

Analysis and simulations of metastable systems, CIRM, Marseille

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

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Partly based on joint work with Manon Baudel



Project  
PERISTOCH

## Example 1: Iterated maps with additive noise

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

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

### Question:

Can  $(X_n)_{n \geq 0}$  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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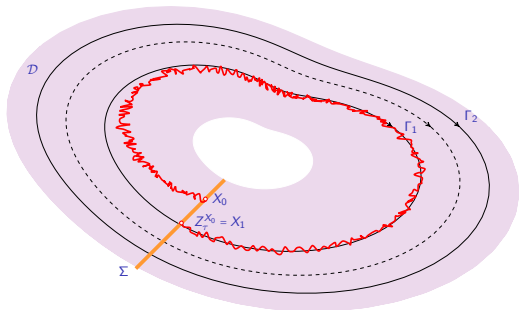
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## Example 2: Random Poincaré maps

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



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

$$\text{Solution: } \tau_0 = 0, \tau'_{n+1} = \inf\{t > \tau_n: Z_t^{X_0} \in \Sigma'\}$$
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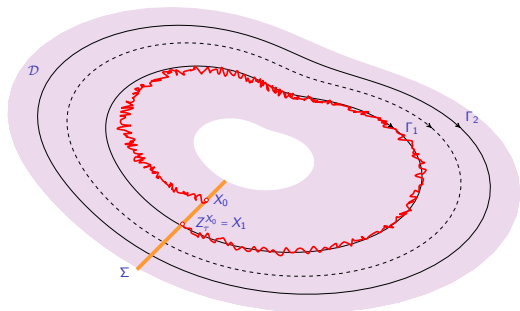
$$X_n = Z_{\tau_n}^{X_0} \in \Sigma \Rightarrow (X_n)_{n \geq 0} \text{ is a Markov chain } K(x, A) := \mathbb{P}^x\{X_1 \in A\}$$

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

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

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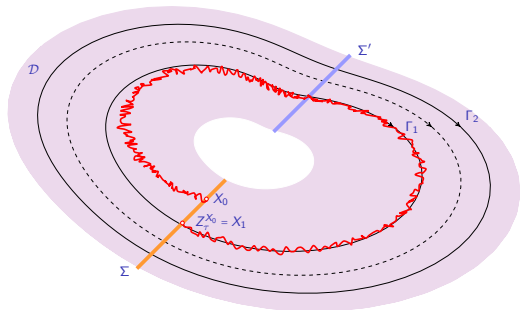
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# Continuous-space Markov chains

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

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

Markov semigroups:

$$(K_\sigma \varphi)(x) = \int_{\mathcal{X}_0} k_\sigma(x, y) \varphi(y) dy = \mathbb{E}^x[\varphi(X_1)] \quad \varphi \in L^\infty$$

$$(\mu K_\sigma)(y) = \int_{\mathcal{X}_0} \mu(x) k_\sigma(x, y) dx = \mathbb{P}^\mu\{X_1 \in dy\} \quad \mu \in L^1$$

- ▶ First-passage time:  $\tau_A = \inf\{n \geq 0: X_n \in A\}$
- ▶ Return time:  $\tau_A^+ = \tau_A^{+,1} = \inf\{n \geq 1: X_n \in A\}$
- ▶  $n$ th return time:  $\tau_A^{+,n} = \inf\{n > \tau_A^{+,n-1}: X_n \in A\}$

## Aim:

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



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## Related work

- ▷ [Freidlin & Wentzell '69–'70]:  $W$ -graphs applications to exit problem, invariant measure, ...
- ▷ [Bovier, Eckhoff, Gaynard & Klein '04–'05]: gradient SDEs, low-lying spectrum, *some* mean transition times are close to those of a Markov chain
- [Landim, Mariani & Seo '18]: extension to non-gradient SDEs application to SDEs with known invariant measure
- [Le Peutrec & Michel '22]: eigenvalues of non-gradient SDEs with known invariant measure
- ▷ [Di Gesù, Lelièvre, Le Peutrec & Nectoux '16, '19, '20, '22]: precise estimates on exit locations from metastable sets
- ▷ [Beltrán & Landim '12, '15], [Landim, Loulakis, Mouragui '18]: trace process, martingale method, convergence of finite-dim distributions for Markov chains on countable state spaces
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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:

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

$\Pi$  has finitely many  $\alpha/\omega$ -limit sets in  $\mathcal{X}$ :

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

▷  $B_i$ : neighbourhood of  $x_i^*$ ,  $\Pi(B_i) \subset B_i$

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## Assumption 2: Large-deviation principle

### Assumption 2:

$K_\sigma$  satisfies an LDP with good rate function  $I$ :

$$\liminf_{\sigma \rightarrow 0} \sigma^2 \log K_\sigma(x, O) \geq - \inf_{y \in O} I(x, y) \quad O \subset \mathcal{X}_0 \text{ open}$$

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

- ▷ True in Example 2, and in Example 1 if  $\xi_n$  satisfy an LDP
- ▷ Quasipotential:

$$H(i, j) = \inf_{n \geq 1} \inf_{x_1, \dots, x_{n-1}} [I(x_i^*, x_1) + I(x_1, x_2) + \dots + I(x_{n-1}, x_j^*)]$$

Then  $\forall \eta > 0$ ,  $\exists \sigma_0, \delta_0 > 0$ , s.t.

$$e^{-[H(i,j)+\eta]/\sigma^2} \leq \mathbb{P}^x \{ \tau_{B_j}^+ < \tau_{B_i}^+ \} \leq e^{-[H(i,j)-\eta]/\sigma^2}$$

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## Assumption 3: Positive Harris recurrence

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For  $\sigma > 0$ ,  $K_\sigma$  has positive density, bdd below

$K_\sigma$  is positive Harris recurrent, in particular  $E_{\mathcal{X}}(\sigma) = \sup_{x \in \mathcal{X}} \mathbb{E}^x[\tau_{\mathcal{X}}^+] < \infty$

- ▶ Harris recurrent means  $\mathbb{P}^x\{\tau_A^+ < \infty\} = 1$  if  $\text{Leb}(A) > 0$   
Then  $\exists$  invariant measure  $\pi_0$   
Positive Harris recurrent means  $\pi_0$  is normalisable  
Then  $\mathbb{E}^x[\tau_A^+] < \infty \forall x \in A$ .
- ▶ [Meyn & Tweedie '92]: Positive Harris rec. if  $\exists$  Lyapunov fct  $U$  s.t.  
 $(K_\sigma U)(x) \leq U(x) - \varepsilon + a\mathbb{1}_{\{x \in \mathcal{X}\}}$ ,  $\varepsilon > 0$
- ▶ LDP  $\Rightarrow E_{\mathcal{X}}(\sigma) \leq e^{\eta/\sigma^2}$  for any  $\eta > 0$  if  $\sigma$  small enough  
Example 1:  $E_{\mathcal{X}}(\sigma) = \mathcal{O}(\log(\sigma^{-1}))$  if  $\xi_n \sim \mathcal{N}$ , no heteroclinic cycles  
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**Example 2:**  $E_{\mathcal{X}}(\sigma) = \mathcal{O}(\log(\sigma^{-1}))$  if no heteroclinic cycles



## Assumption 4: Uniform positivity

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

### Assumption 4:

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

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

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

- ▷ Consequence: spectral gap  $|\lambda_{B_i}^1| / |\lambda_{B_i}^0| = \mathcal{O}((L-1)^{1/n_0(\sigma)})$
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# Spectral gap

## Proposition

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

▷  $K$  has  $N$  eigenvalues outside disc  $\{|\lambda| \leq \rho = e^{-c/E_{\mathcal{X}}(\sigma)}\}$

▷  $N$  leading ev satisfy  $|\lambda - 1| \leq e^{-[H_0 - \eta]/\sigma^2}$  where  $H_0 = \min_{i \neq j} H(i, j)$

▷ Feynman–Kac: If  $u \in \mathbb{C}, |e^{-u}| > \sup_{x \in \mathcal{M}^c} \mathbb{P}^x \{X_1 \in \mathcal{M}^c\},$

$$(K\phi)(x) = e^{-u} \phi(x) \Leftrightarrow \phi(x) = \mathbb{E}^x [e^{u\tau_{\mathcal{M}}} \phi(X_{\tau_{\mathcal{M}}})]$$

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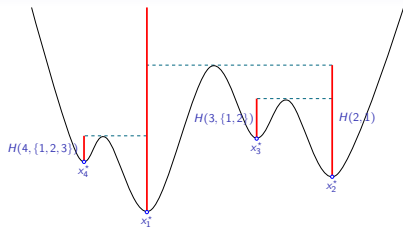
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# Sharper estimates with metastable hierarchy

## Assumption 5

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

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



**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.

$$\lambda_0 = 1$$

$$\lambda_k = 1 - \mathbb{P}^{\pi_{B_{k+1}}^0} \{ \tau_{\mathcal{M}_k}^+ < \tau_{B_{k+1}}^+ \} [1 + \mathcal{O}(e^{-\theta_k/\sigma^2})] \quad 1 \leq k \leq N-1$$

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

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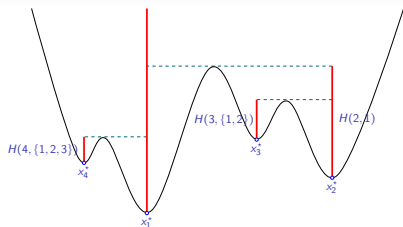


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# Main result: Approximation by finite Markov chain

## Theorem:

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

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

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

$$|\mathbb{P}^x \{X_{\tau_{\mathcal{M}}^+, nm} \in B_j\} - \mathbb{P}^i \{Y_n = j\}| \leq C(e^{-[\widehat{H} - \eta]/\sigma^2} + \varrho^{nm})$$

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

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## Proof ideas

- ▷ Law of  $X_{\tau_{\mathcal{M}}^+, nm}$  approaches  $\text{span}\{\pi_0^0, \dots, \pi_{N-1}^0\}$  where  $\pi_k^0 K^0 = \lambda_k^0 \pi_k^0$

**Problem:**  $\text{span}\{\pi_0^0, \dots, \pi_{N-1}^0\} \neq \text{span}\{\pi_{B_1}^0, \dots, \pi_{B_N}^0\}$

- ▷ Recall  $K^*(x, dy) = \sum_{i=1}^N \mathbb{1}_{\{x \in B_i\}} \mathbb{P}^{\pi_{B_i}^0} \{X_{\tau_{\mathcal{M}}^+} \in dy\}$

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

$$\Pi^* = \sum_{i=1}^N |\mathbb{1}_{B_i}\rangle \langle \pi_{B_i}^0| \quad \Pi^0 = \sum_{k=0}^{N-1} |\phi_k^0\rangle \langle \pi_k^0|$$

- ▷ Changes of basis  $(\{\pi_k^0\}, \{\phi_k^0\}) \rightarrow (\{\mu_i\}, \{\psi_j\})$

### Lemma:

Let  $\Pi_{\perp}^0 = \text{id} - \Pi^0$ . Then

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## Proposition:

- ◇  $\|\psi_j - \mathbb{1}_{B_j}\|_{\infty} \leq e^{-[\hat{H} - \eta]/\sigma^2}$
- ◇  $\mathbb{E}^{\mu_i}[\psi_j(X_{\tau_{\mathcal{M}}^+, nm})] = \mathbb{P}^i\{Y_n = j\}$

where  $(Y_n)_n$  Markov chain with matrix  $P_{ij} = \langle \mu_i | (K^0)^m | \psi_j \rangle$

# Outlook

- ▷ Approximations of the QSDs?
- ▷ Sharper approximation of the  $\mathbb{P}^{\pi_{B_i}^0} \{X_{\tau^+, m} \in B_j\}$ ?
- ▷ 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

Thanks for your attention!

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