Machine Learning for Material Property Simulations

The exercise problem

The aim of this exercise to generate a neural network that classifies LEED-images according to the 2D-Bravais-lattice of the corresponding crystal surface. The exercise consists of three different tasks:

1a) **Discuss** how a neural network could be **designed** that can fulfill the task. How would the necessary input look like? What would the output be? Which kind of (hyper)parameters do you have to choose? For which can you make informed choices, for which would you have to find optimal values via trial and error.

1b) **Produce a simple code** (preferably in python) for such a neural network. It should be geared towards speed (run on your local computer), rather than towards optimal accuracy.

2a) **Discuss** how you would **obtain the training data** for the neural network. Do you have to use first principles methods? If yes, which (first principles) methods would you employ? Discuss which physical effects are incorporated in the simulation and which are neglected. Justify your choices.

2b) **Produce a simple code** that generates LEED-images for different 2D-Bravais lattices.

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3) Train the neural network on your training data and use a test set to determine how well it performs. The network will (very likely) not achieve a 100% accuracy on the test set. Analyze which systems fail often and discuss possible reasons why the network has problems to classify them correctly.

Educational target

The main educational target of the lecture this lecture is to

- get experience in coding and applying machine learning programs and
- independently acquire information required to fulfill a material properties simulation task. This included second-guessing information obtained from sources with questionable reliability.

A secondary (non-mandatory) target is to explore the usage of ChatGPT in teaching. This is currently a relevant topic for the Ethics Commission of the TU Graz, and student experiences are highly welcome. Filling out the lecture evaluation form and reporting your experiences would be highly appreciated.

Execution

To design the network and the general workflow, the use of ChatGPT is encouraged. However, the relevant information can alternatively also be obtained by any other means, e.g. from lecture notes, text books, scientific literature or via the internet. Exercises can be completed in groups of 2-3 people, but the discussion will be in person with each person separately. For the discussion, please make sure to cite the used software and sources. If ChatGPT is used, please also provide the conversation protocol.

Before using ChatGPT (or any other online resources), please inform yourself of the terms and conditions.