Maybe some local algorithms aren't that bad...?

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Overview

How do we efficiently simulate models near criticality?

- Problem: critical slowing-down
- The current state-of-the-art: cluster algorithms
  - Use global moves in clever way
- We will discuss two local algorithms:
  - Sweeny algorithm
    - Simulates the random-cluster model
  - Worm algorithm for the Ising model
    - Simulates the high-temperature graphs
- Both display critical speeding-up and multiple time-scales

References/Collaborators

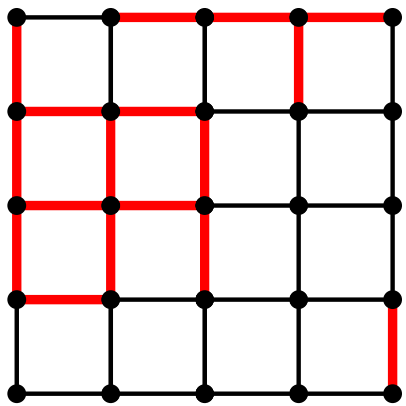
Youjin Deng, Timothy M. Garoni, and Alan D. Sokal, *Critical Speeding-Up in the Local Dynamics of the Random-Cluster Model*, Phys. Rev. Lett. 98, 230602 (2007).

Youjin Deng, Timothy M. Garoni, and Alan D. Sokal, *Dynamic Critical Behavior of the Worm Algorithm for the Ising Model*, Phys. Rev. Lett. 99, 110601 (2007).

Sweeny's algorithm

Random-cluster model

- Fortuin-Kasteleyn 1969
- Fix a finite graph $G = (V, E)$ and real numbers $q, v > 0$



- Pick a random bond configuration $A \subseteq E$ with probability

$$\mathbb{P}(A) \propto q^{k(A)}\, v^{|A|}$$

- $k(A) =$ number of components of (V, A)

- Integer $q \geq 2$ equivalent to q-state Potts model ($q = 2$ Ising)
- $q = 1$ reduces to bond percolation
- $q \to 0$ gives connected spanning subgraphs, spanning forests, spanning trees

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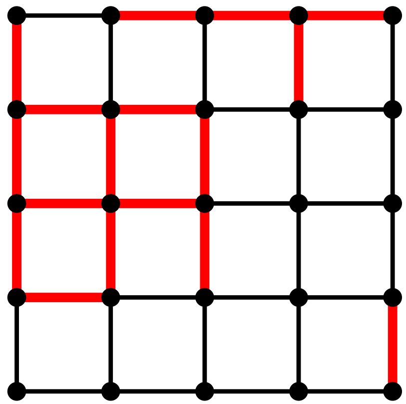
Random-cluster model

- Focus on two observables:



$$\mathcal{N}(A) = |A|$$

$$\mathcal{S}_2(A) = \sum_{\text{clusters } \mathcal{C} \text{ in } (V,A)} |\mathcal{C}|^2$$

- $\mathcal{N}$ is an "energy"
- $\chi = \langle \mathcal{S}_2 \rangle / V$ is the mean cluster size, or "susceptibility"
- Chayes-Machta 1997 devised a cluster algorithm valid for all real $q \geq 1$
  - Simulates a coupled measure of bond and vertex variables
  - Equivalent to Swendsen-Wang when q is an integer

Sweeny's algorithm

- The heat-bath version proceeds as follows:
  - Start with some configuration $A \subseteq E$

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    - If so, occupy xy with probability $v/(1+v)$

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- Valid for all real $q \geq 0$
- Need an efficient way to check connectivity. . .

Sweeny's algorithm

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    - If not, occupy xy with probability $v/(q+v)$
- Valid for all real $q \geq 0$
- Need an efficient way to check connectivity...
- How do we measure the efficiency of an MCMC algorithm?
- Compare Sweeny with Chayes-Machta

General setting for MCMC

- Irreducible, aperiodic, reversible Markov chain
  - State space S, with $|S| < \infty$
  - Transition matrix P
  - Stationary distribution π
- Observable (random variable) X
  - E.g. $X = \mathcal{N}$ or $\mathcal{S}_2 \ldots$
- Simulate Markov chain $\implies$ time series $X_0, X_1, \ldots$
- Define the autocorrelation function

$$\rho_X(t) := \frac{\langle X_s X_{s+t} \rangle_\pi - \langle X \rangle_\pi^2}{\text{var}_\pi(X)}$$

- Stationary process – start "in equilibrium" (or wait "long enough")

Autocorrelation times

- We must consider two distinct autocorrelation times
- The integrated autocorrelation time

$$\tau_{\text{int},X} := \frac{1}{2} \sum_{t=-\infty}^{\infty} \rho_X(t)$$

- If $\widehat{X}$ is the sample mean of $\{X_t\}_{t=1}^{T}$ then we have

$$\text{var}(\widehat{X}) \sim 2\,\tau_{\text{int},X} \frac{\text{var}(X)}{T}, \qquad T \to \infty$$

- We get one "effectively independent" observation every $2\,\tau_{\text{int},X}$ time steps

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Autocorrelation times

- $\rho_X(t)$ typically decays exponentially as $t \to \infty$
- The exponential autocorrelation time

$$\tau_{\exp,X} := \limsup_{t\to\infty} \frac{t}{-\log|\rho_X(t)|} \quad \text{and} \quad \tau_{\exp} := \sup_X \tau_{\exp,X}$$

- Typical observables have $\tau_{\exp,X} = \tau_{\exp}$
- *Nice* chains with $|S| < \infty$ have $\tau_{\exp} < \infty$
- $\tau_{\text{int},X} \leq \tau_{\exp}$ for all X (need NOT be equal)
- Start the chain with arbitrary distribution α
  - Distribution at time t is αP^t
  - αP^t tends to π with rate bounded by $e^{-t/\tau_{\exp}}$

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Critical slowing-down

- Near a critical point the autocorrelation times typically diverge like

$$\tau \sim \xi^z$$

- More precisely, we have a family of exponents:

  z_{exp}, and $z_{\text{int},X}$ for each observable X.

- Different algorithms for the same model can have very different z

- E.g. $d = 2$ Ising model
  - Glauber (Metropolis) algorithm $z \approx 2$
  - Swendsen-Wang algorithm $z \approx 0.2$

Back to Sweeny's algorithm

- Simulated the $d = 2$ critical random-cluster model
  - On $L \times L$ square lattice
  - Simulated a number of values of $0 \leq q \leq 4$
  - Measured:
    - $\mathcal{N}(A) = |A|$
    - $\mathcal{S}_2(A) = \sum_{\text{clusters } \mathcal{C} \text{ in } (V,A)} |\mathcal{C}|^2$
  - Measured observables after every hit

    – i.e. every bond update
  - Natural unit of time is one sweep

    – i.e. L^d hits
  - Cluster algorithms perform one sweep every iteration

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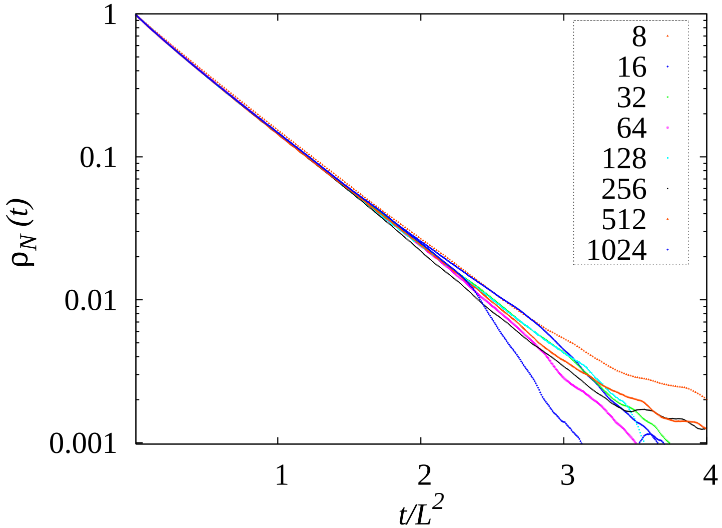
Dynamics of $\mathcal{N}$

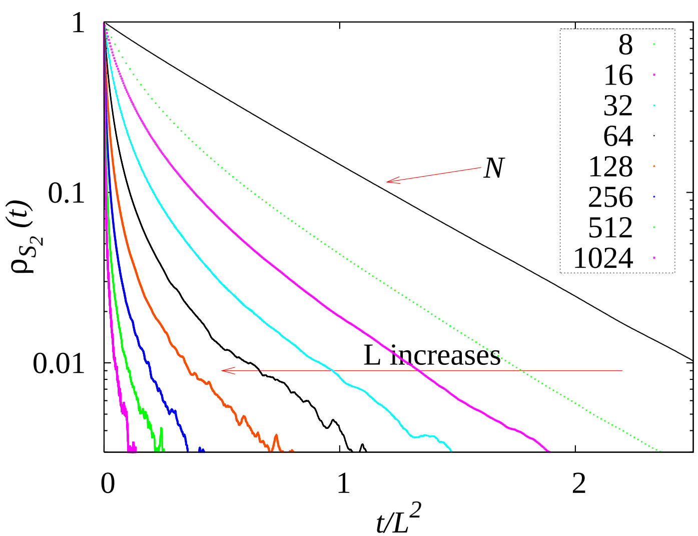


Plot shows $q = 0.2$ and $8 \leq L \leq 1024$

Suggests $\tau_{\text{exp}} \sim L^2$ hits

- Good data collapse
- Empirically $z_{\text{exp}} = 0$ for $q \lessapprox 2$
- $\rho_{\mathcal{N}}(t)$ is almost a perfect exponential
- Li-Sokal bound: $z_{\text{exp}}, z_{\text{int},\mathcal{N}} \geq \alpha/\nu$
  - Applies to Sweeny and Chayes-Machta
  - Empirically $z^{\text{Sweeny}} \approx z^{\text{Chayes-Machta}}$

Dynamics of $\mathcal{S}_2$



- Plot shows $q = 0.2$ and $8 \leq L \leq 1024$
- $\rho_{\mathcal{N}}(t)$ is shown for comparison

- $\rho_{\mathcal{S}_2}(t)$ decays significantly in a time much less than one sweep
- Critical speeding-up

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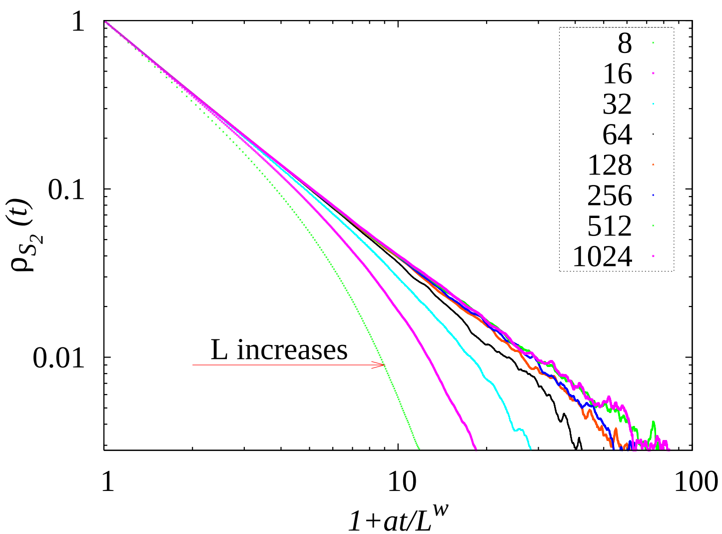
Critical speeding-up



- Plot shows $q = 0.2$ and $8 \leq L \leq 1024$
- $\rho_{\mathcal{S}_2}(t)$ vs $1 + at/L^w$ with $w = 0.99$

- Good data collapse
- $\mathcal{S}_2$ exhibits strong decorrelation on a time scale $O(L^w)$ hits
- Initial decay $\rho_{\mathcal{S}_2}(t) = f(t/L^w)$ with $f(x) \sim x^{-r}$
- Empirically $w < d$ for $q \lessapprox 2$

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Some hand-waving...

- Critical FK clusters are fractal
  - $O(1)$ bond deletions can split a large cluster into two large clusters
  - $O(1)$ bond additions can join two large clusters
- There are $O(L^{d_{\text{red}}})$ edges whose removal would split a big cluster
- There are $O(L^{d_{\text{red}}})$ edges whose addition would connect two big clusters
  - d_{red} is the red bond exponent
  - Coniglio 1989 gives d_{red} for all $0 \leq q \leq 4$ in $d = 2$

A conjecture...

- “The decorrelation of $\mathcal{S}_2$ is due to hitting $O(1)$ red bonds”
  - This takes time $O(L^{d-d_{\mathrm{red}}})$
  - So $w = d - d_{\mathrm{red}}$

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A conjecture...

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  - So $w = d - d_{\mathrm{red}}$

q	z_{exp}	α/ν	w	d_{red}
0.0005	0	-1.9576	0.77	1.2376
0.005	0	-1.8679	0.79	1.2111
0.05	0	-1.6005	0.88	1.1299
0.2	0	-1.2467	0.99	1.0168
0.5	0	-0.8778	1.11	0.8904
1.0	0	-0.5000	1.26	0.7500
1.5	0	-0.2266	1.36	0.6398
2.0	0 (log)	0 (log)	1.49	0.5417
2.5	0.26(1)	0.2036	1.64	0.4474
3.0	0.45(1)	0.4000	1.84	0.3500
3.5	0.636(2)	0.6101	2.04	0.2375

Summary of Sweeny results

- Critical slowing down is absent for small q
- $z_{\exp}, z_{\text{int},\mathcal{N}}$ comparable to their Chayes-Machta values
- $\mathcal{S}_2$ exhibits critical speeding-up for a wide range of q
  - This can lead to $z_{\text{int},\mathcal{S}_2} < 0$
  - Estimating $z_{\text{int},\mathcal{S}_2}$ is tricky ...
- Critical speeding-up and slowing-down can coexist
- All this holds in $d = 3$ too
- It is conceivable that *most* dynamics have a multiple time-scale behavior...

Worm algorithms

How can we simulate the Ising model?

- Glauber dynamics
  - Flip one Ising spin at a time
  - Severe critical slowing-down
- Sweeny dynamics
  - Transform Ising model to $q = 2$ random-cluster model
  - Flip one FK bond at a time
  - Weak critical slowing-down
- Swendsen-Wang (Chayes-Machta) dynamics
  - Transform Ising model to $q = 2$ random-cluster model
  - Simulate joint model of Ising spins and FK bonds
  - Weak critical slowing-down

Worm algorithms

- Worm dynamics
  - Prokof'ev & Svistunov PRL 2001
  - Transform Ising model to high-temperature graphs
  - Simulate high-temperature graphs via *local* moves
  - *worm diffusion*
- Consider simplest case
  - ferromagnetic, zero field, nearest-neighbor, on L^d

State space for worm dynamics

- Fix a finite graph $G = (V, E)$
- For $A \subseteq E$ let ∂A be the set of all vertices with odd degree in (V, A)
- For distinct $x, y \in V$ define

$$\mathcal{S}_{x,y} = \{A \subseteq E | \partial A = \{x, y\}\}$$

and let

$$\mathcal{S}_{x,x} = \{A \subseteq E | \partial A = \emptyset\}$$

- $\mathcal{S}_{x,x}$ is just the cycle space $\mathcal{C}(G)$
- Configuration space of our worm algorithm is

$$\mathcal{S} = \{(A, x, y) | x, y \in V \text{ and } A \in \mathcal{S}_{x,y}\}$$

High temperature expansions

- The standard Ising high-temperature expansions are:

$$Z = \sum_{A \in \mathcal{S}_{x,x}} w^{|A|} \qquad \text{Partition function}$$

$$Z\langle \sigma_x \sigma_y \rangle = \sum_{A \in \mathcal{S}_{x,y}} w^{|A|} \qquad \text{Two-point function}$$

$$Z\langle \mathcal{M}^2 \rangle = \sum_{A \in \mathcal{S}} w^{|A|} \qquad \text{Magnetization}$$

- $\mathcal{M}(\sigma) = \sum_{x \in V} \sigma_x$ is the Ising magnetization
- $w = \tanh(\beta)$
- $0 \leq w \leq 1$

Worm algorithm

- The elementary move of the worm algorithm is as follows:

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  - Pick uniformly at random some $x' \sim x$ (in G)

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  - Propose moving to $(A \triangle xx', x', y)$

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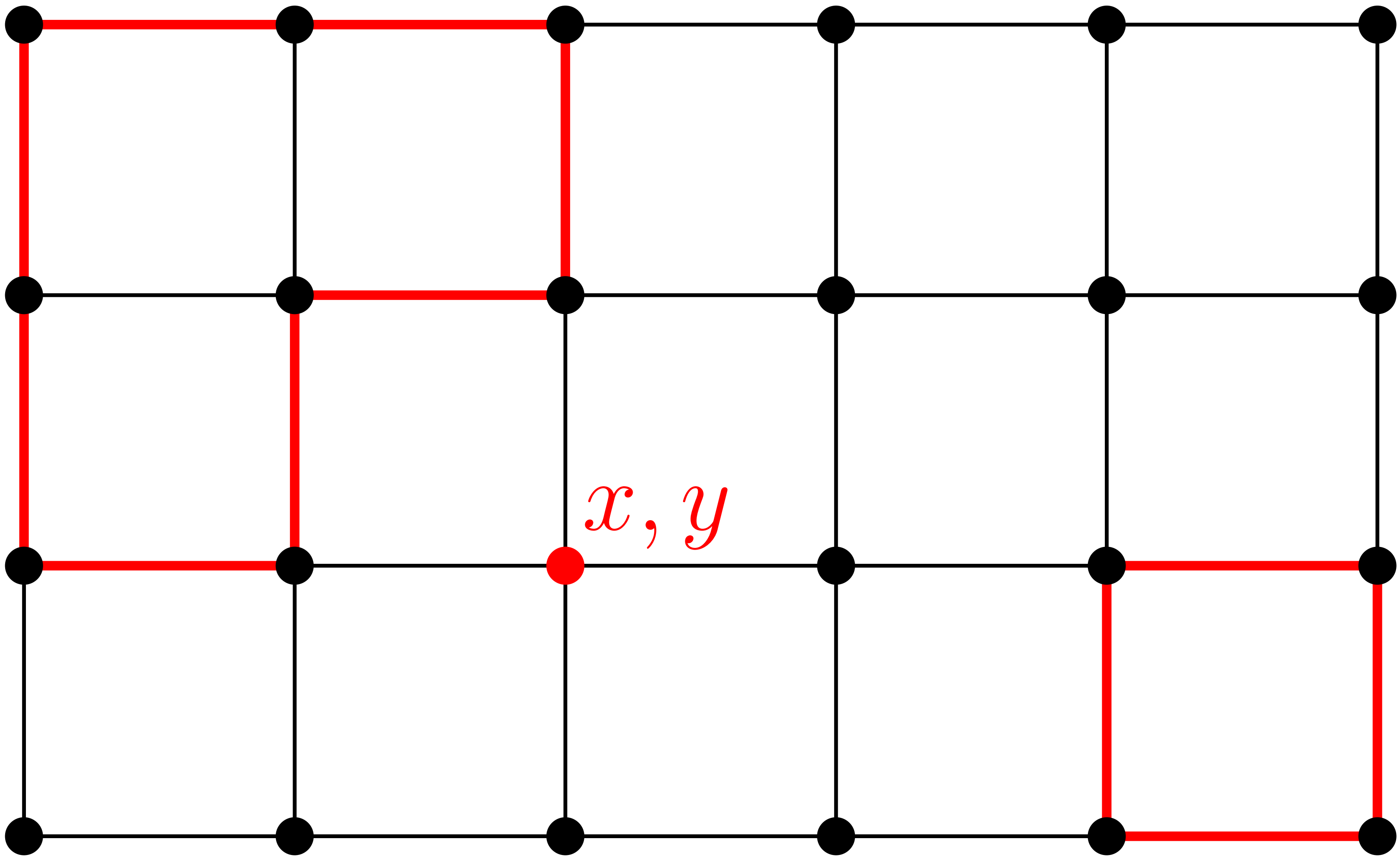
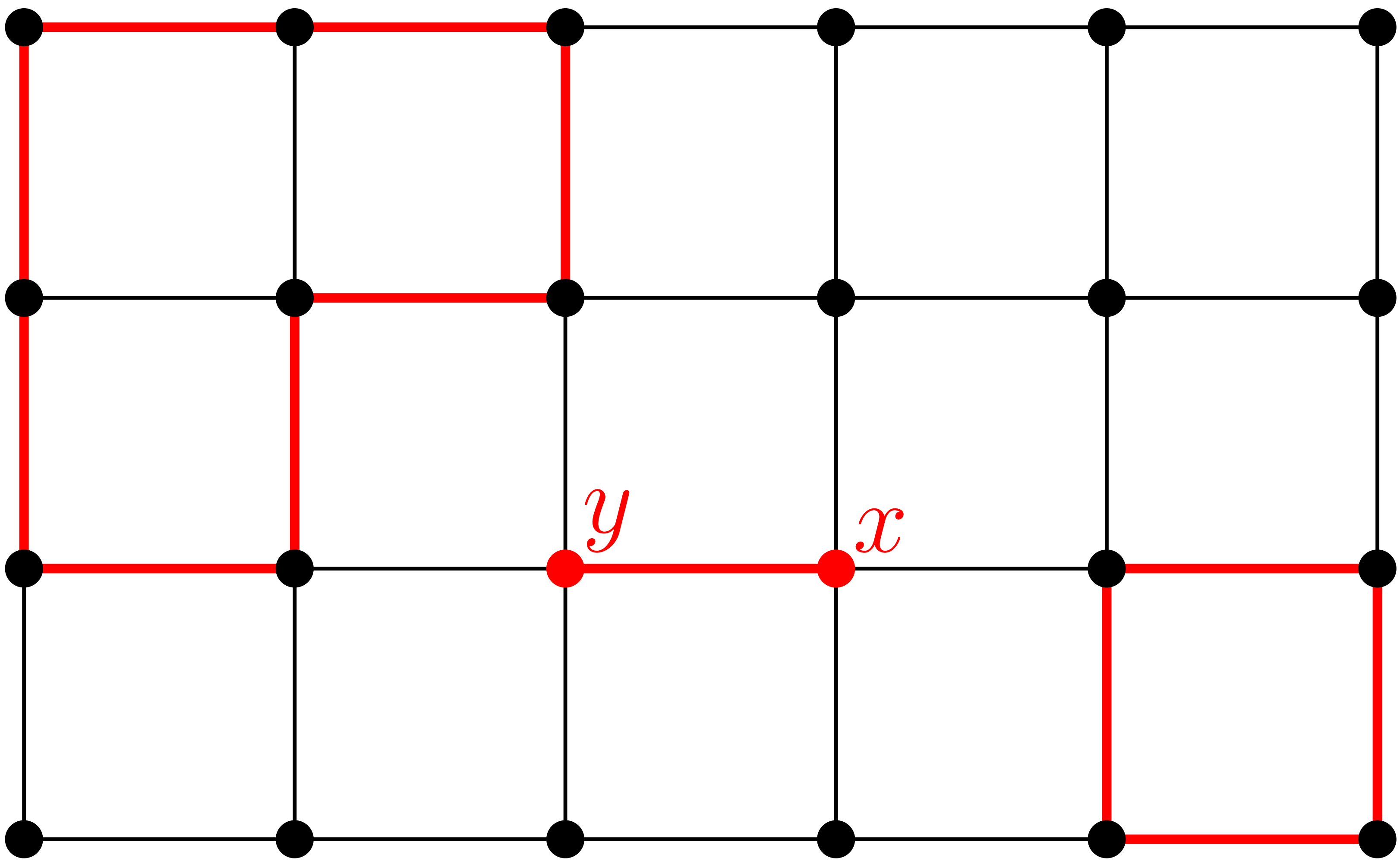
  - Pick uniformly at random either x or y (say, x)
  - Pick uniformly at random some $x' \sim x$ (in G)
  - Propose moving to $(A \triangle xx', x', y)$
    - If proposed transition would add an edge accept with probability w
    - If proposed transition would remove an edge accept with probability 1

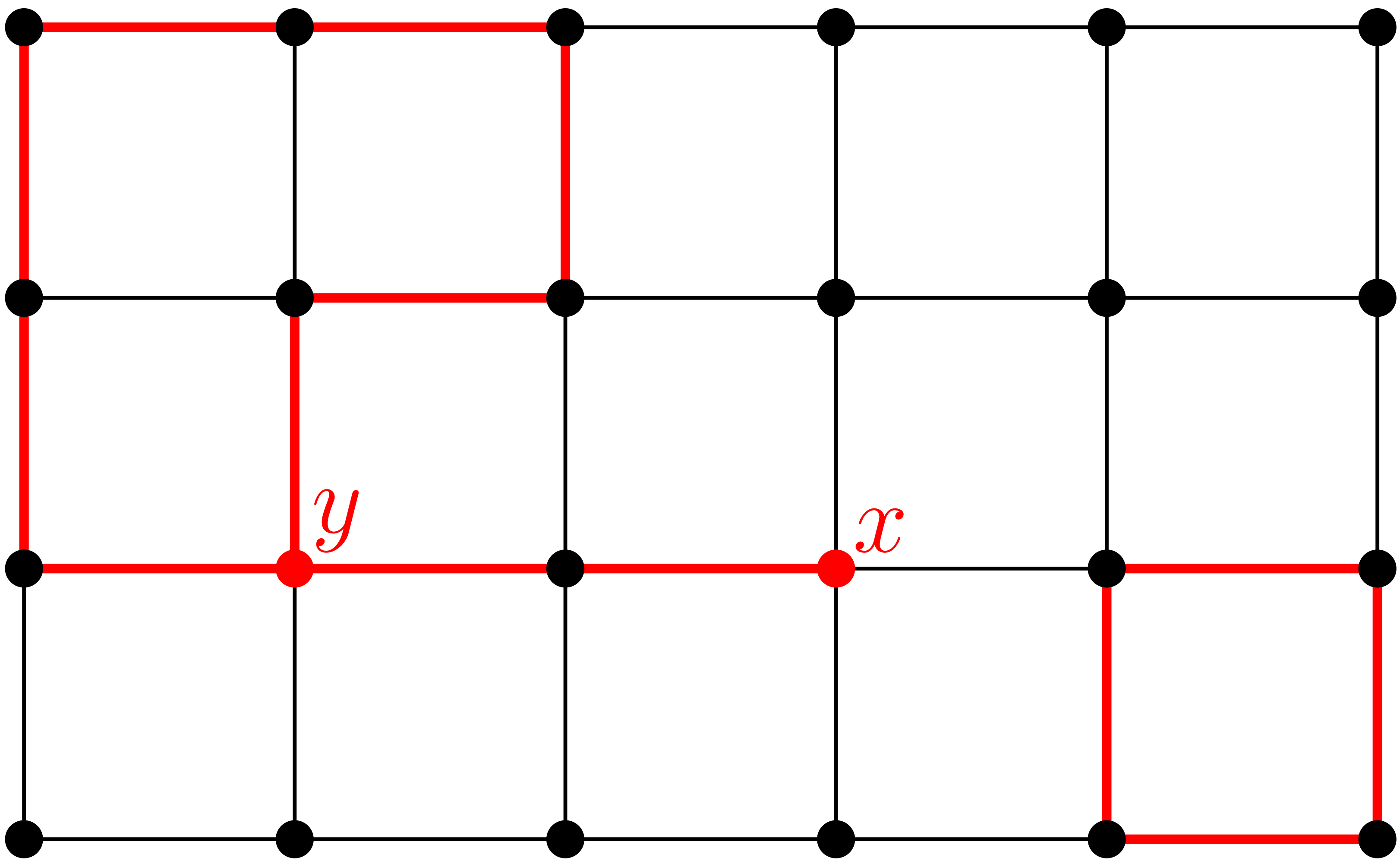
Worm dynamics $t = 0$



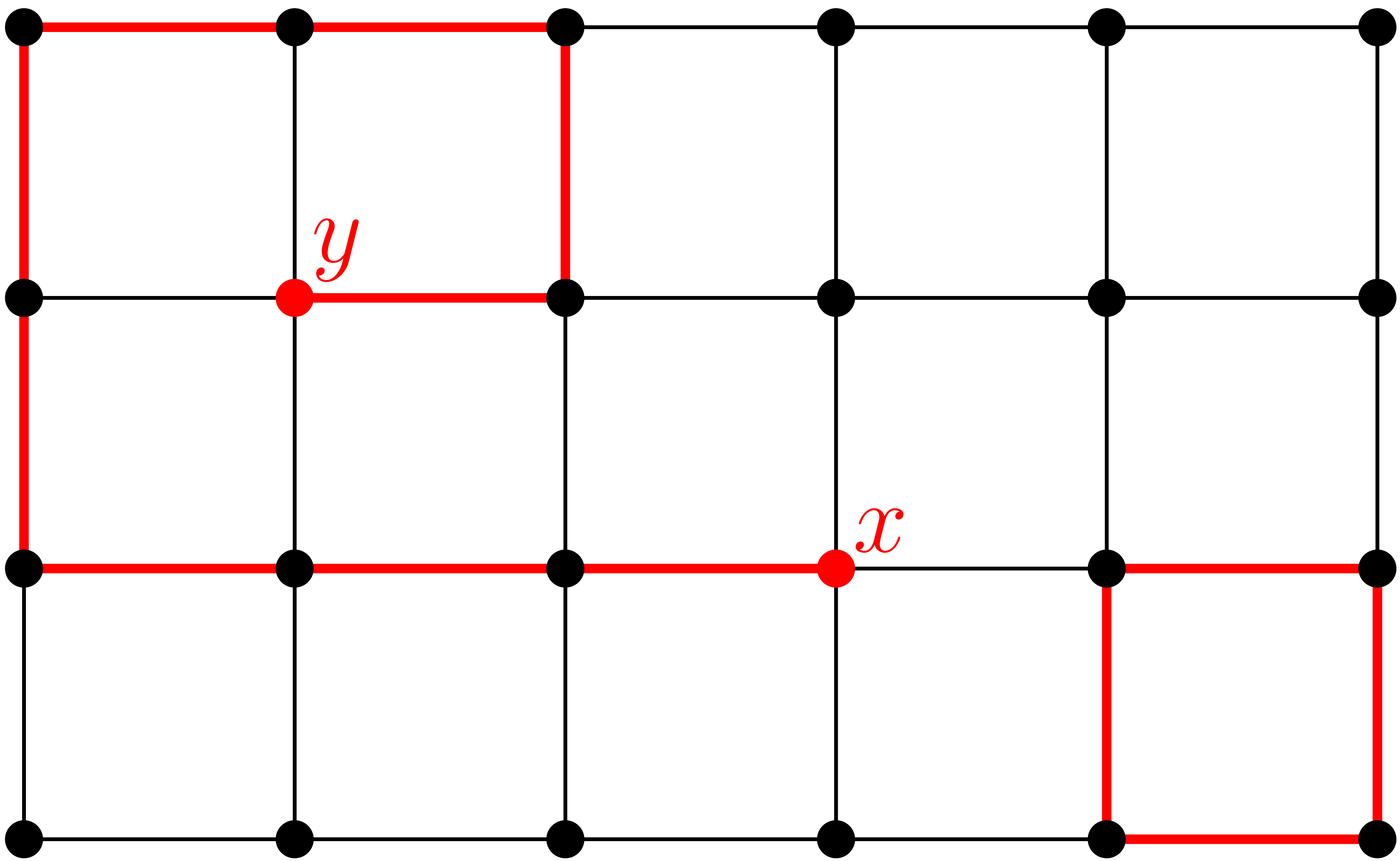
Worm dynamics $t = 1$



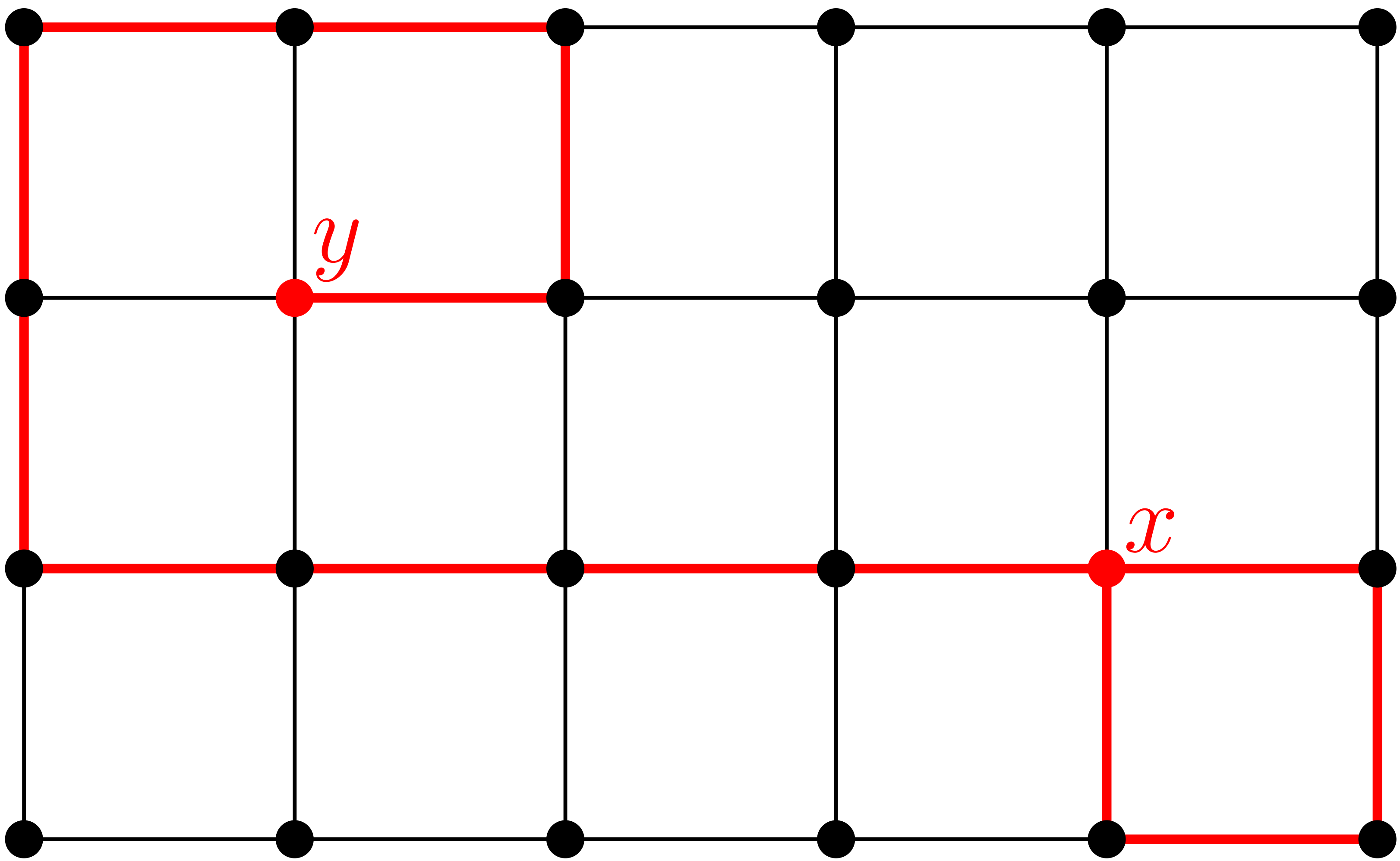
Worm dynamics $t = 2$



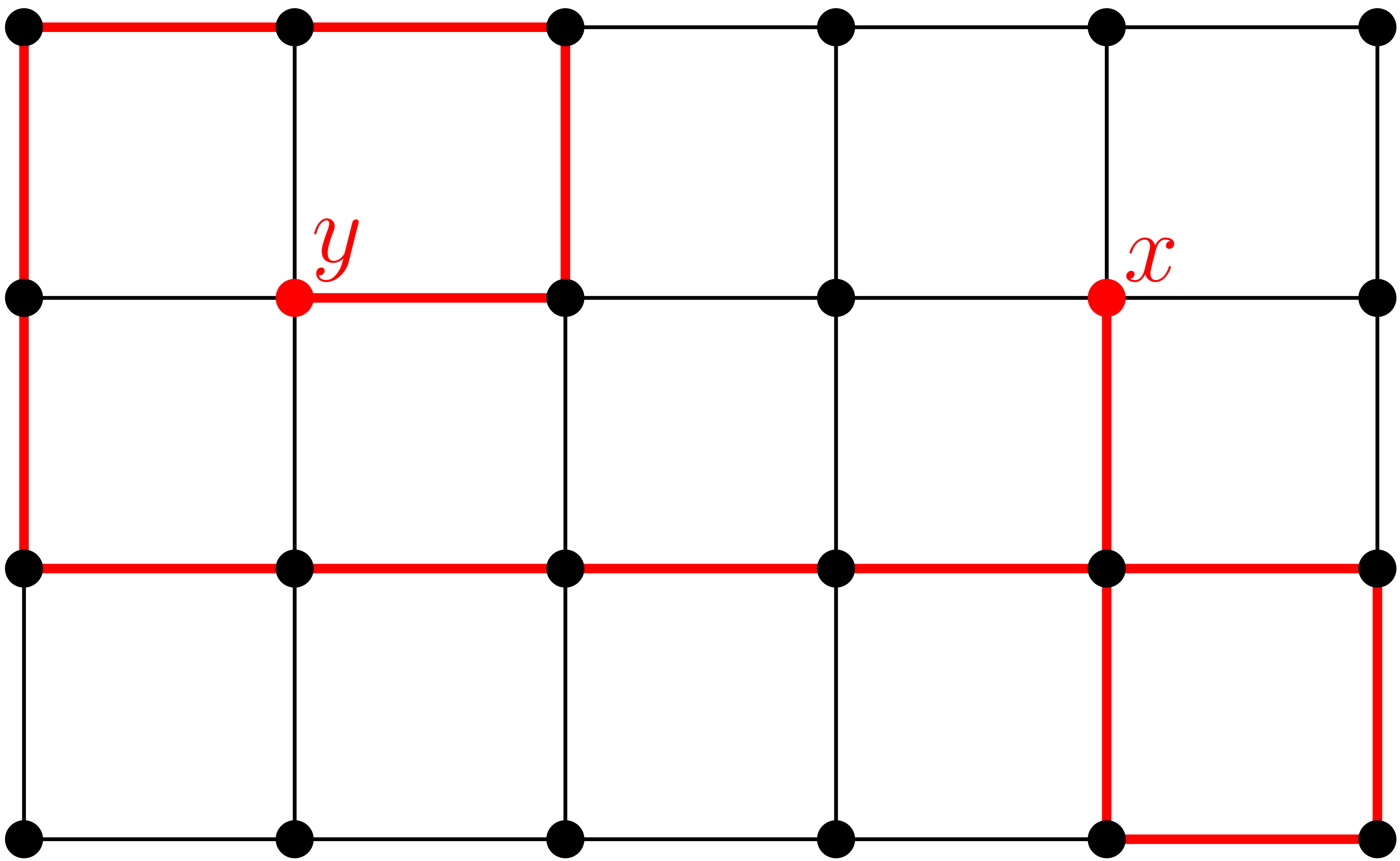
Worm dynamics $t = 3$



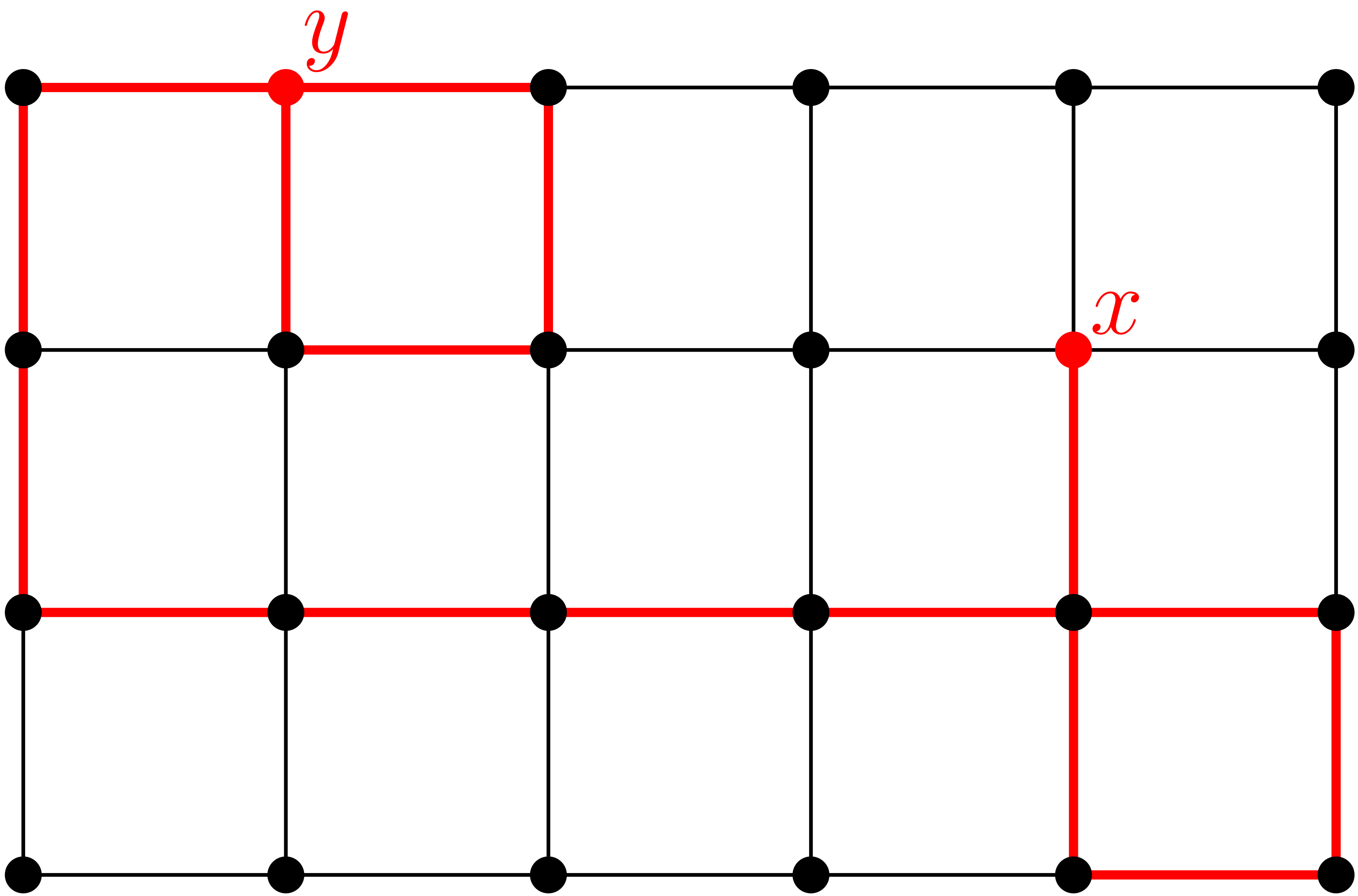
Worm dynamics $t = 4$



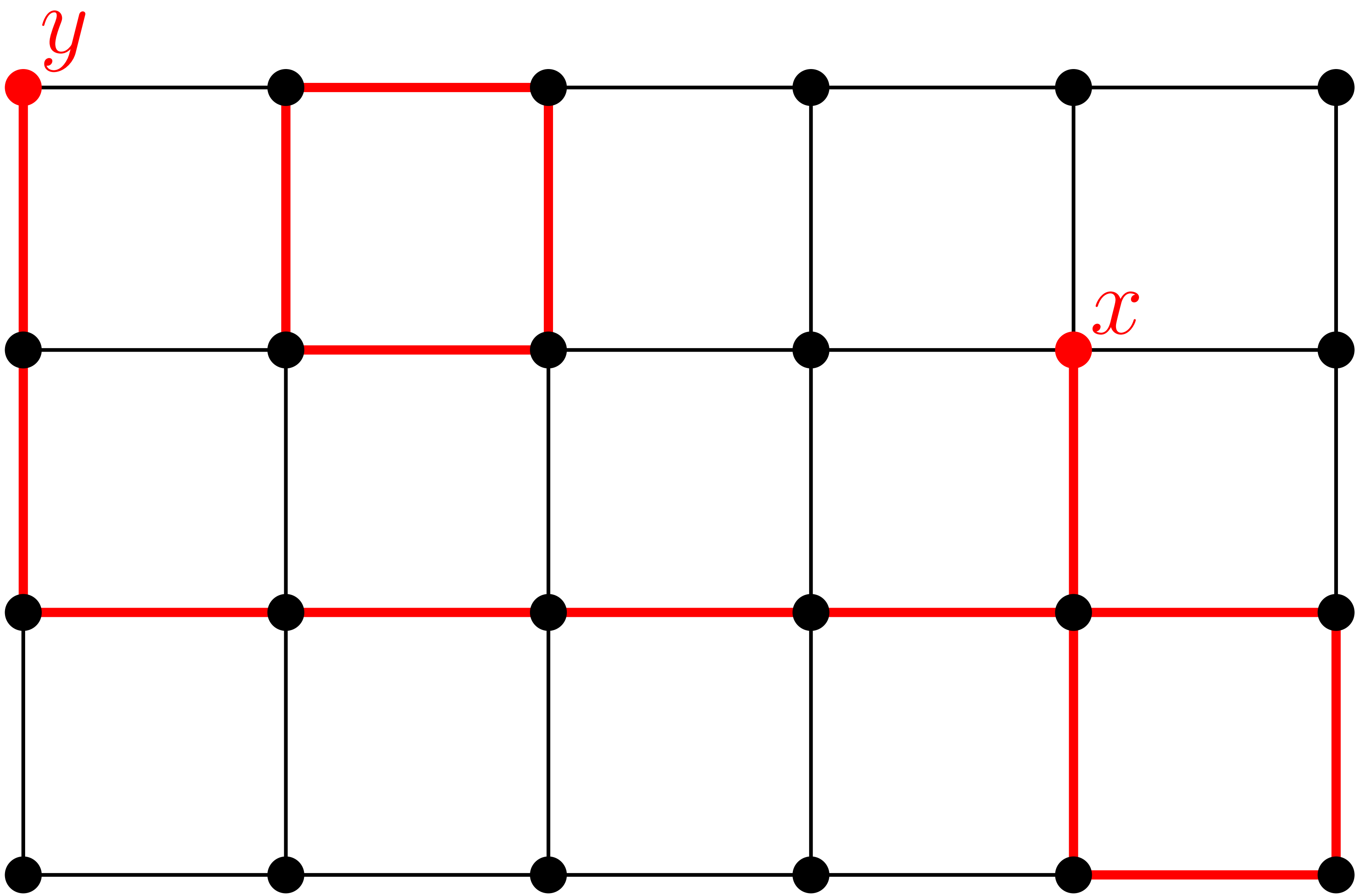
Worm dynamics $t = 5$



Worm dynamics $t = 6$



Worm dynamics $t = 7$



Transition matrix

- Let G be a regular lattice of coordination number z
- Transition matrix P on $\mathcal{S}$ is

$$P[(A,x,y) \to (A\triangle xx', x', y)] = \frac{1}{2}\,\frac{1}{z}\begin{cases} 1, & xx' \in A, \\ w, & xx' \notin A, \end{cases}$$

- And similarly for y moves...
- All other non-diagonal elements of P are zero
- P is in detailed balance with $\pi(A,x,y) = w^{|A|}/Z\langle\mathcal{M}^2\rangle$
- For translation invariant systems $\langle\mathcal{M}^2\rangle = V\,\chi$

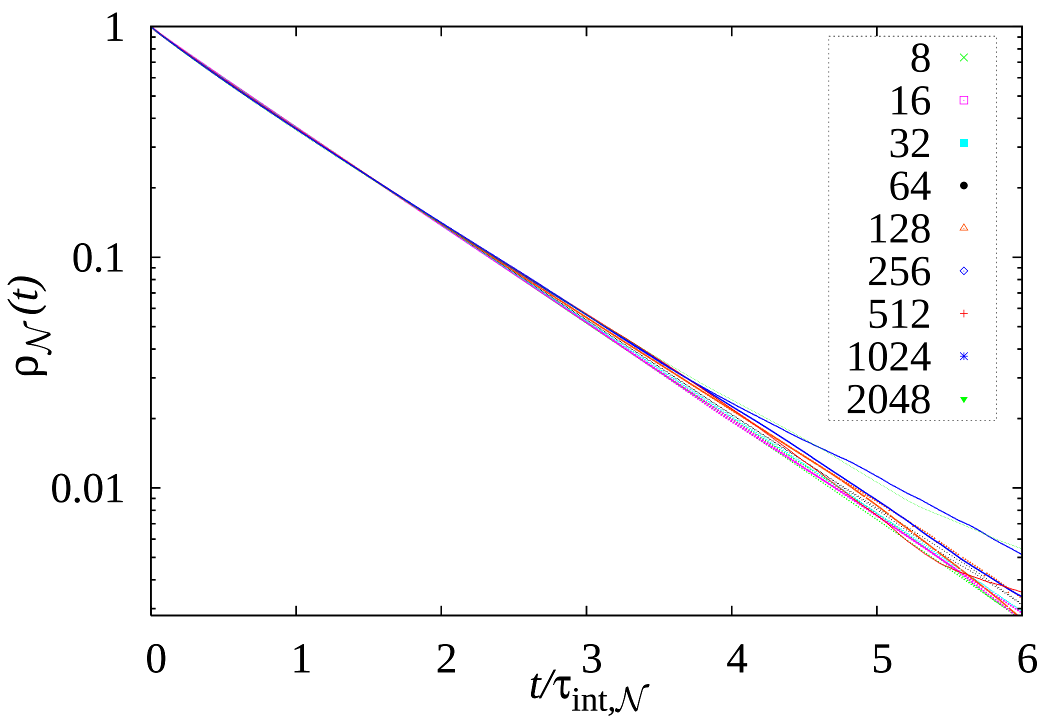
Observables

- Focus on two observables:
  - $\mathcal{N}(A, x, y) = |A|$
  - $\mathcal{D}_0(A, x, y) = \delta_{x,y}$
- $\langle \mathcal{D}_0 \rangle_\pi$ is simply related to χ

$$
\begin{aligned}
\langle \mathcal{D}_0 \rangle_\pi &= \frac{1}{Z\,V\,\chi} \sum_{(A,x,y)\in\mathcal{S}} w^{|A|} \delta_{x,y} \\
&= 1/\chi
\end{aligned}
$$

- Measured observables after every hit (worm update)
- Natural unit of time is one sweep (L^d hits)

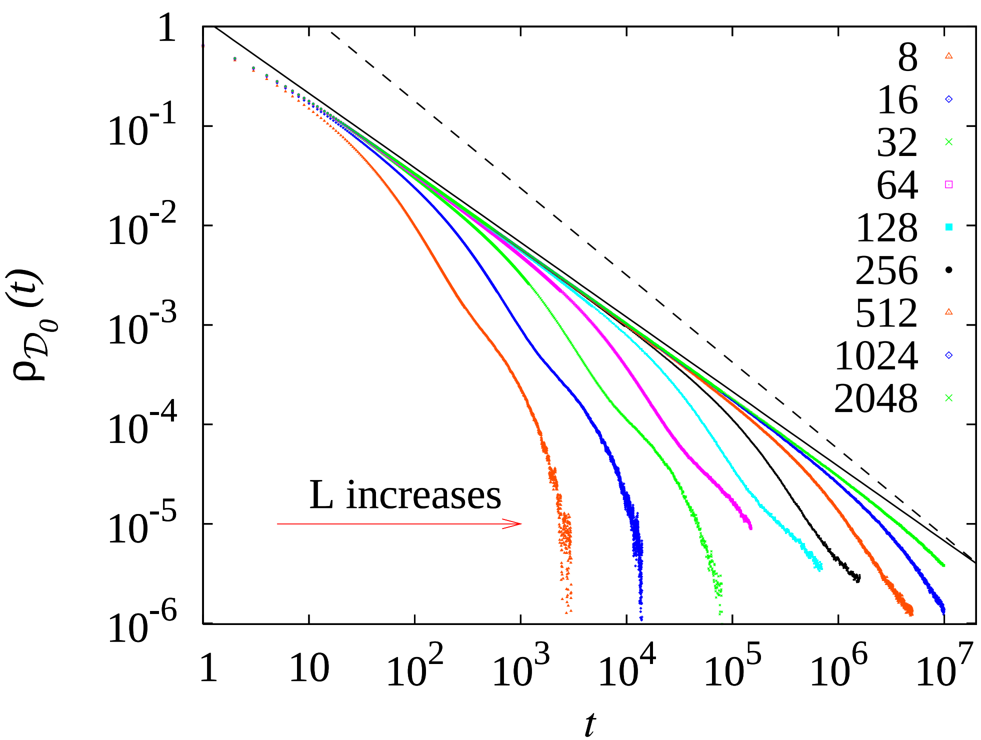
Dynamics of $\mathcal{N}$



- Critical Ising model $d = 2$
- Good data collapse
- $z_{\text{exp}} \approx z_{\text{int},\mathcal{N}} \approx 0.379$

- $\rho_{\mathcal{N}}(t)$ is almost a perfect exponential
- Li-Sokal bound $z_{\text{exp}}, z_{\text{int},\mathcal{N}} \geq \alpha/\nu$ applies to worm too

Dynamics of $\mathcal{D}_0$



Critical Ising model $d = 2$

- $\rho_{\mathcal{D}_0}(t)$ decays significantly in $O(1)$ hits!
- $\rho_{\mathcal{D}_0}(t) \sim t^{-s}$ with $s \approx 0.75$

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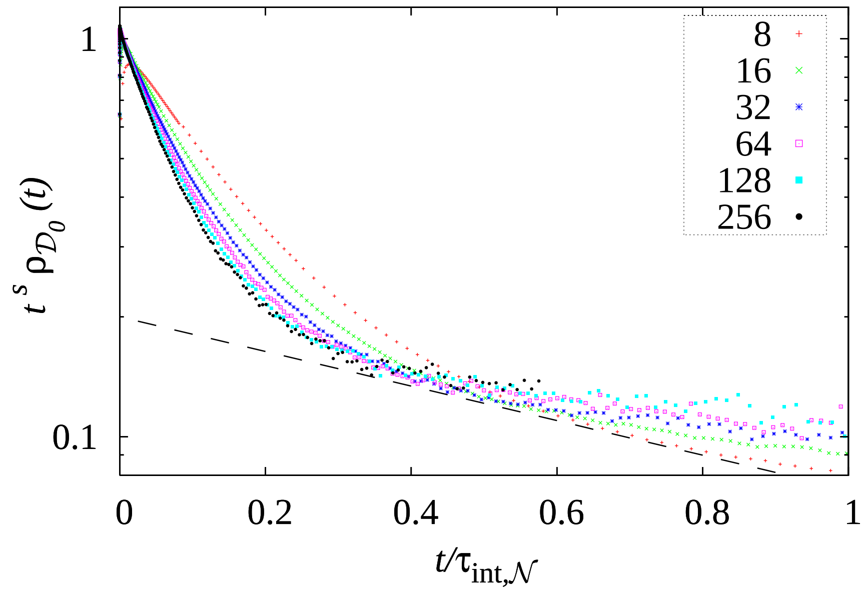
Crossover



Plot $t^s\,\rho_{\mathcal{D}_0}(t)$ versus $t/\tau_{\text{int},\mathcal{N}}$

Reasonable data collapse

- Postulate $\rho_{\mathcal{D}_0}(t) = g(t)h(t/L^{d+z_{\exp}})$ with $g(t) \sim t^{-s}$ and $s < 1$

$$\implies z_{\text{int},\mathcal{D}_0} = -sd + (1-s)z_{\exp}$$

- Gives $z_{\text{int},\mathcal{D}_0} \approx -1.42$

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Three dimensions

Qualitatively similar behavior when $d = 3$:

- $\rho_{\mathcal{D}_0}(t) \sim t^{-s}$
- $s \approx 0.66$
- Implies $z_{\text{int},\mathcal{D}_0} \approx -1.92$
- $\rho_{\mathcal{N}}(t)$ roughly exponential
- $z_{\text{exp}} \approx z_{\text{int},\mathcal{N}} \approx \alpha/\nu \approx 0.174$
- Li-Sokal bound may be sharp for $d = 3$ worm algorithm
- Compare Swendsen-Wang $z_{SW} \approx 0.46$

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Practical efficiency

- Swendsen-Wang seems to outperform worm when $d = 2$
- Efficiency depends on observable, X
- A simple way to compare worm and SW is to compute $\kappa = \sigma^2_{\widehat{X}} T_{CPU}$ for both algorithms
- When $d = 3$ and $X = \chi$ we find $\kappa_{worm}/\kappa_{SW} \approx L^{-0.33}$
  - With the crossover $\kappa_{worm}/\kappa_{SW} \approx 1$ at around $L \approx 20$
- There is also a natural worm estimator for ξ
- Again SW outperforms worm when $d = 2$
  - For $d = 3$ we find $\kappa_{worm}/\kappa_{SW} \approx L^{-0.32}$
  - With the crossover $\kappa_{worm}/\kappa_{SW} \approx 1$ at around $L \approx 45$

Conclusions

- Locality is not a sufficient condition for “badness”
- Sweeny’s algorithm has comparable efficiency to Chayes-Machta
- For $q \lessapprox 2$ Sweeny’s algorithm exhibits critical speeding-up i.e. significant decorrelation in $O(L^w)$ hits with $w < d$
- We can predict w if $\alpha/\nu < 0$ (no critical slowing down)
- The worm algorithm also exhibits decorrelation on multiple time scales
- The worm algorithm outperforms Swendsen-Wang for $d = 3$ Ising model for measuring χ and ξ