First-order phase transitions and efficient sampling algorithms

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Algorithms and phase transitions

• When are phase transitions barriers to efficient algorithms?
• Does the type of phase transition play a role?
• Can we use tools from statistical physics to design new algorithms?
• Can we use the algorithmic perspective to understand phase transitions?
Based on:

- “Efficient sampling and counting algorithms for the Potts model on $\mathbb{Z}^d$ at all temperatures” (joint w/ Borgs, Chayes, Helmuth, Tetali, STOC 2020)

- “Finite-size scaling and phase coexistence for the random cluster model on random graphs” (joint w/ Helmuth, Jenssen on arxiv soon!)
Outline

• Potts model and random cluster model

• What is a phase transition? What is a first-order phase transition?

• Contour representations, Pirogov-Sinai theory

• Algorithms on $\mathbb{Z}^d$ and random graphs
Potts model

Probability distribution on q-colorings $\sigma: V(G) \to [q]$ of the vertices of G:

$$\mu(\sigma) = \frac{e^{\beta m(G, \sigma)}}{Z_G(\beta)}$$

$m(G, \sigma)$ is the number of monochromatic edges of G under $\sigma$

$$Z_G(\beta) = \sum_{\sigma \in [q]^V} e^{\beta m(G, \sigma)}$$ is the partition function.

$\beta$ is the inverse temperature. $\beta \geq 0$ is the ferromagnetic case: same color preferred.
Potts model

High temperature ($\beta$ small)

Low temperature ($\beta$ large)
Phase transitions

- On $\mathbb{Z}^d$ the Potts model undergoes a phase transition as $\beta$ increases.

- For small $\beta$, the influence of boundary conditions diminishes as volume grows; for large $\beta$, influence of boundary conditions persists in infinite volume.

- For small $\beta$, correlations decay exponentially fast, configurations are disordered (on, say, the discrete torus).

- For large $\beta$, we have long range order (and a dominant color in a typical configuration).
Random cluster model

The random cluster model is a generalization of the Potts model.

Probability distribution on subsets of edges of $G$:

$$
\mu_{q,\beta}(A) = q^{c(A)}(e^\beta - 1)^{|A|/Z_G(q, \beta)}
$$

$c(A)$ is the number of connected components of $(V, A)$.

$q > 0$ can be non-integral. $q = 1$ corresponds to independent edge percolation.
Random cluster model

Edwards-Sokal coupling:

1. Pick a set of edges according to the random cluster measure
2. Determine the connected components
Random cluster model

Edwards-Sokal coupling:

1. Pick a set of edges according to the random cluster measure
2. Determine the connected components
3. Assign one of the q colors uniformly and independently to each connected component
Phase transitions

• Another definition of a phase transition: plot the limiting value of an observable against $\beta$. A phase transition occurs at a non-analytic point.
Large q behavior

• For q large enough as a function of d, the random cluster model exhibits a first-order phase transition.

• **No middle ground**: for all $\beta$ typical configurations consist of very few or very many edges (say, $\leq |E|/10$ or $\geq 9|E|/10$ for large enough q).

• Conditioned on number of edges, nice probabilistic properties, including exponential decay of correlations.

• Proved by Laanait, Messager, Miracle-Sole, Ruiz, Shlosman, 1991 using Pirogov-Sinai theory.
Phase transitions and algorithms

• Two main computational problems associated to a statistical physics model: approximate the partition function (counting) and output an approximate sample from the model (sampling)

• Many different approaches including Markov chains, correlation decay method, polynomial interpolation. All are limited by or must bypass phase transitions (slow mixing, long-range correlations, accumulation of zeroes on real axis)
Markov chains

• For the Potts model we have several useful Markov chains:
  • **Glauber dynamics** - pick a random vertex and update color
  • **Swendsen—Wang dynamics** - pick a cluster and update color

• **Glauber dynamics** mix slowly for $\beta \geq \beta_c$ - there is a bottleneck between mostly Red and mostly Green configurations

• **Swendsen-Wang** mixes slowly at $\beta = \beta_c$ - the middle ground is a bottleneck (Gore-Jerrum for $K_n$, Borgs-Chayes-Frieze-Kim-Tetali-Vigoda-Vu and Borgs-Chayes-Tetali for $\mathbb{Z}^d$, Galanis-Stefankovic-Vigoda-Yang for random graphs. Consequence of the **first-order phase transition**
Contour models

- Random cluster model has two **ground states**: the **disordered** state $A = \emptyset$ and the **ordered** state $A = E$.

- In the Potts model these correspond to choosing the color of each vertex independently and choosing a single color for all vertices.

- **Contours** provide a geometric way of separating a RC configuration into ordered and disordered regions.
Contour models

- Idea of Pirogov-Sinai theory is to use **contour models** to separate configurations into mostly ordered and mostly disordered.
- Leads to two **new partition functions** $Z_{\text{dis}}$ and $Z_{\text{ord}}$.
- These can be controlled via the **cluster expansion**.
Free energies

Let \( f_{\text{dis}} = \lim_{n \to \infty} \frac{1}{n} \log \tilde{Z}_{\text{dis}} \) and \( f_{\text{ord}} = \lim_{n \to \infty} \frac{1}{n} \log \tilde{Z}_{\text{ord}} \)

By showing \textbf{no middle ground}, it follows that

\[
f = \lim_{n \to \infty} \frac{1}{n} \log Z = \max\{f_{\text{dis}}, f_{\text{ord}}\}
\]

\( \beta_c \) is the point at which \( f_{\text{dis}} = f_{\text{ord}} \)
Free energies

$\beta_c$
At criticality

• At $\beta = \beta_c$, $Z_{\text{dis}}$ and $Z_{\text{ord}}$ match on an exponential scale.

• On discrete torus, $Z_{\text{ord}}(\beta_c) \approx q \cdot Z_{\text{dis}}(\beta_c)$

• Smaller order corrections in $n$ (volume of torus) are finite-size effects (Borgs—Kotecky—Miracle-Sole, 1991)

• $Z = Z_{\text{ord}} + Z_{\text{dis}} + \exp(-\Theta(n^{(d-1)/d}))$. Typical configurations look either disordered or ordered — no mixtures! unlike in second-order phase transition
What’s new

• The **cluster expansion** (and Pirogov-Sinai theory) can be made algorithmic: approximate $Z_{\text{dis}}$ and $Z_{\text{ord}}$ separately.

• **First-order phase transition** means that this suffices at criticality.

• Efficient sampling and counting for Potts and RC on $\mathbb{Z}^d$ at all temperatures (large $q$) [BCHTP]

• Apply the same approach to other graphs: efficient algorithms at all temperatures on **random $\Delta$-regular graphs** (large $q$) [HJP].

• This gives us a detailed **phase diagram** of the random cluster model on random graphs: correlation decay, local weak convergence, precise phase coexistence etc. (see also Galanis-Stefankovic-Vigoda-Yang)
Rest of the talk

• High-level picture of **contour models** and **cluster expansions**
• How to make these tools **algorithmic**
• What to do for **random graphs**? We lose some geometry but gain **expansion**.
Constructing Contours
Contour representation

We can describe a configuration geometrically:

- **Ordered**: occupied edges
- **Disordered**: unoccupied edges

Boundaries between ordered/disordered regions are **contours**.

Contours are non-intersecting, nested, with **labels** indicating the exterior and interior ground state.
Contour representation

We can describe a configuration geometrically:

- **Ordered**: occupied edges
- **Disordered**: unoccupied edges

A configuration is (dis)ordered if the only region that wraps around the torus (winding number >0) is (dis)ordered.

If any contour wraps around, the configuration is part of the middle ground.
We can express the RC weight of a configuration in terms of its contours.

Ordered regions $B$ have a volume factor $q(e^\beta - 1)^d|B|$.

Disordered regions $B$ have a volume factor $q^{|B|}$.

Contours have a penalty factor exponentially small in their size (number of edges crossing the contour) $e^{-\kappa \|\gamma\|}$.
Contour representation

Weight of this configuration:

\[ (e^\beta - 1)^{nd/2} \cdot e^{-\kappa \| \gamma \|} \cdot \left( \frac{q}{(e^\beta - 1)^d} \right)^{|\text{Int}(\gamma)|} \]

\( \kappa \) is increasing in \( q \). \( \beta_c \approx \log q/d \)
Contour representation

Outer contours
Contour representation

Weight of all configurations with these outer contours:

\[(e^\beta - 1)^{nd} \prod_{\gamma \in \Gamma} e^{-\kappa \|\gamma\|} Z_{dis}(Int(\gamma))(e^\beta - 1)^{-|Int(\gamma)|}\]

where \(Z_{dis}(\Lambda)\) is the partition function with disordered boundary conditions.
Contour representation

Express $Z_{ord}$ as a sum over collections of compatible outer contours:

$$Z_{ord} = q(e^\beta - 1)^{nd} \sum_{\Gamma} \prod_{\gamma \in \Gamma} e^{-\kappa \|\gamma\|} Z_{dis}(Int(\gamma))(e^\beta - 1)^{-|Int(\gamma)|}$$

This looks like a generalized **hard-core model**: sum over `independent set`, product of weights
Contour representation

With some additional manipulations (standard in Pirogov-Sinai theory) we have (sums are over collections of non-intersecting contours):

\[
Z_{ord} = q(e^\beta - 1)^n d \sum_{\Gamma} \prod_{\gamma \in \Gamma} K_{ord}(\gamma)
\]

\[
Z_{dis} = q^n \sum_{\Gamma} \prod_{\gamma \in \Gamma} K_{dis}(\gamma)
\]

For q large, either \( K_{ord}(\gamma) \) or \( K_{dis}(\gamma) \) is exponentially small in \( ||\gamma|| \) \( (\beta \geq \beta_c \) and \( \beta \leq \beta_c \) respectively)
• The cluster expansion is a tool from mathematical physics for analyzing probability laws on ‘dilute’ collections of geometric objects.

• It applies to a very general weighted independent set model — on a graph with inhomogeneous weights and unbounded vertex degrees. Each vertex represents a geometric object, neighboring objects overlap.

\[
Z = \sum_{\Gamma} \prod_{\gamma \in \Gamma} w_\gamma
\]
Cluster expansion

• The cluster expansion says that, under some conditions,

$$\log Z = \sum_{\Gamma_c} \Phi(\Gamma_c) \prod_{\gamma \in \Gamma_c} w_\gamma$$

• The sum is over connected collections of objects. Informally, the conditions say that the weights are exponentially small in the size of the objects.
Making the cluster expansion \textbf{algorithmic} requires:

**Enumerating contours** of size $O(\log n)$: essentially enumerating connected subgraphs in a bounded degree graph

**Computing contour weights** $K_{dis}(\gamma), K_{ord}(\gamma)$: tricky because weights involve ratios of partition functions, but this can be done inductively using the cluster expansion

**Sampling** is done via self-reducibility on the level of contours
Random graphs

We can apply a similar approach to the random cluster model on $\Delta$-regular random graphs.

**Thm** (Helmuth, Jenssen, P.) For $\Delta \geq 5$, $q = q(\Delta)$ large enough:

There are efficient approximate counting and sampling algorithms for the Potts and random cluster models on random $\Delta$-regular graphs at all temperatures.
Random graphs

**Thm** (Helmuth, Jenssen, P.) For $\Delta \geq 5$, $q = q(\Delta)$ large enough:

- Determine distribution of $\frac{Z_{dis}}{Z_{ord}}$ at $\beta_c$
- Exponential decay of correlations for $\beta \neq \beta_c$
- Local convergence of RC measure to free or wired RC measure on infinite $\Delta$-regular tree

Compare to Galanis-Stefankovic-Vigoda; Montanari-Mossel-Sly; Dembo-Montanari-Sly-Sun; Sly-Sun; very different techniques based on verifying the predictions of the **cavity method**; these results are generally on the level of the free energy
Random graphs

Random graphs are very good expanders and are locally tree-like.

We can define $Z_{\text{dis}}$ and $Z_{\text{ord}}$ via polymer models representing deviations from the disordered and ordered ground state.

We don’t have to define weights inductively since the boundary of polymers is proportional to volume. But we lose the geometry of $\mathbb{R}^d$ and have to argue indirectly about the non-local RC interaction via expansion.
Summary

• The **first-order phase transition** in the Potts and Random Cluster model is a barrier to Markov chains like Swendsen-Wang

• But it facilitates a **different type of algorithm** based on approximating / sampling from ordered and disordered configurations separately

• This allows us to find efficient algorithms at **all temperatures**, including critical

• We can follow this framework for **random graphs** as well, obtaining new algorithms and new probabilistic results
Open questions

• Are there provably fast **Markov chain algorithms** to sample from these models at all temperatures?

• Can we deal with boundary conditions and **interfaces** algorithmically?

• How can we deal with **second-order** phase transitions algorithmically?

Thank you!