Advances in Computational Statistical Physics

Trace process and metastability

Nils Berglund

Institut Denis Poisson, Université d'Orléans, France

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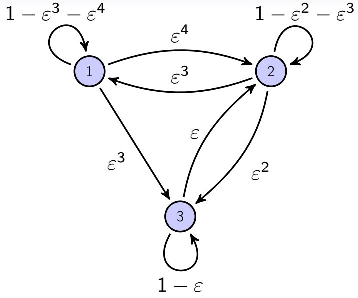
Joint work with Manon Baudel (Ecole des Ponts, Paris)

A simple example



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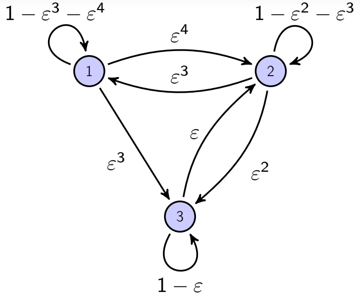

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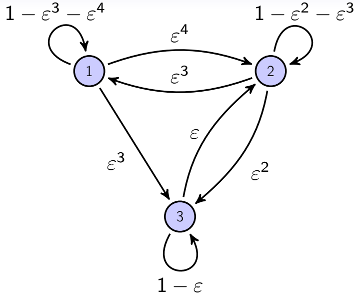

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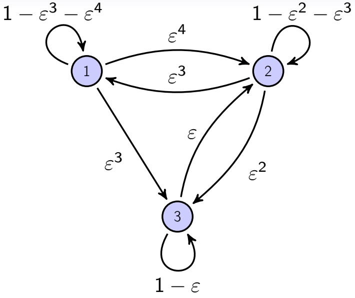

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Eigenvalues of P:

$$\lambda_0 = 1$$
$$\lambda_1 = 1 - 2\varepsilon^3 + \mathcal{O}(\varepsilon^5)$$
$$\lambda_2 = 1 - \varepsilon + \mathcal{O}(\varepsilon^2)$$

Main question

How to easily determine leading term of spectral gap $1 - \lambda_1$?

- Linear algebra/analytic methods (singular perturbation theory), e.g. [Schweitzer 68, Hassin & Haviv 92, Avrachenkov & Lasserre 99]
- Probabilistic methods, e.g. [Wentzell 72, Freidlin & Wentzell 70s, Beltràn & Landim 2010, Cameron & Vanden–Eijnden 2014, Betz & Le Roux 2016, Cameron & Gan 2016]

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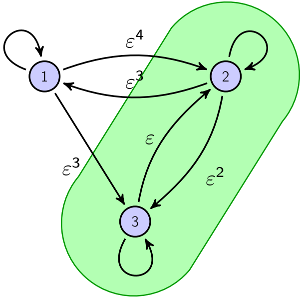
Some probabilistic tools:

- W-graphs
- Lumping of states
- Speeding up time



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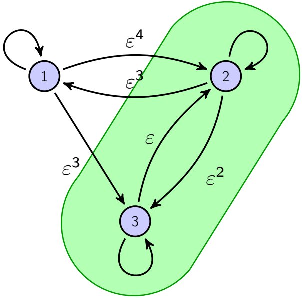
- Here: trace process



Trace process

$\mathcal{X}$ finite, $\{X_n\}_{n\in\mathbb{N}_0}$ irreducible aperiodic M.C., transition matrix P, $A \subset \mathcal{X}$

- Process killed upon leaving A: $P_A(x,y) = P(x,y)\mathbb{1}_{\{x,y\in A\}}$
- Trace process on A: process monitored only when in A

  ${}_AP(x,y) = \mathbb{P}^x\{X_{\tau_A^+=y}\}, \quad \tau_A^+ = \inf\{n \geqslant 1 \colon X_n \in A\}$

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&= P(x,y) + \sum_{z\in A^c} P(x,z) \sum_{n\geqslant 1} \mathbb{P}^z\{\tau_A^+ = n, X_{\tau_A^+=y}\} \\
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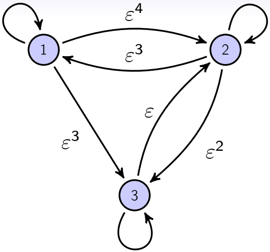
Matrix representation (Schur complement)

$$P = \begin{pmatrix} P_A & P_{AA^c} \\ P_{A^cA} & P_{A^c} \end{pmatrix} \quad \Rightarrow \quad {}_AP = P_A + P_{AA^c}[\mathbb{1} - P_{A^c}]^{-1} P_{A^cA}$$

Application to the example



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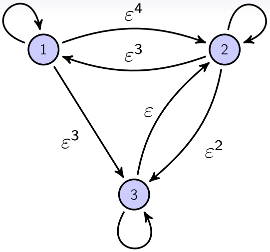

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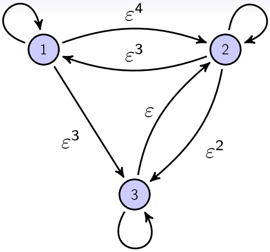

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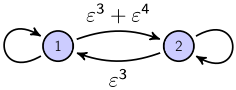

$$\begin{aligned} {}_A\lambda_0 &= 1 \\ {}_A\lambda_1 &= 1 - 2\varepsilon^3 - \varepsilon^4 \end{aligned} \qquad \begin{aligned} \lambda_0 &= 1 \\ \lambda_1 &= 1 - 2\varepsilon^3 + \mathcal{O}(\varepsilon^5) \\ \lambda_2 &= 1 - \varepsilon + \mathcal{O}(\varepsilon^2) \end{aligned}$$

A nice application of the trace process

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- First proof in non-reversible case: [Betz & Le Roux 2016]
  Using $\pi_0(x) = 1/\mathbb{E}^x[\tau_x^+]$
- Alternative proof using trace process:
  Remark: $\pi_0|_A$ is invariant by ${}_AP$
  Take $A = \{x, y\}$. Then

$$\begin{aligned}\pi_0(x) &= (\pi_0 {}_AP)(x)\\ &= \pi_0(x)\mathbb{P}^x\{X_{\tau_A^+} = x\} + \pi_0(y)\mathbb{P}^y\{X_{\tau_A^+} = x\}\\ &= \pi_0(x)\left[1 - \mathbb{P}^x\{\tau_y^+ < \tau_x^+\}\right] + \pi_0(y)\mathbb{P}^y\{\tau_x^+ < \tau_y^+\} \quad \square\end{aligned}$$

Good domains

Definition: For $A \subset \mathcal{X}$, let

$$p_{\text{in}}(A) = \inf_{x \in A^c} \mathbb{P}^x\{X_1 \in A\}$$

$$p_{\text{out}}(A) = \sup_{x \in A} \mathbb{P}^x\{X_1 \in A^c\}$$

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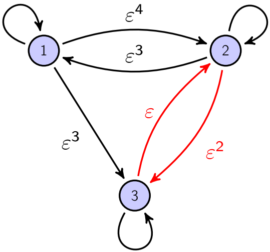
Example:



$$A = \{1, 2\}$$

$$p_{\text{in}}(A) = \varepsilon$$

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A is a good domain

Main idea

For a good domain A,

$P = \begin{pmatrix} P_A & P_{AA^c} \\ P_{A^cA} & P_{A^c} \end{pmatrix}$ is well-approximated by $\widehat{P} = \begin{pmatrix} {}_AP & 0 \\ P_{A^cA} & P_{A^c} \end{pmatrix}$

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Norm: $\|Q\| = \sup_{\|\varphi\|_\infty = 1} \|Q\varphi\|_\infty = \sup_{\|\mu\|_1 = 1} \|\mu Q\|_1 = \sup_{x \in \mathcal{X}} \sum_{y \in \mathcal{X}} |Q(x,y)|$

Lemma: $\|P - \widehat{P}\| = 2p_{\text{out}}(A)$

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Fact from spectral theory (using complex analysis, Riesz projector):
$\hat{\lambda}$ simple eigenvalue of $\widehat{P}$ at distance $> \|P - \widehat{P}\|$ from remaining spectrum
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Consequence: If $A^c = \{x\}$ then $p_{\text{in}}(A) = 1 - P(x,x) = 1 - \hat{\lambda}$
$\Rightarrow 1 - \lambda = 1 - \hat{\lambda} + \mathcal{O}(p_{\text{out}}(A)) = (1-\hat{\lambda})\Big[1 + \mathcal{O}\Big(\frac{p_{\text{out}}(A)}{p_{\text{in}}(A)}\Big)\Big]$

Example: $\hat{\lambda}_2 = 1 - \varepsilon$ perturbs to $\lambda_2 = 1 - \varepsilon + \mathcal{O}(\varepsilon^2)$
The argument does not suffice to compare spectra of P_A and ${}_AP$

Laplace transforms

$u \in \mathbb{C} \Rightarrow \mathbb{E}^x[\mathrm{e}^{u\tau_A^+}]$ exists for $|\mathrm{e}^{-u}| > 1 - p_{\mathrm{in}}(A)$ $(*)$

Proposition [Feynman–Kac type relation]

Under $(*)$,

$$\begin{cases} (P\phi)(x) = \mathrm{e}^{-u}\,\phi(x) & x \in A^c \\ \phi(x) = \bar{\phi}(x) & x \in A \end{cases}$$

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Corollary [Reduction to eigenvalue problem on A]

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Proposition

$$\|{}_AP^u - {}_AP^0\| \leqslant \frac{|1-e^{-u}|\sup_{x\in A}\mathbb{E}^x[\tau_A^+ - 1]}{1-|1-e^{-u}|\sup_{x\in A^c}\mathbb{E}^x[\tau_A^+]} \leqslant \frac{|1-e^{-u}|p_{\text{out}}(A)}{p_{\text{in}}(A)-|1-e^{-u}|}$$

Main result

Theorem

- Non-degenerate case: $\exists A_1 \subset A_2 \subset \cdots \subset A_n = \mathcal{X}$ s.t. $\#(A_{k+1} \setminus A_k) = 1$, each A_k good set for ${}_{A_{k+1}}P$
  Renumber states s.t. $A_k = \{1, \dots, k\}$. Then
  - $\lambda_0 = 1$, $\lambda_k = 1 - \mathbb{P}^{k+1}\{\tau^+_{A_k} < \tau^+_{k+1}\}\Big[1 + \mathcal{O}\Big(\frac{p_{\mathbf{out}}(A_k|A_{k+1})}{p_{\mathbf{in}}(A_k|A_{k+1})}\Big)\Big]$ $\in \mathbb{R}$
  - kth right eigenvector ϕ_k close to $\mathbb{P}^x\{\tau_{k+1} < \tau_{A_k}\}$
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  Use decomposition with blocks of size > 1
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Spectral decomposition in nondegenerate case:

$$P^n(x,y) = \sum_{k=1}^{n} \lambda_k^n \underbrace{\phi_k(x)\pi_k(y)}_{=\Pi_k(x,y)}$$

Continuous-space Markov chains

$(X_n)_{n\in\mathbb{N}_0}$ Markov chain in $\mathcal{X} \subset \mathbb{R}^d$ with kernel K_σ:

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

- $K_0(x, A) = 1_{\{\Pi(x)\in A\}}$ defined by deterministic map $\Pi : \mathcal{X} \to \mathcal{X}$
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Example 1: Randomly perturbed map

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

$(\xi_n)_{n\geqslant1}$ i.i.d. r.v. with density (e.g. $\sigma\xi_n$ Gaussian of variance σ^2)

Continuous-space Markov chains

$(X_n)_{n\in\mathbb{N}_0}$ Markov chain in $\mathcal{X} \subset \mathbb{R}^d$ with kernel K_σ:

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

- $K_0(x, A) = 1_{\{\Pi(x)\in A\}}$ defined by deterministic map $\Pi : \mathcal{X} \to \mathcal{X}$
- For $\sigma > 0$, K_σ admits continuous density k_σ

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Example 2: Random Poincaré map

SDE

$$\mathrm{d}x_t = f(x_t)\,\mathrm{d}t + \sigma g(x_t)\,\mathrm{d}W_t$$

X_n suitably defined location of nth return to surface of section $\Sigma \subset \mathcal{X}$

Assumptions

Assumption 1: Deterministic dynamics

$\Pi : \mathcal{X} \to \mathcal{X}$ admits positively invariant compact set $\mathcal{X}_0 \subset \mathcal{X}$, finitely many limit sets in $\mathcal{X}_0$, all hyperbolic fixed points, N of which are stable

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Assumption 2: Large-deviation principle

K_σ satisfies LDP with good rate function I $(K_\sigma(x, A) \sim \mathrm{e}^{-\inf_A I(x,\cdot)/\sigma^2})$
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Assumption 4: Uniform positivity (Doeblin-type condition)

$\forall x_i^\star$ stable fixed point, $\exists B_i$ nbh of $x_i^\star$ s.t. $k_i = {}_{B_1\cup\dots\cup B_i}k_{B_i}$ satisfies

$$\sup_{x\in B_i} k_i^n(x,y) \leqslant L \inf_{x\in B_i} k_i^n(x,y) \;\; \forall y \in B_i \qquad \text{for some } L \in (1,2),\ n(\sigma) \in \mathbb{N}$$

Main result

Theorem

- Non-degenerate case ($x_1^\star, \dots, x_N^\star$ in metastable order)
  - Eigenvalues of K_σ:

$$\lambda_0 = 1$$

$$\lambda_k = 1 - \mathbb{P}^{\mathring{\pi}_0^{k+1}}\{\tau^+_{B_1\cup\dots\cup B_k} < \tau^+_{B_{k+1}}\}\big[1 + \mathcal{O}(e^{-\theta/\sigma^2})\big] \in \mathbb{R} \qquad 1 \leqslant k < N$$

$$|\lambda_k| < 1 - \frac{c}{\log(\sigma^{-1})} \qquad k \geqslant N$$

where $\mathring{\pi}_0^{k+1}$ is a certain QSD on B_{k+1} and $c, \theta > 0$

  - kth right eigenfunction ϕ_k close to $\mathbb{P}^x\{\tau_{B_{k+1}} < \tau_{B_1\cup\dots\cup B_k}\}$
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- Degenerate case: similar to finite chain...

Approximation result

Theorem: Approximation by a finite Markov chain

$\exists m(\sigma)$, (signed) measures μ_i s.t. $\|\mu_i - \mathring{\pi}_0^{B_i}\|_1 \leqslant \mathrm{e}^{-\theta/\sigma^2}$:

$$\mathbb{P}^{\mu_i}\{X_{\tau^{+,nm}_{B_1\cup\dots\cup B_N}} \in B_j\} = \mathbb{P}^i\{Y_n = j\} + \underbrace{\mathcal{O}(\mathrm{e}^{-\theta/\sigma^2})}_{\text{uniform in } n}$$

where $(Y_n)_{n\in\mathbb{N}_0}$ Markov chain with matrix

$$P_{ij} = \mathbb{P}^{\mathring{\pi}_0^{B_i}}\{X_{\tau^{+,nm}_{B_1\cup\dots\cup B_N}} \in B_j\}[1 + \mathcal{O}(\mathrm{e}^{-\theta/\sigma^2})]$$

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Truncated spectral decomposition of ${}_{B_1\cup\dots\cup B_N}K$:

$$K^0_{\text{trunc}}(x, \mathrm{d}y) = \sum_{k=0}^{N-1} \lambda^0_k \phi^0_k(x) \pi^0_k(\mathrm{d}y)$$

Then $P_{ij} = \mu_i (K^0_{\text{trunc}})^m \psi_j$ where $\|\psi_j - 1\!\!1_{B_j}\|_\infty \leqslant \mathrm{e}^{-\theta/\sigma^2}$

Outlook

- ▹ Finite $\mathcal{X}$ case: simple algorithm to obtain eigenvalues and vectors (complexity $\mathcal{O}(n^2)$, $n = \#(\mathcal{X})$)
- ▹ Continuous-space Markov chains: eigen-elements in terms of committors and QSDs
- ▹ Needed: better ways to approximate QSDs and committors
- ▹ See also poster by Manon Baudel: link between QSD and reactive entrance distribution

Reference:

- ▹ Manon Baudel & N. B., *Spectral theory for random Poincaré maps*, SIAM J. Math. Analysis **49**, 4319–4375 (2017)

Related:

- ▹ N. B. & Damien Landon, *Mixed-mode oscillations and interspike interval statistics in the stochastic FitzHugh–Nagumo model*, Nonlinearity **25**, 2303-2335 (2012)
- ▹ N. B., Barbara Gentz & Christian Kuehn, *From random Poincaré maps to stochastic mixed-mode-oscillation patterns*, J. Dynam. Diff. Eq. **27**, 83–136 (2015)