The cutoff phenomenon for exclusion processes on graphs with open boundaries

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This is based on joint work with

Milton Jara
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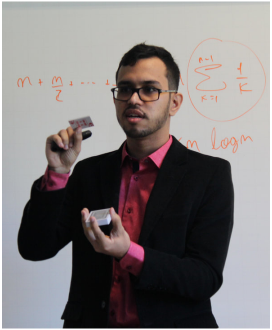


Rodrigo Marinho
(Técnico Lisboa)

Stay tuned for our preprint coming soon on arXiv!

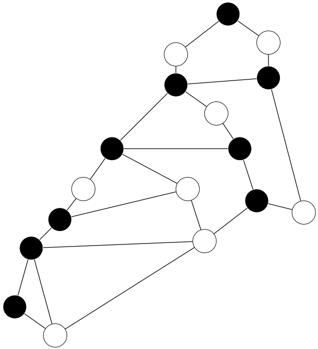
Outline

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?

Outline

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

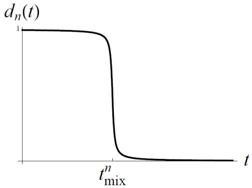
$$d(t) := \sup_{x\in\Omega} \|P_t(x,\cdot)-\pi\|_{\mathrm{TV}} = \sup_{x\in\Omega} \|(e^{tQ}P_0)(x,\cdot)-\pi\|_{\mathrm{TV}}$$

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

Outline

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.
- $d_N(t) := \sup_{\eta\in\Omega_N} \|\mathbb{P}_\eta(\eta_t^N \in \cdot) - \pi^N\|_{\mathrm{TV}}$: distance to stationarity
- A typical graph of $t \mapsto d_N(t)$ looks likes this:

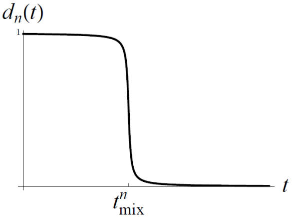


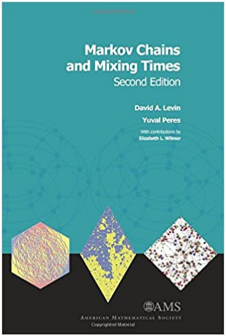
- $t_{\mathrm{mix}}^N(\varepsilon) := \inf\{t \geq 0 : d_N(t) \leq \varepsilon\}$. ε-mixing time.
Some books fix $\varepsilon = \frac{1}{4}$. For us the full range $\varepsilon \in [0, 1]$ is needed.

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

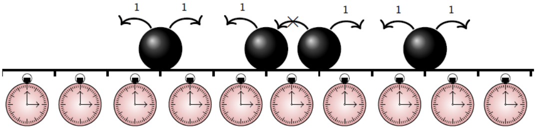




Outline

The exclusion process

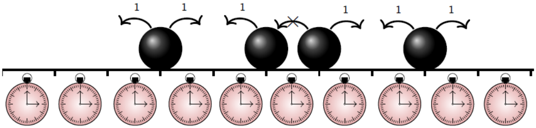
- *Informally:* Lay down k particles on a connected graph $G = (V, E)$. Let the particles move according to random walk rules, subject to the **exclusion rule**: no two particles may occupy the same vertex at any given time.



- 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.

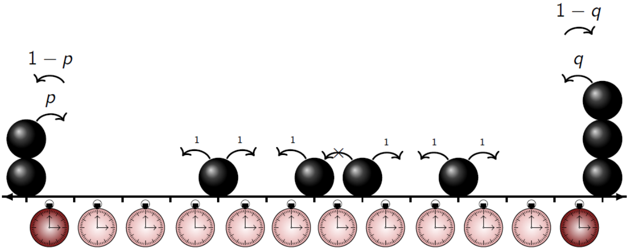
The exclusion process

- *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.

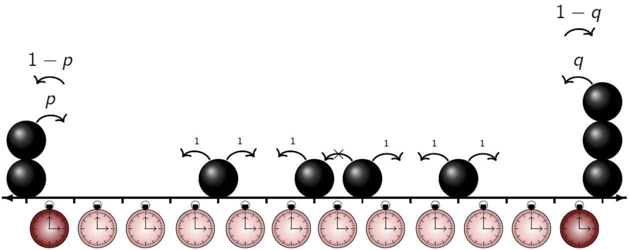


- **Scaling limit**
  Take $G_N = \{0, \frac{1}{N}, \frac{2}{N}, \dots, 1\}$ to be the discrete interval, and define the exclusion process on G_N. Accelerate the process by N^2 (diffusive time scaling, RW $\to$ BM).

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.

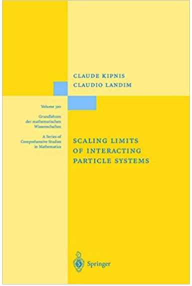
Good observables for exclusion processes

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

Empirical density

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

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

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

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 $-\Delta_N$.

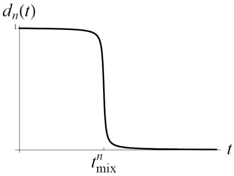
Outline

Cutoffs for 1D symmetric exclusion

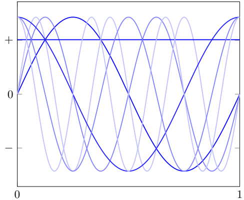
Discrete interval $\{0, \frac{1}{N}, \frac{2}{N}, \ldots, 1\}$
Endpoint boundary condition: Open (Dirichlet), Closed (Neumann), Periodic.

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

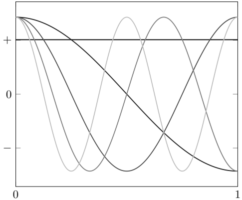
Each purple value is the smallest nonzero eigenvalue of $-u'' = \lambda u$ on $[0, 1]$ with the appropriate boundary condition: $t_N = \dfrac{\log N}{2\lambda_1}$.



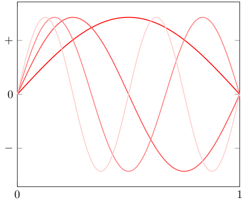
1D Laplacian eigenfunctions: Sines and cosines!



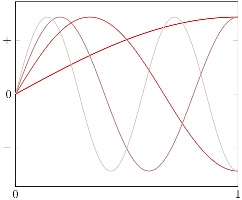
(a) Periodic b.c.



(b) Closed (Neumann) b.c.



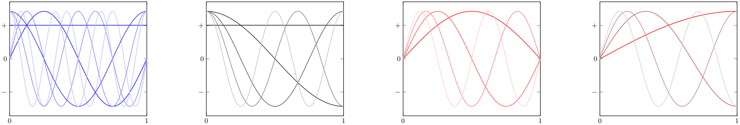
(c) Open (Dirichlet) b.c.



(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!)

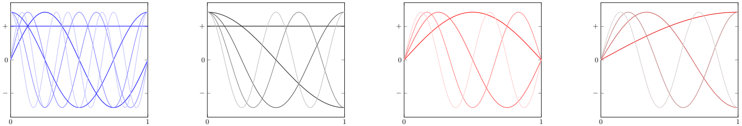
1D **continuous** Laplacian eigensolutions



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 $I_j \in \{P, C, O, OC\}$. Use separation of variables!

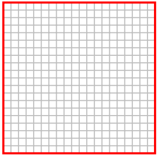
$$\boldsymbol{\psi}_{\mathrm{k}}^{(N)}(x_1, \ldots, x_d) = \prod_{j=1}^{d} \psi_{k_j}^{(N)}(x_j), \qquad \boldsymbol{\lambda}_{\mathrm{k}}^{(N)} = \sum_{j=1}^{d} \lambda_{k_j}^{(N)}.$$

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

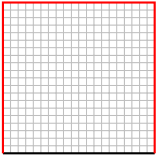
$$\mathcal{T}_N t_N = \frac{N^2 \log(N^d)}{2\lambda_1}$$

assuming the cube has an open codim-1 boundary.

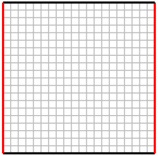
Examples for $d = 2 \longrightarrow$



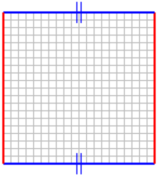
(a) $\lambda_1 = \pi^2 + \pi^2$



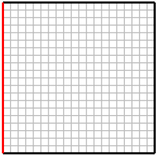
(b) $\lambda_1 = \pi^2 + (\pi/2)^2$



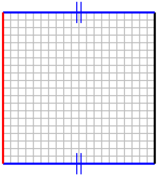
(c) $\lambda_1 = \pi^2 + 0$



(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.

Cutoffs for symm. exclusion on graphs with open boundaries

Exclusion process induced Laplacian

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Set

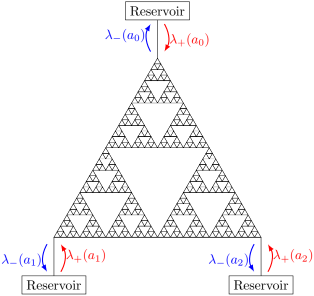
$$t_N := \frac{\log |V_N|}{2\lambda_1^N},$$

$$\kappa^* := \sup\left\{\kappa > 0 : \overline{\lim_{N\to\infty}} \frac{|V_N|^{\kappa-1}}{|\partial V_N|} \sum_{i=1}^{|V_N|} \left(\sup_{b\in\partial V_N} |\partial_N^\perp \psi_i^N(b)|\right) \frac{|\int \psi_i^N \, d\mathfrak{m}_N|}{\lambda_i^N} \sum_{a\in\partial V_N} (\psi_1^N(a))^2 = 0\right\}.$$

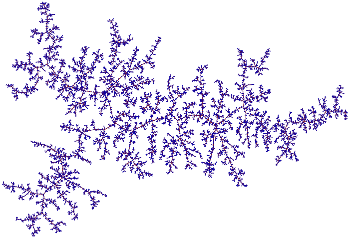
Cutoff Theorem [C.–Jara–Marinho '20+].

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

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.

Outline

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 $N \in \mathbb{N}$,

$$d_N(t\mathcal{T}_N) \geq 1 - \frac{c e^{2\lambda_1^N t}}{|V_N|}.$$

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 $\kappa > 1$,

$$\lim_{N\to\infty} \mathbb{E}_{\mu_{\rm full}}[\chi_\kappa^N(\psi_1^N)]^2 = \infty$$

  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

Cutoffs for exclusion with closed/periodic boundaries

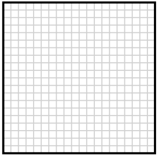
[C.–Marinho '20+]
Adapting the cutoff MG method to prove cutoffs for graphs with closed/no boundaries.
Works in any dimension d.

- 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.

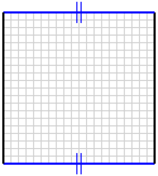
Cutoffs at times

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

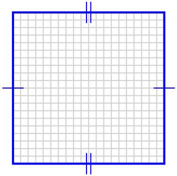
Examples for $d = 2 \longrightarrow$



(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?