Stochastic processes under constraints, Bielefeld

Approximating metastable continuous-space Markov chains by Markov chains on a finite set

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PROJET FINANCÉ PAR L'ANR – PROJECT FUNDED BY THE ANR

Project PERISTOCH

Example 1: Iterated maps with additive noise

$$X_{n+1} = \Pi(X_n) + \sigma\xi_{n+1}$$

- $\Pi : \mathbb{R}^d \to \mathbb{R}^d$ map with N stable fixed points $x_1^\star, \dots, x_N^\star$
- ξ_n iid random variables, e.g. Gaussian
- $0 < \sigma \ll 1$ noise level

Question:

Can $(X_n)_{n \geqslant 0}$ be approximated by a Markov chain on $\{1, \dots, N\}$?

Difficult because

- Time scales can be exponentially different
- Transition probabilities can be exponentially different

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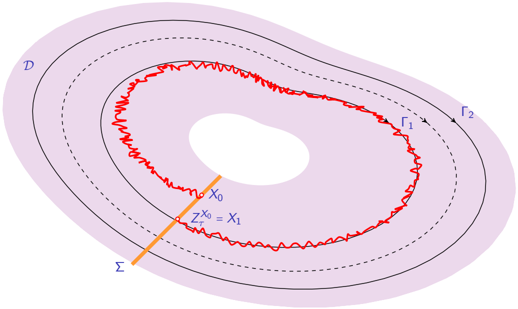
Example 2: Random Poincaré maps

$dz_t = f(z_t)\,dt + \sigma g(z_t)\,dW_t \quad \Rightarrow \quad$ Sample path $(Z_t^{z_0}(\omega))_{t\geqslant 0}$



$$z_0 = X_0 \in \Sigma \quad \Rightarrow \quad \inf\{t > 0 : Z_t^{X_0} \in \Sigma\} = 0$$

Solution: $\tau_0 = 0$, $\tau'_{n+1} = \inf\{t > \tau_n : Z_t^{X_0} \in \Sigma'\}$
$\tau_{n+1} = \inf\{t > \tau'_{n+1} : Z_t^{X_0} \in \Sigma\}$

$X_n = Z_{\tau_n}^{X_0} \in \Sigma \quad \Rightarrow \quad (X_n)_{n\geqslant 0}$ is a Markov chain $\quad K(x, A) := \mathbb{P}^x\{X_1 \in A\}$

$(X_n, \omega) \mapsto X_{n+1}$: random Poincaré map

[J. Weiss, E. Knobloch, 1990], [P. Hitczenko, G. Medvedev, 2009]

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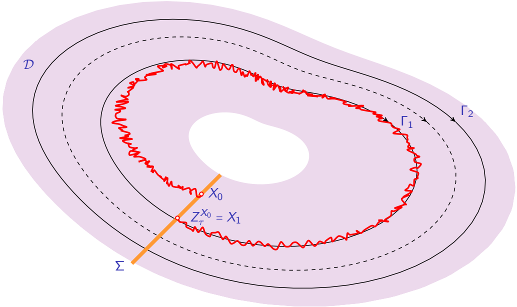

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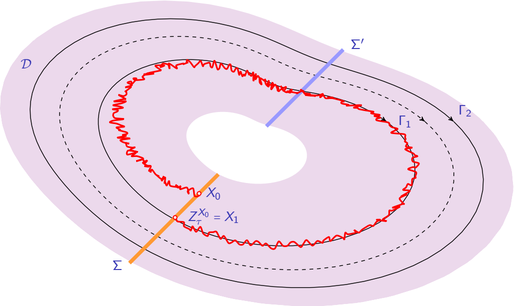

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Continuous-space Markov chains

$(X_n)_{n\geqslant 0}$ Markov chain on $\mathscr{X}_0 \subset \mathbb{R}^d$, of kernel

$$K_\sigma(x,A) = \mathbb{P}\{X_{n+1} \in A | X_n = x\} = \int_A k_\sigma(x,y)\,\mathrm{d}y \qquad (\sigma > 0)$$

Markov semigroups:

$$(K_\sigma\varphi)(x) = \int_{\mathscr{X}_0} k_\sigma(x,y)\varphi(y)\,\mathrm{d}y = \mathbb{E}^x[\varphi(X_1)] \qquad \varphi \in L^\infty$$

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Aim:

Describe $\mathbb{P}^x\{X_{\tau_{\mathscr{M}}^{+,n}} \in B_i\}$ where B_i neighbourhood of $x_i^\star$ and $\mathscr{M} = \bigcup_i B_i$

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Related work

- [Freidlin & Wentzell '69–'70]: W-graphs
  applications to exit problem, invariant measure, ...
- [Bovier, Eckhoff, Gayrard & Klein '04–'05]: gradient SDEs, low-lying spectrum, *some* mean transition times are close to those of a Markov chain

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- [Di Gesù, Lelièvre, Le Peutrec & Nectoux '16, '19, '20, '22]:
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Assumption 1: Deterministic limit

Deterministic limit: $X_{n+1} = \Pi(X_n)$

- $(K_0\varphi)(x) = (\varphi \circ \Pi)(x)$ (Koopman operator)
- $(\mu K_0)(A) = \mu(\Pi^{-1}(A))$
  (pushforward, transfer or Ruelle–Perron–Frobenius operator)

Assumption 1:

$\exists$ bounded, open $\mathscr{X} \in \mathscr{X}_0$, s.t. $\Pi(\mathscr{X}) \subset \mathscr{X}$

Π has finitely many α/ω-limit sets in $\mathscr{X}$:

- $x_1^\star, \dots x_N^\star$ asympt. stable fixed points
- others are unstable fixed points

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Assumption 2: Large-deviation principle

Assumption 2:

K_σ satisfies an LDP with good rate function I:

$$\liminf_{\sigma\to 0} \sigma^2 \log K_\sigma(x, O) \geqslant -\inf_{y\in O} I(x,y) \qquad O \subset \mathscr{X}_0 \text{ open}$$

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$I(x,y) = 0 \Leftrightarrow y = \Pi(x)$, I continuous at $x^\star$ if $\Pi(x^\star) = x^\star$

- True in Example 2, and in Example 1 if ξ_n satisfy an LDP
- Quasipotential:
  $$H(i,j) = \inf_{n\geqslant 1} \inf_{x_1,\dots,x_{n-1}} \Big[I(x_i^\star, x_1) + I(x_1, x_2) + \dots + I(x_{n-1}, x_j^\star) \Big]$$
  Then $\forall \eta > 0$, $\exists \sigma_0, \delta_0 > 0$, s.t.
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For $\sigma > 0$, K_σ has positive density, bdd below
K_σ is positive Harris recurrent, in particular $E_{\mathscr{X}}(\sigma) = \sup_{x \in \mathscr{X}} \mathbb{E}^x[\tau_{\mathscr{X}}^+] < \infty$

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Assumption 4: Uniform positivity

- Trace process on $\mathscr{M}$: $(X_{\tau^{+,n}_{\mathscr{M}}})_{n \geqslant 0}$, kernel ${}_{\mathscr{M}}K_\sigma =: K$
- Process killed upon leaving $A \subset \mathscr{M}$: $k_A(x,y) = k(x,y)\mathbb{1}_{\{x \in A, y \in A\}}$
  Quasistationary distribution (QSD) π_0^A: $(\pi_0^A K_A)(x) = \lambda_0^A \pi_0^A(x)$
  $\lambda_0^A \in (0,1)$ principal eigenvalue, $\lim_{n\to\infty} \mathbb{P}^x\{X_n^A \in B | \tau_{A^c} > n\} = \pi_0^A(B)$

Assumption 4:

$\exists L \in (1,2)$, $n_0(\sigma)$ s.t.

$$\sup_{x \in B_i} k_{B_i}^{n_0(\sigma)}(x,y) \leqslant L \inf_{x \in B_i} k_{B_i}^{n_0(\sigma)}(x,y) \qquad \forall x, y \in B_i, \quad i = 1, \dots N$$

with $n_0(\sigma) \leqslant e^{\eta/\sigma^2}$ for all $\eta > 0$ if $\sigma < \sigma_0(\eta)$

- Consequence: spectral gap $|\lambda_{B_i}^1|/\lambda_{B_i}^0 = \mathcal{O}((L-1)^{1/n_0(\sigma)})$
- Assumption holds for Examples 1 & 2 with $n_0(\sigma) = \mathcal{O}(\log(\sigma^{-1}))$
  (coupling argument and Harnack-type inequaliy)

Assumption 4: Uniform positivity

- Trace process on $\mathscr{M}$: $(X_{\tau^{+,n}_{\mathscr{M}}})_{n\geqslant 0}$, kernel ${}_{\mathscr{M}}K_\sigma =: K$
- Process killed upon leaving $A \subset \mathscr{M}$: $k_A(x,y) = k(x,y)\mathbb{1}_{\{x\in A, y\in A\}}$
  Quasistationary distribution (QSD) π_0^A: $(\pi_0^A K_A)(x) = \lambda_0^A \pi_0^A(x)$
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Spectral gap

Proposition

$\forall \eta > 0$, $\exists \sigma_0, \delta_0 > 0$ s.t. if $\sigma < \sigma_0$, $\operatorname{diam}(B_i) < \delta_0$

- K has N eigenvalues outside disc $\{|\lambda| \leqslant \varrho = e^{-c/E_{\mathscr{X}}(\sigma)}\}$
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- Feynman–Kac: If $u \in \mathbb{C}$, $|e^{-u}| > \sup_{x \in \mathscr{M}^c} \mathbb{P}^x\{X_1 \in \mathscr{M}^c\}$,

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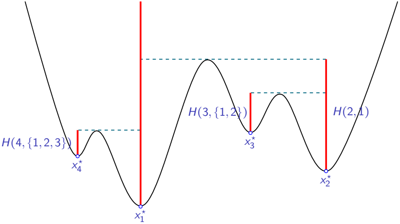
Sharper estimates with metastable hierarchy

Assumption 5

$\exists \theta > 0$ s.t. $\forall\ 2 \leqslant k \leqslant N$

$$\min_{\ell<k} H(k,\ell) \leqslant \min_{\substack{i<k \\ j\neq i}} H(i,j) - \theta$$



Theorem: [Baudel, B, SIAM J. Math. Anal. 2017]

The N largest eigenvalues of K are real and positive. $\exists\ \theta_k, \bar\theta_k, \bar\theta, c > 0$ s.t.

$$\lambda_0 = 1$$

$$\lambda_k = 1 - \mathbb{P}^{\pi^0_{B_{k+1}}}\{\tau^+_{\mathscr{M}_k} < \tau^+_{B_{k+1}}\}[1 + \mathcal{O}(\mathrm{e}^{-\theta_k/\sigma^2})] \qquad 1 \leqslant k \leqslant N-1$$

$$\phi_k(x) = \mathbb{P}^x\{\tau_{B_{k+1}} < \tau_{\mathscr{M}_k}\}[1 + \mathcal{O}(\mathrm{e}^{-\bar\theta/\sigma^2})] + \mathcal{O}(\mathrm{e}^{-\bar\theta_k/\sigma^2})$$

where $\mathscr{M}_k = \bigcup_{i=1}^{k} B_i$

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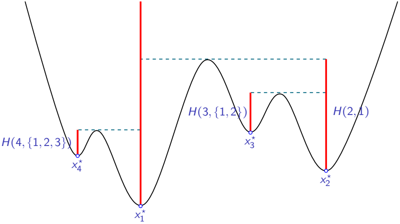

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Main result: Approximation by finite Markov chain

Theorem:

Under Assumptions 1, 2, 3, 4, if time acceleration $m = m(\sigma)$ satisfies

$$\lim_{\sigma \to 0} \sigma^2 \log m(\sigma) = \theta$$

with $\theta > 0$ small enough, for any $\eta > 0$, $x \in B_i$,

$$\left| \mathbb{P}^x \{ X_{\tau^{+,nm}_{\mathscr{M}}} \in B_j \} - \mathbb{P}^i \{ Y_n = j \} \right| \leqslant C \left(\mathrm{e}^{-[\widehat{H} - \eta]/\sigma^2} + \varrho^{nm} \right)$$

uniformly in n, where $\widehat{H} = H_0 - (N-1)\theta$, and $(Y_n)_{n \geqslant 0}$ is N-state Markov chain with matrix

$$P_{ij} = \mathbb{P}^{\pi^0_{B_i}} \{ X_{\tau^{+,m}_{\mathscr{M}}} \in B_j \} \left[1 + \mathcal{O}(\mathrm{e}^{-[\theta - \eta]/\sigma^2}) \right]$$

- $\varrho = \mathrm{e}^{-c/E_{\mathscr{X}}(\sigma)} < 1$ is spectral gap, ϱ^{nm} negligible
- $\mathbb{P}^i Y_n^{-1} = \mathscr{L}(\mathbb{P}^{\mu_i} X^{-1}_{\tau^{+,nm}_{\mathscr{M}}})$ for proba measures μ_i and $\mathscr{L}$ linear map between proba measures on $\mathscr{M}$ and $\{1, \dots, N\}$

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Proof ideas

- Law of $X_{\tau^{+,nm}_{\mathcal{M}}}$ approaches $\mathrm{span}\{\pi^0_0, \dots, \pi^0_{N-1}\}$ where $\pi^0_k K^0 = \lambda^0_k \pi^0_k$

  Problem: $\mathrm{span}\{\pi^0_0, \dots, \pi^0_{N-1}\} \neq \mathrm{span}\{\pi^0_{B_1}, \dots, \pi^0_{B_N}\}$

- Recall $K^\star(x, \mathrm{d}y) = \sum_{i=1}^{N} \mathbb{1}_{\{x \in B_i\}} \mathbb{P}^{\pi^0_{B_i}}\{X_{\tau^+_{\mathcal{M}}} \in \mathrm{d}y\}$

  Projectors on subspaces associated with $K^\star$, resp K^0:

$$\Pi^\star = \sum_{i=1}^{N} |\mathbb{1}_{B_i}\rangle\langle\pi^0_{B_i}| \qquad \Pi^0 = \sum_{k=0}^{N-1} |\phi^0_k\rangle\langle\pi^0_k|$$

- Changes of basis $(\{\pi^0_k\}, \{\phi^0_k\}) \to (\{\mu_i\}, \{\psi_i\})$

Lemma:

Let $\Pi^0_\perp = \mathrm{id} - \Pi^0$. Then

$$\langle\mu_i| = \langle\pi^0_{B_i}|[\mathrm{id} - \Pi^0_\perp \Pi^\star]^{-1}\Pi^0 \qquad |\psi_j\rangle = \Pi^0|\mathbb{1}_{B_j}\rangle$$

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where $\varepsilon_{ij} = \langle \pi^0_{B_i} | \Pi^0_\perp \Pi^\star | \mathbb{1}_{B_j} \rangle = \langle \pi^0_{B_i} | \Pi^\star - \Pi^0 | \mathbb{1}_{B_j} \rangle$

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Proposition:

- $\| \psi_j - \mathbb{1}_{B_j} \|_\infty \leqslant \mathrm{e}^{-[\widehat{H} - \eta]/\sigma^2}$
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Outlook

- Approximations of the QSDs?
- Sharper approximation of the $\mathbb{P}^{\pi^0_{B_i}}\{X_{\tau^{+,m}_{\mathscr{M}}} \in B_j\}$?
- Can the approach be transposed to the general SDE case?

References

- Manon Baudel & N. B., *Spectral theory for random Poincaré maps*, SIAM J. Math. Analysis **49**, 4319–4375 (2017)
- N. B., *Reducing metastable continuous-space Markov chains to Markov chains on a finite set*, arXiv/2303.12624. To appear in Annales de l'Institut Henri Poincaré

Thanks for your attention!

Slides available at https://www.idpoisson.fr/berglund/Bielefeld_2024.pdf