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Sampling and approximation algorithms for Gibbs point processes

Tobias Friedrich, **Andreas Göbel**, Max Katzmann, Martin Krejca, Marcus Pappik

Hard-sphere Model

distribution of particles with *hard constraints* in (Euclidean) space

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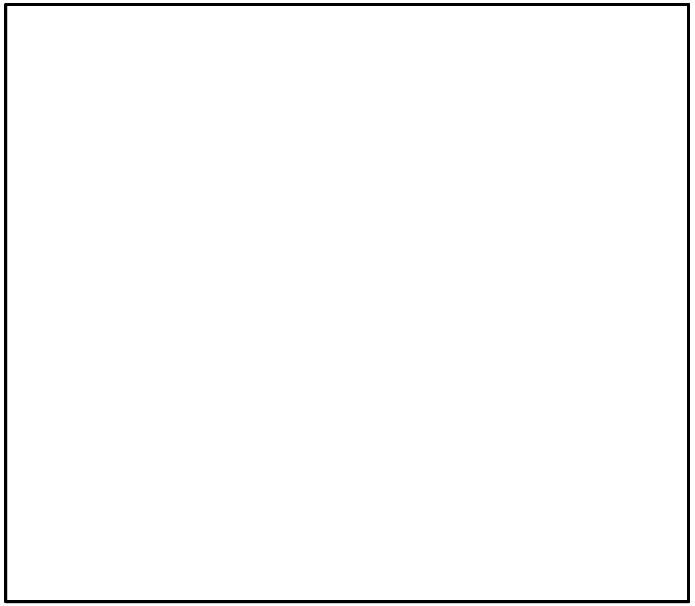

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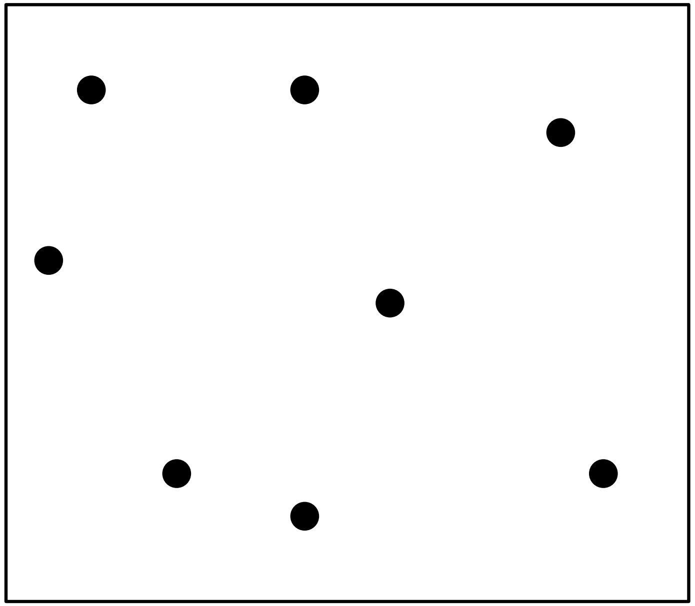

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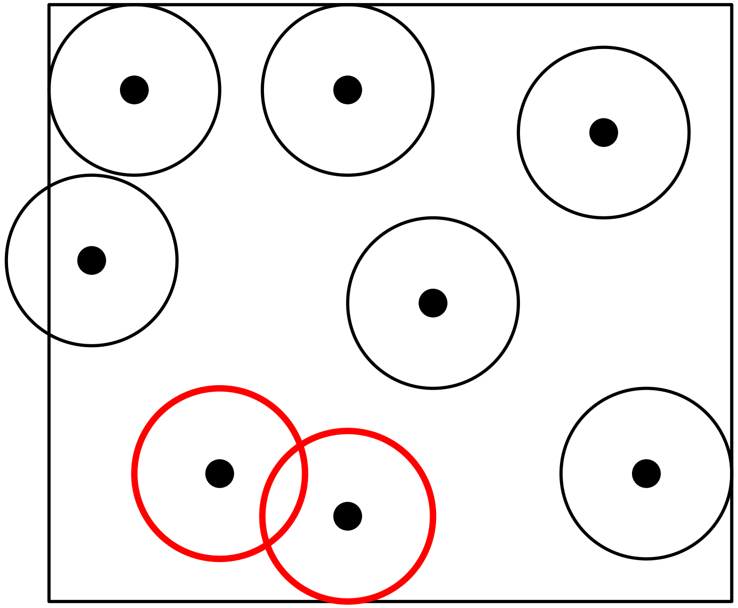

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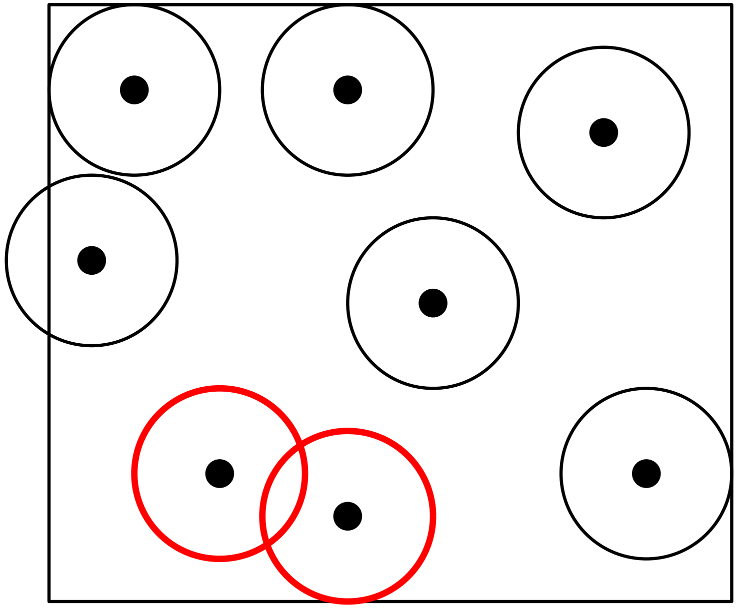

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Gibbs measure:

$$\frac{dP_{\mathbb{V}}^{(\lambda,r)}}{dQ_\lambda}(x_1, \ldots, x_k) = \frac{D_r(x_1, \ldots, x_k) e^{\lambda \nu(\mathbb{V})}}{\Xi_{\mathbb{V}}(\lambda, \phi)}$$

Partition function:

$$\Xi_{\mathbb{V}}(\lambda, r) = 1 + \sum_{k \in \mathbb{N}_{\geq 1}} \frac{\lambda^k}{k!} \int_{\mathbb{V}^k} D_r(x_1, \ldots, x_k) \nu^k(d\mathbf{x})$$

Computational problems

Results:

- Metropolis et al. 1953
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Rigorous run-time guarantees: run-time polynomial in $\nu(\mathbb{V})$

approximately sample

Can we sample from the Gibbs distribution

approximate

Can we compute the partition function

For which parameter range

Phase Transitions:

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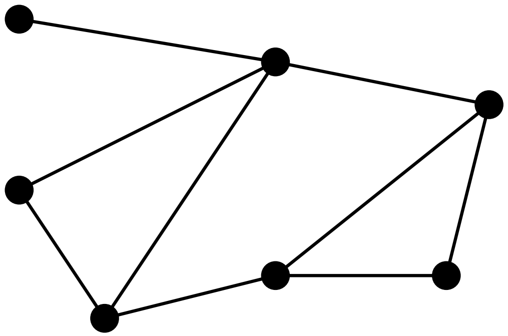
Recent breakthroughs by translating CS methods used on discrete spin systems.

- Helmuth et al. 2020: no phase transition for $\lambda < \frac{2}{\nu(B_{2r})}$
  - Decay of correlations
- Michelen et al. 2020: no phase transition for $\lambda < \frac{e}{\nu(B_{2r})}$
  - Analiticity of the pressure
- Michelen et al. 2021: no phase transition for $\lambda < \frac{e}{(1-8^{-d-1})\nu(B_{2r})}$
  - Potential weighted constant

Discrete world: Hard-core Model

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



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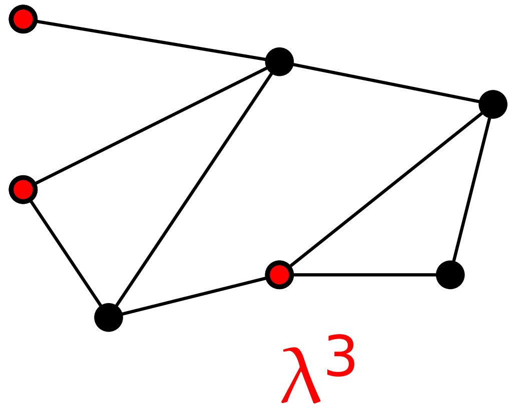

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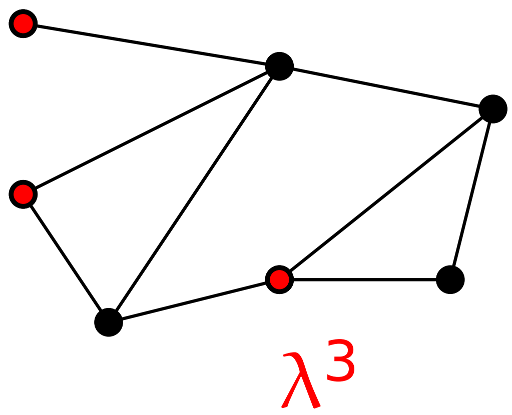

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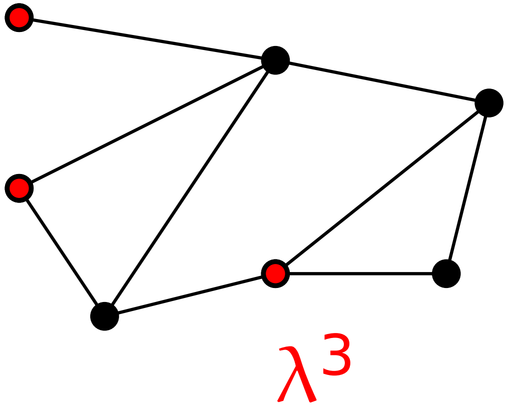

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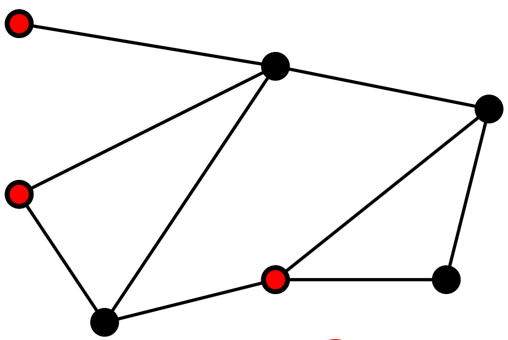

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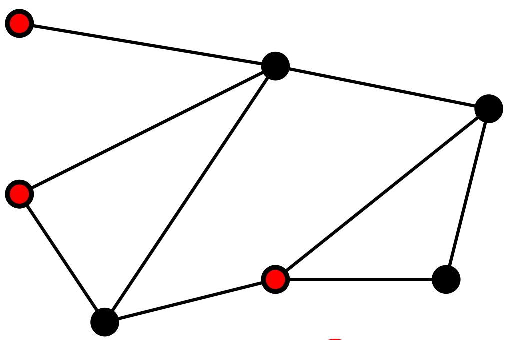

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NP-hard to approximate if $\lambda > \lambda_c(\Delta)$
(Sly 2010, Galanis et al. 2011)

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take hard-sphere instance $(\mathbb{V}, \lambda)$

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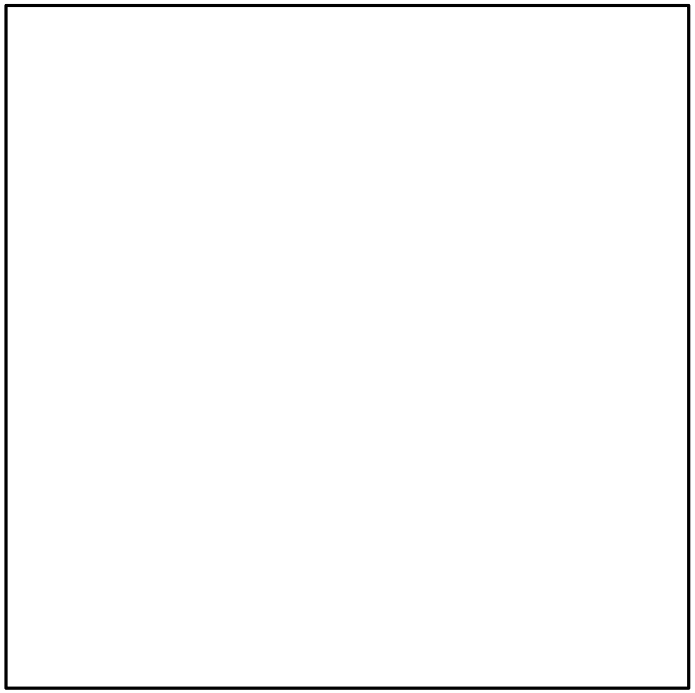
approx. $Z\left(G_{\rho}, \lambda_{\rho}\right)$

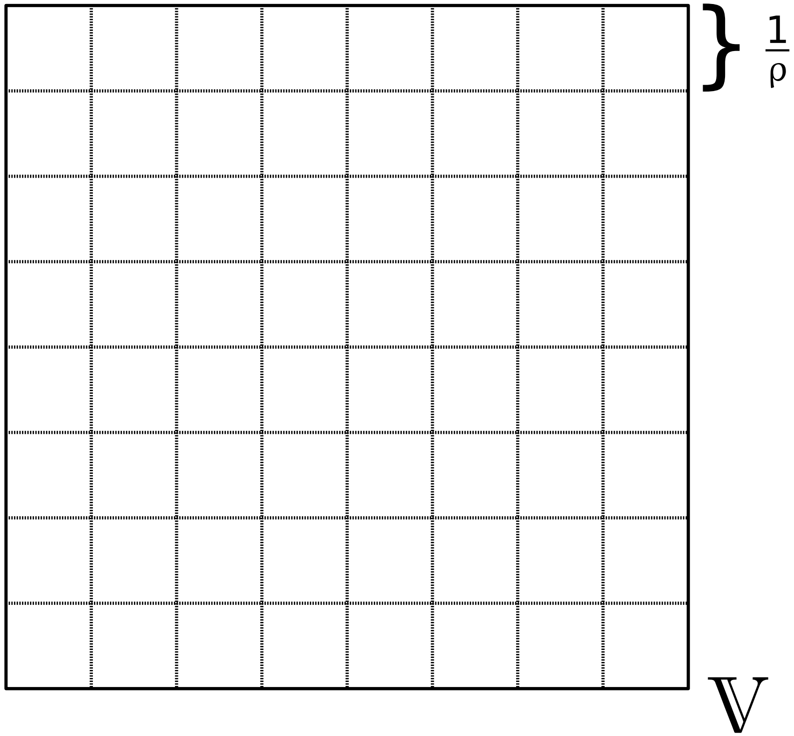
Result is also approximation for $\Xi_{\mathbb{V}}(\lambda, r)$!

1st result: Discretization



$\mathbb{V}$

resolution $\rho \in \mathbb{R}_{\geq 1}$



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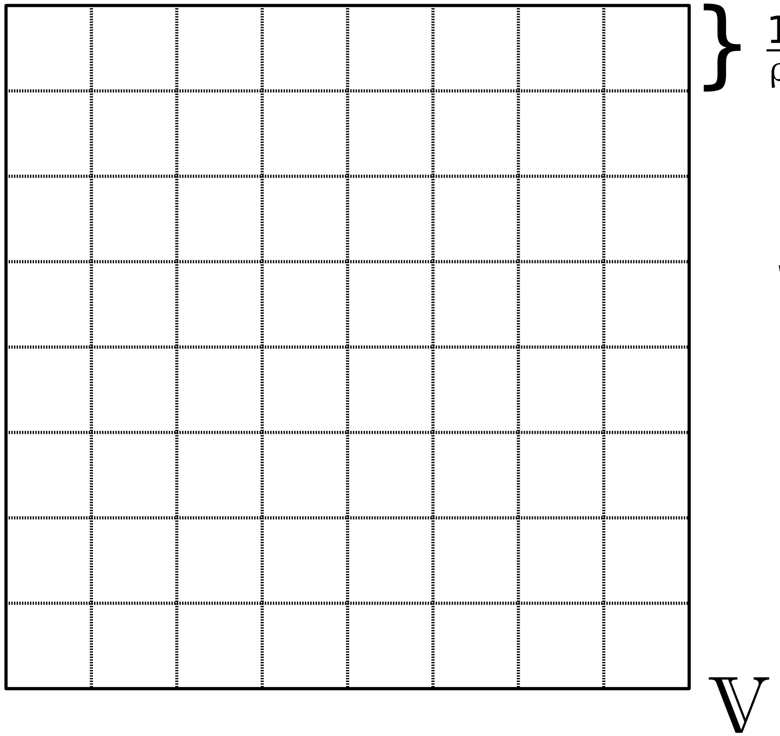

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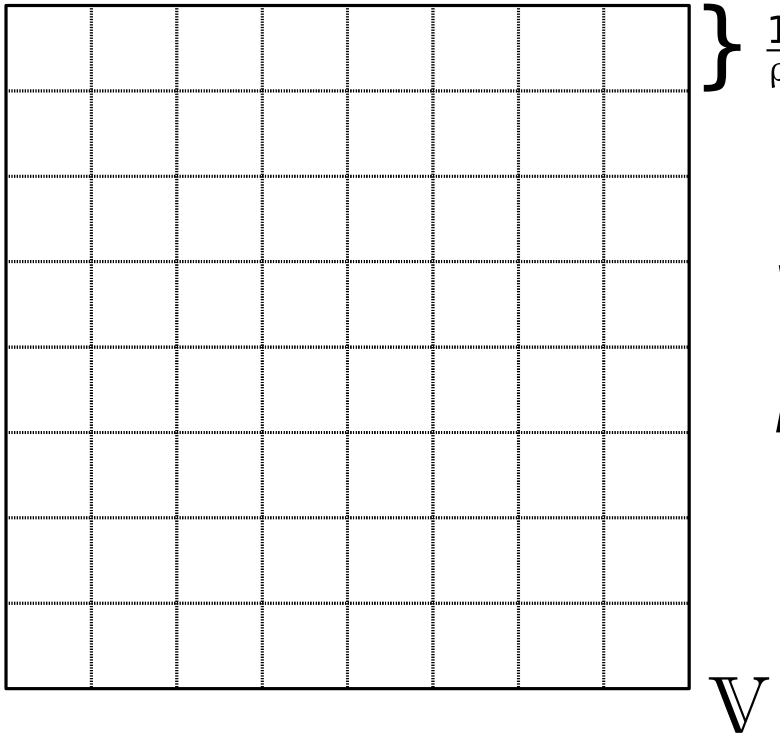

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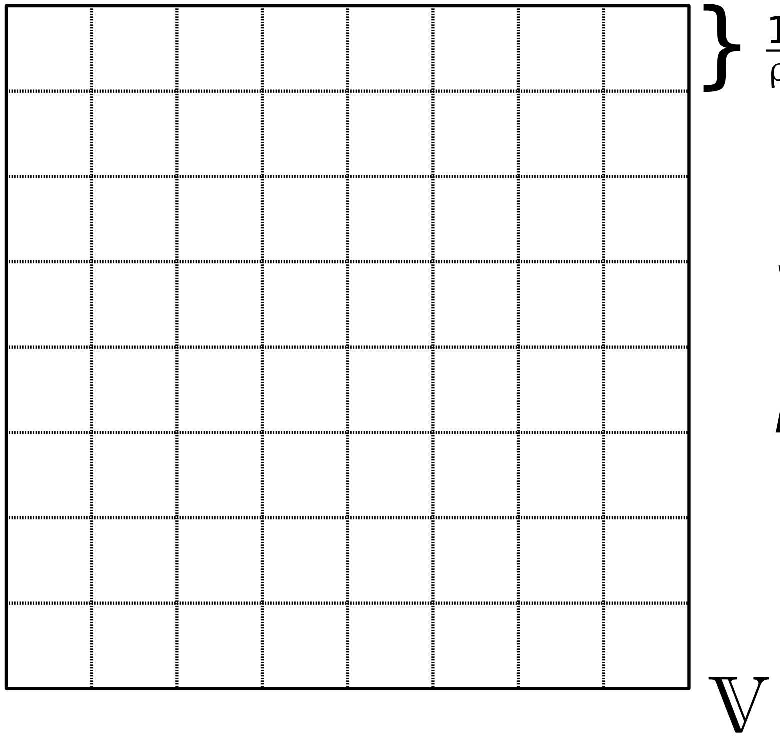

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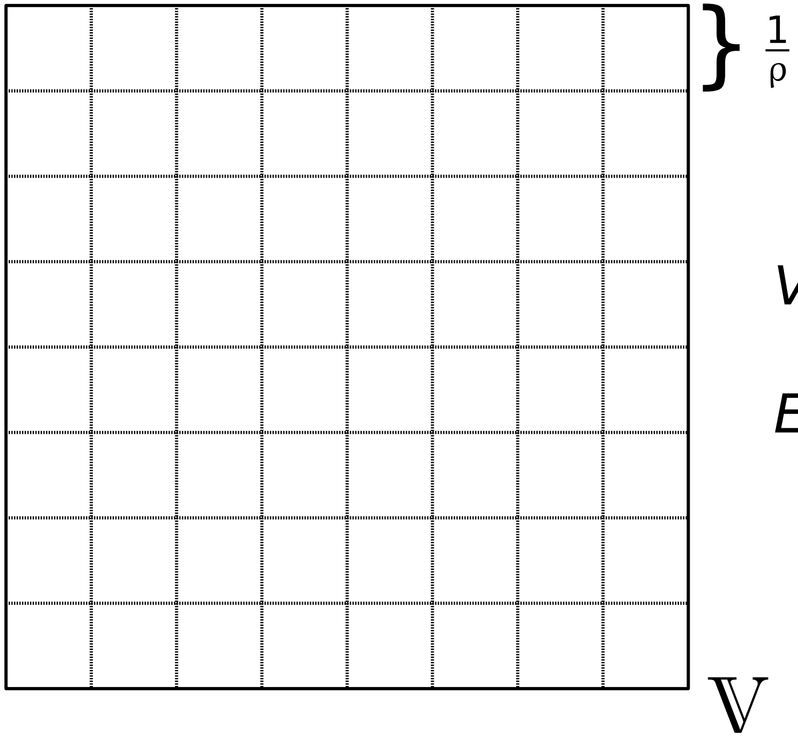

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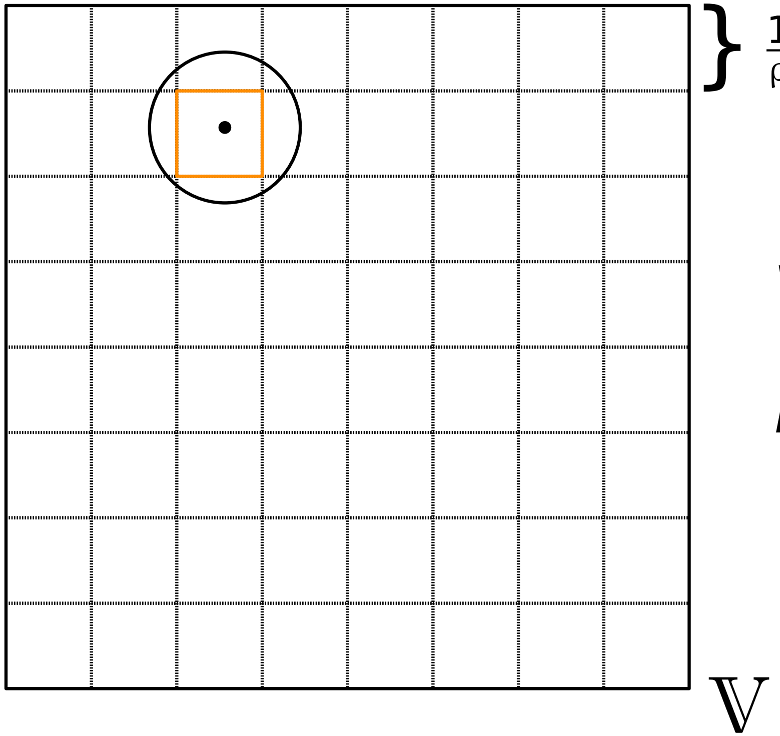

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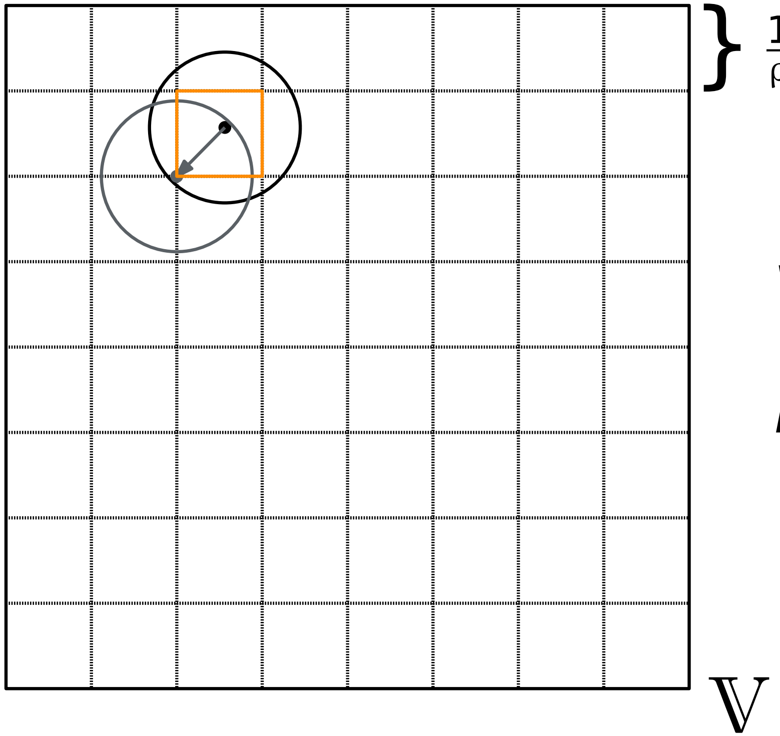

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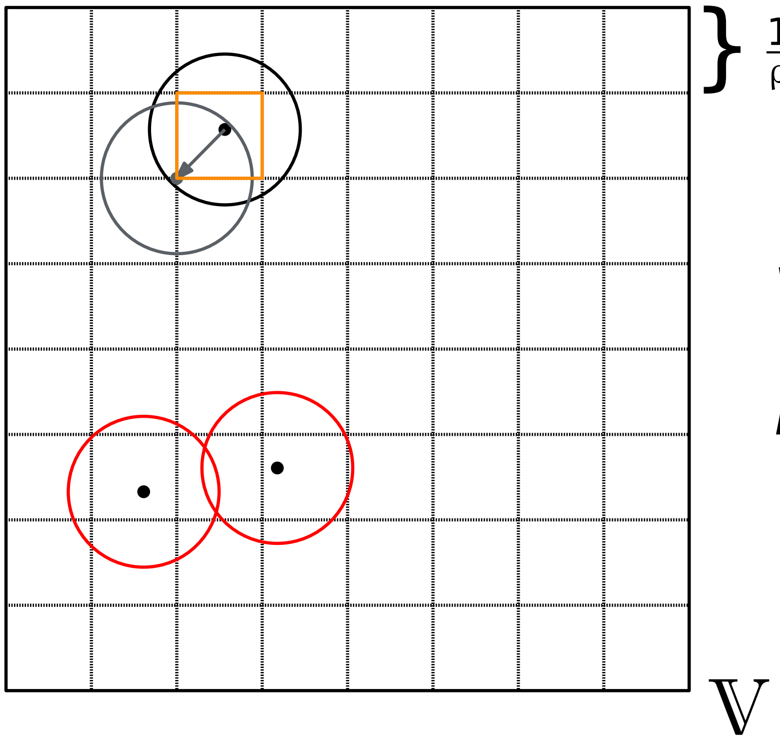

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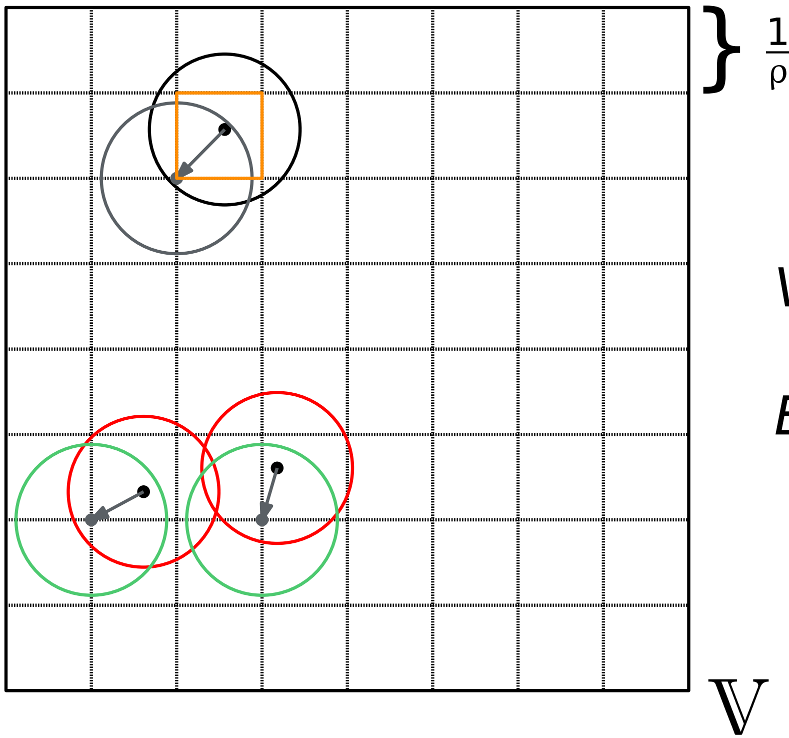

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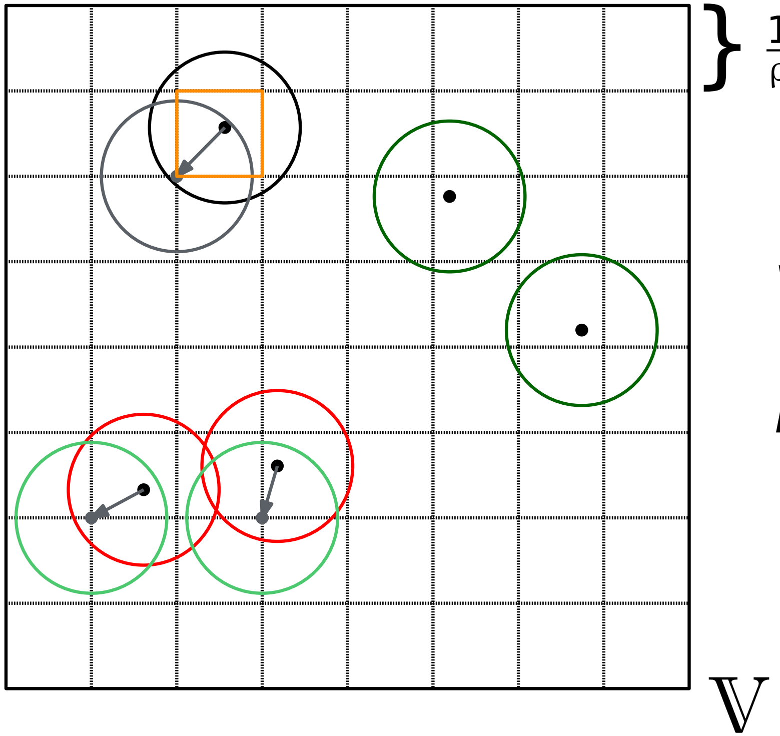

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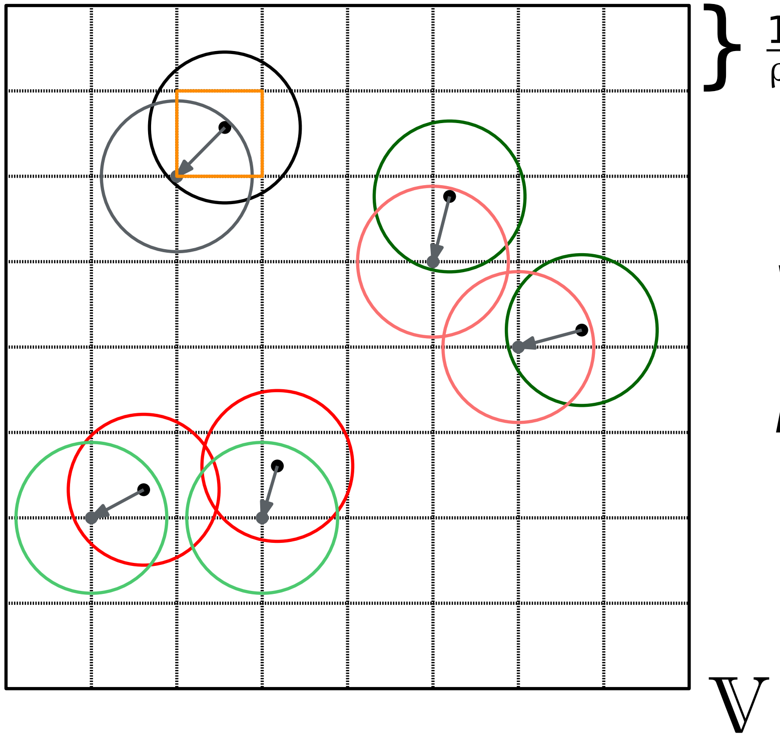

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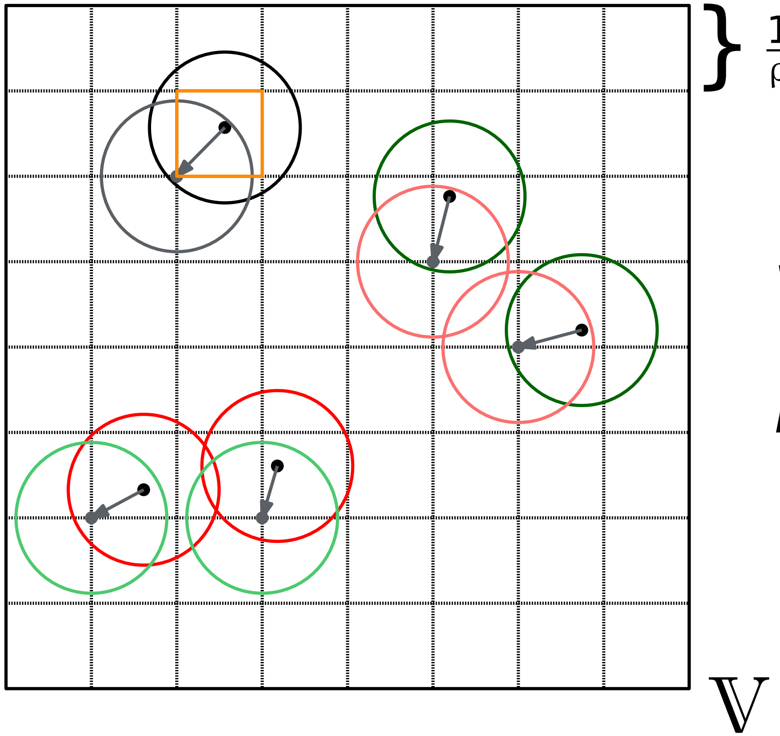

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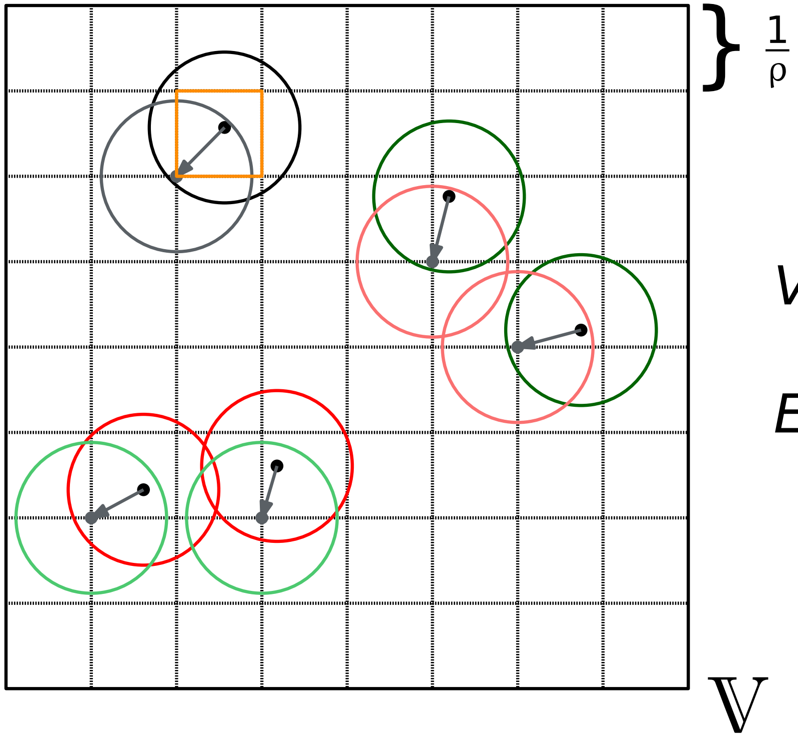

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1st Result: Bounding the volume of erratic configs

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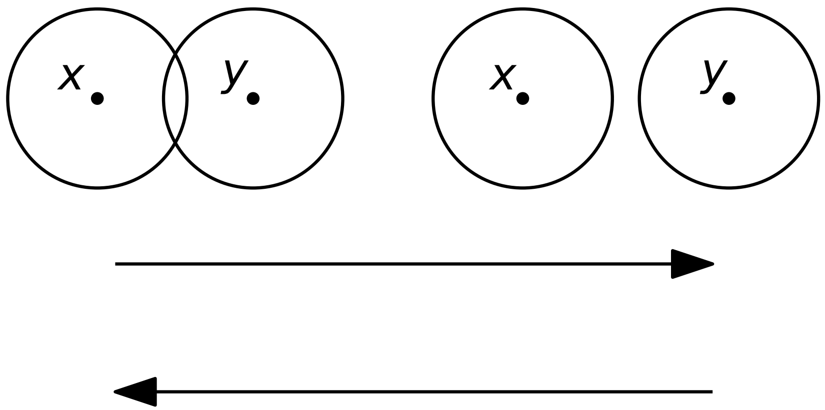

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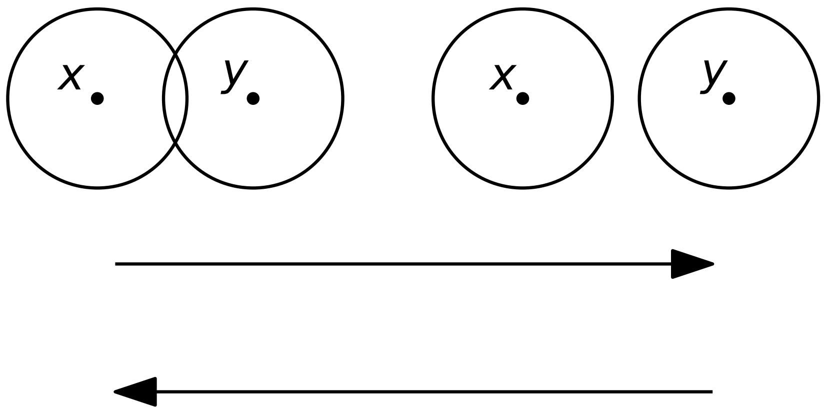

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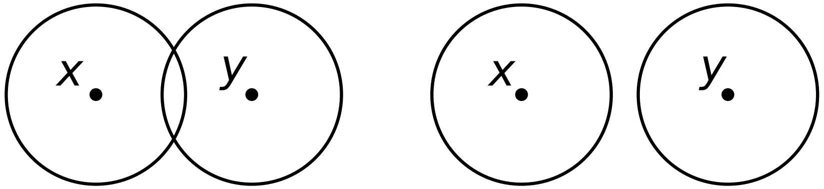

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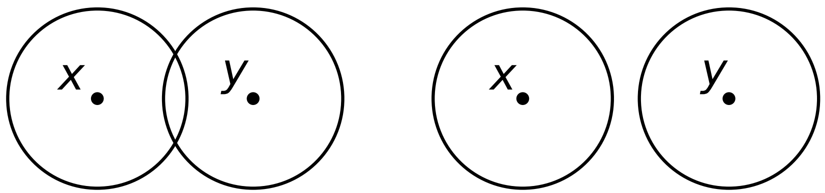

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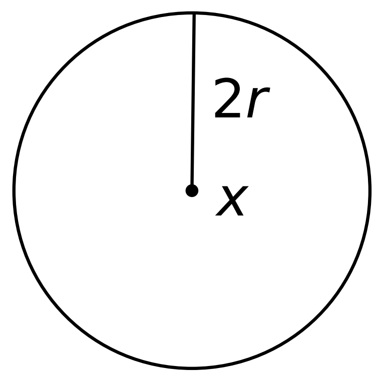

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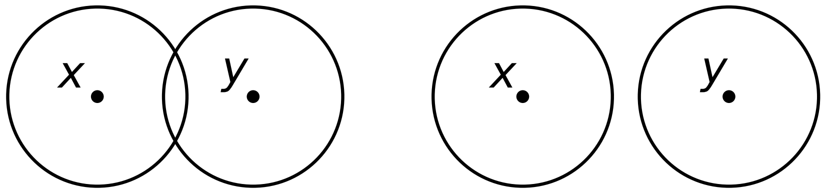

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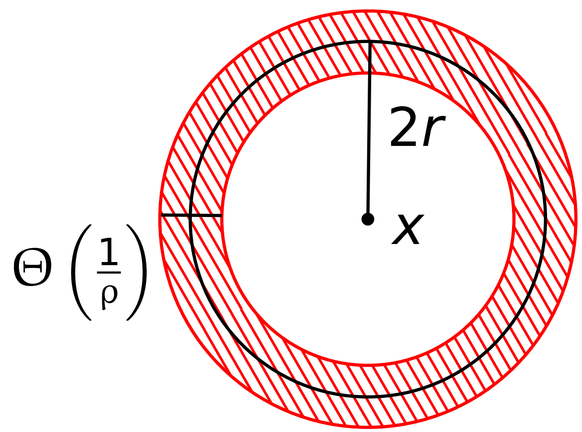

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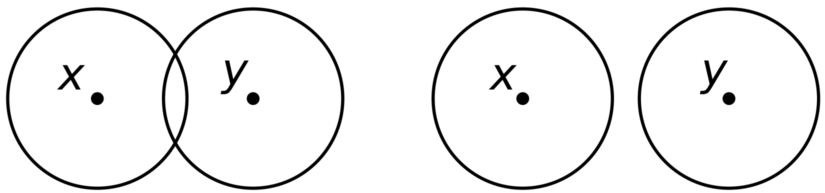

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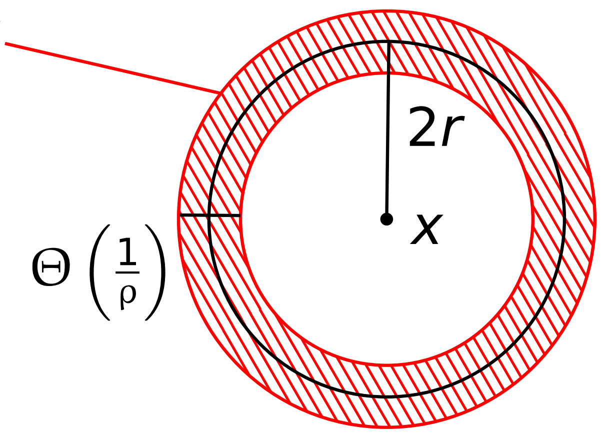

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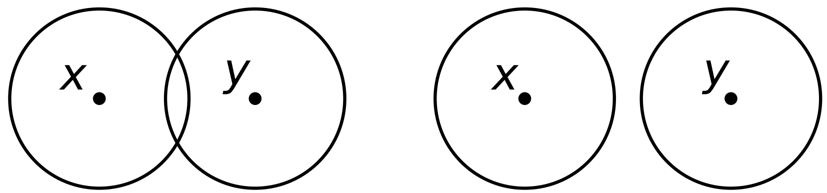

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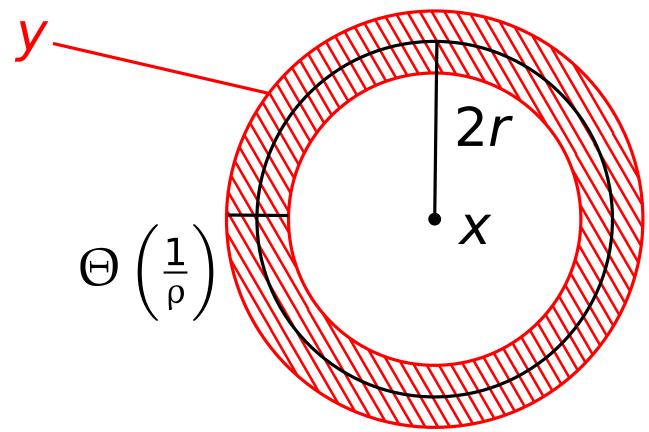

Theorem: $\left|\Xi_{\mathbb{V}}(\lambda, r) - Z\left(G_{\rho}, \lambda_{\rho}\right)\right| \leq \frac{\exp\left(\mathrm{vol}(\mathbb{V}) \ln\left(\mathrm{vol}(\mathbb{V})\right)\right)}{\rho} \cdot \Xi_{\mathbb{V}}(\lambda, r)$

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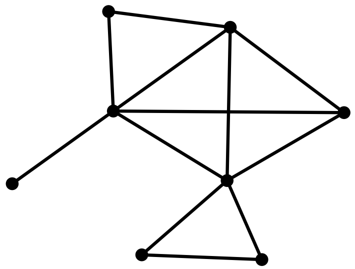
we have $|V_\rho| \approx \rho^d \mathrm{vol}\left(\mathbb{V}\right)$ we would need $\rho \in \Theta\left(\exp\left(\mathrm{vol}\left(\mathbb{V}\right) \ln\left(\mathrm{vol}\left(\mathbb{V}\right)\right)\right)\right)$

Existing algorithms would not run in time poly $\left(\mathrm{vol}\left(\mathbb{V}\right)\right)$!

Glauber Dynamics



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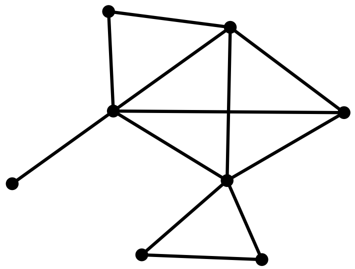
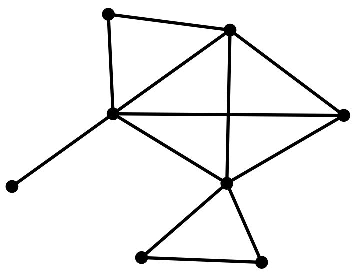


start with some (deterministic) independent set

Glauber Dynamics



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repeat: choose vertex uniformly at random

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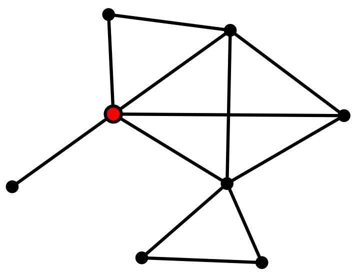

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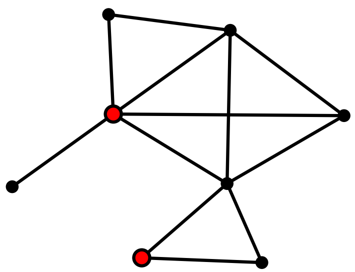

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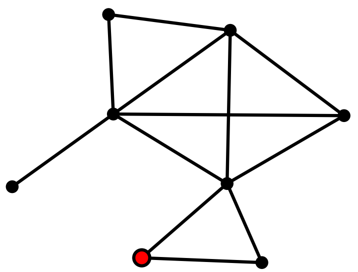

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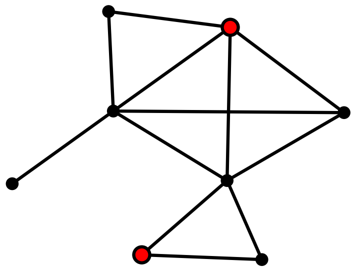

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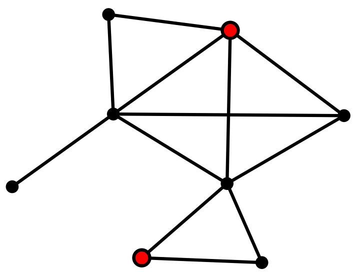

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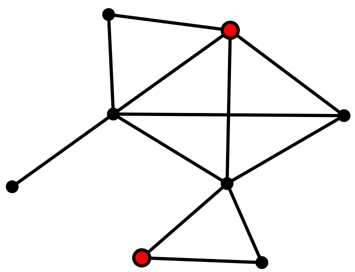

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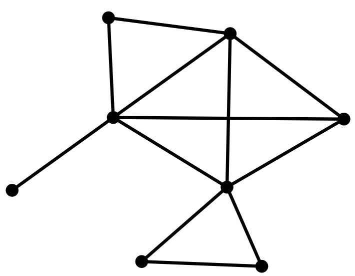

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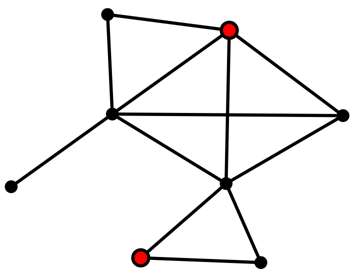

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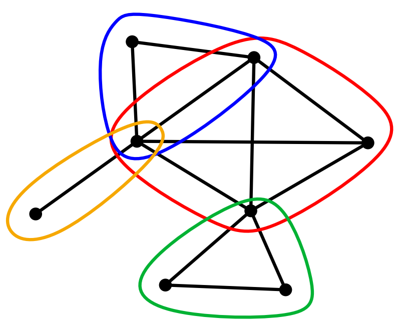
idea: use clique cover to update multiple vertices



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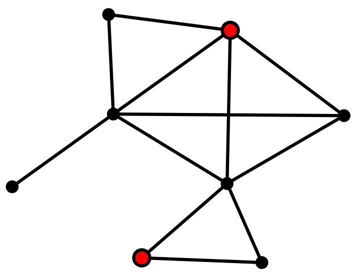

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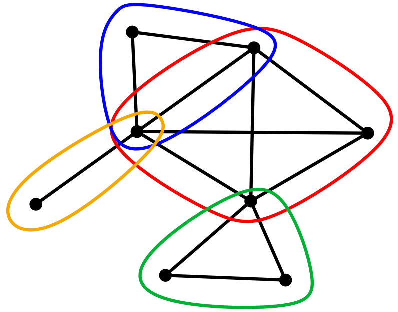

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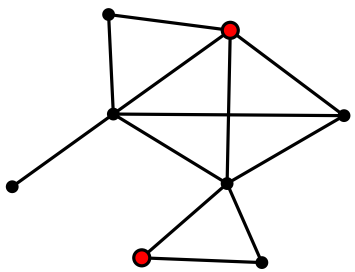

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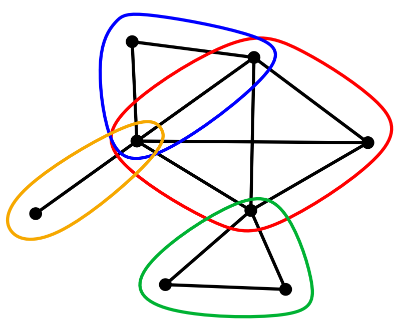

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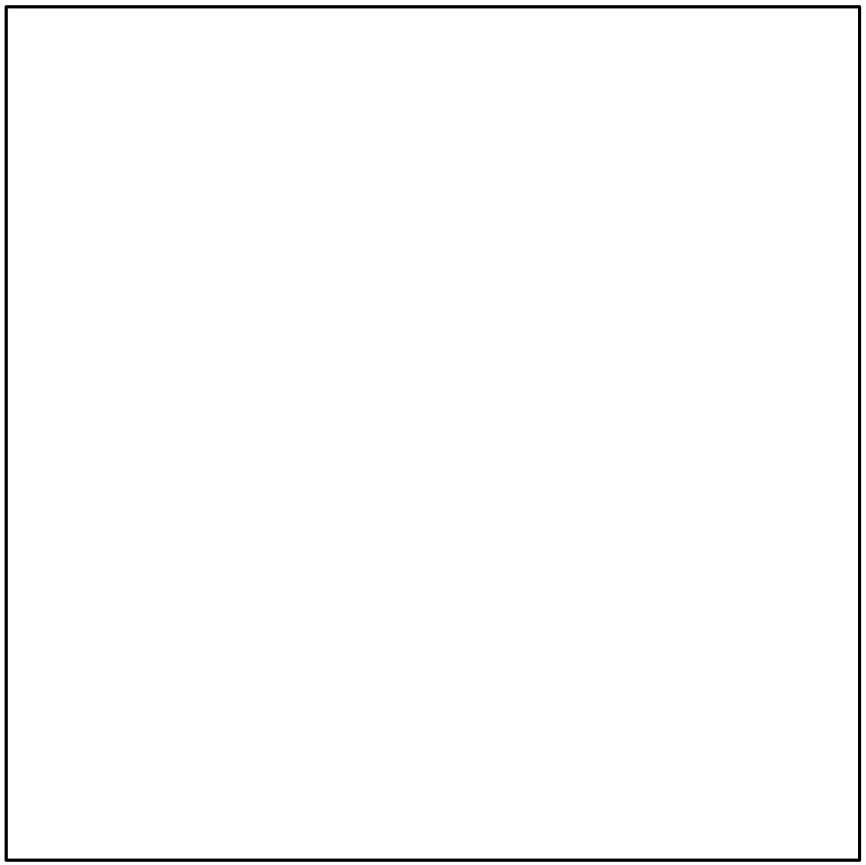
Runtime only depends on the size of the clique cover!

1st Result: Cliques in our Discretization

$\mathbb{V}$



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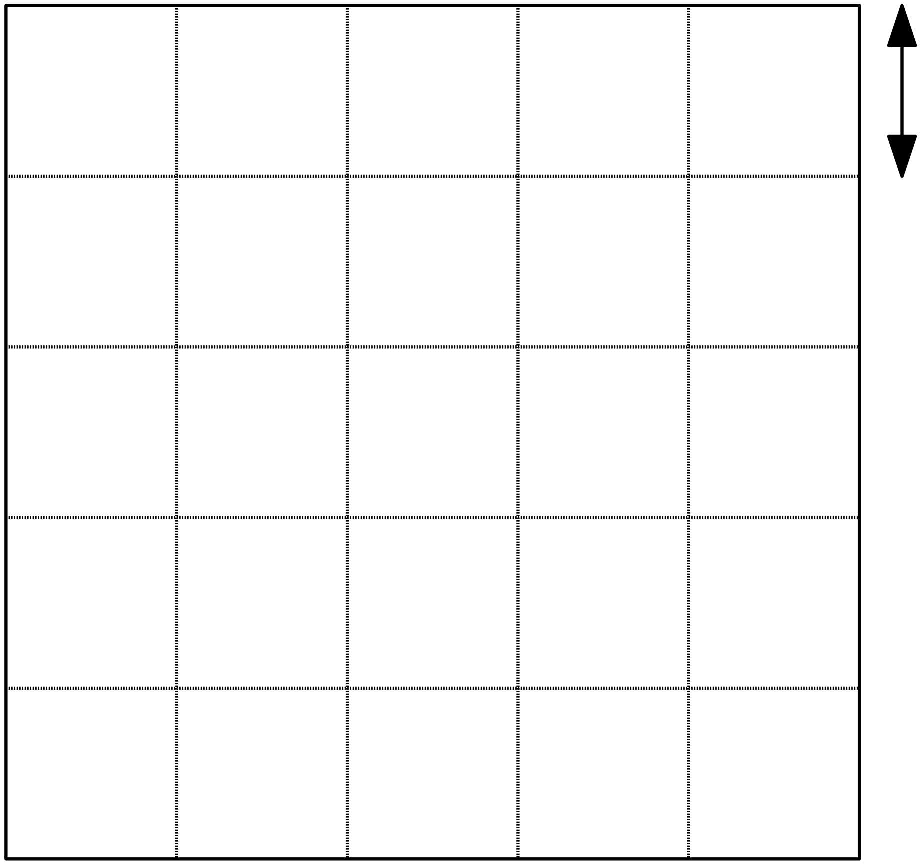

$< \frac{2r}{\sqrt{d}}$

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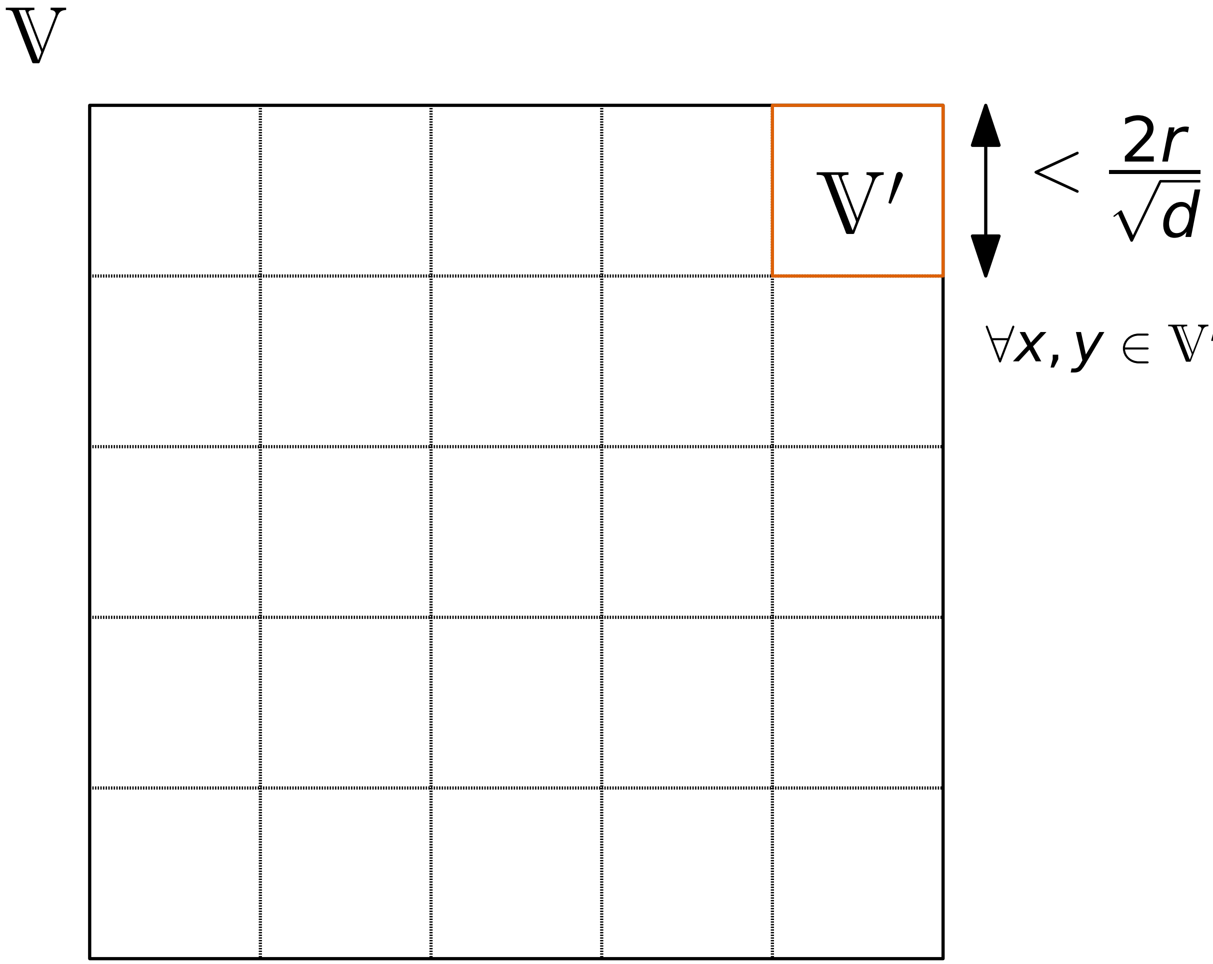

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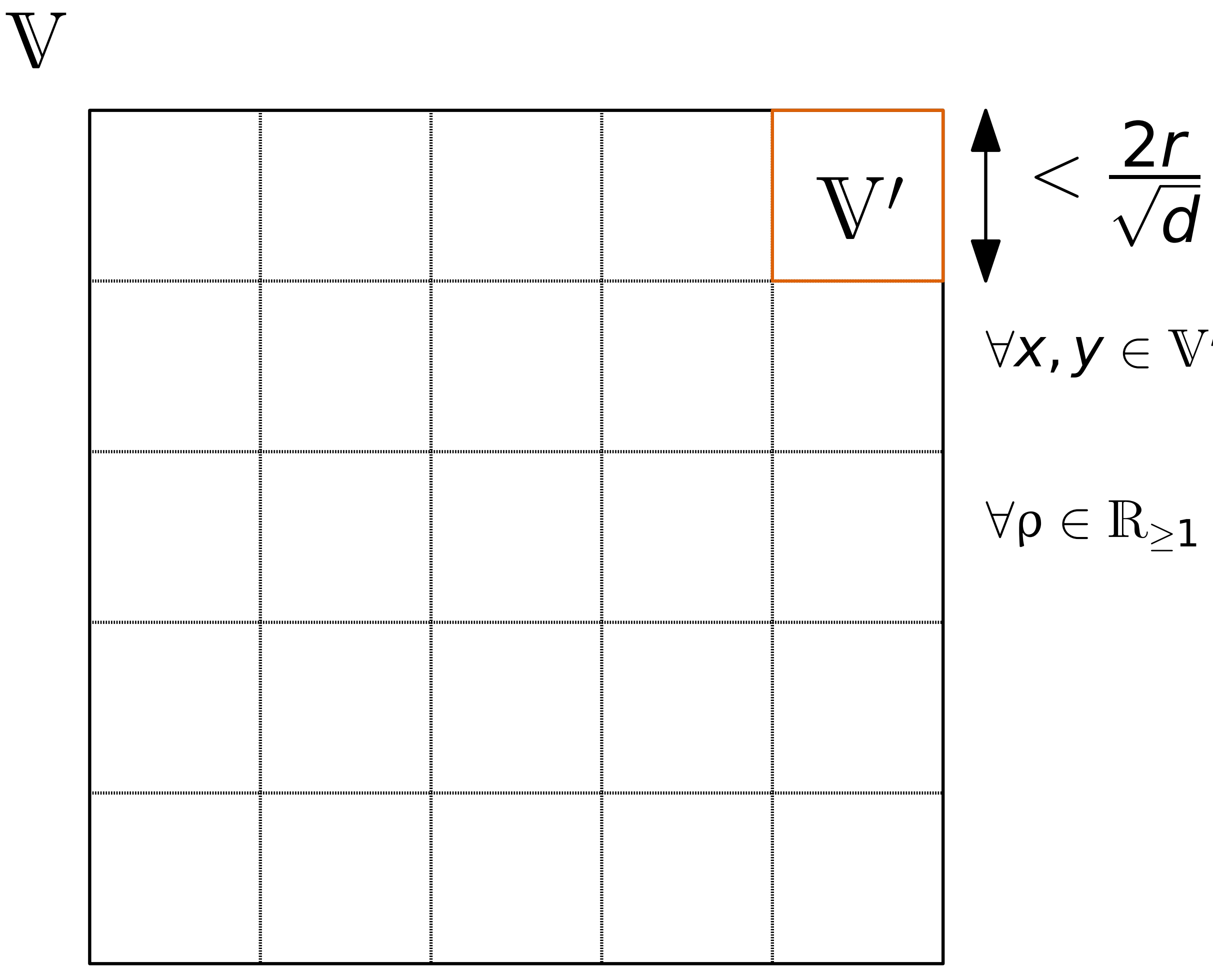

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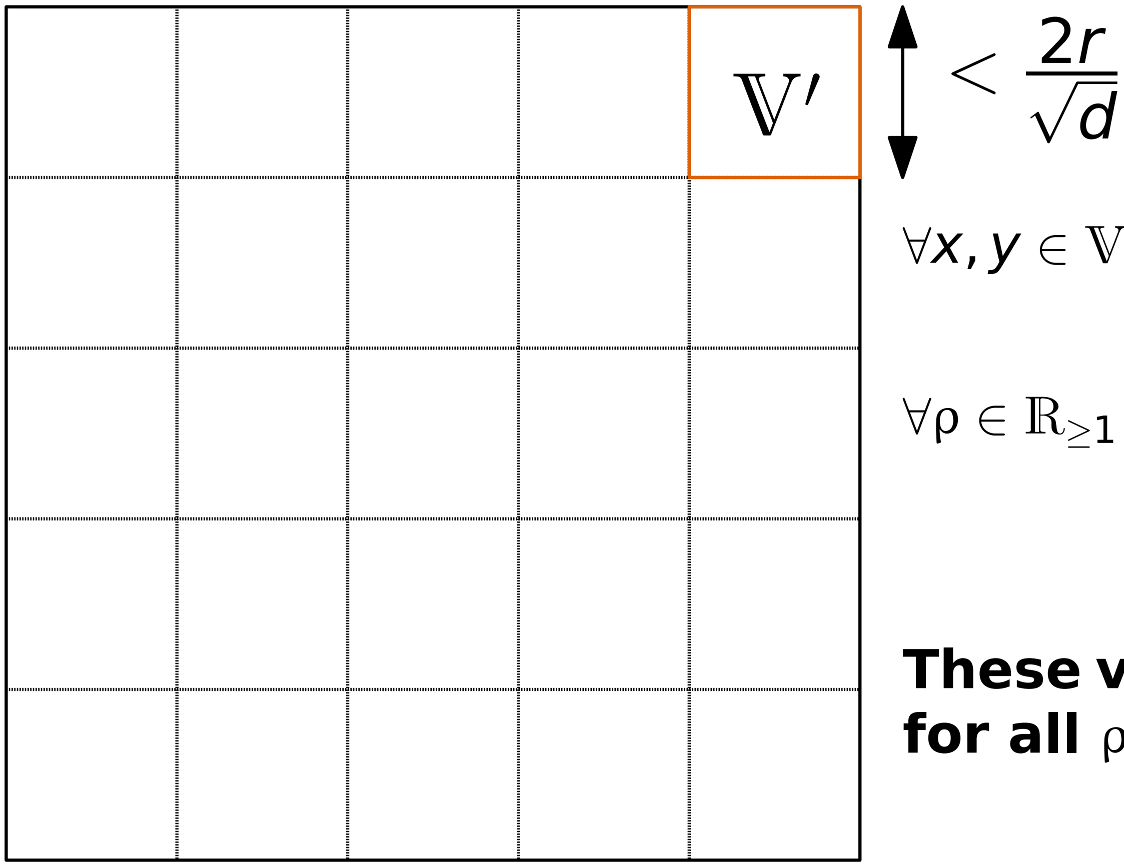

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These vertices form a clique in G_ρ for all ρ!

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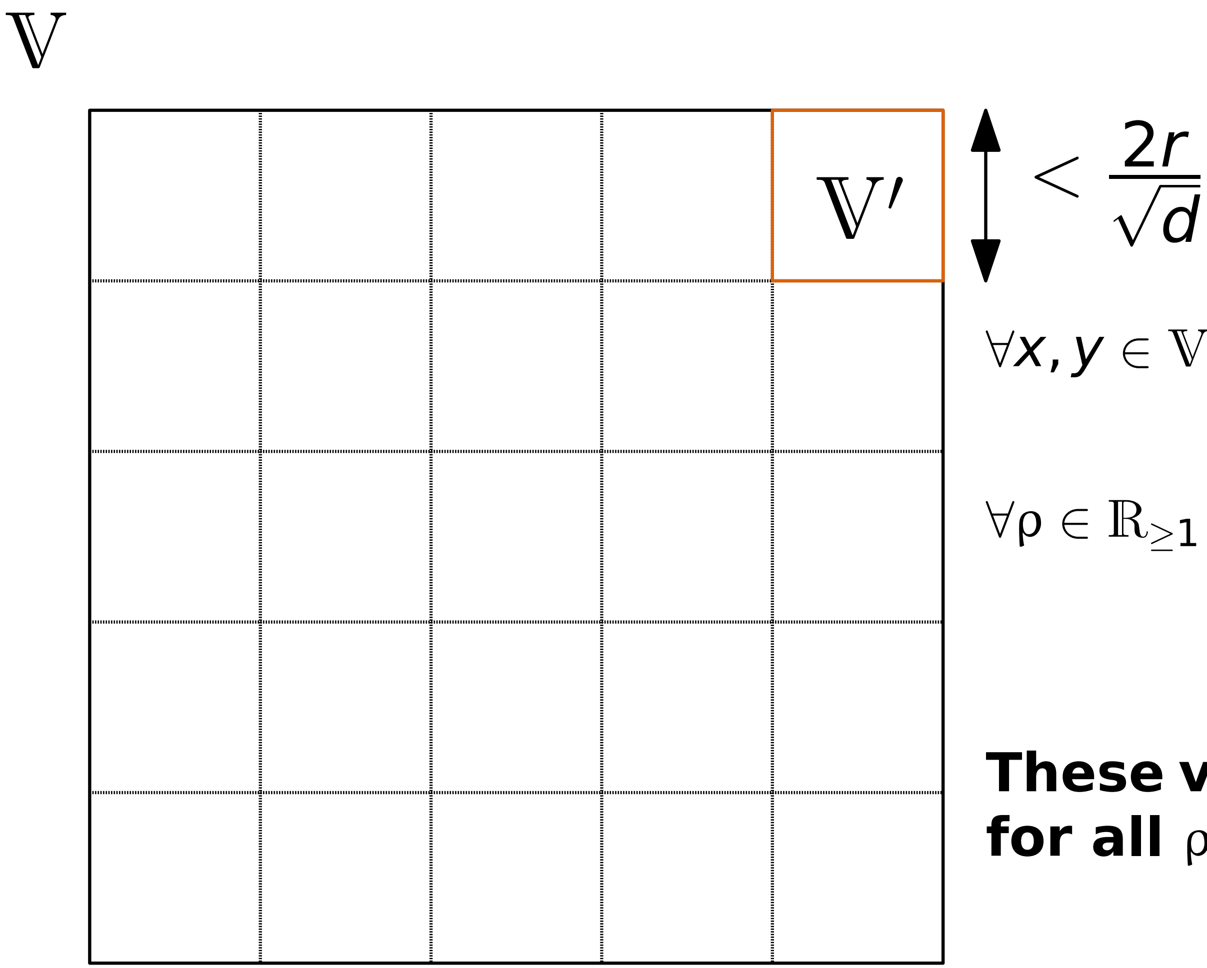

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natural clique cover of size $\Theta\left(\mathrm{vol}\left(\mathbb{V}\right)\right)$

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Are clique dynamics rapidly converging for $\lambda < \lambda_{\mathbf{c}}(\Delta)$?

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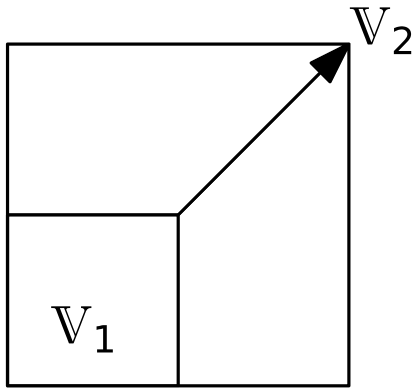
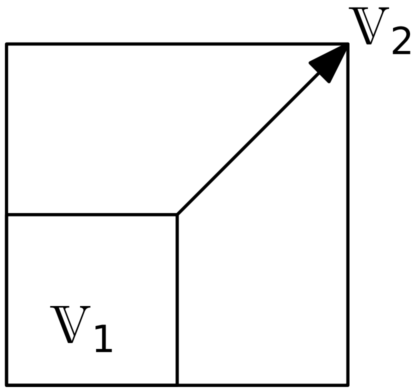
Theorem: Clique dynamics for a clique cover of size m converge in time poly(m) for $\lambda < \lambda_c(\Delta)$.

2nd Result: Properties of the partition function





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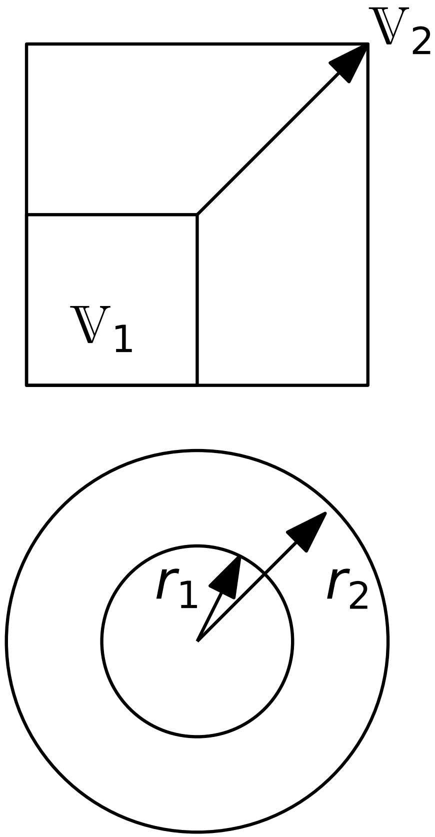

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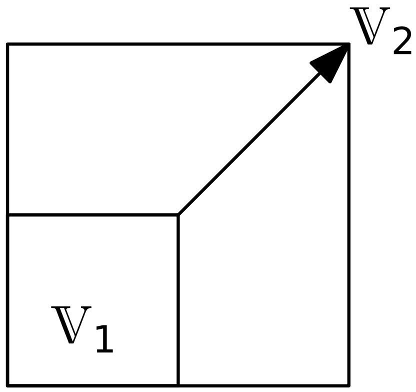

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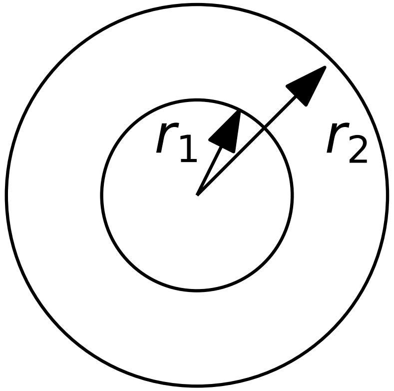

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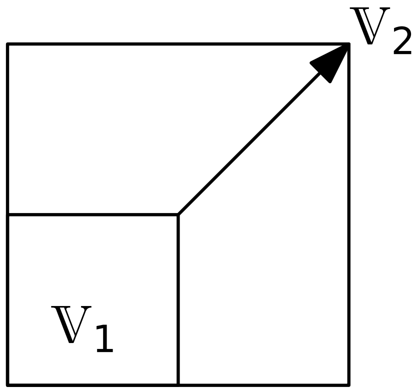

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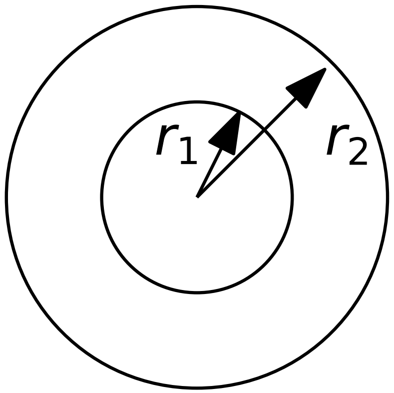

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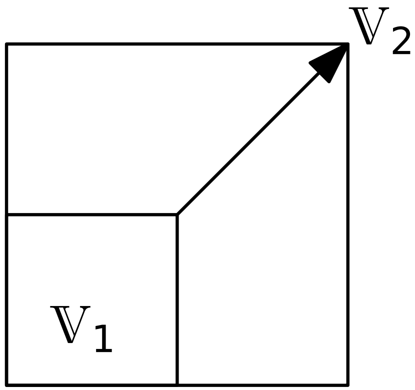

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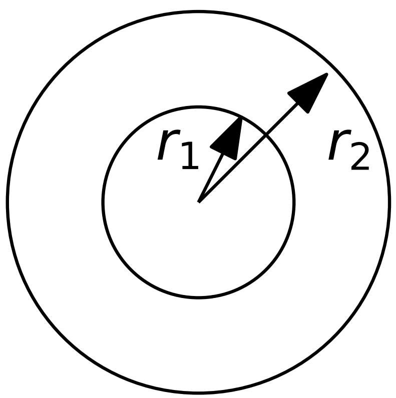

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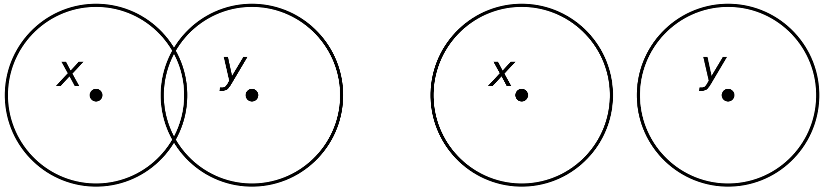

invalid to valid → increase $r \mapsto r_+$

valid to invalid ← decrease $r \mapsto r_-$

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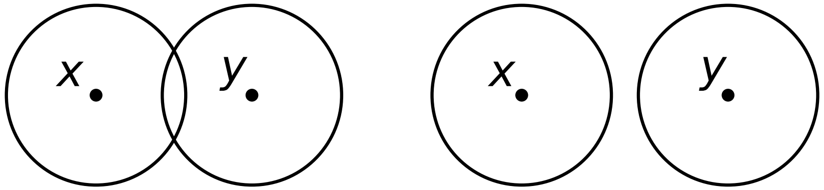

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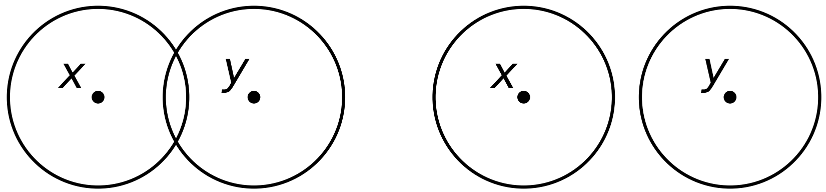

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$$\Xi_{\mathbb{V}}(\lambda, \frac{1}{\alpha} r) = \Xi_{\alpha\mathbb{V}}(\frac{1}{\alpha^d}\lambda, r)$$

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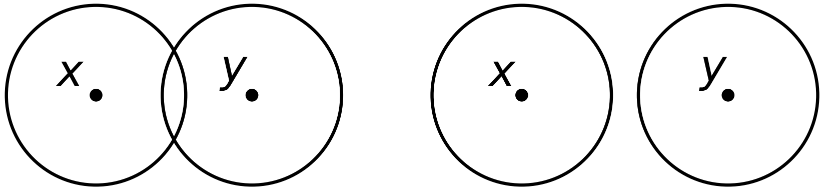

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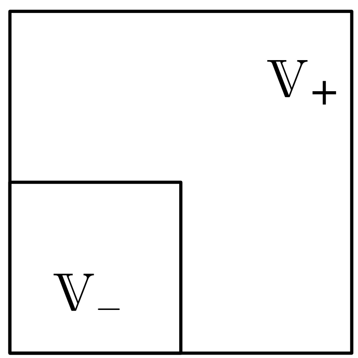

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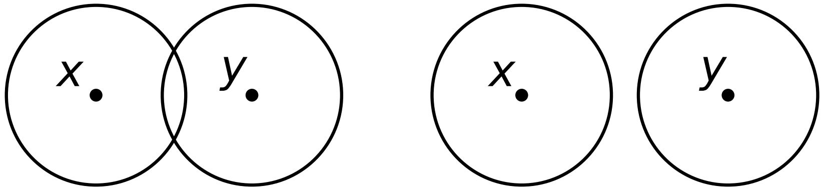

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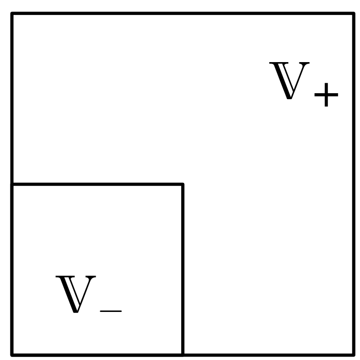

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G_{ρ} now only needs quadratic number of points in $\nu(\mathbb{V})$

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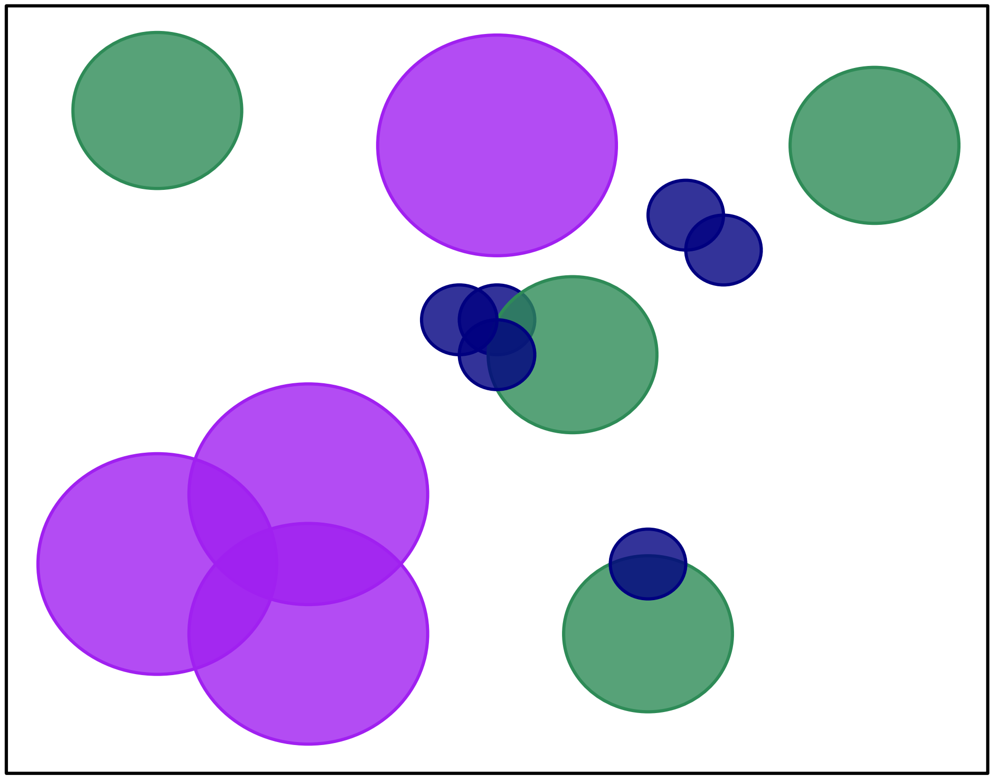
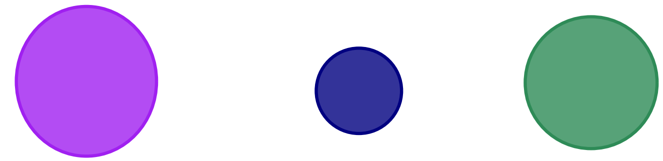
Approximate sampling:

1. Use an approximate sampler to obtain an independent set of G_ρ
2. Recover the points in $\mathbb{V}$ that correspond to the vertices of the independent set
3. Randomly perturb the positions of these points

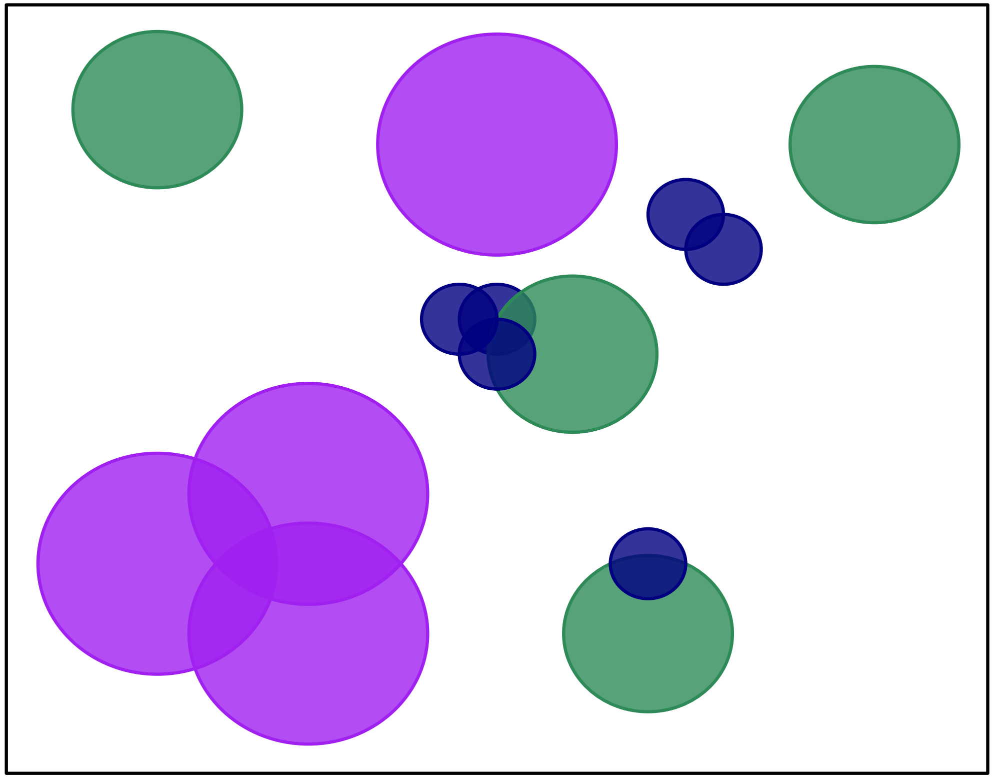
2nd Result: Multiple types of particles

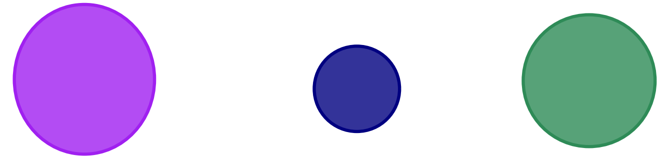




Interaction Matrix

$$\begin{bmatrix} 0 & r_1 + r_2 & r_1 + r_3 \\ r_1 + r_2 & 0 & 0 \\ r_1 + r_3 & 0 & 2r_3 \end{bmatrix}$$





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Approximation + Sampling Algorithms for :

$$\lambda_{\text{max}} < \frac{e}{\|B\|_1}$$

Where B is the volume exclusion matrix, with entries $\nu(B_{r_{ij}})$

2nd Result: Random point allocations

The previous arguments work for any δ-ε-allocation $\Phi : \mathbb{V} \to X$

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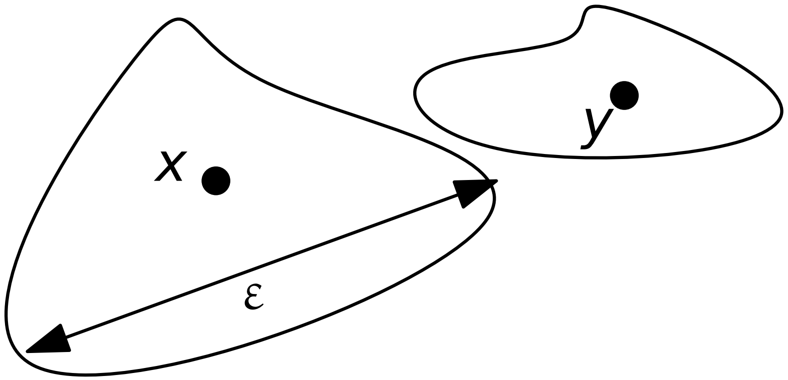

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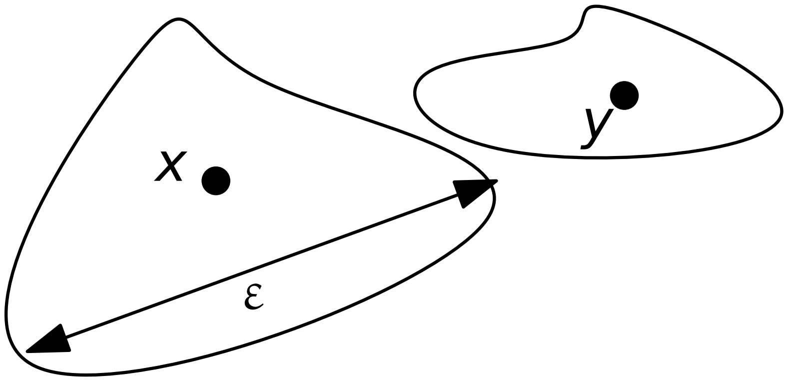

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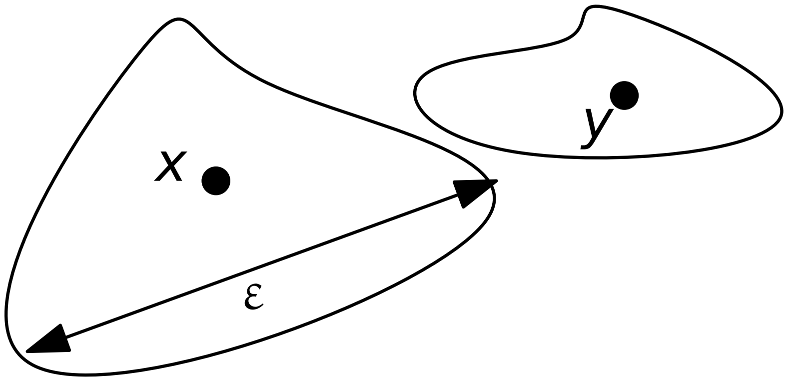

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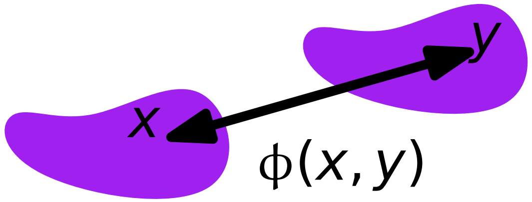
Theorem:

The hard-core model with fugacity $\lambda\nu(\mathbb{V})/n$ of $(\mathbb{V}, r)$-geometric random graphs concentrates around $\Xi_{\mathbb{V}}(\lambda, r)$

Gibbs point processes

Spatial process, where the particles interact via repulsive forces

On any complete, separable measure space $\mathbb{X}$. $\phi(x, y) \geq 0$



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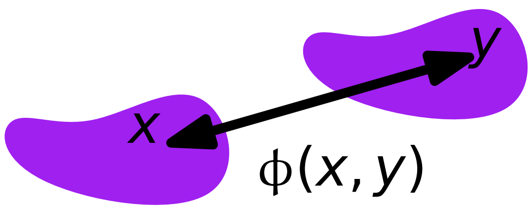

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$$\frac{dP_{\mathbb{V}}^{(\lambda,\phi)}}{dQ_\lambda}(x_1, \ldots, x_k) = \frac{\mathbb{1}_{\forall i \in [k]:\, x_i \in \mathbb{V}} \cdot \mathrm{e}^{-H(x_1,\ldots,x_k)} \mathrm{e}^{\lambda \nu(\mathbb{V})}}{\Xi_{\mathbb{V}}(\lambda, \phi)}$$

Partition function:

$$\Xi_{\mathbb{V}}(\lambda, \phi) = 1 + \sum_{k \in \mathbb{N}_{\geq 1}} \frac{\lambda^k}{k!} \int_{\mathbb{V}^k} \mathrm{e}^{-H(x_1,\ldots,x_k)} \nu^k(d\mathbf{x})$$

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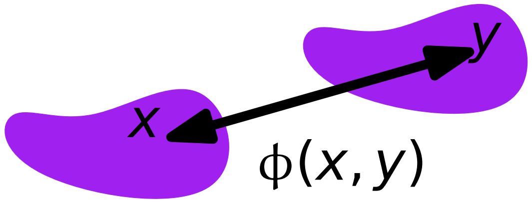

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Hard-sphere model:

$$\phi(x,y) = \begin{cases} \infty, & \text{if } \mathrm{dist}(x,y) < r \\ 0, & \text{otherwise} \end{cases}$$

Temperedness constant:

$$C_\phi = \operatorname{ess\,sup}_x \int_{\mathbb{X}} \left| 1 - e^{-\phi(x,y)} \right| \nu(dy)$$

measures the strength of interactions between points

Phase transitions

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Question: Can we get efficient approximation and sampling algorithms?

The model $\zeta^{(n)}_{\mathbb{V},\phi}$

- n vertices and bounded measurable region $\mathbb{V} \subseteq \mathbb{X}$
- for each $i \in [n]$ draw a point $x_i \sim \text{unif}_{\mathbb{V}}$ independently
- For all $i, j \in [n]$, with $i \neq j$, connect i and j with an edge with probability $p_{\phi} = 1 - \mathrm{e}^{-\phi(x_i, x_j)}$ independently

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Encompasses:

- Erdős–Rényi random graphs
- Geometric random graphs
- Hyperbolic random graphs

Result 3: Hard-core model on $\zeta_{\mathbb{V},\phi}^{(n)}$

Can we show that the hard-core model on $G \sim \zeta_{\mathbb{V},\phi}^{(n)}$ with fugacity $\lambda\nu(\mathbb{V})/n$ concentrates around $\Xi_{\mathbb{V}}(\lambda, \phi)$, its expected value?

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Randomized approximation for the partition function when $\lambda < \frac{e}{C_\phi}$

Result 3: Approximate sampler

1. Sample the graph G from $\zeta^{(n)}_{\mathbb{V},\phi}$, with $n \in \Theta\left(\nu(\mathbb{V})\right)$
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To prove that the two densities have small total variation density, we compare each one of them to a Poisson point process of intensity λ utilizing a theorem of Rényi–Mönch

Independent work and open problems

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- Can we get deterministic approximation of Ξ in poly($\nu(\mathbb{V})$)?
- Can we get approximation for $\lambda < \frac{e}{\Delta_\phi}$ without finite range assumption?
- What about other potentials (e.g. Lennard–Jones)?
- Is there a way to show hardness or approximation for some parameter range?