

1 Results & discussion

In the following section, all results are produced with the following parameters for the RBM and the Hamiltonian:

$$N_{\text{visible}} = 12, \quad N_{\text{hidden}} = 12, \quad J = 1.0, \quad \mu = 1.0, \quad \text{learning rate} = 0.1, \quad \text{number of epochs} = 25$$

1.1 Ising model

As we know from the analytical solution of the 1D Ising model, the ground state is the configuration with all spins aligned in the same direction. This is the state with the lowest energy, and we can use this as a benchmark for our RBM implementation.

1.1.1 Importance of enough samples

The Monte-Carlo sampling is the bread and butter of our implementation, and the number of samples we use is crucial for the accuracy of our results. To illustrate the necessity of a large "enough" sample size, we have plotted the energy of the Ising model as a function of the number of samples in figure(??). In figure(??), we see that the energy of the Ising model converges to the analytical value *only* for the

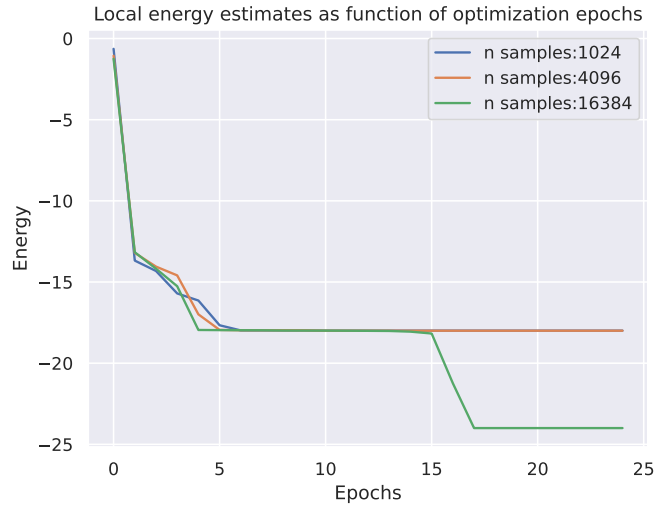


Figure 1: Energy of the Ising model as a function of the number of samples.

largest samplesize, $n = 2^{14}$, whereas it is stuck in a local minima for the smaller samplesizes. With too few samples, the Monte-Carlo sampler will not propely traverse the spin-configuration landscape well enough to properly identify the ground state, and subsequently it will yield the wrong results.

We can also do a statistical analysis of this problem, showcasing the variance and standard error, in the following plot From these two error plots, figure (??) and figure (??), we can see where the higher sample size "breaks out" of the local minima, there is a bump in the statistical errors - and this is where the model leaves the local minima, and progresses onwards to the true minima - the ground state of the 12 spin system with a ground state energy of -24 (with $J = 1.0, \mu = 1.0$).

There is also a clear link between the number of samples and the number of visible units (spins) in our system. With too many spins, and not enough samples - we get the wrong results shown in figure(??) for $n = 2^{10}, 2^{12}$.

For illustrative purposes, we can show the convergence of the system with a larger spin-chain of 20 spins, with the same parameters as before, using 2^{14} samples. The results are shown in figure (??).

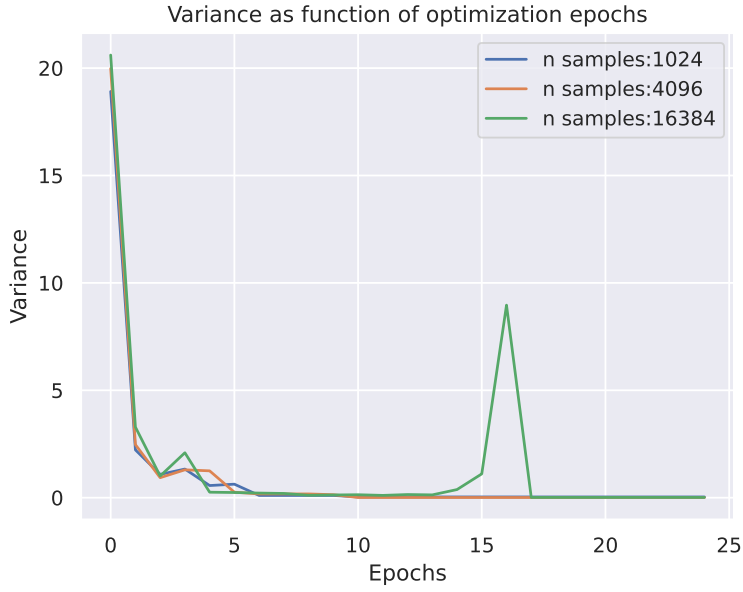


Figure 2: Variance of the Ising model as a function of the number of samples.

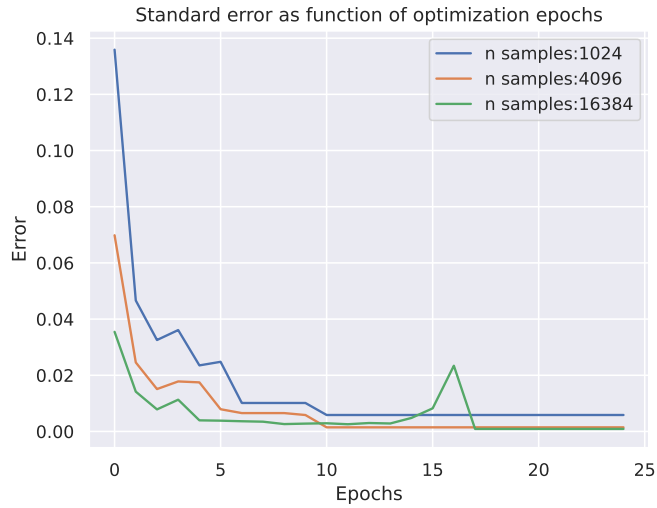


Figure 3: Standard error of the Ising model as a function of the number of samples.

1.1.2 RBM complexity

The complexity of the RBM is also a crucial parameter to consider, even if the hidden layers are not directly visible in the probability distributions, due to use tracing them out - but they are still important for the learning process. More hidden units will introduce more parameters to optimize, and the learning process will be more complex. In figure(??), we see the energy of the Ising model as a function of the number of hidden units in the RBM. Here we see an interesting result. The RBM performs much better for a simpler model, with fewer hidden units. This is likely due to the fact that the model is too complex, and the problem itself is quite simple - and the model is trying to overfit the data. We see that both 4 and 12 hidden units converge to the ground state energy, but with 12 hidden units the convergence is much quicker. This seems to hit the "sweet spot" for model complexity - but this is a tradeoff - as the model complexity increases, the learning becomes more computationally demanding.

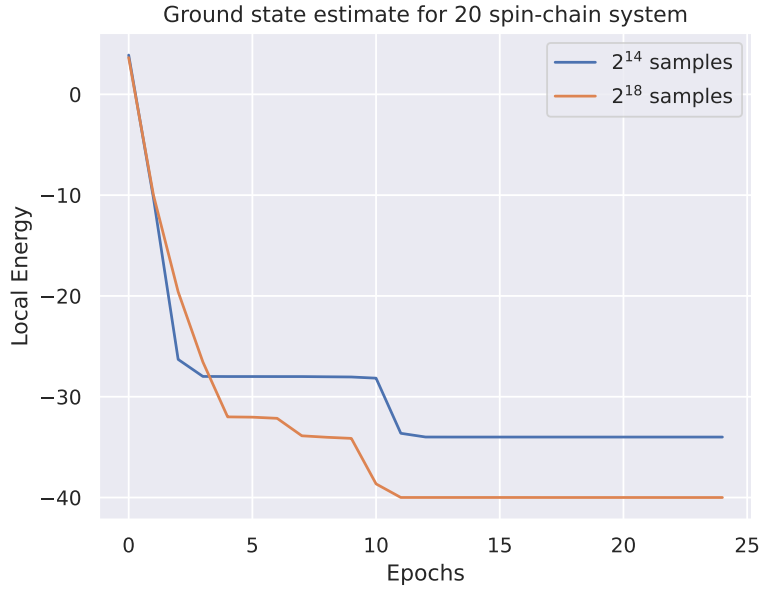


Figure 4: Energy of the Ising model as a function of the number of samples for a larger spin-chain.

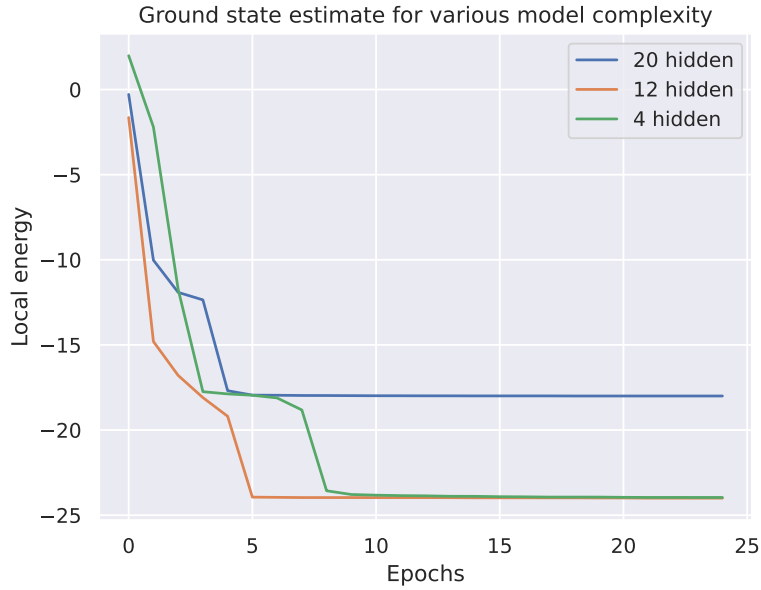


Figure 5: Energy of the Ising model as a function of the number of hidden units in the RBM.

1.1.3 Varying the temperature

The temperature of the system is also an important parameter to consider. We stated that we usually ignore this (see (??)), but it is still interesting to see how the RBM performs for different temperatures. In figure (??), we see the energy-convergence of the Ising model as a function of the temperature, for 50 epochs. Here we see that the RBM performs well for lower temperatures, but that the convergence *rate* is affected more and more as the temperature rises. At $T = 10.0K$, the model does not converge to the ground state within the 50 epochs, but it does not seem that it is stuck in a local minima, rather, it seems that the rate of convergence is too slow. This is likely due to the fact that the system is too "hot" to properly converge to the ground state, and needs more time to properly "find" the ground state.

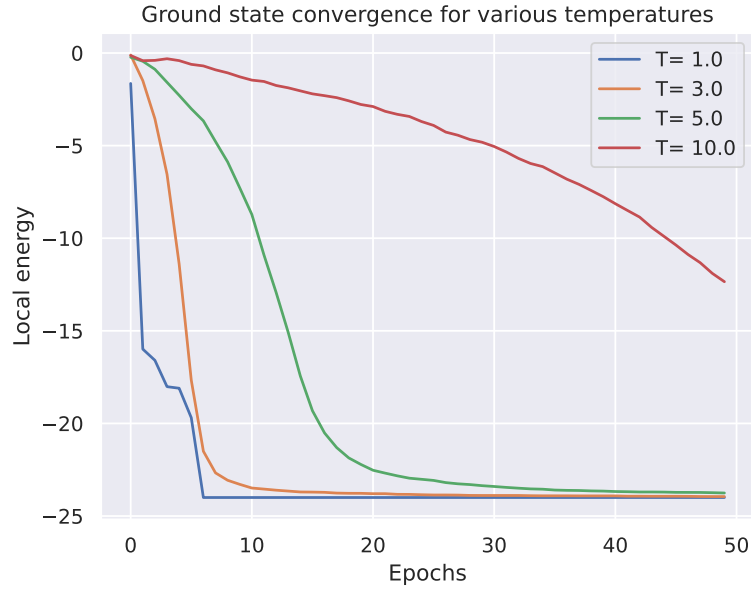


Figure 6: Energy of the Ising model as a function of the temperature.

1.2 Long-range interactions

Adding long-range interactions, it is interesting to see how this affect the ground state of the system. Following the implementations in section (??), we can see how the energy of the system changes as a function of the range of the interaction, n_v , for a constant $\alpha = 1.0$. The result of adding more complex interactions are presented in figure (??).

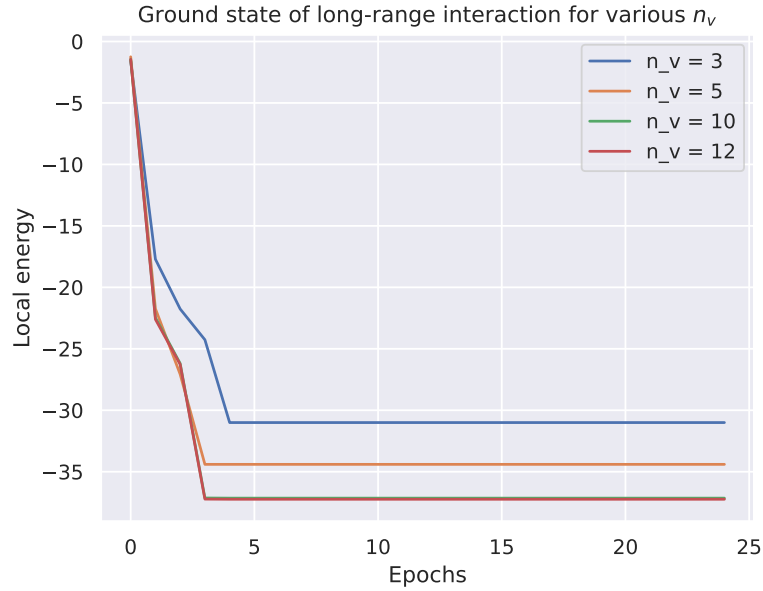


Figure 7: Energy of the Ising model as a function of the range of interaction.