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Error estimates for Feynman-Kac semi-groups.

ICTS - Large Deviation Theory

Grégoire FERRÉ – Gabriel STOLTZ

CERMICS - ENPC, INRIA PARIS & LABEX BEZOUT

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1. Problem and motivation
2. Error estimates on ergodic averages
3. Error estimates for Feynman-Kac semi-groups



1. Problem and motivation

Large deviations

- Consider an ergodic dynamics on the torus with invariant measure ν :

$$dX_t = b(X_t)dt + \sqrt{2\beta^{-1}}dB_t.$$

- Idea of large deviations:

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

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where l is the **rate function**.

- Donsker-Varadhan [1975]**: if one sets

$$\lambda(k) := \sup_{a \in \mathbb{R}} \{ka - l(a)\},$$

then $\lambda(k)$ is the largest eigenvalue of $\mathcal{L} + kW$ where $\mathcal{L}$ is the generator of (X_t) .

Feynman-Kac semi-groups

- Consider (λ, ν_W) the principal eigenvalue and eigenfunction of $\mathcal{L}^\dagger + W$. Feynman-Kac formula gives

$$\lambda = \lim_{t \rightarrow \infty} \frac{1}{t} \log \mathbb{E} \left[e^{\int_0^t W(X_s) ds} \right].$$

- We then consider, for an observable φ ,

$$\Phi_t(\mu)(\varphi) = \frac{\mathbb{E}_\mu \left[\varphi(X_t) e^{\int_0^t W(X_s) ds} \right]}{\mathbb{E}_\mu \left[e^{\int_0^t W(X_s) ds} \right]} \xrightarrow{t \rightarrow \infty} \int_{\mathcal{D}} \varphi d\nu_W.$$

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- Problem related to [Markov processes conditioned on large deviations](#) (Chetrite & Touchette – Tsobgni-Nyawo & Touchette – Angeletti & Touchette).
- [Discretization and error estimates](#) for such semi-groups ?

Problem: error estimates

- We discretize the process (X_t) into a Markov chain (x_n) of time step Δt . Consider for example the estimator:

$$\Phi_{\Delta t, n}(\mu)(\varphi) = \frac{\mathbb{E}_{\mu} \left[\varphi(x_n) e^{\Delta t \sum_{i=0}^{n-1} W(x_i)} \right]}{\mathbb{E}_{\mu} \left[e^{\Delta t \sum_{i=0}^{n-1} W(x_i)} \right]} \xrightarrow{n \rightarrow \infty} \int_{\mathcal{D}} \varphi d\nu_{W, \Delta t}.$$

- Natural question: is $\nu_{W, \Delta t}$ close to ν_W ? Can we find $C > 0$, $p \geq 1$ such that, for all φ regular,

$$\left| \int_{\mathcal{D}} \varphi d\nu_{W, \Delta t} - \int_{\mathcal{D}} \varphi d\nu_W \right| \leq C \Delta t^p,$$

depending on the numerical scheme?

2. Error estimates on ergodic averages

Error estimates on the time step bias

- Ergodic average:

$$\frac{1}{N_{\text{iter}}} \sum_{n=0}^{N_{\text{iter}}-1} \varphi(x_n) \xrightarrow{n \rightarrow \infty} \int_{\mathcal{D}} \varphi d\nu_{\Delta t}.$$

- Systematic error (Talay & Tubaro – Mattingly, Stuart & Tretyakov – Debussche & Faou – Abdule, Vilmart, Konstantinos & Zygalakis – Leimkuhler, Matthews & Stoltz ...)

Theorem

There exists $p \geq 1$ and f regular such that for all smooth φ ,

$$\int_{\mathcal{D}} \varphi d\nu_{\Delta t} = \int_{\mathcal{D}} \varphi d\nu + \Delta t^p \int_{\mathcal{D}} \varphi f d\nu + O(\Delta t^{p+1})$$

- The function f is solution to the Poisson equation of the form $\mathcal{L}^* f = g$, where g and p depend on the numerical scheme.

Sketch of proof

Idea: $Q_{\Delta t}$ defined by $Q_{\Delta t}\varphi(x) = \mathbb{E}[\varphi(x_{n+1})|x_n = x]$ approximates the exact flow $e^{t\mathcal{L}}$ over a time step Δt . We assume that:

$$Q_{\Delta t}\varphi = \varphi + \Delta t \mathcal{A}_1\varphi + \dots + \Delta t^p \mathcal{A}_p\varphi + \Delta t^{p+1} \mathcal{A}_{p+1}\varphi + O(\Delta t^{p+2})$$

The proof relies on the stationarity equations,

$$\int_{\mathcal{D}} P_t \varphi d\nu = \int_{\mathcal{D}} \varphi d\nu, \quad \int_{\mathcal{D}} Q_{\Delta t} \varphi d\nu_{\Delta t} = \int_{\mathcal{D}} \varphi d\nu_{\Delta t}.$$

Idea: expand $\nu_{\Delta t}$ as a function of ν , i.e. search f s.t.

$$\int_{\mathcal{D}} (Q_{\Delta t}\varphi)(1 + \Delta t^p f) d\nu = \int_{\mathcal{D}} \varphi(1 + \Delta t^p f) d\nu + \Delta t^{p+2} R_{\Delta t}\varphi.$$

Then, if $\int_{\mathcal{D}} \mathcal{A}_k \varphi d\nu = 0$ for $k = 1, \dots, p$ we have at order $p+1$

$$\int_{\mathcal{D}} [\mathcal{A}_{p+1}\varphi + (\mathcal{A}_1\varphi)f] d\nu = 0, \text{ so } f = -(\mathcal{A}_1^*)^{-1} \mathcal{A}_{p+1}\mathbb{1}.$$

3. Error estimates for Feynman-Kac semi-groups

A double discretization

- We want to discretize the flow

$$\mathbb{E} \left[\varphi(X_t) e^{\int_0^t W(X_s) ds} \right] = e^{t(\mathcal{L}+W)} \varphi$$

over a time step Δt .

- We need to discretize both the process *and* the integral. We denote $Q_{\Delta t}^W$ the approximated flow, for example

$$(Q_{\Delta t}^W \varphi)(x) = e^{\Delta t W(x)} (Q_{\Delta t} \varphi)(x), \quad (Q_{\Delta t}^W \varphi)(x) = e^{\frac{\Delta t}{2} W(x)} (Q_{\Delta t} \varphi e^{\frac{\Delta t}{2} W})(x).$$

- Same strategy for the long time error, show that

$$Q_{\Delta t}^W \approx e^{\Delta t(\mathcal{L}+W)}$$

with an expansion in Δt .

Main result

We assume that:

$$Q_{\Delta t}^W \varphi = \varphi + \Delta t \mathcal{A}_1^W \varphi + \dots + \Delta t^p \mathcal{A}_p^W \varphi + \Delta t^{p+1} \mathcal{A}_{p+1}^W \varphi + O(\Delta t^{p+2}).$$

Theorem: error estimate on the invariant measure

Under «mild» assumptions, if for $k = 1, \dots, p$ there exists $a_k \in \mathbb{R}$ s.t. for any smooth φ ,

$$\forall \varphi \in \mathcal{C}^\infty, \quad \int_{\mathcal{D}} \mathcal{A}_k^W \varphi d\nu_W = \mathbf{a}_k \int_{\mathcal{D}} \varphi d\nu_W,$$

then

$$\int_{\mathcal{D}} \varphi d\nu_{W, \Delta t} = \int_{\mathcal{D}} \varphi d\nu_W + \Delta t^p \int_{\mathcal{D}} \varphi f d\nu_W + O(\Delta t^{p+1})$$

Sketch of proof

Again, start from stationarity equations:

$$\int_{\mathcal{D}} e^{t(\mathcal{L}+W)} \varphi d\nu_W = e^{t\lambda} \int_{\mathcal{D}} \varphi d\nu_W,$$

and

$$\int_{\mathcal{D}} Q_{\Delta t}^W \varphi d\nu_{W,\Delta t} = \underbrace{\left(\int_{\mathcal{D}} Q_{\Delta t}^W(\mathbf{1}) d\nu_{W,\Delta t} \right)}_{\text{creation of probability: } e^{\Delta t \lambda \Delta t}} \left(\int_{\mathcal{D}} \varphi d\nu_{W,\Delta t} \right).$$

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Next steps:

- identify f solution to a Poisson equation s. t. $\nu_{W,\Delta t} \approx (1 + \Delta t^p f) \nu_W$,
- build an approximate eigenvector $\hat{h}_{W,\Delta t}$ s.t. $Q_{\Delta t}^W \hat{h}_{W,\Delta t} \approx e^{\Delta t \lambda \Delta t} \hat{h}_{W,\Delta t}$,
- a priori estimate on the creation of probability $e^{\Delta t \lambda \Delta t}$,
- technical details.

Useful corollary

- We are mainly interested in the eigenvalue λ . We define:

$$e^{\Delta t \lambda_{\Delta t}} := \int_{\mathcal{D}} Q_{\Delta t}^W(\mathbb{1}) d\nu_{W, \Delta t}.$$

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Error estimate on the eigenvalue

If $Q_{\Delta t}^W$ is consistent at order p , then

$$\lambda_{\Delta t} := \frac{1}{\Delta t} \log \left[\int_{\mathcal{D}} Q_{\Delta t}^W(\mathbb{1}) d\nu_{W, \Delta t} \right] = \lambda + \Delta t^p C + O(\Delta t^{p+1}),$$

where $C \in \mathbb{R}$ is a constant depending on f .

Applications to statistical physics and Diffusion Monte Carlo:

- If the dynamics is discretized with a **second order scheme** $Q_{\Delta t}$, then the splitting

$$Q_{\Delta t}^W = e^{\frac{\Delta t}{2}W} \left(Q_{\Delta t} \left(e^{\frac{\Delta t}{2}W} \cdot \right) \right)$$

provides a **second-order discretization** of the Feynman-Kac semi-group.

- For Diffusion Monte Carlo, the dynamics (X_t) is a **brownian motion**, so the **flow $Q_{\Delta t}$ is exact**. The above splitting is immediately second order.

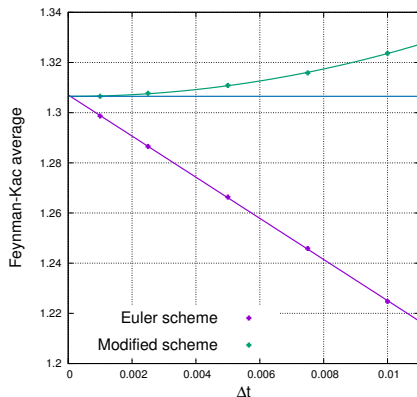
Statistical approximation

- Path average over a set of replicas $(x_n^m)_{m=1}^M$,

$$\Phi_{\Delta t, n}(\varphi) \approx \frac{\frac{1}{M} \sum_{m=1}^M \varphi(x_n^m) e^{\sum_{k=0}^{n-1} W(x_k^m) \Delta t}}{\frac{1}{M} \sum_{m=1}^M e^{\sum_{k=0}^{n-1} W(x_k^m) \Delta t}}$$

- Important variance of the exponential weights.
- Population dynamics over the M replicas of the systems. For each step:
 - 1 evolve the replicas with kernel $Q_{\Delta t}$,
 - 2 compute probabilities $(p_m)_{m=1}^M$ from the weights $e^{\Delta t W}$,
 - 3 kill or clone each replica with probability p_m and resize the population,
 - 4 average φ over the replicas.

Overdamped Langevin dynamics on a one dimensional torus.



Estimation of $\lambda_{\Delta t}$ for:

- $dX_t = -V'(X_t)dt + dB_t$,
- $V(x) = \cos(2\pi x)$,
- $W = |V|^2$,
- Euler-Maruyama scheme and 2nd order modified scheme,
- comparison to Galerkin discretization.

We indeed observe first and second order convergence.

Conclusion

Summary:

- a numerical large deviation problem,
- discretization of SDE's and error on the invariant measure,
- new error estimates on the invariant measure of Feynman-Kac semi-groups,
- alternative representation of the principal eigenvalue.

Perspectives

- convergence of Feynman-Kac semi-groups for an unbounded state space,
- adaptative scheme, variance reduction.

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