Homework 4 due Wednesday, May 13 at 7 PM.
Office hours today 5-6 PM, tomorrow 6-7 PM.

Take care to acknowledge collaborations!

Three broad classes of techniques to approach SDEs in complex models that can’t be solved by elementary techniques.

- **Dynamical systems analysis**
  - identify equilibria, and linearize about them
  - bifurcation theory, phase portraits, ... gets a bit tricky to extend to SDEs, but partially possible

- **Numerical computation**
  - Euler-Marayama is broadly fine as a basic method
  - But the Monte Carlo simulations are often too expensive if directly implemented. Two types of approaches to make the simulations more efficient:
    - Multiscale simulation
    - Multi-level Monte Carlo
  - Polynomial chaos (sort of like trying to extend finite elements to stochastic problems); we won’t discuss (see for example book by Dongbin Xiu, Numerical Methods for Stochastic Computations: A Spectral Method Approach)

- **Asymptotic analysis**
  - Exploit large/small parameters to obtain simplified approximations
    - example: small noise approximation to escape time problem.
  - **Stochastic mode reduction**
    - Simplified approximations to "slow/fast" systems
    - the theoretical basis for multiscale simulation

To illustrate stochastic mode reduction, let’s return to the Langevin equation with external force.

\[
dX(t) = V(t) dt \\
m \, dV(t) = -\gamma V(t) dt + F(X(t)) dt + \sqrt{2k_B T \gamma} \, dW(t)
\]

We want to consider a “overdamped limit” where this equation can be approximated by the Smoluchowski dynamics:

\[
dX(t) = \gamma^{-1} F(X(t)) dt + \sqrt{\frac{k_B T}{\gamma}} \, dW(t)
\]

To systematize the analysis of equations with small/large parameters (here small mass or large friction), **nondimensionalize**.

In this case, appropriate reference length scale for nondimensionalization is:

\[
L = \ell_F, \text{the length scale of the force, i.e., } F(x) = F \left( \frac{x}{\ell_F} \right)
\]

and reference time scale is:

\[
T = \frac{\ell_T}{m} = \frac{\ell_T}{k_B T} \quad (\text{other choices fine, just as long as it doesn’t involve } m)
\]

Then performing the nondimensionalization, i.e.,

\[
\frac{X(t)}{L} = \frac{\xi(t)}{T}\]

\[
X(t) = \xi(t) \frac{L}{T}
\]
Overdamped limit really means $\epsilon \ll 1$.

How do asymptotic analysis for SDE's when we can't solve exactly?

The most widely used approach is to map the SDE onto backward Kolmogorov equations, then do singular perturbation theory on the resulting deterministic PDE. The alternative is to do a "direct method" on the SDE's but this is hard to explain in general terms.

Formally one could just as well map the SDE's onto Fokker-Planck equations and do singular perturbation theory on those, but backward Kolmogorov equations are technically nicer. Backward Kolmogorov equation is just the adjoint of Fokker-Planck equation.

So to do the small $\epsilon$ analysis of the Langevin equation with force, write down the corresponding BKE:
Now one can do the small $\varepsilon$-analysis on this deterministic PDE using singular perturbation techniques. There would result that:

$$f(x, v, t) = \tilde{f}(x, t) + O(\varepsilon)$$

$$\frac{\partial \tilde{f}(x, t)}{\partial t} = \left( \mu \tilde{f}(x) \right) \nabla \tilde{f}(x,t) + \sigma \tilde{f}(x,t)$$

But this is the BKE for the following SDE:

$$d \tilde{X}(t) = \mu \tilde{f}(\tilde{X}(t)) dt + \sqrt{2} d\tilde{W}(t) \quad \text{or} \quad O(\mu^{-1/2})$$

which is the nondimensionalized Smoluchowski equation.

Two key advantages of the simplified system:

- fewer variables ($d$ vs $2d$)
- remove the stiffness from the fast momentum dynamics

A useful broad generalization of these ideas: stochastic averaging

- Arnold, "Hasslemann's Program Revisited: The Analysis of Stochasticity in Deterministic Climate Models"
- Deutch and Oppenheim, "The Concept of Brownian Motion in Modern Statistical Mechanics"
- Bocquet, "From a Stochastic to a Microscopic Approach to Brownian Motion"

Examples:

- If one describes Brownian motion by including solvent molecules in addition to the solute molecule, then solvent molecules are fast and the solute molecule is slow
  - Deutch and Oppenheim, "The Concept of Brownian Motion in Modern Statistical Mechanics"
  - Bocquet, "From a Stochastic to a Microscopic Approach to Brownian Motion"

- Molecular dynamics: momentum variables are fast, position variables are slow
  - see for example K and Majda 2003

- Climate models:
  - weather/clouds operate on fast time scale, global mean temperature would be slow

- Complex fluids (polymers mixed into fluids):
  - polymer dynamics is fast, fluid motion is slow
• Active optical media: amplitude of light wave is slow, electronic transitions are fast

In any case, simulating the system will be expensive if we want to see $X$ dynamics because it is coupled to $Y$ dynamics that require time step $\ll \epsilon$ to resolve. One can make the simulations more efficient if somehow we didn’t have to simulate $Y$ directly. To this end, the following stochastic averaging result is useful:

$$
\hat{X}(t) = \hat{X}^H(t) + O(\epsilon^{1/2})
$$

This SDE involves an averaged drift:

$$
\hat{X}^H(t) = \int \hat{a}(\hat{X},\hat{Y},t) \, \bar{P}_{Y|X}(\hat{Y}|\hat{X}) \, d\hat{Y}
$$

where

$$
\bar{P}_{Y|X}(\hat{Y}|\hat{X})
$$

can be interpreted as the conditional probability density for the fast variable $\hat{Y}$, given that the slow variable is $\hat{X}(t) = \hat{x}$.

It is determined by solving the corresponding stationary Fokker-Planck equation:

$$
- \hat{a}_{\gamma} \cdot (\hat{b}(\hat{X},\hat{Y}) \bar{P}_{Y|X}(\hat{Y}|\hat{X})) + \frac{1}{2} \hat{a}_{\gamma} \hat{a}_{\gamma}^T \left( \hat{b}(\hat{X},\hat{Y}) \hat{b}(\hat{X},\hat{Y})^T \bar{P}_{Y|X}(\hat{Y}|\hat{X}) \right) = 0
$$

along with the normalization:

$$
\int \bar{P}_{Y|X}(\hat{Y}|\hat{X}) \, d\hat{Y} = 1
$$

Note that to solve for $\bar{P}_{Y|X}(\hat{Y}|\hat{X})$, the $X$ appear as parameters. The PDE is only w.r.t. the $Y$ variables.

Intuition:

One could generalize this idea to the case where $\Sigma = \Sigma(X(t),Y(t),t)$, but the averaged noise coefficient has a more complicated formula.

Example: Overdamped dynamics:
Think of this as a nondimensionalized description of overdamped dynamics in a potential $\phi(x,y)$, where the time scale of the $y$ variables is much faster ($c \ll 1$) than the $x$ variables. This happens for example in molecular dynamics: fast vibrations, slower rotations.

Let's see how we could average out the fast variables and obtain an approximate equation only for the slow variables.

To calculate the averaged drift coefficient, we first need the conditional stationary distribution for $y$ given $x$. The corresponding steady-state FP equation is:

\[
0 = -\nabla_y \left( -\nabla_y \phi(x,y) \frac{\mathbb{P}_Y}{\mathbb{P}_X} (x|y) \right) + \nabla_y \nabla_y \left( \frac{1}{2} \sigma^2 \frac{\mathbb{P}_Y}{\mathbb{P}_X} (y|x) \right)
\]

In three dimensions, divergence-free fields must be expressible as the sum of a constant (w.r.t. $y$) and a curl of a "vector potential" $\psi(x,y)$

\[
\left( \nabla_y \phi(x,y) \frac{\mathbb{P}_Y}{\mathbb{P}_X} (y|x) \right) + \frac{1}{2} \sigma^2 \nabla_y \frac{\mathbb{P}_Y}{\mathbb{P}_X} (y|x) = \nabla \psi(x,y)
\]

We'll look for a solution with $c(x) = 0, \psi(x,y) \equiv 0$; this can be justified either by:

- showing (tediously) that otherwise one cannot obtain a normalizable solution
- arguing that the stationary Fokker-Planck equation has a unique solution, so if we find one solution, it's the only one. (Standard well-posedness results for elliptic equations have to be adapted to having unbounded domain.)

Proceeding then to solve:

\[
\nabla \phi(x,y) \frac{\mathbb{P}_Y}{\mathbb{P}_X} (y|x) + \frac{1}{2} \sigma^2 \nabla \frac{\mathbb{P}_Y}{\mathbb{P}_X} (y|x) = 0
\]

This is a first order PDE which could be generally solved by method of characteristics. But we can take an easier approach, by using the separation method from ordinary first order differential equations. (This doesn't usually work for PDE's, but here it does)
Divide by $p_{Y|X}(y|x)$:

$$\nabla \phi(x, y) + \frac{1}{2} \sigma^2 \nabla p_{Y|X}(y|x) \nabla \log p_{Y|X}(y|x) = 0$$

$$\nabla \phi(x, y) + \frac{1}{2} \sigma^2 \nabla \log p_{Y|X}(y|x) = 0$$

For this gradient to vanish everywhere, the function in $[\ ]$ must be constant (w.r.t. $y$):

$$\phi(x, y) + \frac{1}{2} \sigma^2 \log p_{Y|X}(y|x) = k(x)$$

Solving for $p_{Y|X}(y|x)$:

$$p_{Y|X}(y|x) = Z(x)^{-1} \exp \left( -\frac{2\phi(x, y)}{\sigma^2} \right)$$

where $Z(x) = e^{-\frac{2\phi(x, y)}{\sigma^2}}$ can be determined by the normalization condition

$$\int p_{Y|X}(y|x) dy = 1$$

which implies

$$Z(x) = \int \exp \left( -\frac{2\phi(x, y)}{\sigma^2} \right) dy$$

essentially a partition function from statistical mechanics

Now substituting the solution for $p_{Y|X}(y|x)$ into the effective drift formula, noting the bare drift is:

$$a(x, y, t) = -\nabla_x \phi(x, y), \text{ we have:}$$

$$a^g(x, t) = \int a(x, y, t) p_{Y|X}(y|x) dy = \int \left( -\nabla_x \phi(x, y) \right) Z(x)^{-1} \exp \left( -\frac{2\phi(x, y)}{\sigma^2} \right) dy$$

$$= Z(x)^{-1} \left[ \frac{\sigma^2}{2} \nabla_x \exp \left( -\frac{2\phi(x, y)}{\sigma^2} \right) dy = \frac{\sigma^2}{2} Z(x)^{-1} \nabla_x \exp \left( -\frac{2\phi(x, y)}{\sigma^2} \right) dy \right]$$

$$= \frac{\sigma^2}{2} Z(x)^{-1} \nabla_x Z(x) = \frac{\sigma^2}{2} \nabla_x \log Z(x)$$

That is the effective drift

$$a^g(x) = -\nabla_x \tilde{F}(x)$$

where $\tilde{F}(x) = -\frac{\sigma^2}{2} \log Z(x) = -\frac{\sigma^2}{2} \log \exp \left( -\frac{2\phi(x, y)}{\sigma^2} \right) dy$ is the free energy.

To make the connection with the terminology from equilibrium statistical mechanics, when the noise in the system represents thermal noise, then (in dimensional form) $\sigma^2 = \frac{k_B T}{2}$, and $\tilde{F}(x) = -k_B T \log Z(x)$.

In any case, the slow-fast dynamics in a potential can be well approximated by the following equation involving only the slow variables:

$$dX(t) = -\nabla_x \tilde{F}(X(t)) dt + \Sigma(X(t), t)dW_x(t)$$

The potential $\phi(x, y)$ in the slow-fast system has been replaced by the free energy, which is a suitably averaged version of the potential (with
respect to the dynamics of the fast variables $Y(t)$. 