Sampling up to the *Uniqueness* Threshold

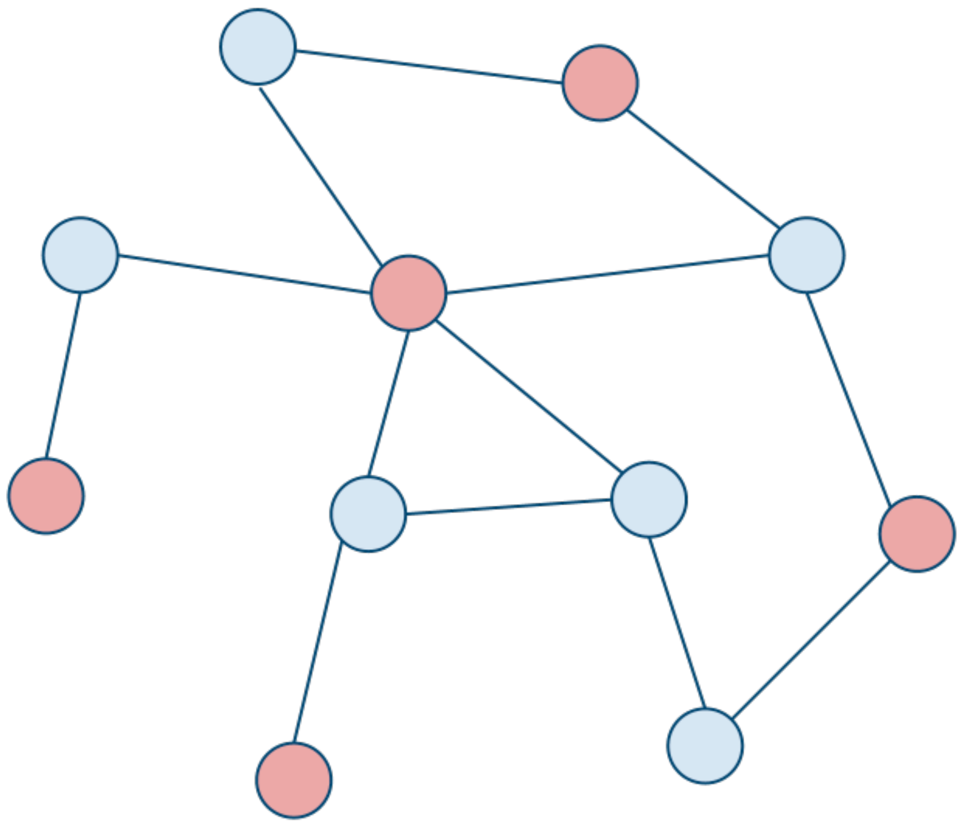
Yitong Yin
Nanjing University

Joint work with: Charis Efthymiou (Goethe-Universität Frankfurt)
Thomas P. Hayes (UNM)
Daniel Štefankovič (Rochester)
Eric Vigoda (Georgia Tech)

Sampling Independent Set

undirected graph $G(V, E)$ of max-degree Δ

- Sample (*nearly*) uniform random independent set.



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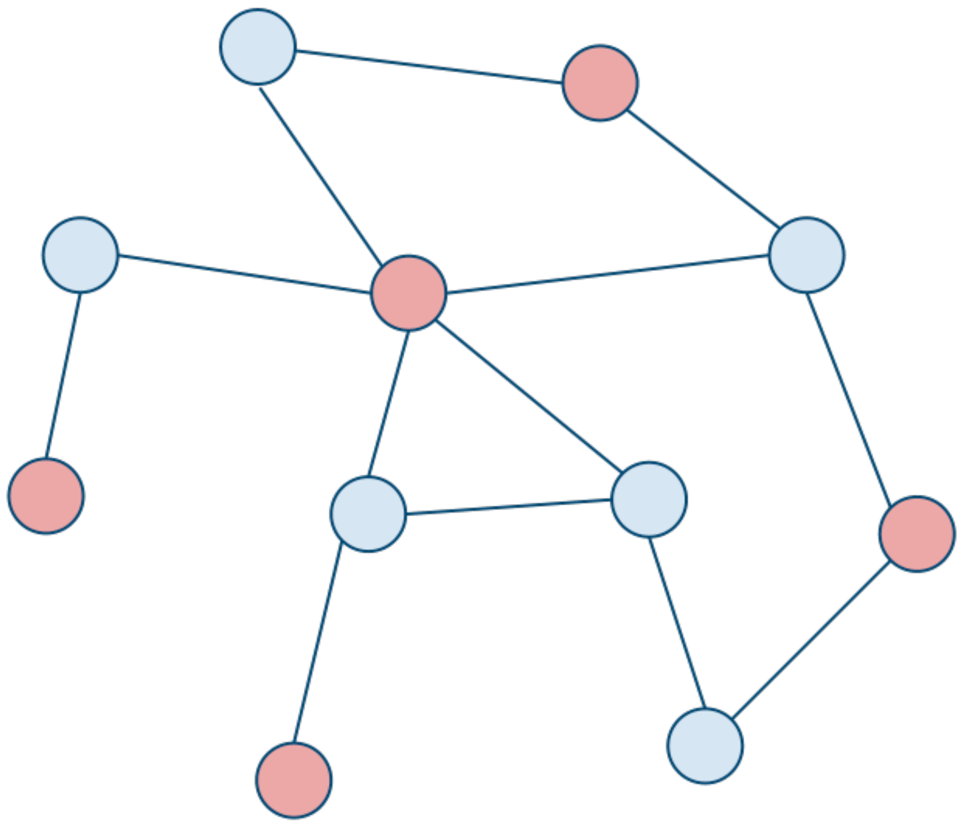
undirected graph $G(V,E)$ of max-degree Δ

- Sample (*nearly*) uniform random independent set.
- $\Delta \leq 5 \Rightarrow$ poly-time

  Conjecture: $O(n \log n)$ time
- $\Delta \geq 6 \Rightarrow$ NP-hard



Hardcore Model

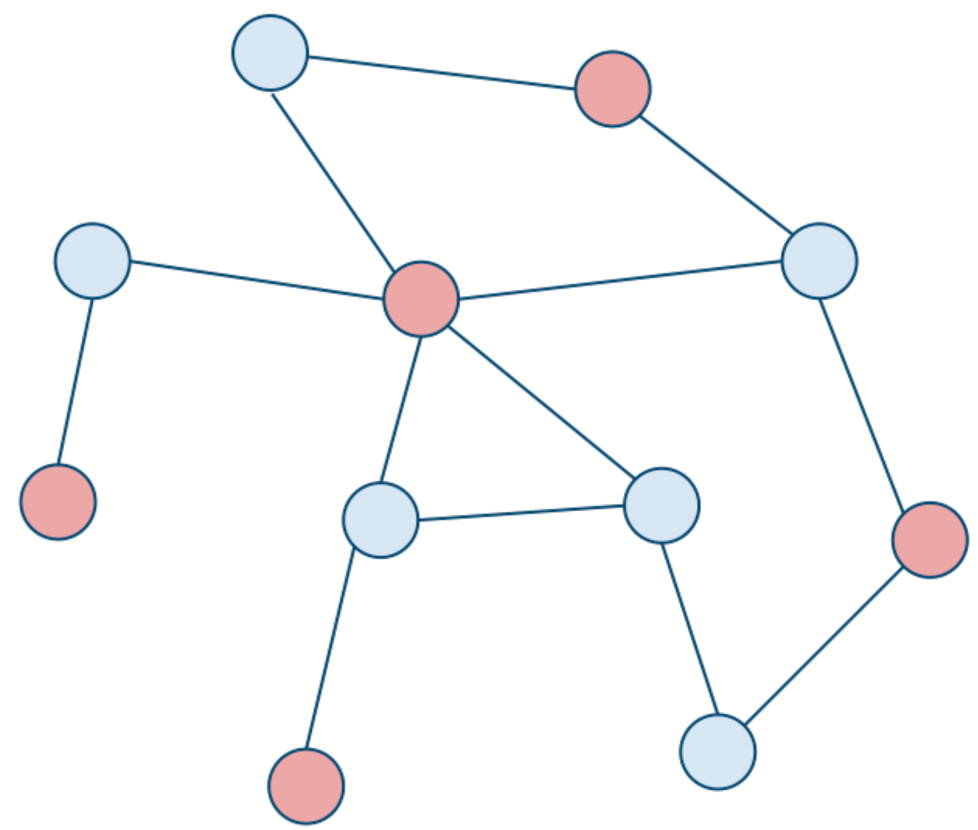
undirected graph $G(V, E)$ of max-degree Δ

- fugacity parameter $\lambda > 0$
- each independent set I in G is assigned a weight:

$$w(I) = \lambda^{|I|}$$

- distribution μ over all independent sets in G:

$$\mu(I) = \frac{w(I)}{\sum_I w(I)}$$

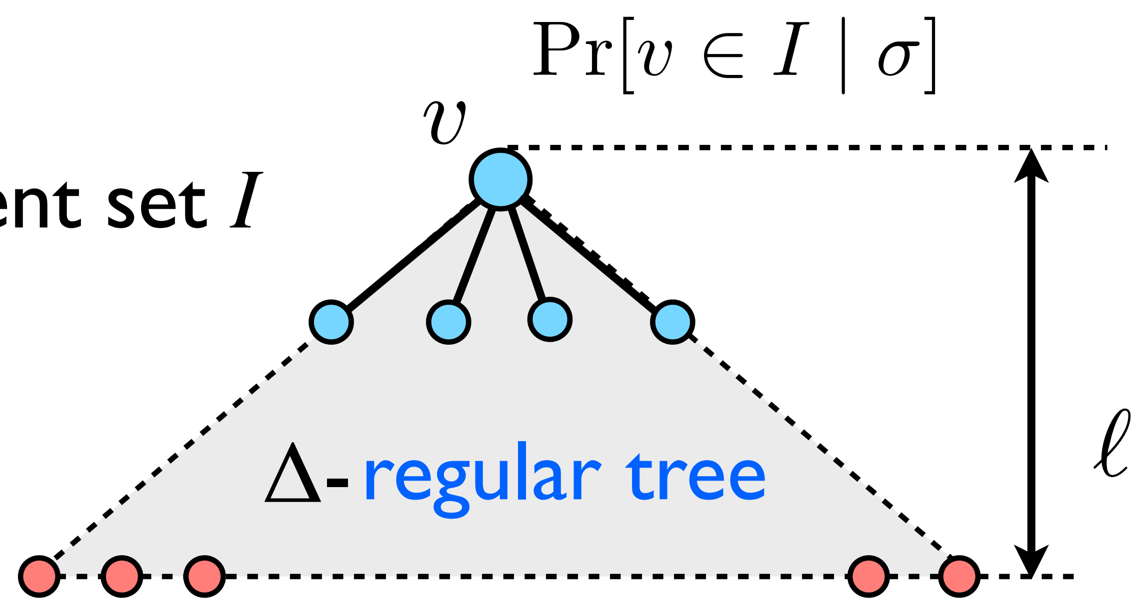


- $\lambda = 1$: uniform distribution over independent sets

Uniqueness Threshold

random independent set I

$\mu(I) \propto \lambda^{|I|}$



σ: boundary condition fixing each leaf $\in I$ or $\notin I$

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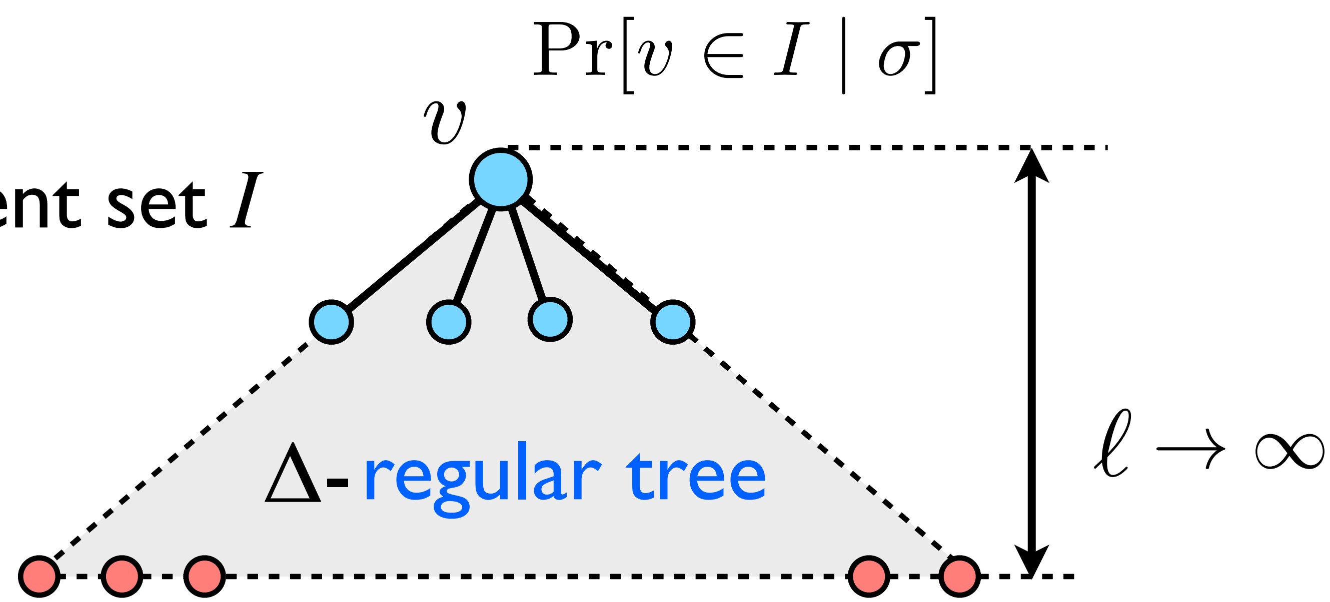

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Critical phenomenon:

$\Pr[v \in I \mid \sigma]$ is independent of σ when $l \to \infty$

iff $\lambda \leq \lambda_c(\Delta) = \frac{(\Delta-1)^{(\Delta-1)}}{(\Delta-2)^{\Delta}}$

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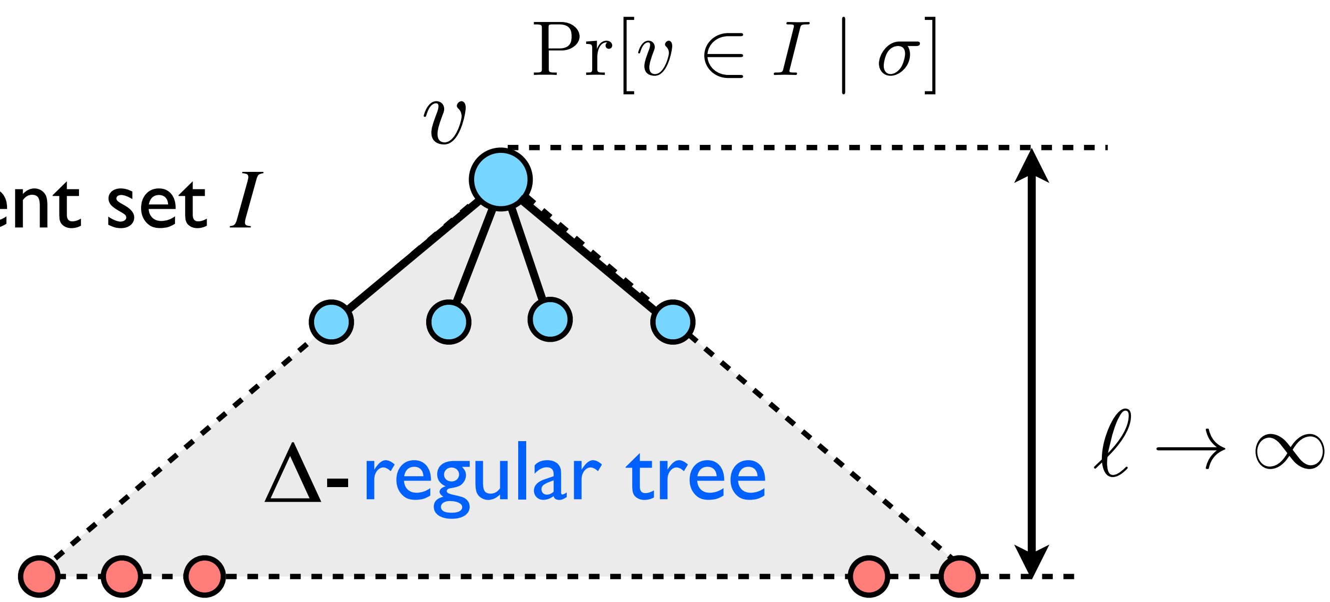

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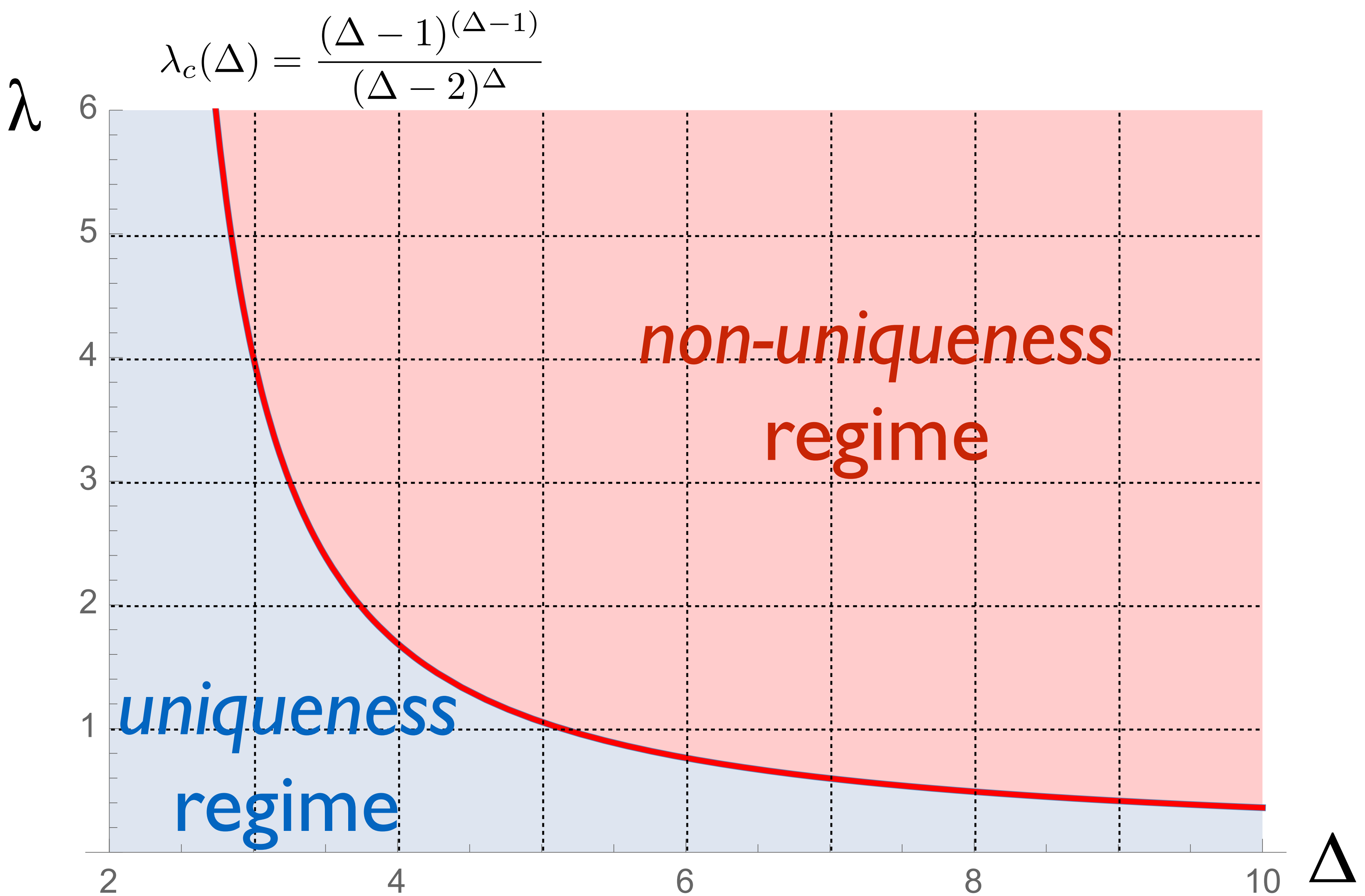
Uniqueness threshold

Phase Transition



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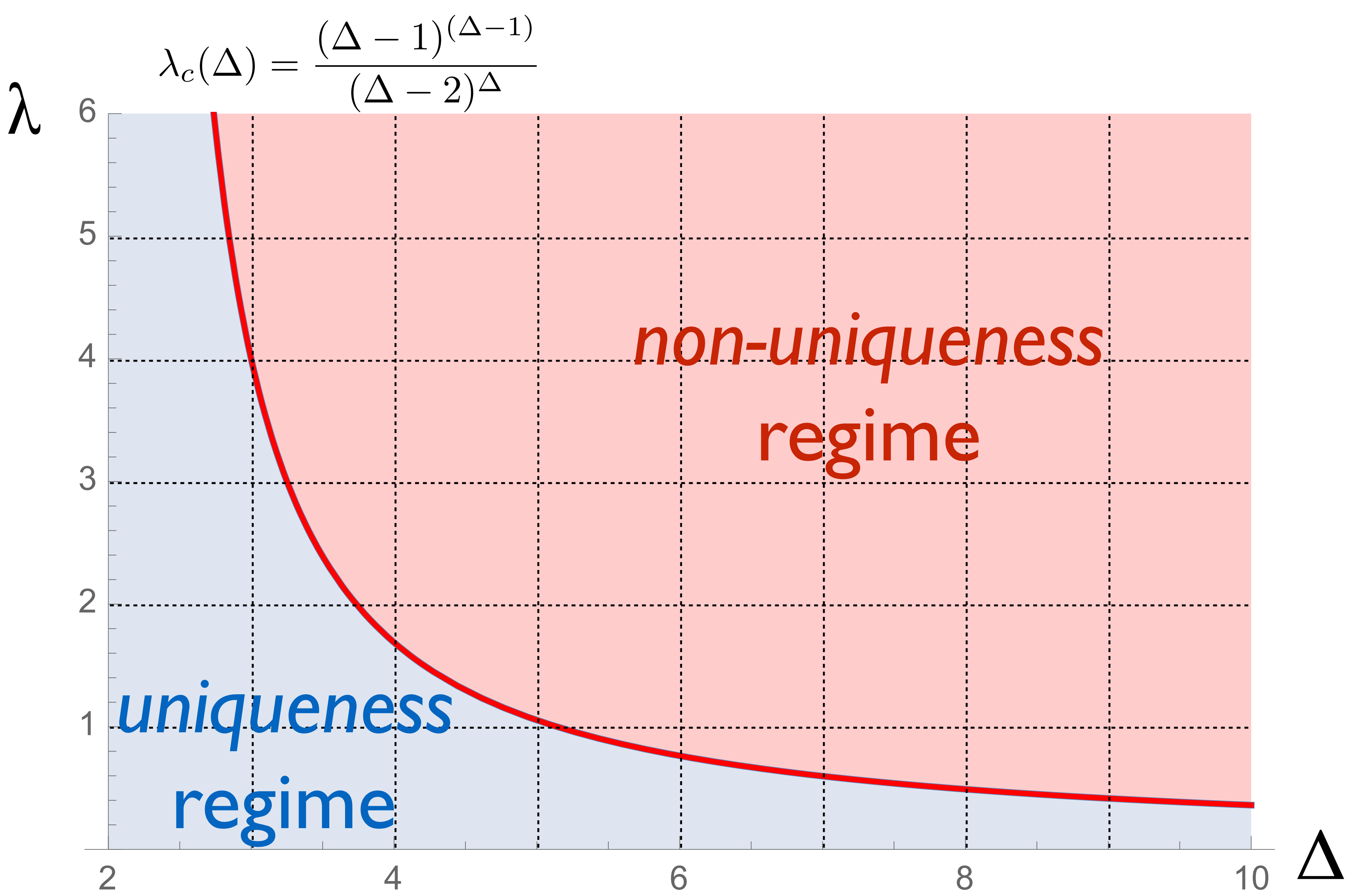


sampling (with bounded error) from the hardcore model on graphs of max-degree Δ and fugacity $\lambda>0$

Glauber Dynamics

[Glauber'63]

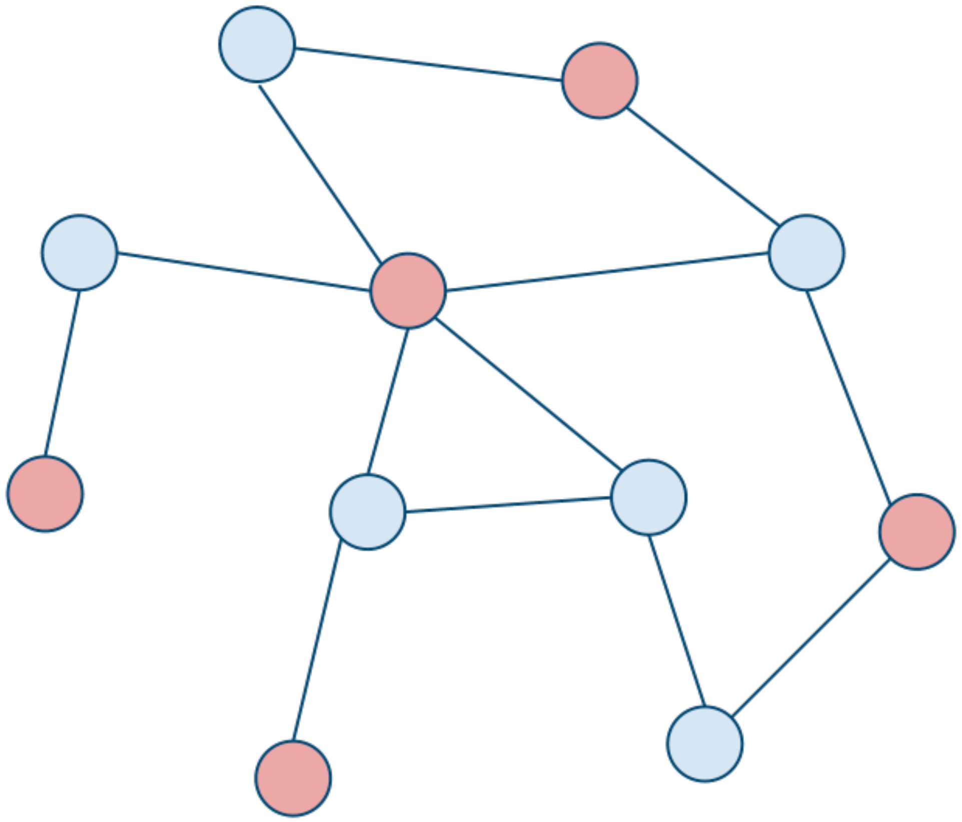
Markov chain $\{X_t\}_{t=0,1,2,\ldots}$ over independent sets in $G(V,E)$

transition $X_t \to X_{t+1}$:

pick a uniform random vertex v;
if $u \notin X_t$ for all v's neighbors u:

$$X_{t+1} = \begin{cases} X_t \cup \{v\} & \text{with prob. } \frac{\lambda}{1+\lambda} \\ X_t \setminus \{v\} & \text{with prob. } \frac{1}{1+\lambda} \end{cases}$$

else $X_{t+1} = X_t$;



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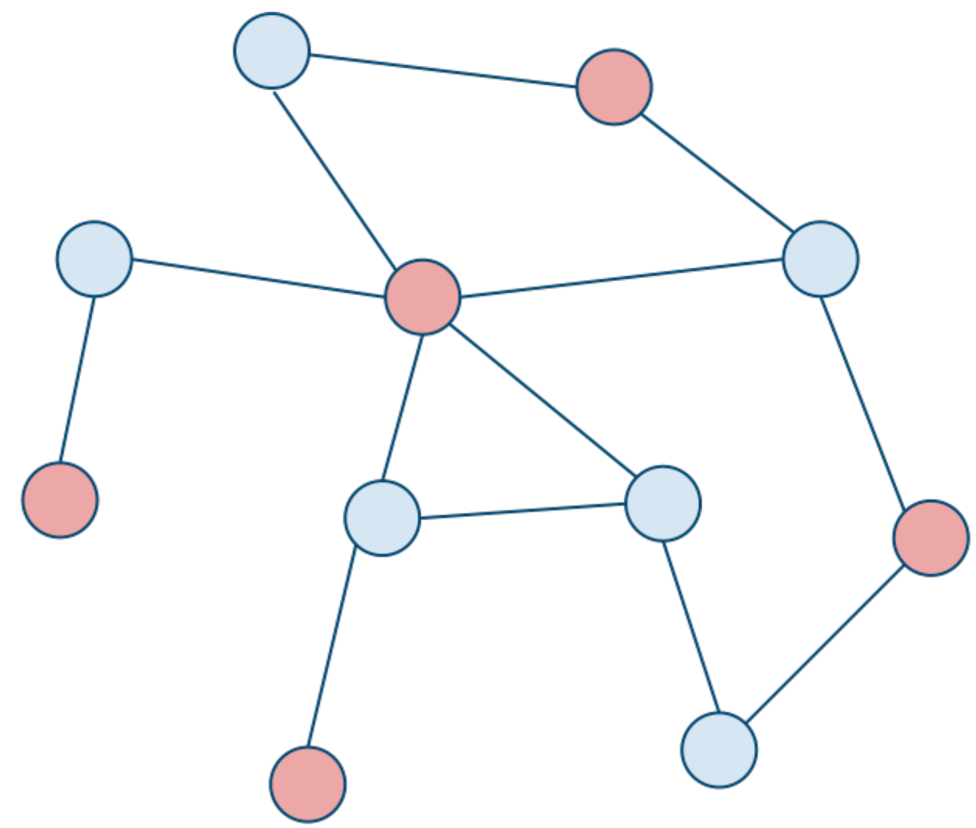

ergodic, *irreducible*
time-reversible w.r.t. μ

Markov chain convergence Thm ⟹

$X_t \to \mu$ as $t \to \infty$

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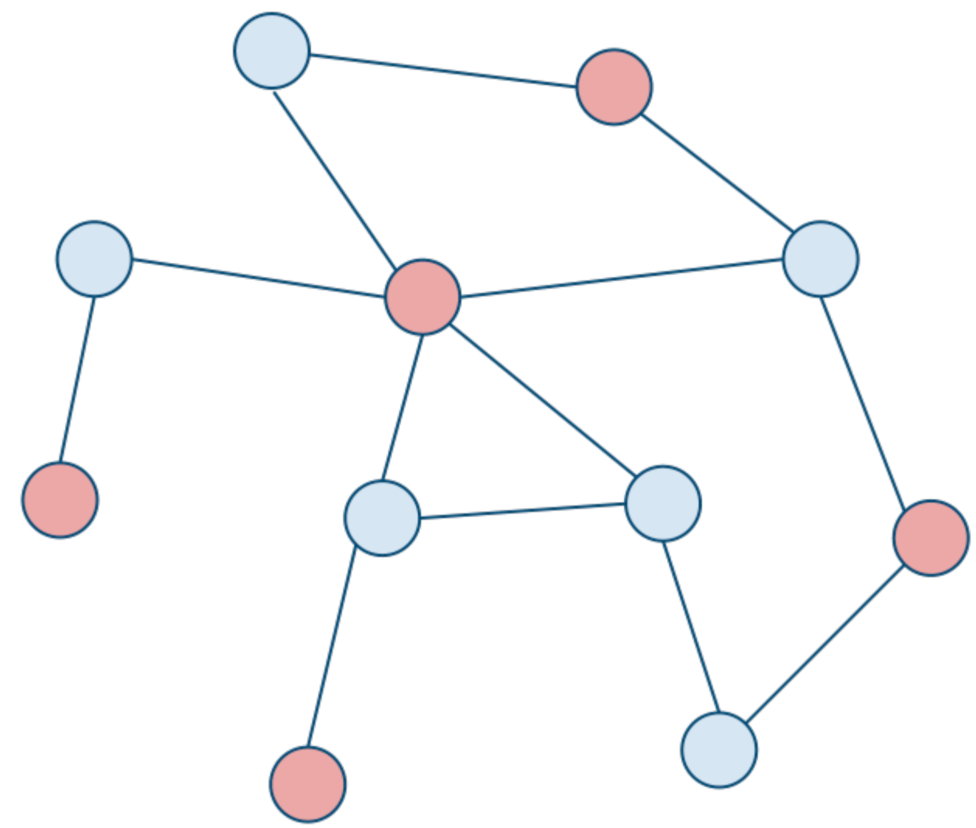

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mixing time: $\tau_{\text{mix}} = \max_{X_0} \min\{t \mid d_{\text{TV}}(X_t, \mu) < 0.1\}$

sampling (with bounded error) from the hardcore model on graphs with max-degree Δ and fugacity $\lambda>0$

uniqueness threshold: $\lambda_c(\Delta) = \frac{(\Delta-1)^{(\Delta-1)}}{(\Delta-2)^{\Delta}} \approx \frac{\mathrm{e}}{\Delta-2}$

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Theorem (Efthymiou-Hayes-Štefankovič-Vigoda-Y.'16):

$\tau_{\text{mix}}=O(n\log n)$ for Glauber dynamics when $\lambda<\lambda_c(\Delta)$,

if Δ is sufficiently large, and there is no small cycles.

sampling (with bounded error) from the hardcore model on graphs with max-degree Δ and fugacity $\lambda>0$

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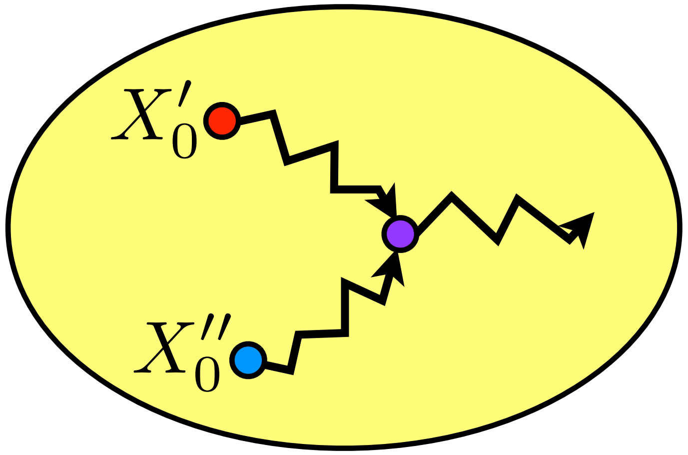
Theorem (Efthymiou-Hayes-Štefankovič-Vigoda-Y.'16):
$\forall\delta>0$, $\exists\Delta_0$ s.t. $\tau_{\text{mix}}=O(n \log n)$ for all graphs of max-degree $\Delta\geq\Delta_0$ and girth ≥ 7 when $\lambda\leq(1-\delta)\lambda_c(\Delta)$.

Coupling

a coupling of a Markov chain X_t is a joint Markov chain (X'_t, X''_t):

- both X_t' and X_t'' follow the same transition rule as X_t
- once collides, makes identical moves thereafter

$$X'_t = X''_t \Rightarrow X'_{t+1} = X''_{t+1}$$



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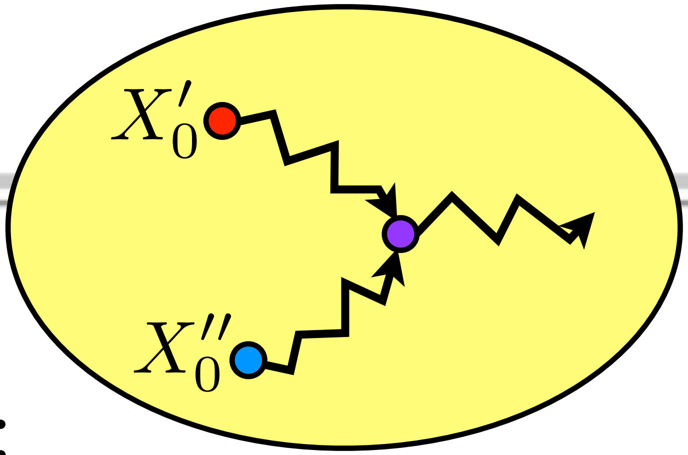

Theorem (Griffeath'78, Aldous'83):

$\forall$ coupling (X_t', X_t'') of Markov chain X_t :

$$\tau_{\text{mix}} \le \max_{X'_0, X''_0} \min\{t \mid \Pr[X'_t \neq X''_t] < 0.1\}$$

Path Coupling

Theorem (Bubley-Dyer'97):

If there is a metric $\Phi(\cdot,\cdot)$ over all states for the chain and a coupling $(X_t, Y_t) \rightarrow (X_{t+1}, Y_{t+1})$ for *adjacent* (X_t, Y_t)

s.t.: $$\mathbb{E}[\Phi(X_{t+1}, Y_{t+1}) \mid X_t, Y_t] \leq (1 - \frac{\alpha}{n})\Phi(X_t, Y_t)$$

$$\Rightarrow \quad \tau_{\mathsf{mix}} = O\left(\frac{n}{\alpha}\log n\right)$$

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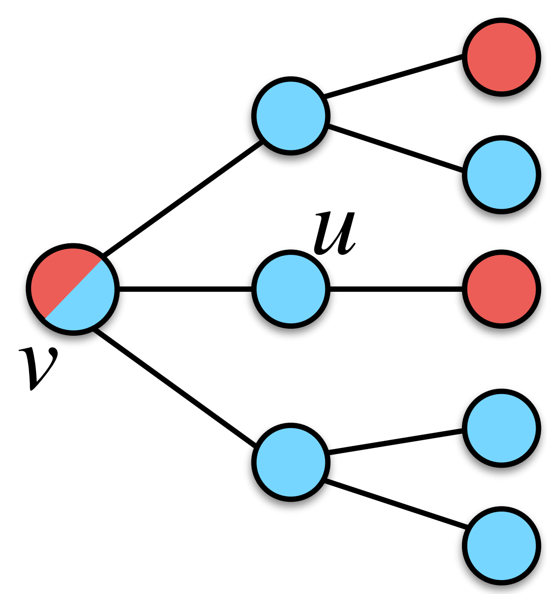

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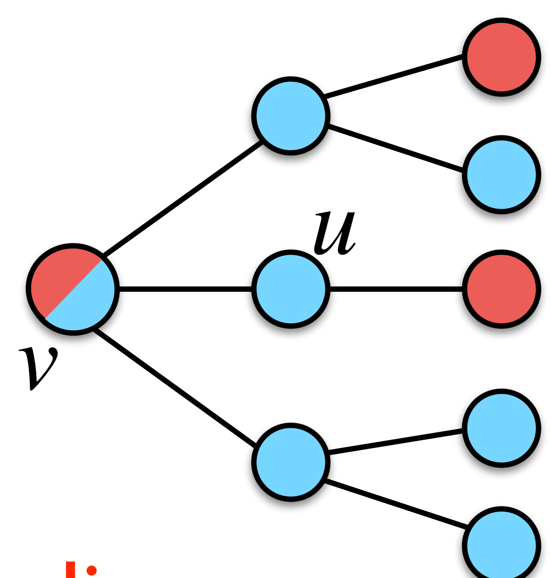
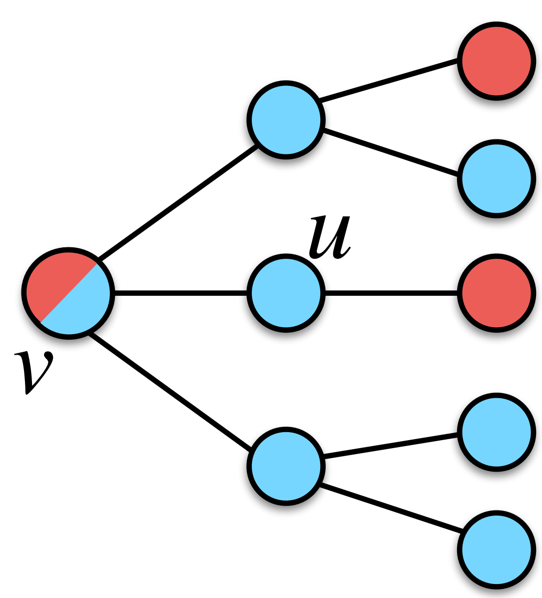


one-step optimal coupling:

$\Pr[X_t(u) \neq X_t(u) \mid u \text{ is picked in step } t]$ is minimized one-step optimal coupling for (X_t, Y_t) that $X_t \oplus Y_t = \{v\}$

Goal: $\mathbb{E}[\Phi(X_{t+1}, Y_{t+1}) \mid X_t, Y_t] \leq (1 - \frac{\alpha}{n})\Phi(X_t, Y_t)$



metric $\Phi(\cdot,\cdot)$ is a weighted Hamming distance:

$$\Phi(X,Y) = \sum_{v \in X \oplus Y} \Phi_v$$ where $\Phi_v \geq 1$ is v's weight

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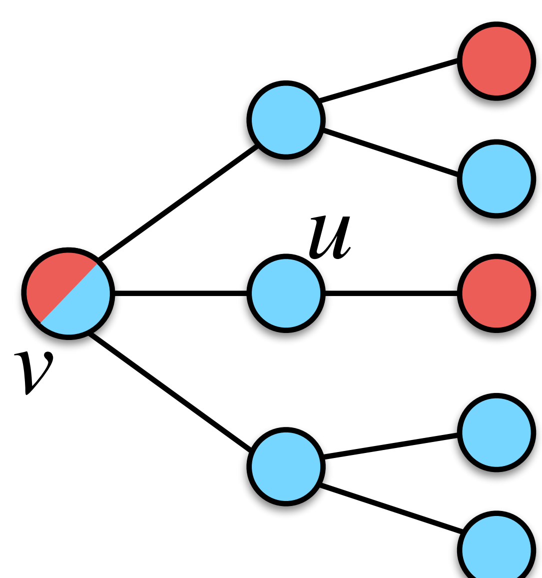

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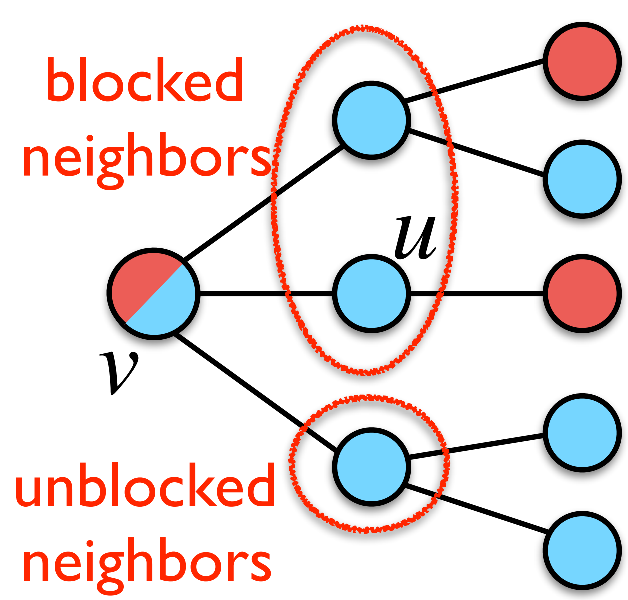

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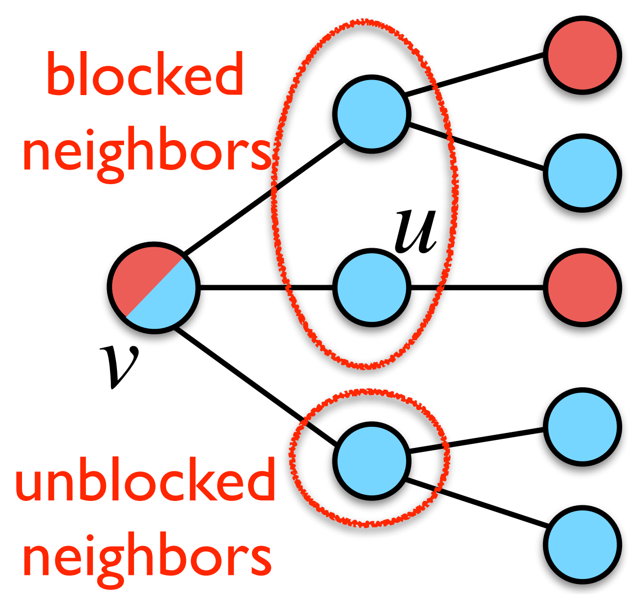

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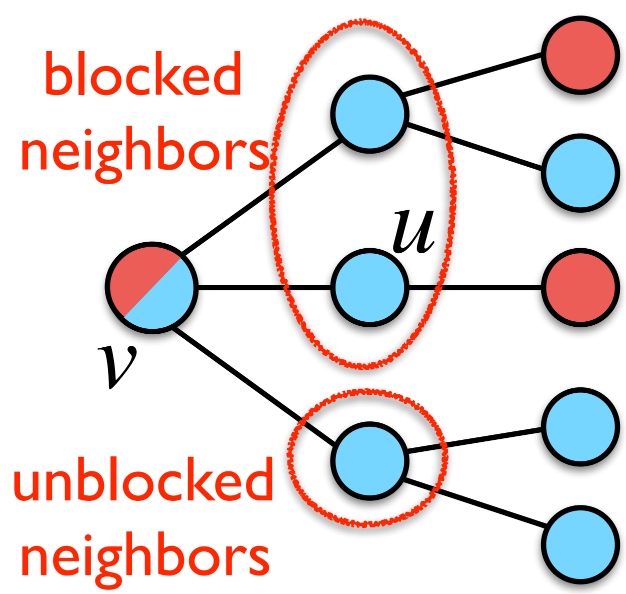

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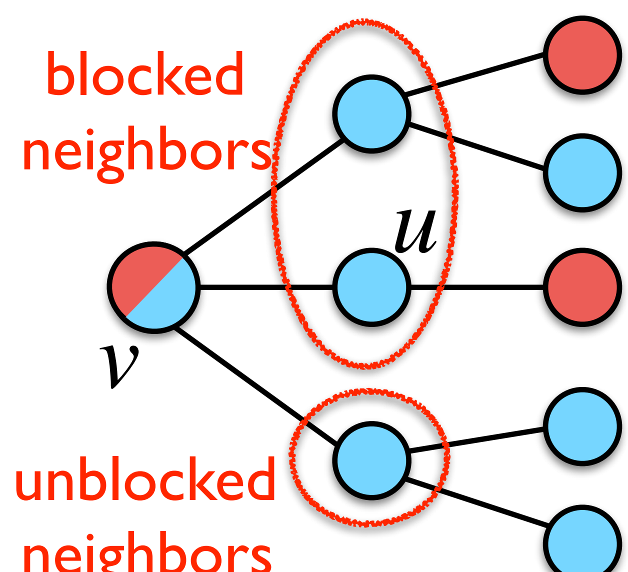

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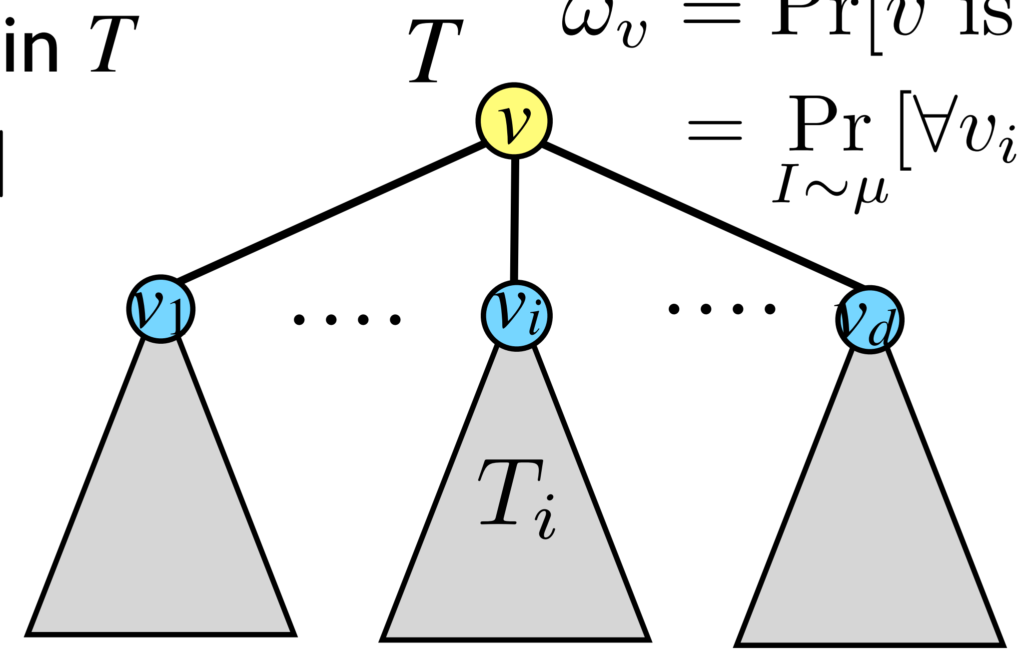
Belief Propagation

[Pearl'82]

independent set I in T

$$\mu(I) \propto \lambda^{|I|}$$

$$\omega_v = \Pr[v \text{ is unblocked } \mid v \notin I]$$
$$= \Pr_{I\sim\mu}[\forall v_i \in N(v), v_i \notin I \mid v \notin I]$$



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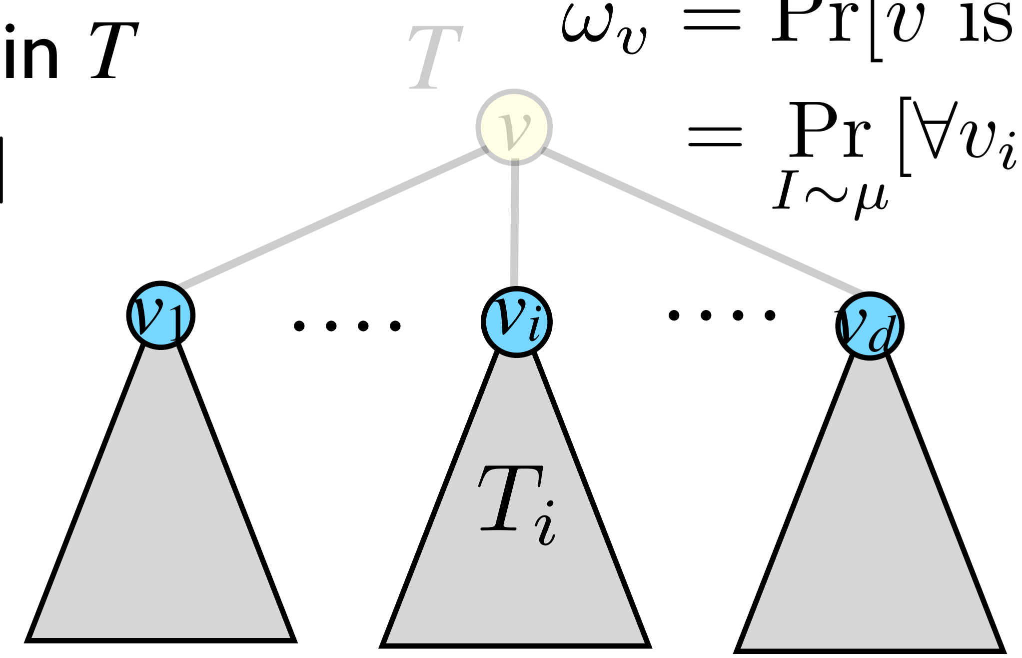

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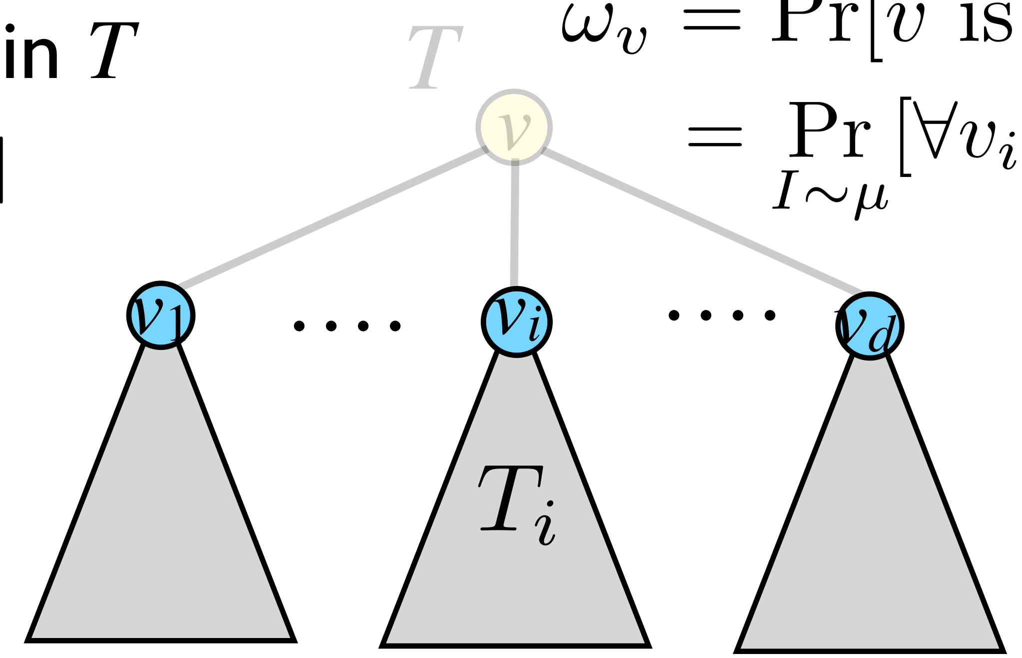

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Belief propagation (BP):

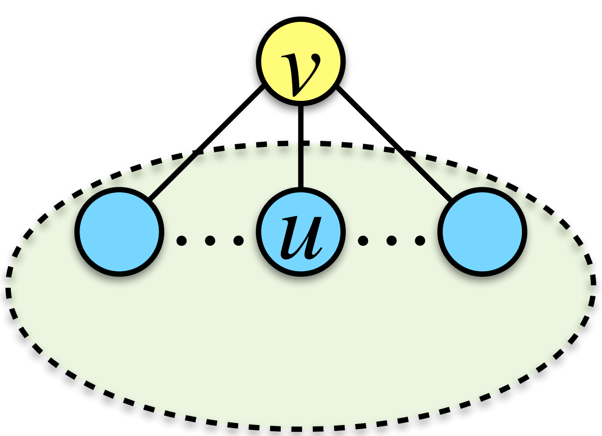
$$\omega_v = \prod_{i=1}^{d} \frac{1}{1 + \lambda \omega_i}$$

Loopy Belief Propagation

graph $G(V, E)$ with max-degree ≤Δ $\qquad \vec{\omega} \in [0,1]^V$

loopy BP: $\vec{\omega}^{(t+1)} = F(\vec{\omega}^{(t)})$

where ∀v: $\omega_v^{(t+1)} = \prod_{u \in N(v)} \frac{1}{1 + \lambda \omega_u^{(t)}}$

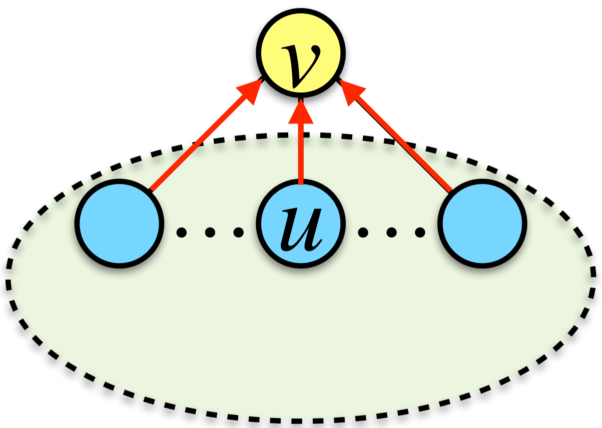


Loopy Belief Propagation

graph $G(V, E)$ with max-degree $\leq\Delta$ $\qquad \vec{\omega} \in [0,1]^V$

loopy BP: $\vec{\omega}^{(t+1)} = F(\vec{\omega}^{(t)})$

where $\forall v$: $\omega_v^{(t+1)} = \prod_{u \in N(v)} \frac{1}{1 + \lambda \omega_u^{(t)}}$



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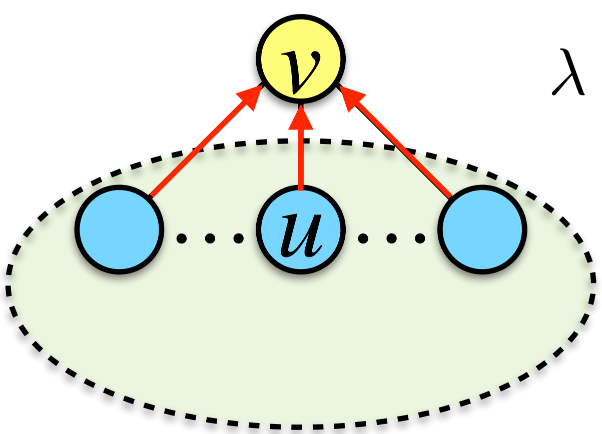


$\lambda < \frac{\Delta^\Delta}{(\Delta-1)^{\Delta+1}}$

$\approx \frac{\mathrm{e}}{\Delta-1}$

$\forall$initial values $\vec{\omega}^{(0)}\in[0,1]^V$

$\vec{\omega}^{(t)}$ converges to a unique fixpoint $\omega^* = F(\omega^*)$

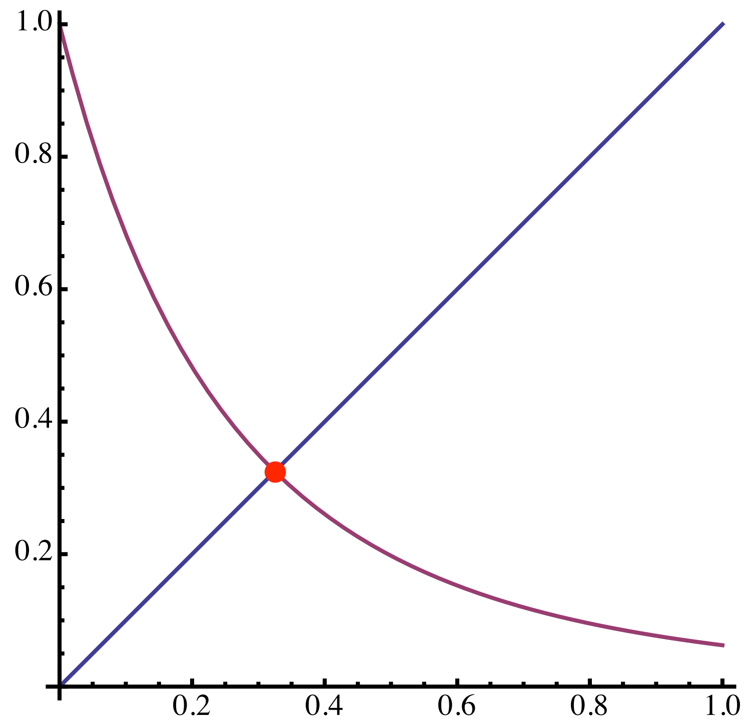
at an exponential rate.

BP Convergence

$$\omega_v^{(t+1)} = \prod_{u \in N(v)} \frac{1}{1 + \lambda \omega_u^{(t)}}$$

univariate dynamical system:

$$f(x) = (1 + \lambda x)^{-\Delta}$$



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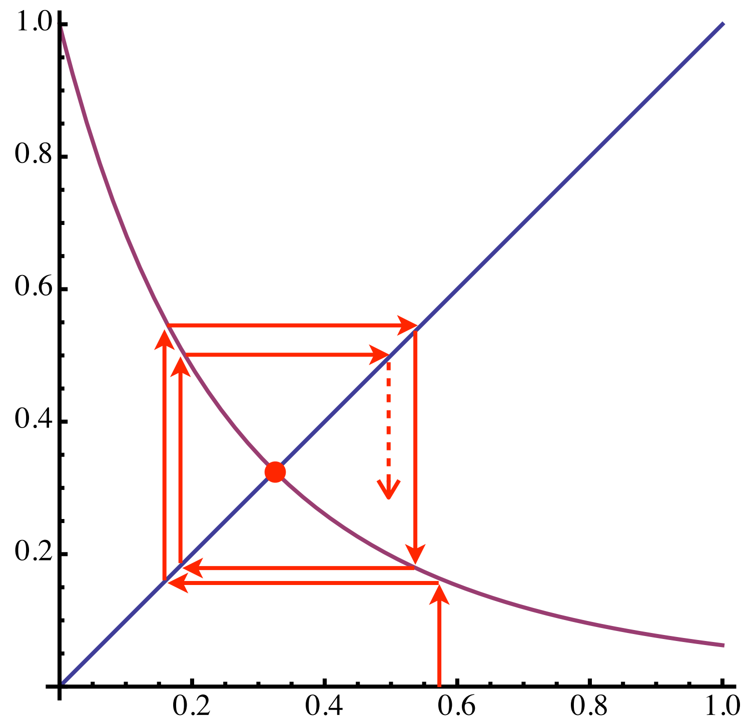

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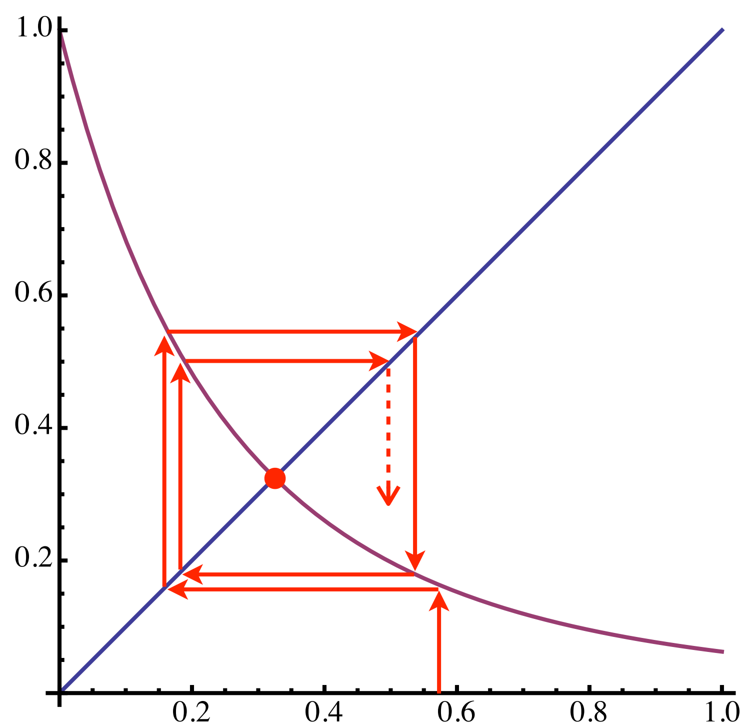

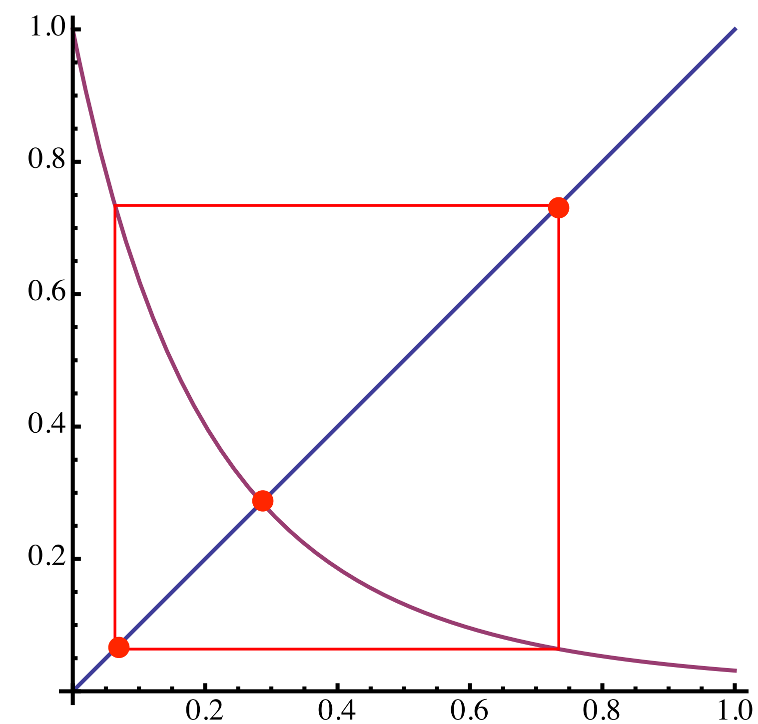

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Potential Method

$$f(x) = (1 + \lambda x)^{-\Delta}$$

$\uparrow$

x

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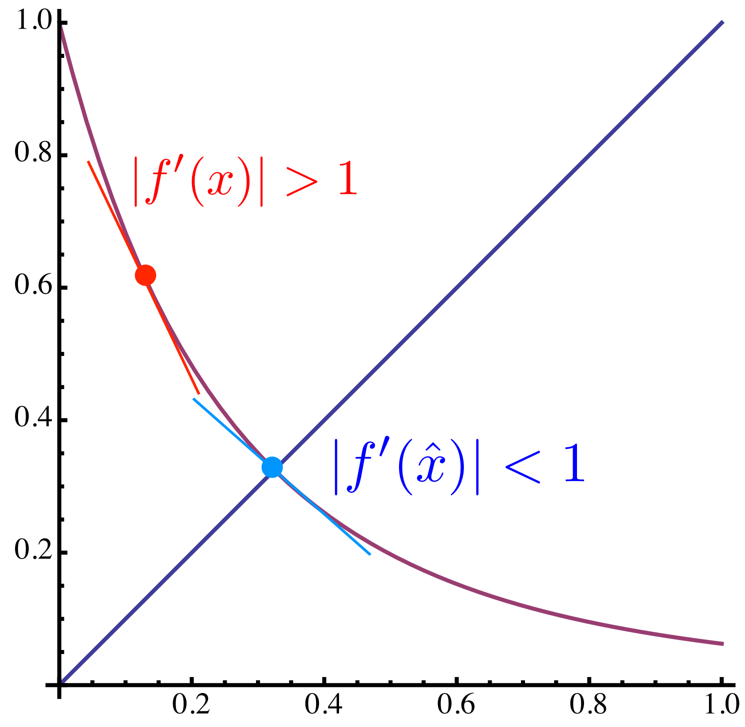


Potential Method

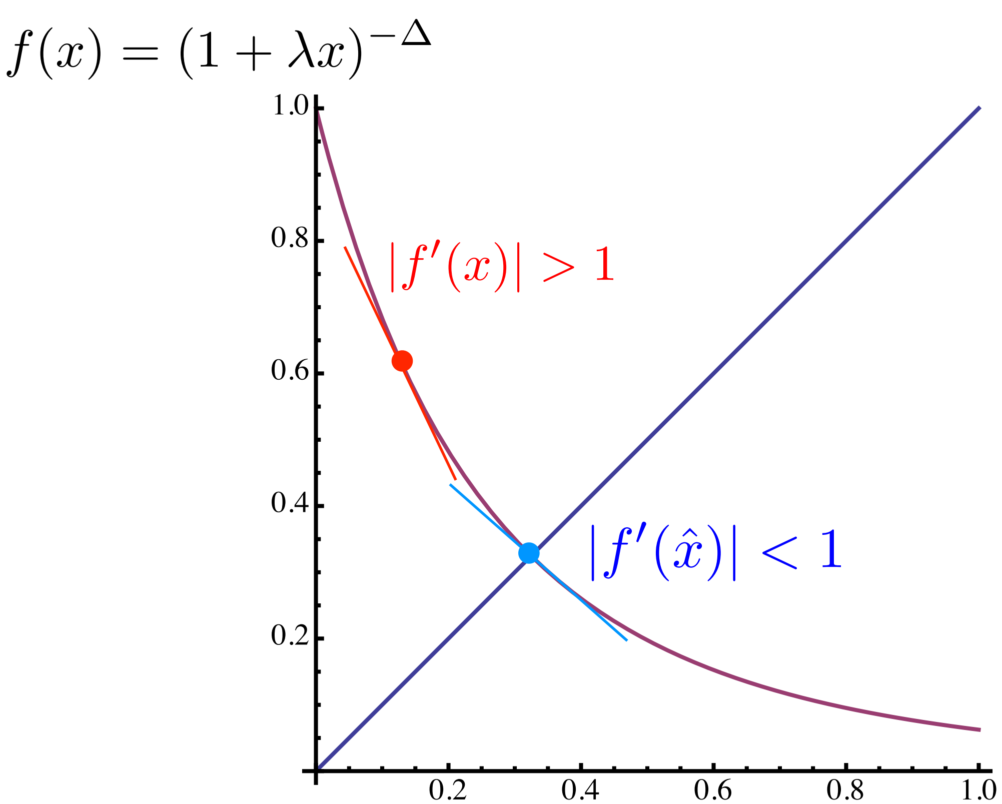
$$f(x) = (1+\lambda x)^{-\Delta} \xrightarrow{\ \psi\ } g(y)$$

$$\uparrow$$

$$x \xrightarrow{\ \psi(x) = \operatorname{arcsinh}(\sqrt{\lambda x})\ } y$$

used in

[Li-Lu-Y.'13] [Sinclair-Srivastava-Y.'13] [Sinclair-Srivastava-Štefankovič-Y.'15]



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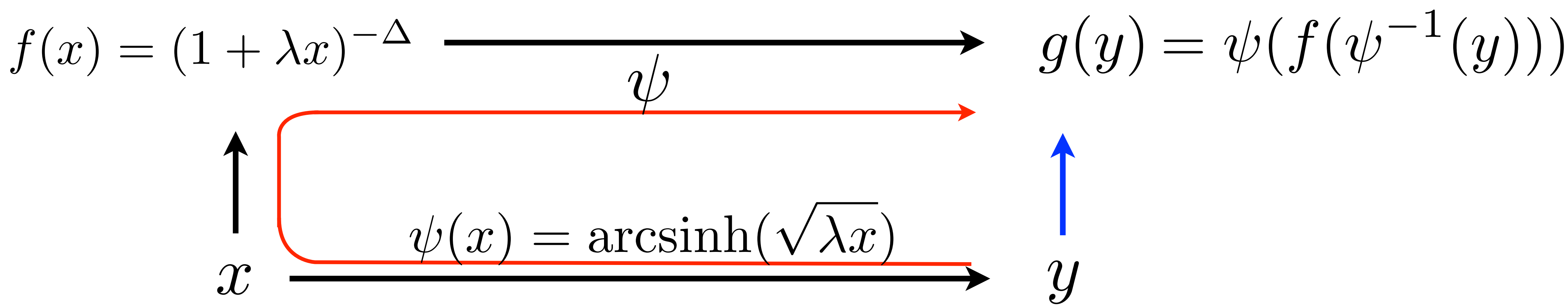

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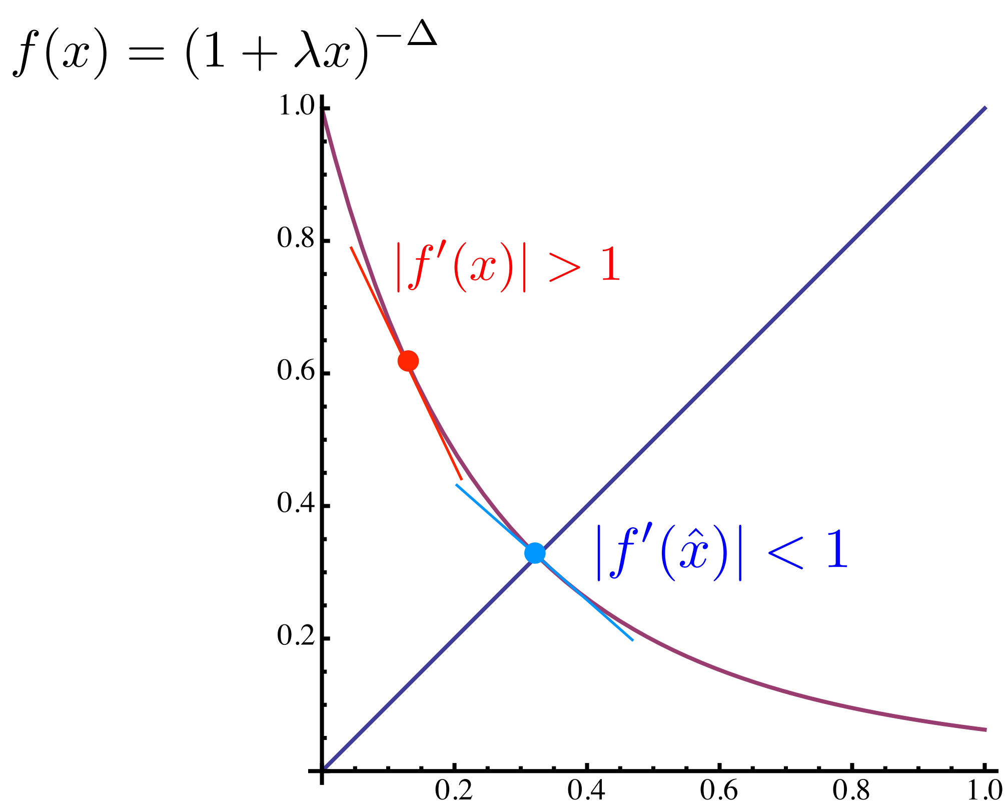

Potential Method

$$f(x) = (1+\lambda x)^{-\Delta} \xrightarrow{\psi} g(y) = \psi(f(\psi^{-1}(y)))$$

$$x \longrightarrow y$$

$$\psi(x) = \operatorname{arcsinh}(\sqrt{\lambda x})$$

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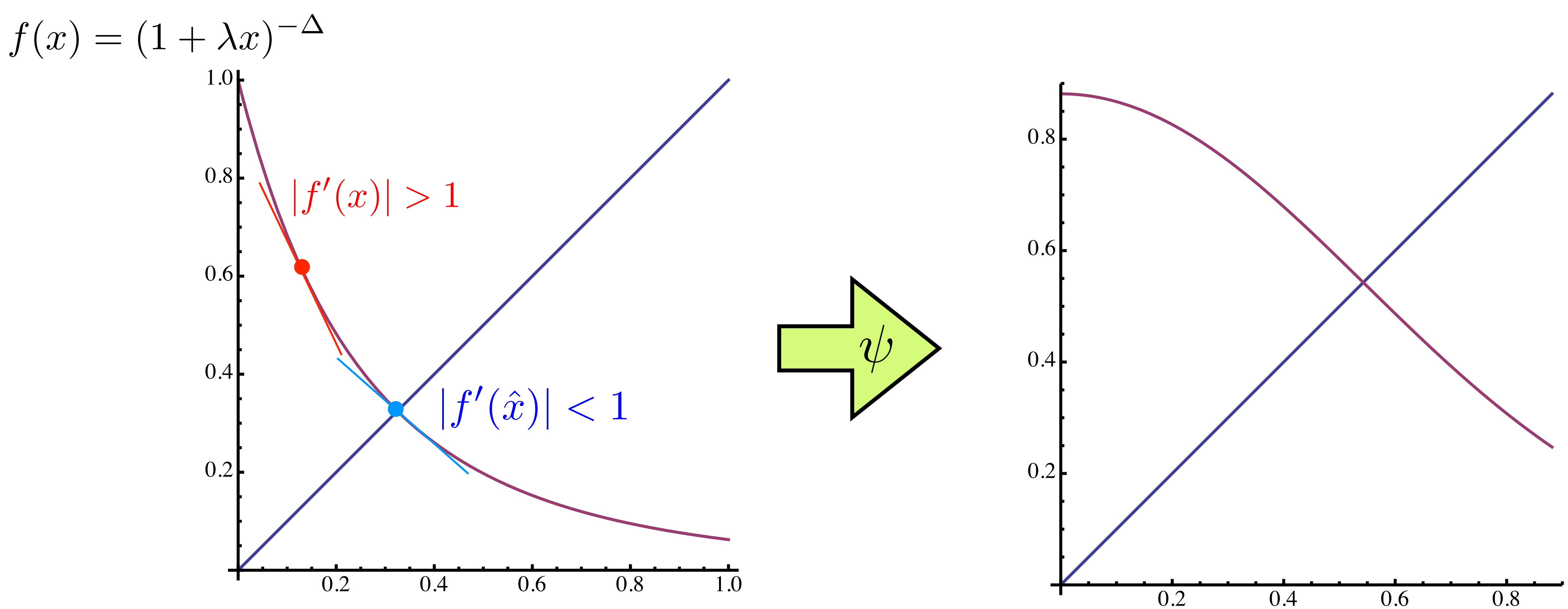

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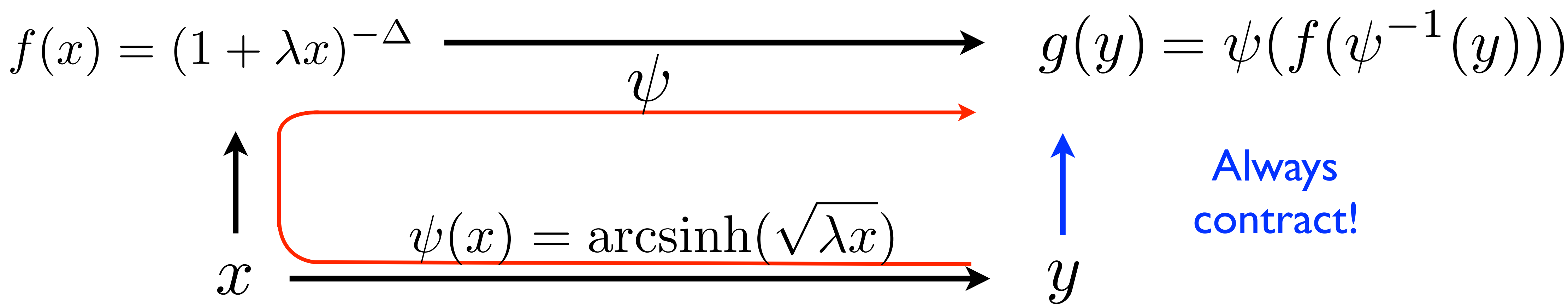

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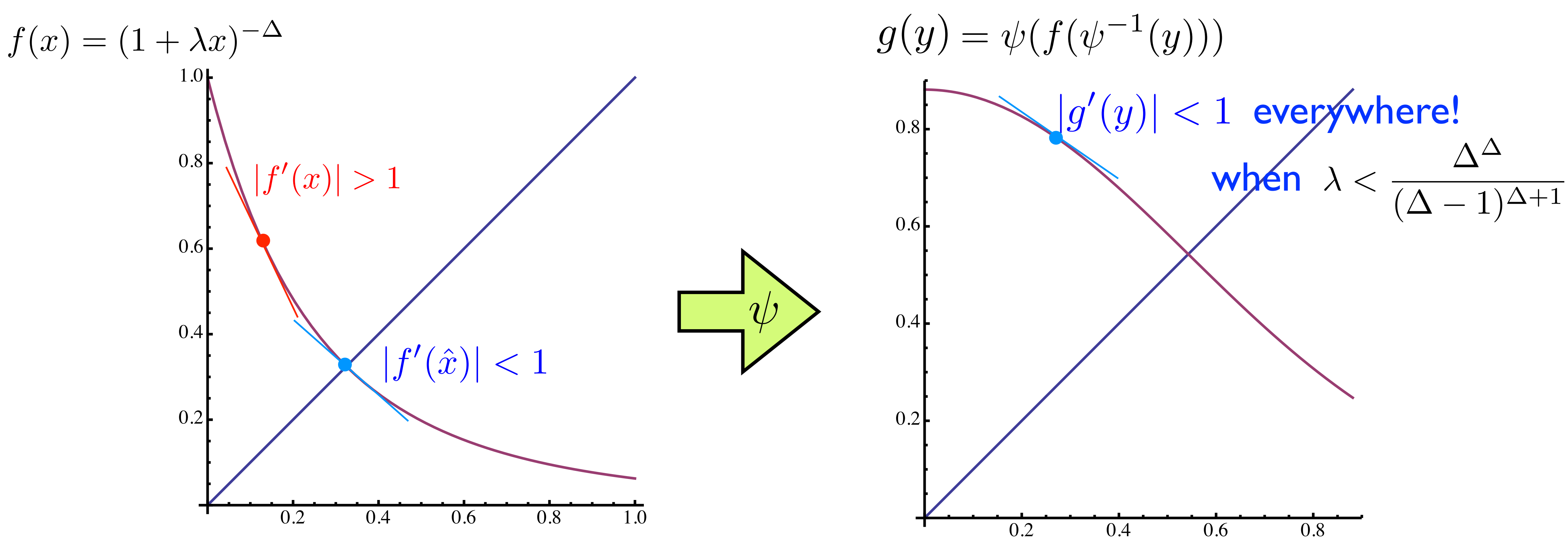

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Φ_u Φ_v

define $\Phi_v \triangleq \frac{1}{\omega_v^* \cdot \psi'(\omega_v^*)} = 2\sqrt{\frac{1+\lambda\omega_v^*}{\lambda\omega_v^*}}$

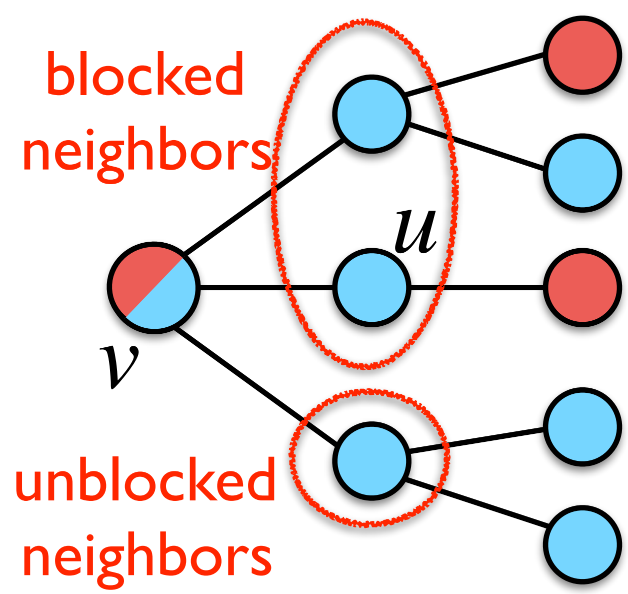
metric $\Phi(\cdot,\cdot)$ is a weighted Hamming distance:

$$\Phi(X,Y) = \sum_{v \in X \oplus Y} \Phi_v$$ where $\Phi_v \geq 1$ is v's weight

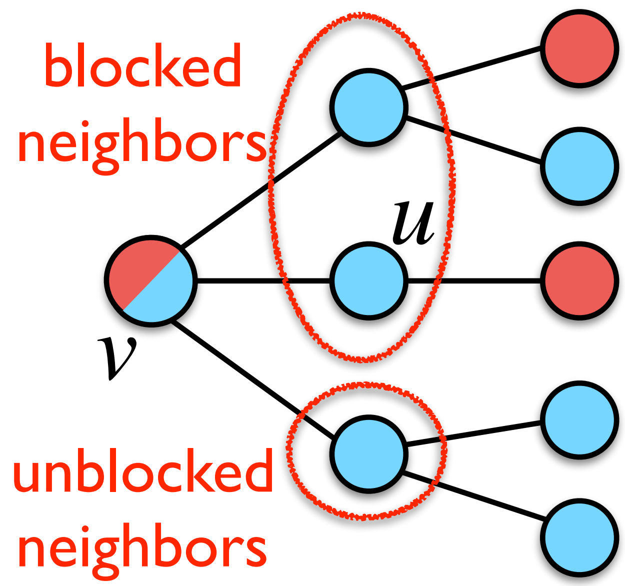
one-step optimal coupling for (X_t, Y_t) that $X_t \oplus Y_t = \{v\}$

Goal: $\mathbb{E}[\Phi(X_{t+1}, Y_{t+1}) \mid X_t, Y_t] \leq (1 - \frac{\alpha}{n})\Phi(X_t, Y_t)$

$$\sum_{u \in N(v)} \frac{\lambda W_u^{(t)}}{1 + \lambda W_u^{(t)}} \Phi_u \leq (1-\alpha)\Phi_v$$



$W_u^{(t)} = I[u \text{ is unblocked in } X_t]$

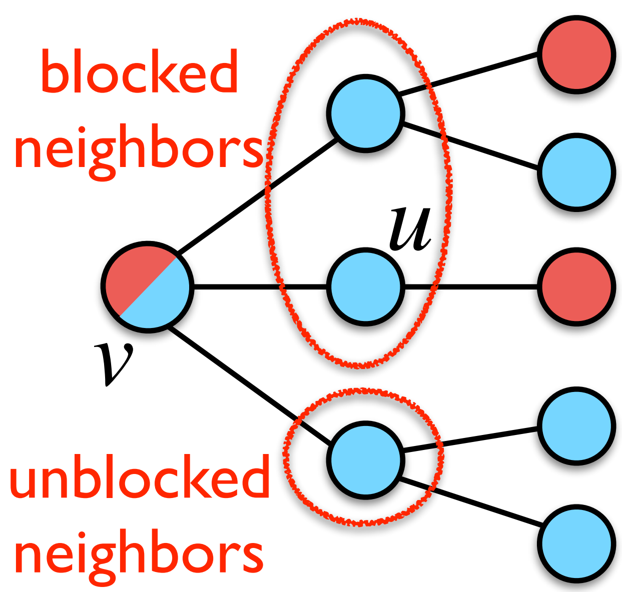


for coupling of Glauber dynamics (X_t, Y_t) that $X_t \oplus Y_t = \{v\}$

$$W_u^{(t)} = I[u \text{ is unblocked in } X_t]$$

$\exists$ vertex weights Φ_v :

$$\sum_{u \in N(v)} \frac{\lambda W_u^{(t)}}{1 + \lambda W_u^{(t)}} \Phi_u < \Phi_v$$



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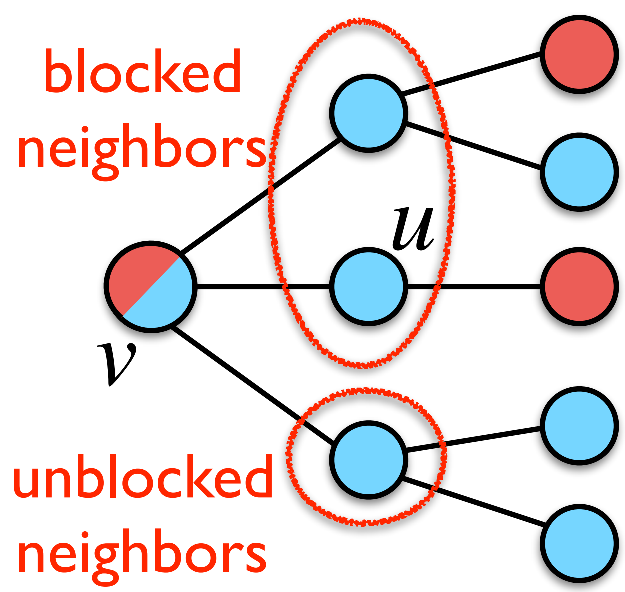
$$\sum_{u \in N(v)} \frac{\lambda W_u^{(t)}}{1 + \lambda W_u^{(t)}} \Phi_u < \Phi_v \quad \Rightarrow \quad \tau_{\text{mix}} = O(n \log n)$$

loopy BP: $\omega_v^{(t+1)} = \prod_{u \in N(v)} \frac{1}{1+\lambda\omega_u^{(t)}}$ fixpoint: $\omega_v^{*} = \prod_{u \in N(v)} \frac{1}{1+\lambda\omega_u^{*}}$

$$\lambda < \frac{\Delta^\Delta}{(\Delta-1)^{\Delta+1}} \Rightarrow \sum_{u \in N(v)} \frac{\lambda\omega_u^*}{1+\lambda\omega_u^*}\Phi_u < \Phi_v$$

where $\Phi_v = 2\sqrt{\frac{1+\lambda\omega_v^*}{\lambda\omega_v^*}}$



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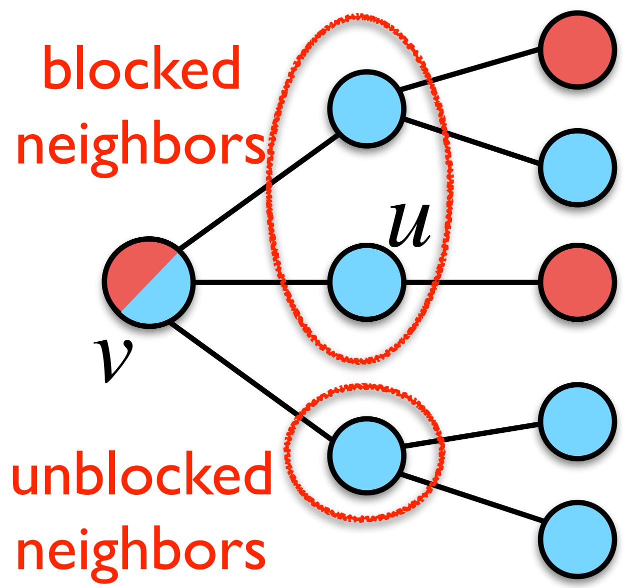
Local Uniformity



Glauber dynamics X_t

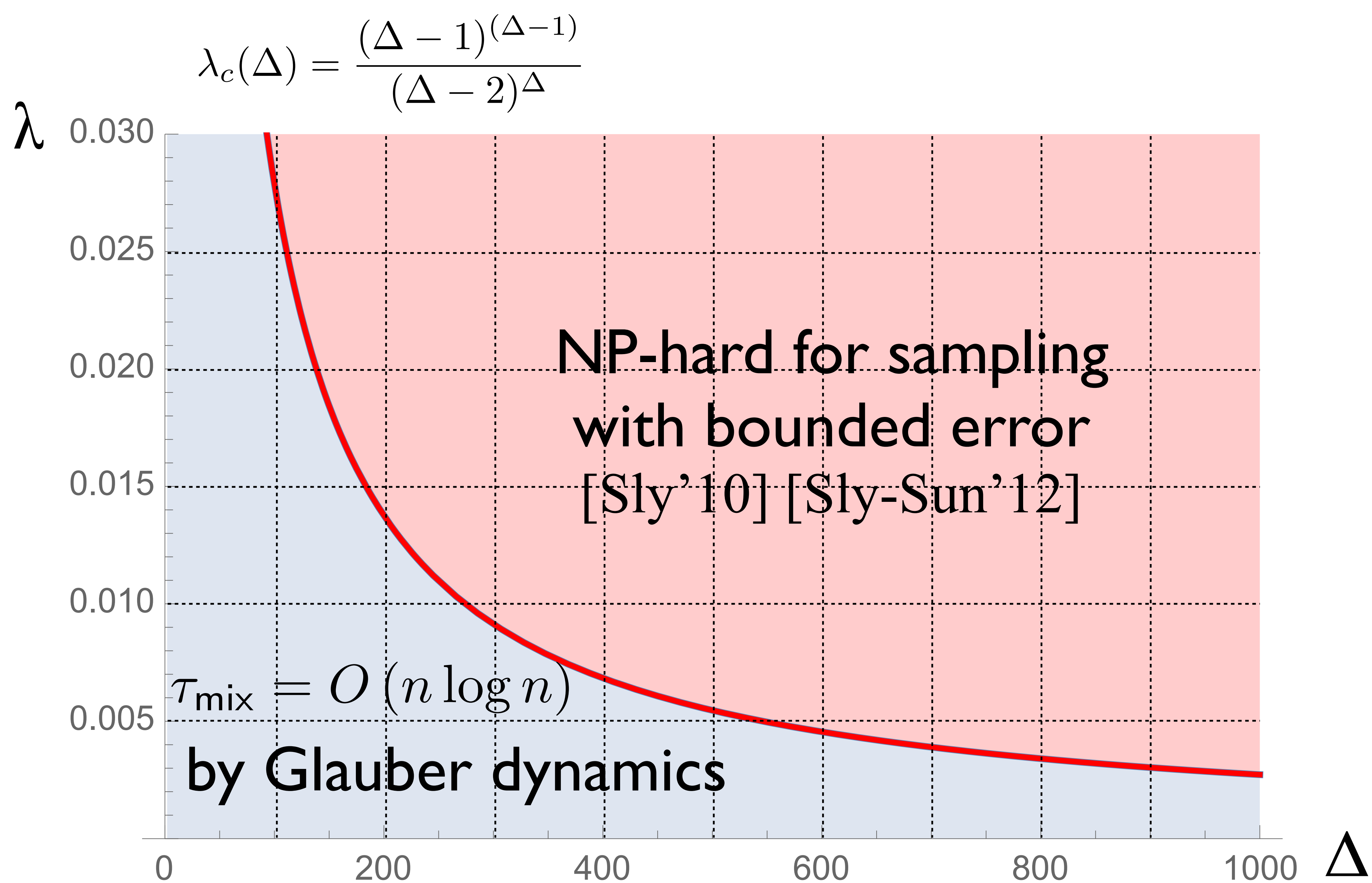
$$W_u^{(t)} = I[u \text{ is unblocked in } X_t]$$

$\forall \epsilon, \delta > 0$, $\exists \Delta_0$ and $\mathcal{I} = [O(n \log \Delta), n \exp(\Omega(\Delta))]$ s.t.
for all graphs of max-degree $\Delta \geq \Delta_0$ and girth ≥ 7:
$\lambda \leq (1-\delta)\lambda_c(\Delta)$ ⇒ $\forall$ vertex v:

$$\Pr\left[\forall t \in \mathcal{I}: \sum_{u \in N(v)} \frac{\lambda W_u^{(t)}}{1+\lambda W_u^{(t)}} \Phi_u < \sum_{u \in N(v)} \frac{\lambda \omega_u^*}{1+\lambda \omega_u^*} \Phi_u + \epsilon\right] \geq 1 - \exp(-\Omega(\Delta))$$

proved by concentration using the arguments in:

[Dyer-Frieze-Hayes-Vigoda'04] [Hayes-Vigoda'05] [Hayes'13]



$\lambda_c(\Delta) = \frac{(\Delta-1)^{(\Delta-1)}}{(\Delta-2)^{\Delta}}$
λ
0.030
0.025
0.020
0.015
0.010
0.005
0
200
400
600
800
1000
Δ
NP-hard for sampling
with bounded error
[Sly'10] [Sly-Sun'12]
$\tau_{\text{mix}} = O(n \log n)$
by Glauber dynamics

Summary

- Optimal mixing time for Glauber dynamics for the hardcore model in the *uniqueness* regime (when degree is big enough and there is no small cycle).

- Connecting rapid mixing of MCMC sampling with BP convergence:
  - If BP converges, there probably is contraction for Markovian coupling.
  - Path coupling "*from art to science*".

- Open problem: get rid of the degree and girth requirements.

Charis Efthymiou, Thomas P. Hayes, Daniel Štefankovič, Eric Vigoda, Yitong Yin. *Convergence of MCMC and Loopy BP in the Tree Uniqueness Region for the Hard-Core Model*. **FOCS'16**. arxiv: 1604.01422.

Thank you!

Any questions?