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Variational autoencoder analysis of phase transitions

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An important part of quantum condensed matter physics deals with the calculation of phase diagrams of interacting many-body systems. A novel approach for studying these systems is to utilize representation learning. This technique enables the study of quantum states in a human independent manner, as the representation of quantum phenomena is decided on by the AI. Therefore, this approach promises a new perspective into the study of phase diagrams and new insight into the description of quantum states.

In general, representation learning is a technique that allows a system to automatically discover the representations needed to perform a task from data. This is achieved by compressing the input into a smaller set of latent variables. In my thesis, variational autoencoders (VAEs) are used. An autoencoder is a type of neural network that learns an efficient encoding of data through refinement by attempting to regenerate the input from the encoding. The compression is achieved by passing the input through the latent space of smaller dimension.

The variational autoencoder adds the idea of constraining the latent variables to be normally distributed. This allows new output to be generated by sampling. Other types of constraints can also be applied to the latent space, all with the goal of "disentangling" the latent variables and encouraging them to be independent and learn unique features of the input. This disentanglement of latent variables is a key feature of representation learning.

One of the research goals in this thesis is the targeted representation learning of entangled states. In this problem, a dataset of groundstates of a spin-1 Hamiltonian with various degrees of entanglement entropy is used. By training a VAE on this dataset and disentangling its latent space, it is investigated how the entanglement entropy is meaningfully represented by the latent variables.

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