Math 217: Topics in Applied Mathematics, Spring 2019

Course Project

Due: 2:30 pm, Thursday, June 13, 2019

Instructions

1. You need only to do one project, and you need to turn in your project report on time.
2. Your project report should include:
   (a) description of the problem;
   (b) the method you use to solve the problem;
   (c) simulation data in graphs or tables, or analytical proofs of theorems; and
   (d) brief conclusions.

   Please spell-check your report.
3. Please contact the instructor if you have any questions.

Suggested Projects

1. Monte Carlo integration, i.e., evaluate a multi-dimensional integral using Monte Carlo simulation.
   (a) Design a function $g(x)$ on $[0,1]^d$ with $d = 5$ for which you know the exact value of the integral
   $$I = \int_{[0,1]^d} g(x)\,dx.$$
   (b) Reformulate the integral as the expectation of some random variable (or the function of a randome variable) with respect to some known probability density function $f(x)$.
   (c) Generate random variables $X_1, X_2, \ldots$ and estimate the integral value.
   (d) Plot the sample mean $\overline{X}_N = (1/N)\sum_{k=1}^{N} X_k$ vs. N, together with the value I. Plot the variance of $\overline{X}_N$ vs. N.
   (e) Discuss the convergence and accuracy.
2. Monte Carlo optimization with the simulated annealing. You can study the knapsack problem with a relatively small system, say, $m = 100$.
   (a) Design your own vectors $\vec{v}$ and $\vec{w}$, pick some $b > 0$, and define your set S of feasible solutions.
   (b) Generate the Markov chain (which has time-dependent transition probabilities) using the simulated annealing algorithm with $\beta(t) = \ln(t+1)$.
   (c) Determine approximately the size of the set $S_{\max}$.
   (d) Estimate the maximal value of $\vec{v} \cdot \vec{z}$ for $\vec{z} \in S$.

   You can also design a different cost function and find its global minimum value.
3. Use the Metroplis–Hastings Monte Carlo algorithm to simulate an ionic system to study the ionic size effect.
   (a) Set up the system by defining a simulation box $[-L, L]^3$, fixing a large ball in the center with -10-charge at the center of the ball, fixing the number of mobile $+1$-charge ions of the same radius 3, and fixing the number of mobile -1-charged ions of the same radius

    3. Make sure your have the total charge value 0. You can add ions with +2 charges, with different sizes, but you may want to make the system simple.
   (b) Define the interaction potential. Once two balls touch, the energy is ∞. Otherwise, use the Coulomb energy and pairwise interaction.
   (c) Do Monte Carlo simulations in two stages: equilibration and statistical analysis.
   (d) Calculate the density of ions around the sphere. Use histograms to plot the densities.
   (e) Analyze the convergence.

4. Molecular dynamics simulations with GROMACS of the solvation of a spherical non-charged molecule in water.
   (a) Compute the solvation free energy.
   (b) Compute the water density profile.
   (c) Define using different methods the radius of the spherical molecule using your simulation data.
5. Monte Carlo simulations of the binding of two molecules treated as rigid bodies.
   (a) Design the system, and in particular, the interaction potential. Only the solute-solute interaction energy should be enough.
   (b) Implement the Metropolis–Hastings algorithm to simulate the system.
   (c) Show the binding process (a short movie) if you can.
   (d) Discuss briefly the result.
6. Prove the continuum electrostatic energy is the limit of a sequence of discrete electrostatic energies.
   (a) Let $\Omega = (0,1)^3$. Given a continuous function on $\overline{\Omega}$ and and discretize Ω uniformly to define a sequence of point charges (at the centers of uniform grid cells) and the corresponding discrete Coulomb energies.
   (b) Define the continuum energy using Poisson's equation.
   (c) Prove that the discrete energies converge to the continuum one.