The cutoff phenomenon for exclusion processes on graphs with open boundaries

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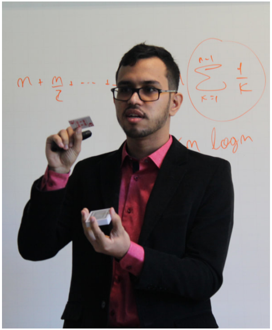
This is based on joint work with

Milton Jara
(IMPA)



Rodrigo Marinho
(Técnico Lisboa)

Stay tuned for our preprint coming soon on arXiv!

Outline

Motivations

Convergence of Markov chains

The cutoff phenomenon

The exclusion process on graphs with boundaries

Cutoffs for exclusion processes

Proof ideas

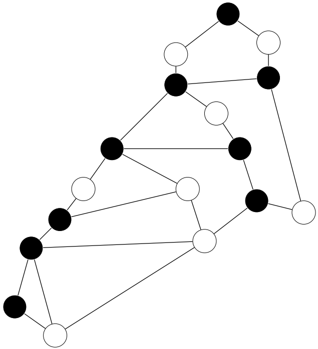
Thank you for listening!

Mixing a deck of cards

- Deck with n cards $\Rightarrow$ $n!$ permutations
- Deck with 52 cards $\Rightarrow \sim 10^{68}$ permutations
- A deck will be considered **mixed** whenever all permutations are equally probable.

Question: How long does it take to mix a deck of 52 cards, using your preferred shuffle method?

Mixing road traffic



- ● = Position occupied by a vehicle; ○ = Position vacant.
- A vehicle is allowed to move to an adjacent position provided that it is vacant.

Questions: How long does it take to mix the vehicles on this road network, according to the random adjacent moves?

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Markov chains

- Fix a finite state space Ω. To each $x, y \in \Omega$, $x \neq y$, we assign a transition rate $Q(x, y) \geq 0$, and define $Q(x, x) = -\sum_{y \neq x} Q(x, y) =: -\lambda_x$.
- The continuous-time Markov chain (MC) with rate matrix Q — "hold-jump" construction
- Q is the infinitesimal generator ("Laplacian") for the Markov chain. A negative semidefinite operator.
- If $P_t(x, y)$ denotes the probability of moving from x to y over time $t \geq 0$, then it satisfies the backward/forward Kolmogorov's equation $\partial_t P_t(x, y) = (QP_t)(x, y) = (P_t Q)(x, y)$. $\Longrightarrow P_t(x, y) = e^{tQ} P_0(x, y)$

Convergence of Markov chains

- **Ergodic theorem for MCs.** Under irreducibility, there exists a unique prob. measure π (stationary distribution) s.t. $\lim_{t\to+\infty} P_t(x,y)=\pi(y)$ for all $x,y\in\Omega$.
- Can we state this convergence more quantitatively?
  Assume that Q is self-adjoint w.r.t. π (that is, the MC is reversible). By linear algebra, $-Q =: L$ has all $\mathbb{R}$-valued eigenvalues $\{\lambda_i\}_{i=0}^{|\Omega|-1}$, listed in increasing order; and corresponding $L^2(\pi)$-orthonormal eigenfunctions $\{\psi_i\}_{i=0}^{|\Omega|-1}$.

Spectral decomposition $$(e^{tQ}f)(x)=\sum_{i=0}^{|\Omega|-1} e^{-t\lambda_i}\langle f,\psi_i\rangle_{L^2(\pi)}\psi_i(x).$$

- $\lambda_0=0$ ALWAYS. (Q is a singular matrix.)
- Rate of convergence is governed by λ_1 (the spectral gap), which is positive by irreducibility and Perron-Frobenius.

Convergence of Markov chains

- **Ergodic theorem for MCs.** Under irreducibility, there exists a unique prob. measure π (stationary distribution) s.t. $\lim_{t\to+\infty} P_t(x,y) = \pi(y)$ for all $x, y \in \Omega$.
- Can we state this convergence more quantitatively?
  Use the **total variation distance** between two probability measures μ and ν:

$$\|\mu - \nu\|_{\mathrm{TV}} := \sup_{S\subset\Omega} |\mu(S) - \nu(S)| = \frac{1}{2}\sum_{x\in\Omega} |\mu(x) - \nu(x)| \in [0,1].$$

TV distance to stationarity

$$d(t) := \sup_{x\in\Omega} \|P_t(x,\cdot) - \pi\|_{\mathrm{TV}} = \sup_{x\in\Omega} \|(e^{tQ}P_0)(x,\cdot) - \pi\|_{\mathrm{TV}}$$

We shall be interested in how $d(t)$ drops from 1 to 0 as t increases.

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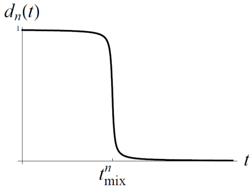
Cutoff := sharp transition in convergence to stationarity

- Let $\{\{\eta_t^N : t \geq 0\}\}_{N\in\mathbb{N}}$ be a family of irreducible MCs, each of which has state space Ω_N, with $|\Omega_N| \uparrow \infty$.
- π^N: Stationary distribution of the Nth chain.
- $d_N(t) := \sup_{\eta\in\Omega_N} \|\mathbb{P}_\eta(\eta_t^N \in \cdot) - \pi^N\|_{\rm TV}$: distance to stationarity
- A typical graph of $t \mapsto d_N(t)$ looks likes this:

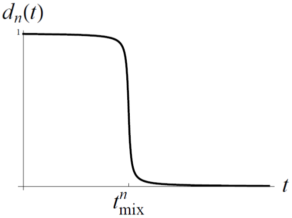


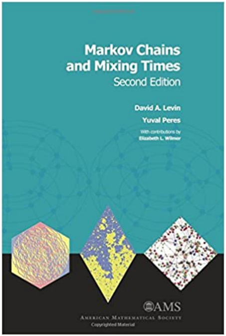
- $t^N_{\rm mix}(\varepsilon) := \inf\{t \geq 0 : d_N(t) \leq \varepsilon\}$. ε-mixing time.
  Some books fix $\varepsilon = \frac{1}{4}$. For us the full range $\varepsilon \in [0,1]$ is needed.

Cutoff := sharp transition in convergence to stationarity

Def. $\{\{\eta_t^N : t \geq 0\}\}_{N\in\mathbb{N}}$ is said to exhibit **total variation cutoff** at times $\{t_N\}_{N\in\mathbb{N}}$ if:

- For every $\varepsilon \in (0,1)$, $\displaystyle\lim_{N\to\infty} \frac{t_{\text{mix}}^N(\varepsilon)}{t_N} = 1.$
- Equivalently, $\displaystyle\lim_{N\to\infty} d_N(\kappa t_N) = \begin{cases} 1, & \text{if } \kappa < 1, \\ 0, & \text{if } \kappa > 1. \end{cases}$





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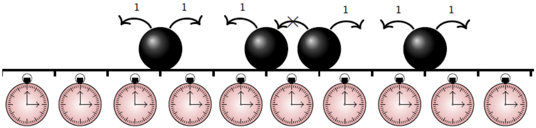
The exclusion process

- *Informally:* Lay down k particles on a connected graph $G = (V, E)$. Let the particles move according to random walk rules, subject to the **exclusion rule**: no two particles may occupy the same vertex at any given time.



- This is a MC $\{\eta_t : t \geq 0\}$ with state space $\{0,1\}^V$. Total particle number is conserved.
- Any product Bernoulli measure $\bigotimes_{x \in V} \mathrm{Bern}(\alpha)$ of constant density $\alpha \in [0,1]$ is stationary for the process.

The exclusion process

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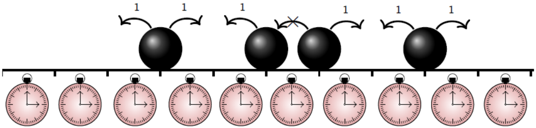
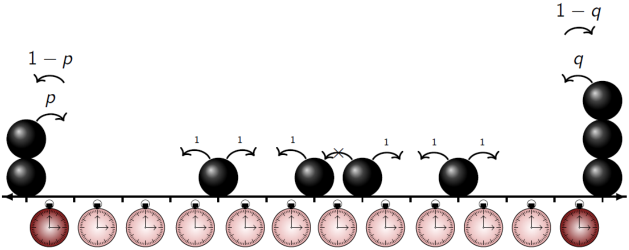


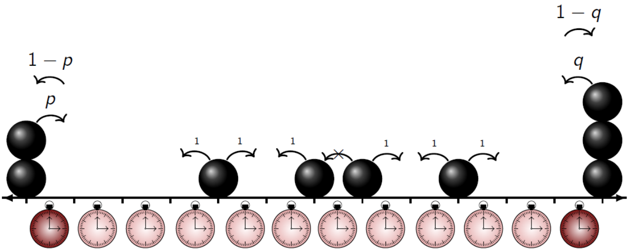
- **Scaling limit**

  Take $G_N = \{0, \frac{1}{N}, \frac{2}{N}, \dots, 1\}$ to be the discrete interval, and define the exclusion process on G_N. Accelerate the process by N^2 (diffusive time scaling, RW $\to$ BM).

Bulk exclusion + boundary reservoirs



Bulk exclusion + boundary reservoirs



The cutoff problem for exclusion on the d-dim lattice

- $d = 1$ Cutoffs have been established in several **exclusion** models and the related **adjacent transposition shuffle**.
  [Wilson '04; Oliveira '13; Lacoin '16, '17; Labbé–Lacoin '19, '20; Nam–Nestoridi '19; Gantert–Nestoridi–Schmid '20]
  Proofs take advantage of special properties of 1D particle systems: height function representations, stochastic monotonicity, censoring inequality, ...
- $d \geq 2$ Lower bound on mixing time ✓. Upper bound ? [off by 2×]
  Tools specific to $d = 1$ do not generalize to higher dimensions.

Good observables for exclusion processes

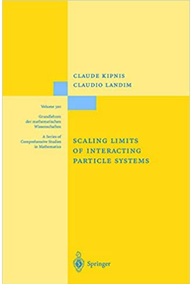
Let $F : V_N \to \mathbb{R}$ be a test function (from a suitable Banach space).

Empirical density

$$\pi_t^N(F) = \frac{1}{|V_N|} \sum_{x \in V_N} \eta_{N^2 t}^N(x) F(x).$$

Reason: To obtain a **L**aw of **L**arge **N**umbers (LLN).
$\pi_t^N \Rightarrow \pi_t$, where $\frac{d\pi_t}{dx} = \rho_t$ solves the heat equation $\partial_t \rho_t = \Delta \rho_t$.

Mean density $\rho_t^N(x) := \mathbb{E}_{\mu_N}[\eta_t^N(x)]$.



Density fluctuation field

$$\mathcal{Y}_t^N(F) = \frac{1}{\sqrt{|V_N|}} \sum_{x \in V_N} \left(\eta_{N^2 t}^N(x) - \rho_{N^2 t}^N(x) \right) F(x).$$

Reason: To obtain a **C**entral **L**imit **T**heorem (CLT).
$\mathcal{Y}_t^N \Rightarrow \mathcal{Y}_t$, an Ornstein-Uhlenbeck (Gaussian) process.

- To prove scaling limits, need to consider *all* F in the said Banach space.
- To prove cutoff, suffice to take $F = \psi_1^N$, the eigenfunction corresponding to the smallest nonzero eigenvalue of $-\Delta_N$.

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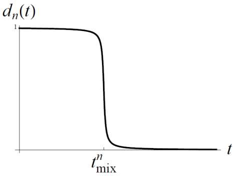
Cutoffs for 1D symmetric exclusion

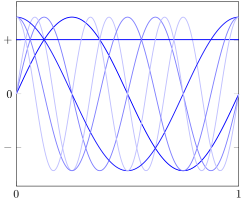
Discrete interval $\{0, \frac{1}{N}, \frac{2}{N}, \dots, 1\}$
Endpoint boundary condition: Open (Dirichlet), Closed (Neumann), Periodic.

Boundary condition	*Cutoff times $N^2 t_N$*	*#1 proof*
	$\frac{N^2 \log N}{2\pi^2}$	[Lacoin '16]
	$\frac{N^2 \log N}{2(2\pi)^2}$	[Lacoin '16, '17]
	$\frac{N^2 \log N}{2(\pi/2)^2}$	[Gantert–Nestoridi–Schmid '20]
	$\frac{N^2 \log N}{2\pi^2}$	**[C.–Jara–Marinho '20+]**

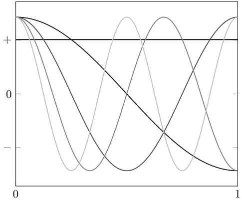
Each purple value is the smallest nonzero eigenvalue of $-u'' = \lambda u$ on $[0,1]$ with the appropriate boundary condition: $t_N = \dfrac{\log N}{2\lambda_1}$.



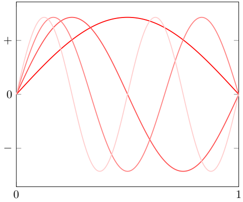
1D Laplacian eigenfunctions: Sines and cosines!



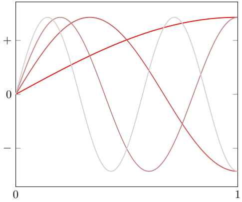
(a) Periodic b.c.



(b) Closed (Neumann) b.c.



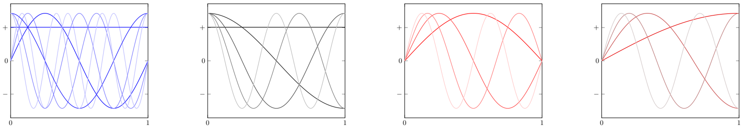
(c) Open (Dirichlet) b.c.



(d) Open at $\{0\}$, Closed at $\{1\}$

Taught in undergrad (P)DE courses! (I did this for an intro engineering DiffEq course at Cornell in 2010!)

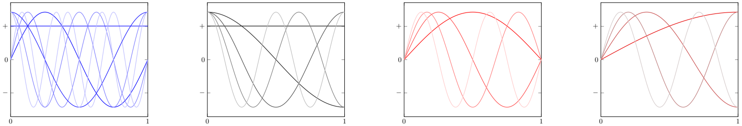
1D **continuous** Laplacian eigensolutions



Unit interval $[0,1]$, $-\Delta u := -u''$.
Endpoint boundary condition: Open (Dirichlet), Closed (Neumann), Periodic.

Boundary condition	*Eigenvalue* λ_k	*Eigenfunction* $\psi_k(x)$	*Index & range*
	$(2k\pi)^2$	$\cos(2k\pi x)$, $\sin(2k\pi x)$	$k \in \mathbb{N} \cup \{0\}$
	$(k\pi)^2$	$\cos(k\pi x)$	$k \in \mathbb{N} \cup \{0\}$
	$(k\pi)^2$	$\sin(k\pi x)$	$k \in \mathbb{N}$
	$(k\pi/2)^2$	$\sin\left(\frac{k\pi x}{2}\right)$	$k \in 2\mathbb{N} - 1$

1D **discrete** Laplacian eigensolutions



Discrete interval $\{0, \frac{1}{N}, \frac{2}{N}, \dots, 1\}$, $(-\Delta_N u)(x) := N^2 \left[2u(x) - u(x+\frac{1}{N}) - u(x - \frac{1}{N})\right]$.
Endpoint boundary condition: Open (Dirichlet), Closed (Neumann), Periodic.

Boundary condition	*Eigenvalue* λ_k^N	*Eigenfunction* $\psi_k^N(x)$ $(x \in \{0, \frac{1}{N}, \frac{2}{N}, \dots, 1\})$	*Index & range*
	$2N^2\left(1-\cos\left(\frac{2k\pi}{N}\right)\right)$	$\cos(2k\pi x)$, $\sin(2k\pi x)$	$k \in \{0, 1, \dots, N-1\}$ (*Note:* $\lambda_k^N = \lambda_{N-k}^N$)
	$2N^2\left(1-\cos\left(\frac{k\pi}{N}\right)\right)$	$\cos(k\pi x)$	$k \in \{0, 1, \dots, N\}$
	$2N^2\left(1-\cos\left(\frac{k\pi}{N}\right)\right)$	$\sin(k\pi x)$	$k \in \{1, 2, \dots, N\}$
	$2N^2\left(1-\cos\left(\frac{k\pi}{2N}\right)\right)$	$\sin\left(\frac{k\pi x}{2}\right)$	$k \in \{1, 3, \dots, 2N-1\}$

Spectral convergence: For each k, $\lambda_k^N \xrightarrow[N\to\infty]{} \lambda_k$, and $\psi_k^N \xrightarrow[N\to\infty]{} \psi_k$ in $C([0,1])$.

Cutoffs for d-dim symm. exclusion with open boundaries NEW!

Take $I_1 \times I_2 \times \ldots \times I_d$, where each $I_j \in \{\mathrm{P}, \mathrm{C}, \mathrm{O}, \mathrm{OC}\}$. Use separation of variables!

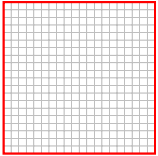
$$\psi_{\mathbf{k}}^{(N)}(x_1, \ldots, x_d) = \prod_{j=1}^{d} \psi_{k_j}^{(N)}(x_j), \qquad \boldsymbol{\lambda}_{\mathbf{k}}^{(N)} = \sum_{j=1}^{d} \lambda_{k_j}^{(N)}.$$

Cutoffs established
[C.–Jara–Marinho '20+]
at times

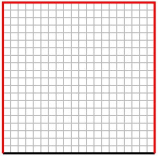
$$\mathcal{T}_N t_N = \frac{N^2 \log(N^d)}{2\lambda_1}$$

assuming the cube has an open codim-1 boundary.

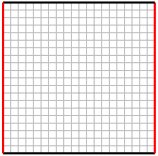
Examples for $d = 2 \longrightarrow$



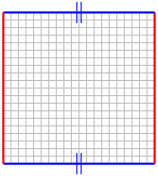
(a) $\lambda_1 = \pi^2 + \pi^2$



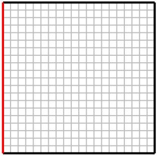
(b) $\lambda_1 = \pi^2 + (\pi/2)^2$



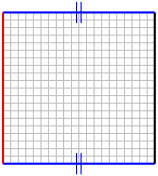
(c) $\lambda_1 = \pi^2 + 0$



(d) $\lambda_1 = \pi^2 + 0$



(e) $\lambda_1 = (\pi/2)^2 + 0$



(f) $\lambda_1 = (\pi/2)^2 + 0$

Cutoffs for symm. exclusion on graphs with open boundaries

Basic idea

Let $(K, d, \mathfrak{m})$ be a compact metric measure space with boundary ∂K equipped with a normalized surface measure $\mathfrak{s}$.

Approximate $(K, d, \mathfrak{m}, \partial K, \mathfrak{s})$ by an increasing family of bounded-degree graphs $\{G_N = (V_N, E_N)\}_{N\in\mathbb{N}}$, each having a boundary vertex set $\partial V_N \subset V_N$.

Assumption 1 (Geometric convergence).

(a) For every $N \in \mathbb{N}$, $V_N \subseteq K$ and $\partial V_N \subseteq \partial K$.

Moreover, as $N \to \infty$:

(b) $|\partial V_N|/|V_N| \to 0$.

(c) $\mathfrak{m}_N := \frac{1}{|V_N|} \sum_{x\in V_N} \delta_x$ converges weakly to $\mathfrak{m}$.

(d) $\mathfrak{s}_N := \frac{1}{|\partial V_N|} \sum_{a\in\partial V_N} \delta_a$ converges weakly to $\mathfrak{s}$.

Cutoffs for symm. exclusion on graphs with open boundaries

Exclusion process induced Laplacian

$\{\mathcal{T}_N\}_N$ is the diffusive time scale $\uparrow \infty$.

$$(\Delta_N f)(x) = \mathcal{T}_N \sum_{\substack{y \in V_N \\ y \sim x}} (f(y) - f(x)) - \mathcal{T}_N \lambda_{\Sigma,N}(x) f(x) \mathbb{1}_{\{x \in \partial V_N\}}, \qquad x \in V_N.$$

The operator $-\Delta_N$ is self-adjoint on $L^2(\mathfrak{m}_N)$. Denote the $L^2(\mathfrak{m}_N)$-orthonormal eigensolutions of $-\Delta_N$ by $\{(\lambda_i^N, \psi_i^N)\}_i$, where $0 < \lambda_1^N < \lambda_2^N \leq \lambda_3^N \leq \dots$.

Assumption 2 (Spectral convergence).

(a) There exist $\{\lambda_i\}_{i=1}^\infty \subseteq \mathbb{R}_+$ such that $\lim_{N\to\infty} \lambda_i^N = \lambda_i$ for each $i \in \mathbb{N}$.

(b) There exist $\{\psi_i\}_{i=1}^\infty \subseteq C(K)$ such that $\psi_i^N \to \psi_i$ in $C(K)$ for each $i \in \mathbb{N}$.

(c) ψ_1 is Lipschitz continuous on K.

(d) Each ψ_i has bounded normal derivative on ∂K.

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The operator $-\Delta_N$ is self-adjoint on $L^2(\mathfrak{m}_N)$. Denote the $L^2(\mathfrak{m}_N)$-orthonormal eigensolutions of $-\Delta_N$ by $\{(\lambda_i^N, \psi_i^N)\}_i$, where $0 < \lambda_1^N < \lambda_2^N \le \lambda_3^N \le \dots$.

Set

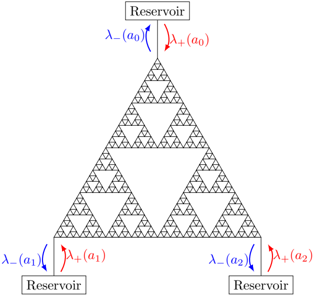
$$t_N := \frac{\log |V_N|}{2\lambda_1^N},$$

$$\kappa^* := \sup\left\{ \kappa > 0 : \overline{\lim_{N\to\infty}} \frac{|V_N|^\kappa}{\mathcal{T}_N |\partial V_N|} \sum_{i=1}^{|V_N|} \frac{|\int \psi_i^N \, d\mathfrak{m}_N|}{\lambda_i^N} = 0 \right\}.$$

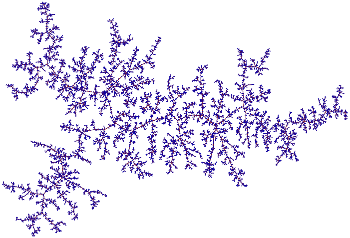
Cutoff Theorem [C.–Jara–Marinho '20+].

Suppose $\kappa^* > 1$. Then for every $\varepsilon \in (0,1)$, $\lim_{N\to\infty} \frac{t^N_{\rm mix}(\varepsilon)}{t_N \mathcal{T}_N} = 1$.

Cutoff examples: non-lattice graphs NEW!



(a) Sierpinski gasket



(b) Aldous' continuum random tree

Geometric convergence ✓
Spectral convergence ✓ [Barlow–Perkins '89, Kigami '90s, ...; Croydon-Hambly '08]

Cutoff can also be established on d-fold product of these graphs.

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Coupling

Couple the following three MCs:

- $\eta_t^{1,N}$ - original exclusion process, initialized from η.
  Boundary rate: $\lambda_{+,N}(a)$ [in], $\lambda_{-,N}(a)$ [out].
- $\eta_t^{2,N}$ - indep. copy of $\eta_t^{1,N}$, initialized from η'.
  Boundary rate: $\lambda_{+,N}(a)$ [in], $\lambda_{-,N}(a)$ [out].
- ξ_t^N - indep. copy of $\eta_t^{1,N}$, initialized from η.
  Boundary rate: 0 [in], $\lambda_{+,N}(a) + \lambda_{-,N}(a)$ [out]. (pure annihilation)

$\rightarrow$ Same bulk dynamics; boundary dynamics differ between $\{\eta_t^{1,N}, \eta_t^{2,N}\}$ and ξ_t^N.

Let

- $\eta_{\rm full}$ denote the all-1 config: $\eta_{\rm full} \equiv 1$. Initialize from the fully occupied config.
- $T_N := \inf\{t \geq 0 : \xi_t^N(x) = 0 \quad \forall x \in V_N\}$. #1 time the graph is empty of particles.

Prop. $d_N(t) = \mathbb{P}_{\eta_{\rm full}}[T_N > t]$.

From this point on, the analysis is performed on this worst-case model.

Lower bound on mixing times: Wilson's method

Well-known method from [Wilson '04].

- Use the empirical density observable
$$\pi_t^N(\psi_1^N) = \frac{1}{|V_N|} \sum_{x \in V_N} \eta^N_{\mathcal{T}_N t}(x)\psi_1^N(x).$$
- Apply Dynkin's formula: $\exists$ martingale $\{\mathcal{M}_t^N : t \geq 0\}$ s.t.
$$\pi_t^N(\psi_1^N) = \pi_0^N(\psi_1^N)e^{-\lambda_1^N t} + \mathcal{M}_t^N.$$
- Compute the mean and the variance of $\pi_t^N(\psi_1^N)$, deduce that there exists $c > 0$ s.t. for every $t \geq 0$ and every $N \in \mathbb{N}$,
$$d_N(t\mathcal{T}_N) \geq 1 - \frac{ce^{2\lambda_1^N t}}{|V_N|}.$$

This implies that for any $\kappa < 1$, $d_N(\kappa t_N \mathcal{T}_N) \xrightarrow[N\to\infty]{} 1$ (desired lower bound).

Upper bound on mixing times: the "cutoff martingale" method NEW!

- Use the density fluctuation field observable, suitably rescaled:
  (mean zero) **Cutoff martingale**
  $$\mathcal{X}_\kappa^N(\psi_1^N) = |V_N|^{\frac{\kappa}{2}-1} \sum_{x\in V_N} (\eta^N_{\kappa t_N \mathcal{T}_N}(x) - \rho^N_{\kappa t_N \mathcal{T}_N}(x))\psi_1^N(x) \qquad \left[t_N = \frac{\log|V_N|}{2\lambda_1^N}\right]$$
- On the one hand, by expanding ρ_t^N in a spectral series, we find that w.p. 1, $\forall \kappa \geq 0$,
  $$\mathcal{X}_\kappa^N(\psi_1^N) = |V_N|^{\frac{\kappa}{2}-1} \sum_{x\in V_N} \eta^N_{\kappa t_N \mathcal{T}_N}(x)\psi_1^N(x) - \int \psi_1^N \, d\mathfrak{m}_N.$$
  If $\kappa t_N \mathcal{T}_N$ is the time that all particles are annihilated (reach stationarity), then $\chi_\kappa^N(\psi_1^N) = \Theta_N(1)$ w.p. 1.
- On the other hand, a laborious computation shows that for every $\kappa > 1$,
  $$\lim_{N\to\infty} \mathbb{E}_{\mu_{\text{full}}}[\chi_\kappa^N(\psi_1^N)]^2 = \infty$$
  Laborious computation = analysis of the mean quadratic variation ($\mathbb{E}$QV) of the cutoff MG. $\mathbb{E}$QV is expanded in a complete Fourier series, then simplified using Dirichlet forms and Γ-calculus. We also need the negativity of the two-point correlation function in the exclusion process.
- So all particles must have been annihilated by time $t_N\mathcal{T}_N$. *i.e.*, for any $\kappa > 1$, $d_N(\kappa t_N \mathcal{T}_N) \xrightarrow[N\to\infty]{} 0$ (desired upper bound). Q.E.D.

Outline

Motivations

Convergence of Markov chains

The cutoff phenomenon

The exclusion process on graphs with boundaries

Cutoffs for exclusion processes

Proof ideas

Thank you for listening!

Cutoffs for exclusion with closed/periodic boundaries

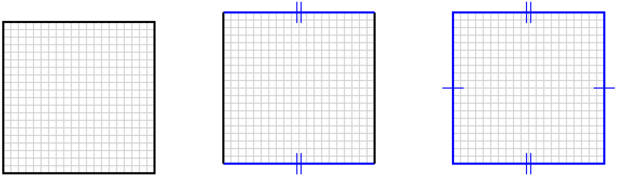
[C.–Marinho '20+]
Adapting the cutoff MG method to prove cutoffs for graphs with closed/no boundaries.
Works in any dimension d.

- A revised coupling argument.
- A revised cutoff MG which removes the nonzero stationary density, and therefore captures the fluctuations about stationarity.
- Analysis of the cutoff MG is similar to the open boundary case.

Cutoffs at times

$$\mathcal{T}_N t_N = \frac{N^2 \log(N^d)}{2\lambda_1}$$

Examples for $d = 2 \longrightarrow$



(g) $\lambda_1 = \pi^2 + 0$ (h) $\lambda_1 = \pi^2 + 0$ (i) $\lambda_1 = (2\pi)^2 + 0$

Open questions: Can the cutoff MG method be applied to prove the cutoff window? What about other prob. models on graphs, such as asymmetric exclusion processes?