Numerical methods in stochastic modeling and simulations:

Miniproject 2

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In this miniproject you will implement the fundamental Ising model and investigate its behavior with respect to properties of interest. The idea is to also give a feeling for *how to actually investigate* these kinds of models. As a minimum you are to submit the (draft) report on the mandatory part before the next seminar.

If you wish to also take the extended part you are to present your results towards the end of the course (but feel invited to actively help me schedule this presentation on a suitable occasion where the material still feels fresh!).

Note: to pass the course you need to take *one* extended part from one of the three miniprojects during the course.

Mandatory part

Reading For this project I suggest to read and implement at the same time. Refine your understanding and formulations when preparing the written report.

- I have based the present project mainly on Newman and Barkema [1999], in particular, see §1–3[1].
- There are some additional and openly available texts linked from the course web-page.

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[1] The formulation was also inspired by a similar laboration in the SeSE-course *"Stochastic Methods in Computational Sciences"* from 2013.

- Finally, most technical terms (I try to use *emphasized* text for those below) can be found on Wikipedia and there are also several starting implementations available on the web. *It is ok to be inspired and adapt, but bluntly stealing and/or making a poor job in citing other's efforts is either cheating (unacceptable) or a sign of poor habits (also unacceptable).*

The Ising model We will consider the classical Ising model on a 2D square lattice of size 100×100 under periodic boundary conditions. The state (or *spin*) in each lattice consists of the two values ± 1 only and the Hamiltonian is given by

$$H(s) = -J \sum_{\langle i,j \rangle} s_i s_j,$$

where the sum runs over neighboring sites only.

The equilibrium distribution is then just the Boltzmann distribution $P(s) \propto \exp(-\beta H(s))$ with $\beta = 1/(k_B T)$. The *order parameter* for this system is the (absolute) magnetization,

$$M = \left| N^{-1} \sum_i s_i \right|,$$

and switches in a *phase transition* from ordered (1) to unordered (0) when the temperature T increases above a certain critical value. This value is known analytically for the Ising model,

$$T_c = \frac{2J}{k_B \log(1 + \sqrt{2})} \approx 2.27J.$$

Implementation and usage Following the pieces of advice in [Newman and Barkema, 1999, §3.1–3.4, §3.7] very closely,

- Start at either $T = 0$ or ∞. In the first case, all $s_i = 1$ (or -1), and the Ising model is in its *ground state*. In the other case you can select s_i randomly such that all spins are uncorrelated. If you are performing a sweep of simulations over different temperatures, selecting the end-state of the previous run is natural.

- Run the Metropolis algorithm at your temperature of interest and monitor its convergence to steady-state with respect to, for example, the order parameter. Reasonably, try with a different stream of random numbers and check that you get comparable results. Measure also the *auto-correlation* time to ensure that you get a meaningful ergodic average in the end.

- Finally, estimate the magnetization by an ergodic (time series) average and the error in this estimate by $\pm 2\sigma/\sqrt{N}$ (say), with σ the sample standard deviation.

Task 1: critical temperature Implement the Metropolis algorithm for the Ising model and investigate M as a function of T around the critical temperature. When reporting back on this, make an effort into convincing the reader that your computations are reasonably accurate (compare above).

Task 2: the 5-state Potts model Modify your code to *the 5-state Potts model*, where the spins take the 5 values $\{\pm 1, \pm 1/2, 0\}$ instead. Determine the critical temperature and the phase transition behavior anew.

Extra task, competition! Make a GIF-movie (or similar format) of the phase-transition process in one of the cases above, suitable to eg. a web-page. Who makes the best animation?

Extended part

For the extended part, perform and report on *at least one* of the tasks below (there is only one task described here!).

The task is very openly described and the intent here is that you undertake a bit of research and take the role of a critical reviewer. *Take your job seriously!*

Task 3: the cellular Potts model Implement the *cellular Potts model* Graner and Glazier [1992] for simulating a few human cells on a lattice. First implement the Hamiltonian terms corresponding to volume- and boundary targets. Other terms of interest: adhesion/repulsion between cells, cellular migration in the direction of an on-lattice gradient, cells that grow and divide...

References

F. Graner and J. A. Glazier. Simulation of biological cell sorting using a two-dimensional extended potts model. *Phys. Rev. Lett.*, 69:2013–2016, 1992. doi:10.1103/PhysRevLett.69.2013.

M. E. J. Newman and G. T. Barkema. *Monte Carlos Methods in Statistical Physics*. Clarendon Press, Oxford, 1999.