Dense packing on uniform lattices

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Introduction

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The Hard Core model

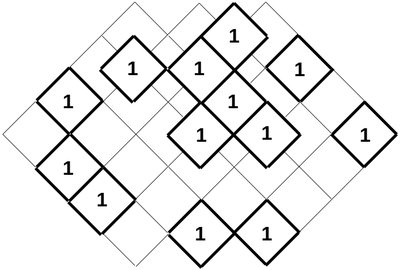
Let **G** be a graph and let the nearest neighbors on in be defined by the hop count.

Definition

The subset of the configurations $\{0,1\}^{\mathbf{G}}$ *with the restriction that no two nearest neighbors both carry 1's form the configurations of the Hard Core Model on* **G**.

This model is called Independent Sets/Golden Mean Subshift in Theoretical Computer Science/Dynamical Systems respectively.

Often the graph has additional structure; if it is e.g. a lattice, then some geometry enters. On $\mathbf{Z}^2$ the model is known as the Hard Square Model:



On the hexagonal (i.e. honeycomb) lattice and on triangular lattice it becomes the Hard Hexagon Model etc.

Regimes

- In the high temperature/loose packing regime the geometry of the configurations is not a distinct feature. There is an exponential number of configurations in the size of the domain and solving the **topological entropy** as well as the correlation decay are major open problems. For the set of legal configurations X_0 the entropy is defined as

$$h_{top}^{X_0} = \lim_{n\to\infty} \frac{1}{n} \ln |\{x|_{A_n} \mid x \in X_0\}|$$

  where $|A_n| = n$ and the sequence of domains $\{A_n\}$ grows in a sufficiently regular fashion. Estimates on many different lattices for the topological entropy and the measure of maximal entropy are available ([E2], 2009).

- In the low temperature/high density regime the Hard Core is essentially a **packing model**. If the graph has e.g. a lattice structure, as the density of 1's increases, the geometry of the lattice imposes itself on the packing in qualitatively different ways. Phase transition may or may not appear as the packing gets denser and the residual entropy may be zero or positive.

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Packing types

Three qualitatively different types of densest packings appear in Hard Core configurations defined on uniform lattices (as well as on a number of other graphs). The distinct optimal packing classes are:

- **Laminated packings (L):** Undeformable, layered packings. Seven of the eleven uniform lattices only have (a finite number of) these.
- **2d-random packings (R):** Three uniform lattices allow **local moves** in the optimal packing (akin to domino flip/phason exchange in lozenge tiling) and hence have positive 2-d entropy (residual entropy, positivity implies exponential degeneracy of the ground state).
- **Random laminated packings (RL):** Borderline cases where the lattice allows a **non-local move** of the layers resulting in positive 1-dimensional entropy but vanishing 2-dimensional entropy. Their non-transitivity and long range order can be analyzed ([E3]). The optimal packing of spheres in 3-d Euclidean space is of this type.

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Archimedean or Uniform lattices

- Using only one type of regular convex polygon, the plane can be tiled using either squares, triangles and hexagons. The vertex and edge sets of these tilings form the **regular lattices**: the **square, triangular and hexagonal (honeycomb) lattices** ($\mathbf{Z}^2$, **T** and **H**).
- If at most two regular convex polygons are allowed to be used so that at each vertex the same arrangement of the polygons appears (upto rotation), there are 11 different ways of tiling the plane. These tilings yield the **Archimedean or Uniform lattices**. The code of the lattice is the numbering of the adjacent *n*-gons recorded clockwise around a vertex.

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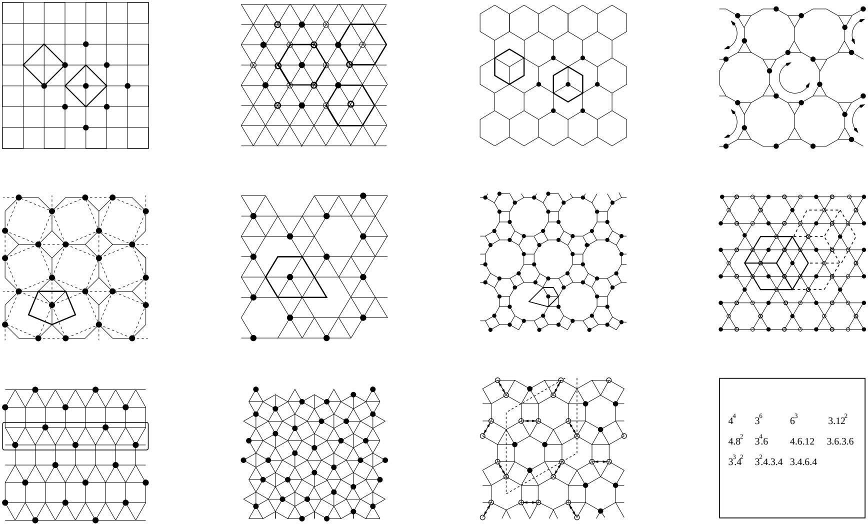
4^4 3^6 6^3 3.12^2
4.8^2 $3^4.6$ $4.6.12$ $3.6.3.6$
$3^3.4^2$ $3^2.4.3.4$ $3.4.6.4$

Densities

The **density of** 1's in a configuration c is

$$\rho = \lim_{n\to\infty} \frac{1}{|D_n|} \sum_{x \in D_n} c(x)$$

where the limit must agree for all sequences $\{D_n\}$ retaining their two dimensional shape as $n \to \infty$ (D_n is a domain of size n lattice points on **G**). This number, when existing, is always between 0 and 1 and for Hard Core on a connected graph obviously at most $1/2$.

Let N_x be the set of nearest and $N_x^{(2)}$ the second nearest neighbors of x. Let n be the average number of nearest neighbor 1's that $y \in N_x$ has in $N_x^{(2)}$.

Proposition

On an Archimedean graph of degree d and second neighbor mean occupancy n the global configuration density of 1's is bounded from above by

$$\overline{\rho} = \frac{1}{1 + \frac{d}{n+1}} \quad .$$

- The result is more general than our set-up and also applies e.g. to homogeneous trees: $n = d - 1$, hence $\overline{\rho} = 1/2$ always.
- The bound is often tight: for example for the square lattice we have $d = 4$, $n_y \equiv 3$ hence $n = 3$ and $\overline{\rho} = 1/2$. Indeed it is tight for seven of the Archimedean lattices.

For the remaining Archimedean lattices the density bounds can be argued individually:

Proposition

For $(3^2.4.3.4)$, $(3^4.6)$, $(3^3.4^2)$ and $(3.4.6.4)$ the maximal density is $1/3$.

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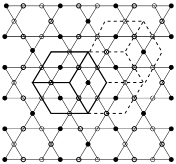
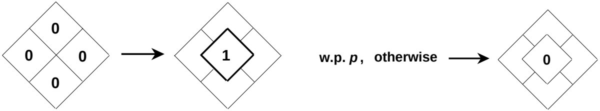
Sublattices

- Square or hexagonal lattices as a bipartite graphs split in two sublattices; e.g. $\mathbf{Z}^2$ has $2\mathbf{Z}^2$ ($\mathbf{Z}^2$ scaled & rotated) and its shifted copy inside it. Triangular and Kagomé lattices as tripartite graphs split into three scaled copies of themselves, $\mathbf{Z}^2$ with Moore neighborhood (i.e. eight nearest neighbors) divides up in four parts etc.
- Each 1 on a sublattice vertex blocks the nearest neighbor vertices on the other sublattice(s) i.e. forces them to carry 0's. Conversely if a sublattice vertex has no 1's as nearest neighbors on the other sublattices it is free.
- The optimal densities can be realized by the full occupation of one sublattice alone; these are the most regular densest packings. But they may not be the only optimal packings; a **local move** may prevail, like in the Kagomé case:



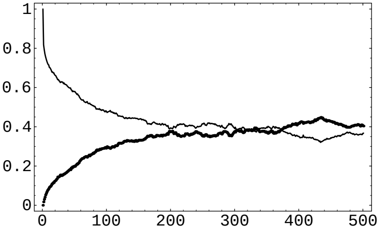
Fill-in scheme: PCA

- The idea is to fill-in all but one of the sublattices according to some distribution and then update the remaining sublattice using a **Probabilistic Cellular Automaton** with **packing pressure** p. For example for the square lattice the Local Rule (rendered using unit diamonds) is:



- Applying the local rule at each sublattice vertex one updates the entire configuration on the sublattice. All the sublattices are updated cyclically and the combined map of these sublattice update maps is this the global map, the PCA.

- Once $p \neq \{0, 1\}$ iterating the PCA generates eventually all legal configurations (a.s. on a finite lattice). The initial condition can be arbitrary as the PCA corrects an illegal one in one step.
- The equilibrium state of the PCA is the measure of maximal entropy at the given p-level for the Hard Core model.
- The relaxation to the equilibrium is in most cases exponentially fast. But for some lattices there is a critical probability p_c near which there is critical slowing down.



Density relaxation under PCA iteration on the two sublattices of the hexagonal lattice. 5000 full cycles on a torus of size 200×200 vertices, $p \approx 0.859$ is in the subcritical phase.

Non-critical case

- If, as $p \uparrow 1$, there is no threshold beyond which the equilibrium configurations of the PCA concentrate 1's on one (or several) of the sublattices, the lattice has **dynamically non-critical Hard Core**.
- On three of the uniform lattices the PCA is non-critical: these are the Kagomé lattice (3.6.3.6), (3.4.6.4) and (3.12^2).
- In each case there is an allowed perturbation, a **local move** left on the optimal packings at the limit $p = 1$. It transforms optimal configurations to each other without affecting the number of 1's. Because of local moves there is an uncountable number of best packings (on the infinite lattice) and they are essentially **random packings**. Due to the local moves there is positive 2-d **residual entropy** in this case.

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Critical case

- If there is a **critical value** $p_c < 1$ beyond which the equilibrium configurations start concentrating on a sublattice the Hard Core has a **dynamic phase transition at** p_c.
- There are seven uniform lattices with this property: the three regular lattices together with (4.8^2), $(4.6.12)$, $(3^2.4.3.4)$ and $(3^4.6)$.
- The limiting ($p = 1$) densest packings are **rigid**: there is no local move. Consequently there is only a finite number of optimal packings which are all **laminated packings**.

Borderline critical case

- On the Trellis lattice ($3^3.4^2$) yet another phenomenon appears: the densest packings do not admit local moves but they are **slide deformable**. The optimal configurations are stacks that permit **non-local moves**: only infinite two-rows to be slid. Hard Core is borderline critical here: it has zero 2-d but positive 1-d residual entropy.
- Another example of this behavior appears in Hard Core on $\mathbf{Z}^2$M (each lattice site has eight neighbors). Here the densest packings allow either infinite column- or row-slides but not both. Again 2-d entropy vanishes but 1-d does not. $p_c \approx 0.98$ but is rather hard to compute.
- This case is analogous to the Barlow packing, the densest packing of spheres in $\mathbf{R}^3$; in it only certain infinite planes of spheres can be slid.

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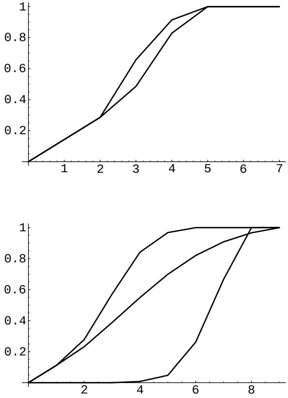
- There is an **embedded Voter rule** in all the critical cases. In the hexagonal case the local PCA rule *squared* is a map from a 7-tuple (extended neighborhood) to $\{0, 1\}$. Count the fraction of these neighborhoods that map to 1 as $p = 1$. This is plotted on the right, top curve. On the triangular lattice do the same while restricted to any one sublattice; this results in a map from 7-tuples as well, rendered second from the top. $\mathbf{Z}^2$ works analogously on 9-tuples. $\mathbf{Z}^2$M requires further argument.
- Sufficiently steep Voter curves imply criticality. This mechanism seems behind the criticality here as well.



The Voter curves: top: **H** and **T**, bottom: $\mathbf{Z}^2$ and $\mathbf{Z}^2$M (2).

Graph	Optimal subgraphs, multiplicity, tiles	Type	ρ	Critical prob. and dens., residual entropy
$(4^4)(\mathbf{Z}^2)$	$\sqrt{2}\ \mathbf{Z}^2$, 2, diamond	L	$1/2$	$p_c \approx 0.79,\ \rho(p_c) \approx 0.36$
(6^3) (**H**)	$\sqrt{3}\ \mathbf{T}$, 2, hexagon	L	$1/2$	$p_c \approx 0.87,\ \rho(p_c) \approx 0.4$
(3^6) (**T**)	$\sqrt{3}\ \mathbf{T}$, 3, hexagon	L	$1/3$	$p_c \approx 0.90,\ \rho(p_c) \approx 0.26$
(4.8^2)	$\simeq (3^2.4.3.4)$, 2, 5-gon	L	$1/2$	$p_c \approx 0.90,\ \rho(p_c) \approx 0.4$
$(4.6.12)$	$\simeq (3^4.6)$, 2, 5-gon	L	$1/2$	$p_c \approx 0.91,\ \rho(p_c) \approx 0.42$
$(3^2.4.3.4)$	$\simeq$ **T**, 3, 6-gon	L	$1/3$	$p_c \approx 0.99,\ \rho(p_c) \approx 0.3$
$(3^4.6)$	$\sqrt{3}\ (3^4.6)$, 3, 5-gon	L	$1/3$	$p_c \approx 0.97,\ \rho(p_c) \approx 0.29$
$(3^3.4^2)$	3 **Z** stack, ∞	RL	$1/3$	$h^{(1)} = \frac{1}{2} \log 2$
$(3.4.6.4)$	$\simeq (3^4.6)$, ∞, 5-gon	R	$1/3$	$h^{(2)} \geq \frac{3}{16} \log 2$
$(3.6.3.6)$ (**K**)	$\sqrt{3}\ (3.6.3.6)$, ∞, $\diamondsuit$	R	$1/3$	$h^{(2)} \approx 0.323$
(3.12^2)	$\simeq (3^4.6)$, ∞, 5-gon	R	$1/3$	$h^{(2)} \geq \frac{1}{18} \log 2$
$\mathbf{Z}^2\mathrm{M}$	2 **Z** stack, ∞, square	RL	$1/4$	$p_c \approx 0.98?$, $h^{(1)} = \frac{1}{2} \log 2$
$[4.8^2]$ (**UJ**)	$\mathbf{Z}^2$, 1,sq., $\sqrt{2}\ \mathbf{Z}^2$, 2,$\diamond$	L	$1/2$	increasing critical curve
Quilt (**Q**)	$\sqrt{2}\ \mathbf{Z}^2$, 3, diamond	L	$1/3$	increasing critical curve

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Thank you!