It is standard to model the dynamics of physical systems by differential equations, such as $X' = f(X)$ for a finite dimensional problem where $X(t)$ is a N-by-1 vector. Practical systems, however, are usually subject to noisy perturbations from the environment, and a common stochastic model can be written non-rigorously as $X' = f(X) + \varepsilon\xi_t$, where ξ_t is called a white noise process, which can be intuitively understood as i.i.d. N-dimensional standard Gaussian random variable at each time. It is important to understand how small noise may affect the dynamics.

Let us consider an easiest situation in which $f(X) = -\nabla V(X)$, i.e. the gradient of some scalar-valued potential function. Then, in the system $X' = -\nabla V(X)$, X will always try to move to a lower potential value in the sense that $\frac{d}{dt}V(X(t)) \leq 0$. Given two local minima of V, say X_a and X_b, it is thus impossible to have a trajectory that goes from X_a to X_b (i.e., satisfying boundary conditions $X(0) = X_a$ and $X(T) = X_b$).

In the system with noise, i.e. $X' = f(X) + \varepsilon\xi_t$, however, it is possible to have rare events in which X moves from X_a to X_b with the aid of noise. These rare events are important because they correspond to chemical reactions, changes of material configurations, etc. In fact, there will be multiple trajectories satisfying those boundary conditions, corresponding to different probability densities. In the $\varepsilon \to 0$ limit, Freidlin-Wentzell large deviation theory says that the rare transition from X_a to X_b that one can most likely observe is given by the minimizer of an action functional, defined as

$$S[X] := \frac{1}{2}\int_0^T \|X'(t) - f(X(t))\|_2^2 dt$$

among all trajectories $X(t)$ that satisfy the boundary conditions.

The minimizer of the action can be shown by calculus of variation to be the solution of the ODE $X''(t) = \mathrm{Hess}V(X(t))\nabla V(X(t))$, where $\mathrm{Hess}V$ is the Hessian of V which is an N-by-N matrix, and ∇V is an N-by-1 vector. Therefore, to quantify the rare transitions which fundamentally differ from what happens in the deterministic system, one can solve the boundary value problem:

$$X''(t) = \mathrm{Hess}V(X(t))\nabla V(X(t)), \quad X(0) = X_a, X(T) = X_b.$$

If central difference is used to discretize this equation, one can obtain a system of nonlinear equations:

$$\begin{cases} (X_{i-1} - 2X_i + X_{i+1})/h^2 = \mathrm{Hess}V(X_i)\nabla V(X_i), \quad i = 1, \cdots, M-1 \\ X_0 = X_a, X_M = X_b. \end{cases}$$

where X_i is a vector for each i, and $Mh = T$.

In this project, you are asked to, in a specific setting, find the trajectory that minimizes the action and thus corresponds the most likely transition, by solving this above system using an iterative method of your choice.

Consider $N = 2$ and X expressed in coordinates as $X = [x; y]$, $V(X) = (1 - x^2)^2/4 + (y + x^2 - 1)^2/2$, and $X_a = [-1; 0]$, $X_b = [1; 0]$. Try at least $T = 5, 10, 20$ with $h = 0.1$, and plot $x(t)$ versus $y(t)$ on a background of a contour plot of $V(x, y)$. Can you make h smaller and T larger? (Hint: a sanity check is, one can actually prove that as $T \to \infty$, the transition path will intersect with the point $[0; 1]$).