18.325 Topics in Applied Mathematics, Spring 2001, Prof. Bazant.

Problem Set 2

Due at lecture on Tuesday, March 20.

1. **Inelastic Diffusion**. Consider a ball bouncing on a rough surface. Each time the ball hits the surface it is scattered in a random direction. For any real surface, the collision is *inelastic*, i.e. the ball only retains a fraction $0 < r < 1$ of its kinetic energy ($r =$ "the coefficient of restitution"). Therefore, the ball's expected height and horizontal displacement are reduced by factors of r and $\sqrt{r}$, respectively, with each successive bounce.

   A reasonable model for this situation is an "inelastic random walk", with exponentially decreasing step lengths. Let ΔX_n be iid random variables with zero mean and cumulants $c_l < \infty$ ($l \geq 2$), which represent the typical displacement after an elastic bounce. The inelastic nature of the collisions is reflected in a rescaling of this distribution with each step. Specifically, our model is the random walk

   $$X_N = \sum_{n=1}^{N} a^n \Delta X_n$$

   with non-identical steps, where $0 < a < 1$ is a constant ($a = \sqrt{r}$).

   Do the analysis below for the case of one dimension (which would model transverse diffusion on a surface with random parallel grooves), but keep in mind that your results are easily generalized to higher dimensions.

   (a) Express the PDF $P_N(x)$ of X_N as an inverse Fourier transform.

   (b) Find the cumulants $C_{N,l}$ of X_N (in terms of c_l).

   (c) Let $C_l = \lim_{N\to\infty} C_{N,l}$ and $a = 1-\epsilon$ ($\epsilon > 0$). Show that $C_{2m}/C_2^m = O(\epsilon^{m-1})$ as $\epsilon \to 0$.

   (d) Let $\phi(\zeta,\epsilon) = C_2^{1/2} P_\infty(\zeta C_2^{1/2})$, and show that "the Central Limit Theorem holds" as $a \to 1$. In other words, show that

   $$\phi(\zeta,\epsilon) \to \phi_o(\zeta) = e^{-\zeta^2/2}/\sqrt{2\pi}$$

   as $\epsilon \to 0$ with ζ fixed. This, of course, agrees with the limit of a simple random walk ($a = 1$).

   (e) Compute a few terms in the Gram-Charlier expansion $\phi(\zeta,\epsilon) = \phi_o(\zeta)(1+\epsilon^{1/2} f_{1/2}(\zeta) + \epsilon f_1(\zeta) + \ldots)$. The functions $f_l(\zeta)$ may look familiar...

   (f) Simulate this walk in one dimension (or in two dimensions, if you want to use your code from PS#1a), and compute $\phi(\zeta,\epsilon)$ for $\epsilon = 0.25, 0.1, 0.01$. Check the accuracy of the first three Gram-Charlier approximations above with a plot for each value of ϵ.

2. **Normal Diffusion with Fat-Tailed Transitions.** Consider a random flight (iid steps) with transition probability density

   $$p(x) = \frac{A}{(1+x^2)^2}$$

(A = constant to be determined), which is a "student t distribution" with a "fat" (power-law).

This kind of random flight, which has an infinite kurtosis, could have relevance for financial time series with large fluctuations (but finite volatility).

(a) Find exact expressions for the structure function $\hat{p}(k)$ and the Fourier transform of the position after n steps, $\hat{P}_n(k)$.

(b) Show that "the Central Limit Theorem holds" with the usual diffusive scaling,

$$\sigma\sqrt{n}P_n(\zeta\sigma\sqrt{n}) \sim \frac{e^{-\zeta^2/2}}{\sqrt{2\pi}}$$

as $n \to \infty$ with ζ fixed. (What is σ?)

3. **Anomalous Diffusion with Very Fat-Tailed Transitions.** Consider a random flight (iid steps) with the transition probability density

$$p(x) = \frac{A}{1+x^2}$$

(A = constant), which is a "Cauchy (or Lorenz) distribution". In this case the tail is so "fat" that the variance is infinite, so the Central Limit Theorem does not hold. Find the exact probability density function for the position of after n steps, $P_n(x)$. Show that the diffusion is "anomalous" because the width of $P_n(x)$ scales like N^α with $\alpha > 1/2$. (What is α?)

This is the simplest example of a "**Lévy flight**", exhibiting "super-diffusion". Lévy flights have been applied to financial time series, foraging ants, Drospohila flies, and albatross migrations.

4. **Non-Reversing Random Walk.** Consider a correlated random walk on the d-dimensional integer (or simple cubic) lattice ($d \geq 2$) starting from the origin where the walker's transition probability distribution is uniform over the $2d-1$ neighboring sites other than his location at the previous time step.

This kind of "persistent" random walk is a reasonable model for transport in a turbulent fluid because the non-reversal mimics the effect of short-time linear advection in the flow. (A continuum version of this model was first proposed by G. I. Taylor in 1925.)

(a) Calculate the root-mean-square distance from the origin after n steps $< |\vec{X}_n|^2 >^{1/2}$. Is the scaling diffusive, and if so what is the diffusion constant?

(b) Show that the "Central Limit Theorem holds" (Gaussian limiting distribution).

5. **Self-Trapping Walk.** Consider a correlated random walk on the d-dimensional integer (or simple cubic) lattice ($d \geq 2$) starting from the origin which does not self-intersect, i.e. the walker will not visit the same site twice. Specifically, the transition probability is uniform over all neighboring sites which have not previously been visited. The walk ends when the walker is "trapped" or surrounded by previously visited sites.

This is a reasonable model for the diffusion of a reactive object (e.g. a volatile liquid drop) in a substrate (e.g. a surface) which is altered so as to be chemically repulsive after the object passes.

Simulate the self-trapping walk in $d = 2$ dimensions, and measure the probability distribution $p(n_{trap})$ of the number of steps n_{trap} before trapping occurs. Does it appear that the mean and variance are finite? Also, compute the probability distribution $P_n(\vec{x}) = \psi_n(r = |\vec{x}|)$ for the position after n steps, including realizations where the walker is trapped before step n. [Extra credit: repeat for $d = 3, 4$ and see how the distribution changes, particularly the mean and variance of n_{trap}.]

6. **Self-Avoiding Walk.** The set of self-avoiding walks (SAW) of length n is equal to the set of non-self-intersecting random walks of length n (on a lattice, starting from the origin). Every step of a self-trapping walk (STW) *before trapping* generates a self-avoiding walk, but there is a very subtle difference in the probability measures. For the self-trapping walk, there is equal probability for each (initially) non-self-intersecting path of n steps, including those which get trapped and stay in place for steps between n_{trap} and $n > n_{trap}$. The latter paths, however, are all assigned zero probability as self-avoiding walks. In other words, the SAW position distribution $P_n^{SAW}(\vec{x})$ is the *conditional probability* that a STW reaches position $\vec{x}$ without being trapped,

$$P_n^{SAW}(\vec{x}) = \text{Prob}(X_n^{STR} = \vec{x} | X_{n-1}^{STR} \neq X_n^{STR}).$$

The self-avoiding walk is the standard model for the equilibrium structure of a polymer chain, which takes into account *excluded volume interactions* between monomers in the chain. The number C_n of self-avoiding walks of length n determines the entropy $S_n = k_b \log C_n$ and the free energy of $F = -k_B T \log C_n$ of the polymer. More realistic random-walk models for polymers could also take into account other energetic interactions between sites (e.g. short-range chemical-bonding forces due to cross linking, long-range forces electrostatic forces due to ionic charges, hydrophobic/hydrophilic interactions with a water solvent, etc.).

Simulate the self-avoiding walk in $d = 3$ and compute the distribution of the position $P_n^{SAW}(\vec{x})$. Also, determine the scaling of the root-mean-square end-to-end length

$$r_n = < |\vec{X}_n|^2 >^{1/2} \sim N^\nu = n^{1/D_f}$$

where D_f is the fractal dimension, by plotting $\log r_n$ versus $\log n$ and getting the slope of a (hopefully) straight line. How does your result compare with the Flory prediction $\nu = 3/(d+2) = 3/5$ and the recent numerical estimate 0.5877 ± 0.0006?

It is difficult to generate SAW for large n (because most end up "trapped"), so to see the scaling above, you may need to think about more sophisticated sampling algorithms.