Model reduction in stochastic dynamics and applications to Molecular Dynamics

Frédéric Legoll

Ecole des Ponts & project-team MATHERIALS, INRIA Paris

Joint with T. Lelièvre (ENPC and INRIA), U. Sharma (ENPC) and S. Olla (CEREMADE)

IPAM long program on Complex High-Dimensional Energy Landscapes

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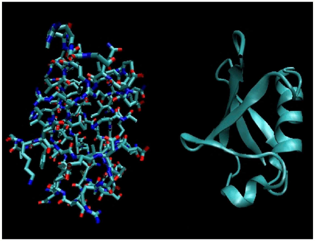
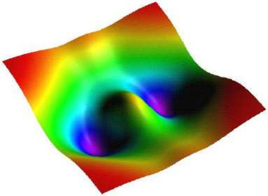
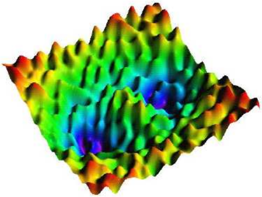
Molecular systems







All the physics is encoded in the potential energy function,

$$V : \mathbb{R}^n \to \mathbb{R}$$

Molecular simulation

Quantities of interest in molecular dynamics:

- thermodynamical averages wrt Gibbs measure:

$$\langle \Phi \rangle = \int_{\mathbb{R}^n} \Phi(X) \, d\mu_{\rm Gibbs}, \quad d\mu_{\rm Gibbs} = Z^{-1} \exp(-\beta V(X)) \, dX$$

- or dynamical quantities (diffusion coefficients, rate constants, ...).

Consider the dynamics (overdamped Langevin equation)

$$dX_t = -\nabla V(X_t) \, dt + \sqrt{2\beta^{-1}} \, dW_t \quad \text{in } \mathbb{R}^n,$$

prototypical of those used in MD (e.g. ergodic for the Gibbs measure).

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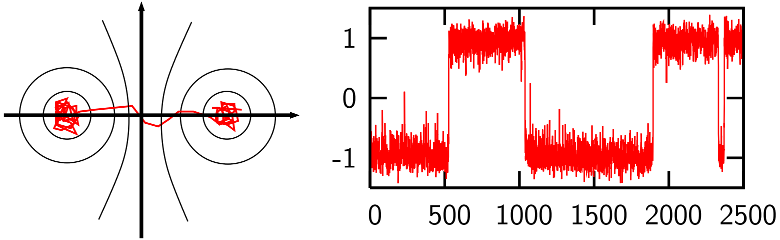
In practice, quantities of interest often depend on a few variables.

Reduced description of the system, that still includes some dynamical information?

Metastability and reaction coordinate

$$dX_t = -\nabla V(X_t)\,dt + \sqrt{2\beta^{-1}}\,dW_t, \quad X_t \equiv \text{position of all atoms}$$

- in practice, the dynamics is metastable: the system stays a long time in a well of V before jumping to another well:



- we assume that wells are fully described through a well-chosen reaction coordinate

$$\xi : \mathbb{R}^n \mapsto \mathbb{R}$$

$\xi(x)$ may be e.g. the coordinate of some particular atom.

Quantity of interest: path $t \mapsto \xi(X_t)$.

Our aim

$$dX_t = -\nabla V(X_t)\,dt + \sqrt{2\beta^{-1}}\,dW_t \quad \text{in } \mathbb{R}^n$$

Given a reaction coordinate $\xi : \mathbb{R}^n \mapsto \mathbb{R}$,
propose a dynamics z_t that approximates $\xi(X_t)$.

- preservation of equilibrium properties:
  when $X \sim d\mu_{\rm Gibbs}$, then $\xi(X)$ is distributed according to $\exp(-\beta A(z))\,dz$, where A is the free energy.

  The dynamics z_t should be ergodic wrt $\exp(-\beta A(z))\,dz$.

- recover in z_t some dynamical information included in $\xi(X_t)$.

- what about non-reversible cases:
  $$dX_t = \mathcal{F}(X_t)\,dt + \sqrt{2\beta^{-1}}\,\sigma(X_t)\,dW_t, \qquad \mathcal{F} \text{ not gradient}$$

Related works: Mori-Zwanzig approaches, Schuette, Pavliotis and Stuart, Hartmann, Papanicolaou, E & Vanden-Eijnden, ...

Construction of an effective dynamics

Effective dynamics using conditional expectations - 1

$$dX_t = -\nabla V(X_t)\,dt + \sqrt{2\beta^{-1}}\,dW_t, \qquad \xi : \mathbb{R}^n \to \mathbb{R}$$

From the dynamics on X_t, we obtain (chain rule)

$$d\left[\xi(X_t)\right] = \left(-\nabla V \cdot \nabla \xi + \beta^{-1}\Delta\xi\right)(X_t)\,dt + \sqrt{2\beta^{-1}}\;\; |\nabla\xi|(X_t)\;\; dB_t$$

where B_t is a 1D brownian motion.

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where B_t is a 1D brownian motion.

Introduce the average of the drift term:

$$\begin{aligned} b(z) \ &:= \ \int \left(-\nabla V \cdot \nabla \xi + \beta^{-1} \Delta \xi\right)(X) \ \psi_{\rm Gibbs}(X)\, \delta_{\xi(X)-z}\, dX \\ &= \ \mathbb{E}_{\rm Gibbs}\left[\left(-\nabla V \cdot \nabla \xi + \beta^{-1} \Delta \xi\right)(X) \ \Big| \ \xi(X) = z\right] \end{aligned}$$

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and likewise for the diffusion term:

$$\sigma^2(z) := \int |\nabla \xi(X)|^2\;\; \psi_{\rm Gibbs}(X)\,\delta_{\xi(X)-z}\,dX$$

Effective dynamics using conditional expectations - 2

Chain rule:

$$d\left[\xi(X_t)\right] = \left(-\nabla V \cdot \nabla \xi + \beta^{-1} \Delta \xi\right)(X_t)\, dt + \sqrt{2\beta^{-1}}\ \ |\nabla \xi|(X_t)\ \ dB_t$$

Average of the drift and diffusion terms:

$$b(z) \ := \ \int \left(-\nabla V \cdot \nabla \xi + \beta^{-1} \Delta \xi\right)(X)\ \psi_{\rm Gibbs}(X)\, \delta_{\xi(X)-z}\, dX$$

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Eff. dyn. we propose: $\boxed{dz_t = b(z_t)\, dt + \sqrt{2\beta^{-1}}\, \sigma(z_t)\, dB_t}$

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The approximation makes sense if, in the manifold

$$\Sigma_z = \left\{X \in \mathbb{R}^n, \quad \xi(X) = z\right\},$$

X_t quickly reaches equilibrium: no metastability in Σ_z.

Remarks

$$dz_t = b(z_t)\, dt + \sqrt{2\beta^{-1}}\, \sigma(z_t)\, dB_t$$

- OK from the statistical viewpoint: the dynamics is ergodic wrt $\exp(-\beta A(z))dz$.

- Reformulation:

$$dz_t = \left[-\sigma^2(z_t)A'(z_t) + 2\beta^{-1}\sigma'(z_t)\sigma(z_t)\right]\, dt + \sqrt{2\beta^{-1}}\, \sigma(z_t)\, dB_t$$

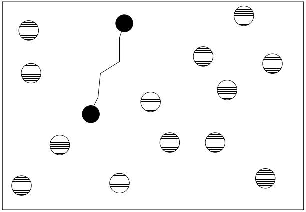
  with A the free energy associated to ξ, and $\quad \sigma^2(z) = \langle |\nabla \xi|^2 \rangle_{\Sigma_z}$.

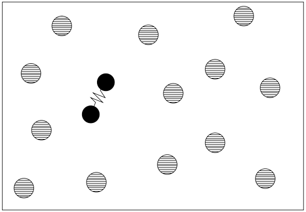
- Interesting particular case: $\xi(X) = X^1$

  Then $b = -A'$ and the effective dynamics reads

$$dz_t = -A'(z_t)\, dt + \sqrt{2\beta^{-1}}\, dB_t$$

An example without clear time-scale separation





- solvent-solvent, solvent-monomer: truncated LJ on $r = \|x_i - x_j\|$:
  $V_{WCA}(r) = 4\varepsilon \left(\frac{\sigma^{12}}{r^{12}} - 2\,\frac{\sigma^6}{r^6} \right)$ if $r \leq \sigma$, 0 otherwise (repulsive potential)
- monomer-monomer: double well on $r = \|x_1 - x_2\|$

Reaction coordinate: the distance between the two monomers

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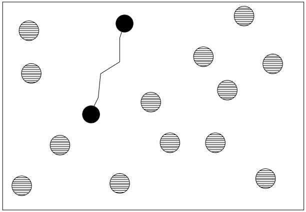

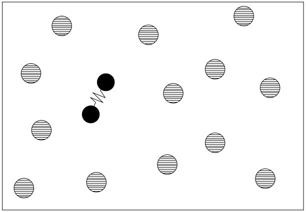

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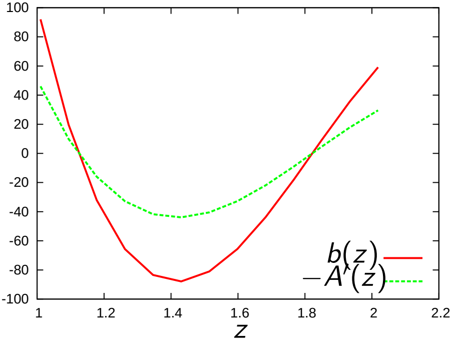
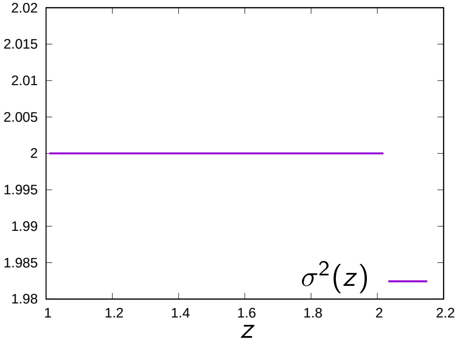
Reaction coordinate: the distance between the two monomers

β	Reference	Eff. dyn.	Dyn. based on A
0.5	262 ± 6	245 ± 5	504 ± 11
0.25	1.81 ± 0.04	1.68 ± 0.04	3.47 ± 0.08





$$b(z) = \mathbb{E}_{\rm Gibbs}\left[-\nabla V \cdot \nabla \xi + \beta^{-1} \Delta \xi \ \Big| \ \xi(X) = z \right]$$

$$-A'(z) = \mathbb{E}_{\rm Gibbs}\left[-\frac{\nabla V \cdot \nabla \xi}{|\nabla \xi|^2} + \beta^{-1} \text{div} \left(\frac{\nabla \xi}{|\nabla \xi|^2} \right) \ \Big| \ \xi(X) = z \right]$$

$$\sigma^2(z) = \mathbb{E}_{\rm Gibbs}\left[|\nabla \xi|^2 \ \Big| \ \xi(X) = z \right]$$

Accuracy of the effective dynamics: the entropy approach

FL, T. Lelièvre, Nonlinearity 2010
FL, T. Lelièvre, Springer LN Comput. Sci. Eng., vol. 82, 2012

- Our effective dynamics is ergodic wrt $\exp(-\beta A(z))dz$
- At any time t, law of $z_t \approx$ law of $\xi(X_t)$?

A convergence result

$$dX_t = -\nabla V(X_t)\, dt + \sqrt{2\beta^{-1}} dW_t, \quad \text{consider } \xi(X_t)$$

Let $\psi_{\rm exact}(t,z)$ be the probability distribution function of $\xi(X_t)$:

$$\mathbb{P}\left(\xi(X_t) \in I\right) = \int_I \psi_{\rm exact}(t,z)\ dz$$

We have introduced the effective dynamics

$$dz_t = b(z_t)\, dt + \sqrt{2\beta^{-1}}\, \sigma(z_t)\, dB_t$$

Let $\phi_{\rm eff}(t,z)$ be the probability distribution function of z_t.

Introduce the error

$$E(t) := \int_{\mathbb{R}} \psi_{\rm exact}(t,\cdot) \ln \frac{\psi_{\rm exact}(t,\cdot)}{\phi_{\rm eff}(t,\cdot)}$$

We would like $\psi_{\rm exact} \approx \phi_{\rm eff}$, i.e. E small ...

Error estimate (FL, T. Lelièvre, Nonlinearity 2010)

$$E(t) = \text{error} = \int_{\mathbb{R}} \psi_{\rm exact}(t,\cdot) \ln \frac{\psi_{\rm exact}(t,\cdot)}{\phi_{\rm eff}(t,\cdot)}$$

Under some assumptions that formalize the fact that

- fast ergodicity in Σ_z (quantified by some $\rho \gg 1$),
- small coupling between dynamics in Σ_z and on z_t (quantified by some $\kappa \ll 1$),

we have, for all $t \geq 0$,

$$E(t) \leq C \frac{\kappa^2}{\rho^2}$$

The effective dynamics is accurate in the sense that

at any time t, law of $\xi(X_t) \approx$ law of z_t.

Remark 1: this is not an asymptotic result, and this holds for any ξ.
Remark 2: this estimate does not contain any information about correlations in time ...

Accuracy of the effective dynamics: a pathwise approach

FL, T. Lelièvre, S. Olla, Stoch. Processes and their Applications 127, 2017

Setting

- For the sake of simplicity, we restrict ourselves to the case $\xi(X) = X^1$.
- The reference dynamics is

$$dX_t = -\nabla V(X_t)\,dt + \sqrt{2\beta^{-1}}dW_t$$

while the effective dynamics approximating $t \mapsto \xi(X_t) = X_t^1$ is

$$dz_t = b(z_t)\,dt + \sqrt{2\beta^{-1}}\,dW_t^1$$

- We aim at controlling $\mathbb{E}\left[\sup_{0\leq t\leq T} |\xi(X_t) - z_t|\right] = \mathbb{E}\left[\sup_{0\leq t\leq T} \left|X_t^1 - z_t\right|\right]$.

Exact and approximate dynamics

- Non-closed dynamics:
$$dX_t^1 = -\nabla_1 V(X_t)\,dt + \sqrt{2\beta^{-1}}dB_t, \qquad B_t = W_t^1.$$

- Effective dynamics:
$$dz_t = b(z_t)\,dt + \sqrt{2\beta^{-1}}dB_t$$
with
$$-b(z) = \mathbb{E}_{\rm Gibbs}\left(\partial_1 V(X) \,\middle|\, X^1 = z\right) = \int_{\mathbb{R}^{n-1}} \partial_1 V(z, x_2^n)\,\psi^z_{\rm Gibbs}(x_2^n)\,dx_2^n$$
where
$$\psi^z_{\rm Gibbs}(x_2^n) = \frac{\psi_{\rm Gibbs}(z, x_2^n)}{\displaystyle\int_{\mathbb{R}^{n-1}} \psi_{\rm Gibbs}(z, x_2^n)\,dx_2^n}, \qquad x_2^n = (x^2, \dots, x^n)$$

- The above non-closed dynamics can be written
$$dX_t^1 = b(X_t^1) + f(X_t)\,dt + \sqrt{2\beta^{-1}}dB_t, \quad \text{mean of } f \text{ vanishes}$$

Assumptions – 1

For any z, the conditional probability measures $\psi^z_{\rm Gibbs}(x_2^n)$ satisfy a Poincaré inequality for a constant ρ independent of z: for any $v \in H^1(\psi^z_{\rm Gibbs})$,

$$\int_{\mathbb{R}^{n-1}} \left(v - \int_{\mathbb{R}^{n-1}} v \, \psi^z_{\rm Gibbs} \right)^2 \psi^z_{\rm Gibbs} \leq \frac{1}{\rho} \int_{\mathbb{R}^{n-1}} \left| \widehat{\nabla} v \right|^2 \psi^z_{\rm Gibbs}$$

where $\widehat{\nabla} v = (\partial_2 v, \dots, \partial_n v)$.

Recall that a Poincaré inequality holds on a probability measure $\exp(-\beta W(x)) \, dx$ under relatively mild assumption on W.

Assumptions – 2

The cross derivative $\widehat{\nabla}\partial_1 V$ is in $L^2(\psi_{\rm Gibbs})$:

$$\kappa^2 := \int_{\mathbb{R}^n} \left| \widehat{\nabla}\partial_1 V(x) \right|^2 \psi_{\rm Gibbs}(x) dx < \infty.$$

Assumptions – 2

The cross derivative $\widehat{\nabla}\partial_1 V$ is in $L^2(\psi_{\rm Gibbs})$:

$$\kappa^2 := \int_{\mathbb{R}^n} \left|\widehat{\nabla}\partial_1 V(x)\right|^2 \psi_{\rm Gibbs}(x) dx < \infty.$$

The effective drift b is one-sided Lipschitz on $\mathbb{R}$: there exists $L_b > 0$ such that

$$\forall x \in \mathbb{R}, \quad b'(x) \leq L_b$$

This assumption is satisfied if b is Lipschitz on bounded domains and decreasing at infinity, which corresponds to a case when the associated free energy is smooth and convex at infinity.

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For any $x > 0$, introduce $\alpha(x) = \sup_{s \in [-x,x]} |b'(s)|$. We assume that

$$\mathbb{E}\left[\Big(\alpha \left(|X^1| \right) \Big)^2 \right] < \infty.$$

This assumption is satisfied e.g. if V has polynomial growth.

Error estimate

We work under the above assumptions, and we assume that the system starts under equilibrium:

$$X_0 \sim \psi_{\rm Gibbs}. \qquad (\star)$$

Consider $(X_t)_{0 \leq t \leq T}$ solution to the reference dynamics and $(z_t)_{0 \leq t \leq T}$ solution to the effective dynamics over a bounded time interval $[0, T]$. Then, there exists a constant C, independent of ρ and κ, such that

$$\mathbb{E}\left[\sup_{0 \leq t \leq T} \left| X_t^1 - z_t \right| \right] \leq C \, \frac{\kappa}{\rho}.$$

Remark: assumption $(\star)$ *can be relaxed if assume* $\left\| \frac{\psi_0}{\psi_{\rm Gibbs}} \right\|_{L^\infty(\mathbb{R}^n)} < \infty.$

Ingredients of the proof

$$\begin{aligned} dX_t^1 &= b(X_t^1) + f(X_t)\, dt + \sqrt{2\beta^{-1}} dB_t, \quad \text{mean of } f \text{ vanishes} \\ dz_t &= b(z_t)\, dt + \sqrt{2\beta^{-1}} dB_t \end{aligned}$$

which implies that

$$X_t^1 - z_t = \int_0^t \left(b(X_s^1) - b(z_s) \right) \, ds + \int_0^t f(X_s)\, ds$$

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- through the introduction of a Poisson equation (with f as right-hand side), and using an argument due to T. Lyons and T. Zhang, we get an estimate on $\mathbb{E}\left(\sup_{0\le t\le T}\left|\int_0^t f(X_s)ds\right|^2\right)$;

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- Gronwall type argument to deduce a bound on $\mathbb{E}\left(\sup_{0 \le t \le T} \left| X_t^1 - z_t \right| \right)$.

Gronwall type argument

$$dX_t = b(X_t)dt + \sigma\, dB_t, \qquad dY_t = b(Y_t)dt + \sigma\, dB_t + f_t dt$$

- The standard Gronwall Lemma gives an estimate of the difference $(|X_t - Y_t|)_{t\in[0,T]}$ in terms of $(|f_t|)_{t\in[0,T]}$.
- We have an estimate on $(|f_t|)_{t\in[0,T]}$, but we have a much better one on $\left(\left|\int_0^t f_s ds\right|\right)_{t\in[0,T]}$ that we wish to use.
- This is why, in addition to the one-sided Lipschitz assumption on b, we assume that

$$C_\alpha(\beta) = \mathbb{E}\left[\left(\alpha\left(|X^1|\right)\right)^2\right] = \int_{\mathbb{R}} \left(\sup_{s\in[-|x|,|x|]} |b'(s)|\right)^2 \varphi_{\rm Gibbs}(x)\, dx < \infty$$

The Gronwall argument is of interest by its own.

Conclusions on the reversible case

- We proposed a "natural" way to obtain a closed equation on $\xi(X_t)$
- Encouraging numerical results and rigorous error bounds
- Our approach can also be applied to the standard problem

$$\begin{cases} dX_t^{\varepsilon,1} = -\partial_1 V(X_t^\varepsilon)\,dt + \sqrt{2\beta^{-1}}\,dW_t^1 \\ dX_t^{\varepsilon,i} = -\varepsilon^{-1}\,\partial_i V(X_t^\varepsilon)\,dt + \sqrt{2\beta^{-1}\varepsilon^{-1}}\,dW_t^i \qquad \text{for } i = 2,\dots,n \end{cases}$$

without Lipschitz assumptions on ∇V.

FL, T. Lelièvre, Nonlinearity 23, 2010
FL, T. Lelièvre, Springer LN Comput. Sci. Eng., vol. 82, 2012
FL, T. Lelièvre, S. Olla, Stoch. Processes and their Applications 127, 2017

See also works by Duong, Lamacz, Pelletier, Schlichting and Sharma.

Extension to some non-reversible cases

$$dX_t = \mathcal{F}(X_t)\, dt + \sqrt{2}\, dW_t, \qquad \mathcal{F} \text{ is not a gradient}$$

FL, T. Lelièvre, U. Sharma, ongoing works

A motivating example – 1

$$dX_t = \mathcal{F}(X_t)\,dt + \sqrt{2}\,dW_t \qquad \text{on } \mathbb{T}^2$$

for a $\mathbb{Z}^2$ periodic function $\mathcal{F}$ of the form

$$\mathcal{F}(x,y) = (-\partial_y \psi(x,y), \partial_x \psi(x,y)).$$

- Unique stationary measure:

$$\mu(x,y) = 1$$

- Conditional stationary measure:

$$\mu^x(y) = \frac{\mu(x,y)}{\int \mu(x,y)\,dy} = 1$$

- Free energy associated to the reaction coordinate $\xi(x,y) = x$:
  - in non-reversible cases, there is no obvious definition
  - one possible definition (reversible setting spirit):

$$\exp(-A(x)) = \int \mu(x,y)\,dy$$

  and hence $A(x) = 1$ here.

A motivating example – 2

$$dX_t = \mathcal{F}(X_t)\,dt + \sqrt{2}\,dW_t \quad \text{on } \mathbb{T}^2, \qquad \mathcal{F} = (-\partial_y \psi, \partial_x \psi)$$

and with $\xi(X) = \xi(x,y) = x$, we have

$$dx_t = -\partial_y \psi(x_t, y_t)\,dt + \sqrt{2}\,dW_t^1$$

- Closure procedure:

  $$dz_t = b(z_t)\,dt + \sqrt{2}\,dW_t^1$$

  with

  $$b(z) = \mathbb{E}_\mu \Big[\text{ drift } \Big| \ \xi(X) = z \ \Big] = \int \Big(-\partial_y \psi(z,y) \Big) \mu^z(y)\,dy$$

- In the simple case

  $$\psi(X) = \psi_{\rm per}(X) + L \cdot X, \qquad L \text{ constant},$$

  we get $b(z) = -L_2$.

A motivating example – 3

$$dX_t = \mathcal{F}(X_t)\,dt + \sqrt{2}\,dW_t \text{ on } \mathbb{T}^2, \qquad \mathcal{F} = (-\partial_y \psi, \partial_x \psi)$$

and

$$\xi(x,y) = x, \qquad \psi(X) = \psi_{\rm per}(X) + L \cdot X$$

- Following our general procedure, we propose the effective dynamics

$$dz_t = -L_2\,dt + \sqrt{2}\,dW_t^1$$

- On the other hand:
  - In the reversible case with $\xi(x,y) = x$, the effective dynamics is

$$dz_t = -A'(z_t)\,dt + \sqrt{2}\,dW_t^1$$

  - A natural definition of A here leads to $A' = 0$.

- The two propositions differ! Which one is accurate?

Setting (non-reversible case)

- For the sake of simplicity, we restrict ourselves to the case $\xi(X) = X^1$.
- Reference dynamics:

$$dX_t = \mathcal{F}(X_t)\, dt + \sqrt{2} dW_t, \qquad \text{unique stat. measure } \mu$$

- Non-closed dynamics:

$$dX_t^1 = \mathcal{F}_1(X_t)\, dt + \sqrt{2} dB_t, \qquad B_t = W_t^1$$

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- Effective dynamics:

$$dz_t = b(z_t)\,dt + \sqrt{2}dB_t$$

with

$$b(z) = \mathbb{E}_\mu\Big(\mathcal{F}_1(X) \,\Big|\, X^1 = z\Big) = \int_{\mathbb{R}^{n-1}} \mathcal{F}_1(z, x_2^n)\ \mu^z(x_2^n)\,dx_2^n$$

where

$$\mu^z(x_2^n) = \frac{\mu(z, x_2^n)}{\displaystyle\int_{\mathbb{R}^{n-1}} \mu(z, x_2^n)\,dx_2^n}, \qquad x_2^n = (x^2, \dots, x^n)$$

Assumptions (non-reversible case)

Similar assumptions as in the reversible case:

- For any z, the conditional probability measures $\mu^z(x_2^n)$ satisfy a Poincaré inequality for a constant ρ independent of z.
- The cross derivative $\widehat{\nabla}\mathcal{F}_1$ is in $L^2(\mu)$:

$$\kappa^2 := \int_{\mathbb{R}^n} \left| \widehat{\nabla}\mathcal{F}_1 \right|^2 \mu < \infty.$$

- The effective drift b is one-sided Lipschitz on $\mathbb{R}$.
- For any $x > 0$, introduce $\alpha(x) = \sup_{s \in [-x,x]} |b'(s)|$. We assume that

$$\mathbb{E}\left[\left(\alpha\left(|X^1|\right) \right)^2 \right] < \infty.$$

Error estimate (non-reversible case)

We work under the above assumptions, and we assume that the system starts under equilibrium:

$$X_0 \sim \mu \equiv \text{stationary measure.}$$

Consider $(X_t)_{0 \leq t \leq T}$ solution to the reference dynamics and $(z_t)_{0 \leq t \leq T}$ solution to the effective dynamics over a bounded time interval $[0, T]$. Then, there exists a constant C, independent of ρ and κ, such that

$$\mathbb{E}\left[\sup_{0 \leq t \leq T} \left| X_t^1 - z_t \right|\right] \leq C \, \frac{\kappa}{\rho}.$$

The proof essentially follows the same steps as in the reversible case.

On-going works and open questions

- Ongoing work: general non-reversible SDE of the form

$$dX_t = \mathcal{F}(X_t)\,dt + \sqrt{2}\,\sigma(X_t)\,dW_t$$

for a non-degenerate diffusion coefficient σ.

- Open question: SDEs with degenerate noise, such as the Langevin equation:

$$dX_t = P_t\,dt, \qquad dP_t = \mathcal{F}(X_t)\,dt - P_t\,dt + \sqrt{2}\,\sigma(X_t)\,dW_t$$

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