Properties and error analysis of the effective dynamics for diffusion processes

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Outline

- Effective dynamics
- Properties of effective dynamics on time scales
- Pathwise error estimates

Diffusion process

SDE on $\mathbb{R}^n$

$$dx(s) = -a\nabla V\, ds + \frac{1}{\beta}(\nabla \cdot a)\, ds + \sqrt{2\beta^{-1}}\sigma\, dw(s)\,, \quad s \geq 0\,.$$

Infinitesimal generator

$$\begin{aligned}\mathcal{L} =& - a\nabla V \cdot \nabla + \frac{1}{\beta}(\nabla \cdot a) \cdot \nabla + \frac{1}{\beta} a : \nabla^2 \\ =& \frac{e^{\beta V}}{\beta} \sum_{1\leq i,j\leq n} \frac{\partial}{\partial x_i}\Big(e^{-\beta V} a_{ij} \frac{\partial}{\partial x_j}\Big)\,.\end{aligned}$$

Invariant measure

$$d\mu = \rho(x)dx\,, \quad \rho(x) = \frac{1}{Z} e^{-\beta V}\,,$$

where $Z = \int_{\mathbb{R}^n} e^{-\beta V} dx$.

Assumptions: smooth coefficients, $a = \sigma\sigma^T$ is elliptic, $\cdots$.

Effective dynamics

Reaction coordinate: $\xi : \mathbb{R}^n \to \mathbb{R}^m$.

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Ito's formula

$$d\xi_l(x(s)) = \mathcal{L}\xi_l(x(s))ds + \sqrt{2\beta^{-1}} \sum_{i=1}^{n} \sum_{j=1}^{d} \frac{\partial \xi_l}{\partial x_i} \sigma_{ij}(x(s))\, dw_j(s)\,.$$

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This motivates the effective dynamics[1]

$$\boxed{dz(s) = \widetilde{b}(z(s))\, ds + \sqrt{2\beta^{-1}} \widetilde{\sigma}(z(s))\, dw(s)\,.}$$

For $z \in \mathbb{R}^m$, $1 \leq l, k \leq m$,

$$\widetilde{b}_l(z) = \mathbf{E}_{\mu_z}(\mathcal{L}\xi_l)\,,$$

$$(\widetilde{a})_{lk}(z) = (\widetilde{\sigma}\widetilde{\sigma}^T)_{lk}(z) = \mathbf{E}_{\mu_z}\Big(\sum_{i,j=1}^{n} a_{ij} \frac{\partial \xi_l}{\partial x_i} \frac{\partial \xi_k}{\partial x_j}\Big)\,.$$

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$$\Longleftrightarrow \quad \widetilde{b} = \mathbf{E}_{\mu_z}(\mathcal{L}\xi), \quad \widetilde{\sigma} = \Big[\mathbf{E}_{\mu_z}(\nabla\xi a \nabla\xi^T)\Big]^{\frac{1}{2}}.$$

1. Legoll and Lelièvre, Nonlinearity, 2010 .

Conditional expectation μ_z

On the level set $\Sigma_z = \left\{ x \in \mathbb{R}^n \;\middle|\; \xi(x) = z \right\}$, given by

$$d\mu_z(x) = \frac{1}{Q(z)} \rho(x) \Big[\det(\nabla \xi \nabla \xi^T)(x) \Big]^{-\frac{1}{2}} \, d\nu_z(x) \, .$$

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$\forall\, f : \mathbb{R}^n \to \mathbb{R}$, co-area formula gives

$$\begin{aligned}\int_{\mathbb{R}^n} f(x)\rho(x)\,dx &= \int_{\mathbb{R}^m}\Big(\int_{\Sigma_z} f(x)d\mu_z\Big)Q(z)\,dz \\ &= \int_{\mathbb{R}^m}\Big(\int_{\mathbb{R}^n} f(x)\rho(x)\delta(\xi(x)-z)dx\Big)\,dz\end{aligned}$$

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$$\begin{aligned}\implies \quad \mathbf{E}_{\mu_z}(f) &= \int_{\Sigma_z} f(x) d\mu_z \\ &= \frac{1}{Q(z)} \int_{\mathbb{R}^n} f(x)\rho(x)\delta(\xi(x) - z) dx \\ &= \mathbf{E}_{\mu}(f \,|\, \xi(x) = z)\,.\end{aligned}$$

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- Effective dynamics
- Properties of effective dynamics on time scales
- Pathwise error estimates

Generator of effective dynamics

$$\widetilde{\mathcal{L}} = \sum_{l=1}^{m} \widetilde{b}_l \frac{\partial}{\partial z_l} + \frac{1}{\beta} \sum_{l,l'=1}^{m} \widetilde{a}_{ll'} \frac{\partial^2}{\partial z_l \partial z_{l'}} \,.$$

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Suppose $f(x) = \widetilde{f}(\xi(x))$, $g(x) = \widetilde{g}(\xi(x))$. Using chain rules,

$$\mathcal{L}f = \sum_{l=1}^{m} (\mathcal{L}\xi_l) \frac{\partial \widetilde{f}}{\partial x_l} + \frac{1}{\beta} \sum_{l,l'=1}^{m} \Big(\sum_{i,j=1}^{n} a_{ij} \frac{\partial \xi_l}{\partial x_i} \frac{\partial \xi_{l'}}{\partial x_j} \Big) \frac{\partial^2 \widetilde{f}}{\partial z_l \partial z_{l'}}$$

$$\Longrightarrow \quad \int_{\mathbb{R}^n} (\mathcal{L}f)\, g \rho dx = \int_{\mathbb{R}^m} \mathbf{E}_{\mu_z} (\mathcal{L}f)\, \widetilde{g} Q(z)\, dz = \int_{\mathbb{R}^m} (\widetilde{\mathcal{L}}\widetilde{f})\, \widetilde{g} Q(z)\, dz \,.$$

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Proposition 1

The effective dynamics is both reversible and ergodic. And the invariant measure $\widetilde{\mu}$ is given by $d\widetilde{\mu} = Q(z)\, dz$.

Time scales

Let φ_i be the orthonormal eigenfunctions of operator $-\mathcal{L}$, i.e., $-\mathcal{L}\varphi_i = \lambda_i \varphi_i$, with eigenvalues

$$0 = \lambda_0 < \lambda_1 \leq \lambda_2 \leq \cdots .$$

Similarly, let $\widetilde{\varphi}_i$ be the orthonormal eigenfunctions of operator $-\widetilde{\mathcal{L}}$ corresponding to eigenvalues $\widetilde{\lambda}_i$, where

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Theorem 1 (Min-Max)

$$\lambda_i = \min_{H_{i+1}} \max_{f \in H_{i+1},\, |f|_\mu = 1} \langle -\mathcal{L} f, f \rangle_\mu ,$$

for $i \ge 0$, where H_{i+1} is $(i+1)$-dimensional subspaces.

Time scales

Proposition 2

$$\lambda_i \leq \widetilde{\lambda}_i \leq \lambda_i + \frac{1}{\beta}\langle a\nabla(\varphi_i - \widetilde{\varphi}_i \circ \xi), \nabla(\varphi_i - \widetilde{\varphi}_i \circ \xi)\rangle_\mu \,.$$

Time scales

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$$\lambda_i \leq \widetilde{\lambda}_i \leq \lambda_i + \frac{1}{\beta}\langle a\nabla(\varphi_i - \widetilde{\varphi}_i \circ \xi), \nabla(\varphi_i - \widetilde{\varphi}_i \circ \xi)\rangle_\mu \,.$$

Particularly, if

$$\begin{aligned} \boldsymbol{\varphi}(x) &= \big(\varphi_1(x), \varphi_2(x), \cdots, \varphi_m(x)\big) \in \mathbb{R}^m\,, \\ \xi(x) &= F \circ \boldsymbol{\varphi}(x) \in \mathbb{R}^m\,, \end{aligned}$$

we have

$$\widetilde{\lambda}_i = \lambda_i\,, \quad 0 \leq i \leq m\,.$$

1. Zhang, Hartmann and Schütte, Faraday Discuss., 2016.
2. Nüske, 2018.

Reaction rate

Disjoint sets $A, B \subset \mathbb{R}^n$.

k_{AB}: transition rate between A and B in TPT theory [1,2] :

$$k_{AB} = \frac{1}{\beta} \int_{(A\cup B)^c} \sum_{i,j=1}^{n} a_{ij}(x) \frac{\partial q(x)}{\partial x_i} \frac{\partial q(x)}{\partial x_j} \rho(x)\, dx \,,$$

where q is the committor satisfying

$$\begin{aligned} \mathcal{L}q &= 0, \quad x \in (A \cup B)^c \\ q|_A &= 0, \quad q|_B = 1 \,, \end{aligned}$$

1. Vanden-Eijnden, 2006.
2. E and Vanden-Eijnden, Annu. Rev. Phys. Chem. , 2010.

Reaction rate

Suppose $A = \xi^{-1}(\widetilde{A})$, $B = \xi^{-1}(\widetilde{B})$.

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Proposition 3

$$k_{AB} \leq \widetilde{k}_{\widetilde{A}\widetilde{B}} = k_{AB} + \frac{1}{\beta} \int_{(A\cup B)^c} \sum_{i,j=1}^{n} a_{ij} \frac{\partial(q - \widetilde{q} \circ \xi)}{\partial x_i} \frac{\partial(q - \widetilde{q} \circ \xi)}{\partial x_j} \rho \, dx \,,$$

where $\widetilde{q}$ is committor of effective dynamics.

Again, if $\xi(x) = q(x)$, then $\widetilde{k}_{\widetilde{A}\widetilde{B}} = k_{AB}$.

1. Lu and Vanden-Eijnden, J. Chem. Phys., 2014.

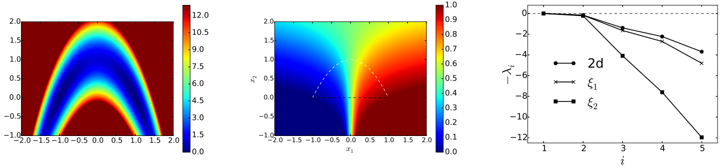
2. Zhang, Hartmann and Schütte, Faraday Discuss., 2016.

Simple 2D Example

$$V_\epsilon(x_1, x_2) = \left(x_1^2 - 1\right)^2 + \frac{1}{\epsilon}\left(x_1^2 + x_2 - 1\right)^2 ,$$

$$\xi_1(x_1, x_2) = x_1 \exp(-2x_2) \quad \text{and} \quad \xi_2(x_1, x_2) = x_1$$

$$\beta = 2.0 , \quad \epsilon = 0.1 .$$



(a) Potential (b) Committor (c) Eigenvalues

k_{AB}	ξ_1	ξ_2
3.0×10^{-2}	3.3×10^{-2}	4.8×10^{-2}

Table: Reaction rate k_{AB}

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Pathwise error estimates

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$$d\xi(x(s)) = (\mathcal{L}\xi)(x(s))\,ds + \sqrt{2\beta^{-1}}(\nabla\xi\sigma)\big(x(s)\big)\,dw(s)\,,$$

$$\begin{aligned} dz(s) &= \widetilde{b}(z(s))\,ds + \sqrt{2\beta^{-1}}\widetilde{\sigma}(z(s))\,d\widetilde{w}(s) \\ &= \mathbf{E}_{\mu_z}(\mathcal{L}\xi)(z(s))\,ds + \sqrt{2\beta^{-1}}\big[\mathbf{E}_{\mu_z}(\nabla\xi a \nabla\xi^T)\big]^{\frac{1}{2}}(z(s))\,d\widetilde{w}(s)\,. \end{aligned}$$

Two guiding examples: linear case 1

Linear reaction coordinate:

$$\xi(x) = (x_1, x_2, \cdots, x_m)^T = z\,, \qquad x = (z, y) \in \mathbb{R}^m \times \mathbb{R}^{n-m}\,.$$

Choose

$$V(z,y) = V_0(z,y) + \frac{1}{\epsilon} V_1(y), \quad 0 < \epsilon \ll 1$$
$$a = \sigma = I_{n\times n}$$

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$\Longrightarrow$ SDE becomes

$$dz_i(s) = -\frac{\partial V_0}{\partial z_i}\big(z(s), y(s)\big)\,ds + \sqrt{2\beta^{-1}}dw_i(s)\,,$$
$$dy_j(s) = -\frac{\partial V_0}{\partial y_j}\big(z(s), y(s)\big)\,ds - \frac{1}{\epsilon}\frac{\partial V_1}{\partial y_j}\big(y(s)\big)\,ds + \sqrt{2\beta^{-1}}\,dw_j(s)\,.$$

Two guiding examples: linear case 2

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Choose

$$\sigma \equiv \begin{pmatrix} I_{m\times m} & 0 \\ 0 & \frac{1}{\sqrt{\delta}} I_{(n-m)\times(n-m)} \end{pmatrix}\,, \quad 0 < \delta \ll 1$$

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(1) is the "averaging system" in the study of multiscale dynamics.

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Facts:

1. $\mathbb{R}^n = \mathbb{R}^m \times \mathbb{R}^{n-m}$.
2. $\rho_z(y) \propto e^{-\beta V(z,y)}$ is the density used to perform "averaging", for fixed z.
3. $\mathcal{L} = \frac{1}{\delta}\mathcal{L}_0 + \mathcal{L}_1$, s.t. $\int_{\mathbb{R}^{n-m}} (\mathcal{L}_0 f)\rho_z dy = 0$, $\forall f$ on $\mathbb{R}^{n-m}$.
4. δ: time scale separation.

1. Pavliotis and Stuart, 2008.

General case

For a general mapping $\xi : \mathbb{R}^n \to \mathbb{R}^m$, we have

1. $\Sigma_z = \left\{ x \in \mathbb{R}^n \;\middle|\; \xi(x) = z \right\}$.
2. $d\mu_z(x) = \frac{1}{Q(z)}\rho(x)\Big[\det(\nabla\xi\nabla\xi^T)(x)\Big]^{-\frac{1}{2}} d\nu_z(x)\,.$

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3. $\mathcal{L} = \mathcal{L}_0 + \mathcal{L}_1$, where

$$\mathcal{L}_0 = \frac{e^{\beta V}}{\beta} \sum_{1\le i,j\le n} \frac{\partial}{\partial x_i}\left(e^{-\beta V} (a\Pi)_{ij} \frac{\partial}{\partial x_j} \right),$$

$$\Pi = I - \sum_{1\le i,j\le m} (\Phi^{-1})_{ij} \nabla\xi_i \otimes (a\nabla\xi_j), \quad \Phi = \nabla\xi a \nabla\xi^T.$$

$$\Longrightarrow \quad \int_{\Sigma_z} (\mathcal{L}_0 f) d\mu_z = 0, \quad \forall\, f : \Sigma_z \to \mathbb{R}.$$

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$$\Longrightarrow \quad \int_{\Sigma_z} (\mathcal{L}_0 f) d\mu_z = 0, \quad \forall\, f : \Sigma_z \to \mathbb{R}.$$

4. $\mathcal{E}_z(f, h) = -\int_{\Sigma_z} (\mathcal{L}_0 f)\, h\, d\mu_z = \frac{1}{\beta}\int_{\Sigma_z} (a\Pi\nabla f)\cdot(\Pi\nabla h)\, d\mu_z$.

1. Lelièvre and Zhang, 2018.

Pathwise error estimates: Assumptions

1. $|\widetilde{b}(z) - \widetilde{b}(z')| \leq L_b|z - z'|\,, \quad \left\|\widetilde{\sigma}(z) - \widetilde{\sigma}(z')\right\|_F \leq L_\sigma|z - z'|\,.$

2. Define $A = \left(\nabla\xi a \nabla\xi^T\right)^{\frac{1}{2}}$, and
$$\kappa_1^2 := \sum_{i=1}^{m} \int_{\mathbb{R}^n} (\Pi\nabla\mathcal{L}\xi_i)\cdot(a\Pi\nabla\mathcal{L}\xi_i)\, d\mu < +\infty\,,$$
$$\kappa_2^2 := \sum_{1\leq i,j\leq m} \int_{\mathbb{R}^n} (\Pi\nabla A_{ij})\cdot(a\Pi\nabla A_{ij})\, d\mu < +\infty\,.$$

3. μ_z and $\mathcal{E}_z$ satisfy the Poincaré inequality with a uniform constant $\rho > 0$, i.e.,
$$\int_{\Sigma_z} f^2\, d\mu_z - \Big(\int_{\Sigma_z} f\, d\mu_z\Big)^2 \leq \frac{1}{\rho}\mathcal{E}_z(f,f)\,, \quad \forall\, f : \Sigma_z \to \mathbb{R}\,.$$

Pathwise error estimates

Theorem 2

$x(s)$ satisfies

$$dx(s) = -a\nabla V\, ds + \frac{1}{\beta}(\nabla\cdot a)\, ds + \sqrt{2\beta^{-1}}\sigma\, dw(s)\,,\quad s \geq 0\,,$$

starting from $x(0)\sim\mu$, and $z(s)$ is the effective dynamics

$$dz(s) = \widetilde{b}(z(s))\, ds + \sqrt{2\beta^{-1}}\widetilde{\sigma}(z(s))\, d\widetilde{w}(s)\,,$$

with $z(0)=\xi(x(0))$. For all $t\geq 0$,

$$\mathbf{E}\Big(\sup_{0\leq s\leq t}\big|\xi(x(s)) - z(s)\big|^2\Big) \leq \frac{3t}{\beta\rho}\Big(\frac{27\kappa_1^2}{2\rho} + \frac{32\kappa_2^2}{\beta}\Big)e^{Lt}\,,$$

where $L = 3L_b^2 + \frac{48L_\sigma^2}{\beta} + 1$.

1. Lelièvre and Zhang, 2018.

Pathwise error estimates: proof

1. Coupling of noise: $d\widetilde{w}(s) = \left(A^{-1}\nabla\xi\sigma\right)(x(s))\,dw(s)$, $A = \left(\nabla\xi a \nabla\xi^T\right)^{\frac{1}{2}}$.

1. Legoll, Lelièvre and Olla, Stoch. Process. Appl., 2017.
2. Lyons and Zhang, Ann. Probab., 1994.

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2. $\varphi(x) = (\mathcal{L}\xi)(x) - \widetilde{b}(\xi(x))\,, \quad \forall\, x \in \mathbb{R}^n$.

$$d\big(\xi(x(s)) - z(s)\big)$$
$$= \varphi(x(s))\,ds + \Big[\widetilde{b}(\xi(x(s))) - \widetilde{b}(z(s))\Big]\,ds + \sqrt{2\beta^{-1}}\Big[A(x(s)) - \widetilde{\sigma}(z(s))\Big]\,d\widetilde{w}(s)\,.$$

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3. Forward-backward Martingale approach[1,2]

$$\Longrightarrow \qquad \mathbf{E}\bigg[\sup_{0\le t'\le t}\Big|\int_0^{t'}\varphi(x(s))\,ds\Big|^2\bigg] \le \frac{27\kappa_1^2 t}{2\beta\rho^2}\,.$$

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2. Lyons and Zhang, Ann. Probab., 1994.

Pathwise error estimates: proof

1. Coupling of noise: $d\widetilde{w}(s) = \left(A^{-1}\nabla\xi\sigma\right)(x(s))\,dw(s)$, $A = \left(\nabla\xi a \nabla\xi^T\right)^{\frac{1}{2}}$.
2. $\varphi(x) = (\mathcal{L}\xi)(x) - \widetilde{b}(\xi(x))\,, \quad \forall\, x \in \mathbb{R}^n$.
$$\begin{aligned} & d\big(\xi(x(s)) - z(s)\big) \\ = & \varphi(x(s))\,ds + \Big[\widetilde{b}(\xi(x(s))) - \widetilde{b}(z(s))\Big]\,ds + \sqrt{2\beta^{-1}}\Big[A(x(s)) - \widetilde{\sigma}(z(s))\Big]\,d\widetilde{w}(s)\,. \end{aligned}$$
3. Forward-backward Martingale approach[1,2]
$$\Longrightarrow \qquad \mathbf{E}\left[\sup_{0\le t'\le t}\left|\int_0^{t'}\varphi(x(s))\,ds\right|^2\right] \le \frac{27\kappa_1^2 t}{2\beta\rho^2}\,.$$
4. $\widetilde{\sigma} = \left[\mathbf{E}_{\mu_z}(A^2)\right]^{\frac{1}{2}}$. Lieb's concavity theorem
$$\Longrightarrow \quad \mathbf{E}_{\mu_z}\left\|A - \widetilde{\sigma}\circ\xi\right\|_F^2 \le 2\,\mathbf{E}_{\mu_z}\left\|A - (\mathbf{E}_{\mu_z}A)\circ\xi\right\|_F^2\,.$$

1. Legoll, Lelièvre and Olla, Stoch. Process. Appl., 2017.
2. Lyons and Zhang, Ann. Probab., 1994.

Pathwise error estimates: linear cases

Corollary 3

Let $x = (z, y)$ *and* $\xi(x) = z$*.* $L = 3L_b^2 + \frac{48L_\sigma^2}{\beta} + 1$*.*

1. *(Case 1) Potential* $V = V_0 + \frac{1}{\epsilon}V_1$*.* $\exists \epsilon_0 \geq 0$*, s.t. when* $\epsilon \leq \epsilon_0$*,*

$$\mathbf{E}\Big(\sup_{0\leq s\leq t}\big|\xi(x(s)) - z(s)\big|^2\Big) \leq \frac{C_2\epsilon^2 t}{K^2}e^{Lt}\,,$$

   for some $C_2 > 0$ *independent of* ϵ *and* K*.*

2. *(Case 2) We have*

$$\mathbf{E}\Big(\sup_{0\leq s\leq t}\big|\xi(x(s)) - z(s)\big|^2\Big) \leq \frac{C_2\delta t}{\rho_0^2}e^{Lt}\,,$$

   for some $C_2 > 0$ *independent of* δ *and* ρ_0*.*

Conclusion

Summary

1. effective dynamics
2. properties on eigenvalues and reaction rates
3. pathwise estimates (nonlinear, vector-valued ξ)

Related topics

1. numerical methods
2. non-reversible case   (U. Sharma)

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Thank you !