Path Coupling and Belief Propagation

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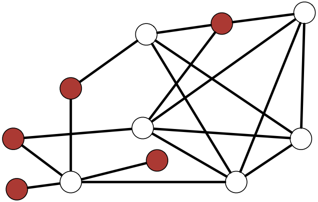
joint work with:
C. Efthymiou, T. Hayes, D. Štefankovič, Y. Yin [FOCS '16]

Martin Dyer Celebration, July '18

Independent Set

Undirected graph $G = (V, E)$:



Independent set: subset of vertices with no adjacent pairs.

Let $\Omega =$ all independent sets (of all sizes).

Our Goal:

1. *Counting problem:* Estimate $|\Omega|$.
2. *Sampling problem:* Sample uniformly at random from Ω.

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restricted classes of graphs

Bounded Degree Graphs

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Given input graph $G = (V, E)$ with maximum degree Δ
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Exact computation of $|\Omega|$ is #P-complete, even for $\Delta = 3$.

[Greenhill '00]

What about approximating $|\Omega|$?

Hard-Core Gas Model

Graph $G = (V, E)$, *fugacity* $\lambda > 0$, for $\sigma \in \Omega$:

Gibbs distribution: $$\mu(\sigma) = \frac{\lambda^{|\sigma|}}{Z}$$

where

Partition function: $$Z = \sum_{\sigma} \lambda^{|\sigma|}$$

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Inuition: Small λ easier: for $\lambda < 1$ prefer smaller sets.
Large λ harder: for $\lambda > 1$ prefer max independent sets.

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FPRAS for Z: Given G, $\epsilon, \delta > 0$, output EST where:

$$\mathbf{Pr}\left(\text{EST}(1-\epsilon) \leq Z \leq \text{EST}(1+\epsilon)\right) \geq 1 - \delta,$$

in time poly$(|G|, 1/\epsilon, \mathit{log}(1/\delta))$.

FPTAS for Z: FPRAS with $\delta = 0$.

FPAUS for μ: Given G, $\delta > 0$, output X from distribution ν:

$$d_{\text{TV}}(\nu, \mu) := \frac{1}{2} \sum_{\sigma \in \Omega} |\nu(\sigma) - \mu(\sigma)| \leq \delta,$$

in time poly$(|G|, \mathit{log}(1/\delta))$.

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Then $T_{\text{mix}}(\epsilon) \leq \log(1/\epsilon)\, T_{\text{mix}}$.

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Recall, $d_{\mathrm{TV}}(\mu, \nu) = \frac{1}{2} \sum_{\sigma \in \Omega} |\mu(\sigma) - \nu(\sigma)|$.

Approximating Partition Function

- For $\lambda < \frac{2}{\Delta - 2}$, $T_{\text{mix}} = O(n \log n)$ ($\lambda = 1, \Delta = 4$, poly(n))

  [Luby,V '97],[Dyer,Greenhill '00]

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Statistical physics phase transition on infinite Δ-regular tree!

Our Results

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Theorem

For all $\delta > 0$, *there exists* $\Delta_0 = \Delta_0(\delta)$:

all $G = (V, E)$ *of max degree* $\Delta \geq \Delta_0$ *and girth* ≥ 7,

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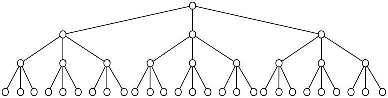
Corollaries

- An $O^*(n^2)$ FPRAS for estimating the partition function Z.
- $T_{mix} = O(n \log n)$ when $\lambda \leq (1 - \delta)\lambda_c(\varDelta)$ for:
  - random $\varDelta$-regular graphs
  - random $\varDelta$-regular bipartite graphs

Phase Transition on Trees

For Δ-regular tree of height ℓ:

$$\text{Let } p_\ell := \mathbf{Pr}\,(\text{root is occupied})$$



Extremal cases: even versus odd height.

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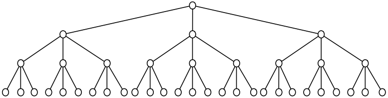

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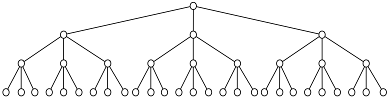

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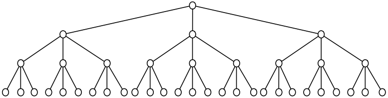

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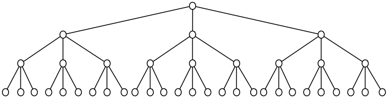

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Example: $\Delta = 5$, $\lambda = 1$:

$$p_{even} = .245, \ p_{odd} = .245$$

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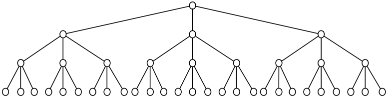

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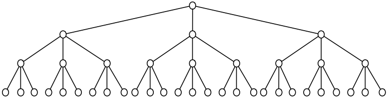

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Example: $\Delta = 5$, $\lambda = 1.06$:

$$p_{even} = .283, \; p_{odd} = .219$$

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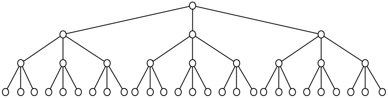

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Tree/BP recursions: $p_{\ell+1} = \frac{\lambda(1-p_\ell)^{\Delta-1}}{1+\lambda(1-p_\ell)^{\Delta-1}}$

Key: Unique vs. Multiple fixed points of 2-level recursions.

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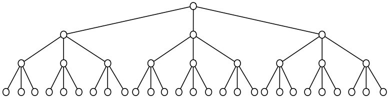

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For 2-dimensional integer lattice $\mathbb{Z}^2$:

Conjecture: $\lambda_c(\mathbb{Z}^2) \approx 3.79$

Best bounds: $2.53 < \lambda_c(\mathbb{Z}^2) < 5.36$

Coupling of Markov Chains

Consider a Markov chain (Ω, P).

Coupling is a joint process $\omega = (X_t, Y_t)$ on $\Omega \times \Omega$ where:

$$X_t \sim P \text{ and } Y_t \sim P$$

More precisely, for all $a, b, c \in \Omega$,

$$\mathbf{Pr}\left(X_{t+1} = c \mid X_t = a, Y_t = b\right) = P(a, c)$$
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Intuition:

$(X_t \to X_{t+1}) \sim P$ and $(Y_t \to Y_{t+1}) \sim P$ can correlate by ω.

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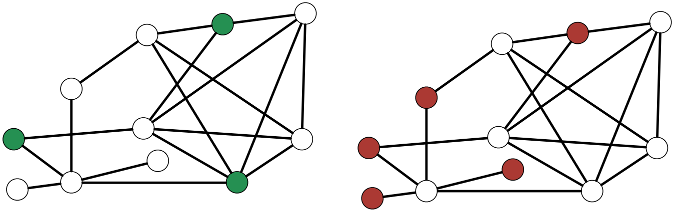
Coupling time:

$$T_{\text{couple}} = \max_{a,b} \min\{t : \mathbf{Pr}\left(X_t \neq Y_t \mid X_0 = a, Y_0 = b\right) \leq 1/4.\}$$

$$T_{\text{mix}} \leq T_{\text{couple}}$$

Coupling for Independent Sets

Consider a pair of independent sets X_t and Y_t:



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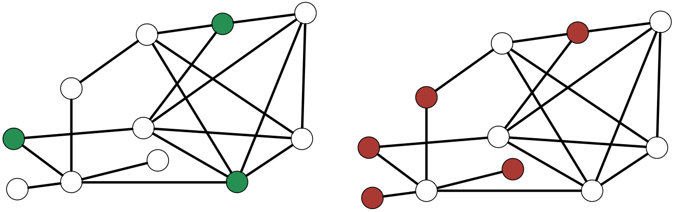

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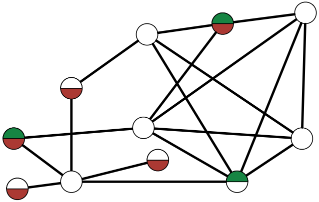

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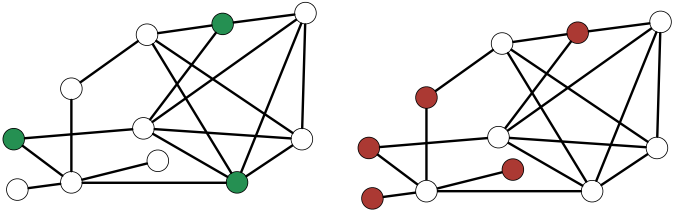

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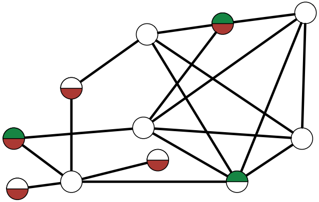

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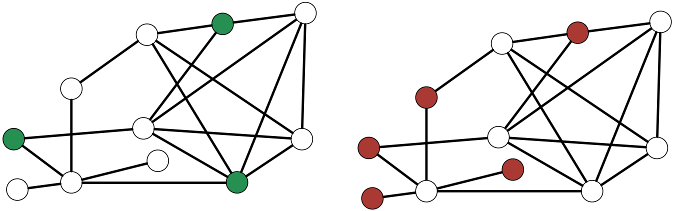

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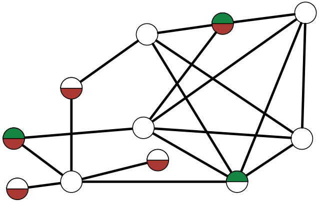

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How to analyze???

Coupling for bounding T_{mix}

For all X_t, Y_t, define a coupling: $(X_t, Y_t) \to (X_{t+1}, Y_{t+1})$.

Look at Hamming distance: $H(X_t, Y_t) = |\{v : X_t(v) \neq Y_t(v)\}|$.

If for all X_t, Y_t,

$$\mathbb{E}\left[H(X_{t+1}, Y_{t+1}) \middle| X_t, Y_t \right] \leq (1 - 1/n) H(X_t, Y_t),$$

then $T_{\mathrm{mix}} = O(n \log n)$.

Path coupling: Suffices to consider pairs where $H(X_t, Y_t) = 1$.

Path Coupling [Bubley and Dyer '97]

Let $S \subset \Omega^2$ denote pairs (X_t, Y_t) where $H(X_t, Y_t) = 1$.
Define a coupling ω for all $(X_t, Y_t) \in S$ where:

$$\mathbb{E}\left[H(X_{t+1}, Y_{t+1}) \mid X_t, Y_t\right] \leq 1 - C/n.$$

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For arbitrary $(A_t, B_t) \in \Omega^2$:

In graph (Ω, S), consider a shortest path X_t to Y_t:

$$(A_t, W_t^1, W_t^2, \ldots, W_t^{\ell-1}, B_t),\ \ell = H(A_t, B_t).$$

Couplings: $\omega^1 = (W_t^0, W_t^1), \ldots, \omega^\ell = (W_t^{\ell-1}, W_t^\ell)$.
Compose: $\omega = \omega^1 \circ \omega^2 \circ \cdots \circ \omega^\ell$ gives coupling (A_t, B_t).

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Algorithmic View:

1. Choose $W_t^0 \to W_t^1$ by P,
2. Apply ω^1 to get $W_t^2 \to W_{t+1}^2$,
3. Apply ω^2 to get $W_t^3 \to W_{t+1}^3, \ldots,$
4. Get $W_t^\ell \to W_{t+1}^\ell$.

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$$\begin{aligned}
\mathbb{E}\left[H(A_{t+1}, B_{t+1})\right] &\leq \mathbb{E}\left[\sum_i H(W_{t+1}^{i-1}, W_{t+1}^i)\right] \\
&\leq \sum_i \mathbb{E}\left[H(W_{t+1}^{i-1}, W_{t+1}^i)\right] \\
&\leq \sum_i (1 - C/n) \\
&\leq H(A_t, B_t)(1 - C/n).
\end{aligned}$$

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Then for arbitrary $(A_t, B_t) \in \Omega^2$, can construct coupling where:

$$\mathbb{E}\left[H(A_{t+1}, B_{t+1})\right] \leq H(A_t, B_t)(1 - C/n).$$

$$\begin{aligned}
\mathbf{Pr}\left(A_T \neq B_T\right) &\leq \mathbb{E}\left[H(A_T, B_T)\right] \\
&\leq H(A_0, B_0)(1 - C/n)^T \\
&\leq n \exp(-C/n) \\
&\leq 1/4 \quad \text{for } T = O(n \log n).
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Hence, $T_{\mathrm{mix}} = O(n \log n)$.

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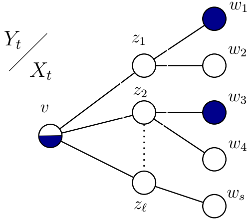
Can replace $H()$:

For $\Phi : V \to \mathbb{R}_{\geq 1}$, let $\Phi(X, Y) = \sum_{v \in X \oplus Y} \Phi_v$.

Key: if $X \neq Y$ then $\Phi(X, Y) \geq 1$ and $\mathbf{Pr}\left(X_t \neq Y_t\right) \leq \mathbb{E}\left[\Phi(X_t, Y_t)\right]$.

Path Coupling with Hamming Distance

$$\mathbb{E}\left[H(X_{t+1}, Y_{t+1})\right] = H(X_t, Y_t) - \frac{1}{n} + \sum_{z_i} \Pr[z_i \in Y_{t+1}]$$



Coupling: update same vertex, attempt add $\frac{\lambda}{1+\lambda}$, remove $\frac{1}{1+\lambda}$.

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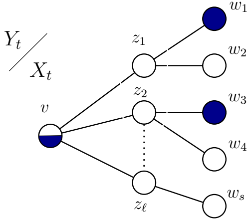

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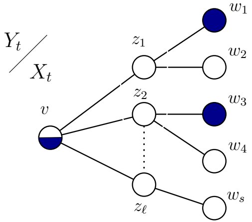

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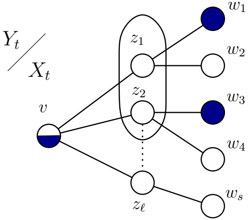

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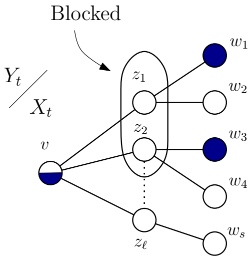

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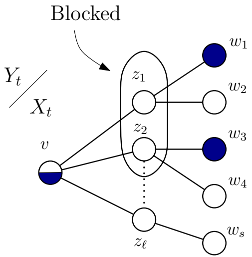
&= (1 - \frac{1}{n}) + \frac{1}{n} \sum_{z_i} \mathbf{1}\{z_i \text{ unblocked}\} \frac{\lambda}{1+\lambda} \\
&\leq 1 - \frac{1}{n} + \frac{\Delta}{n} \frac{\lambda}{1+\lambda}
\end{aligned}$$



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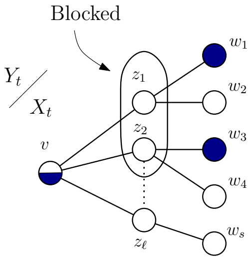
$$= (1 - \frac{1}{n}) + \frac{1}{n} \sum_{z_i} \mathbf{1}\{z_i \text{ unblocked}\} \frac{\lambda}{1+\lambda}$$

$$\leq 1 - \frac{1}{n} + \frac{\Delta}{n} \frac{\lambda}{1+\lambda} \quad < 1$$

Requires: $\lambda < 1/(\Delta - 1)$



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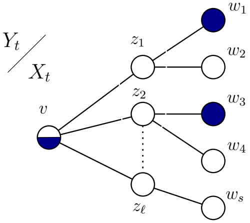

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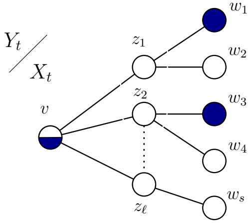

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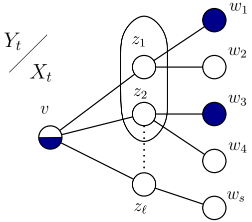

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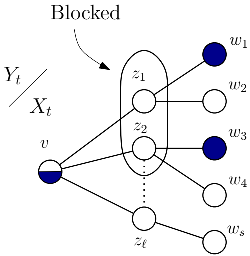

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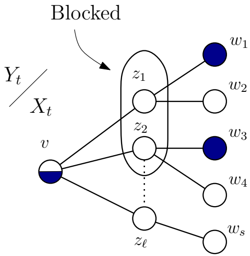

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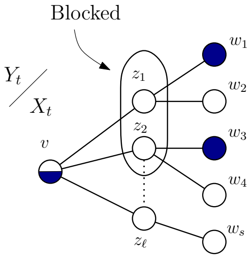
Want: $\Phi_v > \frac{\lambda}{1+\lambda}\sum_{z_i} \mathbf{1}\{z_i \text{ unblocked in } Y_t\} \cdot \Phi_{z_i}$



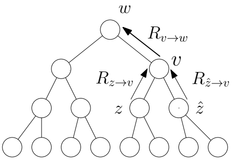
Belief Propagation on trees

For tree T and given λ, compute:

$q(v, w) = \mu(v \text{ occupied} | w \text{ unoccupied})$

$$R_{v\to w} = \frac{q(v,w)}{1-q(v,w)}$$

$$R_{v\to w} = \lambda \prod_{z\in N(v)\setminus\{w\}} \frac{1}{1+R_{z\to v}}$$



BP starts from arbitrary $R^0_{v\to w}$,
then iterates:

$$R^i_{v\to w} = \lambda \prod_{z\in N(v)\setminus\{w\}} \frac{1}{1+R^{i-1}_{z\to v}}$$

BP and Gibbs distribution on trees

Convergence on trees

For $i >$ max-depth, for every initial (R^0):

$$R^i_{v\to w} = R^*_{v\to w}$$

In turn

$$\mu(v \text{ occupied}|w \text{ unoccupied}) = q^* = \frac{R^*_{v\to w}}{1 + R^*_{v\to w}}$$

BP is an elaborate version of *Dynamic Programing*

BP Convergence for girth ≥ 6

Loopy Belief Propagation: Run BP on general $G = (V, E)$. For all $v \in V, w \in N(v)$:

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For $\lambda < \lambda_c$: $R()$ has a unique fixed point R^*.

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Theorem

Let $\delta, \epsilon > 0$, $\Delta_0 = \Delta_0(\delta, \epsilon)$ and $C = C(\delta, \epsilon)$.
For G of max degree $\Delta \geq \Delta_0$ and girth ≥ 6, all $\lambda < (1 - \delta)\lambda_c(\Delta)$:
for $i \geq C$, for all $v \in V$, $w \in N(v)$,

$$\left| \frac{q^i(v, w)}{\mu(v \text{ is occupied} \mid w \text{ is unoccupied})} - 1 \right| \leq \epsilon$$

Unblocked Neighbors and loopy BP

Recall, loopy BP estimate that z is unoccupied:

$$R_z^i = \lambda \prod_{y \in N(v)} \frac{1}{1 + R_y^{i-1}}$$

Loopy BP estimate that z is unblocked:

$$\omega_z^i = \prod_{y \in N(z)} \frac{1}{1 + \lambda \cdot \omega_y^{i-1}}$$

For $\lambda < \lambda_c$:

Since R converges to unique fixed point R^*,

thus ω converges to unique fixed point ω^*.

We'll prove (but don't know a priori):

$$\omega^*(z) \approx \mu(z \text{ is unblocked})$$

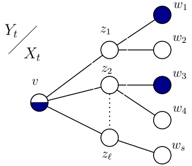
Back to Path Coupling

worst case condition

$$\Phi_v > \frac{\lambda}{1+\lambda} \sum_{z_i} \mathbf{1}\{z_i \text{ unblocked}\} \cdot \Phi_{z_i}$$

when X_t, Y_t "behave" like ω^*

$$\Phi_v > \frac{\lambda}{1+\lambda} \sum_{z_i} \omega^*(z_i) \cdot \Phi_{z_i}$$



Finding Φ

Reformulation

Goal: Find Φ such that

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Define $n \times n$ matrix $\mathcal{C}$

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Rephrased: Find vector $\Phi \in \mathbb{R}^V_{\geq 1}$ such that

$$\mathcal{C} \, \Phi < \Phi$$

Connections with Loopy BP

Recall, BP operator for unblocked: $F(\omega)(z) = \prod_{y \in N(z)} \frac{1}{1 + \lambda\omega(y)}$

It has Jacobian: $J(v,u) = \left| \frac{\partial F(\omega)(v)}{\partial \omega(u)} \right| = \begin{cases} \frac{\lambda F(\omega)(v)}{1+\lambda\omega(u)} & \text{if } u \in N(v) \\ 0 & \text{otherwise} \end{cases}$

Let $J^* = J|_{\omega=\omega^*}$ denote the Jacobian at the fixed point ω^*.

Key fact: $\mathcal{C} = D^{-1} J^* D$,

where D is diagonal matrix with $D(v,v) = \omega^*(v)$

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Fixed point ω^* is Jacobian attractive so all eigenvalues < 1.

Principal eigenvector Φ is good coupling distance.

Outline

Problem: We don't know good Φ for worst-case X_t, Y_t.

Proof approach:

- Find good Φ when locally X_t, Y_t "behave" like ω^*
  –dynamics gets "*local uniformity*" builds on [Hayes '13]
  which builds on [Dyer,Frieze '03]

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  For any X_0, when $\lambda < \lambda_c$ and girth ≥ 7,
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  For (X_0, Y_0) differ only at v, for $T = O(n \log \Delta)$, $r = O(\sqrt{\Delta})$,

$$\mathbf{Pr}\left(X_T \oplus Y_T \subset B_r(v)\right) \geq 1 - \exp(\Omega(\sqrt{\Delta}))$$

Local Uniformity Result

Main result: For Glauber (X_t), when $\lambda < \lambda_c$ and girth ≥ 7, with prob. $\geq 1 - \exp(-\Omega(\Delta))$, for $t = \Omega(n \log \Delta)$:

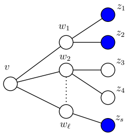
$$\#\{\text{Unblocked Neighbors of } v \text{ in } X_t\} < \sum_{z \in N(v)} \omega^*(z) + \epsilon\Delta.$$

Proof idea: Chain behaves locally like loopy BP.

Local Uniformity Proof Idea

For $v \in V$, fix σ on its grandchildren $S_2(v)$, let

$$\mathbf{R}_v(\sigma) := \Pr_{Y \sim \mu}\left[v \text{ is unblocked in } Y \mid v \notin Y,\ Y(S_2(v)) = \sigma(S_2(v))\right]$$



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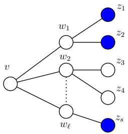

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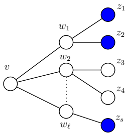

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Key result: for Gibbs dist. μ when girth ≥ 6, for $X \sim \mu$. whp:

$$\left| \mathbf{R}_v(X) - \prod_{w \sim v} \left(1 - \frac{\lambda}{1+\lambda} \mathbf{R}_w(X)\right) \right| < \gamma,$$

Proof: Conditions on $S_3(v)$ and uses girth ≥ 6 so $\mathbf{R}_w(X)$ is independent across $w \in N(v)$.

Similarly for Glauber dynamics when girth ≥ 7.

Key Results

Proof approach:

- Find good Φ when locally X_t, Y_t "behave" like ω^*
- Glauber dynamics converges locally to ω^*
  - dynamics gets "*local uniformity*" builds on [Hayes '13]
- This Φ + local uniformity $\rightarrow$ rapid mixing

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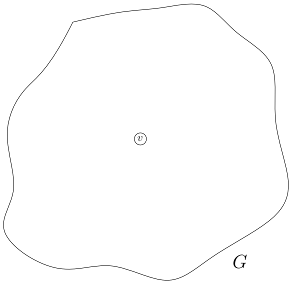
Rapid Mixing with Uniformity [Dyer-Frieze-Hayes-V '13]



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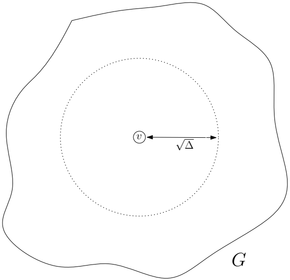

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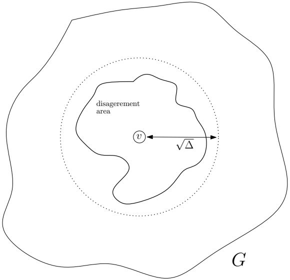

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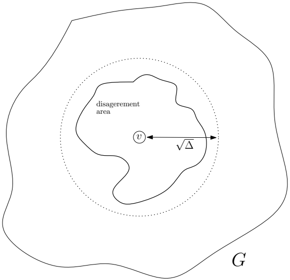

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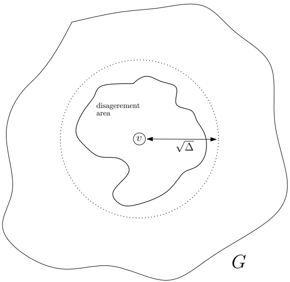

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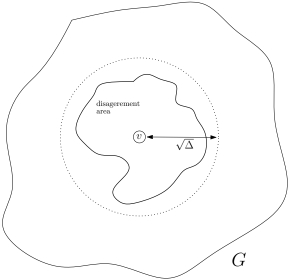

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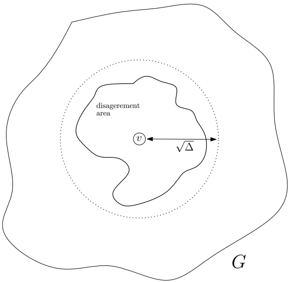

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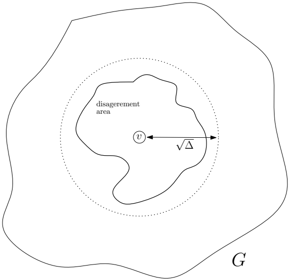

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7. Run $O(n)$ steps to get expected # of disagreements $< 1/8$.

Questions

Interesting directions:

- Remove girth assumptions: Modified form of BP to deal with short cycles?
- Conjecture: Glauber dynamics is rapidly mixing for any model in "uniqueness".
- Rapid mixing for independent sets for $\Delta = 5$?
- Extend from hard-core to general (anti-ferromagnetic) 2-spin models.
- Rapid mixing (or some approx. counting scheme) for k-colorings when $k \geq \Delta + 2$.
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THANK YOU!

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Convergence with Ψ

Potential function

$$\Psi(x) = (\lambda)^{-1}\mathrm{arcsinh}(\sqrt{\lambda x})$$

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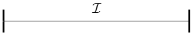

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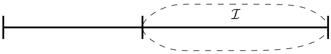

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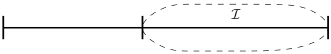

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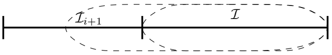

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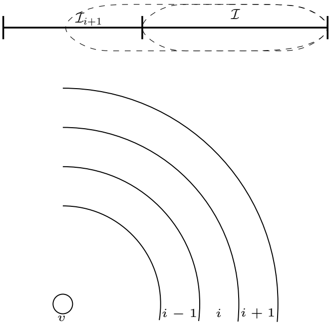

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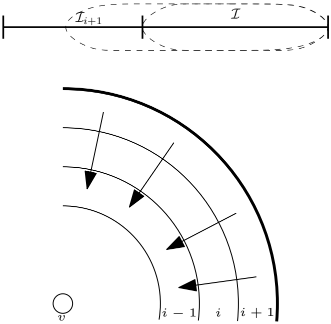

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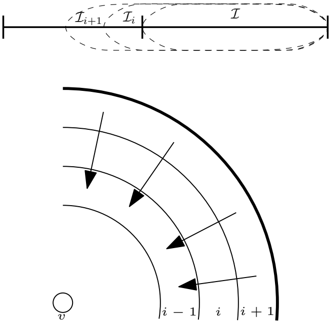

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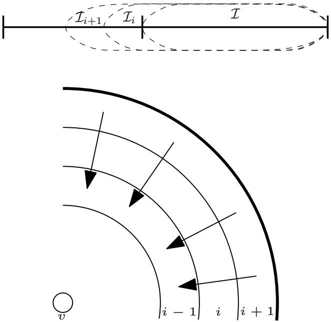

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