Take-home final exam. Due Wednesday, May 22, 11:59 PM.

Guidelines

- Working on this final, you can use any sources you wish. Please provide proper references to your sources.
- You **may not** discuss solutions to these problems with anyone.
- Please upload your files on ELMS.
- **Theoretical problems 1 and 2.** Submit a pdf file with your solution to each theoretical problem. It should be done in latex or any other text editor suitable for math formulas. If you submit a handwritten solution, your score will be reduced by 10% of the maximum.
- **Computational problems 3 and 4.** Programming must be done in MATLAB. Submit a single `.m` file with your code for each problem. I will run your codes. Your codes should not be too slow. Vectorize your codes (to a reasonable extent) and avoid symbolic commands. Then your runtimes will be small. I will penalize for too large runtimes even if the results are correct.

Problems

1. **(10 points)** The Freidlin-Wentzel action for the Langevin dynamics

$$\ddot{x} = -\dot{x} - \nabla V(x) + \sqrt{2\beta^{-1}}\eta(t), \quad \text{where} \quad \eta(t) \quad \text{is the white noise} \tag{1}$$

and $\dot{x} \equiv dx/dt$, $\ddot{x} \equiv d^2x/dt^2$, is given by

$$S_T(\phi) = \frac{1}{2}\int_0^T \|\ddot{\phi} + \dot{\phi} + \nabla V(\phi)\|^2 dt.$$

(a) Let $V(x)$ be a double-well potential with two stable equilibria at x_A and x_B and a saddle point at x_S. Prove that the maximum likelihood from $(x = x_A, \dot{x} = 0)$ to $(x = x_S, \dot{x} = 0)$ is the path $\phi_\star$ satisfying

$$\ddot{\phi}_\star = \dot{\phi}_\star - \nabla V(\phi_\star). \tag{2}$$

What is the infimum of $S_T(\phi)$ in all times and all paths?

(b) Suppose $x \in \mathbb{R}^1$. Let $V(x) = 0.25(1 - x^2)^2$. Then $x_A = -1$, $x_B = 1$, $x_S = 0$. Write a program that plots the level sets of the full energy $V(x) + \dot{x}^2/2$ and the maximum likelihood transition path from $(-1, 0)$ to $(1, 0)$ in the phase plane $(x, \dot{x})$. *Hint: the part of the path connecting* $(-1, 0)$ *and* $(0, 0)$ *is obtained by integrating Eq.* (2) *backward in time starting from an appropriate point near the saddle.*

Submit a single pdf file with your proof, your plot, and a copy of your code.

2. **(10 points)** Consider the SDE

$$\begin{bmatrix} dx \\ dy \end{bmatrix} = \begin{bmatrix} b_1(x,y) \\ b_2(x,y) \end{bmatrix} dt + \sqrt{\epsilon} \begin{bmatrix} dw_1 \\ dw_2 \end{bmatrix} \tag{3}$$

where ϵ is a small parameter. The corresponding ODE

$$\frac{d}{dt} \begin{bmatrix} x \\ y \end{bmatrix} = \begin{bmatrix} b_1(x,y) \\ b_2(x,y) \end{bmatrix} \tag{4}$$

rewritten in polar coordinates splits into two independent ODEs:

$$\frac{dr}{dt} = f(r), \tag{5}$$

$$\frac{d\theta}{dt} = g(\theta). \tag{6}$$

Suppose that f and g are smooth, $g(\theta)$ is strictly positive, and $f(r)$ has zeros at $r = 0$ and $r = r_0$, and $f(r) > 0$ for $0 < r < r_0$ and $f(r) < 0$ for $r > r_0$. Hence, the only attractor of ODE (4) is the limit cycle C at $r = r_0$.

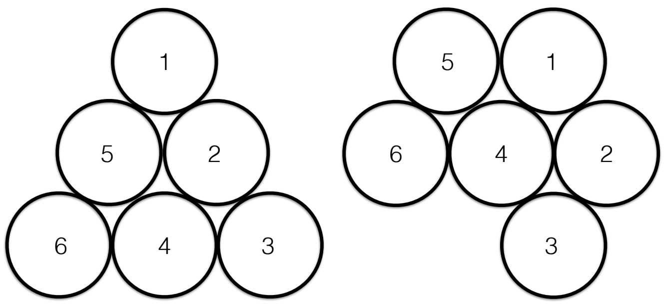
Find the quasipotential of SDE (3) with respect to C and justify your result by showing that (i) the proposed quasipotential is indeed the infimum of the Freidlin-Wentzell action and (ii) the minimizing path from C to every point (x, y) exists. *Hint: Start with expressing b_1 and b_2 via f and g, spot an orthogonal decomposition...*

Submit a single pdf file with your solution.

3. **(10 points)** Consider 6 atoms in 2D interacting according to the Lennard-Jones pair potential. The potential energy of this system is given by

$$V = 4\sum_{i=1}^{5}\sum_{j=i+1}^{6}(r_{ij}^{-12} - r_{ij}^{-6}), \quad r_{ij} = \sqrt{(x_i - x_j)^2 + (y_i - y_j)^2}.$$

(a) Use the string method to find the Minimum Energy Path connecting the following two configurations:



Plot the energy along the found Minimum Energy Path.

(b) Use the shrinking dimer method to find all of the saddle points encountered by the found Minimum Energy Path. Make your code display the found saddles and the potential energy at them and indicate the norm of the gradient of the potential at them (it should be small, less than your tolerance, but it will not be exactly zero).

Hint: The endpoints for the string method, functions for computing the gradient and the potential energy, and a function for visualizing configurations and transition paths are provided in `LJ6in2Dsetup.m`.

Submit a single .m file with your code.

4. **(10 points)** The goal of this problem is to understand the Geometric Minimum Action Method (GMAM) [1] and observe its strengths (relatively simple, applicable to high-dimensional SDEs and SPDEs) and its weaknesses (e.g., slow convergence). Use GMAM to find the Minimum Action Path connecting the two asymptotically stable equilibria of the Lorenz system at $\rho = 5$, $\sigma = 10$, $\beta = 8/3$. Your time step should be sufficiently small. For example, for 100 images along the path a good size of τ is $5.0e-3$. Mark the stable equilibria a_1 and a_2 (they are available in the Wiki's article, click on the link above) and the origin O in your 3D plot. For comparison, shoot trajectories of the Lorenz system from appropriate points of the found path located near the origin to the equilibria. The exact Minimum Action Path must coincide with the trajectory on its way from O to the stable equilibrium a_2. On the way from the stable equilibrium a_1 to O, the exact Minimum Action Path should be sort of symmetric to the trajectory. It is likely that your computed approximation to the Minimum Action Path meets these expectations only approximately (not so great but not a disaster).

   Submit a single .m file with your code.

References

[1] Heymann, M. and Vanden-Eijnden, E., Pathways of maximum likelihood for rare events in non-equilibrium systems, Application to nucleation in the presence of shear, Phys. Rev. Letters **100** 14, 140601 (2008)