An Occupancy Approach to the Hard-core Model

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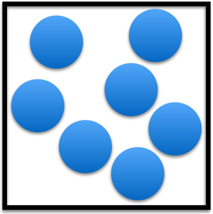
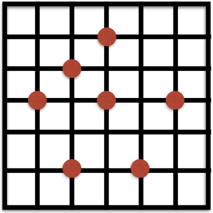
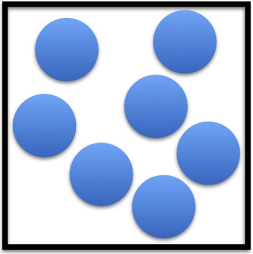




The Hard Sphere Model

Place αn spheres of volume 1 uniformly at random in the d-dimensional torus of volume n, conditioned on no overlap.



Question Is there a phase transition in this model?

For background, read 'Fun With Hard Spheres' (Löwen).

The Hard Sphere Model

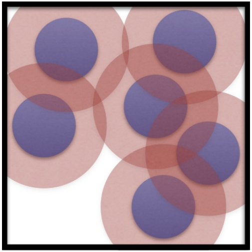
Difficulty seems to stem from:

1. Uncountably many ground states.
2. Ground states are sphere packings which aren't easy to understand.

Can we say anything useful at high densities?

The Hard Sphere Model

The excluded volume is the volume of the union of spheres of volume 2^d around the centers.



How to related expected excluded volume to the density α?

The Hard Sphere Model

The partition function is:

$$Z(\alpha, n) = \int_{\mathcal{T}_d(n)} \int_{\mathcal{T}_d(n)} \cdots \int_{\mathcal{T}_d(n)} \mathbf{1}_{d(x_i, x_j) > 2r \forall i \neq j} \, dx_1 \cdots dx_{\alpha n}$$

$$Z(\alpha, n) = \Pr[G_{\mathcal{T}_d(n)}(n, 2r) \text{ is empty}]$$

Probability that a random geometric graph is empty.

The Hard Sphere Model

Let

$$E_k = \{d(x_i, x_j > 2r \forall 1 \leq i < j \leq k\}$$
$$V_k = \frac{1}{n} \text{vol} \cup_{i=1}^{k} B(x_i, 2r) \text{ (the excluded volume fraction)}$$

Then

$$\begin{aligned} Z(\alpha, n) &= \Pr[E_{\alpha n}] \\ &= \Pr[E_{\alpha n - 1}] \cdot \mathbb{E}[1 - V_{\alpha n - 1} | E_{\alpha_n - 1}] \\ &= \prod_{k=1}^{\alpha n - 1} (1 - \mathbb{E}[V_k | E_k]) \end{aligned}$$

The Hard Sphere Model

Theorem

For $\alpha < 4^{-d}$,

$$Z(\alpha, n) \leq (1-p)^{\binom{\alpha n}{2}}.$$

where $p = 2^d \alpha / n$.

Enough to show, for $1 \leq k \leq \alpha n - 1$,

$$\mathbb{E}[V_k | E_k] \geq \mathbb{E}[V_k].$$

Call this the **Repulsion Inequality**.

Holds at low enough densities ($k < 4^{-d} n$). Holds in dimension 1 at all densities, and in all dimensions at high enough density.

The Repulsion Inequality

Theorem

In dimension 24, the repulsion inequality **fails** *for some* $0 < \alpha < \alpha_{max}$.

Conditioning on the pairwise repulsion of the centers of spheres can decrease the expected volume of their union!

The Repulsion Inequality

Conjecture

The repulsion inequality holds in the fluid phase of the hard sphere model.

Would imply a phase transition in dimension 24.

The Hard-Core Model

Let G be a d-regular graph. Define the hard-core model on G to be a random independent set I drawn according to

$$\Pr(I) = \frac{\lambda^{|I|}}{Z_G(\lambda)}$$

where the partition function is

$$Z_G(\lambda) = \sum_I \lambda^{|I|}$$

The Hard-Core Model

The occupancy fraction is

$$\alpha_G(\lambda) = \frac{1}{n}\sum_{v} \Pr[v \in I] = \frac{\lambda Z'(\lambda)}{n Z(\lambda)} = \frac{\lambda}{n}(\log Z)'$$

What is the relationship between λ and α?

Bounding the occupancy fraction

By integrating, bounds on α give bounds on the free energy $\frac{1}{n}\log Z$.

Used e.g. by Dembo, Montanari, Sun in the context of locally tree-like graphs.

I will show an application of the occupancy fraction in combinatorics.

Any algorithmic applications?

Bounding the occupancy fraction

Theorem (Kahn, Galvin-Tetali, Zhao)

For any d-regular G,

$$\frac{1}{n}\log Z_G(\lambda) \leq \frac{1}{2d}\log Z_{K_{d,d}}(\lambda).$$

Proved by counting homomorphisms using the 'entropy method'.

Theorem (Davies, Jenssen, P., Roberts)

For any d-regular G,

$$\alpha_G(\lambda) \leq \alpha_{K_{d,d}}(\lambda).$$

Strengthening of Kahn, Galvin-Tetali, Zhao, with a probabilistic proof.

Bounding the occupancy fraction

Proof: Assume triangle-free.
Call v uncovered if $N(v) \cap I = \emptyset$.

1. $\Pr[v \in I | v \text{ uncovered}] = \frac{\lambda}{1+\lambda}$.
2. $\Pr[v \text{ uncovered} | v \text{ has j uncovered neighbors}] = (1+\lambda)^{-j}$.

Let Y be the number of uncovered neighbors of a random vertex v.

$$\mathbb{E} Y = d \mathbb{E}\left[(1+\lambda)^{-Y}\right]$$

Bounding the occupancy fraction

Same proof gives:

Theorem

Let G be d-regular, bipartite, transitive. Then

$$\alpha_G(\lambda) > \alpha_{T_d}(\lambda)$$

where α_{T_d} is the occupancy fraction of the translation invariant hard-core measure on the infinite regular tree.

For $\lambda > \lambda_c(T_d)$ which graphs are minimizers?

A repulsion inequality

In the fugacity model, the repulsion inequality is

$$\alpha/\lambda \leq e^{-(d+1)\alpha}$$

1. Holds for all graphs, small enough λ.
2. Fails for bipartite graphs $d \geq 6$ and in some range of λ - $\lambda = \Omega(1/d)$.
3. Holds for the translation invariant measure on T_d, all λ.
4. Fails for semi-translation-invariant measure on T_d, $d \geq 6$, at λ approaching λ_c as $d \to \infty$.

Monomer-dimer model

Choose a random matching M from a d-regular graph G.

$$M_G(\lambda) = \sum_M \lambda^{|M|}$$

$$\alpha_G^M(\lambda) = \frac{1}{nd/2} \sum_e \Pr[e \in M]$$

Monomer-dimer model

Theorem (Davies, Jenssen, P., Roberts)

For all d-regular G,

$$\alpha_G^M(\lambda) \le \alpha_{K_{d,d}}^M(\lambda).$$

Corollary 1. $\frac{1}{n} \log M_G(\lambda)$ maximized by $K_{d,d}$ + 'Asymptotic Upper Matching Conjecture' of Friedland, Krop, Lundow, and Markström.

Corollary 2. Repulsion inequality holds in monomer-dimer model on all regular graphs, for all λ.

A conjecture

Conjecture

The repulsion inequality holds in the hard-core model on $\mathbb{Z}^d$ in the uniqueness phase.

$$\alpha/\lambda \leq e^{-(2d+1)\alpha}$$

for $\lambda < \lambda_c(\mathbb{Z}^d)$.

A conjecture

Would imply optimal bound of $\lambda_c(\mathbb{Z}^d) = O(1/d)$. Current bound is $O(d^{-1/3})$ by Peled and Samotij.

$\mathbf{d}$	2	3	4	5	6
$\lambda_\mathbf{c}$	3.79625517391234	1.05601	0.58372	0.40259	0.308217
$\alpha(\lambda_\mathbf{c})$	0.367743000	0.210490	0.143334	0.109392	0.088948
$e^{-(2d+1)\alpha} / \frac{\alpha}{\lambda}$	1.6415	1.1495	1.1210	1.1048	1.0902

Figure: Numerical data collected in Butera and Pernici.

Thank you!