Ergodicity and Lyapunov functions for Langevin dynamics with singular potentials

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(joint with B. Cooke, S.A. McKinley, S.C. Schmidler, J.C. Mattingly)

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Introduction

A familiar setting

An ODE on $\mathbf{R}^d$:

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- **First Answer**: Apply iteration scheme and show it has a unique fixed point!
- **Problem**: This assumes b is globally Lipschitz.
- **Solution**. Find a *Lyapunov function*.

Lyapunov functions

- Suppose that $V \in C^1(\mathbf{R}^d : [0, \infty))$ satisfies

$$\frac{d}{dt} V(x_t) = b(x_t) \cdot \nabla V(x_t) \leq C V(x_t).$$

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- Therefore if we can find a $V \in C^1(\mathbf{R}^d : [0, \infty))$ satisfying satisfying
  - $V(x) \to \infty$ as $|x| \to \infty$;
  - $b(x) \cdot \nabla V(x) \leq CV(x)$ for some constant $C > 0$,

we are done.

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Today: Existence of and convergence to the invariant measure for Hamiltonian dynamics with singular potentials?

Langevin dynamics

SDE on $(\mathbf{R}^k)^N \times (\mathbf{R}^k)^N$:

$$\begin{aligned} dq(t) &= p(t)\,dt \\ dp(t) &= -\gamma p(t)\,dt - \nabla U(q(t))\,dt + \sqrt{2\gamma k_B T}\,dB(t). \end{aligned}$$

- $q(t) = (q_1(t), \ldots, q_N(t)),\ p(t) = (p_1(t), \ldots, p_N(t)) \in (\mathbf{R}^k)^N$ are the position and momentum vectors;
- U is the potential function; $\gamma, k_B, T > 0$ are constants.
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Main Questions: Relaxation to Gibbs measure? If so, how fast?

Point: Requires nontrivial understanding of how dissipation spreads through the system.

Singular U?

$$U(q) = \underbrace{\sum_{i=1}^{N} U_{\mathcal{E}}(q_i)}_{\text{environmental forces}} + \underbrace{\sum_{i<j} U_{\mathcal{I}}(q_i - q_j)}_{\text{interaction forces}}$$

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(3) $U_{\mathcal{E}}(x) = a\|x\|^{2j} + p_{2j-1}(x); \quad U_{\mathcal{I}}(x) = \frac{b}{\|x\|^{12}} - \frac{c}{\|x\|^{6}} = \text{LJ}.$

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Point: Mathematics literature almost exclusively restricted to potentials like those in (1) and (2). How does one handle singular potentials like (3) and (4)? How do (1)-(4) fit together? How is the dynamics different?

The dynamics

Example: $k = N = \gamma = k_B = 1$, $U(q) = \frac{q^4}{4} + \frac{1}{2q^2}$, $q_0 = 8, p_0 = 1$, $T = 25$

The dynamics

Example: $k = 1,\ N = 2,\ \gamma = 1,\ k_B = 1,\ T = 25,$
$U_{\mathcal{Q}}(q) = q^2,\ U_{\mathcal{I}}(q) = \frac{1}{|q|^{1.3}}$

The dynamics

Example: $k = 1,\ N = 3, \gamma = 1,\ k_B = 1,\ T = 25,$
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Previous Work and Main Results

Previous Work

Theorem (Mattingly, Stuart, Hingham '02)
Suppose that $U \in C^\infty((\mathbf{R}^k)^N; (0,\infty))$ *satisfies the global bound*

$$\frac{1}{2}\nabla U(q)\cdot q \geq \beta U(q) + \gamma^2 \frac{\beta(2-\beta)}{8(1-\beta)}\|q\|^2 - \alpha$$

for some $\alpha > 0$ *and* $\beta \in (0,1)$*. Then for every* $\ell \geq 1$ *there exists* $C = C(\ell) > 0, \lambda = \lambda(\ell) > 0$ *such that*

$$\left|\mathcal{P}_t\phi(q,p) - \int \phi \, d\mu\right| \leq CV(q,p)^\ell e^{-\lambda t}$$

for all $t \geq 0$*,* $|\phi| \leq V^\ell$*. Here* $V \sim H + 1$*.*

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- (Talay '02) Similar conclusion provided $U \in C^\infty((\mathbf{R}^k)^N; (0,\infty))$ is essentially a polynomial.

Previous Work

Point: In both works, there is an explicit Lyapunov function V which satisfies

$$V(q, p) = H(q, p) + \psi(q, p)$$

where $\psi(q, p) = \epsilon p \cdot q$, $\epsilon > 0$ small.

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Theorem (Villani '06)

Assumes $U \in C^2((\mathbf{R}^k)^N; (0,\infty))$ grows "at least linearly at infinity" and satisfies $|\nabla^2 U| \leq C(1 + |\nabla U|)$. Then there exist $C, \lambda > 0$ for which

$$\left\| \mathcal{P}_t \phi - \int \phi \, d\mu \right\|_{H^1(\mu)} \leq C e^{-\lambda t} \|\phi\|_{H^1(\mu)}$$

for all $t \geq 0$, $\phi \in H^1(\mu)$.

- Strengthens work of Helffer and Nier ('05).

Previous Work

- Hypocoercivity approach vs Lyapunov approach. Makes use of existence of an invariant measure, handles a different norm.
- (Conrad, Grothaus '10) Under appropriate growth of U and assuming

$$|\nabla^2 U| \leq C(1 + |\nabla U|^\alpha)$$

for some $C > 0$ and $\alpha \in [1, 2)$, then there exists a constant $D > 0$ such that for all $t > 0$, $\phi \in L^2(\mu)$

$$\mathbf{E}_\mu \left(\frac{1}{t} \int_0^t \bar{\phi}(q(s), p(s))\, ds \right)^2 \leq \frac{D}{t} \|\bar{\phi}\|^2_{L^2(\mu)}.$$

In the above, $\bar{\phi} = \phi - \int \phi \, d\mu$.

  - Includes singular cases since α can be greater than 1.

Previous work

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Question: Does a Lyapunov function exist in the singular case? Can we improve convergence results? How does it all fit together?

Main Results

Theorem (Cooke, H., Mattingly, McKinley, Schmidler '17)
Suppose $N = k = 1$ *and* $U : (0, \infty) \to (0, \infty)$ *is of the form*

$$U(q) = \sum_{i=1}^{J} \beta_i q^{\alpha_i}$$

where $\beta_1, \beta_J > 0$, $\alpha_1 > \alpha_2 > \cdots > \alpha_J$, *and* $\alpha_1 > 2, \alpha_J < 0$. *Then there exist constants* $C, \lambda > 0$ *such that*

$$\left| \mathcal{P}_t \phi(q,p) - \int \phi \, d\mu \right| \leq CV(q,p) e^{-\lambda t}$$

for all $t \geq 0$, $|\phi| \leq V$. *Here* $V \sim \exp(\delta H)$ *where* $\delta < \beta$.

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- Result makes use of an explicit construction of a Lyapunov function of the form $V = H + \psi$, $\psi = o(H)$ as $H \to \infty$.
- Works for two particles in $\mathbf{R}^1$. What about N particles on $\mathbf{R}^k$?

Main Results

Definition

Let $U : (\mathbf{R}^k)^N \to [0, +\infty]$ and $\mathcal{O} = \{q : U(q) < \infty\}$. We call U **admissible** if

- $\mathcal{O}$ is non-empty, open, connected. Moreover, for each $R > 0$ the set

  $$\{q : U(q) < R\}$$

  has compact closure in $(\mathbf{R}^k)^N$.
- $U \in C^\infty(\mathcal{O})$ and $\int_{\mathcal{O}} e^{-\beta U(q)}\, dq < \infty$.
- For any sequence $\{q_k\} \subset \mathcal{O}$ for which $U(q_k) \to \infty$ as $k \to \infty$ we have

  $$|\nabla U(q_k)| \to \infty \text{ and } \frac{|\nabla^2 U(q_k)|}{|\nabla U(q_k)|^2} \to 0$$

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- Explicit Lyapunov function. Proof is relatively simple.
- Can relax regularity to $U \in C^2(\mathcal{O})$ in construction.
- Construction does not need apriori knowledge of the invariant measure.

Heuristics and Proof

Propagation of dissipation

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If $H(q,p) = \frac{\|p\|^2}{2} + U(q)$ and $x_0 = (q_0, p_0)$, then

$$\mathbf{E}_{x_0} H(q(t), p(t)) - H(x_0) = \mathbf{E}_{x_0} \int_0^t \underbrace{-\gamma \|p(s)\|^2 + \gamma k_B T k N}_{\mathcal{L}H(q(s),p(s))} \, ds.$$

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Problem: H is NOT pointwise contractive.

- $\mathcal{L}H(q,p) > 0$ for $|p|^2 > 0$ small enough. Is dissipation possible?
- Yes, but must be due to averaging effects:

$$A_{p^2}(x_0, t, R) := \frac{1}{t} \int_0^t \|p(s)\|^2 \mathbf{1}\{H(q(s), p(s)) \geq R\} \, ds$$

where for fixed x_0, t and $R \gg 1$ we hope

$$\frac{1}{2} A_{p^2}(x_0, t, R) \gg 1.$$

Averaging

Example: $k = N = \gamma = k_B = 1$, $U(q) = \frac{q^4}{4} + \frac{1}{2q^2}$, $q_0 = 8, p_0 = 1$, $T = 25$

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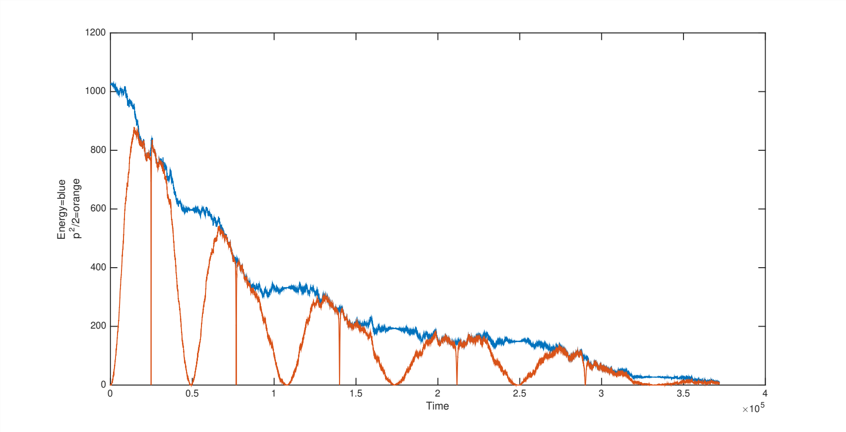

Figure 1: $H(q(t), p(t))$ and $\frac{p^2(t)}{2}$ plotted for $t \in [0, 4]$. We have $A_H((8,1), 10, 8) \approx 82.04$ and $\frac{1}{2}A_{p^2}((8,1), 10, 8) \approx 53.62$

Averaging ($N = 2,\ T = 25,\ U_{\mathcal{E}}(q) = q^2,\ U_{\mathcal{I}}(q) = \frac{1}{|q|^{1.3}}$)

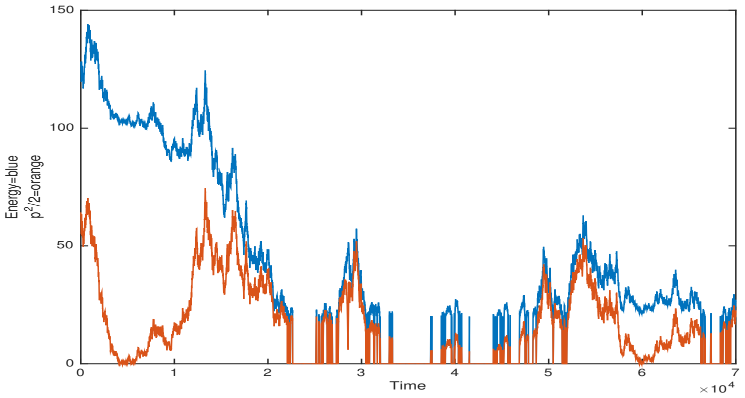

Figure 2: $H(q(t), p(t))$ and $\frac{p^2(t)}{2}$ plotted for $t \in [0, 70]$. We have $A_H((8, -8, 1, .5), 70, 20) \approx 3.94$ and $\frac{1}{2} A_{p^2}((8, -8, 1, .5), 70, 20) \approx 1.58$

Construction outline

Goal: Find $\psi \in C^2$ with $\psi = o(H)$ as $H \to \infty$ and such that

$$\mathcal{L}\psi(q, p) \leq -\kappa \qquad \text{for} \qquad H \geq R$$

for some constants $\kappa > 2\gamma k_B TkN$, $R \gg 1$.

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for some constants $\kappa > 2\gamma k_B T k N, R \gg 1$.

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- Does not imply geometric convergence, however!
- Existence of invariant measure (if we perturb γ and noise coefficients within reason) follows from Hasminskii's cycle trick.

Faster return times?

Point: Should be the case that $W = e^{\delta(H+\psi)} \approx e^{\delta H}$ satisfies

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Conclusion: Exponentiate δV and control quadratic variation terms by picking $0 < \delta < 1/(k_B T)$.

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For simplicity: Set $k = N = 1$ and $U(q) = q^{\alpha} + 1/q^{\beta}$ for $q > 0$ where $\alpha > 1, \beta > 0$.

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Conclusion: We don't need ψ if p^2 is large enough. Need to analyze the behavior of process at large energies when p^2 is bounded (i.e. p^2 is bounded while $U(q)$ is large).

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- For general k, N, one can repeat the analysis to conclude

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$\implies$ competition with $-\gamma p^2$ unless condition is satisfied.

The end

THANK YOU!!!