Metastability of random processes and solution of resolvent equations

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Webminar of French-Korean IRL in Mathematics

March 18th, 2022

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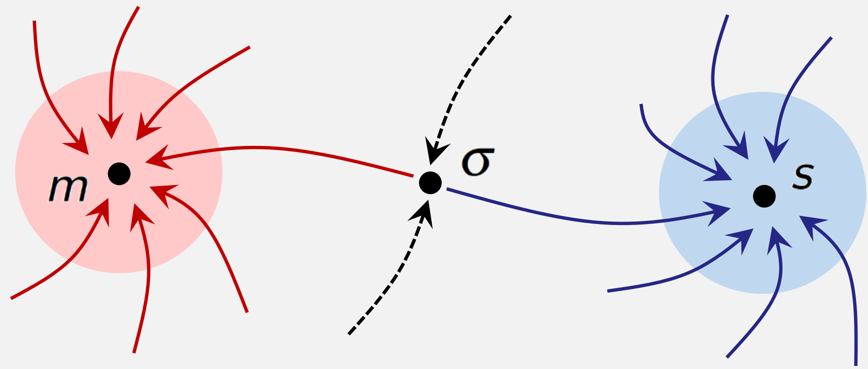
Small random perturbation of dynamical systems



- **Dynamical system** $dx_t = b(x_t)dt$
- Equilibria: m, s (stable) and σ (unstable, saddle)

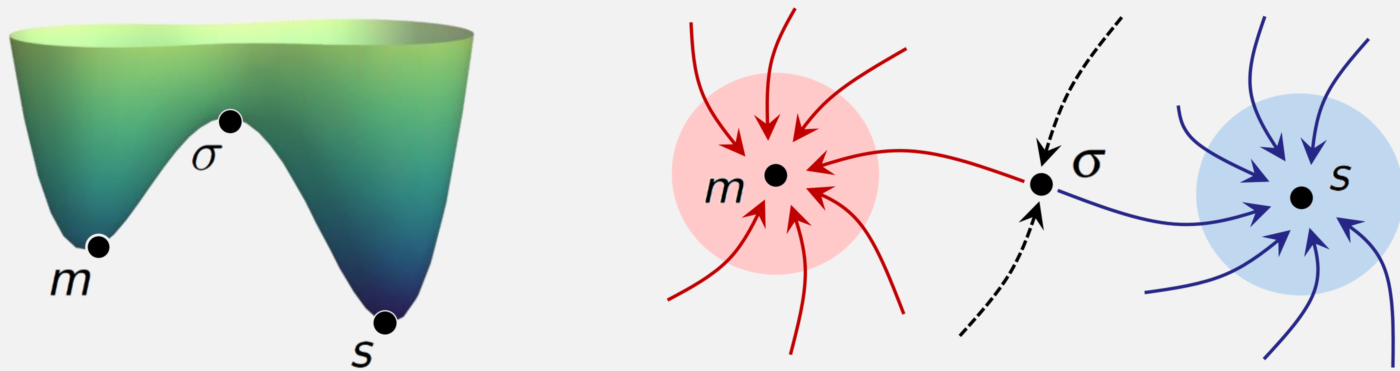
Small random perturbation of dynamical system (SRPDS)

- Stochastic dynamical system

$$dx_t = b(x_t)dt + \sqrt{2\epsilon}\, dW_t$$

- $\epsilon > 0$: small parameter (temperature), W_t: Brownian motion
- Metastability: rare transition from m to s

SRPDS: gradient case



- **Dynamical system** $dx_t = -\nabla U(x_t)dt$
- U: double-well potential (left figure above)

Special case: $b = -\nabla U$

- Stochastic dynamical system

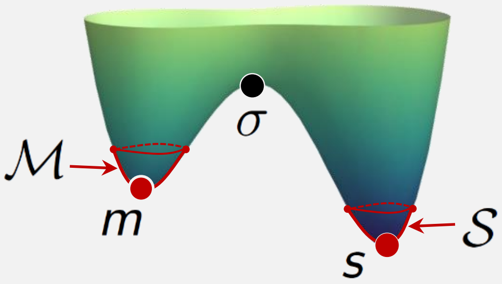
$$dx_t = -\nabla U(x_t)dt + \sqrt{2\epsilon}\, dW_t$$

- $\epsilon > 0$: small parameter (temperature), W_t: Brownian motion
- Metastability: rare transition from m to s

Metastability of SRPDS: mean transition time

Model: gradient SRPDS

$$dx_t = -\nabla U(x_t)dt + \sqrt{2\epsilon}\,dW_t$$



Question: How long does it take to go from m to s?

- $\tau_{m\to\mathcal{S}}$: transition time from m to $\mathcal{S}$
- $\mathbb{E}(\tau_{m\to\mathcal{S}})$: mean transition time

Large-deviation type estimate (Freidlin-Wentzell, 60s-70s)

$$\log \mathbb{E}(\tau_{m\to\mathcal{S}}) \simeq \frac{U(\sigma)-U(m)}{\epsilon}$$

Remark. Sharp estimate is missing:

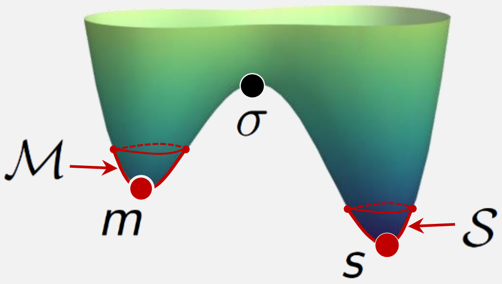
$$\mathbb{E}(\tau_{m\to\mathcal{S}}) \simeq c_\epsilon\, e^{\frac{U(\sigma)-U(m)}{\epsilon}}$$

where c_ϵ can be any sub-expoential term (e.g. ϵ^k or $e^{1/\sqrt{\epsilon}}$)

Metastability of SRPDS: mean transition time

Model: gradient SRPDS

$$dx_t = -\nabla U(x_t)dt + \sqrt{2\epsilon}\, dW_t$$



Question: How long does it take to go from m to s?

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Eyring-Kramers formula (Bovier et. al., 2004)

$$\mathbb{E}(\tau_{m \to \mathcal{S}}) \simeq \frac{-\mu_\sigma}{2\pi} \sqrt{\frac{\det(\nabla^2 U)(m)}{-\det(\nabla^2 U)(\sigma)}}\, e^{\frac{U(\sigma)-U(m)}{\epsilon}}$$

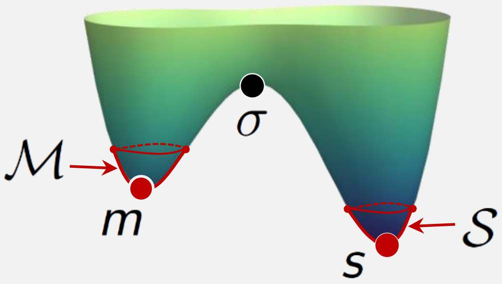
- μ_σ: unique negative e.v. of $(\nabla^2 U)(\sigma)$
- The **self-adjointness** of associated generator $\mathcal{L}_\epsilon$ is crucially used:

$$\mathcal{L}_\epsilon f = -\nabla U \cdot \nabla f + \epsilon \Delta f$$

Metastability of SRPDS: spectral gap

Model: gradient SRPDS

$$dx_t = -\nabla U(x_t)dt + \sqrt{2\epsilon}\, dW_t$$



Eyring-Kramers formula (Bovier et. al., 2004)

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- μ_σ: unique negative e.v. of $(\nabla^2 U)(\sigma)$
- The **self-adjointness** of associated generator $\mathcal{L}_\epsilon$ is crucially used:

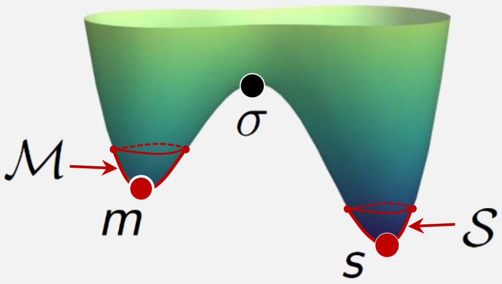
$$\mathcal{L}_\epsilon f = -\nabla U \cdot \nabla f + \epsilon \Delta f$$

- λ_ϵ: smallest non-zero eigenvalue of $-\mathcal{L}_\epsilon$ (spectral gap)
- $\lambda_\epsilon \simeq \mathbb{E}(\tau_{m\to\mathcal{S}})^{-1}$ (exponentially small)

Metastability of SRPDS: distributions

Model: gradient SRPDS

$$dx_t = -\nabla U(x_t)dt + \sqrt{2\epsilon}\, dW_t$$



Question: $x_0 \in \mathcal{M}$ ➡ Estimate of $\mathbb{P}(x_t \in \mathcal{M})$ and $\mathbb{P}(x_t \in \mathcal{S})$

Observation: something will happen around $\theta_\epsilon = e^{\frac{U(\sigma)-U(m)}{\epsilon}}$

Landim-Lee-Seo, forthcoming

- $t_\epsilon \ll \theta_\epsilon$ ➡ $\mathbb{P}(x_{t_\epsilon} \in \mathcal{M}) \simeq 1$
- $t_\epsilon = t\theta_\epsilon$ ➡ $\mathbb{P}(x_{t_\epsilon} \in \mathcal{M}) \simeq p(t)$ and $\mathbb{P}(x_{t_\epsilon} \in \mathcal{S}) \simeq 1 - p(t)$
- $t_\epsilon \gg \theta_\epsilon$ ➡ $\mathbb{P}(x_{t_\epsilon} \in \mathcal{S}) \simeq 1$

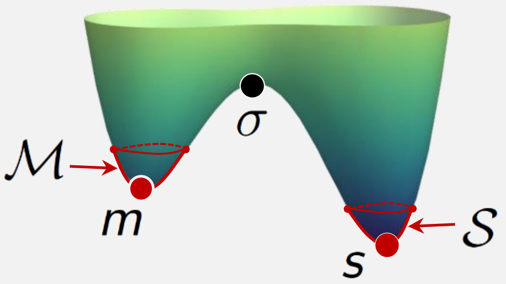
Remark. $p(t)$ can be computed explicitly

Connection to parabolic equations

Model: gradient SRPDS

$$dx_t = -\nabla U(x_t)dt + \sqrt{2\epsilon}\,dW_t$$

with generator $\mathcal{L}_\epsilon = -\nabla U \cdot \nabla + \epsilon\Delta$



Parabolic equation: for continuous and bounded g,

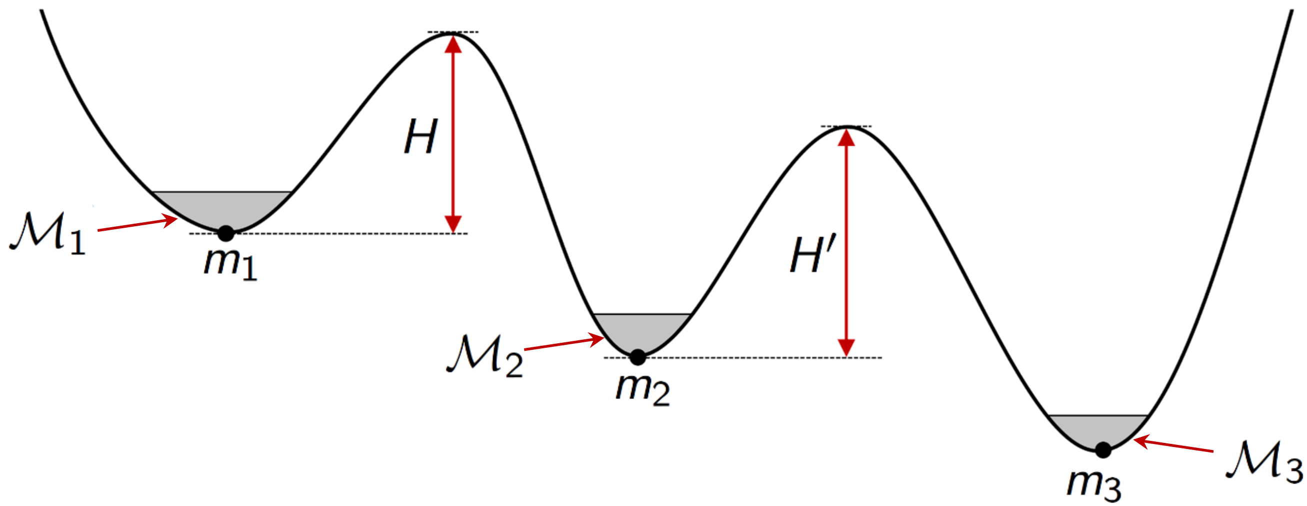
$$\begin{cases} u_t = \mathcal{L}_\epsilon u & \text{for } (t,x) \in (0,\infty) \times \mathbb{R}^d \\ u(0,x) = g(x) & \text{for } x \in \mathbb{R}^d \end{cases}$$

Probabilistic expression: $u(t,x) = \mathbb{E}[g(x_t) \,|\, x_0 = x]$

Landim-Lee-Seo, forthcoming

$$x \in \mathcal{M} \Rightarrow u(t_\epsilon, x) \simeq \begin{cases} g(m) & \text{if } t_\epsilon \ll \theta_\epsilon \\ p(t)g(m) + 1 - p(t)g(s) & \text{if } t_\epsilon = t\theta_\epsilon \\ g(s) & \text{if } t_\epsilon \gg \theta_\epsilon \end{cases}$$

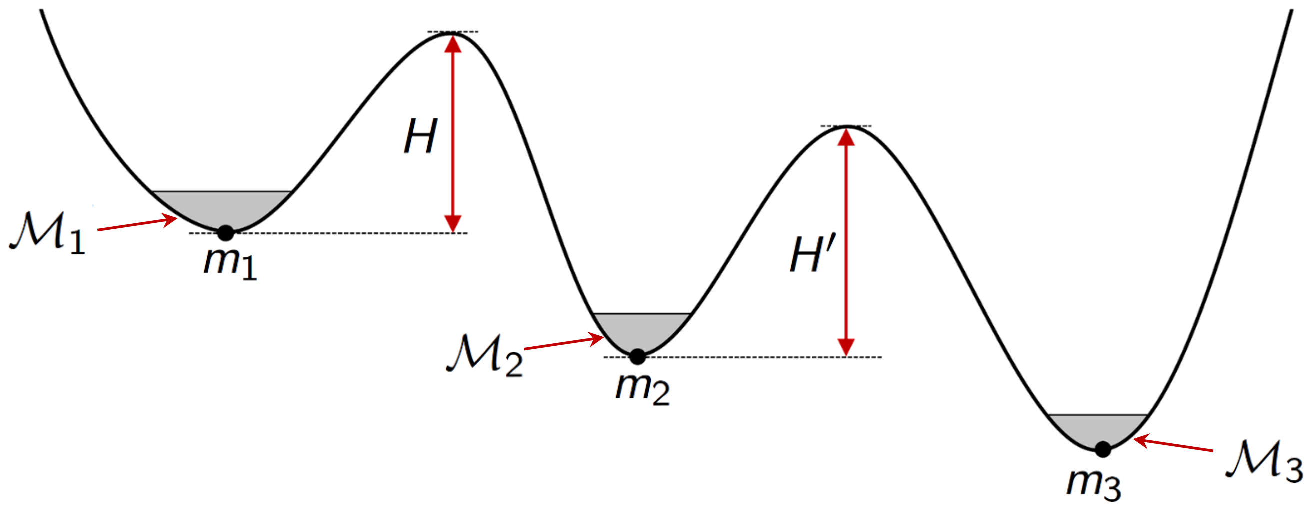
Difficulty in complex potential



(Case 1) $H < H'$: two-scales $\theta_\epsilon = e^{H/\epsilon}$ and $\sigma_\epsilon = e^{H'/\epsilon}$

- $t_\epsilon \ll \theta_\epsilon$ ➡ $\mathbb{P}(x_{t_\epsilon} \in \mathcal{M}_1) \simeq 1$
- $t_\epsilon = t\theta_\epsilon$ ➡ $\mathbb{P}(x_{t_\epsilon} \in \mathcal{M}_1) \simeq p(t)$ and $\mathbb{P}(x_{t_\epsilon} \in \mathcal{M}_2) \simeq 1 - p(t)$
- $\theta_\epsilon \ll t_\epsilon \ll \sigma_\epsilon$ ➡ $\mathbb{P}(x_{t_\epsilon} \in \mathcal{M}_2) \simeq 1$
- $t_\epsilon = t\sigma_\epsilon$ ➡ $\mathbb{P}(x_{t_\epsilon} \in \mathcal{M}_2) \simeq q(t)$ and $\mathbb{P}(x_{t_\epsilon} \in \mathcal{M}_3) \simeq 1 - q(t)$
- $t_\epsilon \gg \sigma_\epsilon$ ➡ $\mathbb{P}(x_{t_\epsilon} \in \mathcal{M}_3) \simeq 1$

Difficulty in complex potential



(Case 2) $H = H'$: complex behavior at scale $\theta_\epsilon = e^{H/\epsilon}$

- $t_\epsilon \ll \theta_\epsilon \implies \mathbb{P}(x_{t_\epsilon} \in \mathcal{M}_1) \simeq 1$
- $t_\epsilon = t\theta_\epsilon \implies \mathbb{P}(x_{t_\epsilon} \in \mathcal{M}_i) \simeq p_i(t)$ for $i = 1, 2, 3$
- $t_\epsilon \gg \theta_\epsilon \implies \mathbb{P}(x_{t_\epsilon} \in \mathcal{M}_3) \simeq 1$

Discussion on general SRPDS

Same questions for the **general** SRPDS

$$dx_t = b(x_t)dt + \sqrt{2\epsilon}dW_t$$

are widely open because of the following difficulties:

1. Complexity of the invariant measure
2. Generator is not self-adjoint

Remarks on invariant measure:

- Gradient model ($b = -\nabla U$) has Gibbs invariant measure $e^{-U(x)/\epsilon}$
- Friedlin-Wentzell decomposition: $b = -\nabla U + \ell$ with $\nabla U \cdot \ell \equiv 0$
- Gibbs invariant measure if and only if $\nabla \cdot \ell \equiv 0$
- Without condition $\nabla \cdot \ell \equiv 0$, invariant measure is highly complex; Bouchet-Reygner, 2016

Discussion on general SRPDS

Same questions for the **general** SRPDS

$$dx_t = b(x_t)dt + \sqrt{2\epsilon}dW_t$$

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- Friedlin-Wentzell decomposition: $b = -\nabla U + \ell$ with $\nabla U \cdot \ell \equiv 0$
- Gibbs invariant measure if and only if $\nabla \cdot \ell \equiv 0$

Metastability under Gibbs invariant measure

- Eyring-Kramers formula: Lee-Seo, 2022
- Spectral gap: Le Peutrec-Michel, 2021
- Distributions: Landim-Lee-See, forthcoming

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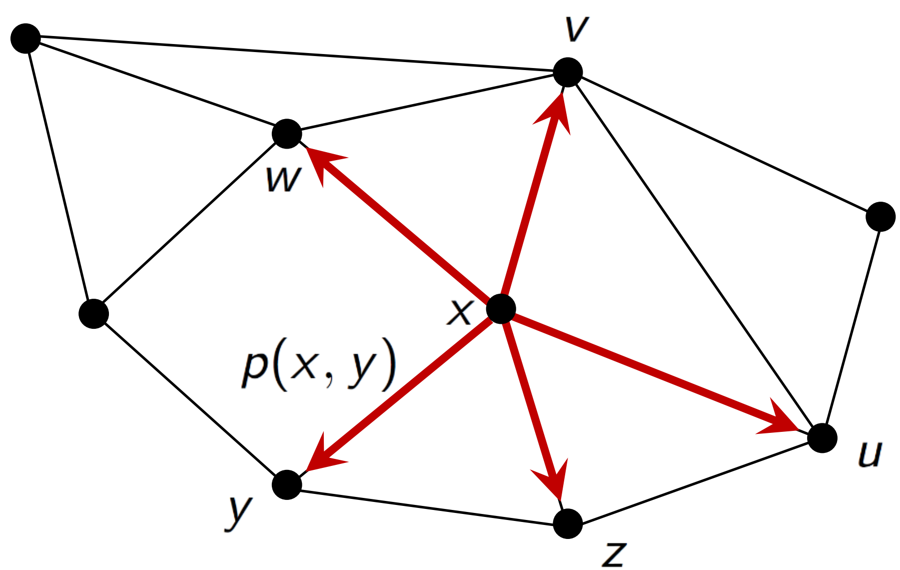
Markov process: discrete time

Discrete time Markov chain on finite set

$X_1, X_2, \ldots$ is called a **Markov chain** with jump probability $p(x, y)$ if it jumps from x to y with probability $p(x, y)$:

$$\mathbb{P}(X_{t+1} = y \,|\, X_t = x) = p(x, y)$$



$$p(x, y) + p(x, z) + p(x, w) + p(x, u) + p(x, v) = 1$$

Markov process: discrete time

Discrete time Markov chain on finite set

$X_1, X_2, \ldots$ is called a **Markov chain** with jump probability $p(x, y)$ if it jumps from x to y with probability $p(x, y)$:

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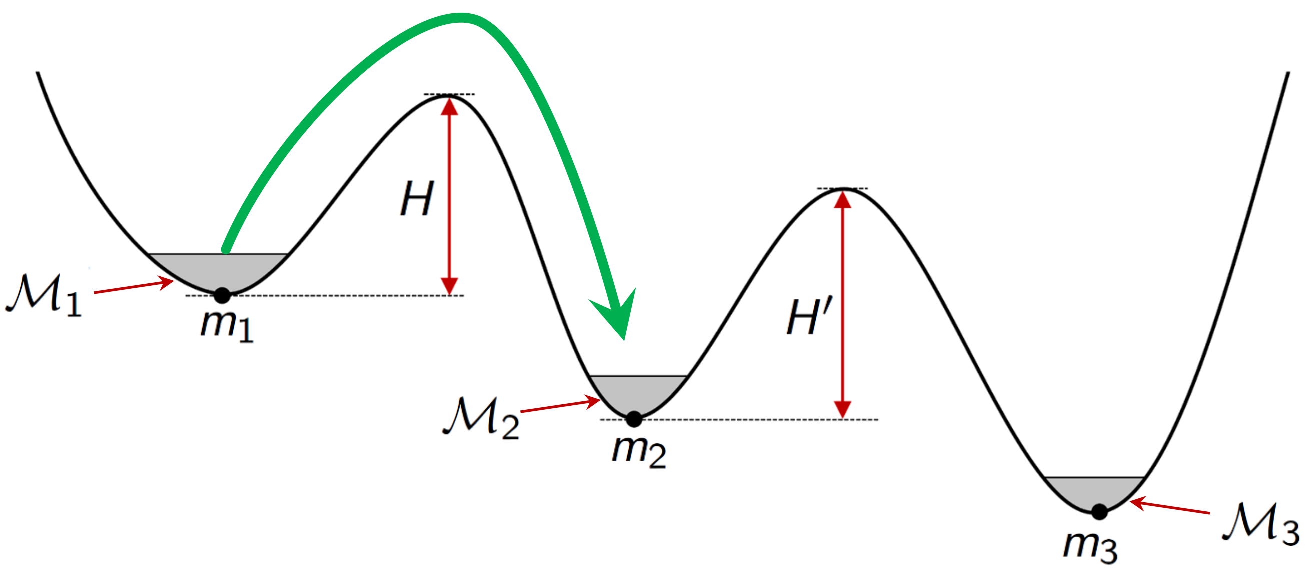


Jump from $\mathcal{M}_1$ to $\mathcal{M}_2$ after waiting a random amount of time

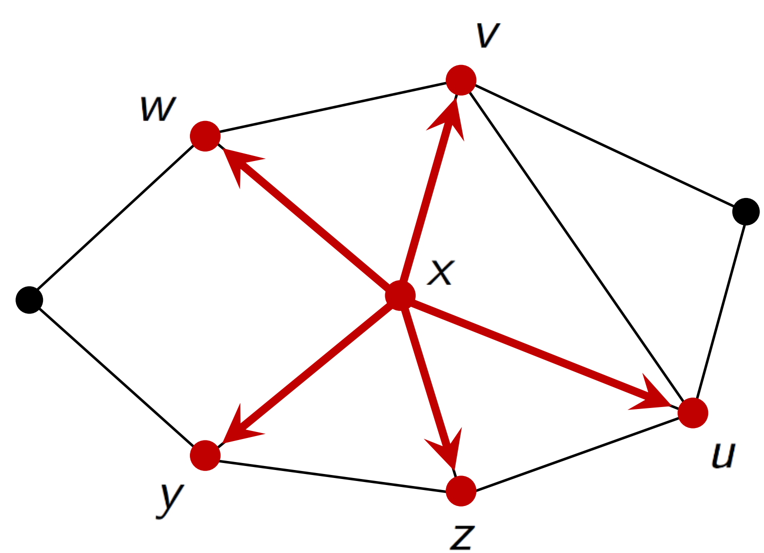
Markov process: continuous time

Continuous time Markov process on finite set

$(X_t)_{t\geq 0}$ is called a **Markov process** with jump rate $r(x,y)$ if

1. the process at x waits for random time of mean $\frac{1}{\sum_u r(x,u)}$
2. and then jumps to y with probability $\frac{r(x,y)}{\sum_u r(x,u)}$

- By increasing $r(\cdot,\cdot)$, not only jump probability is increased but also the jump occurs more quickly



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2. and then jumps to y with probability $\frac{r(x,y)}{\sum_u r(x,u)}$

- By increasing $r(\cdot,\cdot)$, not only jump probability is increased but also the jump occurs more quickly
- Associated generator L:

$$(Lf)(x) = \sum_u r(x,u)(f(u) - f(x))$$

- The generator L contains all the essential information

Markov process: continuous time

Continuous time Markov process on finite set

$(X_t)_{t\geq 0}$ is called a **Markov process** with jump rate $r(x, y)$ if

1. the process at x waits for random time of mean $\frac{1}{\sum_u r(x,u)}$
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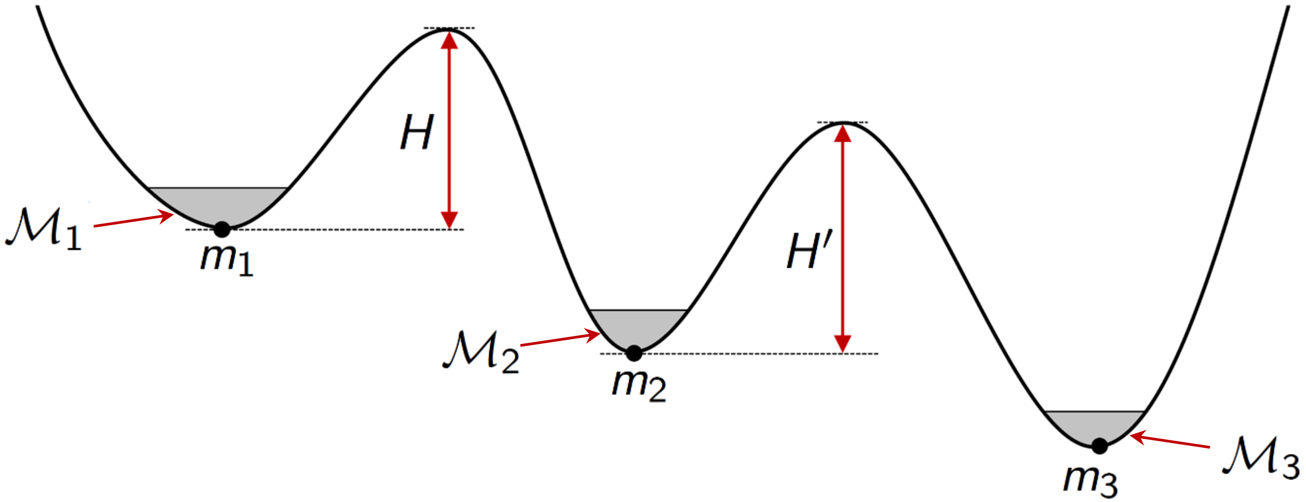
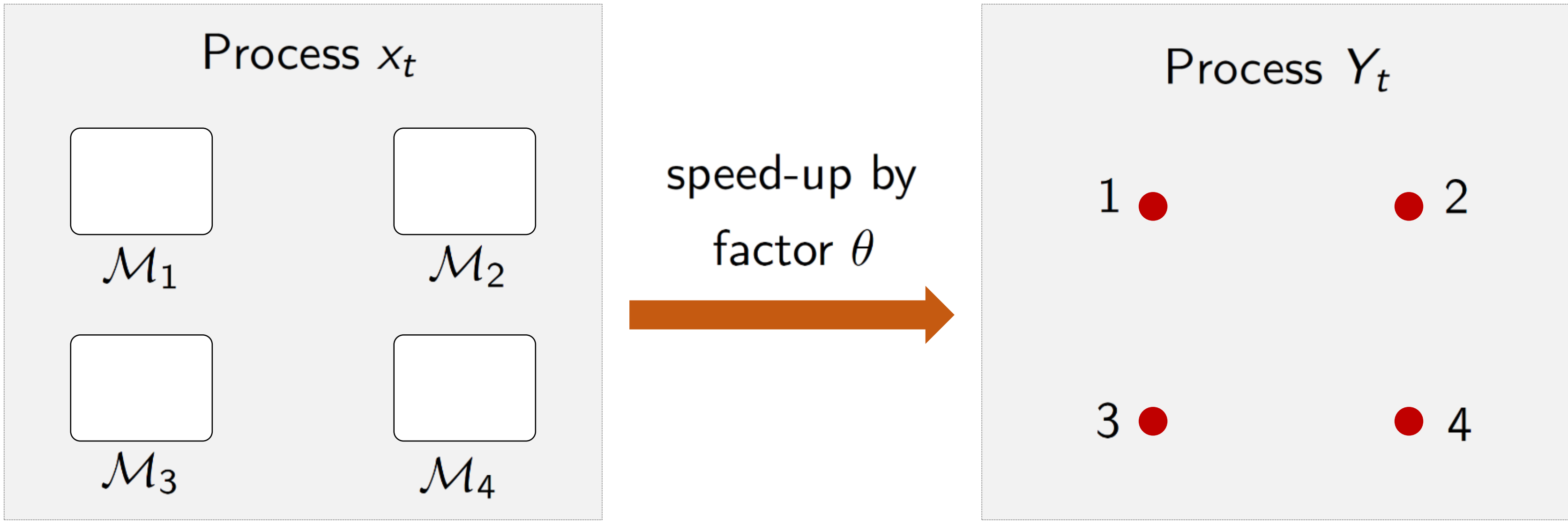


Metastable behavior of x_t is described by a MP on $\{1, 2, 3\}$

Description of metastable behavior



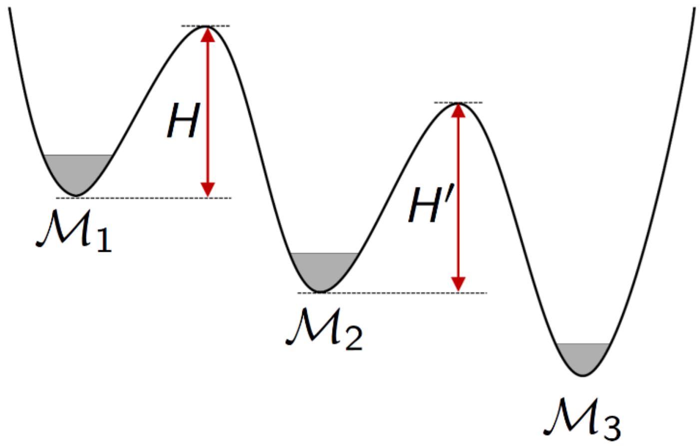
- x_t: metastable process
- Y_t: continuous time Markov process on $\{1, 2, 3, 4\}$

Description of metastable behavior

Metastable behavior of x_t is described by MP Y_t at time scale θ:

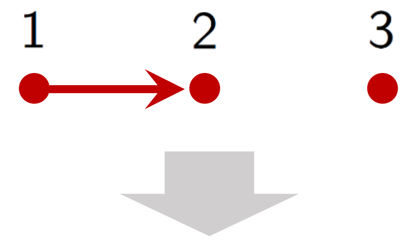
$$\mathbb{P}(x_{\theta t} \in \mathcal{M}_i) \simeq \mathbb{P}(Y_t = i)$$

Concluding remarks



Scale θ_ϵ

Markov process Y_t

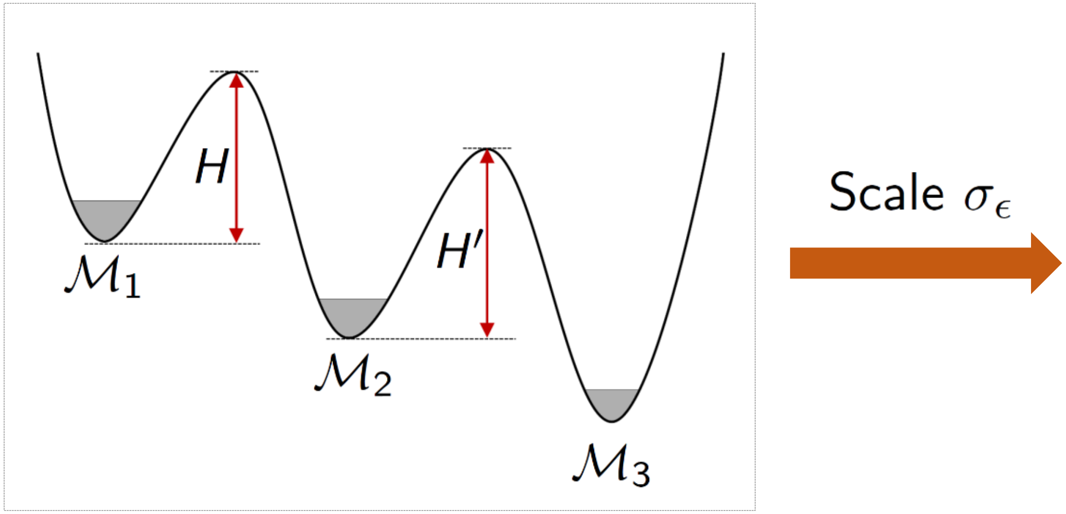


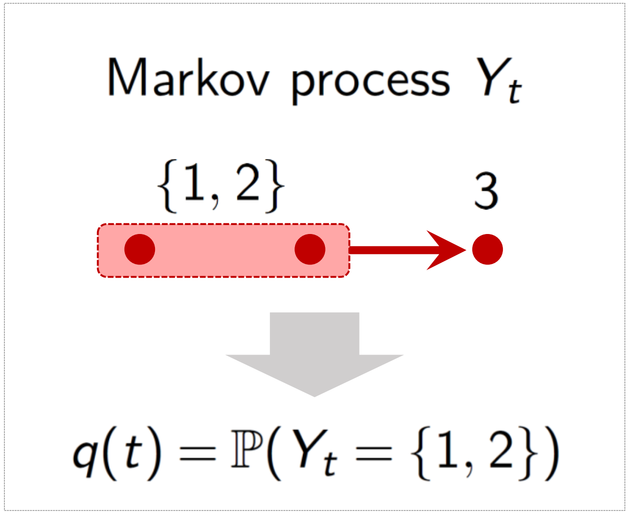
$p(t) = \mathbb{P}(Y_t = 1)$

(Case 1) $H < H'$: two-scales $\theta_\epsilon = e^{H/\epsilon}$ and $\sigma_\epsilon = e^{H'/\epsilon}$

- $t_\epsilon \ll \theta_\epsilon \Rightarrow \mathbb{P}(x_{t_\epsilon} \in \mathcal{M}_1) \simeq 1$
- $t_\epsilon = t\theta_\epsilon \Rightarrow \mathbb{P}(x_{t_\epsilon} \in \mathcal{M}_1) \simeq p(t)$ and $\mathbb{P}(x_{t_\epsilon} \in \mathcal{M}_2) \simeq 1 - p(t)$
- $\theta_\epsilon \ll t_\epsilon \ll \sigma_\epsilon \Rightarrow \mathbb{P}(x_{t_\epsilon} \in \mathcal{M}_2) \simeq 1$

Concluding remarks





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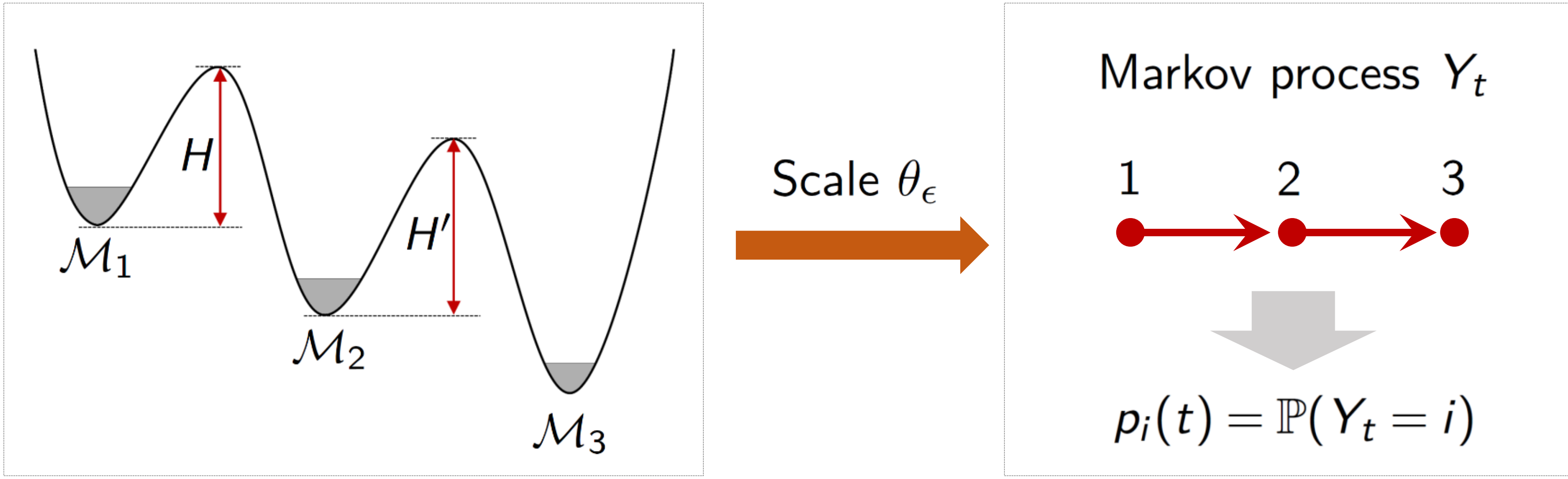
- $t_\epsilon \gg \sigma_\epsilon \Rightarrow \mathbb{P}(x_{t_\epsilon} \in \mathcal{M}_3) \simeq 1$

Concluding remarks



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- $t_\epsilon \gg \theta_\epsilon \Rightarrow \mathbb{P}(x_{t_\epsilon} \in \mathcal{M}_3) \simeq 1$

Remark. Jump rate of Y_t can be inferred from Eyring-Kramers formula

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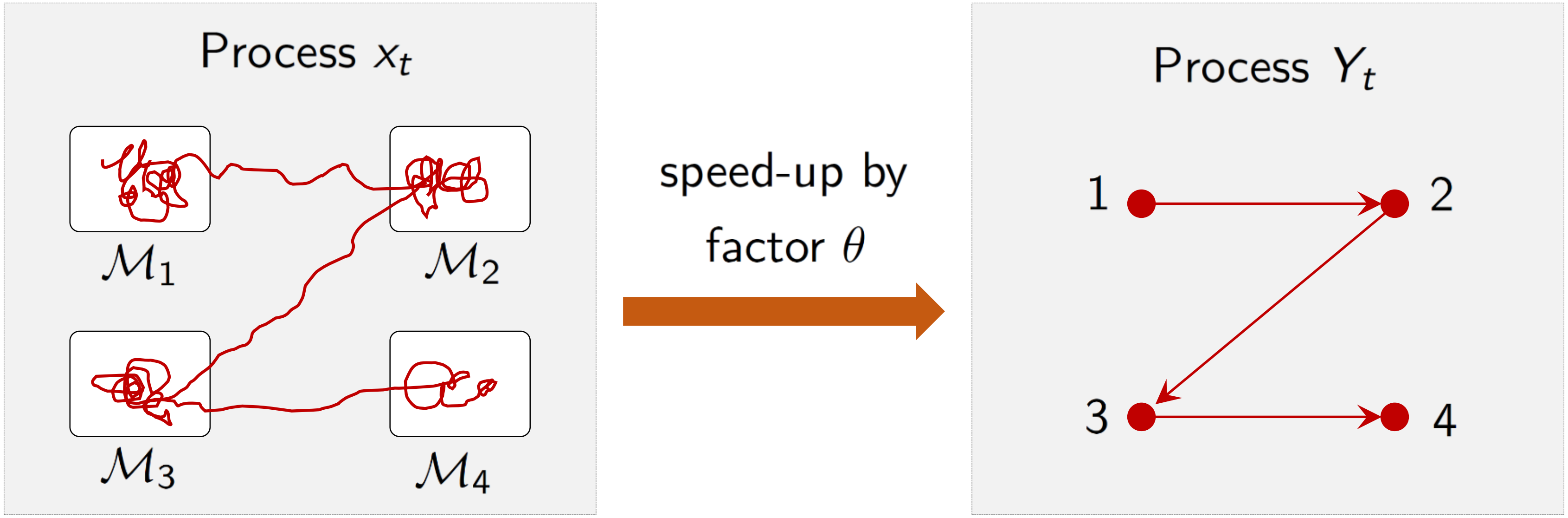
Negligibility of excursions

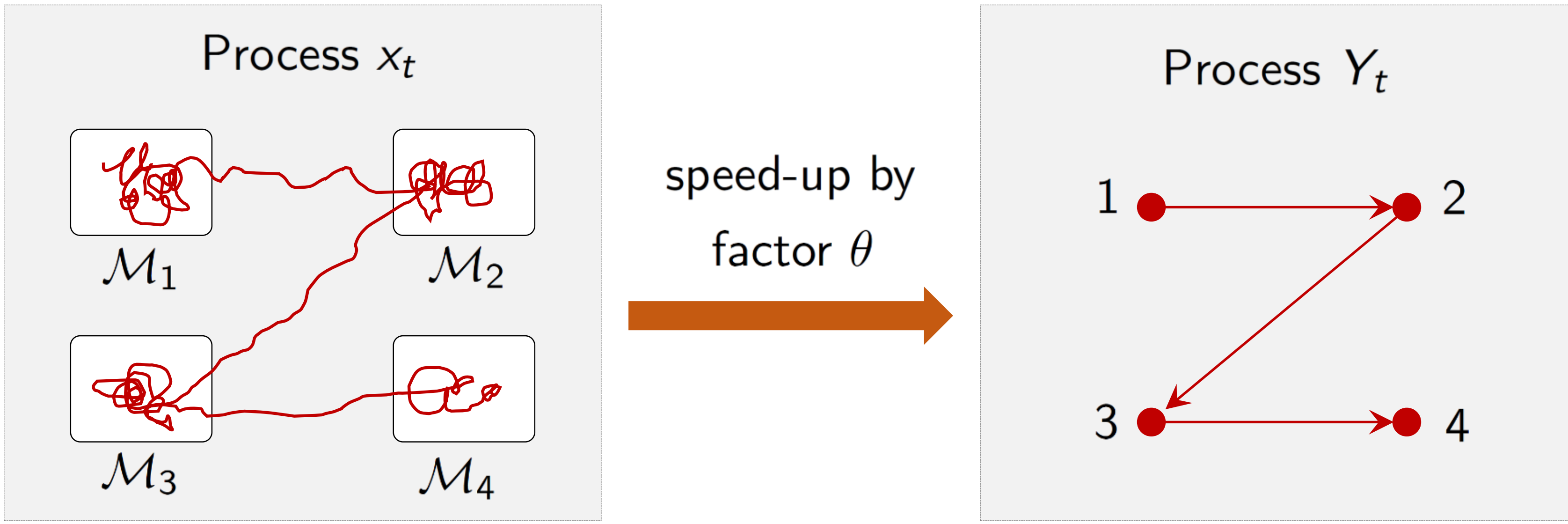


- Condition **(N)**: if the process x_t starts at a metastable set,

$$\mathbb{E}\left[\int_0^T \mathbf{1}\left(x_{\theta t} \notin \bigcup \mathcal{M}_i\right)\right] \simeq 0$$

Meaning: speeded-up process spends negligible amount of time outside of metastable sets

Description of metastable behavior

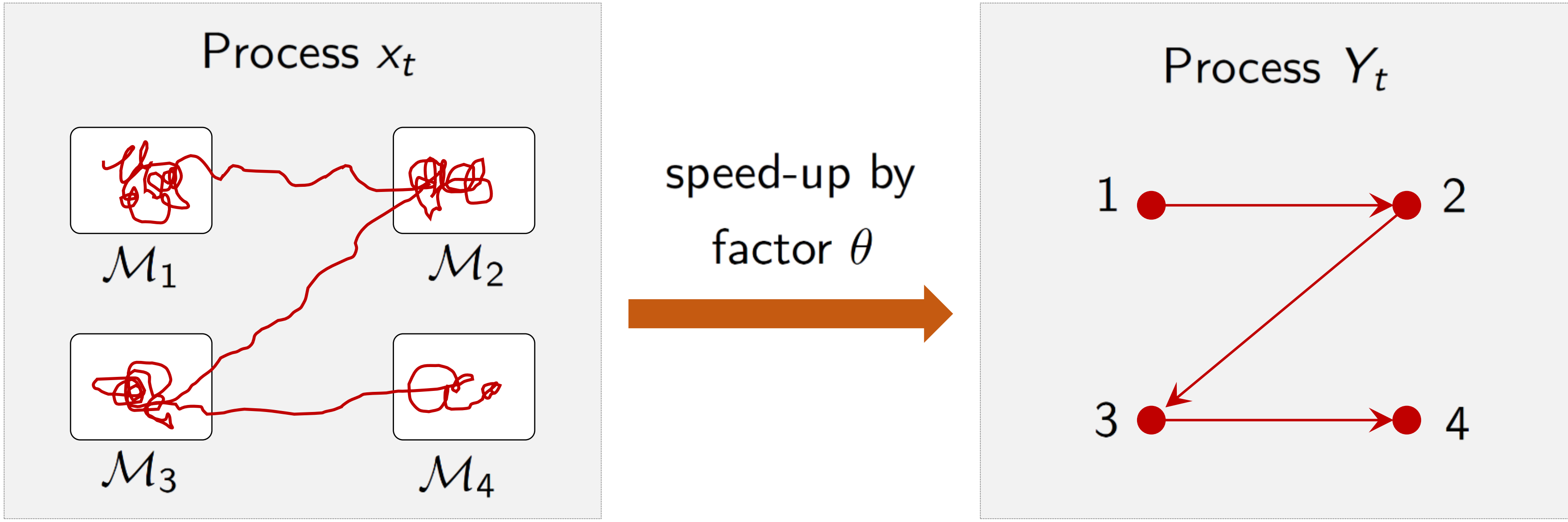


- Condition **(C)**: For all $t_1 < \cdots < t_k$ and $i_1, \ldots, i_k$,

$$\mathbb{P}(x_{\theta t_1} \in \mathcal{M}_{i_1}, \ldots, x_{\theta t_k} \in \mathcal{M}_{i_k}) \simeq \mathbb{P}(Y_{t_1} = i_1, \ldots, Y_{t_k} = i_k)$$

Meaning: the MP Y_t describes metastable behavior of the process x_t at time scale θ

Resolvent equation



- Condition **(R)**: For any $f : S \to \mathbb{R}$, the solution F of

$$\lambda F(x) - \theta(\mathcal{L}F)(x) = \sum_{i \in S} (\lambda f - Lf)(i) \mathbf{1}_{\mathcal{M}_i}(x)$$

satisfies $F(x) \simeq f(i)$ on each $\mathcal{M}_i$

- S: state space of Y_t (e.g., $S = \{1, 2, 3, 4\}$ for example above)
- $\mathcal{L}$: generator of x_t
- L: generator of Y_t

Main results

Landim-Marcondes-Seo, 2021

Under the condition **(N)**, the conditions **(C)** and **(R)** are equivalent

- Condition **(C)**: For all $t_1 < \cdots < t_k$ and $i_1, \ldots, i_k$,

$$\mathbb{P}(x_{\theta t_1} \in \mathcal{M}_{i_1}, \ldots, x_{\theta t_k} \in \mathcal{M}_{i_k}) \simeq \mathbb{P}(Y_{t_1} = i_1, \ldots, Y_{t_k} = i_k)$$

- Condition **(R)**: For any $f : S \to \mathbb{R}$, the solution F of

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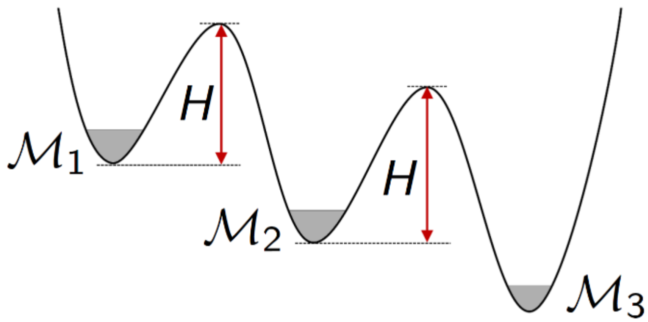
satisfies $F(x) \simeq f(i)$ on each $\mathcal{M}_i$

Remarks.

1. Condition **(N)** is a technical one and can be proven independently
2. Condition **(R)** implies condition **(N)**

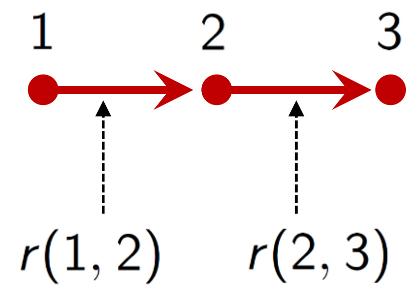
Application to SRPDS

$$dx_t = -\nabla U(x_t)dt + \sqrt{2\epsilon}\, dW_t$$



Scale θ_ϵ →

Markov process Y_t



- Generator of x_t ➡ $\mathcal{L}_\epsilon F = -\nabla U \cdot \nabla F + \epsilon \Delta F$
- Generator of Y_t ➡ $Lf(i) = \sum_j r(i,j)(f(j) - f(i))$
- Y_t decribes the metastable behavior of x_t at scale $\theta_\epsilon = e^{H/\epsilon}$ iff

  Condition **(R)** holds

The solution F of

$$(\lambda - \theta_\epsilon \mathcal{L}_\epsilon)F(x) = \sum_{i=1}^{3} (\lambda f - Lf)(i) \mathbf{1}_{\mathcal{M}_i}(x)$$

satisfies $\|F(x) - f(i)\|_{L^\infty(\mathcal{M}_i)} \to 0$ as $\epsilon \to 0$

Flatness of solutions

Condition **(R)**: For any $f : S \to \mathbb{R}$, the solution F of

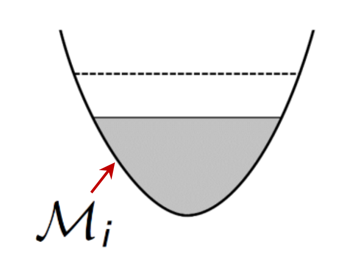
$$\lambda F(x) - \theta(\mathcal{L}F)(x) = \sum_{i \in S} (\lambda f - Lf)(i) \mathbf{1}_{\mathcal{M}_i}(x)$$

satisfies $F(x) \simeq f(i)$ on each $\mathcal{M}_i$

General flatness: Landim-Marcondes-Seo, 2021

There exists $c(i) \in \mathbb{R}$ such that $F(x) \simeq c(i)$ on $\mathcal{M}_i$ if

$$\text{mixing time} \ll \text{escape time} \qquad (1.1)$$



- Self-adjoint case: mixing time can be replaced with spectral gap^{-1}
- (1.1) has been verified for SRPDS
- Proving $c(i) \simeq f(i)$ is model dependent part

Concluding remarks

1. We developed several robust methods to prove $c(i) \simeq f(i)$

2. This method is also applied to
   - (Landim-Lee-Seo, forthcoming) SRPDS
     $$dx_t = b(x_t) + \sqrt{2\epsilon} W_t \tag{1.2}$$
     with Gibbs invariant measure, i.e. $b = -\nabla U + \ell$ with
     $$\nabla U \cdot \ell \equiv \nabla \cdot \ell \equiv 0$$
   - (Landim-Marcondes-Seo, 2021) Condensing interacting particle system with weak mixing property

3. We believe that the methodology is robust and can be applied to general SRPDS (1.2) as well

End of Presentation