Effective dynamics using conditional expectations

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Classical n-body system

Atomistic system whose position is given by $X = \left(X^1, \ldots, X^n\right) \in \mathbb{R}^n$

Potential energy: $V(X),$ which contains all the physics of the system

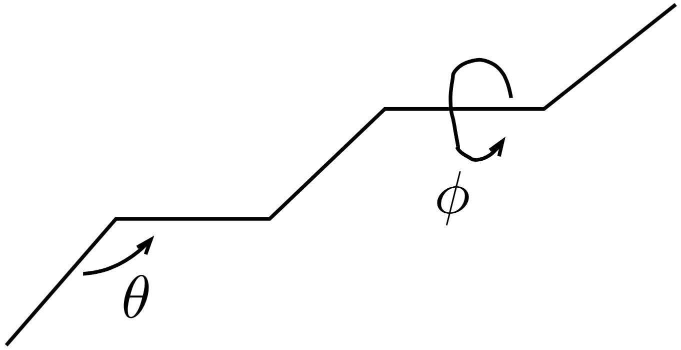
A standard task in molecular dynamics is to compute thermodynamical averages wrt Gibbs measure:

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

with $\beta = 1/(k_B T)$ and $Z = \int_{\mathbb{R}^n} \exp(-\beta V(X))\, dX$.

A simple example

- Chain-like molecules (biological molecules, polymers, . . .):



$$V(X) = \sum_i V_2\left(X^{i+1} - X^i\right) + \sum_i V_3(\theta_i) + \sum_i V_4(\cos\phi_i)$$

with

$$V_2\left(X^{i+1} - X^i\right) = \frac{k_2}{2}\left(\left|X^{i+1} - X^i\right| - d_{eq}\right)^2, \quad V_3(\theta_i) = \frac{k_3}{2}(\theta_i - \theta_{eq})^2$$

- end-to-end distance $\langle\left|X^n - X^1\right|\rangle$

Other examples: pressure in a liquid, . . .

Dynamics

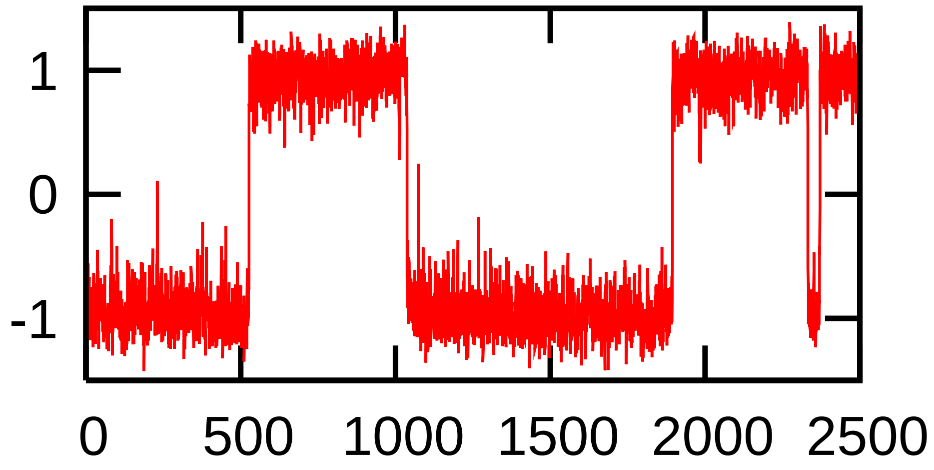
Consider the dynamics (overdamped Langevin equation)

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

which is ergodic for $d\mu$: for a.a. initial conditions X_0, and a.s.,

$$\forall \text{ smooth } \phi, \quad \frac{1}{T}\int_0^T \phi(X_t)\,dt = \int \phi(X)\,d\mu + O\left(\frac{1}{\sqrt{T}}\right).$$

In practice, the constant in the $O(\cdot)$ may be big (metastability). Reduced description of the system, that still includes some dynamical information?



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 is distributed according to $d\mu$, then $\xi(X)$ distributed according to $\exp(-\beta A(z))\, dz$:

$$\forall \text{ smooth } \phi_r, \quad \int_{\mathbb{R}^n} \phi_r(\xi(X))\, d\mu = \int_{\mathbb{R}} \phi_r(z) \exp(-\beta A(z))\, dz$$

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

- estimation of the distance between z_t and $\xi(X_t)$.

Some related works

- Mori-Zwanzig projection formalism
- Normal modes decomposition
- system reduction in the framework on SDEs (E, Vanden-Eijnden, ...):

$$\begin{aligned} dx_t &= f(x_t, y_t)\,dt + \sqrt{2\beta^{-1}}\,dB_t^1 \\ dy_t &= \frac{1}{\varepsilon} g(x_t, y_t)\,dt + \sqrt{\frac{2\beta^{-1}}{\varepsilon}}\,dB_t^2 \end{aligned}$$

If x_t is held fixed, then y_t is ergodic w.r.t. a measure independant of ε.

Our framework:

- cartesian coordinates not adapted to slow/fast splitting.
- even if $\xi(x,y) = x$, the fast dynamics is different:

$$\begin{aligned} dx_t &= f(x_t, y_t)\,dt + \sqrt{2\beta^{-1}}\,dB_t^1 \\ dy_t &= \frac{1}{\varepsilon} g(x_t, y_t)\,dt + \sqrt{2\beta^{-1}}\,dB_t^2 \end{aligned}$$

Convergence to equilibrium: Fokker-Planck equation

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

The pdf $\psi(t, X)$ of X_t satisfies the Fokker-Planck equation:

$$\partial_t \psi = \text{div}\, \left(\psi \nabla V\right) + \beta^{-1} \Delta \psi$$

Introduce the equilibrium density

$$\psi_\infty(X) = Z^{-1} \exp(-\beta V(X)), \quad d\mu = \psi_\infty(X)\, dX$$

We have $\nabla \psi_\infty = -\beta \psi_\infty \nabla V$. Hence the Fokker-Planck equation reads

$$\partial_t \psi = \beta^{-1} \text{div}\, \left[\psi_\infty \nabla \left(\frac{\psi}{\psi_\infty} \right) \right]$$

We wish to prove that $\psi(t, \cdot) \to \psi_\infty(\cdot)$ as $t \to \infty$. Relative entropy argument.

Convergence to equilibrium: relative entropy

Introduce $e(t) = H(\psi|\psi_\infty) := \int_{\mathbb{R}^n} \ln\left(\frac{\psi(t,x)}{\psi_\infty(x)}\right)\psi(t,x)\,dx$. Then

$$
\begin{aligned}
\frac{de}{dt} &= \int \ln\left(\frac{\psi}{\psi_\infty}\right)\partial_t\psi + \frac{\psi_\infty}{\psi}\,\frac{\partial_t\psi}{\psi_\infty}\,\psi \\
&= \int \ln\left(\frac{\psi}{\psi_\infty}\right)\beta^{-1}\mathrm{div}\,\left[\psi_\infty\nabla\left(\frac{\psi}{\psi_\infty}\right)\right] \\
&= -\beta^{-1}\int \nabla\left[\ln\left(\frac{\psi}{\psi_\infty}\right)\right]\psi_\infty\nabla\left(\frac{\psi}{\psi_\infty}\right) \\
&= -\beta^{-1}\int \left|\nabla\left[\ln\left(\frac{\psi}{\psi_\infty}\right)\right]\right|^2\psi =: -\beta^{-1}I(\psi|\psi_\infty)
\end{aligned}
$$

Assume that ψ_∞ satisfies a Log-Sobolev Inequality (LSI): there exists $\rho > 0$ such that, for any probability measure of density ν,

$$H(\nu|\psi_\infty) \le (2\rho)^{-1} I(\nu|\psi_\infty)$$

Then $\quad \frac{de}{dt} \le -2\rho\beta^{-1}e(t)$, hence $e(t) \to 0$.

Outline of the talk

- Construction of an effective dynamics
- Assessment of its quality in terms of marginals
- Pathwise convergence in a specific case
- Numerical examples

A non-constructive closure

From the dynamics on X_t, we obtain

$$\begin{aligned} d\xi(X_t) &= \nabla\xi(X_t)\cdot dX_t + \beta^{-1}\Delta\xi(X_t)\,dt \\ &= \left(-\nabla V\cdot\nabla\xi + \beta^{-1}\Delta\xi\right)(X_t)\,dt + \sqrt{2\beta^{-1}}\,\nabla\xi(X_t)\cdot dW_t \\ &= \left(-\nabla V\cdot\nabla\xi + \beta^{-1}\Delta\xi\right)(X_t)\,dt + \sqrt{2\beta^{-1}}\,|\nabla\xi|(X_t)\,dB_t \end{aligned}$$

where $dB_t = \dfrac{\nabla\xi(X_t)\cdot dW_t}{|\nabla\xi|(X_t)}$: B_t is a 1D standard noise.

$$\begin{aligned} \widetilde{b}(t,z) &:= \mathbb{E}\left[\left(-\nabla V\cdot\nabla\xi + \beta^{-1}\Delta\xi\right)(X_t)\;|\;\xi(X_t)=z\right] \\ \widetilde{\sigma}^2(t,z) &:= \mathbb{E}\left[|\nabla\xi|^2(X_t)\;|\;\xi(X_t)=z\right] \end{aligned}$$

and consider

$$d\widetilde{z}_t = \widetilde{b}(t,\widetilde{z}_t)\,dt + \sqrt{2\beta^{-1}}\,\widetilde{\sigma}(t,\widetilde{z}_t)\,dB_t, \quad \widetilde{z}_0 = \xi(X_0)$$

Then, for any t, the law of $\widetilde{z}_t$ is equal to the law of $\xi(X_t)$ (Gyongy 1986)

But $\widetilde{b}(t,z)$ and $\widetilde{\sigma}(t,z)$ are extremely difficult to compute . . .

An approximate closure

Need for approximation:

$$
\begin{aligned}
\widetilde{b}(t,z) &= \mathbb{E}\left[\left(-\nabla V\cdot\nabla\xi+\beta^{-1}\Delta\xi\right)(X_t)\;\middle|\;\xi(X_t)=z\right]\\
b(z) &:= \mathbb{E}_\mu\left[\left(-\nabla V\cdot\nabla\xi+\beta^{-1}\Delta\xi\right)(X)\;\middle|\;\xi(X)=z\right]
\end{aligned}
$$

Idea: $\widetilde{b}(t,z)\approx b(z)$ if, in the manifold

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

X_t quickly reaches equilibrium. $\xi(X_t)$ much slower than evolution of X_t in Σ_z.

Consider the effective dynamics

$$
dz_t=b(z_t)\,dt+\sqrt{2\beta^{-1}}\,\sigma(z_t)\,dB_t,\quad z_0=\xi(X_0)
$$

with $\sigma^2(z):=\mathbb{E}_\mu\left[|\nabla\xi|^2(X)\;\middle|\;\xi(X)=z\right]$.

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

Accuracy of the effective dynamics

- In the general case, obtain estimates between the law of z_t and the law of $\xi(X_t)$, for any t, in terms of relative entropy.

- the potential V is frequently of the form

$$V_\varepsilon(X) = V_0(X) + \frac{1}{\varepsilon} q^2(X)$$

  - rough dependence of the above estimate in ε?
  - exploit this structure to properly define $\xi(X)$?
  - consider a more restrictive case to obtain stronger results (pathwise convergence):

$$\mathbb{E}\left[\sup_{t \in (0,T)} \left|\xi(X_t) - z_t\right|^2\right].$$

An entropy convergence result

$$dX_t = -\nabla V(X_t)\,dt + \sqrt{2\beta^{-1}}dW_t, \quad \text{pdf } \psi(t,X)$$

The pdf of $\xi(X_t)$ is

$$\overline{\psi}(t,z) = \int_{\mathbb{R}^n} \psi(t,X)\ \delta(\xi(X) - z)$$

On the other hand, we have introduced the effective dynamics

$$dz_t = b(z_t)\,dt + \sqrt{2\beta^{-1}}\,\sigma(z_t)\,dB_t, \quad z_0 = \xi(X_0)$$

Let $\phi(t,z)$ be the pdf of z_t. Introduce the relative entropy:

$$E(t) := H(\overline{\psi}|\phi) = \int_{\mathbb{R}} \ln\left(\frac{\overline{\psi}(t,z)}{\phi(t,z)}\right)\overline{\psi}(t,z)\,dz.$$

We would like $\overline{\psi} \approx \phi$, e.g. E small ...

Decoupling assumptions

$$\Sigma_z = \{X \in \mathbb{R}^n,\ \xi(X) = z\}, \quad d\mu_z \propto \exp(-\beta V(X))\, \delta(\xi(X) - z)$$

- assume that the conditioned probability measures $d\mu_z$ satisfy a log-Sobolev inequality with a large constant ρ (uniform in z). They can be quickly sampled.

- assume that the coupling between the dynamics of $\xi(X_t)$ and the dynamics in Σ_z is weak:

  At equilibrium, $\xi \sim \exp(-\beta A(z))\, dz$ with $A'(z) = \int_{\Sigma_z} F(X) d\mu_z$

  We assume that $\|\nabla_{\Sigma_z} F\|_{L^\infty} \leq \kappa$.

  When $\xi(x, y) = x$, $\nabla_{\Sigma_z} F = \partial_{xy} V$: weak-coupling between x and y.

- assume that $|\nabla \xi|$ is close to a constant on each Σ_z, e.g.

$$\lambda = \left\| \frac{|\nabla \xi|^2(X) - \sigma^2(\xi(X))}{\sigma^2(\xi(X))} \right\|_{L^\infty} < +\infty$$

A bounded entropy result

$$E(t) := H(\overline{\psi}|\phi) = \int_{\mathbb{R}} \ln\left(\frac{\overline{\psi}(t,z)}{\phi(t,z)}\right)\overline{\psi}(t,z)\,dz.$$

Under the above assumptions, for all $t \geq 0$,

$$E(t) \leq \frac{\|\nabla\xi\|_{L^\infty}^2}{4}\left(\lambda + \frac{\beta^2\kappa^2}{\rho^2}\right) H(\psi(0,\cdot)|\psi_\infty)$$

Hence, if ξ is such that

- ρ is large (strong mixing in Σ_z),
- κ is small (small coupling between dynamics in Σ_z and on z_t),
- λ is small ($|\nabla\xi|$ is close to a constant on each Σ_z),

then the effective dynamics z_t obtained by conditional expectations is close to the real dynamics $\xi(X_t)$ in the sense of relative entropy.

A particular case

Standard expression in MD: $V_\varepsilon(X) = V_0(X) + \frac{1}{\varepsilon} q^2(X)$

- LSI estimate for the measure μ restricted on $\{X; \xi(X) = z\}$:
  This measure essentially looks like a gaussian measure of variance $O(\varepsilon)$.
  Such gaussian measures satisfy a LSI with $\rho_\varepsilon = O(1/\varepsilon)$.

- Mean-force $F(X)$ estimation: $A'(z) = \int_{\Sigma_z} F(X)\, d\mu_z$, $\kappa_\varepsilon = \|\nabla_{\Sigma_z} F\|_{L^\infty}$?

$$\begin{aligned} F(X) &= \frac{\nabla V \cdot \nabla \xi}{|\nabla \xi|^2} - \beta^{-1} \text{div} \left(\frac{\nabla \xi}{|\nabla \xi|^2} \right) \\ &= \frac{2q(X)}{\varepsilon} \frac{\nabla q \cdot \nabla \xi}{|\nabla \xi|^2} + O(1), \quad \text{assuming that } \nabla \xi = O(1). \end{aligned}$$

If $\nabla \xi \cdot \nabla q = 0$, then $\kappa_\varepsilon = O(1)$, otherwise $\kappa_\varepsilon = O(1/\varepsilon)$.

Explicit entropy bounds

$$E(t) \leq \frac{\|\nabla \xi\|_{L^\infty}^2}{4} \left(\lambda + \frac{\beta^2 \kappa^2}{\rho^2} \right) H(\psi(0,\cdot)|\psi_\infty)$$

where λ measures how much $|\nabla \xi|$ deviates from a constant on Σ_z.

$$\rho_\varepsilon = O(1/\varepsilon).$$

- If $\nabla \xi \cdot \nabla q = 0$, then $\kappa_\varepsilon = O(1)$, hence $\kappa_\varepsilon / \rho_\varepsilon = O(\varepsilon)$, and “good” estimate. In the absence of λ,

  $$E(t) = O(\varepsilon^2).$$

- If $\nabla \xi \cdot \nabla q \neq 0$, then $\kappa_\varepsilon = O(1/\varepsilon)$, hence $\kappa_\varepsilon / \rho_\varepsilon = O(1)$, and

  $$E(t) = O(1),$$

  hence the laws of $\xi(X_t)$ and of z_t are not close one to each other.

Can we get stronger results?

A commutative diagram?

$$V_\varepsilon(X) = V_0(X) + \frac{1}{\varepsilon} q^2(X), \quad X \in \mathbb{R}^2$$

2D dynamics on X_t^ε	$\longrightarrow_{\varepsilon\to 0}$ [pathwise cv]	1D limit dynamics on $\overline{X}_t$
$\downarrow$		$\downarrow$
Itô computation		$\downarrow$
$\downarrow$		$\downarrow$
Nonclosed dynamics on $\xi(X_t^\varepsilon)$		*One-to-one change of variable*
$\downarrow$		$\xi_t = \xi(\overline{X}_t)$
Conditional expectations		$\downarrow$
$\downarrow$		$\downarrow$
Dynamics on $z_t^\varepsilon \approx \xi(X_t^\varepsilon)$	$\longrightarrow_{\varepsilon\to 0}$?	Dynamics on ξ_t
$dz_t^\varepsilon = b_\varepsilon(z_t^\varepsilon)\,dt + \sigma_\varepsilon(z_t^\varepsilon) dB_t$		

Sufficient conditions for the two dynamics to be identical:

$$\nabla \xi(X) \cdot \nabla q(X) = 0 \text{ for all } X \in \mathbb{R}^2$$

Recall $V_\varepsilon(X) = V_0(X) + \dfrac{1}{\varepsilon} q^2(X)$, hence the limit dynamics lives on

$$\mathcal{M} = \{X \in \mathbb{R}^2;\ q(X) = 0\}.$$

We ask that the parametrization ξ of $\mathcal{M}$ is orthogonal to the direction ∇q where sampling is fast.

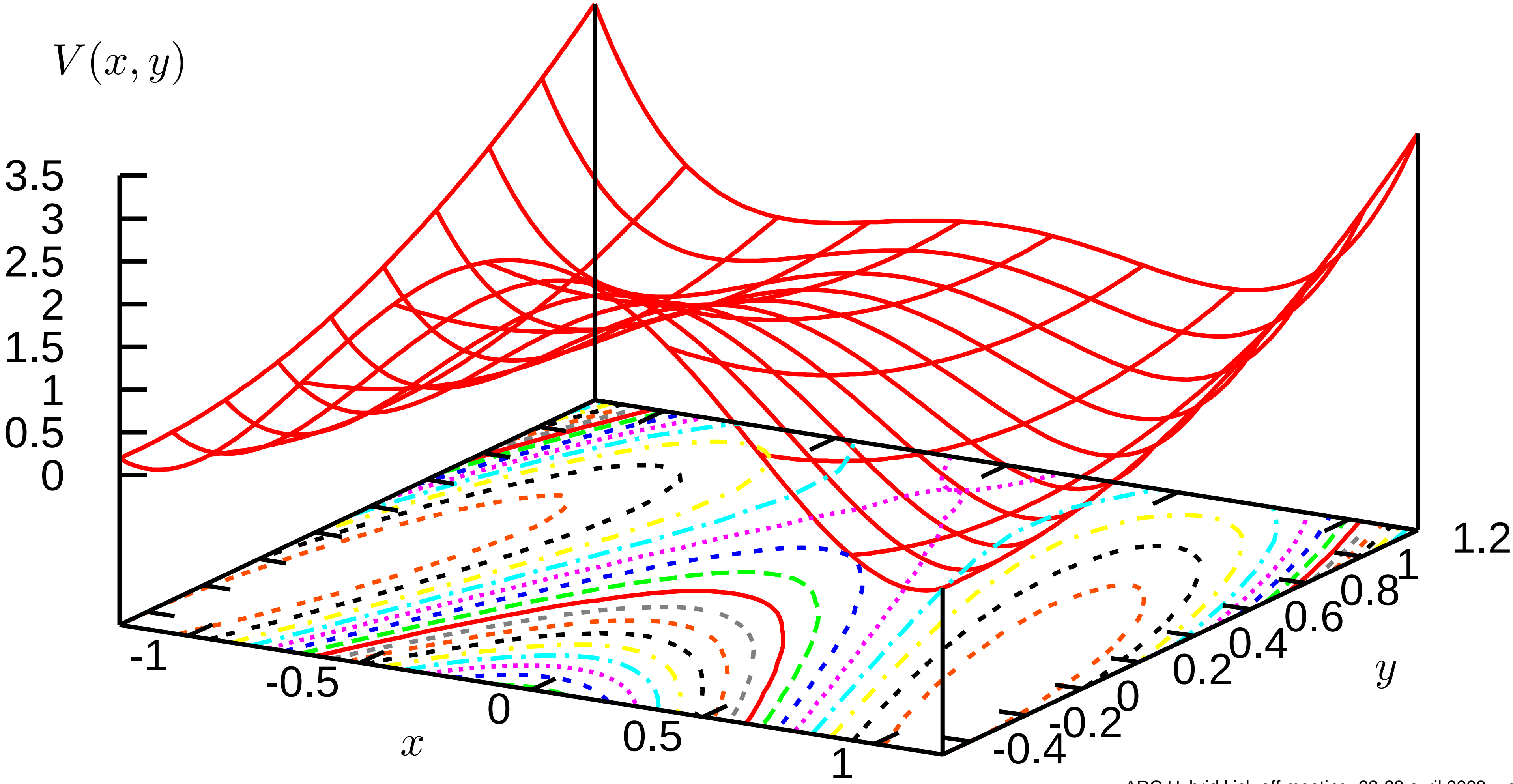
Hence, if the orthogonality condition holds:

- our effective dynamics is a good approximation of the true dynamics $\xi(X_t)$, on finite time intervals ($X \in \mathbb{R}^2$).
- good entropy estimate ($X \in \mathbb{R}^n$).

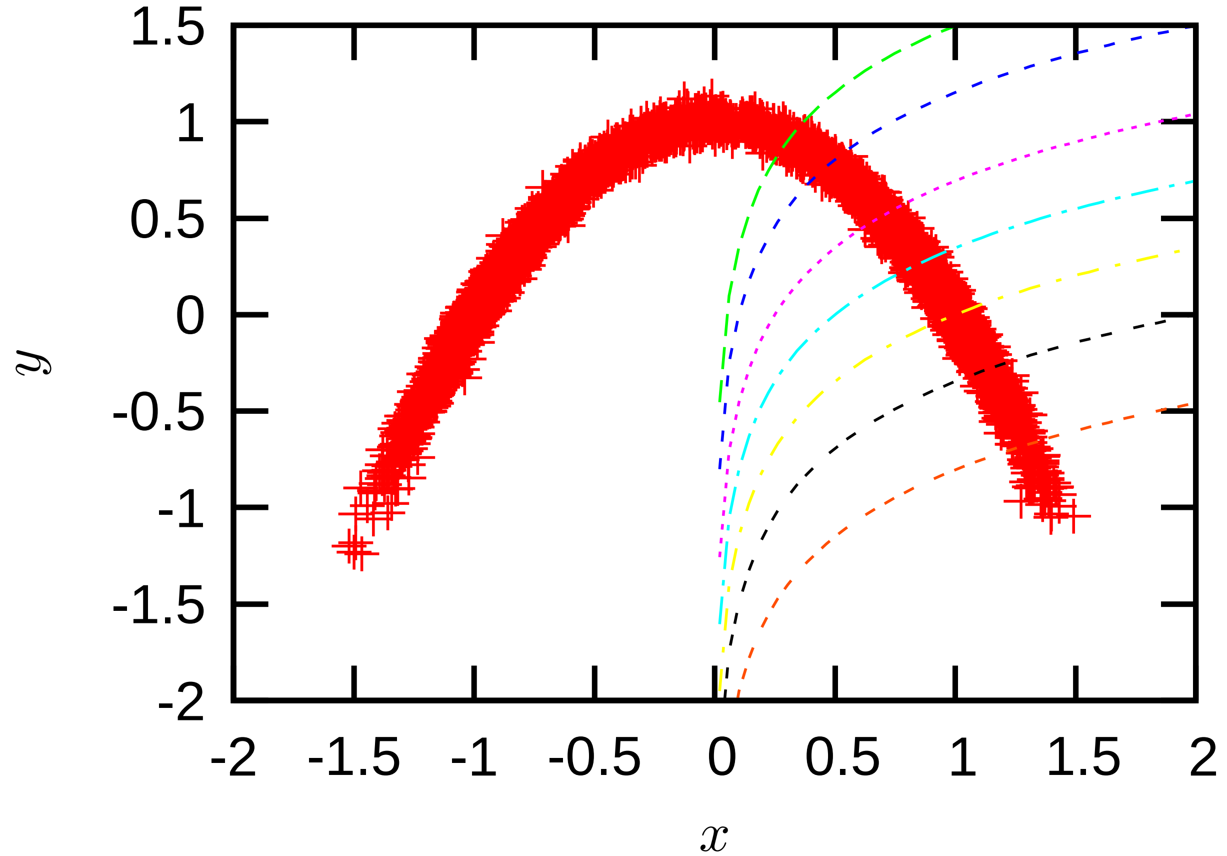
A toy example

$$V(x,y) = (x^2-1)^2 + (y+x^2-1)^2$$

Two wells $V(\pm 1, 0) = 0$, one saddle point $V(0,1) = 1$.

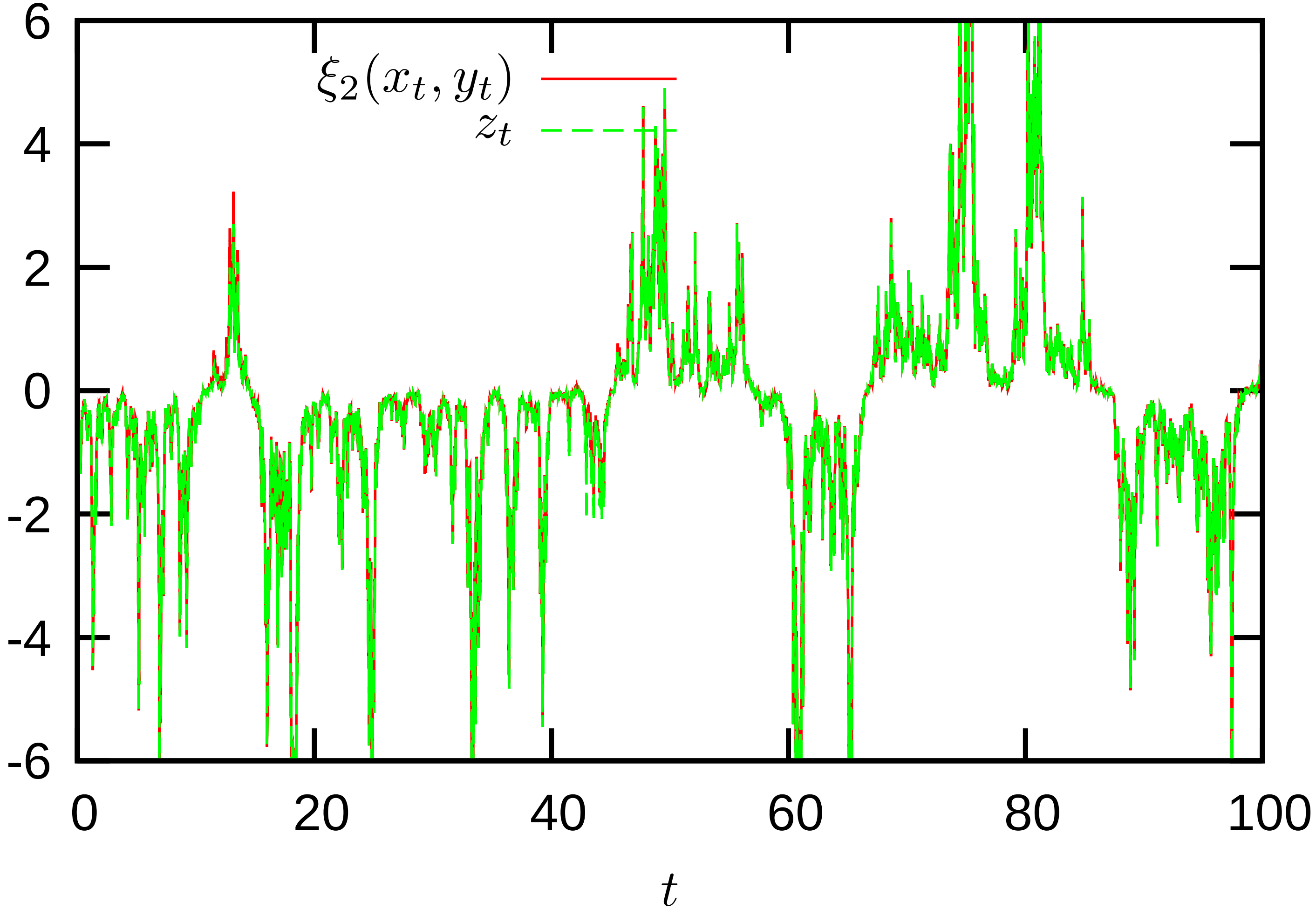


A numerical 2D example: $\varepsilon = 0.01$, $\beta = 3$



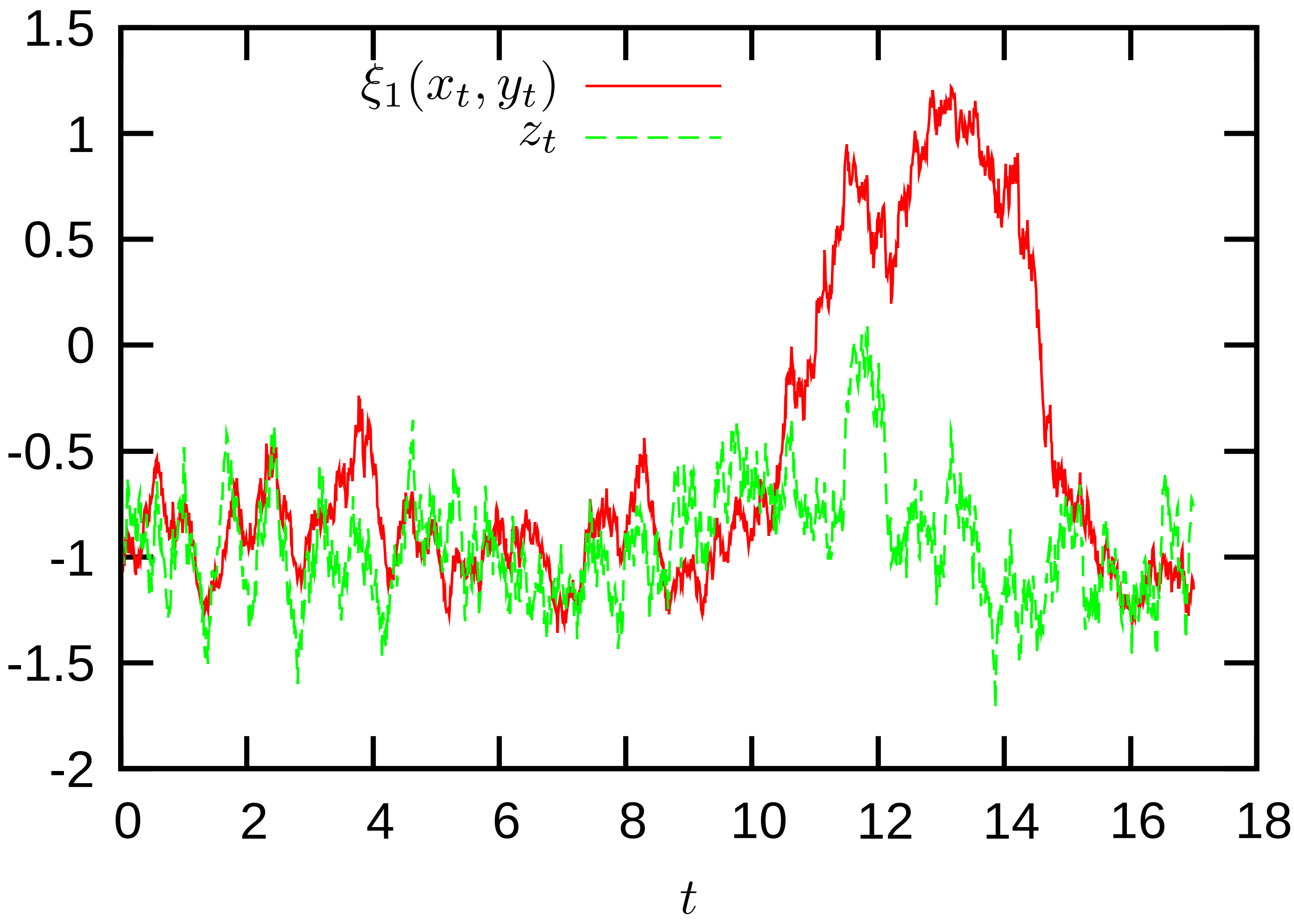
$$V_\varepsilon(x,y) = (x^2-1)^2 + \frac{1}{\varepsilon}(x^2+y-1)^2$$

Two possible reaction coordinates: $\xi_1(x,y) = x, \quad \xi_2(x,y) = x\exp(-2y)$



$$q(x,y) = x^2 + y - 1, \quad \xi_2(x,y) = x\exp(-2y) : \quad \nabla\xi_2 \cdot \nabla q = 0$$

Effective dynamics with the first reaction coordinate



$$q(x,y) = x^2 + y - 1, \quad \xi_1(x,y) = x : \quad \nabla \xi_1 \cdot \nabla q \neq 0$$

Effective dynamics and free energy

Free energy barriers are often associated with residence times in the wells.

Is our effective dynamics the same as

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

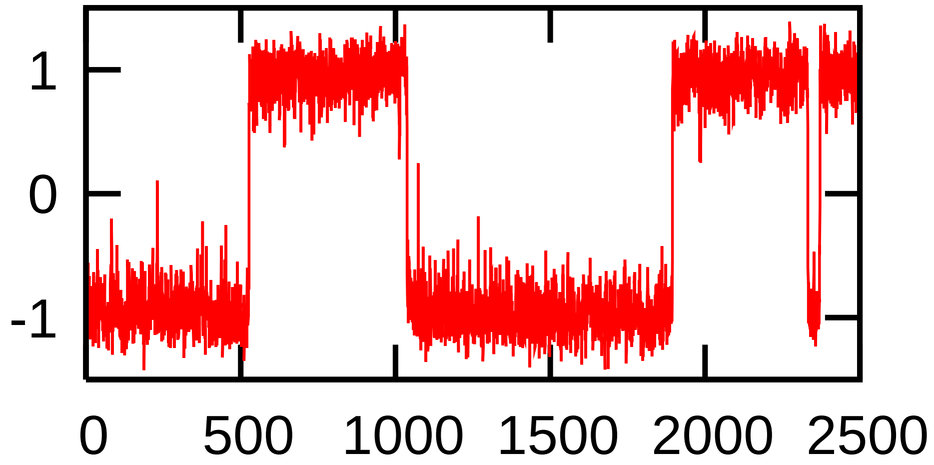
e.g. the dynamics driven by the free energy A associated with the reaction coordinate $\xi(X)$?

$$\text{Recall} \quad \sigma^2(z) = \mathbb{E}_\mu \left[|\nabla\xi|^2(X) \mid \ \xi(X) = z \right]$$

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

- If $|\nabla\xi(X)| = 1$, then $\sigma(z) = 1$, and $b(z) = -A'(z)$. We recover the free energy. An example: $\xi(X) = X^j$.
- In general, $\sigma(z)$ is not a constant, and $b(z) \neq -A'(z)$, even up to a multiplicative constant.

Approximation of residence times ($\varepsilon = 0.01$, $\beta = 3$)



Reac. Coord.	Full dyn.	Reduced dynamics
$\xi_2(x,y) = x\exp(-2y)$	32.5 $\pm$ 0.5	32.7 $\pm$ 0.5 (Eff. dyn.)
$\xi_2(x,y) = x\exp(-2y)$	32.5 $\pm$ 0.5	6.4 $\pm$ 0.3 (based on $A(\xi_2)$)
$\xi_1(x,y) = x$	31.6 $\pm$ 0.5	24.4 $\pm$ 0.4

If $\xi_1(x,y) = x$, effective dynamics $\equiv$ dynamics driven by free energy.

It seems that residence times are well approximated by the reduced dynamics when the “good” reaction coordinate and the “good” dynamics are used.

Conclusions

- We have proposed a “natural” way to obtain a closed equation on $\xi(X_t)$, by conditional expectations (natural extension of the Gyongy result).
- In some cases, we are able to estimate the accuracy of this effective equation.
- Encouraging numerical results on some simple cases.

F. Legoll, T. Lelièvre, *Effective dynamics using conditional expectations*, Arxiv preprint 0906.4865