Due on Wednesday after the break, on November 4th, 2020.

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1. **A non-computer example of the variational method of quantum mechanics.**

   Here is a toy variational approximation we can do by hand.

   Consider a single quantum particle subject to the confining potential $V(x) = kx^4$ (a very anharmonic oscillator). The Hamiltonian is

   $$\hat{H} = -\frac{1}{2}\partial_x^2 + kx^4$$

   where we've chosen units such that $\hbar = m = 1$. This problem cannot be solved analytically. To approximate the ground state energy and ground state eigenfunction, let's use the trial (variational) wavefunction

   $$\psi_T(\sigma, x) = \exp\left[-\frac{x^2}{2\sigma^2}\right]$$

   depending on the single parameter σ. Since it is a localized function with no nodes, it may be a reasonable approximation to the ground state of the quartic trapping potential. I've left it un-normalized; you can use a normalized version if you want.

   (a) Calculate the variational energy

   $$E_T = \frac{\langle \psi_T | \hat{H} | \psi_T \rangle}{\langle \psi_T | \psi_T \rangle}$$

   as a function of σ.

   (b) Find the value of σ which minimizes the energy; let's call this σ_0. This is our best estimate for the spatial width of the ground state wavefunction.

   (c) Explain physically the dependence of σ_0 on k.

   (d) What is the estimate for the ground state energy as a function of k? Explain physically the dependence on k.

   (e) Variational approximations generally get better when the trial wavefunction has more variable parameters. Suggest improved trial wavefunctions. (Hint: plotting or visualizing might help.)

   Of course, if the trial wavefunction is more complicated, the problem can no longer be solved by hand, and you might need a computer to help.

2. **MCMC for 1D Ising.**

Consider the one-dimensional ferromagnetic Ising model

$$H = -\sum_{i=1}^{L-1} \sigma_i \sigma_{i+1} - B \sum_{i=1}^{L} \sigma_i \, .$$

The L classical spins σ_i, arranged linearly, can each take values ± 1.

(Question: why is the upper limit in the first sum $L-1$ rather than L?)

We will use Markov chain Monte Carlo sampling, with Metropolis updates, to extract properties at thermal equilibrium, i.e., when the configurations appear with probability $\propto e^{-\beta H}$.

Given the configuration at the current timestep, the proposed new configuration is obtained by flipping one of the spins, chosen at random. This proposed move is then accepted or rejected, according to the Metropolis ratio.

(a) Write out on paper the algorithm or pseudocode for generating a Markov chain, using the Metropolis algorithm.

Do not submit your first version — this might require a couple of iterations.

Hint 1: first work out what your accept/reject criterion is. Do you need to calculate the total energies of the current state and proposed state? Or is it enough to calculate the local energies near the flipped spin? It might help to draw a configuration of a 3-spin system, and calculate the energy change due to flipping one spin.

Hint 2: You probably don't want to save every full configuration as you proceed through your Markov chain. If L is reasonably large, your computer RAM would be exhausted soon. You only keep in memory the configuration at the current Monte Carlo step. For every step, you only need to save a few properties of the system, rather than the full configuration.

(b) Write a python function that generates a Markov chain according to your plan from the previous step. At each step, calculate and save the magnetization (per site) and the energy. The magnetization is defined as

$$M = \frac{1}{L} \sum_i \sigma_i \, .$$

The energy (= Hamiltonian) is defined at the beginning of this problem.

Use this first for temperature $T = 2$ (i.e., $\beta = 1/2$) and zero field, $B = 0$. You could first use a lattice (chain) size $L = 20$. Increase this later if you can.

Create and present history plots (magnetization vs step and energy vs step).

(c) Calculate the average magnetization $\langle M \rangle$ by averaging over the last x steps. Justify your choice of x.

(d) Keeping the magnetic field B fixed at zero, vary the temperature T in steps of 0.5, from $T = 4$ down to $T = 0.5$. Plot the magnetization $\langle M \rangle$ per site as a function of T.

(Question: What's the problem with zero temperature?)

Plot this curve for at least two different sizes (values of L). Can you guess what the $M(T)$ curve will look like for $L \to \infty$?

The $L \to \infty$ limit is called the *thermodynamic limit*.

(e) Calculate the susceptibility

$$\chi = \beta\Big(\langle M^2 \rangle - \langle M \rangle^2\Big) .$$

(Background question: how does this expression follow from the physical definition $\chi = \dfrac{\partial \langle M \rangle}{\partial B}$? Please do look up.)

It appears that, to calculate the susceptibility, you need to save M^2 at every step, in addition to M. Calculate the susceptilbility as a function of T, keeping B fixed at zero.