Project on Machine Learning

Data Analysis and Machine Learning FYS-MAT3155/FYS4155

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Using results from Monte Carlo models for machine learning

Introduction. The aim of this project is to use an already developed Monte Carlo program (either the ising Model or a variational Monte Carlo code) to produce, in case of the Ising model, the energy as function of temperature. For the variational Monte carlo calculation of interacting electrons in an oscilaltor trap, the data are represented by the ground state energies as functions of the variational parameters.

In its simplest form the energy of the Ising model is expressed as, without an externally applied magnetic field,

$$E = -J \sum_{<kl>}^{N} s_k s_l$$

with $s_k = \pm 1$. The quantity N represents the total number of spins and J is a coupling constant expressing the strength of the interaction between neighboring spins. The symbol $< kl >$ indicates that we sum over nearest neighbors only. We will assume that we have a ferromagnetic ordering, viz $J > 0$. We will use periodic boundary conditions and the Metropolis algorithm only. Alternatively we can use the supplied variational Monte Carlo program which solves Schroedinger's equation for two interacting electrons in a harmonic oscillator trap. Both codes can be found at the webpage of the course under programs.

Part a): Producing the data. $\langle E \rangle$ and $\langle |M| \rangle$, the specific heat C_V and the susceptibility χ as functions of T for $L = 40$, $L = 60$, $L = 100$ and $L = 140$ for $T \in [2.0, 2.3]$ with a step in temperature $\Delta T = 0.05$ or smaller. You may find it convenient narrow the domain for T.

Plot $\langle E \rangle$, $\langle |M| \rangle$, C_V and χ as functions of T.

Part b): Fitting the data using regression analysis and other methods. More text to come

Part c): Introducing Bayesian statistics. More text to come

Part d): Studying the Ising model or the VMC results with Neural networks. More text to come

Background literature

If you wish to read more about the Ising model and statistical physics here are three suggestions.

- M. Plischke and B. Bergersen, *Equilibrium Statistical Physics*, World Scientific, see chapters 5 and 6.
- D. P. Landau and K. Binder, *A Guide to Monte Carlo Simulations in Statistical Physics*, Cambridge, see chapters 2,3 and 4.
- M. E. J. Newman and T. Barkema, *Monte Carlo Methods in Statistical Physics*, Oxford, see chapters 3 and 4.

Introduction to numerical projects

Here follows a brief recipe and recommendation on how to write a report for each project.

- Give a short description of the nature of the problem and the eventual numerical methods you have used.
- Describe the algorithm you have used and/or developed. Here you may find it convenient to use pseudocoding. In many cases you can describe the algorithm in the program itself.
- Include the source code of your program. Comment your program properly.
- If possible, try to find analytic solutions, or known limits in order to test your program when developing the code.
- Include your results either in figure form or in a table. Remember to label your results. All tables and figures should have relevant captions and labels on the axes.
- Try to evaluate the reliabilty and numerical stability/precision of your results. If possible, include a qualitative and/or quantitative discussion of the numerical stability, eventual loss of precision etc.
- Try to give an interpretation of you results in your answers to the problems.

- Critique: if possible include your comments and reflections about the exercise, whether you felt you learnt something, ideas for improvements and other thoughts you've made when solving the exercise. We wish to keep this course at the interactive level and your comments can help us improve it.
- Try to establish a practice where you log your work at the computerlab. You may find such a logbook very handy at later stages in your work, especially when you don't properly remember what a previous test version of your program did. Here you could also record the time spent on solving the exercise, various algorithms you may have tested or other topics which you feel worthy of mentioning.