# Long-time behavior of some Markov processes, and application to stochastic algorithms

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# Contents

# Gibbs measure in Statistical physics

- Gas of $N \gg 1$ particles, temperature $T = \beta^{-1}$, in domain $D \subset \mathbb{R}^3$.
- Potential:
$$U : D^{3N} \to \mathbb{R}_+.$$
- Hamiltonian:
$$H(x, y) = U(x) + \frac{|y|^2}{2}.$$

# Gibbs measure in Statistical physics

- Gas of $N \gg 1$ particles, temperature $T = \beta^{-1}$, in domain $D \subset \mathbb{R}^3$.
- Potential:
$$U : D^{3N} \to \mathbb{R}_+.$$
- Hamiltonian:
$$H(x, y) = U(x) + \frac{|y|^2}{2}.$$
- Gibbs measure:
$$\mu_\beta(\mathrm{d}x, \mathrm{d}y) = Z^{-1} e^{-\beta H(x,y)} \mathrm{d}x\mathrm{d}y.$$
- Goal: numerical simulation of
$$\mu_\beta(f) := \mathbb{E}(f(X, Y)), \quad (X, Y) \sim \mu_\beta.$$

# Example

- Lennard-Jones potential:

$$U(x) = \sum_{1 \leqslant i \neq j \leqslant N} W(|x_i - x_j|), \quad W(r) = 4\varepsilon \left( \frac{\sigma}{r^{12}} - \frac{\sigma}{r^6} \right).$$

Argon: $\varepsilon = 1.66 * 10^{-21} J$, $\sigma = 3.405 \times 10^{-10} m$.

Pressure:

$$P = \mu_\beta(f_P), \qquad f_P(x,y) = \frac{1}{3|D|} \sum_{i=1}^{N} \left( \frac{y_i^2}{m} - x_i \cdot \nabla_{x_i} U(x) \right).$$

- Statistics,. . . :

$$\nu_\beta(\mathrm{d}x) = Z'^{-1} e^{-\beta U(x)} \mathrm{d}x.$$

# Monte-Carlo method

$E$ state space, $(Z_t)_{t\geqslant 0}$ Markov process.

## Semi-group

$$P_t f(z) := \mathbb{E}_z\left(f(Z_t)\right).$$

## Definition

$Z$ is ergodic / $\eta$ if:

$$\frac{1}{t}\int_0^t \delta_{Z_s} \mathrm{d}s \underset{t\to\infty}{\rightharpoonup} \eta, \text{ a.s.}$$

$Z$ converges in law towards $\eta$ if $\forall f$ continuous bounded:

$$P_t f \underset{t\to\infty}{\to} \eta(f).$$

Simulation of a single trajectory

$$\frac{1}{t}\int_0^t f(Z_t) \approx \eta(f).$$

Simulation of a large number of $(Z_t)$:

$$\frac{1}{n}\sum_{k=1}^{n} f(Z_t^k) \approx \mathbb{E}\left(f(Z_t)\right) \approx \eta(f).$$

# Monte-Carlo method

- **Overdamped Langevin Process** :

$$\mathrm{d}X_t = -\nabla U(X_t)\mathrm{d}t + \sqrt{2\beta^{-1}}\mathrm{d}B_t.$$

# Monte-Carlo method

- **Overdamped Langevin Process** :

$$\mathrm{d}X_t = -\nabla U(X_t)\mathrm{d}t + \sqrt{2\beta^{-1}}\mathrm{d}B_t.$$

- **Kinetic Langevin Process** :

$$\begin{cases} \mathrm{d}X_t = Y_t \mathrm{d}t \\ \mathrm{d}Y_t = -\nabla U(X_t)\mathrm{d}t - \gamma Y_t \mathrm{d}t + \sqrt{2\gamma\beta^{-1}}\mathrm{d}B_t. \end{cases}$$

- **Bouncy particle sampler** :

$$\begin{cases} \mathrm{d}X_t = Y_t \mathrm{d}t \\ Y \to y - 2y \cdot \nabla U(x) \nabla U(x)/|\nabla U(x)|^2 \text{ at rate } (y \cdot \nabla U(x))_+. \\ Y \text{resampled according to a Gaussian with variance } \beta \text{ at rate } a > 0. \end{cases}$$

# Numerical scheme

Particles with Lennard-Jones interaction, Coulomb interaction.
A (first-order) splitting scheme:

$$\begin{cases} \tilde{X}_{n+1} = \tilde{X}_n + \delta \tilde{Y}_{n+1}, \\ \tilde{Y}_{n+1} = \tilde{Y}_n - \delta \nabla U(\tilde{X}_n) - \delta\gamma \tilde{Y}_n + \sqrt{2\gamma\beta^{-1}\delta}\, G_n. \end{cases}$$

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$\forall f \notin L^1_{loc}$:

$$\mathbb{E}\left(f(\tilde{X}_n, \tilde{Y}_n)\right) = \infty, \quad \forall n \geqslant 2.$$

# Numerical scheme

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$\forall f \notin L^1_{loc}$:

$$\mathbb{E}\left(f(\tilde{X}_n, \tilde{Y}_n)\right) = \infty, \quad \forall n \geqslant 2.$$

A (first-order) splitting scheme with rejection:

$$\begin{cases} \bar{X}_{n+1} = \bar{X}_n + \mathbb{1}_{E_\delta(\bar{X}_n, \bar{Y}_n, G_n) \in \mathcal{H}_d} \delta \bar{Y}_{n+1}, \\ \bar{Y}_{n+1} = \bar{Y}_n + \mathbb{1}_{E_\delta(\bar{X}_n, \bar{Y}_n, G_n) \in \mathcal{H}_d} \left(-\delta \nabla U(\bar{X}_n) - \delta\gamma \bar{Y}_n + \sqrt{2\gamma\beta^{-1}\delta} G_n\right). \end{cases}$$

$$\mathcal{H}_d = \left\{ V \leqslant e^{b\delta^{-l}} \right\}, V \text{ some Lyapunov function.}$$

# Weak error extension

Particles with Lennard-Jones interaction, Coulomb interaction.

**Theorem (J., accepted in ESAIM: M2AN)**

- $\forall f$ test function, $t = n\delta \geqslant 0$, $\exists (C_i)_i$ explicit such that:

$$\mathbb{E}_{(x,y)}\left(f\left(\bar{X}_n, \bar{Y}_n\right)\right) = \mathbb{E}_{(x,y)}\left(f\left(X_t, Y_t\right)\right) + C_1\delta + \cdots + C_k\delta^k + O\left(\delta^{k+1}\right).$$

- $\forall 0 < \delta < \delta_0$, $\exists$ invariant measure $\mu_{\beta,\delta}$, $\forall f \in \mathcal{F}$:

$$\lim_{n\to\infty} \frac{1}{n}\sum_{k=1}^{n} \mathbb{E}_{(x,y)}\left(f\left(\bar{X}_k, \bar{Y}_k\right)\right) = \mu_{\beta,\delta}(f).$$

- $\forall f$ test function, $\exists (D_i)_i$ explicit such that:

$$\mu_{\beta,\delta}(f) = \mu_\beta(f) + D_1\delta + \cdots + D_k\delta^k + O(\delta^{k+1}).$$

[Talay, Tubaro 90], [Talay 02], [Leimkuhler, Matthews, Stoltz 16].

# Semi-group estimates

Particles with Lennard-Jones interaction, Coulomb interaction.

**Theorem (J., accepted in ESAIM: M2AN)**

$\exists q >$, $\forall f$ test function, $\exists C, b > 0$ such that:

$$|\partial^\alpha (P_t f - \mu_\beta(f))| \leqslant C e^{-qt} e^{bH}.$$

Proof based on hypocoercivity in Sobolev spaces, [Villani, 09], [Baudoin, Gordina, Herzog 21].

$$\begin{aligned} \|h\|^2_{mH^k} &= \int_{\mathcal{X}} h^2 V_k \mathrm{d}\mu_\beta \\ &+ \int_{\mathcal{X}} \sum_{p=1}^{r} \left( \sum_{i=0}^{p-1} \omega_{i,p} |\nabla_x^i \nabla_y^{p-i} h|^2 + \omega_{p,p} |\left(\nabla_x^p - \xi \nabla_x^{p-1} \nabla_y\right) h|^2 \right) \\ &\qquad (1 + \varepsilon_p V_{k-p}) \, \mathrm{d}\mu_\beta. \end{aligned}$$

# The velocity jump Langevin process

Write

$$U = \underbrace{U_0}_{\text{grad easy to compute}} + \overbrace{U_1}^{\text{grad hard to compute}} .$$

## Generator velocity jump Langevin process

$$L = y \cdot \nabla_x - \nabla U_0 \cdot \nabla_y - \gamma y \cdot \nabla_x + \gamma \beta^{-1} \Delta_y + L_J$$

$$L_J h(x,y) := \sum_{i=1}^{d} \lambda_i(x,y) \int_{\mathbb{R}^d} \left(h(x,y') - h(x,y)\right) q_i(x,y,\mathrm{d}y'),$$

$$\lambda_i(x,v) \int_{\mathbb{R}^d} h(x,v') q_i(x,v,\mathrm{d}v')$$

$$= \sqrt{\beta}\frac{1+\theta^2}{\theta^2}\mathbb{E}\left[h\left(x, v - \frac{2\theta}{1+\theta^2}\left(\theta v_i + G/\sqrt{\beta}\right)e_i\right)\right.$$

$$\left.\Psi\left(\sqrt{\beta}\frac{\theta \partial_i U_1(x)}{1+\theta^2}(\theta v_i + G)\right)\right].$$

# $H^k$-convergence

- $U_0 \sim$ quadratic, $\nabla U_1$ and derivatives bounded.
- $\Psi \in \mathcal{C}^\infty\left(\mathbb{R}^d, \mathbb{R}_+\right)$ is such that $\Psi'$ and all its derivative are bounded, and

$$\Psi(s) - \Psi(-s) = s.$$

**Theorem (J., Gouraud, Monmarché)**

- $\mu_\beta$ is the unique stationary measure of the velocity jump Langevin process.
- For all $k \in \mathbb{N}$, there exist $C_k, \rho_k > 0$ such that for all $f \in H^k(\mu_\beta)$ and $t \geqslant 0$

$$\|P_t f - \mu_\beta(f)\|_{H^k(\mu_\beta)} \leqslant C_k e^{-\rho_k t} \|f - \mu_\beta(f)\|_{H^k(\mu_\beta)}.$$

# Contents

# Optimisation

$$U : \mathbb{R}^d \longrightarrow \mathbb{R}_+.$$

Goal :

$$\min_{\mathbb{R}^d} U.$$

- **Molecular dynamics** :

  $U$ = energy, minima = stable states.

$$U(x_1, ...x_N) = \sum_{i<j} W(|x_i - x_j|).$$

- **Statistics** :

  $U$ = log posterior probability, minimum = maximum likelihood.

$$U(\theta) = V(\theta) + \sum_{i=1}^{n} p_\theta(X_i).$$

# Gradient descent

$$x_t' = -\nabla U(x_t).$$

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Solutions:

- Gradient descentS with random initial conditions.
- Exhaustive visit of space.

Sometimes intractable in high dimension.

# Gradient descent

$$x_t' = -\nabla U(x_t) +\text{"}\sqrt{2\beta^{-1}}B_t'\text{"}.$$

$\implies$ local minima.

Solutions:

- Gradient descentS with random initial conditions.
- Exhaustive visit of space.

Sometimes intractable in high dimension.

Solution: add noise
and use the fact that:
$\forall \varepsilon > 0$

$$\lim_{\beta\to\infty} \nu_\beta \left( U > \min_{\mathbb{R}^d} U + \varepsilon \right) = 0.$$

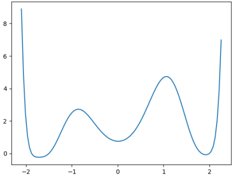


Figure: A non-convex potential

# Simulated annealing

Design stochastic process $(X_t)$ whose law is close to:

$$\nu_{\beta_t}(\mathrm{d}x) \propto e^{-\beta_t U(x)}\mathrm{d}x$$

where $\beta_t \underset{t\to\infty}{\longrightarrow} \infty$. Cooling schedule:

$$\beta_t = \frac{\ln(e^{c\beta_0} + t)}{c}.$$

# Simulated annealing

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$$\beta_t = \frac{\ln(e^{c\beta_0} + t)}{c}.$$

Largest energy barrier:

$$c^* = \sup_{x_1,x_2} E(x_1, x_2),$$

where

$$E(x_1, x_2) = \inf_{\xi} \left\{ \max_{0\leqslant t\leqslant 1} U(\xi(t)) - U(x_1) - U(x_2) \right\}.$$

[Holley, Stroock 88] [Holley, Kusuoka, Stroock 89] [Fournier, Tardif 20]

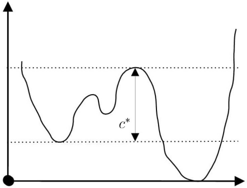
# Convergence of kinetic annealing

$$\begin{cases} dX_t = Y_t dt \\ dY_t = -\nabla U(X_t)dt - \gamma_t Y_t dt + \sqrt{2\gamma_t \beta_t^{-1}} dB_t. \end{cases}$$

**Theorem (J., Monmarché, EJP, 2022)**

$U : \mathbb{R}^d \longrightarrow \mathbb{R}_+$ smooth, $U(\infty) = \infty$, $\int_{\mathbb{R}^d} e^{-\alpha_0 U} < \infty$.

- If $c > c^*$, $H(X_t, Y_t) \to \min U$ in probability.
- If there exists $p$, bottom of a well of height greater than $c$, then $\mathbb{P}(\inf U(X_t) > U(p)) > 0$.



# Saddle point search

$$\mathrm{d}X_t = -\nabla U(X_t)\mathrm{d}t + \sqrt{2\beta^{-1}}\mathrm{d}B_t.$$

**Proposition [Freidlin , Wentzell 84]**

At low temperature, the most probable trajectory from a local minima to another passes through the index-1 saddle point with lowest energy elevation.

# Saddle point search

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At low temperature, the most probable trajectory from a local minima to another passes through the index-1 saddle point with lowest energy elevation.

$\lambda_1(x) \leqslant \lambda_2(x) \leqslant \cdots \leqslant \lambda_d(x)$ eigenvalues of $\nabla^2 U(x)$.

Idealised saddle dynamics:

$$\begin{cases} x_t' = -\left(I - 2v_1(x_t)v_1(x_t)^T\right)\nabla U(x_t) \\ \nabla^2 U(x_t)v_1(x_t) = \lambda_1(x_t)v_1(x_t). \end{cases}$$

**Proposition [Levitt, Ortner 18]**

Any critical point of $U$ is an equilibrium points for the ISD. It is stable if and only if it is a index-1 saddle point.

# The processes

- **Noisy idealised saddle dynamics**:

$$\mathrm{d}X_t = -\left(I - 2v_1(X_t)v_1(X_t)^T\right)\nabla U(X_t)\mathrm{d}t + \sqrt{2\beta^{-1}}\mathrm{d}B_t.$$

- **Idealised switched process**:

$$\mathrm{d}X_t \;=\; H_{I_t}(X_t)\mathrm{d}t + \sqrt{2\beta^{-1}}\mathrm{d}B_t,$$

where $(I_t)$ is a Poisson process on $\{0,1\}$ with jump rate $\nu > 0$ and

$$H_0(x) = -\nabla U(x)\,, \qquad H_1(x) = -(I - 2v_1(x)v_1(x)^T)\nabla U(x).$$

# Numerical result for the switched process

Mixture of Gaussians:
$U(x, y) = -\ln\left(\frac{1}{2}e^{-(x^2+y^2)} + \frac{1}{2}e^{-(x-m_x)^2-3(y-m_y)^2}\right).$

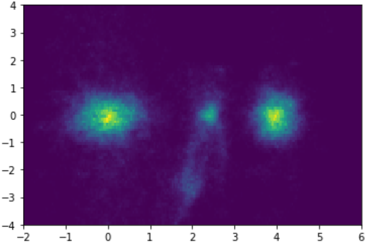

Figure: Invariant measure ISP, $\nu = 0.1$, $\beta^{-1} = 0.05$.

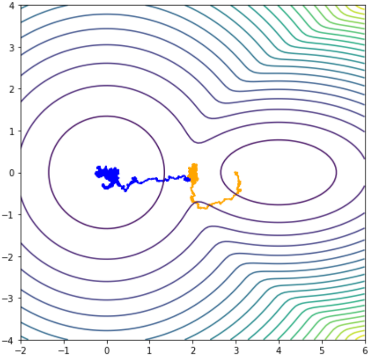

Figure: Trajectory of the switched process.

# The Lennard-Jones potential

$N = 7$ particles in dimension 2.

$$U(x_1, \dots x_N) = \sum_{i<j} W(|x_i - x_j|),$$

where $x_i \in \mathbb{R}^2$ for all $1 \leqslant i \leqslant N$, and for $r > 0$:

$$W(r) = 4\left(\frac{1}{r^{12}} - \frac{1}{r^6}\right).$$

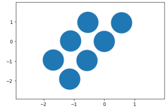


Figure: $U \approx -11,40$

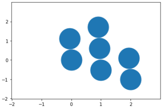


Figure: $U \approx -11,47$

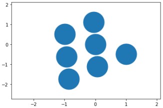


Figure: $U \approx -11,50$

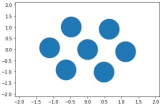

Figure: $U \approx -12,53$

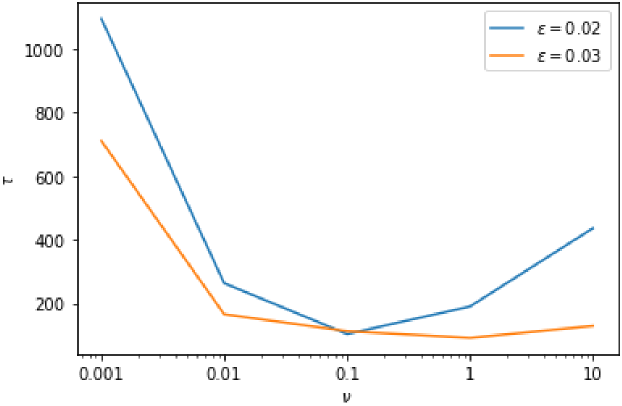


Figure: Time to visit all minima of the Lennard-Jones cluster.

# Contents

# Killed processes

$$\mathbb{P}(X_t \in \cdot) \to \mathbb{P}(X_t \in \cdot | \tau > t).$$

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$$\mathbb{P}\left(X_t \in \cdot\right) \to \mathbb{P}\left(X_t \in \cdot | \tau > t\right).$$

- **Soft killing**:

$$\tau_\lambda = \inf\left\{t \geqslant 0, E_\lambda \leqslant \int_0^t \lambda(X_s)\mathrm{d}s\right\},$$

$\lambda$: death rates, $E_\lambda$ exponential random variable.

- **Hard killing**:

$$\tau_{\partial D} = \inf\left\{t \geqslant 0, X_t \notin D\right\}.$$

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$\lambda$: death rates, $E_\lambda$ exponential random variable.

- **Hard killing**:

$$\tau_{\partial D} = \inf \left\{ t \geqslant 0, X_t \notin D \right\} .$$

Simulation of a large number of independent realisations of $(X_t)$:

$$\sum_{k=1}^n f(X_t^k) \mathbb{1}_{\tau_k > t} / \sum_{k=1}^n \mathbb{1}_{\tau_k > t} \approx \mathbb{E}\left( f(X_t) | \tau > t \right) .$$

# Fleming-Viot process

- $N$ particles $\mathbf{X} = (X^1, \cdots, X^N)$.
- Independent between death events, following the same dynamics as $X$.
- At death events, resurrect on another particles chosen uniformly at random.

# Fleming-Viot process

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- Independent between death events, following the same dynamics as $X$.
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**Empirical measure**:

$$\pi(\mathbf{X}_t) = \frac{1}{N} \sum_{i=1}^{N} \delta_{X_t^i}.$$

## Propagation of chaos

There is propagation of chaos if

$$\mu_0^N = \mu_0^{\otimes N} \implies \forall t \geqslant 0, \lim_{N \to \infty} \pi(\mathbf{X}_t) \to \mathcal{L}aw(X_t | \tau > t).$$

[Burdzy, Hołyst, Marc 00][Rousset 06][Villemonais 14]

# A softly killed diffusion

$$d\bar{X}_t = b(\bar{X}_t)dt + dB_t,\ \bar{X}_t \in \mathbb{T},\ \text{ killed at rate } \lambda.$$

**Theorem (J., Monmarché, ESAIM: P&S, 2022)**

$\exists\, c_0 > 0$ s.t. if $\lambda$ is Lipschitz with constant $L_\lambda < c_0$ then $\exists\, C > 0$ s.t. $\forall\, N \in \mathbb{N}$, $t \geqslant 0$, $\mu_0 \in \mathcal{P}(\mathbb{T}^{dN})$

$$\mathbb{E}\left(\mathcal{W}_1\left(\pi\left(\mathbf{X}_t\right), \mathbb{P}_{\mu_0}\left(X_t \in \cdot | \tau > t\right)\right)\right) \leqslant C\alpha(N),$$

where

$$\alpha(N) = \begin{cases} N^{-1/2} & \text{if } d = 1, \\ N^{-1/2}\ln(1+N) & \text{if } d = 2, \\ N^{-1/d} & \text{if } d > 2. \end{cases}$$

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$$\mathbb{E}\left(\mathcal{W}_1\left(\pi\left(\mathbf{X}_t^\delta\right), \mathbb{P}_{\mu_0}\left(X_t \in \cdot | \tau > t\right)\right)\right) \leqslant C\left(\alpha(N) + \sqrt{\delta}\right),$$

where

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# Metastable exit events

$U : \mathbb{R}^d \to \mathbb{R}_+$, $\beta \gg 1$

$$\mathrm{d}X_t = -\nabla U(X_t)\mathrm{d}t + \sqrt{2\beta^{-1}}\mathrm{d}B_t, \quad \tau_{\partial D} = \inf\left\{t \geqslant 0, X_t \notin D\right\}.$$

Suppose metastability:

$$U_0 = U(\partial D) - \min_D U > c^*,$$

$\implies$

$$\tau_{\partial D} \sim e^{\beta U_0} \underset{\beta\to\infty}{\gg} t_{mix} \approx e^{\beta c^*}.$$

## Theorem (J., Monmarché, 24)

u.s.a., $\forall \mu_0 \in \mathcal{M}^1(D)$, $\exists \beta_0 > 0$, such that $\forall \beta > \beta_0$, $N \in \mathbb{N}$, $\exists C_\beta, \eta_\beta > 0$ such that $\forall f : D \to \mathbb{R}_+$ bounded:

$$\sup_{t\geqslant 0} \mathbb{E}\left(\left|\int_D f \mathrm{d}\pi(\mathbf{X}_t) - \mathbb{E}_{\mu_0}\left(f\left(X_t\right)|\tau > t\right)\right|\right) \leqslant \frac{C_\beta \|f\|_\infty}{N^{\eta_\beta}}.$$

# Convergence through coupling

**Wasserstein distances on compact set [Villani 09]**

$d_N$ be a distance on $E^N$. $\forall\ \mu, \nu \in \mathcal{M}^1(E^N)$:

$$W_d(\mu,\nu) = \inf\left\{\mathbb{E}\left(d(X,Y)\right), \mathcal{L}(X) = \mu, \mathcal{L}(Y) = \nu\right\}.$$

$W_d$ is a distance on $\mathcal{M}^1(E^N)$ and $(\mathcal{M}^1(E^N), W_d)$ is a complete space.

- Fix $t \geqslant 0$. $\forall x, y \in E^N$, construct $(X,Y)$ such that $\mathcal{L}(X) = \delta_x P_t^N$ and $\mathcal{L}(Y) = \delta_y P_t^N$ such that:

$$\mathbb{E}(d_N(X,Y)) \leqslant (1-c)d_N(x,y)$$

- $\implies$ $P_t^N$ is a contraction on $(\mathcal{M}_d^1(E))$.

# A high killing regime

$D$ finite/countable set, $(q(x,y))_{(x,y)\in D}$ jump rates, $\lambda_r : D \to \mathbb{R}_+$ death rates.

$N$ is fixed, $\lim_{r\to\infty} \inf_D \lambda_r = +\infty$, and $\forall x, y \in D$

$$\lim_{r\to\infty} \lambda_r(y)/\lambda_r(x) = \alpha_{x,y,\infty} \in [0,\infty].$$

Biased jump rates:

$$\tilde{q}_\infty(x,y) = \begin{cases} nq(x,y)\dfrac{\alpha_{x,y,\infty}-1}{\alpha^n_{x,y,\infty}-1} & \text{if } \alpha_{x,y,\infty} \neq 1, \\ q(x,y) & \text{otherwise.} \end{cases}$$

**Theorem (J., Lelievre, Reygner, in preparation)**

$\forall \eta \in \mathcal{M}^1_n(D)$, $\exists \bar{\eta} \in \mathcal{M}^1(D)$, $Y_0 \sim \bar{\eta}$, s.t. if $(Y_t)_{t\geqslant 0}$ is a Markov process on $D$ with jump rate $(\tilde{q}_\infty(x,y))_{(x,y)\in D}$ and initial condition $Y_0$, then $\forall t > 0$,

$$\lim_{r\to\infty} \|\mathcal{L}aw\left(\pi(\mathbf{X}^r_t)\right) - \mathcal{L}aw\left(\delta_{Y_t}\right)\|_{TV} = 0.$$

THANK YOU FOR YOUR ATTENTION