Final Exam. Due May 17, 11:59 PM

You are allowed to use textbooks, course materials, and internet resources. You are not allowed to consult with anyone regarding solving the final exam problems.

Please type your solutions using any appropriate text editor.

1. **(10 points)**

   Consider a symmetric random walk over the edges of a d-dimensional unit cube: time is discrete, and at each moment of time, a particle, located at a vertex $(i_1, \ldots, i_d)$ moves to one of its neighbors with equal probability. We select vertices $A := (0, \ldots, 0)$ and $B = (1, \ldots, 1)$. For each vertex $v = (i_1, \ldots, i_d)$, find the probability that the random walk starting at it, will first reach B rather than A, i.e., the value of the committor function $q_{AB}(v)$.

   (a) Give exact numerical values for the committor function $q_{AB}(v)$ for $d = 5$.

   (b) Obtain an exact formula for the committor function $q_{AB}(v)$ for an arbitrary d.

   You can first solve (a) and then generalize your result, or you can first derive the general formula and then use it to get the answer for (a).

2. **(10 points)** Consider the following 2D model for a polymer. We represent the polymer as a sequence of points $\{(x_j, y_j)\}_{j=0}^{n}$ where neighboring points (x_j, y_j) and (x_{j+1}, y_{j+1}), $j = 0, \ldots, n-1$, are connected with edges of length 1. Assume that the direction of each edge is random, i.e., the angles which the edges form with the x-axis are independent uniformly distributed random variables on $[0, 2\pi)$. Find the square root from the expectation of the squared distance between (x_0, y_0) and (x_n, y_n). *This quantity is more amenable for calculation than the expectation for the distance between (x_0, y_0) and (x_n, y_n). at the same time, it is a reasonable approximation to it.*

3. **(10 points)** Consider the SDE describing a genetic switch model:

$$\begin{bmatrix} dx \\ dy \\ dz \end{bmatrix} = \begin{bmatrix} \frac{a_0\gamma_0 + ak_0 z}{\gamma_0 + k_0 z} - \gamma_m x \\ bx - \gamma_n y - 2k_1 y^2 + 2\gamma_1 z \\ k_1 y^2 - \gamma_1 z \end{bmatrix} dt + \sqrt{\epsilon} \begin{bmatrix} dw_1 \\ dw_2 \\ dw_3 \end{bmatrix}. \quad (1)$$

   The parameter values are:

$$k_0 = 1,\ \gamma_0 = 50,\ a0 = 0.4,\ a = 400,\ b = 40,\ \gamma_m = 10,\ \gamma_n = 1,\ k_1 = 0.0002,\ \gamma_1 = 2.$$

The corresponding system has three equilibria: active state

$$(x_a, y_a, y_a) = (29.3768600805981, 1175.07440322392, 138.079985311206),$$

inactive state

$$(x_i, y_i, z_i) = (0.0402067142317042, 1.60826856926817, 0.000258652779089588),$$

and a saddle point

$$(x_s, y_s, z_s) = (10.5829, 423.3173, 17.9198).$$

Implement the geometric minimum action method in 3D and obtain maximum likelihood transition paths from (x_a, y_a, y_a) to (x_i, y_i, z_i) and the other way around. Using these paths, calculate the quasipotential barriers from (x_a, y_a, y_a) to (x_i, y_i, z_i) and from (x_i, y_i, z_i) to (x_a, y_a, y_a) by numerical integration of the geometric action, e.g., using the composite trapezoid rule. *You might find my code* `gmam.m` *with the GMAM in 2D helpful. It is posted on ELMS.*

Submit a figure with the minimum action paths, mark which one of from (x_a, y_a, y_a) to (x_i, y_i, z_i) and which one is from (x_i, y_i, z_i) to (x_a, y_a, y_a). Indicate the found values of the quasipotential barrier, and paste a print-out of your code.