TITLE: Machine learning for accelerating Monte Carlo simulations

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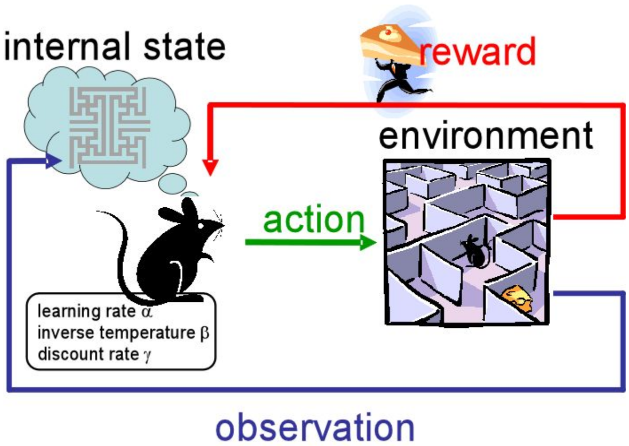
General Context

A common problem in simulating spin systems is the high degree of correlation between samples in a Markov Chain. For some models, specific update algorithms which reduce the correlation time are well known. Yet, finding such an update algorithm is often highly model-dependent and not easily transferable. Several machine learning algorithms are well suited for the purpose of speeding up simulations.

Research goals of the MSc thesis



In particular, reinforcement learning -- where an agent is rewarded or punished for the actions it performs in its environment -- has been shown to be well suited for automatically proposing new Monte Carlo update moves (https://arxiv.org/abs/1808.09095). This is in stark contrast with human-defined Markov Chain Monte Carlo (MCMC) algorithms, which typically take steps according to a physically motivated but fixed scheme.

Alternatively, we can train a model to extract the features that define system configurations and uses these to directly generate new configurations. This comes down to learning a joint probability distribution. Learning such a distribution is typically much more complex than discriminative machine learning, but allows for incredibly efficient sampling of new configurations. Generative adversarial networks (GANs) tackle this problem by having two networks contest with each other, a generator and discriminator. The generator creates fake configurations, which are compared to real ones by the discriminator. A GAN can be trained on simple spin configurations sampled with Monte Carlo (e.g., on the Ising model https://arxiv.org/abs/1710.04987). Understanding which features of a physical data set a GAN captures is a possible thesis subject (e.g. with

InfoGAN https://arxiv.org/abs/1606.03657), as well as applying it to more complex physical models.

We are seeking a student with an outspoken interest in Computational Physics and Statistical Physics and intend to apply the newly developed simulation technique to some challenging problems in physics.

Mobility options for the MSc thesis

Options are for example: research stays in other groups and attending Summer Schools on topics related to simulations, complexity science, sampling techniques, … .