

Practice Exam Questions: Monte Carlo Methods (Bazant)

Directions: Try to solve these problems in the spaces provided *before* looking at the answers at the end. One problem similar to these will appear on the exam, as one of roughly four problems on Particle Methods.

1. Consider simulating a random walk of N independent steps on a cubic lattice in three dimensions, hopping to nearest neighbor sites with equal probability.

(a) Show that the root-mean-square distance from the origin, \overline{R}_N , should satisfy $\overline{R}_N^2 = 3a^2N$.

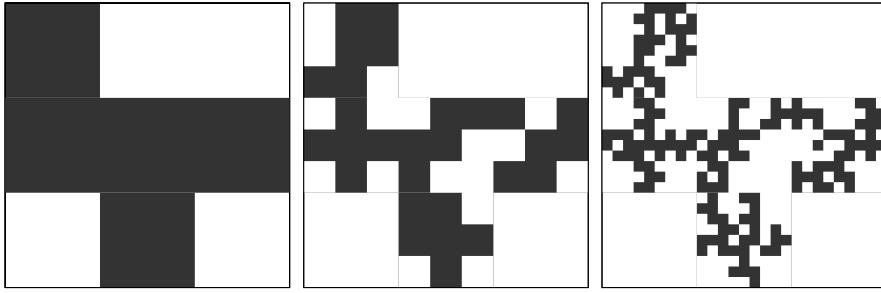
(b) From the Central Limit Theorem, we know that random walk is effectively confined to a sphere of radius $\propto \overline{R}_N$ (the “central region”). Assuming that the walk rarely returns to the same site, calculate the fractal dimension, D_f , of the trail of sites visited by the random walk.

Image removed due to copyright reasons.

2. Above is a photograph of a bacteria colony grown in petri dish with low nutrient concentration. [Reproduced from: E. Ben-Jacob et al., "Cooperative strategies in formation of complex bacterial patterns," *Fractals* 4, 849-868 (1995).]

(a) Explain (physically) why Diffusion-Limited-Aggregation might be a reasonable model for this pattern.

(b) The bacterial colony is clearly not as branched as a DLA cluster. How would you vary the rules of DLA to simulate the bacterial growth?



3. Monte Carlo simulations of critical percolation (and other models) generate random fractal clusters. A simple way to think about such objects is via recursive constructions, analogous to the (non-random) Sierpinski carpet from lecture. As shown in the sequence of images, consider dividing a square into nine smaller squares and keeping a random number n_1 of the smaller squares. For each remaining square, again remove a random number n_2 of smaller squares (out of nine), and repeat this process.

(a) Assuming $\{n_i\}$ is a set of independent, identically distributed random variables with mean \bar{n} , calculate the expected fractal dimension of the set.

(b) How does the set differ from the non-random case, where $n_i = \bar{n}$?

BRIEF ANSWERS:

1. (a) In lecture 3, we noted that the variance is *additive* for independent steps, so the variance after N steps is just N times the variance of each step, which has a contribution of a^2 from each coordinate direction. $\overline{R}_N^2 = N(a^2 + a^2 + a^2) = 3a^2N$.
(b) Neglecting returns to the same site, after N steps, the random walk has visited of order N sites, all of which are roughly confined to a sphere of radius $\overline{R}_N \propto \sqrt{N}$. Since the “mass” of the trail scales like $N \propto \overline{R}_N^2$, the fractal dimension is two. (Although this is an integer, it is smaller than the embedding dimension of three, which implies that the trail has a very complicated “stringy” fractal structure.)
2. (a) A simple model would be to assume that bacteria quickly consume nearby nutrients and slowly grow in the direction of incoming, diffusing nutrient flux (by cell division). The model is then roughly equivalent to DLA where the random walkers arriving at the cluster, and driving the growth, are the nutrient particles.
(b) One way to make the DLA cluster look less “branched” would be to allow for a some positive probability that the random walker does not stick when it meets the cluster, which would model slow eating of nutrients by the bacteria. As shown in class demos, this increases the fractal dimension and reduces branching. Another way, also discussed in class, would be to require that multiple random walkers arrive at the same site before a growth event occurs, which would make sense if each bacteria must eat lots of nutrients before dividing. This is a standard method of “noise reduction” in DLA, which reduces tip splitting and makes the branches grow in a more radial fashion.
3. (a) At each stage of recursion, we keep \overline{n} square regions of linear size l containing a typical mass m , from a larger square region of linear size $3l$ (and area $9l^2$). If we assume that $m \propto l^{D_f}$ at every scale, we have $\overline{n}m = (3l)^{D_f}$, which implies $D_f = \log_3 \overline{n} = \log \overline{n} / \log 3$.
(b) In the non-random case (e.g. the Sierpinski carpet from lecture, $\overline{n} = 8$), there are no fluctuations in the mass of the object and the connectivity is always the same. When the recursive construction is random, there are very large fluctuations in the mass of the cluster, at the same scale as the mass itself, since there is randomness in the number of “occupied” cells at the largest scale. Moreover, the random selection of cells breaks up connectivity of the cluster, as shown in the figures. These kinds of effects of clearly seen in critical percolation clusters.