Summer 2010 NSERC USRA Report: Mean First Passage Time Simulations on Domains with Traps

Philip Mar

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This summer I worked with Dr. Ward to analyze and simulate diffusion of particles on domains with traps. Most of the summer was spent first understanding how to simulate diffusion on various domains and then implementing this on MATLAB. The important feature was being able to incorporate traps on the domain and finding the mean first passage time of many particles from one point, or, later on, many points. A trap is a region in the domain in which, when the particle reaches its boundary, does not return to the rest of the domain, it is 'trapped' in that region. This has been researched before extensively with applications to simulating diffusing proteins on the surface of a cell. The paper written by Dr. Ward and his group contained an analytic formula for the mean first passage time of particles diffuing on a sphere, with one trap at the north pole. The paper also contains formulas for traps that are well separated, so that if the traps are of radius $O(\epsilon)$ with $\epsilon \to 0$, the distance between the centres of the traps on the surface of the sphere are $O(1)$. Dr. Ward was primarily interested in the case where the traps are clustered and not well separated, and was able to get an asymptotic solution for when two traps are clustered close together. The objective of the summer project was to verify past results, and to perform simulations for trap configurations that do not have a clean analytic or asymptotic solution.

The first month of the summer was spent deriving and understanding how to obtain the differential equation of $u(x)$, the mean first passage time given the position x on the domain. The derivation involved manipulation of the probability density of the particle being at point x' at a given time t given that it began at point x at time t. The final result is that $u(x)$ follows the differential equation:

$$\begin{cases} \Delta u = -1 & \text{for } x \in S \\ u = 0 & \text{for } x \in \partial\Omega \end{cases}$$

Where S denotes the domain (taken to be a sphere in our case) and $\partial\Omega$ is the boundary of the trap Ω.

The second and third months of summer was to verify this. MATLAB was used to simulate a diffusing particle on the surface of the sphere. The diffusion was approximated by a random walk of the particle on the sphere which in turn was performed by iterating a random walk on the tangent plane (basically iteration to a random position at a random direction from the current position) of the current position of the particle and then projecting the new position (normalizing it) to obtain the new position on the surface of the sphere. To verify the formula derived in Dr. Ward's paper, I simulated the diffusion from several source points (10-20) distributed over a meridian of the sphere, each with several particles (500-1000) emanating from it, and then averaging the total time it took to get trapped. It seemed that no matter how accurate I made the time steps, the average time always seemed less than the estimated average time (given the source point). Then I tried simulating the situation where there were two traps closely clustered together, and again, the mean first passage time in the simulation was faster than the estimated mean first passage time.

Lastly (the fourth month), I tried performing the simulation on surfaces more general than the sphere; one paper outlined a method to perform a random walk on arbitrary surfaces. The latest simulation allows for any positive order and degree spherical harmonic and performs the diffusion on it. We tried to analyze the effect of having the trap or the source point at a local maximum or minimum; that is, the effect of curvature on the mean first passage time. But since the simulations take very long to run, I have not yet been able to obtain conclusive results for the relationship between trap and source point position and the curvature of the surface around the trap and source point.