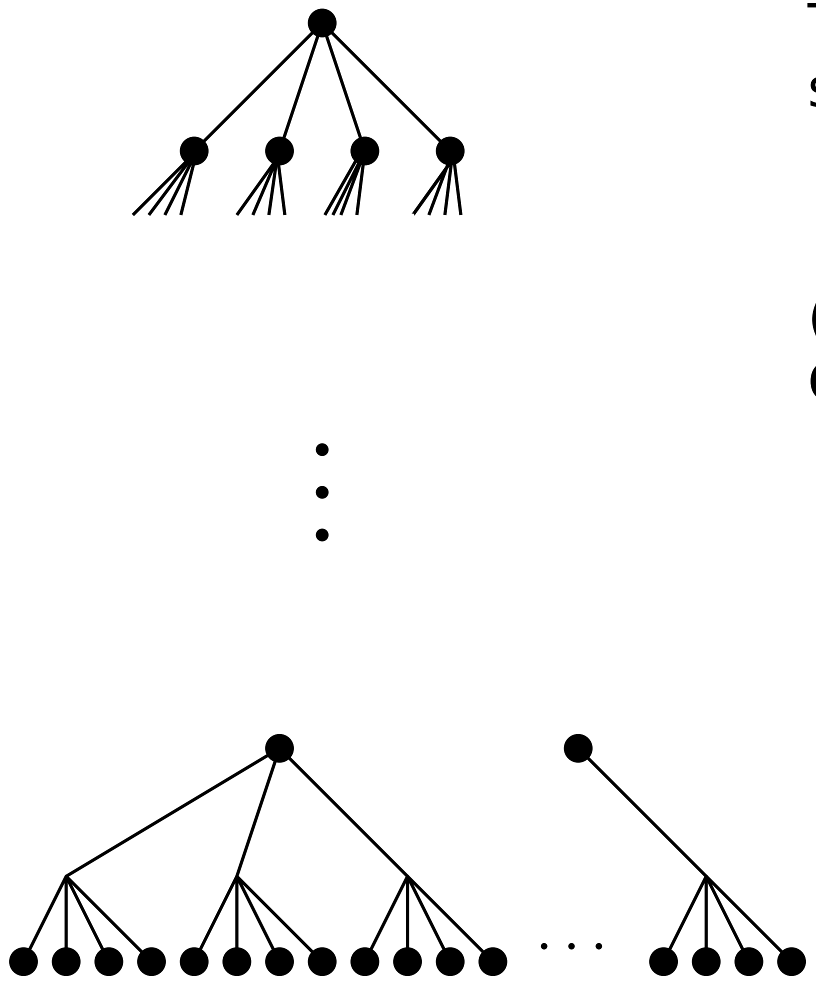
They used a path coupling argument

Hard-core model PT on Δ-regular trees

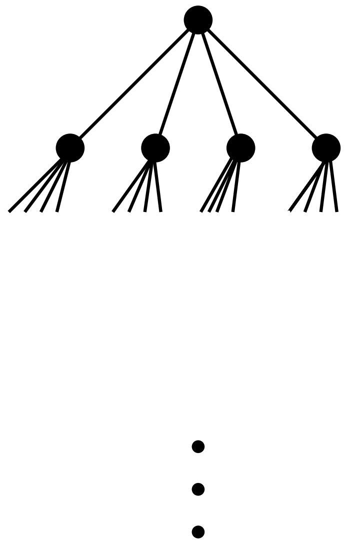




The hard-core model exhibits a phase transition at

$$\lambda_c(\Delta) = \frac{(\Delta-1)^{\Delta-1}}{(\Delta-2)^{\Delta}} \approx \frac{e}{\Delta}$$

(uniqueness vs non-uniqueness of the Gibbs measure) Kelly '85



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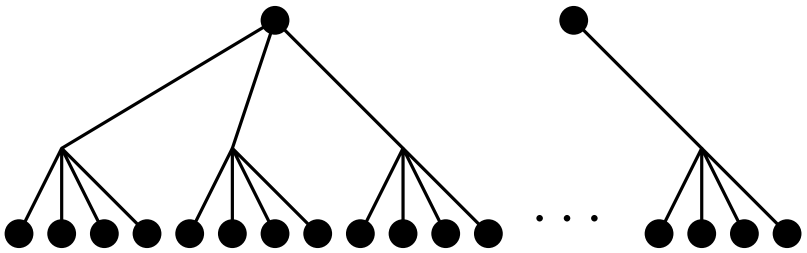
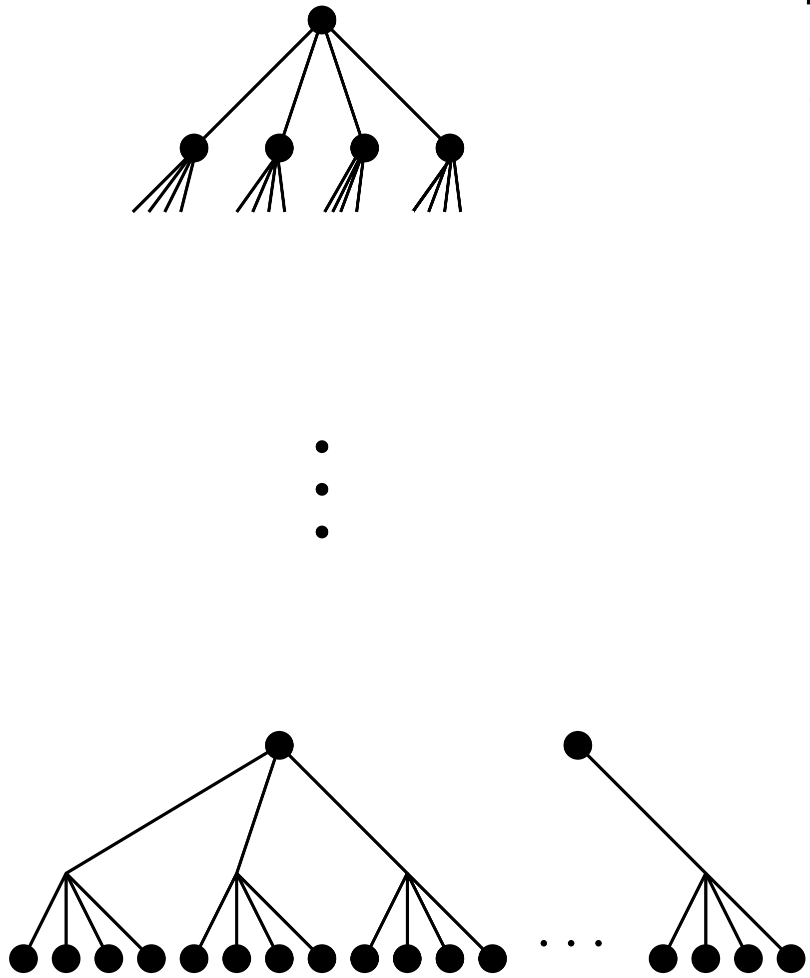


Many results at early 00’s showing that MC’s mix slowly (in exponential time), for $\lambda >> \lambda_c(\Delta)$ in various graphs



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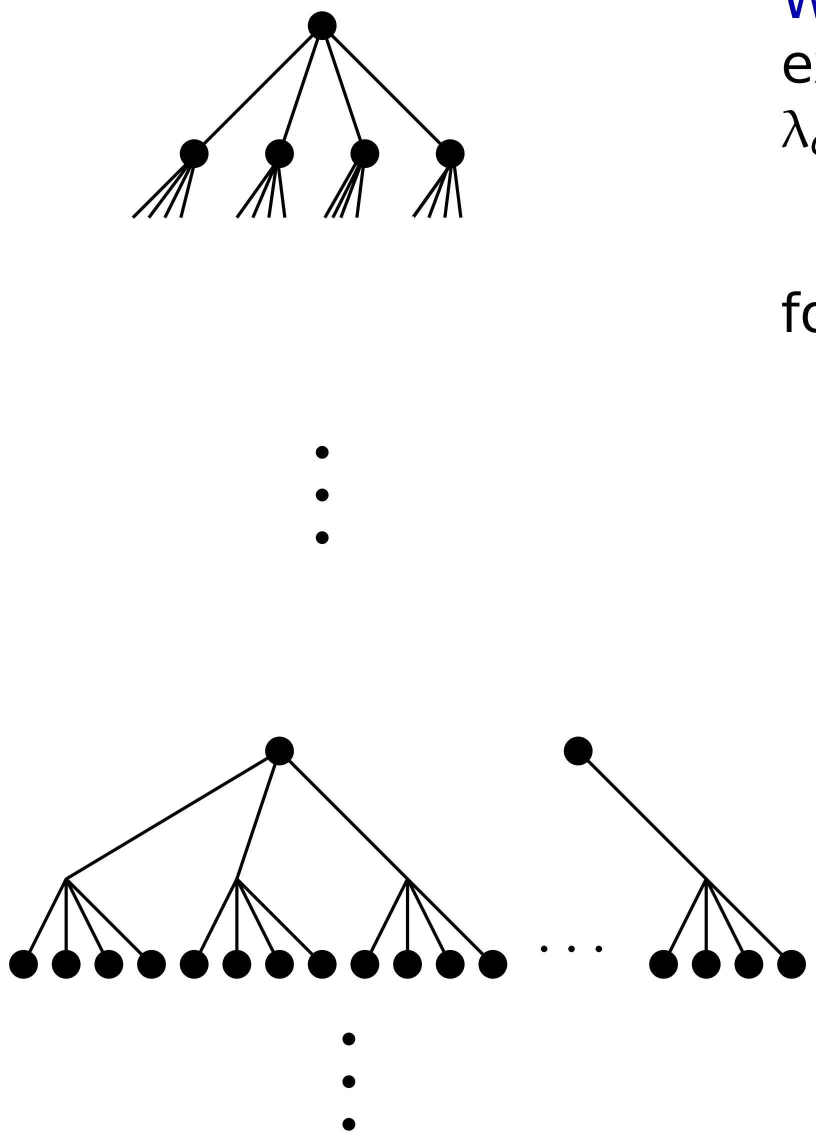
It was conjectured that $\lambda_c(\Delta)$ is a threshold for the mixing time of the MC (rapid mixing vs torpid mixing) for all graphs Sokal '00



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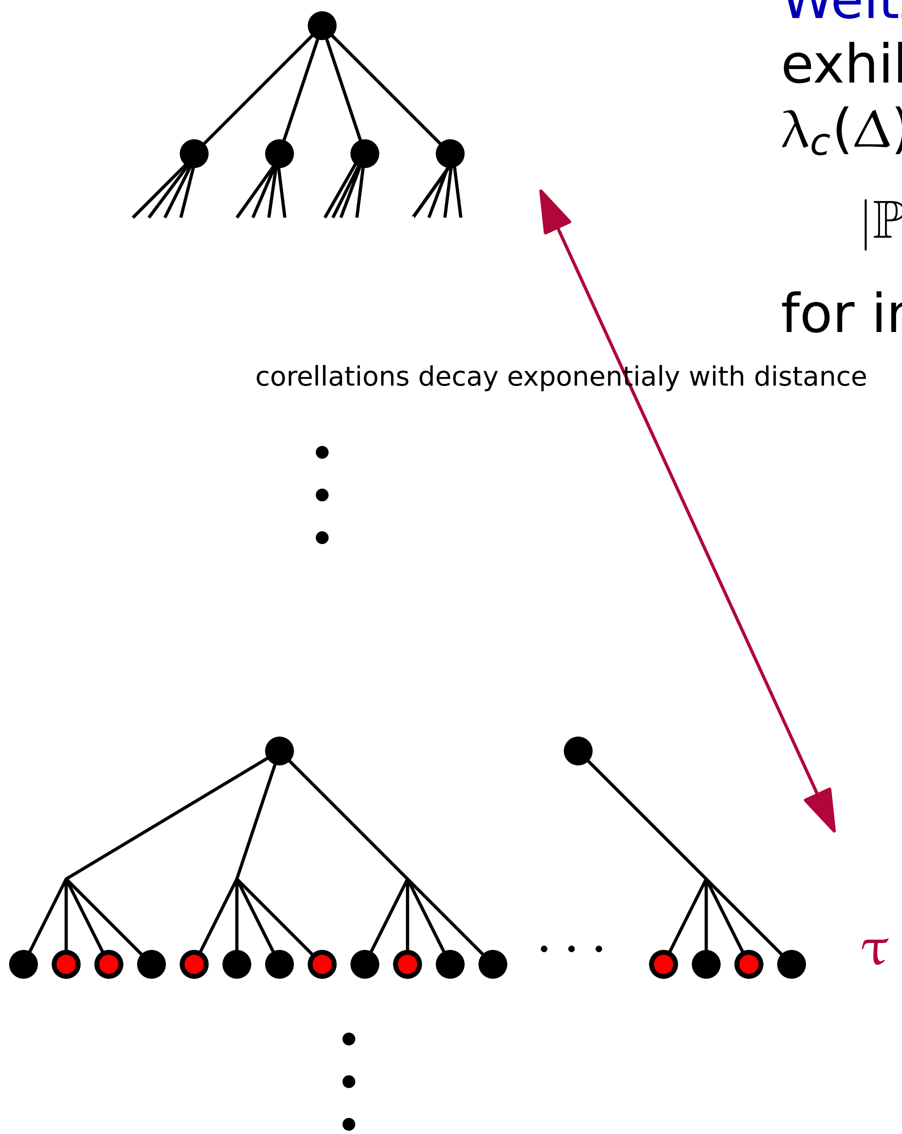
$$|\mathbb{P}_\mu(v \in I \mid \tau) - \mathbb{P}_\mu(v \in I \mid \tau')| \leq Ce^{-d_T(v,\tau \neq \tau')}$$

for independent set configurations τ, τ'.

Weitz's results



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Hasso Plattner Institut

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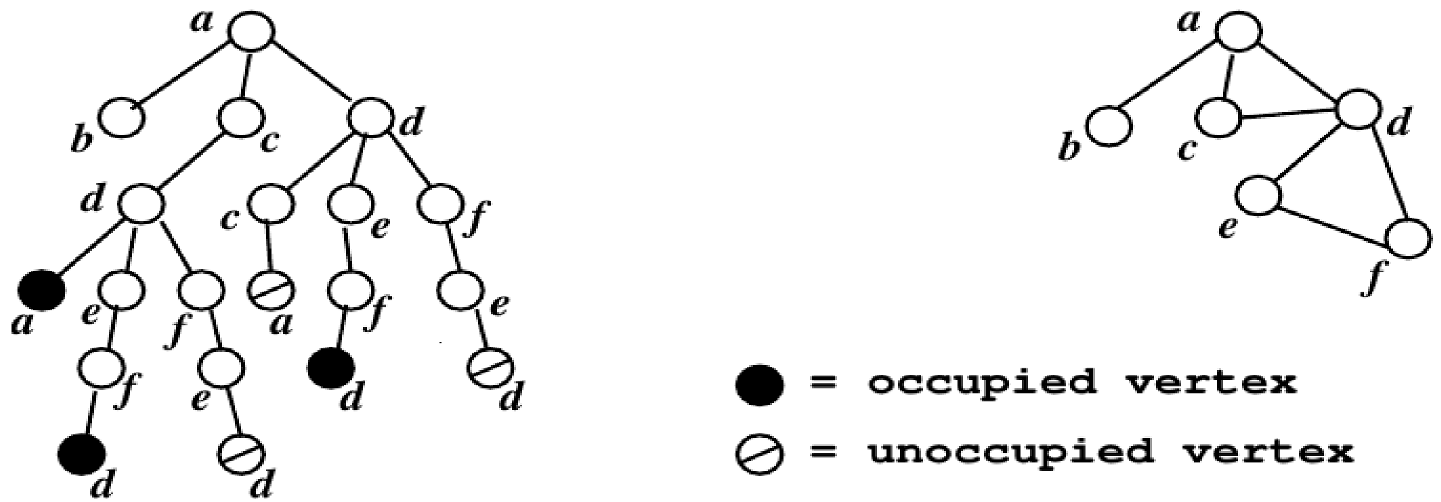

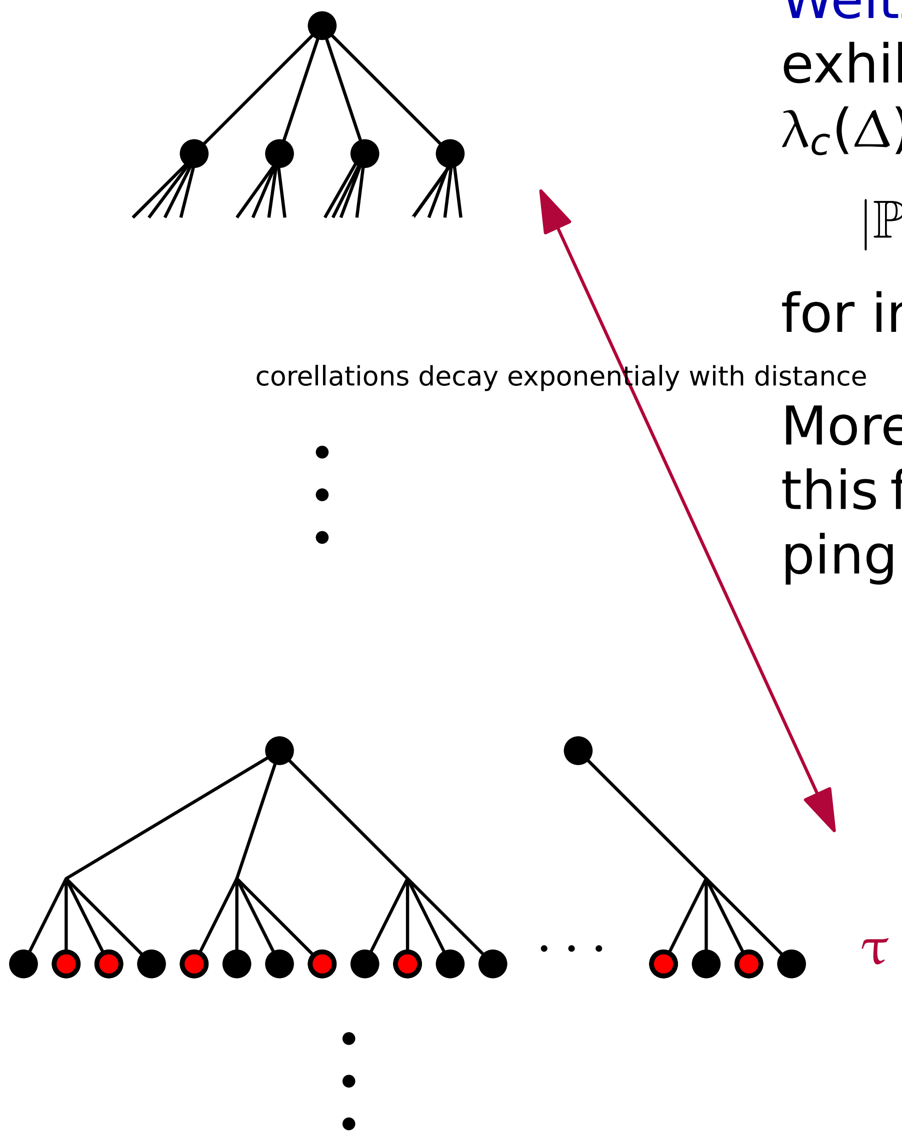

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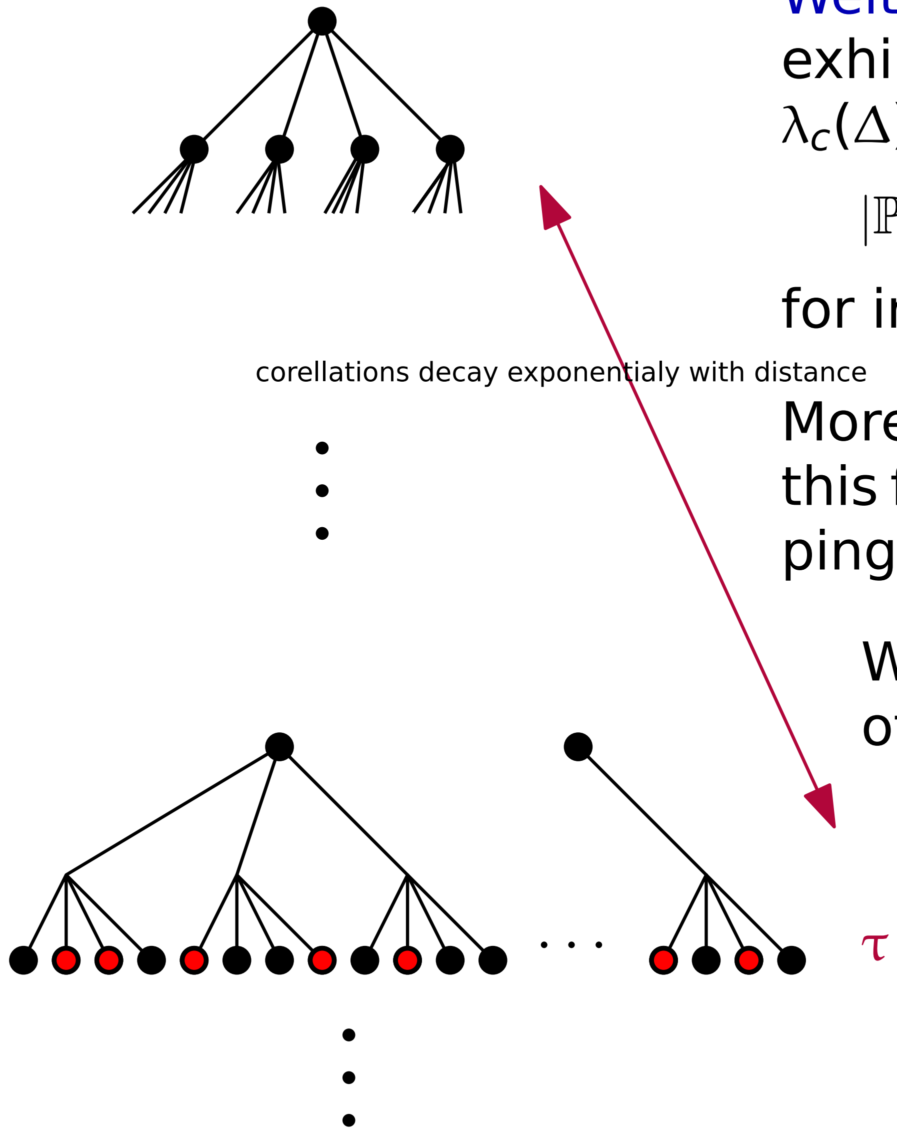

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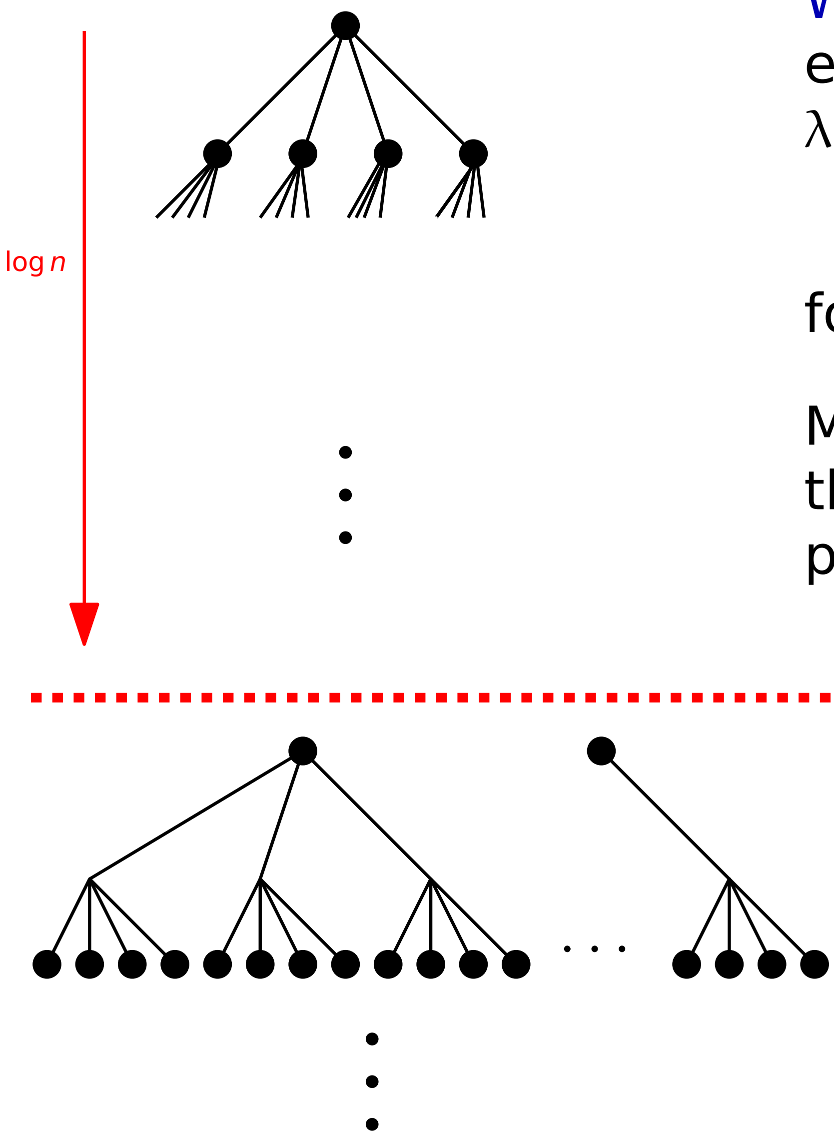

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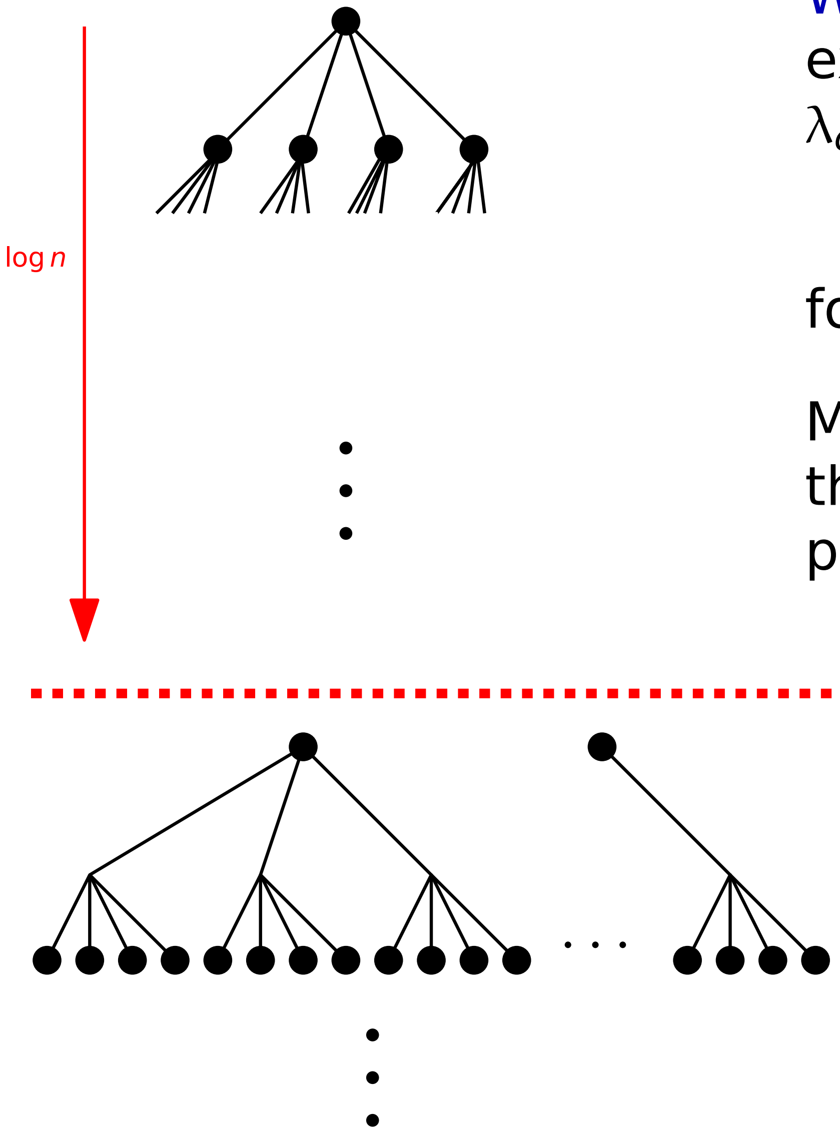

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This results to an algorithm for computing the partition function in $O(n^{\log \Delta})$ for bounded degree graphs

More on Glauber dynamics

On trees Glauber dynamics are fast mixing for all G, λ (Martinelli, Sinclair and Weitz '04)

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On random Δ-regular bipartite graphs Glauber dynamics have exponential mixing time when $\lambda > \lambda_c(\Delta)$ (Mossel, Weitz, Wormald ’09)

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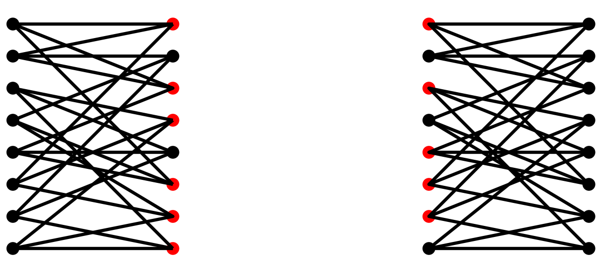
On trees Glauber dynamics are fast mixing for all G, λ (Martinelli, Sinclair and Weitz ’04)

When the graph has subexponential growth:
SSM $\Rightarrow$ rapid mixing of glauber dynamics for $\lambda < \lambda_c(\Delta)$

On random Δ-regular bipartite graphs Glauber dynamics have exponential mixing time when $\lambda > \lambda_c(\Delta)$ (Mossel, Weitz, Wormald ’09)

Moreover, on these graphs when $\lambda > \lambda_c(\Delta)$ the system is with high probability in one of two phases



Computational phase transition at the tree threshold

Sly '10, Galanis et al. '11: When $\lambda > \lambda_c(\Delta)$ it is NP-hard to compute the partition function

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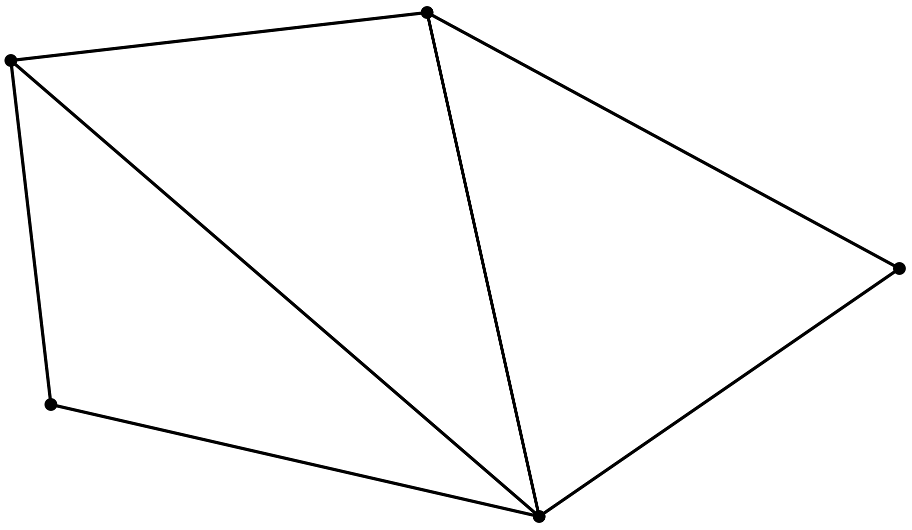
Idea: Reduce from MaxCut



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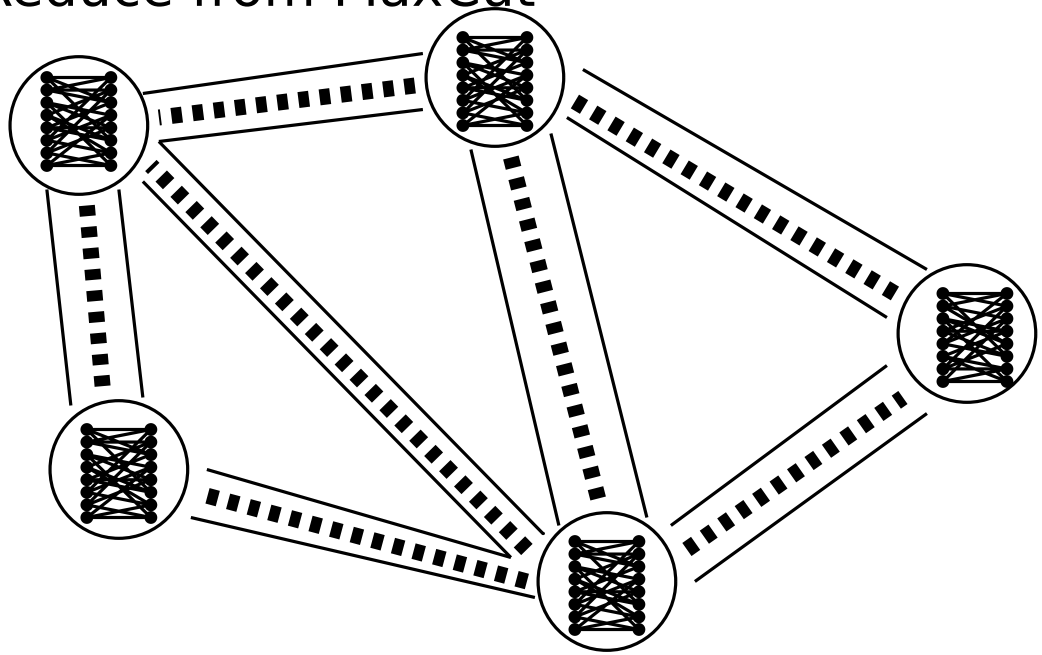

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Reduction: G'

For each edge uv connect left part of the gadget for u to the left part of the gadget for v with "many" edges and the same for the right parts

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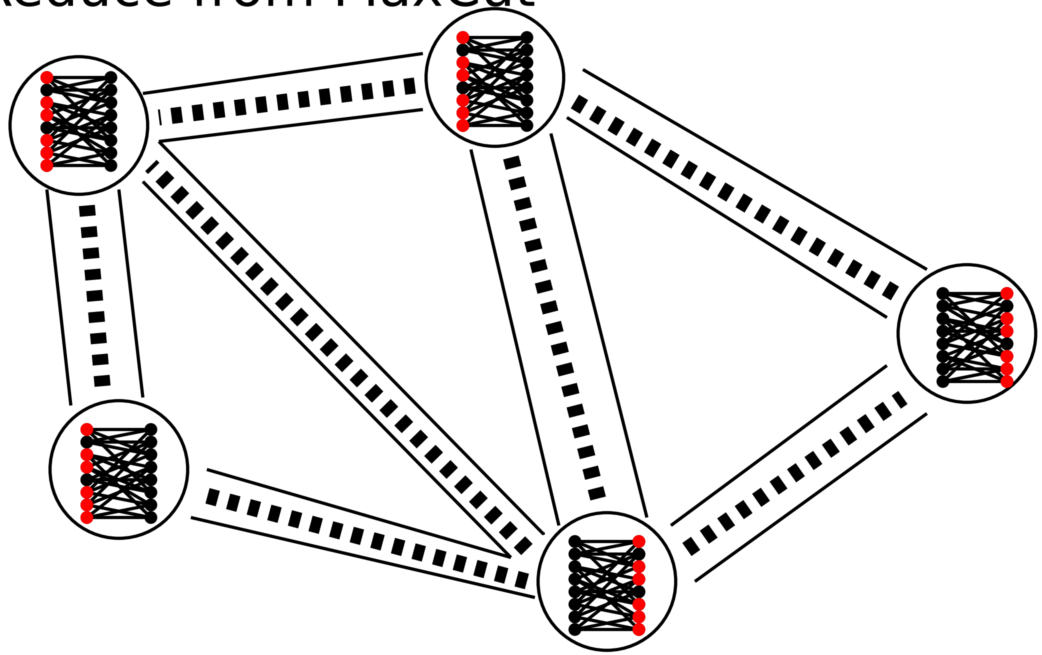

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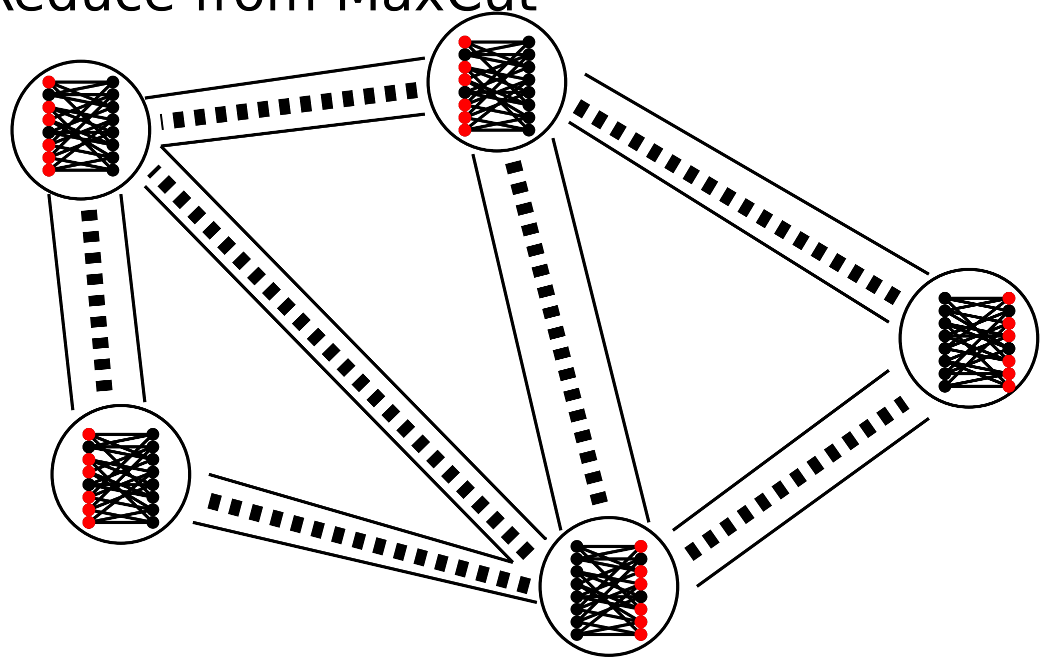

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The hardcore model undergoes a computational phase transition at the tree threshold $\lambda_c(\Delta) \approx e\Delta^{-1}$

Complex λ and Barvinok's method

Let us view $Z(G, \lambda) = \sum_{i=0}^{n} a_i \lambda^i$ as a polynomial where $\lambda \in \mathbb{C}$

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Patel and Regts '17: on graphs of max degree Δ we can ennumerate their connected subgraphs in $O(n^{\log \Delta})$-time

The picture on the complex plane

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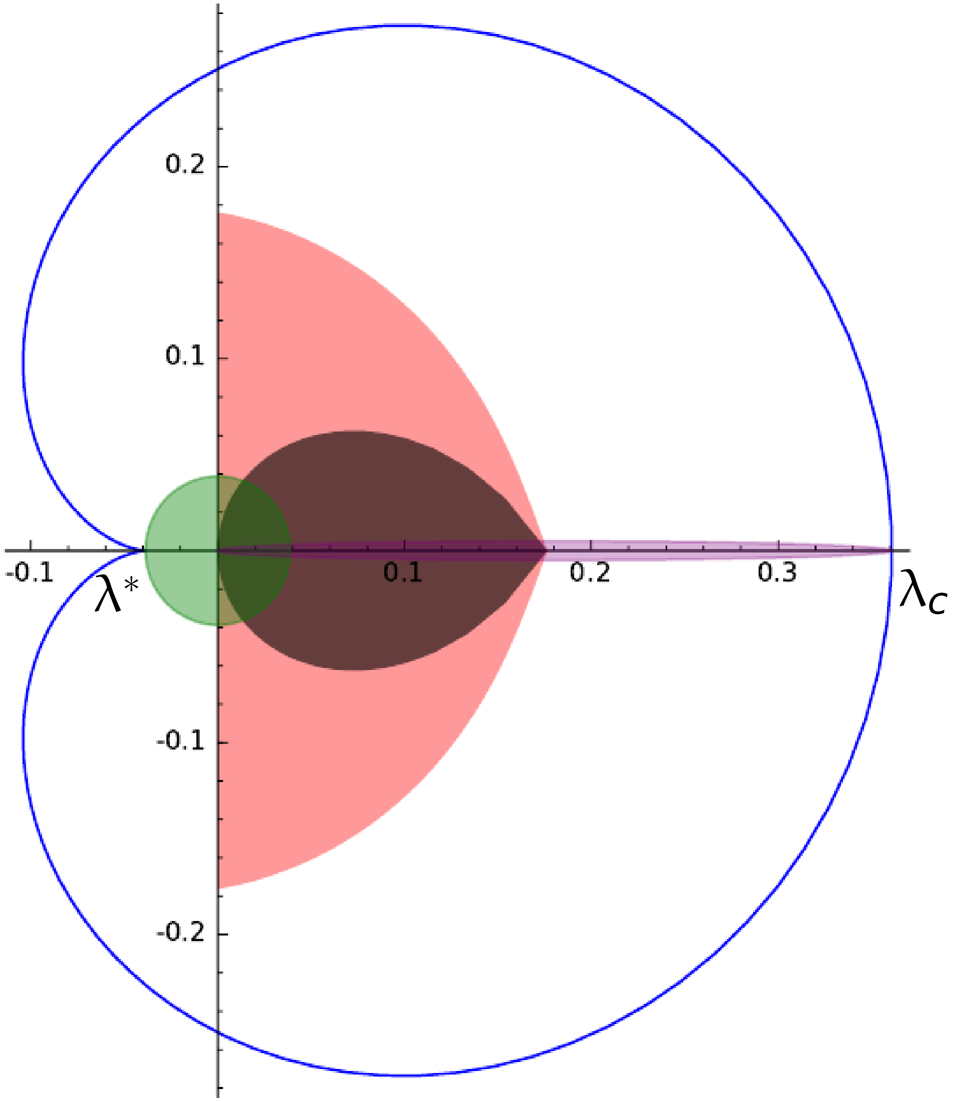

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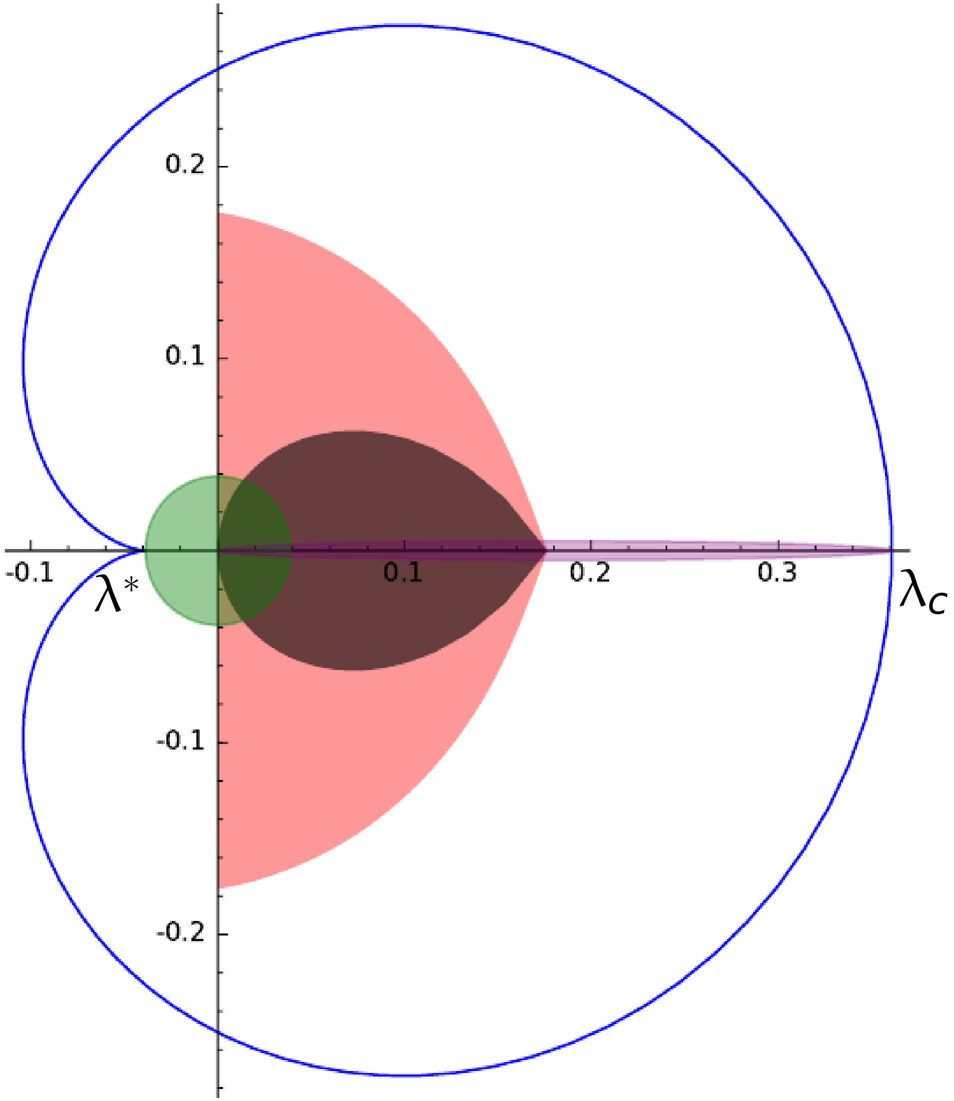

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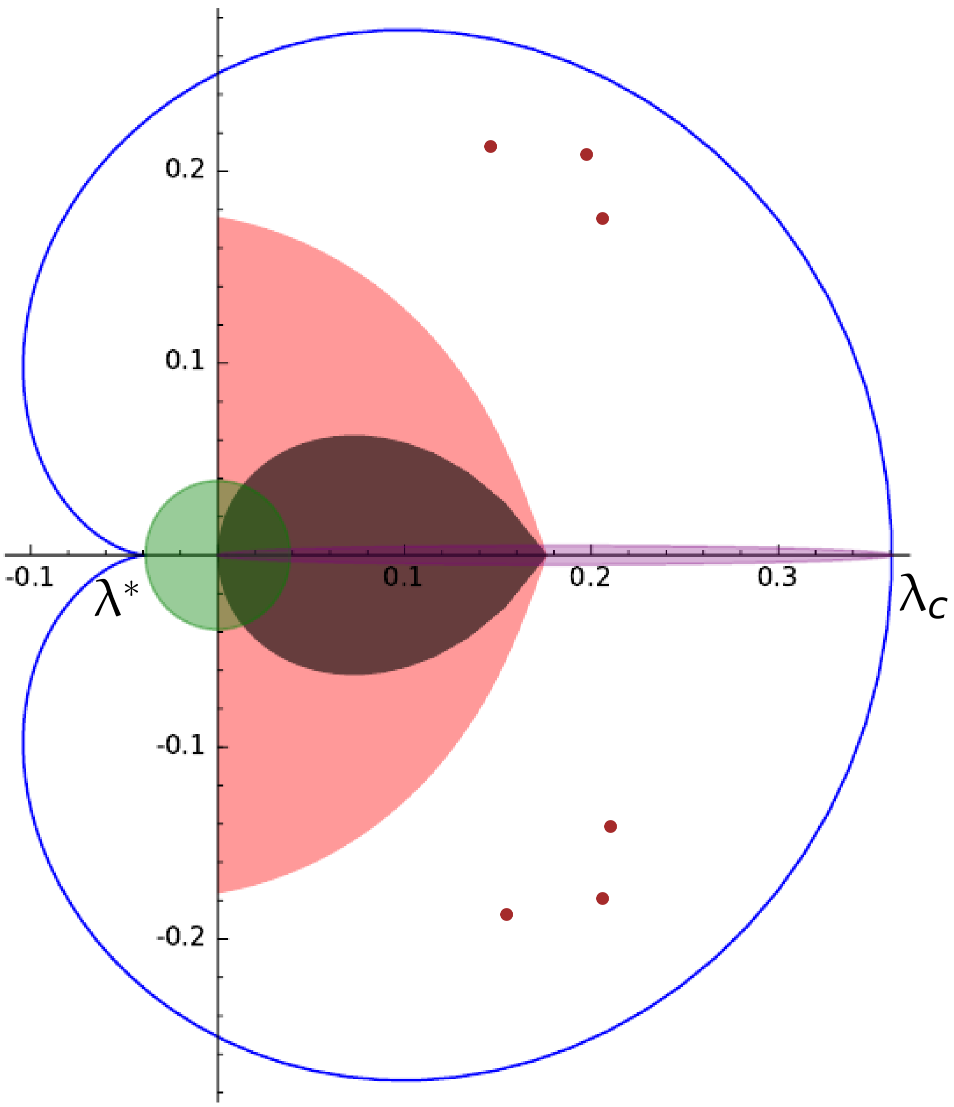

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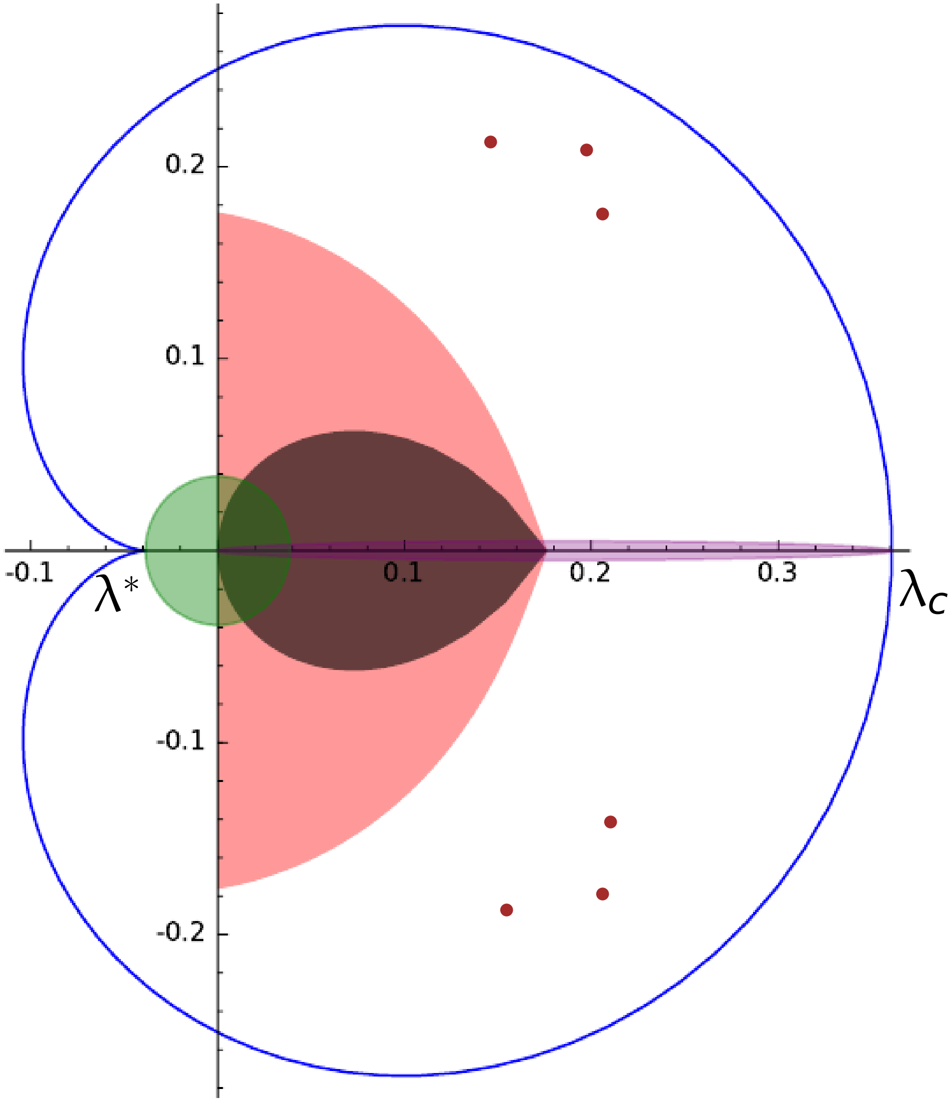

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Sectral independence: back to Glauber dynamics

Diaconis and Strook '91 The mixing time of a MC can be bounded by $\sim \gamma_2^{-1}$, where γ_2 is the second eigenvalue of its transition matrix

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Chen, Feng, Yin and Zhang '22: Mixing time in $O(n^2 \log n)$ and $\Delta = \Delta(n)$

Perfect sampling

When G has subexponential growth

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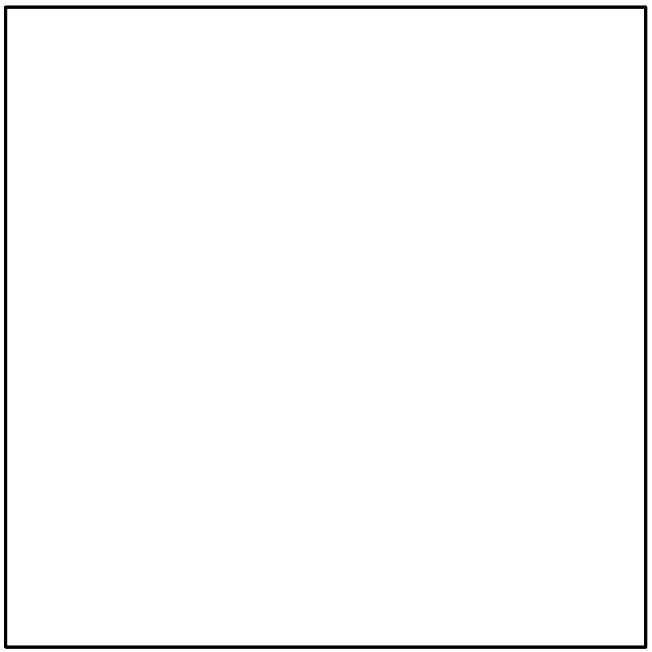
Very high level idea:

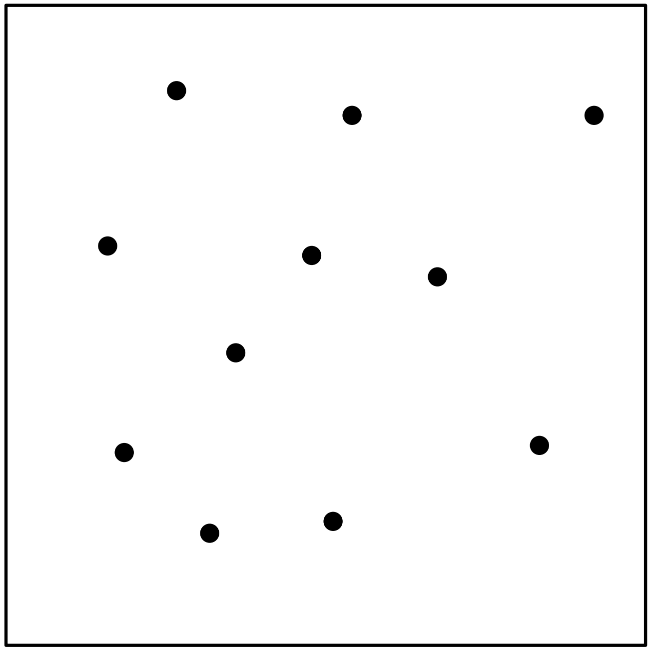
Choose a vertex u.a.r. and update its state using the correct marginal distribution

Part II



bounded mesurable **region** $\mathbb{V} \subset \mathbb{R}^d$

Understanding Gibbs PPs computationally



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configurations: finite point sets in $\mathbb{V}$

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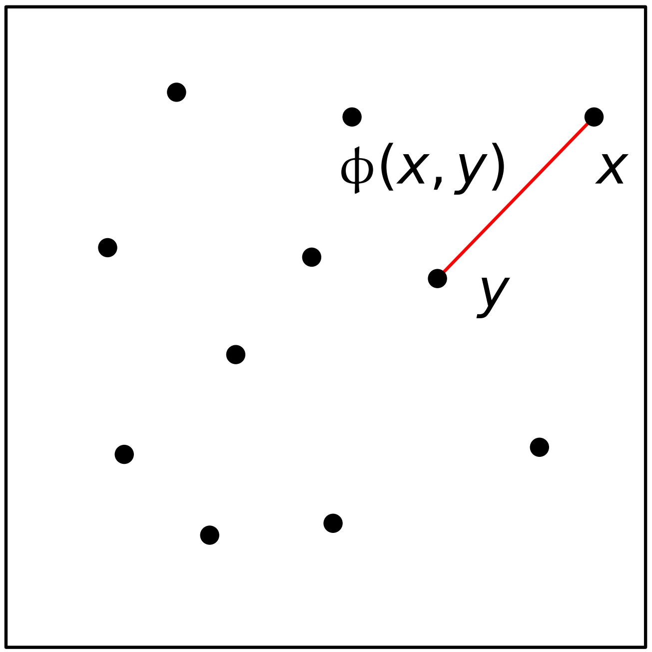

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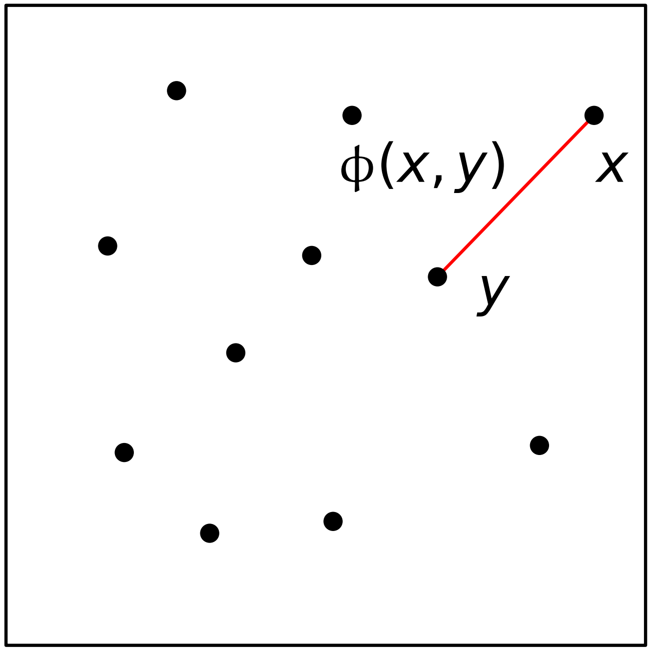

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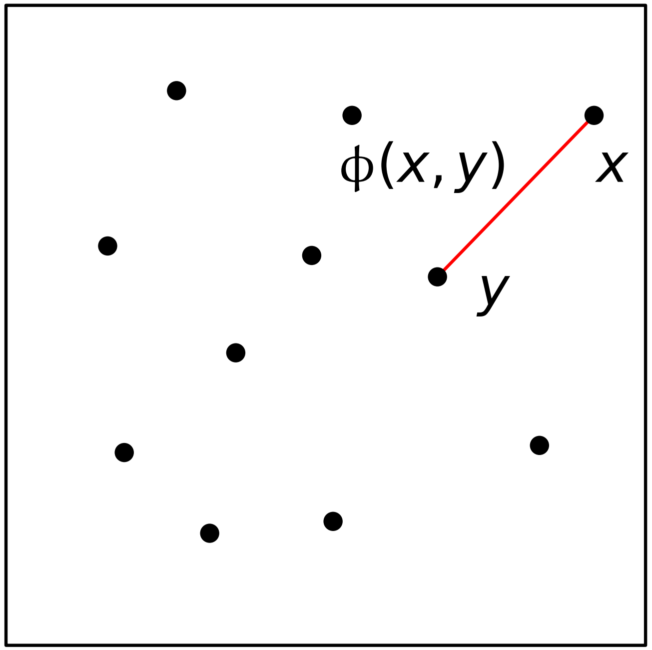

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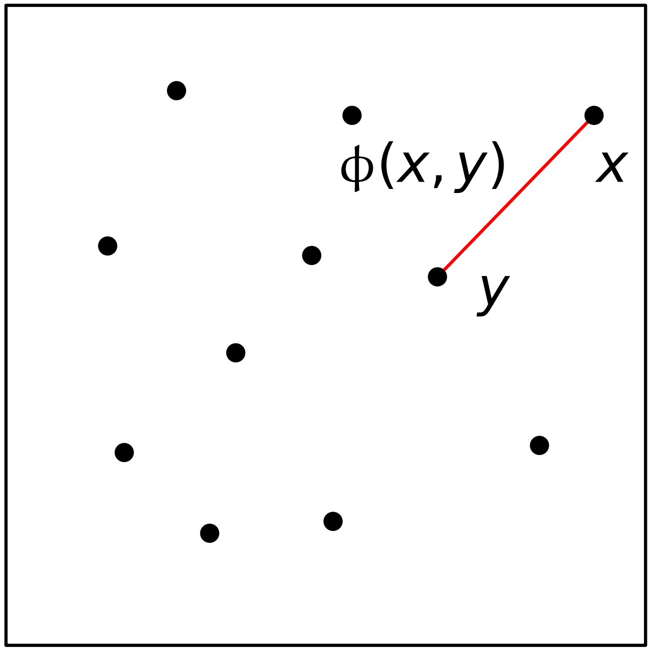
(P: Poisson point process of intensity 1)



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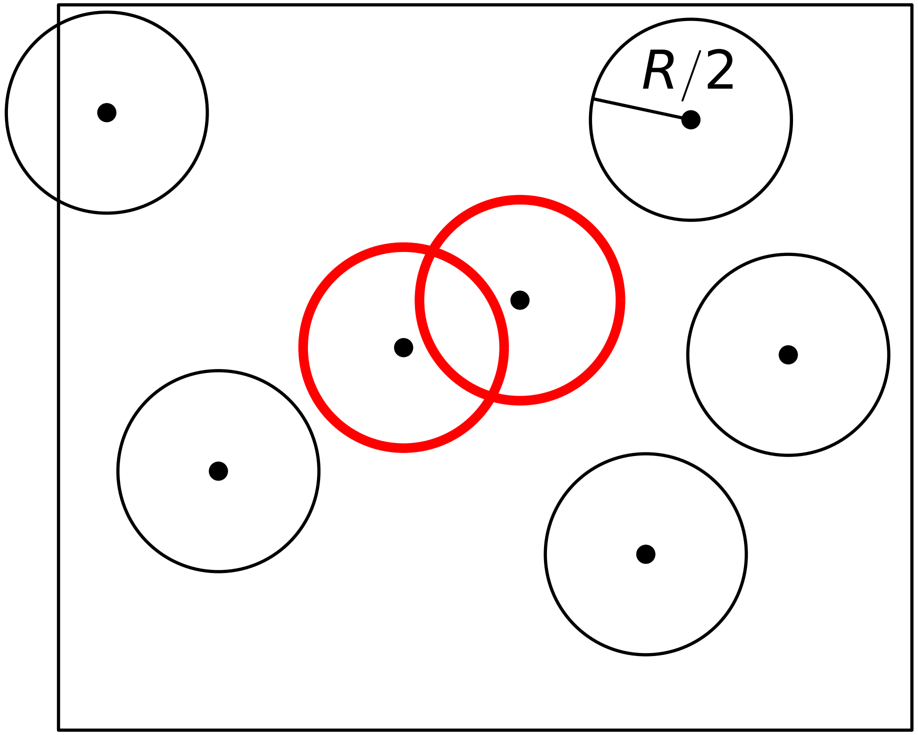
Partition function: $\Xi_{\mathbb{V}}(\phi, \lambda) = \sum_{k \geq 0} \frac{\lambda^k}{k!} \int_{\mathbb{V}^k} e^{-\sum_{i<j} \phi(x_i, x_j)} dx_1 \ldots dx_k$

Hard-sphere model:

Poisson point process of intensity $\lambda \in \mathbb{R}_{\geq 0}$ but $dist(x, y) \geq R \in \mathbb{R}_{\geq 0}$



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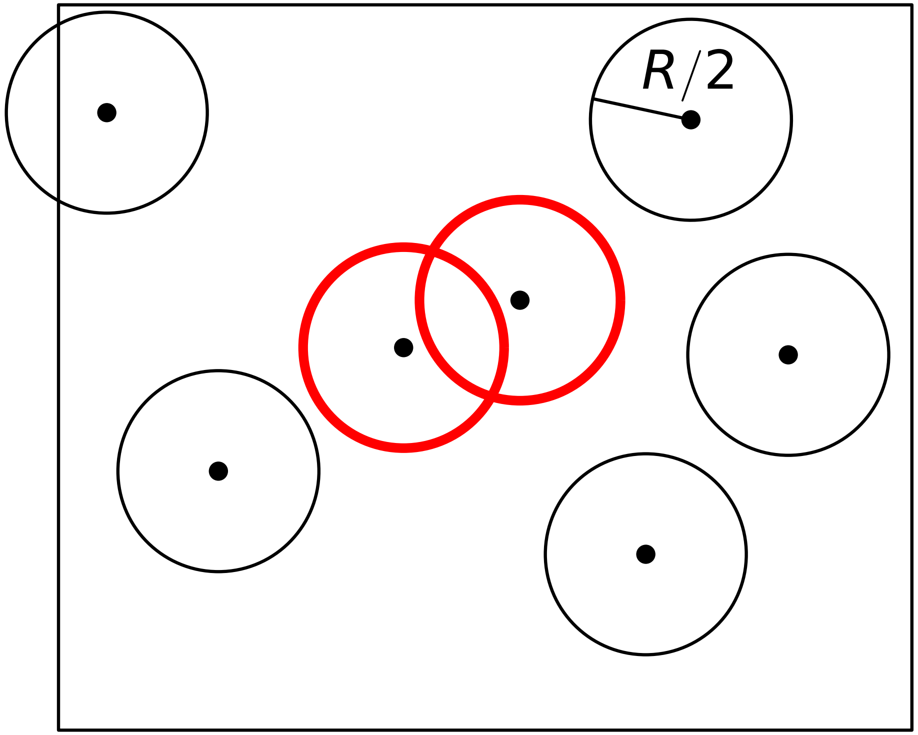

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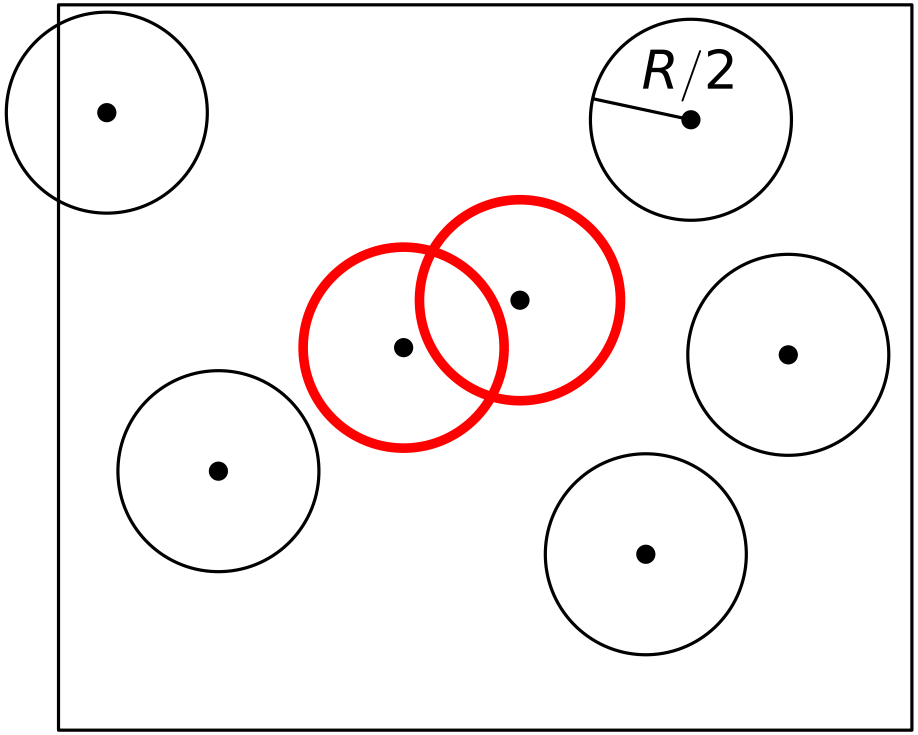

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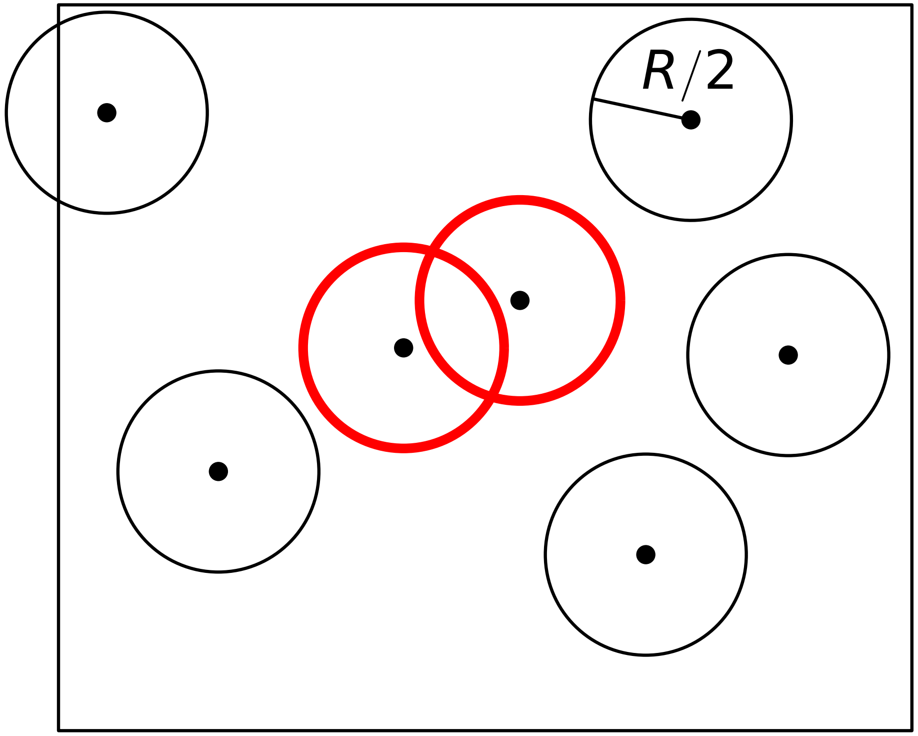

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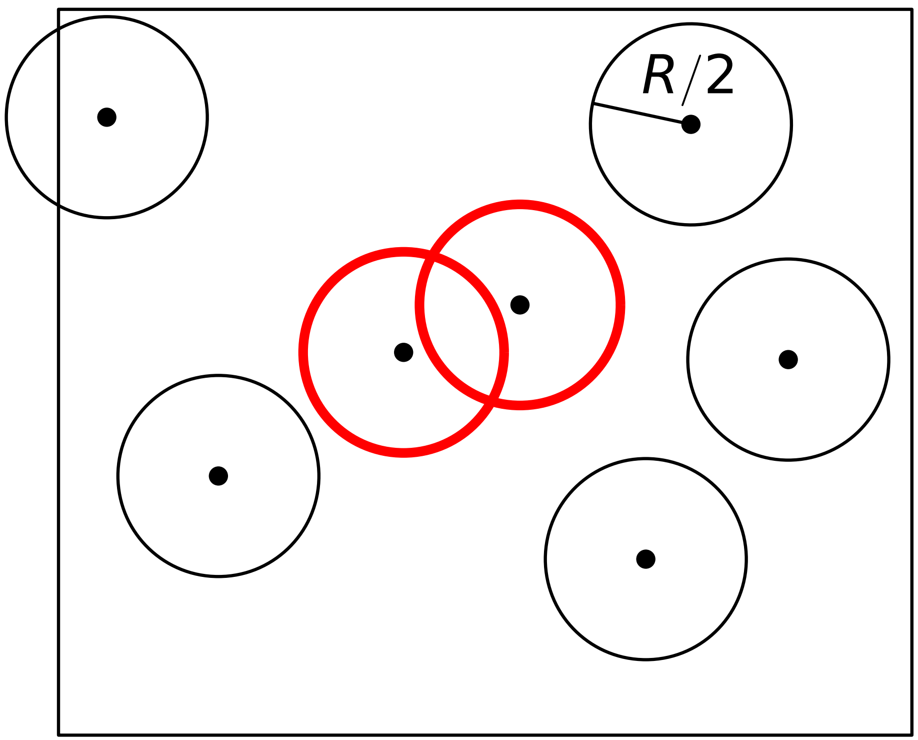

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inspired the hard-core model

Properties of potentials

For a pair potential ϕ, we say:

- ϕ is **repulsive** if $\phi \geq 0$
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hard-sphere model: $C_{\phi_R} = \mathrm{vol}\left(\mathbb{B}\left(R\right)\right)$

Absence of phase transition

Groeneveld ’60, Ruelle ’63, Penrose ’63 :

- analyticity and uniquness for repulsive potentials for $\lambda < \frac{1}{eC_\phi}$

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best known bound is for the hard-sphere model: $\Delta_{\phi_R} \leq \left(1 - (1/8)^{d+1}\right) C_{\phi_R}$

ε-approximation of partition functions:

paper	potentials	regime	running time	type
Friedrich et al. '21	hard-sphere	$\lambda < e/C_{\phi_R}$	$\text{poly}\left(\text{vol}\left(\mathbb{V}\right)\right)$	randomized
Friedrich et al. '22	hard-sphere	$\lambda < e/C_{\phi_R}$	$\widetilde{\mathcal{O}}\left(\text{vol}\left(\mathbb{V}\right)^4\right)$ $\text{vol}\left(\mathbb{V}\right)^{\mathcal{O}\left(\log(\text{vol}(\mathbb{V}))\right)}$	randomized deterministic
Friedrich et al. '22	repulsive	$\lambda < e/C_{\phi}$	$\widetilde{\mathcal{O}}\left(\text{vol}\left(\mathbb{V}\right)^4\right)$	randomized
Michelen et al. '22	repulsive with bounded range	$\lambda < e/\Delta_{\phi}$	$\widetilde{\mathcal{O}}\left(\text{vol}\left(\mathbb{V}\right)^3\right)$	randomized
Jenssen et al. '22	smooth, repulsive with bounded range	$\lambda < e/\Delta_{\phi}$	$\text{vol}\left(\mathbb{V}\right)^{\mathcal{O}\left(\log(\text{vol}(\mathbb{V}))^2\right)}$	deterministic
Anand et al. '23	repulsive with bounded range	$\lambda < e/\Delta_{\phi}$	$\widetilde{\mathcal{O}}\left(\text{vol}\left(\mathbb{V}\right)\right)$	perfect sampler

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Discretization: hard-sphere model

Basic idea: $(\mathbb{V}, \lambda, R) \xrightarrow{\rho \in \mathbb{R}_{>0}} (G_\rho, \lambda_\rho)$

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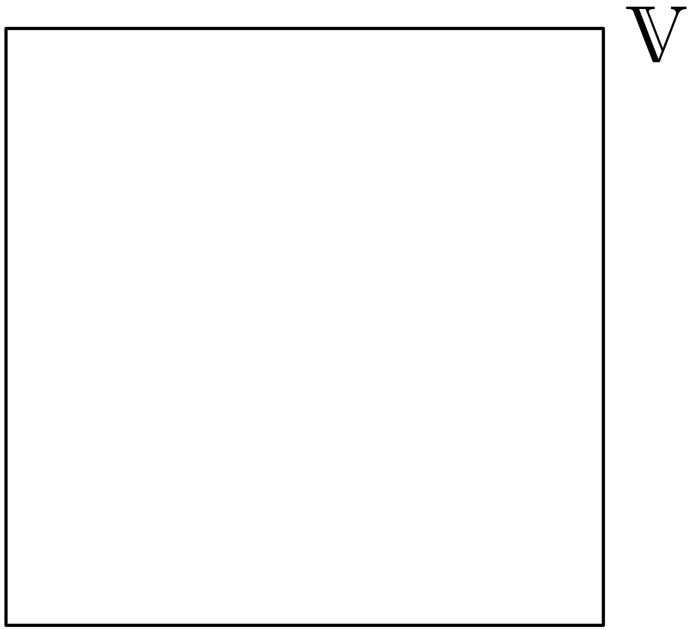

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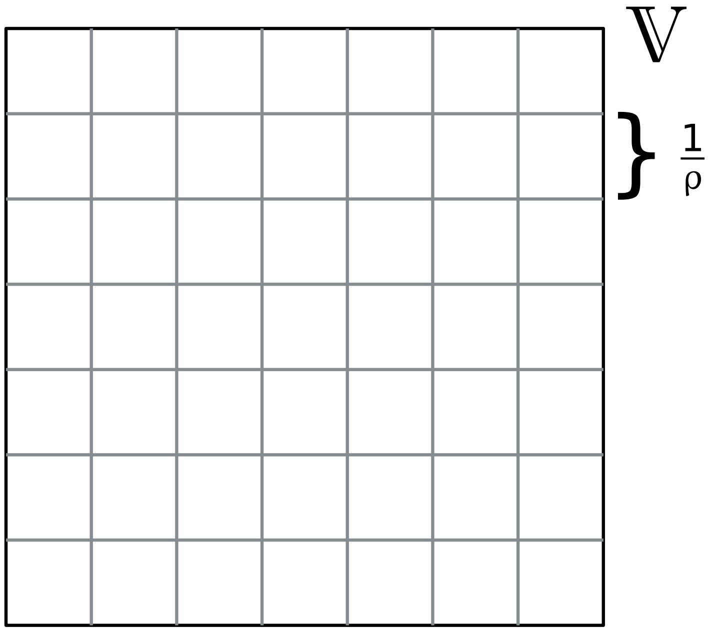

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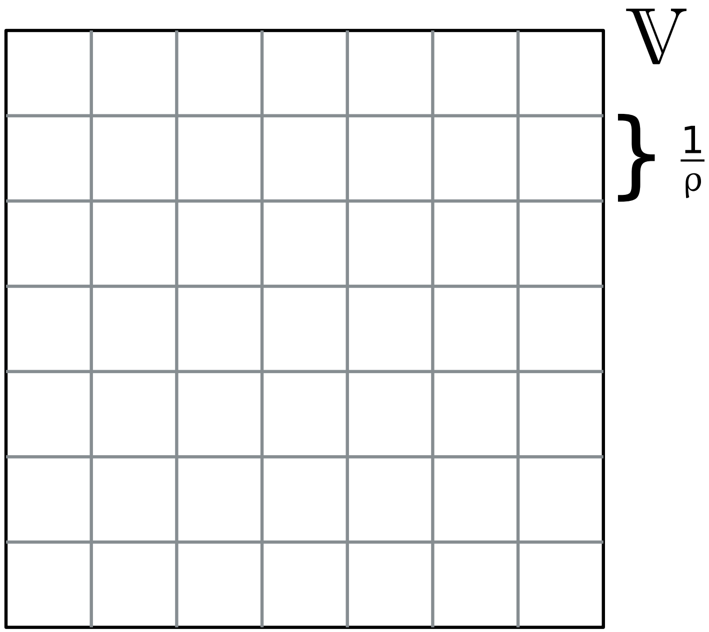

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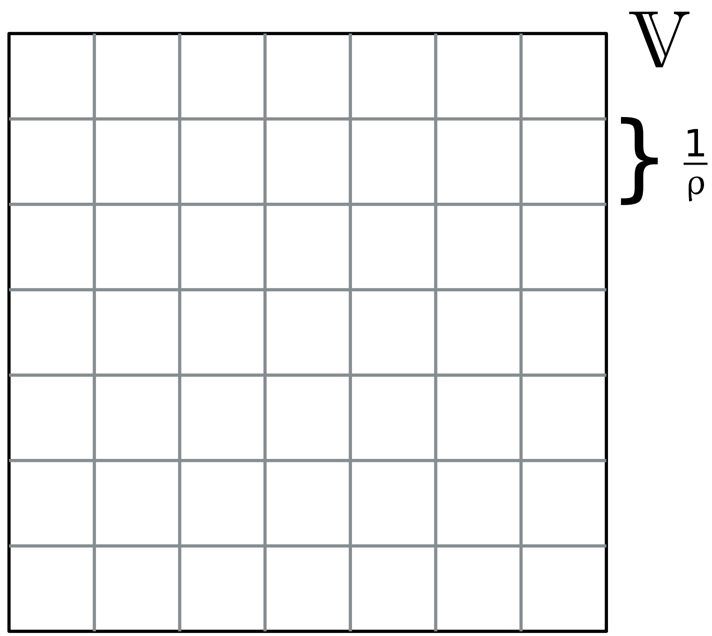

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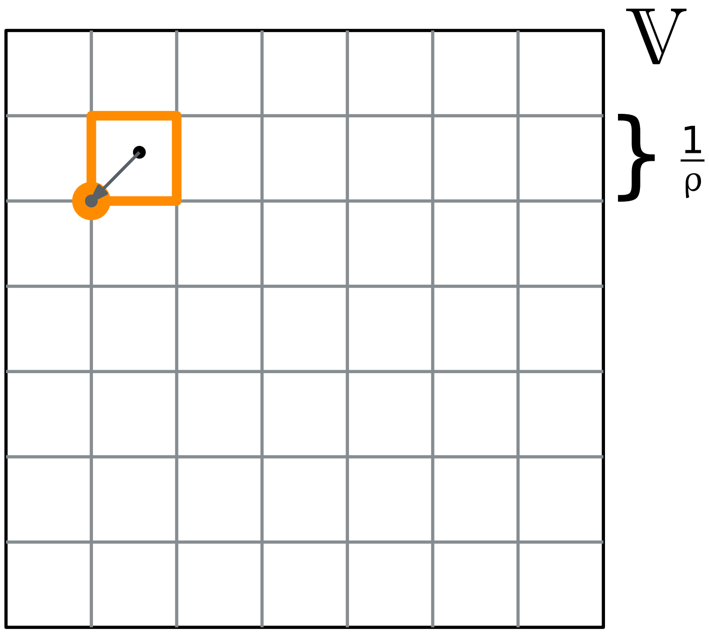

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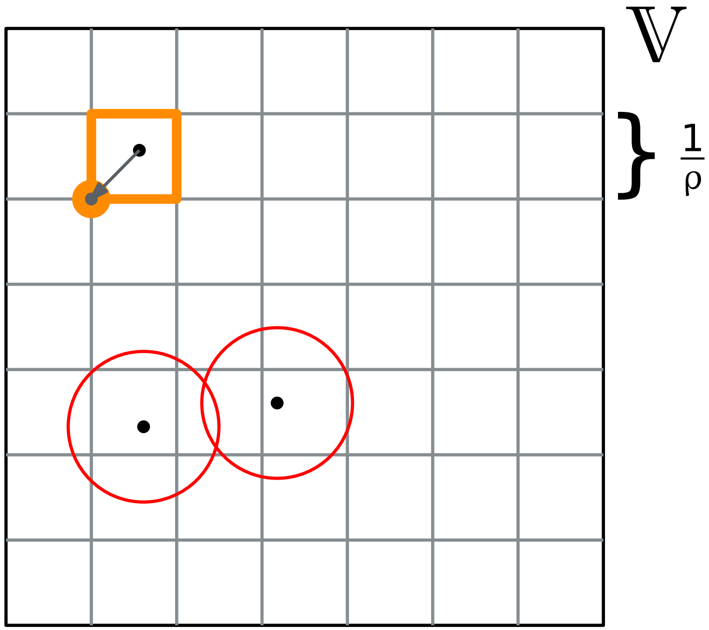

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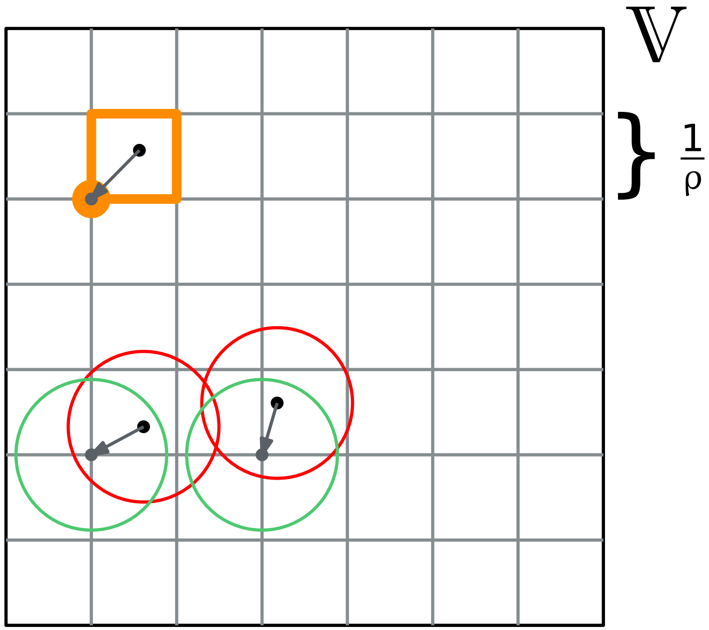

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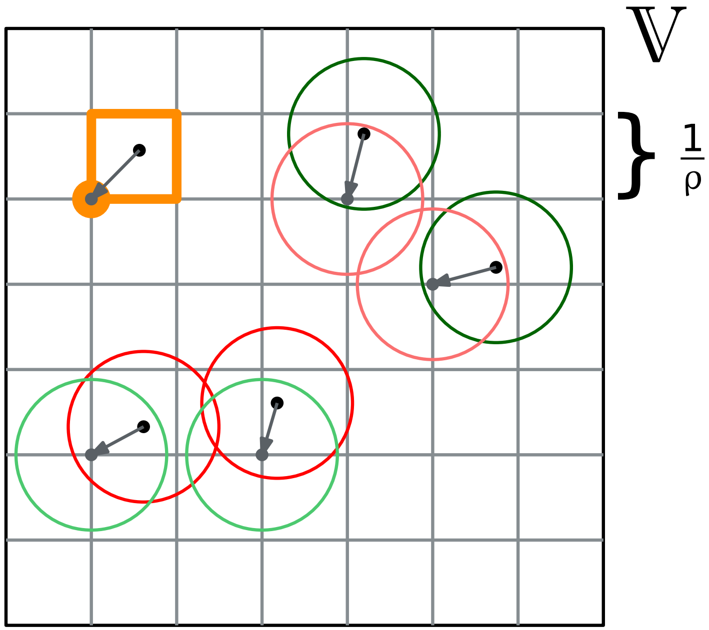

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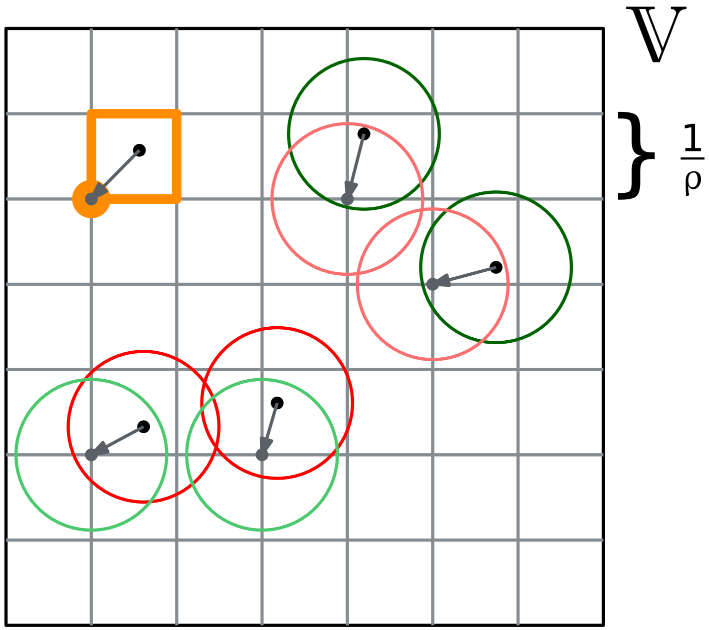

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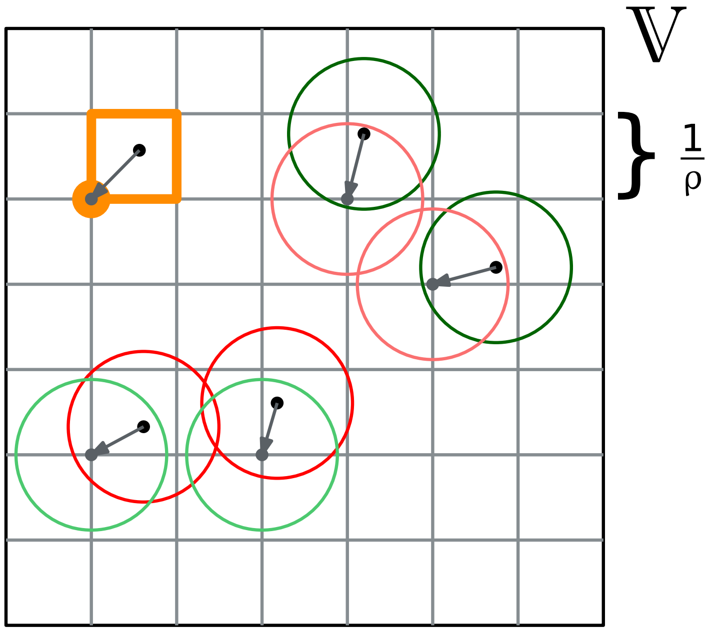

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Friedrich et al. 2022: $\left|\Xi_{\mathbb{V}}\left(\phi_R, \lambda\right) - Z\left(G_\rho, \lambda_\rho\right)\right| \leq \frac{\mathrm{vol}(\mathbb{V})^{1/d}}{\rho} \cdot \Xi_{\mathbb{V}}\left(\phi_R, \lambda\right)$

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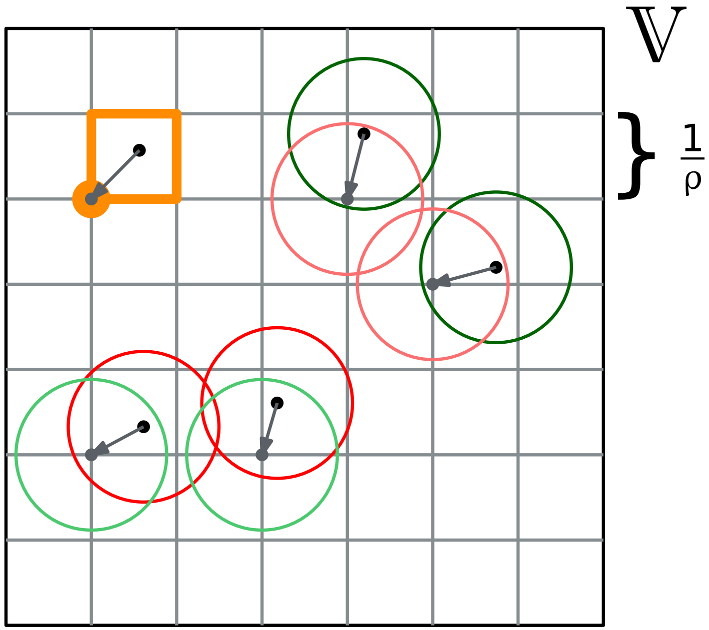

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Observations:

1. for $\rho \in \Theta\left(\text{vol}\left(\mathbb{V}\right)^{1/d}\right)$ we have $|V_\rho| \in \Theta\left(\text{vol}\left(\mathbb{V}\right)^2\right)$ and $\Delta_{G_\rho} \in \Theta\left(\text{vol}\left(\mathbb{V}\right)\right)$
2. for $\lambda < \frac{e}{C_{\phi_R}}$ we have $\lambda_\rho < \frac{e}{\Delta_{G_\rho}} \approx \lambda^*\left(\Delta_{G_\rho}\right)$

Problems with general repulsive potentials:

adversarial potentials

soft interactions

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adversarial potentials → randomize vertices

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Repulsive potentials: random graphs

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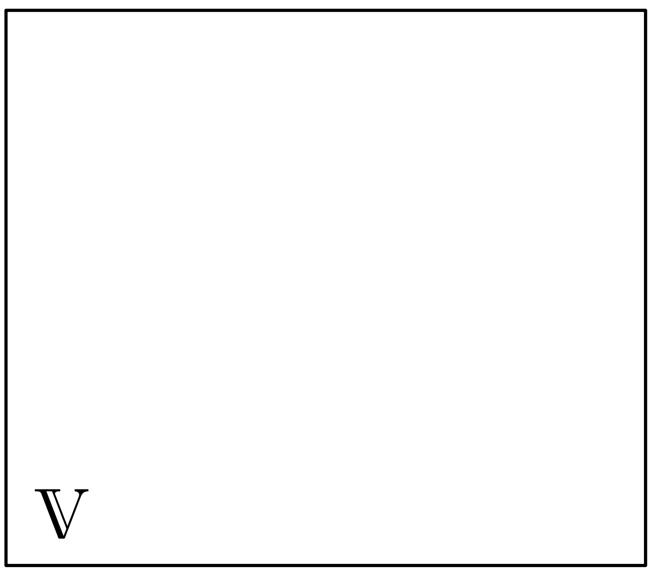
Given $\mathbb{V}$, ϕ, λ and $n \in \mathbb{N}_{\geq 1}$



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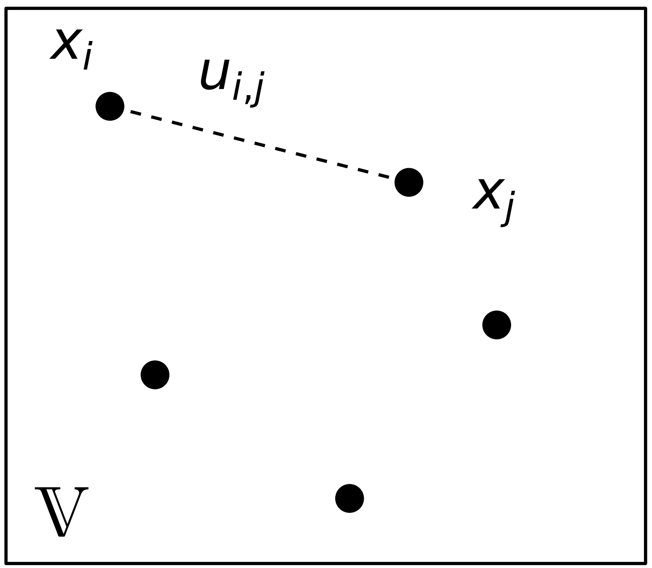

random graph model $\zeta^{(n)}_{\mathbb{V},\phi}$:

$\boldsymbol{x}$: choose $x_1, \cdots, x_n \sim U(\mathbb{V})$ (uniform) i.i.d.

$\boldsymbol{u}$: for $i < j$ choose $u_{i,j} \sim U[0,1]$ i.i.d.

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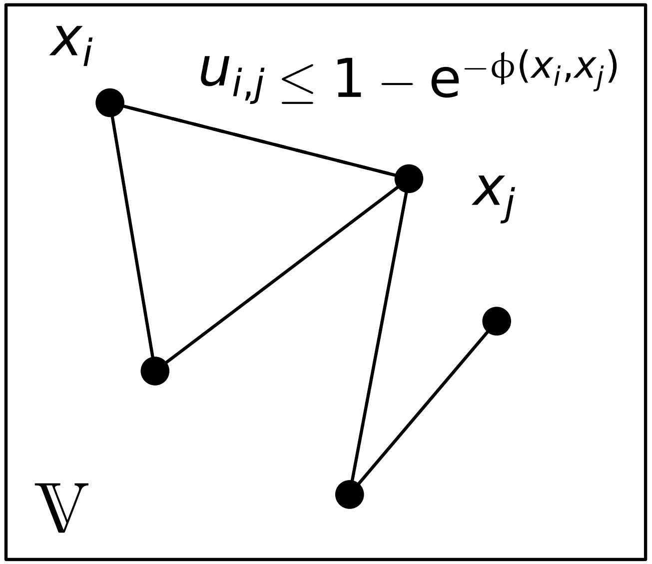

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output $G(\boldsymbol{x}, \boldsymbol{u})$: connect v_i, v_j iff $u_{i,j} \leq 1 - e^{-\phi(x_i,x_j)}$

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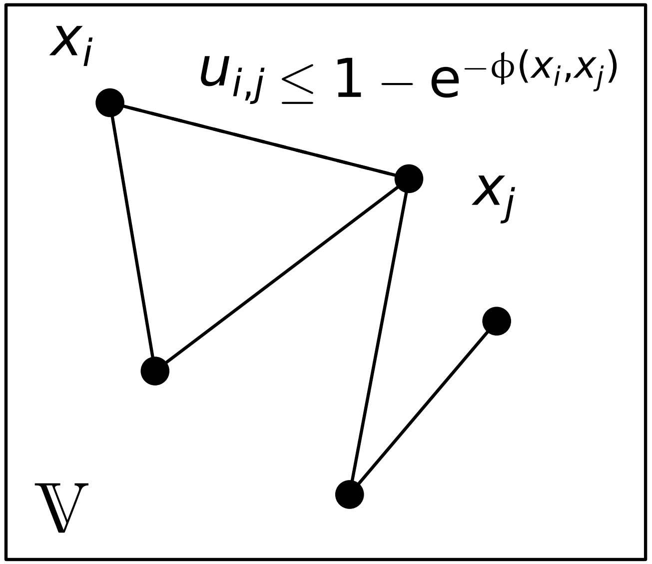

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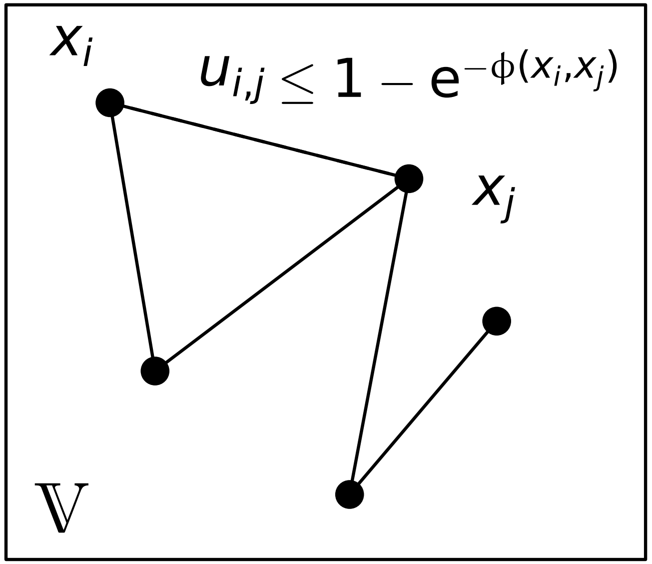

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What can we say about $Z\left(G(\boldsymbol{x}, \boldsymbol{u}), \lambda_n(\lambda)\right)$**?**

Lemma: $\mathbb{E}\left[Z\left(G(\boldsymbol{x}, \boldsymbol{u}), \lambda_n(\lambda)\right)\right] \approx \Xi_{\mathbb{V}}(\phi, \lambda)$ for $n \geq \Theta\left(\mathrm{vol}(\mathbb{V})^2\right)$

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Does $Z\left(G(\boldsymbol{x}, \boldsymbol{u}), \lambda_n(\lambda)\right)$ **concentrate around its expectation?**

Observation: function of independent random variables

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Idea: McDiarmid's inequality (a.k.a. bounded differences)

Requirement: function needs to be c-Lipschitz w.r.t. Hamming distance

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(counter example)

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Observation: $Z\left(G(\boldsymbol{x},\boldsymbol{u}),\lambda_n(\lambda)\right)$ exhibits small relative differences

($|Z - Z'| \leq c(n) \cdot \min\{Z, Z'\}$ for $c(n) \to 0$)

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Theorem:

Let $\mathcal{Y} = \mathcal{Y}_1 \times \cdots \times \mathcal{Y}_m$ and $f : \mathcal{Y} \to \mathbb{R}_{\geq 0}$. If, for all $\boldsymbol{y}, \boldsymbol{y}^{(i)} \in \mathcal{Y}$ that differ only at position i,

$$\left|f(\boldsymbol{y}) - f(\boldsymbol{y}^{(i)})\right| \leq c_i \min\{f(\boldsymbol{y}), f(\boldsymbol{y}^{(i)})\}$$

with $C := \sum_i c_i^2 < 1$ then

$$\mathbb{P}_\nu\left[\left|f - \mathbb{E}_\nu\left[f\right]\right| \geq \varepsilon \mathbb{E}_\nu\left[f\right]\right] \leq C \cdot \varepsilon^{-2}$$

for all $\varepsilon > 0$ and product distributions ν on $\mathcal{Y}$.

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~~**Theorem:**~~ **Corollary of Efron-Stein inequality:**

Let $\mathcal{Y} = \mathcal{Y}_1 \times \cdots \times \mathcal{Y}_m$ and $f : \mathcal{Y} \to \mathbb{R}_{\geq 0}$. If, for all $\boldsymbol{y}, \boldsymbol{y}^{(i)} \in \mathcal{Y}$ that differ only at position i,

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Repulsive potentials: assembling the pieces

Theorem: For $n \geq \Theta\left(\mathrm{vol}\left(\mathbb{V}\right)^2 \delta^{-1} \varepsilon^{-2}\right)$ it holds that

$$\mathbb{P}\left[\left|Z\left(G(\boldsymbol{x}, \boldsymbol{u}), \lambda_n(\lambda)\right) - \mathbb{E}\left[Z\left(G(\boldsymbol{x}, \boldsymbol{u}), \lambda_n(\lambda)\right)\right]\right| \geq \varepsilon \mathbb{E}\left[Z\left(G(\boldsymbol{x}, \boldsymbol{u}), \lambda_n(\lambda)\right)\right]\right] \leq \delta.$$

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Recall that $\mathbb{E}\left[Z\left(G(\boldsymbol{x}, \boldsymbol{u}), \lambda_n(\lambda)\right)\right] \approx \Xi_{\mathbb{V}}\,(\phi, \lambda)$ for $n \geq \Theta\left(\text{vol}\,(\mathbb{V})^2\right)$.

Corollary: For $n \geq \Theta\left(\text{vol}\,(\mathbb{V})^2\, \delta^{-1} \varepsilon^{-2}\right)$ it holds that

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Algorithm (sketch):

1. draw $G \sim \zeta_{\mathbb{V},\phi}^{(n)}$ for $n \in \Theta\left(\text{vol}\,(\mathbb{V})^2\right)$ sufficiently large
2. if $\lambda_n(\lambda) < \lambda^*\left(\Delta_G\right)$: output an approx. of $Z\left(G,\lambda_n(\lambda)\right)$
   else: goto 1

Perfect sampling

Efficient perfect sampling for GPPs:

- Huber '12: perfect sampler for finite-range and repulsive if $\lambda < \frac{2}{C_\phi}$
- Guo et al. '18: perfect sampler for hard-sphere model if $\lambda < \frac{1}{\sqrt{2}C_{\phi_R}}$

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Bounded-range repulsive potentials under SSM

(with Konrad Anand, Marcus Pappik and Will Perkins)

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Idea: adapt perfect samping algorithm for discrete spin systems by Feng et al. ’21 and combine it with Bernoulli factories