Numerical methods II: syllabus for the first part

February 14, 2022

This part of the course will be made up by 2 topics: introduction to Monte Carlo methods (first 4 lectures) and advanced Monte Carlo methods (last 2 lectures).

Monte Carlo methods - Lect 1-6

- brief review of Monte Carlo integration, and a few python examples;
- ergodicity, global balance, and detailed balance conditions in Markov chains;
- Metropolis algorithm;
- Metropolis algorithm for the classical Ising model;
- autocorrelation functions and critical slowing down;
- cluster updates and Wolff algorithm;
- advanced data analysis: the Jacknife method;
- machine learning meets (simple) Monte Carlo: k-means applied to partition functions, and eventually principal component analysis.

Breakdown of the lectures:

1. Lecture 1: introduction to Monte Carlo (MC) integration.
   - a simple example: evaluate the area of a sphere
   - probability function, sampling function
   - direct sampling
   - First MC code: evaluation of π via hit or miss; play a bit and
     a) change the number of points. what does happen?
     b) run the code several times: is the error constant?
   - Brief python reminder: plotting with matplotlib;
   - First exercise : evaluate the volume of a 3D and 10D sphere;
   - comparison with Riemann integration;
2. Lecture 2: variance estimation and importance sampling
   - error scaling: variance of an estimator;

- Second MC code: MC error scaling in the evaluation of π via hit or miss.
- Second exercise : evaluate the volume of a 3D and the corresponding error; show that the latter scales with $O(1/\sqrt{N})$;
- importance sampling: general notion, example with a 1D integral;

3. Lecture 3: Markov Chain Monte Carlo and Metropolis algorithm

   - Exercise review : review of evaluation of 3D and 10D Spheres.
   - Markov chain: definition and connection to the notion of independent sampling;
   - Detailed balance condition;
   - Metropolis algorithm;

4. Lecture 4: Markov Chain Monte Carlo simulations of the Ising model on the square lattice

   - recap of Metropolis;
   - Third MC code: evaluation of π via importance sampling (an overkill!).
   - Fourth MC code: evaluation of multi-dimensional integrals with Metropolis algorithm, error scaling.
   - Third exercise : integrals with Metropolis.
   - Further reading: Monte Carlo algorithms with only global balance.
   - Ising model: review of its basic properties within mean field theory and high-temperature expansions;
   - Why are simulations important? motivation
   - Metropolis algorithm for the Ising model: single spin updates;
   - Fifth MC code: Ising model with single spin updates.
   - a funky way to detect magnetism: clustering of correlations and k-means [if time allows].

5. Lecture 5: critical slowing down

   - correlations in MC data sets: why are they taking place? what are their consequences?
   - autocorrelation functions and critical slowing down in the Ising model: the dynamical critical exponent;
   - Sixth MC code: autocorrelation functions in the Ising model;
   - Jacknife analysis: another method to detect autocorrelations [if time allows].

6. Lecture 6: Cluster algorithms

   - how to fight critical slowing down: detect relevant degrees of freedom;
   - cluster algorithms: Swedsen-Wang [if time allows];
   - cluster algorithm: Wolff's algorithm and cluster updates.