Cluster Algorithms and Interfering Binary Mixtures

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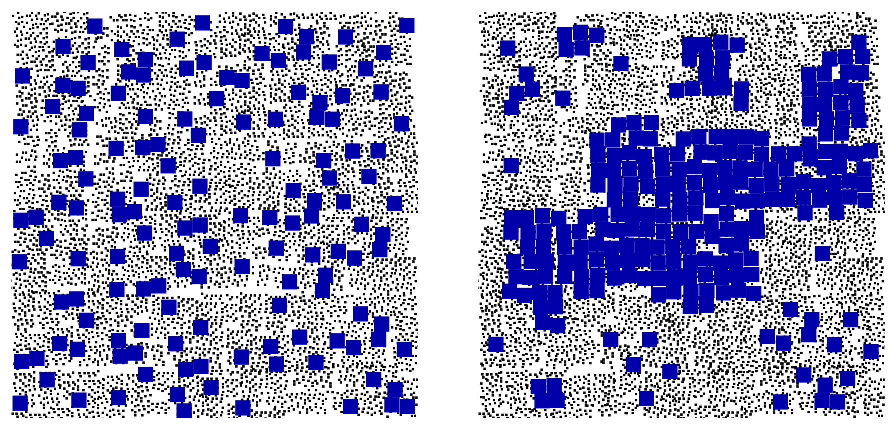
What are Colloids?

- Colloids are mixtures of two types of molecules in suspension. When the density of each type of molecule is low, the mixtures are homogeneous. When the density is high, the two types of molecules separate whereby one type appears to cluster together.
- Physicists have introduced various hard core models to show how this can be caused purely by entropy.

Squares Model:

$\Omega(\varphi) =$ the set of nonoverlapping packings of large squares and small squares of equal density φ in an $n \times n$ torus.



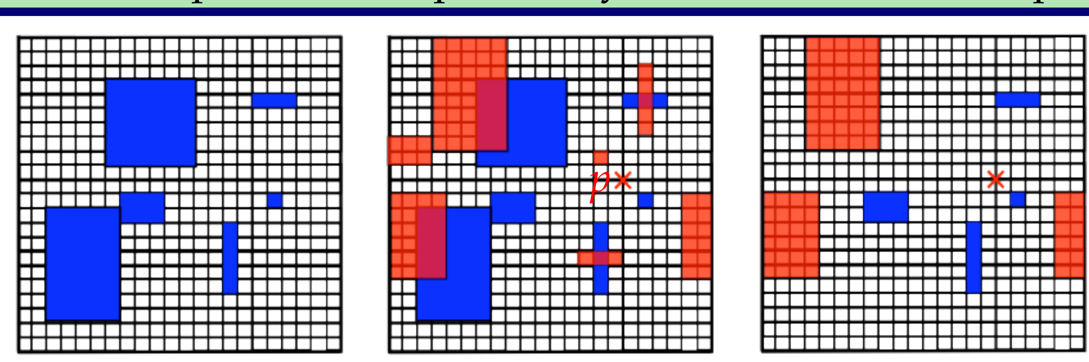
Lower density Higher density

Physicists' Conjecture: If the density φ is large enough then in a uniform sample from $\Omega(\varphi)$, the large squares will clump together.

How to verify? Local sampling algorithms fail when the density is high. A new nonlocal algorithm introduced by Buhot and Krauth (1) provided the first experimental evidence of the colloid effect.

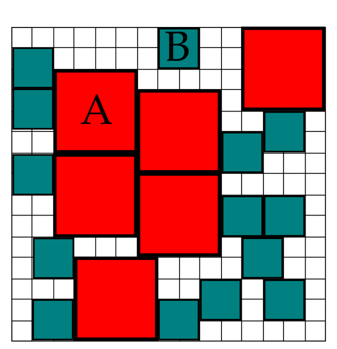
The Dress-Krauth Algorithm

- Given $\sigma_i \in \Omega(\varphi)$, choose a pivot point p uniformly at random.
- Rotate σ_i 180° around p and superimpose on the original to obtain τ.
- For each pair of components independently choose red or blue to produce σ_{i+1}.



σ_i τ σ_{i+1}

General Framework:



Consider Ω, the set of non-overlapping embeddings on a $n \times n$ torus of:

- α type A-tiles
- a variable number of B-tiles

where β is the number of B-tiles and each configuration σ has weight $\pi(\sigma) = \lambda^{\beta}/Z$.

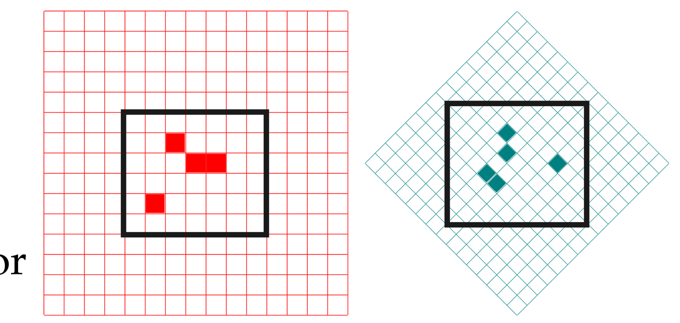
Our Goals

- Understand the stationary distribution.
- Analyze the Dress-Krauth algorithm.

Counting: Interfering Binary Mixtures

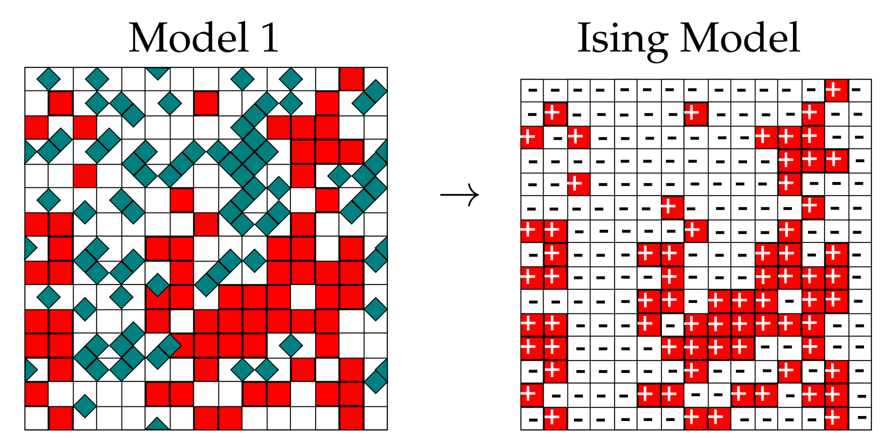
Interfering Binary Mixtures

Consider two planar lattices Δ_A and Δ_B. A-tiles lie on the faces of Δ_A and B-tiles lie on the faces of Δ_B. Take their intersection with some finite region. Interfering Binary Mixtures require that the faces of Δ_A and Δ_B are either disjoint, intersect at a single vertex or intersect at a fixed shape with positive area.

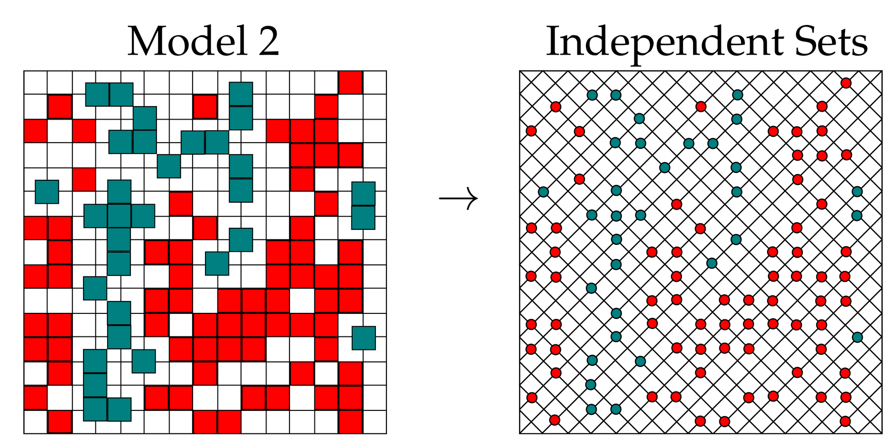


Δ_A Δ_B

Examples



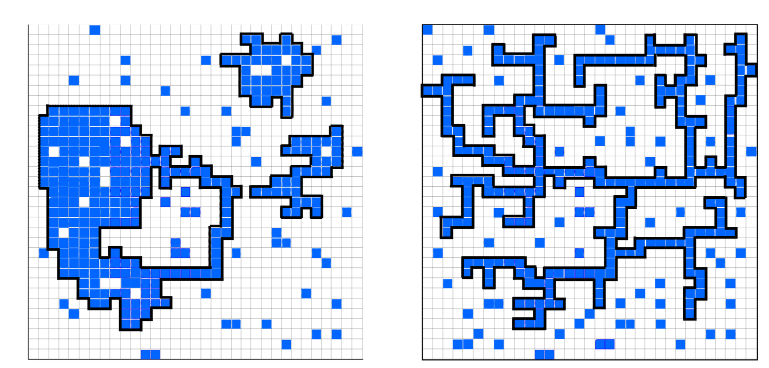
A-tiles: squares on faces; **B-tiles:** diamonds on edges



A-tiles: squares on faces; **B-tiles:** squares on vertices

New Definition - Clustering

A configuration "clusters" if it has the following properties.
- has a large very dense region R
- R is tightly packed (small perimeter : area ratio)
- the rest of the configuration is very sparse



Clustering No Clustering

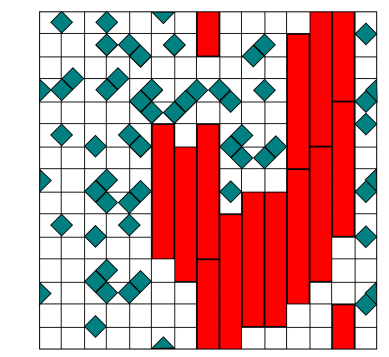
Theorem: For $0 < b \leq 1/2$, there exits constants $\lambda^* = \lambda^*(b) > 1$, $\gamma_1 < 1$ and $n_1 = n_1(b)$ such that for all $n > n_1$, $\lambda \geq \lambda^*$ a random sample from Ω will have the *clustering property* with probability at least $(1 - \gamma_1^n)$.

Theorem: For $0 < b < 1/2$, there exist constant $\lambda_* = \lambda_*(b) > 0$, $\gamma_2 < 1$ and $n_2 = n_2(b)$ such that for all $n > n_2$, $\lambda \leq \lambda_*$ a random sample from Ω will not have the *clustering property* with probability at least $(1 - \gamma_2^n)$.

These theorems apply to Model 1 on an $n \times n$ region with bn^2 A-tiles but hold for all **Interfering Binary Mixtures**.

Sampling: Dress-Krauth Algorithm

Bar Model:

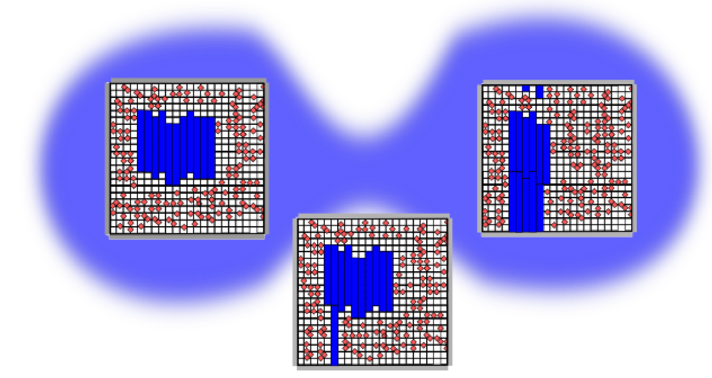


A-tiles: $L \times 1$ bars, where $L = cn$; **B-tiles:** diamonds on edges

Slow Mixing for the Bar Model:

A Markov chain **Mixes Slowly** if it takes time exponential in n to converge to the stationary distribution.

Theorem: If $L = cn$, $L < n/2$, then the Dress-Krauth algorithm is slow mixing.

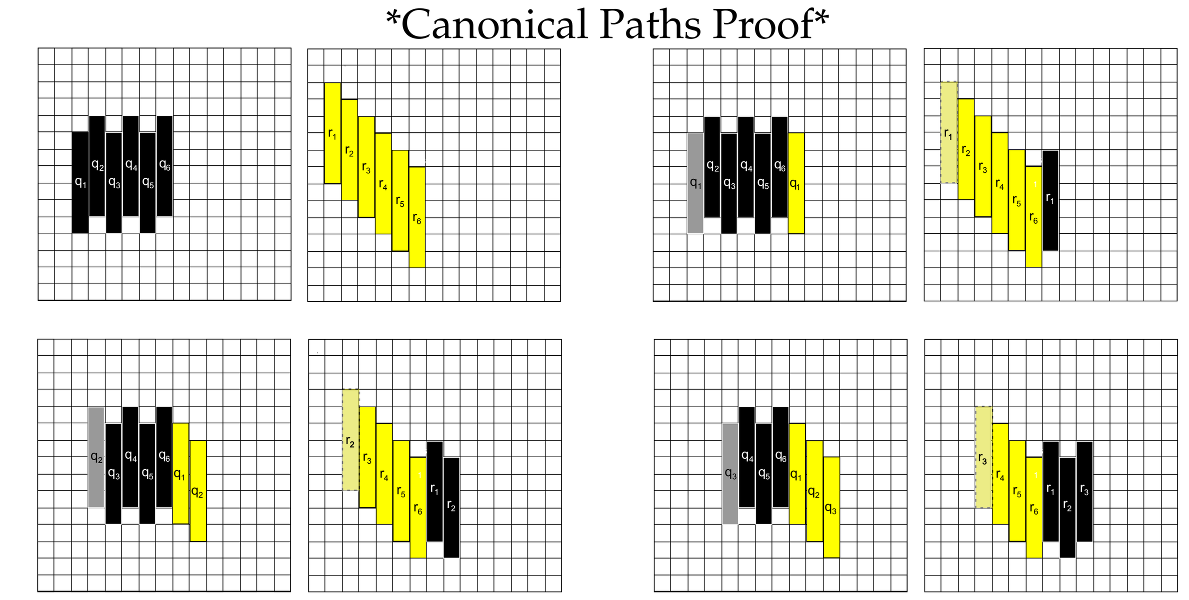


Rapid Mixing for the Bar Model:

A Markov chain **Mixes Rapidly** if it converges to the stationary distribution in time polynomial in n.

Theorem: If $L > n/2$ (at most one bar per column), then the Dress-Krauth algorithm is rapidly mixing.

Canonical Paths Proof



References

[1] A. Buhot, W. Krauth. Phase Separation in Two-Dimensional Additive Mixtures. Phys. Rev. E 59(1990) pp. 2939-2941.

[2] C. Dress and W. Krauth. Cluster Algorithm for Hard Spheres and Rlated Systems. J. Phys. A: Math. Gen. L597 (1995).