Feynman–Kac models

Stability & discretization

MCQMC 2018

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Wednesday July 4th, 2018

Situation

If *this meeting* is about

$$x-\text{Monte Carlo}$$

with

$$x \in \left\{\text{Quasi}, \text{Markov Chain}, \text{Sequential}, \text{Quantum}, \text{Hamiltonian}, \text{Multilevel}, \text{Diffusion}, \text{Langevin}, \text{Multifidelity}\ldots\right\},$$

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summarized as *Feynman–Kac models* (also known as splitting, genealogical, branching models, etc).

A rare event problem

- Consider a dynamics over $\mathcal{X} \subset \mathbb{R}^d$:

$$dX_t = b(X_t)dt + \sigma(X_t)dB_t,$$

with invariant measure μ and generator $\mathcal{L}$.

- Ergodicity: for a test function f

$$\frac{1}{t}\int_0^t f(X_s)ds \xrightarrow{t\to+\infty} \int_{\mathcal{X}} f(x)\,\mu(dx).$$

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- Idea of *large deviations*:

$$\mathbb{P}\left[\frac{1}{t}\int_0^t f(X_s)ds = a\right] \asymp \mathrm{e}^{-tI(a)},$$

where I is the *rate function*, or *generalized entropy creation*.

Duality and importance sampling

- **Donsker-Varadhan** duality [70's]: in many cases it holds

$$I(a) = \sup_{k\in\mathbb{R}} \left\{ ka - \lambda_f(k) \right\},$$

where

$$\lambda_f(k) = \lim_{t\to\infty} \frac{1}{t} \log \mathbb{E}\left[\mathrm{e}^{k\int_0^t f(X_s)ds} \right].$$

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- Similar to study, for an observable φ,

$$\Theta_t(\mu)(\varphi) = \frac{\mathbb{E}_\mu\left[\varphi(X_t)\,\mathrm{e}^{\int_0^t f(X_s)ds}\right]}{\mathbb{E}_\mu\left[\mathrm{e}^{\int_0^t f(X_s)ds}\right]}.$$

- This procedure *weights the trajectories* depending on f.

Natural questions

One may wonder:

- for which class of functions f does λ_f exists?
- under which conditions Θ_t admits a long time limit?
- how can we discretize in time for numerical purposes?
- how to sample efficiently the expectations?

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Link with filtering & Sequential Monte Carlo

In Sequential Monte Carlo/filtering, we generally consider the weighted path measure

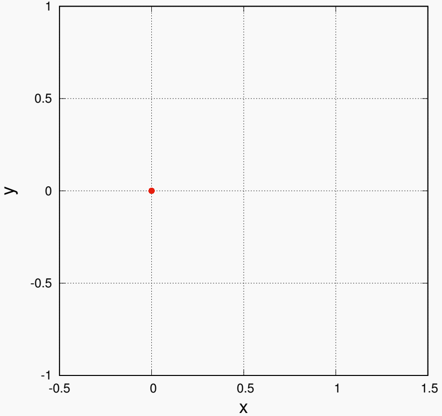
$$\mathbb{Q}_n(dx_{0:n}) = \frac{1}{L_n}\Big\{ G_0(x_0)\prod_{k=1}^{t} G_k(x_{k-1},x_k)\Big\}\mathbb{M}_0(dx_0)\prod_{k=1}^{n} M_k(x_{k-1},x_k).$$

Analogies:

- $G_k(x_{k-1},x_k) \leftrightarrow \mathrm{e}^{f(x_{k-1})}$ with «potential» f,
- $M_k \leftrightarrow Q(x,\cdot) = \mathbb{E}\big[x_k \in \cdot \,\big|\, x_{k-1} = x\big]$ homogeneous transition kernel,
- $L_n \leftrightarrow (\mathrm{e}^f Q)^n \mathbb{1} = \mathbb{E}\big[\mathrm{e}^{\sum_{k=0}^{n-1} f(x_k)}\big]$ accumulated weight up to time n (sometimes written $\gamma_n(1)$).

Numerics – Sequential Monte Carlo

- Dynamics $(x_{n+1}, y_{n+1}) = (x_n, y_n) - 0.1(x_n, y_n) + G_n \in \mathbb{R}^2$,
- Weight function $f(x, y) = x$.



The weight

$$w_m^n = \exp\left(\sum_{k=0}^{n-1} f(x_k^m)\right).$$

of particle m at time n is used for resampling (renormalization).

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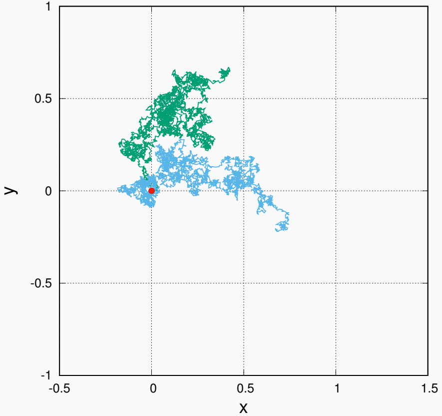

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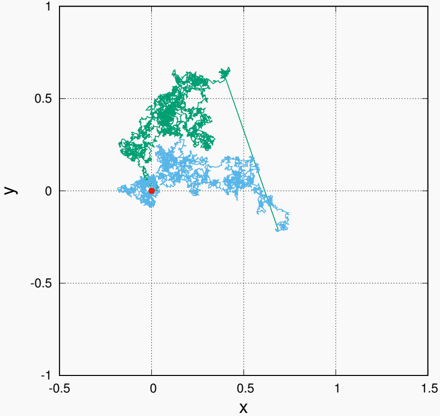

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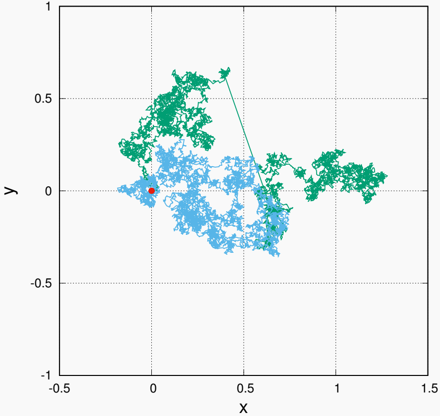

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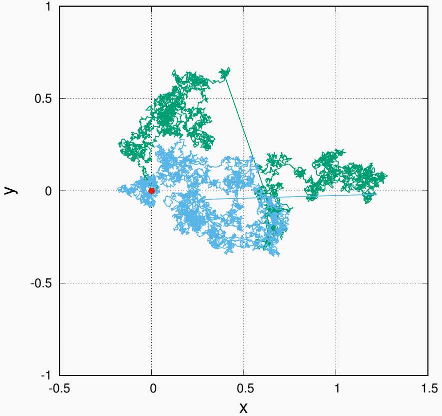

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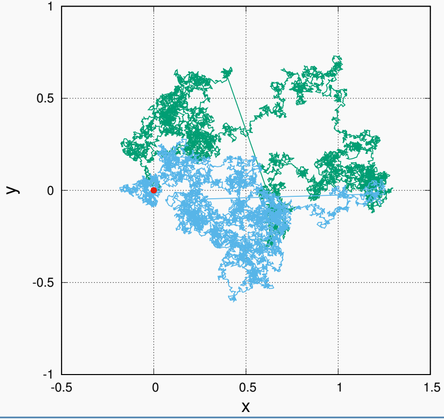

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Conclusion: the particles are selected towards the right.

Markov chains and ergodicity

A homogeneous Markov chain $(x_n)_{n\in\mathbb{N}}$ is defined through its *evolution operator* Q:

$$Q\varphi(x) := \mathbb{E}[\varphi(x_1)\,|\,x_0 = x] = \int_{\mathcal{X}} \varphi(y) Q(x, dy).$$

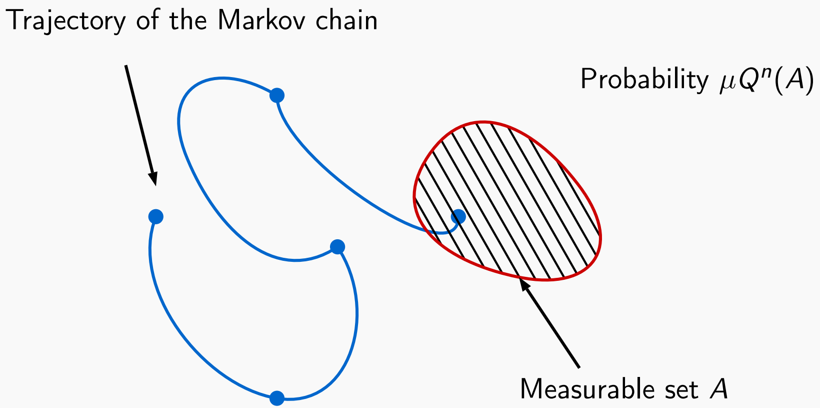
A measure $\mu^* \in \mathcal{P}(\mathcal{X})$ is *invariant* if $\forall\, A \subset \mathcal{X}$:

$$\mu^* Q(A) := \int_{\mathcal{X}} \mu^*(dx) Q(x, A) = \mu(A).$$

The process is *ergodic* when, for any initial distribution μ,

$$\mu Q^n \xrightarrow{n\to+\infty} \mu^*.$$

Big picture I



An ergodic theorem

Theorem [M. Hairer & J. Mattingly]

Assume there exist $W : \mathcal{X} \to \mathbb{R}_+$, $\gamma \in (0,1)$ and $C > 0$ such that

$$(L) \quad PW \leq \gamma W + C,$$

and $\alpha > 0$, $\eta \in \mathcal{P}(\mathcal{X})$ such that

$$(M) \quad \inf_{x \in \mathcal{C}} P(x, \cdot) \geq \alpha \eta(\cdot),$$

for $\mathcal{C}$ a large enough level set of W. Then, there exist a unique $\mu^* \in \mathcal{P}(\mathcal{X})$, $C > 0$ and $\bar{\alpha} \in (0,1)$ such that for any $\mu \in \mathcal{P}(\mathcal{X})$

$$\|P^n \mu - \mu^*\|_W \leq C \bar{\alpha}^n \|\mu - \mu^*\|_W.$$

Here: $\|f\| = \sup_{x \in \mathcal{X}} \frac{|f(x)|}{1 + W(x)}, \quad \|\mu - \nu\|_W = \sup_{\|\varphi\| \leq 1} \int_{\mathcal{X}} \varphi(x)(\mu - \nu)(dx).$

Feynman–Kac models

We consider:

- a kernel operator Q^f with $Q^f \neq \mathbb{1}$;
- a dynamics $\Phi_n : \mathcal{P}(\mathcal{X}) \to \mathcal{P}(\mathcal{X})$ defined by, for tests functions φ

$$\Phi_n(\mu)(\phi) = \frac{\mu\big((Q^f)^n\varphi\big)}{\mu\big((Q^f)^n\mathbb{1}\big)} = (\Phi^n)(\mu)(\varphi) \quad \text{with } \Phi(\mu)(\varphi) = \frac{\mu\big(Q^f\varphi\big)}{\mu\big(Q^f\mathbb{1}\big)}.$$

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Typically

- $Q^f = \mathrm{e}^f Q$, where Q defines a Markov chain $(x_n)_{n\in\mathbb{N}}$;
- then

$$\Phi_n(\mu)(\phi) = \frac{\mathbb{E}_\mu\left[\varphi(x_n)\, \mathrm{e}^{\sum_{k=0}^{n-1} f(x_k)}\right]}{\mathbb{E}_\mu\left[\mathrm{e}^{\sum_{k=0}^{n-1} f(x_k)}\right]}.$$

Ergodicity for Feynman–Kac dynamics

Theorem [G.F., M. Rousset & G. Stoltz, yesterday]

Assumptions:

- Lyapunov condition: there exist $W : \mathcal{X} \to [1, +\infty)$, $\gamma_n \xrightarrow{\infty} 0$, $b_n \geq 0$ and compact sets K_n s.t.

$$(L) \quad Q^f W(x) \leq \gamma_n W(x) + b_n \mathbb{1}_{K_n};$$

- Minorization condition: $\forall\, n \geq 1$, there exist $\alpha_n > 0$, $\eta_n \in \mathcal{P}(\mathcal{X})$ s.t.

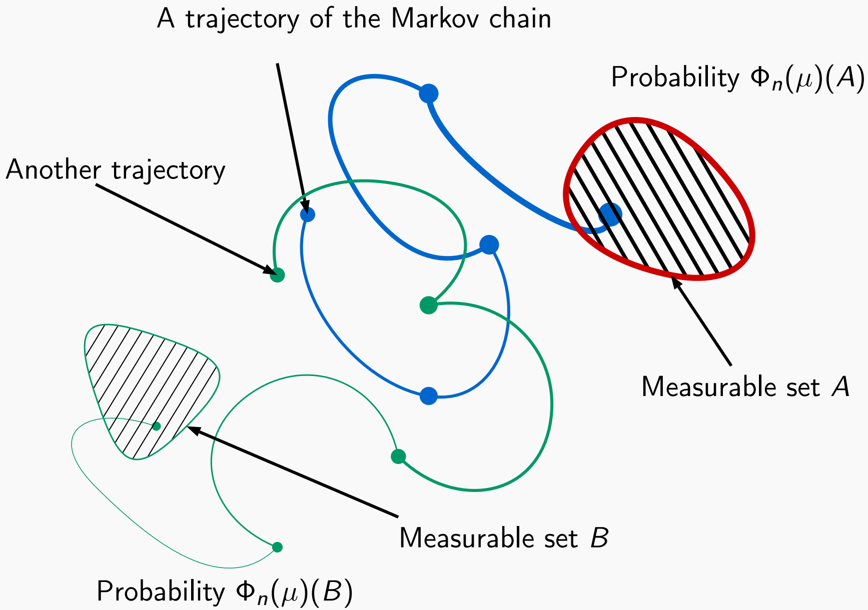
$$(M) \quad \forall\, x \in K_n, \quad Q^f(x, \cdot) \geq \alpha_n \eta_n(\cdot);$$

- $\mathcal{X}$ is Polish and Q^f is «locally strong Feller».

Then, there exist a unique μ_f^* and $\bar{\alpha} \in (0,1)$ such that for any $\mu \in \mathcal{P}(\mathcal{X})$, $\exists C_\mu > 0$ for which

$$\|\Phi_n(\mu) - \mu_f^*\|_W \leq C_\mu \bar{\alpha}^n, \quad \text{and} \quad \Phi(\mu_f^*) = \mu_f^*.$$

Big picture II



Sketch of proof

The steps of the proof are as follows:

- Q^f is quasi-compact in $L^\infty_W(\mathcal{X}) = \{\varphi : \sup |\varphi|/W < +\infty\}$;
- the spectral radius Λ is an eigenvalue with «positive» eigenvector h:

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- define the *Markovian* kernel $Q_h = \Lambda h^{-1} Q^f h$;
- Φ_n is rewritten
$$\Phi_n(\mu)(\phi) = \frac{\mu\big(h(Q_h)^n h^{-1}\varphi\big)}{\mu\big(h(Q^h)^n h^{-1}\big)};$$
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Toy model application

Consider the following Markov chain in $\mathbb{R}^d$:

$$x_{n+1} = \rho x_n + \sigma G_n,$$

with $\rho \in (-1, 1)$, $(G_n)_{n\in\mathbb{N}}$ standard Gaussian r.v.

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Then, the Feynman–Kac dynamics is stable if

$$f(x) \leq a|x|^p + c,$$

with $a > 0$, $c \in \mathbb{R}$, and $0 \leq p < 2$. The *Lyapunov function* is

$$W(x) = \mathrm{e}^{\beta x^2}, \qquad \text{with } 0 < \beta < \frac{1-\rho^2}{2\sigma^2}.$$

Back to O.U. process

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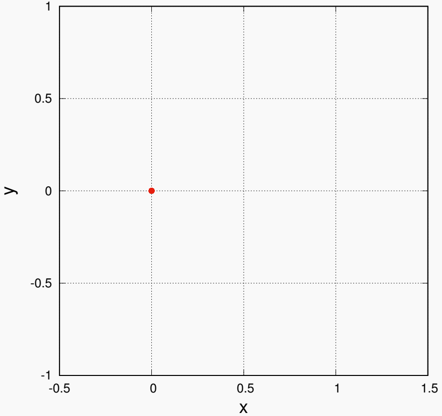

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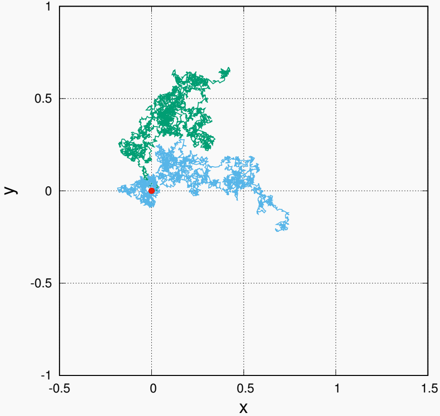

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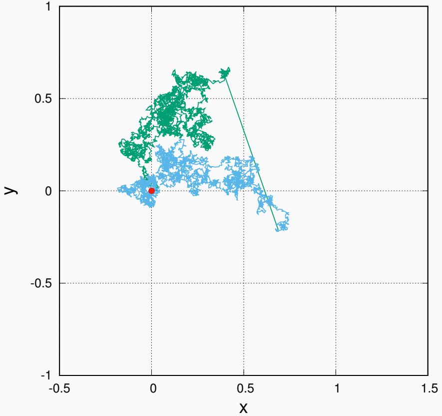

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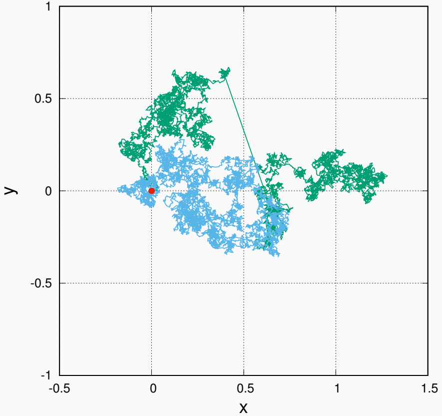

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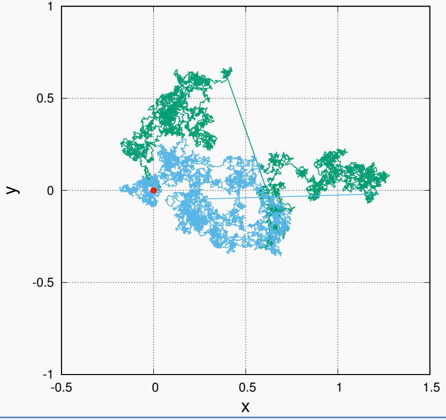

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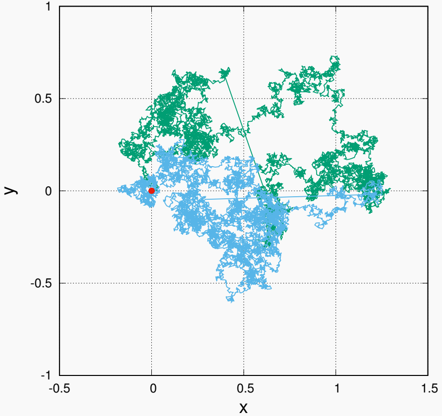

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Discretization

Goal: discretize in time the quantity

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Idea: discretize (X_t) into $x_n \approx X_{n\Delta t}$, and consider *e.g.*

$$\Phi_{n,\Delta t}(\mu)(\phi) = \frac{\mathbb{E}_\mu\left[\varphi(x_n)\,\mathrm{e}^{\sum_{k=0}^{n-1} f(x_k)\Delta t}\right]}{\mathbb{E}_\mu\left[\mathrm{e}^{\sum_{k=0}^{n-1} f(x_k)\Delta t}\right]}.$$

Other possible choice:

$$\Phi_{n,\Delta t}(\mu)(\phi) = \frac{\mathbb{E}_\mu\left[\varphi(x_n)\,\mathrm{e}^{\sum_{k=0}^{n-1} \frac{f(x_k)+f(x_{k+1})}{2}\Delta t}\right]}{\mathbb{E}_\mu\left[\mathrm{e}^{\sum_{k=0}^{n-1} \frac{f(x_k)+f(x_{k+1})}{2}\Delta t}\right]}.$$

Discretization

Under *verifiable conditions* and if $\mathcal{X}$ is bounded, the following theorem holds.

Theorem: error estimate on the invariant measure [G.F., G. Stoltz, 2017]

There exist $\mu_f^*, \mu_{f,\Delta t}^* \in \mathcal{P}(\mathcal{X})$ such that $\forall\, \mu \in \mathcal{P}(\mathcal{X})$

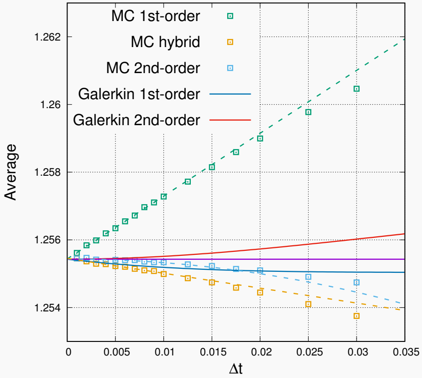
$$\Theta_t(\mu) \xrightarrow{t\to+\infty} \mu_f^*, \quad \Phi_n(\mu) \xrightarrow{n\to+\infty} \mu_{f,\Delta t}^*.$$

Moreover, there exist $p \geq 1$ and ψ solution to a Poisson equation such that

$$\int_{\mathcal{X}} \varphi \, d\mu_{f,\Delta t}^* = \int_{\mathcal{X}} \varphi \, d\mu_f^* + \Delta t^p \int_{\mathcal{X}} \varphi\psi \, d\mu_f^* + O(\Delta t^{p+1}).$$

Application

Overdamped Langevin dynamics on a one dimensional torus.



Average estimate for:

- $dX_t = (-V'(X_t) + 1)dt + dB_t$,
- $V(x) = 0.02 \cos(2\pi x)$,
- $f = |V|^2$,
- $\varphi = \mathrm{e}^f$
- Euler-Maruyama scheme and 2nd order modified scheme,
- comparison to Galerkin discretization.

Conclusion

Take home message:

- new results on the ergodicity of Feynman–Kac dynamics;
- easily verifiable conditions;
- natural extension of the theory for Markov chains;
- numerical analysis for discretizations of SDE's;
- possible directions: applications to SPDE's, link with large deviations theory, application to systems of interacting particles...

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Spectrum of quasi-compact operators