Hard Core entropy: lower bounds

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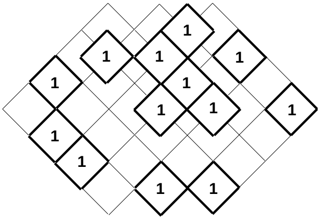
The Hard Core Model/Independent Sets/Golden Mean Subshift

Definition (Hard Core)

Let $\mathbf{L}$ *be a graph with the hop count metric. The set of configurations* $X^{\mathbf{L}}$ *in* $\{0,1\}^{\mathbf{L}}$ *with the restriction that no two nearest neighbors both carry 1's is the Hard Core Model on* $\mathbf{L}$.

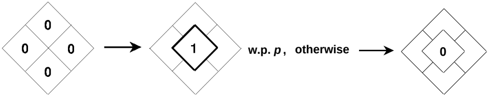
On $\mathbf{Z}^2$ lattice Hard Squares:



(Lattice lines horizontal/vertical, only 1's rendered, each diamond has 0's at corners. On the hexagonal & triangular lattice it is the Hard Hexagon Model etc.)

Dynamics and Regimes

Generating PCA, $p \in (0, 1)$, maps between sublattices. On $\mathbf{Z}^2$ simply



$p \approx 1$, the low temperature/high density regime: a packing model. As $p \uparrow 1$, on some graphs (like the square, hexagonal and triangular lattices) there is a phase transition in the distribution of the 1's. On others like the Kagomé lattice the model is non-critical with positive residual entropy ([E1]).

$p \approx 1/2$, the high temperature/entropic regime. Counting the configurations and solving correlations are central problems.

Definition (Topological entropy)

$$h_{X'}^{top} = \lim_{n \to \infty} \frac{1}{n} \ln \left| \{ x|_{A_n} \mid x \in X' \} \right| = \sup_{\mu \in \mathcal{M}} h_\mu ,$$

$|A_n| = n$ escapes compact sets. In the set of invariant measures $\mathcal{M}$, a maximizing μ is a **measure of maximal entropy** *(mme).*

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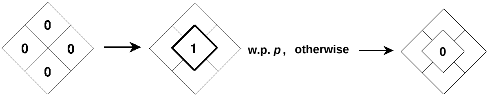

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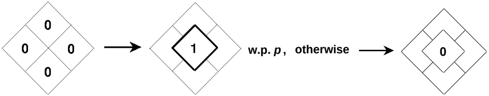

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Results in the entropic regime

- 1-d model is solvable using transfer matrices. Analyzable on Cayley trees (Rozikov&Suhov, Brightwell&Winkler etc.).
- On planar and higher dimensional graphs/lattices little is known rigorously about the entropy except on the triangular lattice where its exact value is known (Baxter, -80). For the uniqueness of the mme there is the Dobrushin-Shlosman -criterion (-85).
- Numerical estimates of very high accuracy exist for the entropy on square, hexagonal and triangular lattices (Baxter, -99, Milosevic et. al., -89) using transfer matrix calculations. They yield little insight on the typical Hard Core configurations. For other numerical approximation approaches see the article references in the Proceedings.
- We will establish a general method to obtain
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Filling in for the entropy

Let $h_\mu^{(e)}$ be the marginal a measure of maximal entropy on the even sublattice and N_e an all-zero 2×2 neighborhood there. Then

Proposition

The topological entropy of the Hard Core Model on a lattice with a two-way sublattice split is given by

$$h^{top} = \frac{1}{2}\left\{ h_\mu^{(e)} + \mathbf{P}\left(N_e\right) \ln 2 \right\} .$$

Idea of the proof: 1. assign the marginal of a measure of maximal entropy to the even sublattice thereby contributing $h_\mu^{(e)}/2$ to the entropy. 2. fill in the non-blocked sites on the odd sublattice optimally: use Bernoulli(1/2).

Procedure for entropy lower bound:

Replace the unknown $h_\mu^{(e)}$ by h_ν with a known distribution ν that allows explicit computation of $\mathbf{P}\left(N_e\right)$. Then optimize the parameter(s) of ν.

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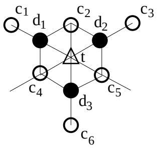
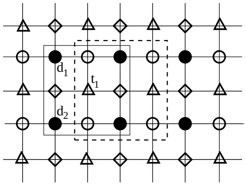
The procedure can be extended from $\mathbf{Z}^2$ to k**-partite graphs**. E.g. in the triangular lattice the sequential fill-in takes place in the order $\circ \rightarrow \bullet \rightarrow \triangle$ as follows (starting from empty lattice):

- Fill-in the $\circ$-sublattice with 1's according to $B(p)$.
- On the sites on the $\bullet$-sublattice that are not blocked by some $\circ$-sublattice 1, fill-in with $B(q)$.
- If the center site $\triangle$ is not blocked by the entries in the $\circ$/$\bullet$-sublattices, fill it in with $B(1/2)$.
- Add up the conditional entropies:

$$\frac{1}{3}\left\{h(\circ) + h(\bullet|\circ) + h(\triangle\;|\circ,\bullet)\right\}$$





Triangular and $\mathbf{Z}^2M$ lattice neighborhoods.

Theorem (First lower bounds)

The topological entropy of the Hard Core model is bounded from below on the square ($n = 4$), hexagonal ($n = 3$), triangular ($m = 3$), Kagomé ($m = 2$) and $\mathbf{Z}^2\mathrm{M}$ lattices by

$$\underline{h}_{\mathbf{Z}^2/\mathbf{H}}(p) = \frac{1}{2}\left\{h_B(p) + (1-p)^n \ln 2\right\} ,$$

$$\underline{h}_{\mathbf{T}/\mathbf{K}}(p,q) = \frac{1}{3}\left\{h_B(p) + (1-p)^m [\, h_B(q) + [1-(1-p)q]^m \ln 2\,]\right\} ,$$

and

$$\underline{h}_{\mathbf{Z}^2\mathrm{M}}(p,q,r) = \frac{1}{4}\Big\{h_B(p) + (1-p)^2\Big[\, h_B(q) + [1-(1-p)q]^4\, h_B(r) + (1-p)^2(1-q)^2\big[1-(1-(1-p)q)^2 r\big]^2 \ln 2\,\Big]\Big\} ,$$

where $p,\ q$ and $r \in (0,1)$. Here $h_B(t) = -t\ln t - (1-t)\ln(1-t)$.

Optimization, first round

For lower bounds compute

$$\max_{p\in(0,1)} \underline{h}_{\mathbf{Z}^2/\mathbf{H}}(p)\ , \qquad \max_{p,q\in(0,1)} \underline{h}_{\mathbf{T}/\mathbf{K}}(p,q) \quad \textit{and} \quad \max_{p,q,r\in(0,1)} \underline{h}_{\mathbf{Z}^2\mathrm{M}}(p,q,r).$$

L	max $\underline{h}_{\mathbf{L}}$	sublattice densities	best estimate in literature
$\mathbf{Z}^2$	0.3924	(0.1702, 0.2370)	0.4074951 (0.2266)[MSS],[B2]
H	0.4279	(0.2202, 0.2371)	0.4360 (0.2424)[B2]
T	0.3253	(0.1457, 0.1559, 0.1517)	0.3332427 (0.1624)[B2]
K	0.3826	(0.1944, 0.1948, 0.1866)	
$\mathbf{Z}^2\mathrm{M}$	0.2858	(0.119, 0.127, 0.130, 0.126)	

Parameters p, q and r can be coupled in such a way that the sublattice densities equal. Resulting optimal entropy bounds decrease very slightly.

Density bounds

Somewhat loose but rigorous bounds for the densities can be derived for the cases involved. For example in the square lattice case where the uniqueness of the measure of maximal entropy guarantees identical sublattice densities we have

Proposition

In the square lattice case the density of 1's at the maximum entropy is a.s. in the interval (0.21367, 0.25806).

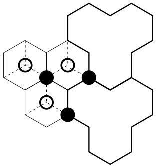
The upper bound is exactly 8/31 and the lower one utilizes the entropy estimate above.

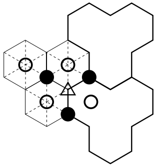
Higher order blocks on hexagonal and triangular lattice

- For improved lower bounds one can use e.g. **extended Bernoulli blocks**.
- Let $B(\mathbf{p})$, $\mathbf{p} = (p_0, p_1, p_2, p_3)$, be the Bernoulli distribution on circle 3-hexes with the probability that the 3-hex has exactly k 1-tiles in it in a given orientation is p_k (so $p_0 + 3p_1 + 3p_2 + p_3 = 1$). Its entropy is

$$h_B^{(3)}(\mathbf{p}) = -p_0 \ln p_0 - 3p_1 \ln p_1 - 3p_2 \ln p_2 - p_3 \ln p_3.$$

  The dot sublattice updates have to account for the three dot locations on the right.
- Triangular and Kagomé lattices: in the sequence $\circ \to \bullet \to \triangle$ the circle 3-hexes first update the dots and then the remaining unforced triangles are updated by B(1/2).





Neighboring circle 3-hexes on the hexagonal and triangular lattices.

Theorem (3-hexes)

Let $a(\mathbf{p}) = p_0 + 2p_1 + p_2$. For the hexagonal lattice the Hard Core entropy is bounded from below by

$$\underline{h}^{(3)}_{\mathbf{H}}(\mathbf{p}) = \frac{1}{6}\left\{h^{(3)}_B(\mathbf{p}) + \left[p_0 + 2a(\mathbf{p})^3\right]\ln 2\right\},$$

and for the triangular lattice a corresponding bound is

$$\underline{h}^{(3)}_{\mathbf{T}}(\mathbf{p}, q) = \frac{1}{9}\Big\{h^{(3)}_B(\mathbf{p}) + \left[p_0 + 2a(\mathbf{p})^3\right] h_B(q) + 3\left[p_1 + p_0(1-q)\right] a(\mathbf{p})^3 (2-q)^2 \ln 2\Big\},$$

where $p_i, q \in (0, 1)$.

Kagomé lattice can be treated analogously to the triangular case.

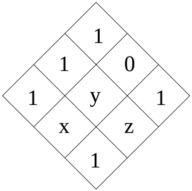
Optimal 3-hexes

Some improvement in the entropy bound and the densities close in...

L	max $\underline{h}_{\mathbf{L}}$	(p_0, p_1, p_2, p_3), q	sublattice densities
H	0.4304	(0.504, 0.110, 0.048, 0.021)	(0.2276, 0.2376)
T	0.3265	(0.64, 0.092, 0,025, 0.010), 0.25	(0.153, 0.155, 0.151)

Higher order blocks on $\mathbf{Z}^2$

- The blocks are chosen to be $n \times n$ diamonds.
- By the uniqueness of the mme (DS-criterion, Radulescu-Styer, -87) we can assume rotation and reflection invariance for the block probabilities. This reduces the number of optimized variables by factor at most 8.
- There is a **further reduction** of the number of variables due to "dummy sites" within blocks. On the right the values at the even sites x, y and z force no further odd sites. Hence the block together with seven other 3×3 -blocks will have exactly the same probability. This reduction compounds the symmetry reduction above.



Dummies in a 3×3 diamond: x, y and z values are irrelevant.

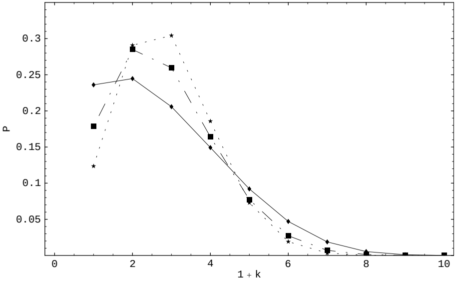
Comparison for higher order blocks on $\mathbf{Z}^2$

First few optimizations done on a desktop & *Mathematica*:

Block size	max $\underline{h}_{\mathbf{Z}^2}$	sublattice densities	reduced/init. variables
1×1	0.392421	(0.1702, 0.2370)	1
2×2	0.39877	(0.1993, 0.2254)	$5/15$
3×3	0.4014	(0.2073, 0.2254)	$46/511$

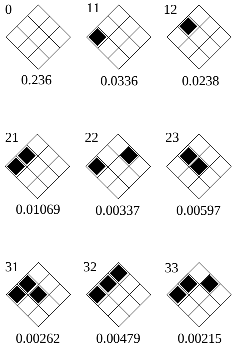
Larger blocks with specialized code. The dummy reduction will be highly significant: e.g. in the next size 4×4 the block count shrinks down to about 1/66th (from 65.535 to 991 free variables).

- 3×3 block occupation probabilities from optimal Bernoulli blocks of dimension 3×3 ($\blacklozenge$), 2×2 ($\blacksquare$), 1×1 ($\bigstar$). $k \in \{0, 1, \ldots, 9\}$ is the number of 1's in the block.
- All distributions have about the same mean $k/9 \approx 0.22$.
- The true 3×3 -block distribution ($\blacklozenge$) has heavier tail indicating longer range order.



Dominant blocks

- The dominant 3×3 -blocks and their probabilities (multiplicities accounted these probabilities sum to about 2/3). At each density level a very small number of blocks carry almost all of the probability mass.
- The fine structure of the optimal blocks as it unfolds in larger block sizes: next denser blocks are "grown" by adding new 1's contiguously to the 1's existing in a dominant lighter block of the same size.



Monotonicity

Let $B_i,\ i = 1, 2$ be $n \times n$-blocks and denote their subsets of 1's by $B_i^{(1)}$. There is a partial order on the B_i-blocks via $B_i^{(1)}$ using the set inclusion. Then

Theorem

Let the blocks $B_i,\ i = 1, 2$ have optimal lower bound probabilities p_i. If $B_1^{(1)} \subset B_2^{(2)}$ then $p_1 \geq p_2$. If $B_2^{(1)} \setminus B_1^{(1)}$ contains only weak sites with respect to $B_1^{(1)}$ then $p_1 = p_2$, otherwise $p_1 > p_2$.

Intuitively “one should favor even blocks which leave more choice to the odd lattice, otherwise weight uniformly”.

Summary

- An alternative method for estimating the entropy in various k-partite graph/lattice set-ups in any dimension. Usefullness beyond Hard Core depends on the computability of conditional probabilities/entropies.
- Numerically not the most efficient but gives explicit block probabilities and thereby insight into the typical configurations (support of mme)
- Depends on/can utilize efficient optimization algorithms.
- The tail behavior of the block probability distributions agrees with the existence of long range order in $\mathbf{Z}^2$ Hard Core. Correlation estimates etc. can be computed from the block probabilities.

Rest

[E1] Eloranta, K.: Dense packing on uniform lattices, *J. of Stat. Phys.*, **130**, pp. 741-55, 2008, `arXiv:0907.4247` [math-ph].

[E2] Eloranta, K.: Hard Core via PCA: Entropy Bounds, *AUTOMATA 2015* (Ed. J. Kari), LNCS **9099**, pp. 85–98, 2015, `arXiv:0907.4035` [math.PR].

`www.math.aalto.fi/∼kve/research.html.en`

Thank you!