Hypoelliptic multiscale Langevin diffusions, large deviations, invariant measure and small mass asymptotics.

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Classical Langevin equation.

Classical Langevin equation:

\[ \tau \ddot{q}_t = b(q_t) - \lambda(q_t) \dot{q}_t + \sigma(q_t) \dot{W}_t. \]  

- \( \tau \) = mass,
- \( b \) = drift (external force),
- \( \lambda \) = friction,
- \( \sigma \dot{W} \) = noise.

(1)
Multiscale Langevin equation.

- Multiscale Langevin equation:

\[
\tau \ddot{q}_t^\varepsilon = \frac{\varepsilon}{\delta} b \left( q_t^\varepsilon, \frac{q_t^\varepsilon}{\delta} \right) + c \left( q_t^\varepsilon, \frac{q_t^\varepsilon}{\delta} \right) - \lambda (q_t^\varepsilon) \dot{q}_t^\varepsilon + \sqrt{\varepsilon} \sigma \left( q_t^\varepsilon, \frac{q_t^\varepsilon}{\delta} \right) \dot{W}_t .
\]

- Parameters \(0 < \varepsilon, \delta \ll 1\) and \(\delta = \delta(\varepsilon) \downarrow 0\) as \(\varepsilon \downarrow 0\).

- Parameter \(\varepsilon\) represents the strength of the noise, whereas \(\delta\) is the parameter that separates the scales.

- We want to send the small parameters \(\varepsilon\) and \(\delta\) to 0 in a way that

\[
\frac{\varepsilon}{\delta} \rightarrow \begin{cases} 
0 & \text{, (large deviation)} \\
\gamma \in (0, 1) & \text{, (intermediate)} \\
\infty & \text{, (homogenization)}
\end{cases}
\]
Background and Motivation.

- **Chemical Physics and Biology.**
- The dynamical behavior of proteins such as their folding and binding kinetics.
- The potential surface of a protein might have a hierarchical structure with potential minima within potential minima. The presence of multiple energy scales associated with the building blocks of proteins implies that the underlying energy landscapes of certain biomolecules can be rugged (i.e., consist of many minima separated by barriers of varying heights).
- As a consequence, the roughness of the energy landscapes that describe proteins has numerous effects on their kinetic properties as well as on their behavior at equilibrium.
We will focus in this work on the homogenization case:

\[
\frac{\varepsilon}{\delta} \to \infty
\]

as \( \varepsilon \downarrow 0 \) and \( \delta = \delta(\varepsilon) \downarrow 0 \) as \( \varepsilon \downarrow 0 \)

Interested in **large deviations** of the process \( \{ q^\varepsilon, \varepsilon > 0 \} \).
Definition. Let \( \{ q^\varepsilon, \varepsilon > 0 \} \) be a family of random variables taking values on a Polish space \( S \) and let \( I \) be a rate function on \( S \). We say that \( \{ q^\varepsilon, \varepsilon > 0 \} \) satisfies the Laplace principle with rate function \( I \) if for every bounded and continuous function \( h : S \rightarrow \mathbb{R} \),

\[
\lim_{\varepsilon \downarrow 0} -\varepsilon \ln E \left[ \exp \left( -\frac{h(q^\varepsilon)}{\varepsilon} \right) \right] = \inf_{x \in S} [I(x) + h(x)].
\]
Weak convergence framework of large deviations.

- We found a parametrization: \( \tau = \tau(\varepsilon, \delta) = m \frac{\delta^2}{\varepsilon}, \, m > 0 \) and we have

  \[
  m \frac{\delta^2}{\varepsilon} \ddot{q}_t^\varepsilon = \frac{\varepsilon}{\delta} b \left( q_t^\varepsilon, \frac{q_t^\varepsilon}{\delta} \right) + c \left( q_t^\varepsilon, \frac{q_t^\varepsilon}{\delta} \right) - \lambda (q_t^\varepsilon) \dot{q}_t^\varepsilon + \sqrt{\varepsilon} \sigma \left( q_t^\varepsilon, \frac{q_t^\varepsilon}{\delta} \right) \dot{W}_t.
  \]

- It is only in this parametrization that we can derive the large deviation principle for \( \{ q^\varepsilon, \varepsilon > 0 \} \).
We can write multiscale Langevin equation into first order diffusion equation

\[
\begin{align*}
\dot{q}^\epsilon_t &= \frac{1}{\sqrt{m\delta}} \frac{\epsilon}{\delta} p^\epsilon_t, \\
\dot{p}^\epsilon_t &= \frac{1}{\sqrt{m\delta}} \left[ \frac{\epsilon}{\delta} b \left( q^\epsilon_t, \frac{q^\epsilon_t}{\delta} \right) + c \left( q^\epsilon_t, \frac{q^\epsilon_t}{\delta} \right) \right] - \frac{\lambda(q^\epsilon_t)}{m} \frac{\epsilon}{\delta^2} p^\epsilon_t \\
&\quad + \frac{\sqrt{\epsilon}}{\delta} \sigma \left( q^\epsilon_t, \frac{q^\epsilon_t}{\delta} \right) \dot{W}_t.
\end{align*}
\]

Initial conditions \( q^\epsilon_0 = q_o \in \mathbb{R}^d, \ p^\epsilon_0 = p_o \in \mathbb{R}^d \).
Weak convergence framework of large deviations.

- Apply classical results of Boué–Dupuis\(^3\) to the above system:

\[-\varepsilon \ln E_{q_0} \left[ \exp \left( -\frac{h(q_\varepsilon)}{\varepsilon} \right) \right] = \inf_{u \in A} E_{q_0} \left[ \frac{1}{2} \int_0^T |u_s|^2 ds + h(q_\varepsilon) \right].\]

- The control set

\[A = \{ u = \{u_s \in \mathbb{R}^d : 0 \leq s \leq T \} \text{ progressively } \mathcal{F}_s-\text{measurable and } E \int_0^T |u_s|^2 ds < \infty \}.\]

- \(q_\varepsilon\): controlled hypoelliptic Langevin diffusion.

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Weak convergence framework of large deviations.

\[
\begin{cases}
\dot{q}_t^\varepsilon = \frac{1}{\sqrt{m \delta}} \varepsilon p_t^\varepsilon,

\dot{p}_t^\varepsilon = \frac{1}{\sqrt{m \delta}} \left[ \frac{\varepsilon}{\delta} b \left( \frac{q_t^\varepsilon, q_t^\varepsilon}{\delta} \right) + c \left( \frac{q_t^\varepsilon, q_t^\varepsilon}{\delta} \right) \right] - \lambda(q_t^\varepsilon) \frac{\varepsilon}{m} \frac{\varepsilon}{\delta^2} p_t^\varepsilon \\
+ \frac{1}{\delta} \frac{\sigma(q_t^\varepsilon, q_t^\varepsilon)}{\sqrt{m}} u_t + \sqrt{\varepsilon} \frac{\sigma(q_t^\varepsilon, q_t^\varepsilon)}{\delta} \sqrt{m} \dot{W}_t.
\end{cases}
\]

Initial conditions \( q_0^\varepsilon = q_0 \in \mathbb{R}^d \), \( p_0^\varepsilon = p_0 \in \mathbb{R}^d \).
Compare the two expressions

\[
\lim_{\varepsilon \downarrow 0} -\varepsilon \ln \mathbb{E} \left[ \exp \left( -\frac{h(q^\varepsilon)}{\varepsilon} \right) \right] = \inf_{x \in S} [I(x) + h(x)],
\]

and

\[
-\varepsilon \ln \mathbb{E}_{q_0} \left[ \exp \left( -\frac{h(q^\varepsilon)}{\varepsilon} \right) \right] = \inf_{u \in A} \mathbb{E}_{q_0} \left[ \frac{1}{2} \int_0^T |u_s|^2 ds + h(\overline{q}^\varepsilon) \right].
\]

Goal: To take the limit as \(\varepsilon \downarrow 0\) of the controlled process \(\{\overline{q}^\varepsilon : \varepsilon > 0\}\) as \(\varepsilon \downarrow 0\).

Fast–slow dynamics, averaging, homogenization...
Large deviations for second order Langevin equation.

- **Condition 1.** The functions $b(q, r)$, $c(q, r)$, $\sigma(q, r)$ are (i) periodic with period 1 in the second variable in each direction, and (ii) $C^1(\mathbb{R}^d)$ in $r$ and $C^2(\mathbb{R}^d)$ in $q$ with all partial derivatives continuous and globally bounded in $q$ and $r$.

- Control space $\mathcal{Z} = \mathbb{R}^d$; Fast variable space $\mathcal{Y} = \mathbb{R}^d \times \mathbb{T}^d$.

- Fast variable is actually $\left( \bar{p}_s^\varepsilon, \bar{q}_s^\varepsilon \right)$. 
Large deviations for second order Langevin equation.

Define an operator

$$\mathcal{L}_q^m \Phi(p, r) = \frac{1}{\sqrt{m}} \left[ p \cdot \nabla_r \Phi(p, r) + b(q, r) \cdot \nabla_p \Phi(p, r) \right]$$

$$+ \frac{1}{m} \left[ -\lambda(q) p \cdot \nabla_p \Phi(p, r) + \frac{1}{2} \alpha(q, r) : \nabla_p^2 \Phi(p, r) \right]$$

where $\alpha(q, r) = \sigma(q, r) \sigma^T(q, r)$.

For each fixed $q$, the operator $\mathcal{L}_q^m$ defines a hypoelliptic diffusion process on $(p, r) \in \mathcal{Y} = \mathbb{R}^d \times \mathbb{T}^d$.

Let $\mu(dpdr|q)$ be the unique invariant measure for this process.

Notice that $\mathcal{L}_q^m$ is effectively the operator corresponding to the fast motion.
Condition 2. (Centering condition) We assume that for every $q \in \mathbb{R}^d$ we have

$$\int_{\mathcal{Y}} b(q, r) \mu(dpdr|q) = 0.$$
Large deviations for second order Langevin equation.

Preliminary cell problem

\[ \mathcal{L}_q^m \Phi(p, r) = -\frac{1}{\sqrt{m}} p , \quad \int_{\mathcal{Y}} \Phi(p, r) \mu(dr dp|q) = 0 , \]

has a unique, smooth solution that does not grow too fast at infinity.

\[ \Phi(p, r) = (\Phi_1(p, r), \ldots, \Phi_d(p, r)) . \]
Theorem 1. Let \( \{q^\varepsilon, \varepsilon > 0\} \) be the unique solution to (3). Under Conditions 1 and 2, \( \{q^\varepsilon, \varepsilon > 0\} \) satisfies the large deviations principle with rate function

\[
S_m(\phi) = \begin{cases} 
\frac{1}{2} \int_0^T (\dot{\phi}_s - r_m(\phi_s))^T Q_m^{-1}(\phi_s)(\dot{\phi}_s - r_m(\phi_s))ds \\
\quad \text{if } \phi \in AC([0, T]; \mathbb{R}^d) \ , \ \phi_0 = q_0 \\
+\infty \ , \ \text{otherwise} 
\end{cases}
\]

where

\[
r_m(q) = \frac{1}{\sqrt{m}} \int_{\mathcal{Y}} \nabla_p \Phi(p, r)c(q, r)\mu(dpdr|q) ,
\]

\[
Q_m(q) = \frac{1}{m} \int_{\mathcal{Y}} \nabla_p \Phi(p, r)\alpha(q, r)(\nabla_p \Phi(p, r))^T \mu(dpdr|q) .
\]
Large deviations for second order Langevin equation.

- **Proof** is based on adapting established methods in previous works such as
- Lots of calculations that I skip here.
Small mass limit: approximation by first order Langevin equation.

Recall the multiscale Langevin equation

\[ m \frac{\delta^2}{\varepsilon} \ddot{q}_t^\varepsilon = \frac{\varepsilon}{\delta} b \left( q_t^\varepsilon, \frac{q_t^\varepsilon}{\delta} \right) + c \left( q_t^\varepsilon, \frac{q_t^\varepsilon}{\delta} \right) - \lambda (q_t^\varepsilon) \dot{q}_t^\varepsilon + \sqrt{\varepsilon} \sigma \left( q_t^\varepsilon, \frac{q_t^\varepsilon}{\delta} \right) \dot{W}_t. \]

Small mass limit: let \( m \to 0 \).

\( q_t^\varepsilon \) is approximated by \( \tilde{q}_t^\varepsilon \):

\[ \tilde{q}_t^\varepsilon = \frac{\varepsilon}{\delta} b \left( \tilde{q}_t^\varepsilon, \frac{\tilde{q}_t^\varepsilon}{\delta} \right) + \frac{c \left( \tilde{q}_t^\varepsilon, \frac{\tilde{q}_t^\varepsilon}{\delta} \right)}{\lambda (\tilde{q}_t^\varepsilon)} + \frac{\nabla \lambda (\tilde{q}_t^\varepsilon)}{2 \lambda^3 (\tilde{q}_t^\varepsilon)} \alpha \left( \tilde{q}_t^\varepsilon, \frac{\tilde{q}_t^\varepsilon}{\delta} \right) + \sqrt{\varepsilon} \frac{\sigma \left( \tilde{q}_t^\varepsilon, \frac{\tilde{q}_t^\varepsilon}{\delta} \right)}{\lambda (\tilde{q}_t^\varepsilon)} \dot{W}_t. \]  

\( \tilde{q}_t^\varepsilon \) the solution of first order Langevin equation.

Large deviations for first order Langevin equation $\tilde{q}^\varepsilon_t$ is well established.

Let $\mu_0(dr|q)$ be the unique invariant measure corresponding to the operator

$$\mathcal{L}_q^0 = \frac{1}{\lambda(q)} b(q, r) \cdot \nabla r + \frac{1}{2\lambda(q)} \alpha(q, r) : \nabla^2 r$$

equipped with periodic boundary conditions in $r$ ($q$ is being treated as a parameter here) on $\tilde{\mathcal{Y}} = \mathbb{T}^d$.

Centering condition:

$$\int_{\tilde{\mathcal{Y}}} b(q, r) \mu_0(dr|q) = 0.$$
Large deviations for first order Langevin equation.

- Cell problem

\[ \mathcal{L}_q^0 \chi_\ell(q, r) = -\frac{1}{\lambda(q)} b_\ell(q, r)\ , \int_{\mathcal{Y}} \chi_\ell(q, r) \mu_0(d r | q) = 0, \]

\( \ell = 1, 2, ..., d, \) has a unique bounded and sufficiently smooth solution \( \chi = (\chi_1, ..., \chi_d). \)
Theorem 2. Let \( \{ \tilde{q}^\varepsilon, \varepsilon > 0 \} \) be the unique solution to the first order Langevin equation. Under Conditions 1 and 2, \( \{ \tilde{q}^\varepsilon, \varepsilon > 0 \} \) satisfies a large deviations principle with rate function

\[
S_0(\phi) = \begin{cases} 
\frac{1}{2} \int_0^T (\dot{\phi}_s - r_0(\phi_s))^T Q_0^{-1}(\phi_s)(\dot{\phi}_s - r_0(\phi_s))ds, & \text{if } \phi \in AC([0, T]; \mathbb{R}^d), \phi_0 = q_0; \\
+\infty, & \text{otherwise.}
\end{cases}
\]

where

\[
r_0(q) = \frac{1}{\lambda(q)} \int_{\tilde{Y}} \left( I + \frac{\partial \chi}{\partial r}(q, r) \right) c(q, r) \mu_0(dr|q)
\]

and

\[
Q_0(q) = \frac{1}{\lambda^2(q)} \int_{\tilde{Y}} \left( I + \frac{\partial \chi}{\partial r}(q, r) \right) \alpha(q, r) \left( I + \frac{\partial \chi}{\partial r}(q, r) \right)^T \mu_0(dr|q).
\]
Approximation of the rate function.

When do we have

\[ \lim_{m \to 0} S_m(\phi) = S_0(\phi) ? \]

This is very hard in general.

We can work out the case when \( \sigma(q, r) = \sqrt{2 \beta \lambda(q)} l, \beta > 0 \) (fluctuation–dissipation balance).
Theorem 1. Let \( \{ q^\varepsilon, \varepsilon > 0 \} \) be the unique solution to (3). Under Conditions 1 and 2, \( \{ q^\varepsilon, \varepsilon > 0 \} \) satisfies the large deviations principle with rate function

\[
S_m(\phi) = \begin{cases} 
\frac{1}{2} \int_0^T \left( \phi_s - r_m(\phi_s) \right)^T Q_m^{-1}(\phi_s) \left( \phi_s - r_m(\phi_s) \right) ds , & \text{if } \phi \in AC([0, T]; \mathbb{R}^d) \ , \ \phi_0 = q_0 \ ; \\
+\infty , & \text{otherwise} .
\end{cases}
\]

where

\[
r_m(q) = \frac{1}{\sqrt{m}} \int_{\mathcal{Y}} \nabla_p \Phi(p, r) c(q, r) \mu(dpdr|q) ,
\]

\[
Q_m(q) = \frac{1}{m} \int_{\mathcal{Y}} \nabla_p \Phi(p, r) \alpha(q, r)(\nabla_p \Phi(p, r))^T \mu(dpdr|q) .
\]
Large deviations for first order Langevin equation.

Theorem 2. Let \( \{\tilde{q}^\varepsilon, \varepsilon > 0\} \) be the unique solution to the first order Langevin equation. Under Conditions 1 and 2, \( \{\tilde{q}^\varepsilon, \varepsilon > 0\} \) satisfies a large deviations principle with rate function

\[
S_0(\phi) = \begin{cases} 
\frac{1}{2} \int_0^T (\dot{\phi}_s - r_0(\phi_s))^T Q_0^{-1}(\phi_s)(\dot{\phi}_s - r_0(\phi_s)) \, ds , & \text{if } \phi \in AC([0, T]; \mathbb{R}^d) , \phi_0 = q_0 ; \\
+\infty , & \text{otherwise .}
\end{cases}
\]

where

\[
r_0(q) = \frac{1}{\lambda(q)} \int_{\mathcal{Y}} \left( (I + \frac{\partial \chi}{\partial r}(q, r)) \right) c(q, r) \mu_0(dr|q)
\]

and

\[
Q_0(q) = \frac{1}{\lambda^2(q)} \int_{\mathcal{Y}} \left( (I + \frac{\partial \chi}{\partial r}(q, r)) \alpha(q, r) \left( (I + \frac{\partial \chi}{\partial r}(q, r)) \right)^T \mu_0(dr|q).
\]
Approximation of the rate function.

Does

\[ r_m(q) = \frac{1}{\sqrt{m}} \int_{\mathcal{Y}} \nabla_p \Phi(p, r) c(q, r) \mu(dpdr|q) \]

converge to

\[ r_0(q) = \frac{1}{\lambda(q)} \int_{\bar{\mathcal{Y}}} \left( I + \frac{\partial \chi}{\partial r}(q, r) \right) c(q, r) \mu_0(dr|q) \]

as \( m \to 0 \)?

Does

\[ Q_m(q) = \frac{1}{m} \int_{\mathcal{Y}} \nabla_p \Phi(p, r) \alpha(q, r) (\nabla_p \Phi(p, r))^T \mu(dpdr|q) \]

converge to \( Q_0(q) = \frac{1}{\lambda^2(q)} \int_{\bar{\mathcal{Y}}} \left( I + \frac{\partial \chi}{\partial r}(q, r) \right) \alpha(q, r) \left( I + \frac{\partial \chi}{\partial r}(q, r) \right)^T \mu_0(dr|q) \) as \( m \to 0 \)?
Approximation of the rate function.

- To establish the convergence of rate functions for the small mass limit it suffices to establish the following two facts.
- **Fact 1.** $\mu(dpdr|q) \to \mu_0(dr|q)$ as $m \to 0$ in a certain sense.
- **Fact 2.** $\frac{1}{\sqrt{m}} \nabla p\Phi \to \frac{1}{\chi(q)}(I + \nabla_r\chi)$ as $m \to 0$ in a certain sense.
Approximation of the rate function.

Write

\[ \mathcal{L}_q^m f(p, r) = \frac{\lambda(q)}{m} Af(p, r) + \frac{1}{\sqrt{m}} B f(p, r), \]

where

\[ Af(p, r) = -p \cdot \nabla p f + \beta \Delta p f \]

and

\[ B f(p, r) = p \cdot \nabla r f + b(q, r) \cdot \nabla p f. \]

Likewise, we have

\[ \mathcal{L}_q^0 f(r) = \frac{1}{\lambda(q)} b(q, r) \cdot \nabla r f(r) + \beta \Delta f(r). \]
Approximation of the rate function.

- We denote by $\mu(dpdr|q) = \rho^m(p, r|q)dpdr$ the invariant measure corresponding to the operator $\mathcal{L}_q^m$. Also, let us write $\mu_0(dr|q) = \rho_0(r|q)dr$ for the invariant measure corresponding to the operator $\mathcal{L}_q^0$.

- Let us also define $\pi(dp) = \rho^{\text{OU}}(p)dp$ to be the invariant measure on $\mathbb{R}^d$ for the Ornstein–Uhlenbeck process with generator $\mathcal{A}$. With this notation, let us write $\rho^m(p, r) = \tilde{\rho}^m(p, r)\rho^0(p, r)$, where $\rho^0(p, r) = \rho^{\text{OU}}(p)\rho_0(r)$, suppressing the dependence on $q$. 
Theorem 3. Let Condition 1 hold and assume that
\[ \sigma(q, r) = \sqrt{2\beta \lambda(q)}l, \beta > 0. \]
Then, for every \( q \in \mathbb{R}^d \), we have
\[
\lim_{m \to 0} \| \tilde{\rho}^m(p, r) - 1 \|_{L^2(\mathcal{Y}; \rho^0)} = 0 .
\]

Theorem 4. Let Conditions 1 and 2 hold and assume that
\[ \sigma(q, r) = \sqrt{2\beta \lambda(q)}l, \beta > 0. \]
Then, for every \( q \in \mathbb{R}^d \), we have
\[
\lim_{m \to 0} \left\| \frac{1}{\sqrt{m}} \nabla_p \Phi - \frac{1}{\lambda(q)} (I + \nabla_r \chi) \right\|_{L^2(\mathcal{Y}; \rho^0)} = 0 .
\]
Ideas in the proof of Theorem 3.

Let $\delta^m(p, r) = \tilde{\rho}^m(p, r) - 1$, want to show

$$\lim_{m \to 0} \|\delta^m\|_{L^2(\mathcal{Y}; \rho^0)} = 0.$$ 

Equation for $\delta^m(p, r)$:

$$\mathcal{L}_q \delta^m(p, r) = \frac{2}{\sqrt{m}} B \delta^m(p, r) - \frac{1}{\sqrt{m}} ph(r)[\delta^m(p, r) + 1].$$

Can be written as

$$\mathcal{L}_q^1 \delta^m(p, r) = (1 + \sqrt{m}) B \delta^m(p, r) - \sqrt{m} ph(r) [\delta^m(p, r) + 1].$$

In other words

$$\mathcal{L}_q^1 \delta^m(p, r) - B \delta^m(p, r) = \sqrt{m} B \delta^m(p, r) - \sqrt{m} ph(r) [\delta^m(p, r) + 1].$$
Ideas in the proof of Theorem 3: hypocoercivity.

\[ \mathcal{L}^1 = A + B \]

where

\[ A = -p \cdot \nabla_p + \Delta_p , \quad B = p \cdot \nabla_r + b(q, r) \cdot \nabla_p . \]

\[ \mathcal{L}^1 \text{ is hypoelliptic.} \]

\[ \mathcal{L}^1 \text{ is hypocoercive}^{5}. \]

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Ideas in the proof of Theorem 3 : hypocoercivity.

\[ L^1 = -AA^* + B \]

where
\[ A = \nabla p, \quad A^* = -(\nabla p - p). \]

Let
\[ C = [A, B] = [\nabla p, p \cdot \nabla r + b(r) \cdot \nabla p] = \nabla r. \]

Introduce a mixed inner–product
\[
((f, f)) = \|f^2\|_{L^2(\mathcal{Y}; \rho^0)} + \alpha\|Af\|_{L^2(\mathcal{Y}; \rho^0)}^2 + 2b\Re \langle Af, Cf \rangle_{L^2(\mathcal{Y}; \rho^0)} + c\|Cf\|_{L^2(\mathcal{Y}; \rho^0)}^2.
\]

Making use of the coercivity of \( L^1 \) with respect to \((\bullet, \bullet))\) and a lot of detailed calculations.
Thank you for your attention!