MagmaDNN: Application in Materials Science

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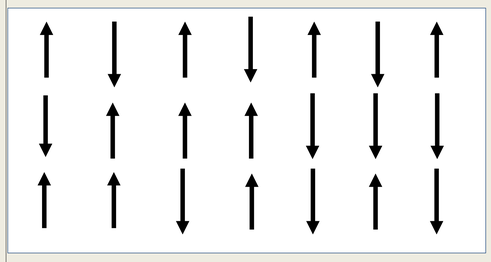
Background

Ising model, for being one of the most basic model in material science for its ability to give estimation on certain physical properties, including the specific heat capacity and the magnetic susceptibility, of a piece of material. .

Example of Ising model on 2D plane
Each arrow represents a spin at direction:
upward: +1
downward: -1



The energy of an Ising configuration, an important quantity for the estimations, can be expressed in terms of the interaction strength of each particle and its neighbour. Without external magnetic field, the energy of an Ising configuration is as following:

$$H = -\sum_{(i,j)} J_{ij} s_i s_j$$

where (i, j) denotes a pair of neighbouring spins, J_{ij} is the interaction strength between different locations and s_i is the spin at location i.

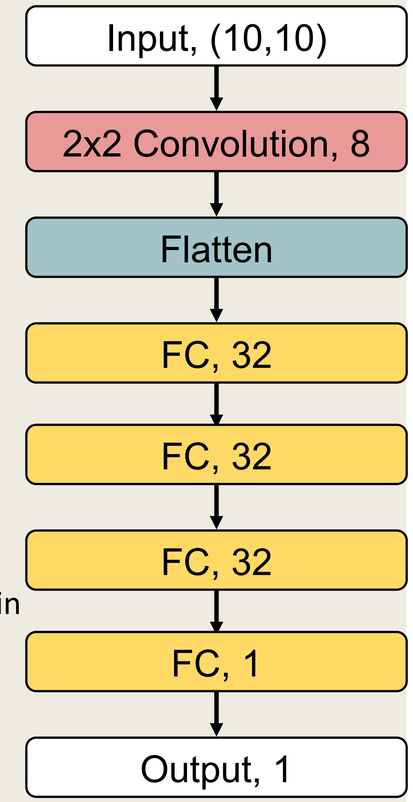
Methodology

With the advance development in high-speed computation in linear algebra, methods of machine learning have presented their power in predicting quantities in batch. Hence we utilize these technologies to predict the energy of Ising configurations.

In our simulations, we focus on a 8x8 square 2D plane with periodic boundary condition and uniform interaction strength.

Since configurations for certain energy levels are scarce in amount, techniques in data argumentation are applied. Period padding is also added to the data.

We have proposed a regression model to predict the energy and is prototyped in Keras. The structure is shown in the graph:



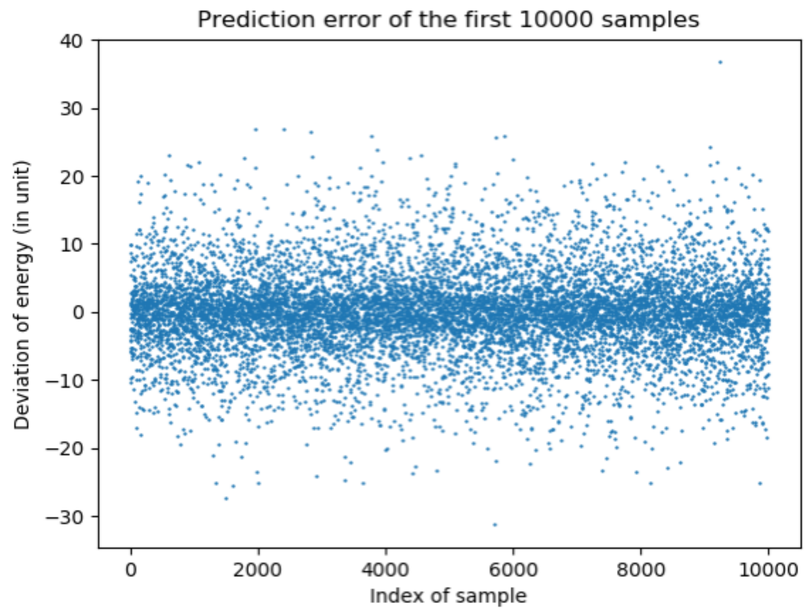
The prediction outcome has mean error -0.012 units, mean absolute deviation 4.46 units, and standard deviation 6.19 units.

As each energy level is 4 units, we consider the model accurate and is a proof of our idea of using machine learning in topics related to materials science.

Analysis

Despite the high accuracy, the model is specialized in one particular setting with no generalisability.he model is specialized in one particular setting with no generalisability.

Also, with the nature of the convolution layer used, the model is confined to plane Ising model but not general crystallographic structure.



Future Work

We are currently searching for a method to generalize the model to different settings.

On the subject of irregular lattice shape, we believe the use of Graph Convolutional Network (GCN) may solve the problem.Graph Convolutional Network is a special type of convolution network that allows doing convolution on non-Euclidean structure. The graph convolution layer are supposed to grant flexibility on how the convolution filter is defined, hence able to capture all 230 crystallography structures. We are implementing such network in MagmaDNN.

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