IRTG Bielefeld–Seoul Winter School - Stochastic Dynamics

Metastable dynamics of Markov processes

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Based on joint works with Manon Baudel, Giacomo Di Gesù, Bastien Fernandez, Barbara Gentz, Damien Landon and Hendrik Weber

What is metastabilty?

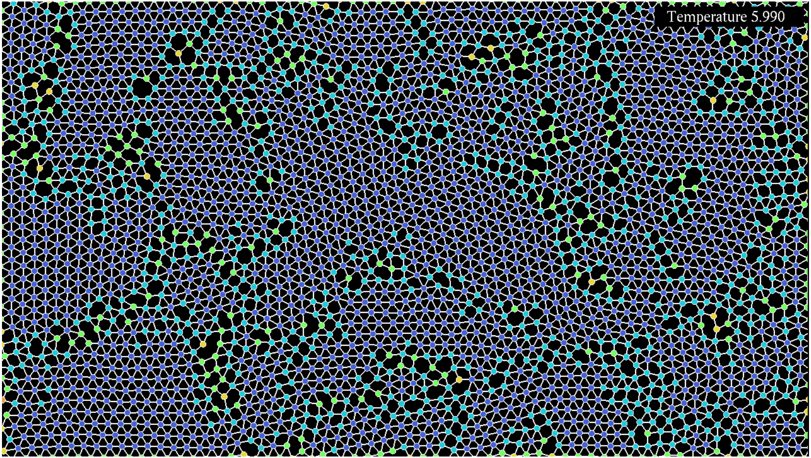
Supercooled water

(Source: https://youtu.be/fSPzMva9_CE)

What is metastabilty?

Ising model with Glauber dynamics at low temperature
(Online: https://youtu.be/_vrtfDcjfxU)

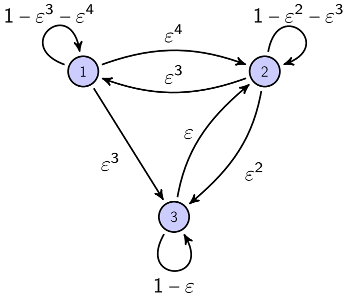
What is metastabilty?



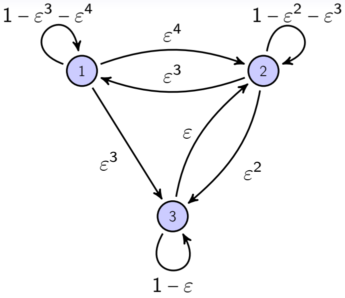
Particles interacting with a Lennard–Jones potential,
coupled to a thermostat (stochastic differential equation, or SDE)

Contents

1. Metastable Markov chains on a finite set



A simple example



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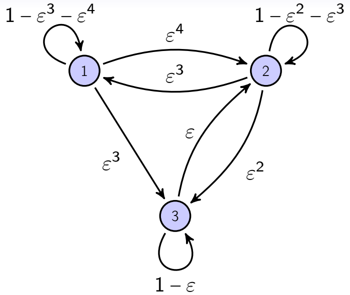

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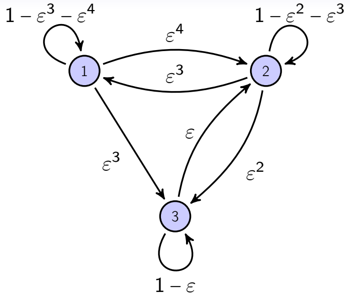

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  Stationary distribution:

  Speed of convergence to π_0?

  Eigenvalues of P:

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, Miclo 95, Beltràn & Landim 2010, Cameron & Vanden–Eijnden 2014, Betz & Le Roux 2016, Cameron & Gan 2016]

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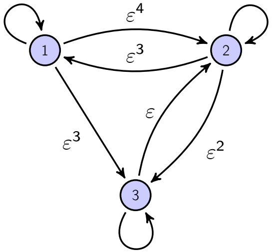
Some probabilistic tools:

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



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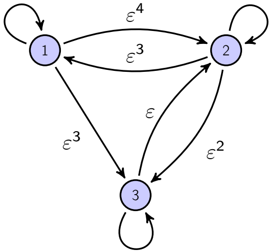
- Here: trace process



Killed 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: $P_A(x,y) = P(x,y)\mathbb{1}_{\{x,y\in A\}}$

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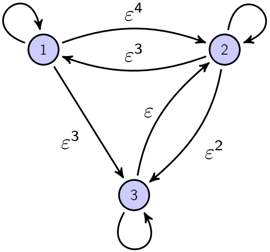

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$$A = \{1,2\}$$

Trace process [Landim, Beltran]

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

- ▷ Trace process on A: process monitored only when in A

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

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Matrix representation (Schur complement)

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

Application to the example

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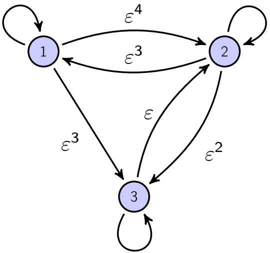

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Recall: the chain in not assumed to be reversible:
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$$\pi_0(x)\mathbb{P}^x\{\tau_y^+ < \tau_x^+\} = \pi_0(y)\mathbb{P}^y\{\tau_x^+ < \tau_y^+\}$$

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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: [Baudel & B 2017]
  Remark: $\pi_0|_A$ is invariant by ${}_AP$

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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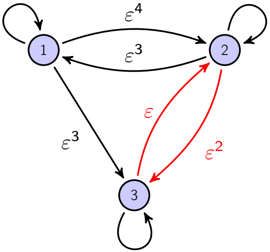
Example:



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

Main idea

Fact from spectral theory (using complex analysis, Riesz projector):
$\hat{\lambda}$ simple eigenvalue of $\widehat{P}$ at distance $> \|P - \widehat{P}\|$ from remaining spectrum
$\Rightarrow P$ has unique eigenvalue at distance $\mathcal{O}(\|P - \widehat{P}\|)$ from $\hat{\lambda}$

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 ${}_AP$

$$\widehat{P} = \begin{pmatrix} 1 - -\varepsilon^3 - \varepsilon^4 & \varepsilon^3 + \varepsilon^4 & 0 \\ \varepsilon^3 & 1 - \varepsilon^3 & 0 \\ 0 & \varepsilon & 1 - \varepsilon \end{pmatrix}$$

Laplace transforms

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

Follows from $\mathbb{P}^y\{\tau_A^+ > n\} \leqslant (1 - p_{\text{in}}(A))^n \ \forall y \in A^c$

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Proposition [Feynman–Kac type relation]

Under $(\star)$,

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

admits unique solution $\phi(x) = \mathbb{E}^x[\mathrm{e}^{u\tau_A}\,\bar{\phi}(X_{\tau_A})]$, $\tau_A = \inf\{n \geqslant 0 \colon X_n \in A\}$

Proof:

Laplace transforms

Corollary [Reduction to eigenvalue problem on A]

Under $(\star)$, $P\phi = e^{-u}\phi$ in $\mathcal{X}$ $\quad\Leftrightarrow\quad$ ${}_AP^u\phi = e^{-u}\phi$ in A
where ${}_AP^u(x,y) = \mathbb{E}^x\bigl[e^{u(\tau_A^+-1)}\,1_{\{X_{\tau_A^+}=y\}}\bigr]$ is such that ${}_AP^0 = {}_AP$

Proof of $\Rightarrow$:

Laplace transforms

Proposition

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

Main result – nondegenerate case

Algorithm in nondegenerate case:

- Assume $\exists x \in \mathcal{X}$ such that $1 - P(x,x) \gg 1 - P(y,y)\ \forall y \neq x$
- Take $A = \mathcal{X} \setminus \{x\}$ (A is a good set)
- Then $\mathbb{1} - P$ has ev $1 - \lambda = P(x,x)\big[1 + \mathcal{O}(p_{\text{in}}(A)/p_{\text{out}}(A))\big] \quad \in \mathbb{R}$
- Compute ${}_AP$ and start again with P replaced by ${}_AP$

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Theorem [Baudel & B, 2017]

- 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
- $\lambda_0 = 1,\ \lambda_k = 1 - \mathbb{P}^{k+1}\{\tau^+_{A_k} < \tau^+_{k+1}\}\Big[1 + \mathcal{O}\Big(\frac{p_{\text{out}}(A_k|A_{k+1})}{p_{\text{in}}(A_k|A_{k+1})}\Big)\Big] \quad \in \mathbb{R}$

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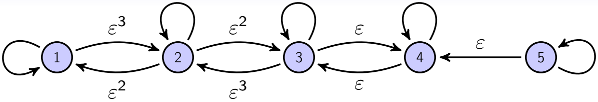
- kth right eigenvector ϕ_k close to $\mathbb{P}^x\{\tau_{k+1} < \tau_{A_k}\}$
- kth left eigenvector π_k close to quasistationary distribution (QSD) of P_{A_k} (left eigenvect of P_{A_k} for Perron–Frobenius principal eigenval)

Algorithm in degenerate case



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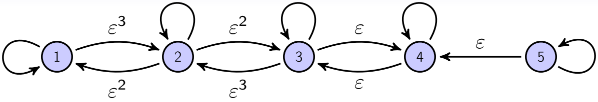
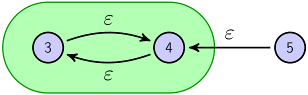


Degenerate part, leading order:

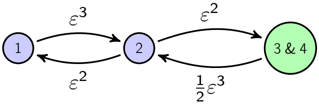


Eigenvalues: 1

$1 - \varepsilon$

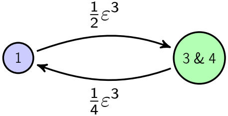
$1 - 2\varepsilon$

Effective trace process:



Eigenvalues: $1 - 2\varepsilon^2$

Trace on $\{1, 3\&4\}$:



$1 - \frac{3}{4}\varepsilon^3$

1

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