Bridging the Gap between Center and Tail for Multiscale Processes

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A **multiscale process** is characterized by multiple coupled processes which evolve at separated time scales.

Event probabilities on the order of greater than one in one thousand are estimated by the Central Limit Theorem.

Event probabilities on the order of less than 10^{-9} are estimated by the Large Deviations Principle.

We focus on the **Moderate Deviations Principle**, which provides estimates for probabilities between these two extremes.

A Model of Protein Folding [Dupuis, et al., 2011]

Define

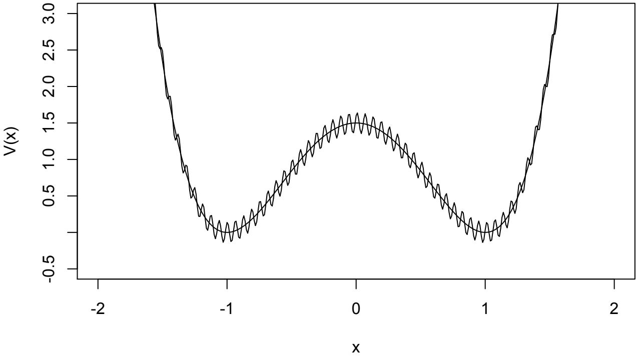
- $X^\varepsilon(t)$ — The configuration of a protein at time t
- $V^\varepsilon(x, x/\delta)$ — The potential surface of a protein

$X^\varepsilon(t)$ satisfies the Langevin equation

$$dX^\varepsilon(t) = -\nabla V^\varepsilon\left(X^\varepsilon(t), \frac{X^\varepsilon(t)}{\delta}\right) dt + \sqrt{\varepsilon}\sqrt{2D}\, dW(t), \quad X^\varepsilon(0) = x_0.$$

where $2D$ is a diffusion constant, $W(t)$ is standard Brownian motion, and δ and ε are small positive parameters.

Graph of a Potential Function



$$V^{\varepsilon}(x, \tfrac{x}{\delta}) = \varepsilon \left(\cos(\tfrac{x}{\delta}) + \sin(\tfrac{x}{\delta})\right) + \tfrac{3}{2}(x^2 - 1)^2,\ \varepsilon = 0.1,\ \delta = 0.01.$$

Definition of Multiscale Processes

Let X_t^ε be a n-dimensional process and Y_t^ε be a k-dimensional process for $0 \leq t \leq 1$ which solve the system

$$\begin{aligned} dX_t^\varepsilon &= c(X_t^\varepsilon, Y_t^\varepsilon)\,dt + \sqrt{\varepsilon}\sigma(X_t^\varepsilon, Y_t^\varepsilon)\,dW_t, & X_0^\varepsilon &= x_0 \\ dY_t^\varepsilon &= \frac{1}{\varepsilon} g(X_t^\varepsilon, Y_t^\varepsilon)\,dt + \frac{1}{\sqrt{\varepsilon}}\tau(X_t^\varepsilon, Y_t^\varepsilon)\,dB_t, & Y_0^\varepsilon &= y_0 \end{aligned}$$

where the coefficient functions $c(x,y)$, $\sigma(x,y)$, $g(x,y)$, and $\tau(x,y)$ are twice differentiable, and all functions, derivatives, and second derivatives are bounded, W_t and B_t are independent m-dimensional Brownian motions, and ε is a small positive parameter.
Furthermore, assume that $\lim_{|y|\to\infty} g(x,y)\cdot y = -\infty$ for all x and that $\tau\tau^{\mathsf{T}}$ is uniformly positive definite.

Law of Large Numbers [Spiliopoulos, 2014]

Consider the Y process with the x variable frozen, that is,

$$d\tilde{Y}_t = g(x, \tilde{Y}_t)\, dt + \tau(x, \tilde{Y}_t)\, dB_t, \quad \tilde{Y}_0 = y_0,$$

where $x \in \mathbb{R}^n$ is a fixed parameter.
This is associated with the operator $\mathcal{L}_x$ defined by

$$\mathcal{L}_x F(y) = \nabla F(y) g(x, y) + \frac{1}{2}\tau\tau^{\mathsf{T}}(x, y) : \nabla\nabla F(y)$$

and the invariant measure $\mu_x(dy)$.

Law of Large Numbers (cont.)

Define the averaged drift

$$\bar{c}(x) = \int_{\mathcal{Y}} c(x,y)\mu_x(dy)$$

and the averaged process $\bar{X}$ as the solution to

$$d\bar{X}_t = \bar{c}(\bar{X}_t)\,dt, \quad \bar{X}_0 = x_0.$$

Then as $\varepsilon \downarrow 0$,

$$X_t^\varepsilon \to \bar{X}_t \text{ in probability.}$$

Central Limit Theorem

Central Limit Theorem

$$\text{As } \varepsilon \downarrow 0,\ \frac{1}{\sqrt{\varepsilon}}(X_t^\varepsilon - \bar{X}_t) \to \bar{\eta}_t \text{ in distribution,}$$

where $\bar{\eta}_t$ is a single scale stochastic process.

This is used to estimate probabilities for X^ε near the center of the distribution.

Definition of Large Deviations

Let X^ε, $\varepsilon > 0$, be a family of random variables parameterized by ε. X^ε satisfies a **large deviations principle** with rate function I if for every closed set F,

$$\limsup_{\varepsilon \downarrow 0} \varepsilon \log P\{X^\varepsilon \in F\} \leq - \inf_{x \in F} I(x)$$

and for every open set G,

$$\liminf_{\varepsilon \downarrow 0} \varepsilon \log P\{X^\varepsilon \in G\} \geq - \inf_{x \in G} I(x).$$

If a family of random variables satisfies a large deviations principle with some rate function, that rate function is unique.

The Laplace Principle [Dupuis and Ellis, 1997]

The family X^ε, $\varepsilon > 0$, satisfies a **Laplace principle** with rate function I if for every bounded continuous function a,

$$\lim_{\varepsilon \downarrow 0} \varepsilon \log E\{\exp[-\frac{1}{\varepsilon} a(X^\varepsilon)]\} = -\inf_x \{I(x) + a(x)\}.$$

The Laplace principle and the large deviations principle are equivalent.

The large deviations principle (or Laplace principle) is used to estimate probabilities in the tail of the distribution.

Definition of Moderate Deviations

Let $h(\varepsilon)$ be a function such that as $\varepsilon \downarrow 0$, $h(\varepsilon) \to \infty$ and $\sqrt{\varepsilon}h(\varepsilon) \to 0$. Consider

$$\eta_t^\varepsilon = \frac{1}{\sqrt{\varepsilon}h(\varepsilon)}(X_t^\varepsilon - \bar{X}_t).$$

A family of stochastic processes X^ε satisfies a **moderate deviations principle** with rate function I if for every bounded continuous function a,

$$\lim_{\varepsilon \downarrow 0} \frac{1}{h^2(\varepsilon)} \log E\{\exp[-h^2(\varepsilon)a(\eta^\varepsilon)]\} = -\inf_x \{I(x) + a(x)\}.$$

Previous results by [Guillin, 2003] and others.

Poisson Equation

Define $\Phi(x,y)$ as the unique solution to

$$\mathcal{L}_x\Phi(x,y) = -\left(c(x,y)-\bar{c}(x)\right), \qquad \int_{\mathcal{Y}} \Phi(x,y)\mu_x(dy) = 0.$$

(Existence and uniqueness due to [Pardoux and Veretennikov, 2003].)

Statement of Theorem

Theorem

Let X^ε and Y^ε as previously defined be a multiscale process. Then X^ε satisfies a moderate deviations principle with rate function

$$I(\phi) = \frac{1}{2}\int_0^1 (\dot{\phi}_s - r(\bar{X}_s, \phi_s))^\mathsf{T} q^{-1}(\bar{X}_s)(\dot{\phi}_s - r(\bar{X}_s, \phi_s))ds$$

if $\phi \in \mathcal{C}([0,1];\mathbb{R}^n)$ is absolutely continuous, and $I(\phi) = \infty$ otherwise, where

$$r(x,\eta) = \nabla \bar{c}(x)\eta$$

and

$$q(x) = \int_\mathcal{Y} \left[\sigma\sigma^\mathsf{T}(x,y) + [\nabla_y \Phi\tau]\,[\nabla_y \Phi\tau]^\mathsf{T}(x,y)\right] \mu_x(dy).$$

Sketch of Proof

The starting point for the proof is a stochastic control representation which follows from [Boué and Dupuis, 1998], which yields

$$-\frac{1}{h^2(\varepsilon)} \log E\left[\exp\{-h^2(\varepsilon)a(\eta^\varepsilon)\}\right] = \inf_{u^\varepsilon} E\left[\frac{1}{2}\int_0^1 \|u^\varepsilon(s)\|^2\, ds + a(\eta^{\varepsilon,u^\varepsilon})\right]$$

where u^ε is a stochastic control and $\eta^{\varepsilon,u^\varepsilon}$ is a controlled process. Then,

1. Prove that $(u^\varepsilon, \eta^{\varepsilon,u^\varepsilon})$ converges in distribution as $\varepsilon \downarrow 0$.
2. Define the rate function I in terms of the limit of the control u^ε, and prove the Laplace principle lower bound,
$$\liminf_{\varepsilon\downarrow 0} -\frac{1}{h^2(\varepsilon)} \log E\left[\exp\left\{-h^2(\varepsilon)a(\eta^\varepsilon)\right\}\right] \geq \inf_{\phi}\left[I(\phi) + a(\phi)\right].$$
3. Rewrite the rate function in the form given in the theorem statement, and use this to prove the Laplace principle upper bound,
$$\limsup_{\varepsilon\downarrow 0} -\frac{1}{h^2(\varepsilon)} \log E\left[\exp\left\{-h^2(\varepsilon)a(\eta^\varepsilon)\right\}\right] \leq \inf_{\phi}\left[I(\phi) + a(\phi)\right].$$

Future Work

1. Importance sampling schemes for accelerated Monte Carlo simulation based on the stochastic control representation.
2. Statistical inference for multiscale processes.

Thank You

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