SIMULATED ANNEALING

Due date: Apr 10, 2024, 9am

1. **Free-hanging necklace.** A necklace features 20 equal beads on a very light string that is suspended from both ends. Every bead can sag to any of the 20 discrete levels and thus decrease its potential energy by one unit per level. However, by doing that, it increases the spring energy to the neighboring beads that is proportional to the square of the level difference.

   a) Determine the equilibrium energy as a function of temperature.

   b) Compare your result with a theoretical shape of the hanging necklace by solving the corresponding differential equation.

   Hint: use random perturbation of a single bead level as your move.

2. **The Ising model.** ferromagnetic and antiferromagnetic materials in two dimensions in the two-state approximation are described by the following Hamiltonian:

$$\mathcal{H} = -J \sum_{\langle ij \rangle} s_i s_j - \mu \sum_i h_i s_i,$$

   where $J > 0$ for ferromagnetic materials, $J < 0$ for antiferromagnetic materials and $J = 0$ for non-interacting materials, $s_i = \pm 1$, the sum $\sum_{\langle ij \rangle}$ runs over nearest neighbors and the sum $\sum_i$ runs over all particles; μ is the magnetic moment of the particle and h_i is the external magnetic field density.

   a) In a typical configuration, are the spins split equally or is there a prevalence of one spin over the other?

   b) If a spin at position i is 1, what is the probability that the spin at position j is also 1?

   c) If there is no external field ($h_i = 0$), the temperature T_c of the phase transition solves the equation:

$$\sinh \frac{2J}{k_B T_c} = 1 \qquad \Rightarrow \qquad T_c \approx 2.269185 \frac{J}{k_B}.$$

   Does your simulation confirm this?

d) Determine the average energy $\langle E \rangle$ and the average self-magnetization $\langle S \rangle$ as a function of temperature, where $S = \sum_i s_i$. Other interesting quantities are the spin susceptibility χ and specific heat c as a function of magnetic field strength:

$$\chi = \frac{\langle S^2 \rangle - \langle S \rangle^2}{N k_B T}, \qquad c = \frac{\langle E^2 \rangle - \langle E \rangle^2}{N k_B T^2}.$$

3. **The traveling salesman problem.** As discussed in class, a salesman needs to figure out an optimal route between N cities.

a) Create an example topology (either randomly or by selecting some real data) and verify the robustness of the Metropolis algorithm by comparing its result to the actual lengths computed by brute force.

b) Randomly place M tolls at certain connections and account for that change in the cost function. How does that change the results? How would you account for the cost of gas?

c) Add other considerations, such as bridge crossings, varying speed limits, haunted forests, bad roads, alien abductions, ..., whatever you deem interesting.