Metastability of overdamped Langevin dynamics

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Analysis and simulations of metastable systems, CIRM

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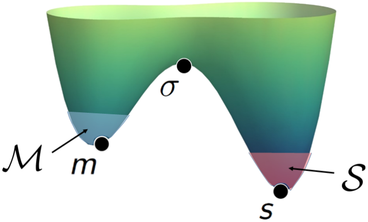
Langevin dynamics

Model: $dx_\epsilon(t) = -\nabla U(x_\epsilon(t))\,dt + \sqrt{2\epsilon}\,dw_t$

Potential U:



- w_t: Brownian motion
- $\epsilon > 0$: small parameter (temperature)

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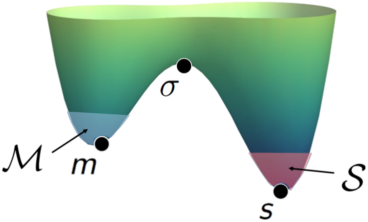
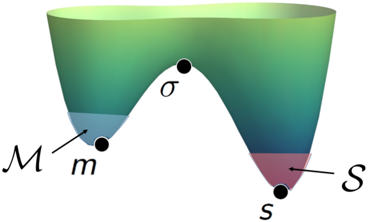


- $\boldsymbol{w}_t$: Brownian motion
- $\epsilon > 0$: small parameter (temperature)
- Gibbs invariant distribution: $\mu_\epsilon(d\boldsymbol{x}) \;=\; \frac{1}{Z_\epsilon}\, e^{-U(\boldsymbol{x})/\epsilon}\, d\boldsymbol{x}$
- Reversible w.r.t. $\mu_\epsilon(d\boldsymbol{x})$

Nonreversible dynamics

Model: $d\boldsymbol{y}_\epsilon(t) \;=\; -(\nabla U + \boldsymbol{\ell})(\boldsymbol{y}_\epsilon(t))\,dt + \sqrt{2\epsilon}\,d\boldsymbol{w}_t$

Quasi-Potential U:



Assumption: non-degenerate $U \in C^3(\mathbb{R}^d)$ and $\nabla U \cdot \boldsymbol{\ell} = 0$

Nonreversible dynamics

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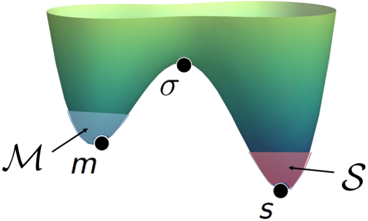

Assumption: non-degenerate $U \in C^3(\mathbb{R}^d)$ and $\nabla U \cdot \boldsymbol{\ell} = 0$

- Gibbs measure $\mu_\epsilon(d\boldsymbol{x})$ is the invariant distribution of $\boldsymbol{y}_\epsilon(\cdot)$ iff $\nabla \cdot \boldsymbol{\ell} = 0$

Expectation of transition time

- $\tau_{\mathcal{S}}$: (random) transition time
- Expectation of transition time: $\mathbb{E}_{\boldsymbol{m}}[\tau_{\mathcal{S}}]$
- Freidlin–Wentzell 70's:

$$\log \mathbb{E}_{\boldsymbol{m}}[\tau_{\mathcal{S}}] \simeq \frac{U(\boldsymbol{\sigma}) - U(\boldsymbol{m})}{\epsilon}$$

$\Rightarrow \mathbb{E}_{\boldsymbol{m}}[\tau_{\mathcal{S}}] \simeq f(\epsilon) \exp \frac{U(\boldsymbol{\sigma}) - U(\boldsymbol{m})}{\epsilon}$

- Eyring–Kramers formula: sharp asymptotics of $f(\epsilon)$.

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  - Reversible dynamics: Bovier–Eckhoff–Gayrard–Klein '04
  - Nonreversible dynamics: Landim–Marinai–Seo '19, L.–Seo '22
  - Degenerate saddle: Avelin–Julin–Vitasaari '22
  - Underdamped dynamics: S.Lee–Ramil–Seo '23+
  - General drift: Bouchet–Reygner '15

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- Spectral asymptotics
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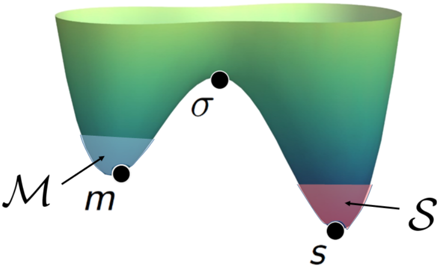
    - Nonreversible dynamics: Le Peutrec–Michel '20

Single transition

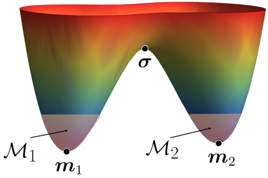


$$\log \mathbb{E}_{\boldsymbol{m}}[\tau_{\mathcal{S}}] \simeq \frac{U(\boldsymbol{\sigma}) - U(\boldsymbol{m})}{\epsilon}$$

$$\log \mathbb{E}_{\boldsymbol{s}}[\tau_{\mathcal{M}}] \simeq \frac{U(\boldsymbol{\sigma}) - U(\boldsymbol{s})}{\epsilon}$$

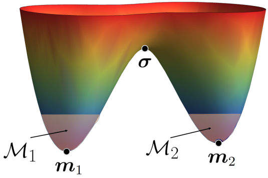
$$\mathbb{E}_{\boldsymbol{m}}[\tau_{\mathcal{S}}] \ll \mathbb{E}_{\boldsymbol{s}}[\tau_{\mathcal{M}}]$$

Successive transitions



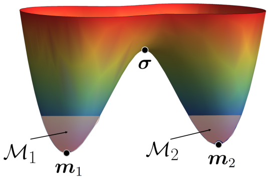
- $D = U(\boldsymbol{\sigma}) - U(\boldsymbol{m}_1)$: depth of wells

Successive transitions



- $D = U(\boldsymbol{\sigma}) - U(\boldsymbol{m}_1)$: depth of wells
- Successive transitions between $\boldsymbol{m}_1$ and $\boldsymbol{m}_2$ occur in time scale $\theta_\epsilon = e^{D/\epsilon}$
- Markov chain model reduction: describing successive transitions by much simpler Markov chain (macroscopic behavior)
  - Markov chain description: Beltrán–Landim '10 '12
  - Martingale approach: Beltrán–Landim '15
  - Reversible Langevin dynamics: Rezakhanlou–Seo '19
  - Nonreversible Langevin dynamics: L.–Seo '22

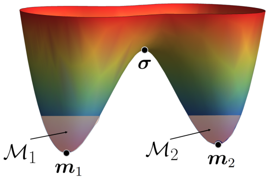
Markov chain model reduction



- $D = U(\boldsymbol{\sigma}) - U(\boldsymbol{m}_1)$ and $\theta_\epsilon = e^{D/\epsilon}$
- Limiting Markov chain **y**:

$$\boldsymbol{m}_1 \longleftrightarrow \boldsymbol{m}_2$$

Markov chain model reduction



- $D = U(\boldsymbol{\sigma}) - U(\boldsymbol{m}_1)$ and $\theta_\epsilon = e^{D/\epsilon}$
- Limiting Markov chain $\mathbf{y}$:

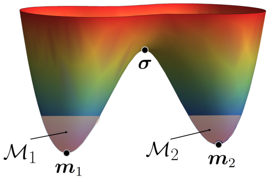
$$\boldsymbol{m}_1 \longleftrightarrow \boldsymbol{m}_2$$

Theorem ([Rezakhanlou–Seo '19], [L.–Seo '22])

Let $\mathbf{Q}_i$ be the law of $(\mathbf{y}(t))_{t\geq 0}$ starting at $i \in \{1, 2\}$. For $\boldsymbol{z} \in \mathcal{M}_i$,

$$\lim_{\epsilon\to 0} \mathbb{P}_{\boldsymbol{z}} \left[\boldsymbol{x}_\epsilon(\theta_\epsilon\, t_1) \in \mathcal{M}_{i_1}, \cdots, \boldsymbol{x}_\epsilon(\theta_\epsilon\, t_k) \in \mathcal{M}_{i_k}\right]$$
$$= \mathbf{Q}_i \left[\mathbf{y}(t_1) = i_1, \cdots, \mathbf{y}(t_k) = i_k\right] .$$

Markov chain model reduction



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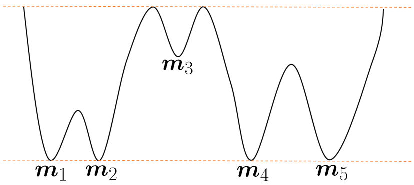
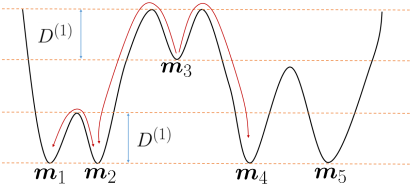
Metastable behavior of the process $\mathbf{x}_\epsilon$ in time scale θ_ϵ is described by Markov chain $\mathbf{y}$.

Complex potential



- Multiple time scales
- Hierarchical structure of metastability

Metastability in multiple time scales: 1st time scale



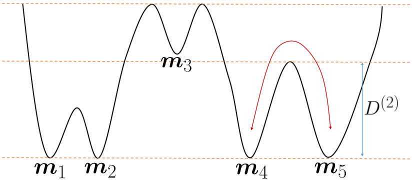
- $D^{(1)} = U(\sigma_1) - U(m_1)$ and $\theta_\epsilon^{(1)} = e^{D^{(1)}/\epsilon}$
- Limiting Markov chain $\mathbf{y}^{(1)}$:

$$m_1 \longleftrightarrow m_2 \leftarrow m_3 \rightarrow m_4 \quad m_5$$

Theorem ([L.–Landim–Seo '23+])

Metastable behavior of the process x_ϵ in time scale $\theta_\epsilon^{(1)}$ can be described by Markov chain $\mathbf{y}^{(1)}$.

Metastability in multiple time scales: 2nd time scale



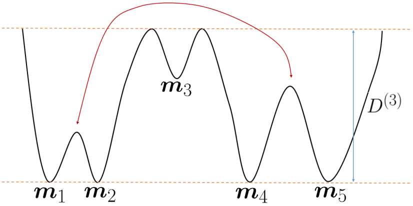
- $D^{(2)} = U(\sigma_4) - U(m_4)$ and $\theta_\epsilon^{(2)} = e^{D^{(2)}/\epsilon}$
- Limiting Markov chain $\mathbf{y}^{(2)}$:

$$\{m_1,\ m_2\} \quad m_4 \longleftrightarrow m_5$$

Theorem ([L.–Landim–Seo '23+])

Metastable behavior of the process x_ϵ in time scale $\theta_\epsilon^{(2)}$ can be described by Markov chain $\mathbf{y}^{(2)}$.

Metastability in multiple time scale: 3rd time scale



- $D^{(3)} = U(\boldsymbol{\sigma}_2) - U(\boldsymbol{m}_2)$ and $\theta_\epsilon^{(3)} = e^{D^{(3)}/\epsilon}$
- Limiting Markov chain $\mathbf{y}^{(3)}$:

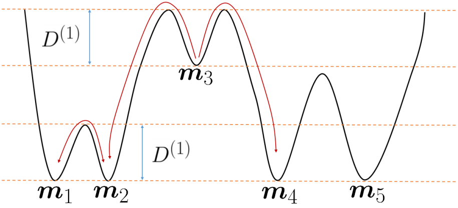
$$\{\boldsymbol{m}_1,\ \boldsymbol{m}_2\} \longleftrightarrow \{\boldsymbol{m}_4,\ \boldsymbol{m}_5\}$$

Theorem ([Rezakhanlou–Seo '19], [L.–Seo '22])

Metastable behavior of the process $\mathbf{x}_\epsilon$ in time scale $\theta_\epsilon^{(3)}$ can be described by Markov chain $\mathbf{y}^{(3)}$.

Hierarchy of metastability: 1st step

$\boldsymbol{m}_1 \quad \boldsymbol{m}_2 \quad \boldsymbol{m}_4 \quad \boldsymbol{m}_5 \quad \boldsymbol{m}_3$

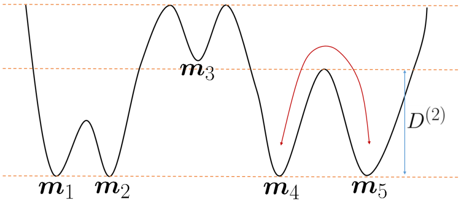


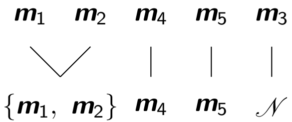
$$\boldsymbol{m}_1 \longleftrightarrow \boldsymbol{m}_2 \leftarrow \boldsymbol{m}_3 \rightarrow \boldsymbol{m}_4 \qquad \boldsymbol{m}_5$$

$\mathcal{M}_0$

- $\mathscr{V}^{(1)} = \{\boldsymbol{m}_1, \boldsymbol{m}_2, \boldsymbol{m}_3, \boldsymbol{m}_4, \boldsymbol{m}_5\}$
- $\mathscr{N}^{(1)} = \emptyset$

Hierarchy of metastability: 2nd step



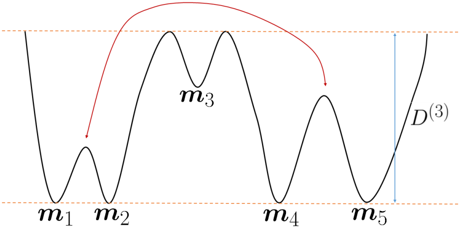


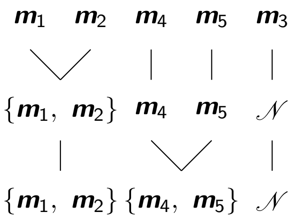
$\{m_1,\ m_2\}$ $m_4 \longleftrightarrow m_5$

$\mathcal{M}_0$

- $\mathscr{V}^{(2)} = \{\{m_1, m_2\}, m_4, m_5\}$
- $\mathscr{N}^{(2)} = \{m_3\}$

Hierarchy of metastability: 3rd step

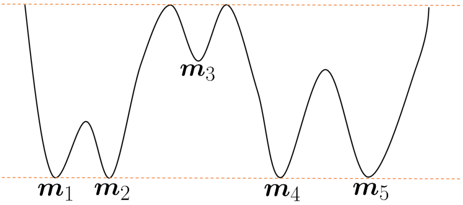




$$\{m_1,\ m_2\} \longleftrightarrow \{m_4,\ m_5\}$$

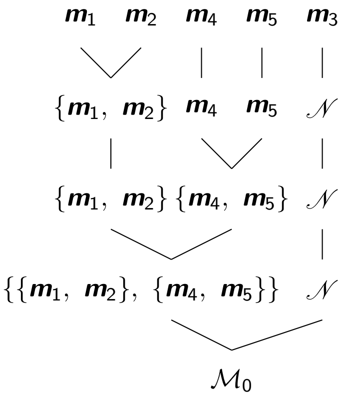
$\mathcal{M}_0$

- $\mathscr{V}^{(3)} = \{\{m_1,\ m_2\},\ \{m_4,\ m_5\}\}$
- $\mathscr{N}^{(3)} = \{m_3\}$



m_3
m_1 m_2 m_4 m_5

$\{m_1, m_2, m_4, m_5\}$



m_1 m_2 m_4 m_5 m_3
$\{m_1, m_2\}$ m_4 m_5 $\mathscr{N}$
$\{m_1, m_2\}$ $\{m_4, m_5\}$ $\mathscr{N}$
$\{\{m_1, m_2\}, \{m_4, m_5\}\}$ $\mathscr{N}$
$\mathcal{M}_0$

Generators of Markov processes

- Generator of $\boldsymbol{x}_\epsilon$:

$$\mathscr{L}_\epsilon f(\boldsymbol{x}) = -\nabla U(\boldsymbol{x}) \cdot \nabla f(\boldsymbol{x}) + \epsilon \Delta f(\boldsymbol{x})$$

- Generator of $\mathbf{y}$:

$$L_{\mathbf{y}} \mathbf{f}(i) = \sum_{j \in S} r(i, j) \mathbf{f}(i)$$

Proof: Resolvent equation approach

- Resolvent equation:

$$(\lambda - \theta_\epsilon \mathscr{L}_\epsilon)\, u(\boldsymbol{x}) = \sum_{i \in S} ((\lambda - L_{\mathbf{y}})\,\mathbf{f})\,(i)\mathbf{1}_{\mathcal{M}_i}(\boldsymbol{x})$$

- $\phi_\epsilon^{\mathbf{f},\,\lambda}$: unique solution of the resolvent equation

Theorem ([Landim–Marcondes–Seo '22])

If, for any $\mathbf{f} : S \to \mathbb{R}$ *and* $\lambda > 0$, $\phi_\epsilon^{\mathbf{f},\,\lambda}$ *satisfies*

$$\sup_{i \in S} \lim_{\epsilon \to 0} \|\phi_\epsilon^{\mathbf{f},\,\lambda} - \mathbf{f}(i)\|_{L^\infty(\mathcal{M}_i)} = 0 \;,$$

metastable behavior of the process $\boldsymbol{x}_\epsilon$ *in time scale* θ_ϵ *can be described by Markov chain* $\mathbf{y}$.

Proof: Resolvent equation approach

Theorem ([L.–Landim–Seo '23+])

Fix $\mathbf{f} : S \to \mathbb{R}$ *and* $\lambda > 0$. *Let* $\phi_\epsilon^{\mathbf{f},\lambda}$ *be the unique solution of*

$$(\lambda - \theta_\epsilon \mathscr{L}_\epsilon)\, u(\boldsymbol{x}) = \sum_{i \in S} ((\lambda - L_{\mathbf{y}})\, \mathbf{f})\,(i) \mathbf{1}_{\mathcal{M}_i}(\boldsymbol{x}) \ .$$

Then, for all $i \in S$, *we have*

$$\lim_{\epsilon \to 0} \| \phi_\epsilon^{\mathbf{f},\lambda} - \mathbf{f}(i) \|_{L^\infty(\mathcal{M}_i)} = 0 \ .$$

We can prove Markov chain convergence if we have the tightness and,

$$\text{(N)} \quad \lim_{\epsilon \to 0} \sup_{\boldsymbol{x} \in \bigcup_{i \in S} \mathcal{M}_i} \mathbb{E}_{\boldsymbol{x}}^\epsilon \left[\int_0^T \mathbf{1} \left\{ \boldsymbol{x}_\epsilon(\theta_\epsilon\, s) \notin \bigcup_{i \in S} \mathcal{M}_i \right\} ds \right] = 0 \text{ for all } T \geq 0 \, .$$

Identification of the limit point

- For all $\mathbf{f} : S \to \mathbb{R}$, $(M_\epsilon(t))_{t\geq 0}$ is a martingale where

$$M_\epsilon(t) = e^{-\lambda t}\phi_\epsilon^{\mathbf{f},\lambda}(\mathbf{x}_\epsilon(\theta_\epsilon t)) - \phi_\epsilon^{\mathbf{f},\lambda}(\mathbf{x}_\epsilon(0)) + \int_0^t e^{-\lambda s}(\lambda - \theta_\epsilon \mathscr{L}_\epsilon)\phi_\epsilon^{\mathbf{f},\lambda}(\mathbf{x}_\epsilon(\theta_\epsilon s))\, ds$$

- (Order process) $\xi_\epsilon(t) = i \quad \mathbf{x}_\epsilon(\theta_\epsilon t) \in \mathcal{M}_i$ so that

$$\sum_{i\in S} \mathbf{g}(i)\mathbf{1}_{\mathcal{M}_i}(\mathbf{x}_\epsilon(\theta_\epsilon t)) \simeq \mathbf{g}(\xi_\epsilon(t))$$

$$(\lambda - \theta_\epsilon \mathscr{L}_\epsilon)\,\phi_\epsilon^{\mathbf{f},\lambda}(\mathbf{x}) = \sum_{i\in S} ((\lambda - L_{\mathbf{y}})\,\mathbf{f})\,(i)\mathbf{1}_{\mathcal{M}_i}(\mathbf{x})$$

$$\int_0^t e^{-\lambda s}(\lambda - \theta_\epsilon \mathscr{L}_\epsilon)\,\phi_\epsilon^{\mathbf{f},\lambda}(\mathbf{x}_\epsilon(\theta_\epsilon s))\, ds = \int_0^t e^{-\lambda s} \sum_{i\in S} ((\lambda - L_{\mathbf{y}})\,\mathbf{f})\,(i)\mathbf{1}_{\mathcal{M}_i}(\mathbf{x}_\epsilon(\theta_\epsilon s)) \simeq \int_0^t e^{-\lambda s}\,((\lambda - L_{\mathbf{y}})\,\mathbf{f})\,(\xi_\epsilon(t))$$

Identification of the limit point

$$M_\epsilon(t) = e^{-\lambda t}\phi_\epsilon^{\mathbf{f},\lambda}(\mathbf{x}_\epsilon(\theta_\epsilon t)) - \phi_\epsilon^{\mathbf{f}}(\mathbf{x}_\epsilon(0)) + \int_0^t e^{-\lambda s}(\lambda - \theta_\epsilon \mathscr{L}_\epsilon)\phi_\epsilon^{\mathbf{f},\lambda}(\mathbf{x}_\epsilon(\theta_\epsilon s))\, ds$$

$$\lim_{\epsilon\to 0} \|\phi_\epsilon^{\mathbf{f},\lambda} - \mathbf{f}(i)\|_{L^\infty(\mathcal{M}_i)} = 0 ,$$

$$e^{-\lambda t}\phi_\epsilon^{\mathbf{f}}(\mathbf{x}_\epsilon(\theta_\epsilon t)) - \phi_\epsilon^{\mathbf{f}}(\mathbf{x}_\epsilon(0)) \simeq e^{-\lambda t}\mathbf{f}(\boldsymbol{\xi}_\epsilon(t)) - \mathbf{f}(\boldsymbol{\xi}_\epsilon(0))$$

$$M_\epsilon(t) \simeq e^{-\lambda t}\mathbf{f}(\boldsymbol{\xi}_\epsilon(t)) - \mathbf{f}(\boldsymbol{\xi}_\epsilon(0)) + \int_0^t e^{-\lambda s}\left((\lambda - L_{\mathbf{y}})\,\mathbf{f}\right)(\boldsymbol{\xi}_\epsilon(s))\, ds$$

$$\Longrightarrow \boldsymbol{\xi}_\epsilon(t) \simeq \mathbf{y}(t)$$

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$$\lim_{\epsilon\to 0} \|\phi_\epsilon^{\mathbf{f},\lambda} - \mathbf{f}(i)\|_{L^\infty(\mathcal{M}_i)} = 0\ ,$$

$$e^{-\lambda t}\phi_\epsilon^{\mathbf{f}}(\mathbf{x}_\epsilon(\theta_\epsilon\, t)) - \phi_\epsilon^{\mathbf{f}}(\mathbf{x}_\epsilon(0)) \simeq e^{-\lambda t}\mathbf{f}(\boldsymbol{\xi}_\epsilon(t)) - \mathbf{f}(\boldsymbol{\xi}_\epsilon(0))$$

$$M_\epsilon(t) \simeq e^{-\lambda t}\mathbf{f}(\boldsymbol{\xi}_\epsilon(t)) - \mathbf{f}(\boldsymbol{\xi}_\epsilon(0)) + \int_0^t e^{-\lambda s}\left((\lambda - L_{\mathbf{y}})\,\mathbf{f}\right)(\boldsymbol{\xi}_\epsilon(s))\, ds$$

$\implies \boldsymbol{\xi}_\epsilon(t) \simeq \mathbf{y}(t)$

Remark. $\mathbf{x}(\cdot)$ is a Markov Process with generator $L_{\mathbf{y}}$ if and only if

$$e^{-\lambda t}\mathbf{f}(\mathbf{x}(t)) - \mathbf{f}(\mathbf{x}(0)) + \int_0^t e^{-\lambda s}(\lambda - L_{\mathbf{y}})\,\mathbf{f}(\mathbf{x}(s))\, ds$$

is a martingale for all $\mathbf{f} : S \to \mathbb{R}$, for some $\lambda > 0$.

Other ingredients of proof

- Resolvent equation approach: Landim–Marcondes–Seo ’22

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- Resolvent equation approach: Landim–Marcondes–Seo '22
- Mixing condition: Barrera–Jara '20
- Finite dimensional convergence: Landim–Loulakis–Mourragui '18
- Exit from neighborhood of saddle point: Kifer '81

Thanks for your attention!
Merci beaucoup!