Opponent's review of the diploma thesis

Name and surname of the review author: doc. RNDr. Iveta Mrázová, CSc.

Name and surname of the thesis author: Elguja Archemashvili

The title of the thesis: Construction of phase diagrams of spin models using unsupervised machine learning

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The text of the review:

Elguja Archemashvili's diploma thesis studies the applicability of contemporary machine learning means to constructing phase diagrams, a concept central to understanding how materials behave under varying conditions like temperature, pressure, and composition. Phase diagrams are indispensable for synthesizing and developing new materials like alloys, polymers, and composites with desired properties. Phase diagrams indicate conditions under which different material phases are stable and pinpoint circumstances leading to phase transitions. Thus, they can be used to control production processes involving phase changes in various fields, ranging from materials science through chemistry and metallurgy to geology.

For the above reasons, the submitted thesis aimed to explore the viability of machine learning-based approaches to construct phase diagrams of spin models using simulated data. According to the assignment, the objective of the thesis was to analyze the configurations obtained through numerical simulations of the Falicov-Kimball model through simple machine learning methods. Further, the student was expected to implement the neural network models designed for an automatic classification of spin configurations. Finally, the trained models had to be applied to classify the data from numerical simulations and analyze the performance behavior of the respective models.

I see the main contribution of the thesis in reviewing, analyzing, and applying adequate unsupervised machine learning methods to study phase transitions in the Falicov-Kimball model. In addition to surveying the selected data analysis mechanisms, the text also debates machine learning approaches used to detect phase transitions in previous studies – DBSCAN, convolutional, and RBM networks. Integrating dimensionality reduction techniques, clustering, and energy-based learning of modern Hopfield networks clearly has the potential to yield promising results advancing the area. The solutions' performance was experimentally evaluated using synthetic data modeling real-world processes and was interpreted from the point of view of phase transition physics.

The thesis is written in English, accompanied by many supporting figures, and is well-organized. Unfortunately, it contains quite a few grammatical, typographical, and spelling errors. For instance, see the third line of the paragraph 'f Electrons' on p. 11, the incorrect citation (Noguer I Alonso, 2024) on p. 30, the last line of the second paragraph on p. 50, the last sentence of the first paragraph and missing ')' in Formula 6.1 on p. 53, the last paragraph on p. 64, the first paragraph on p. 69 the third line on p. 75. Conclusions are not included in the Contents (p. 5-6). The abbreviation FG is not explained in Figure 2.1. Typographical errors include line 4 on p. 18, line 4 of Section 5.1.1 on p. 40, text in Step 3 on p. 41, the first line on p. 56 and 58, resp. The algorithm DBSCAN discussed on p. 37 is not referenced in the thesis.

The work also suffers from several factual inconsistencies. Often, the data processing steps taken are not sufficiently explained, the experiment settings used are missing (e.g., t-SNE in Section 6.2, or autoencoders and their CNN-based version in Section 6.3), and their results are discussed vaguely only (lacking the information, e.g., on the involved time and memory costs, confidence intervals obtained for the loss function values, etc.), and some decisions are questionable right away, see below:

- In the dimensionality reduction experiments involving t-SNE (basically a non-linear dimensionality reduction technique), it is unclear why the PCA preprocessed data was used and not the original one. PCA is, namely, a linear transformation (unlike mentioned in the second paragraph of p. 61) using in the underlying experiments only the first 10, resp. 50 components.
- On p. 71, the author claims that 'All Hopfield experiments were implemented in PyTorch 2.15.' Unfortunately, I have not found any reference to the location of the data or implementation used. Similarly, concerning the introductory paragraphs of Section 5, it is unclear whether the development of the Monte Carlo simulator should also have been a part of the thesis.
- In Section 5.2.1, the author states that the dataset is comprised of results from 19 independent simulation runs denoted as versions. Anyway, from the description below, it is not clear what the actual division of the data was into the training, testing, and validation sets. The following paragraph namely considers only 10 versions in total. Also, the last paragraph of the section is quite confusing (the size of the training set mentioned for the majority of experiments states 1000000 examples, while the following sentence considers, in general, the initial number of 10000 training samples).
- On p. 39, the author states: 'Based on the advantages of ML, it will be possible to continue to uncover exotic phases and refine phase diagrams, especially for models such as the Falicov-Kimball system, which is the main focus of this thesis.' However, the text does not mention any examples of such exotic phases.
- On p. 44, it is unclear why 12x12 arrays have been chosen to represent the electron configurations considered. For Figures 5.1-5.12, it should be clearly stated, which illustrate the ordered states, and which are the disordered states. These claims seem to be done based on a visual assessment but do not offer any hint for a formal evaluation.
- Further on p. 60, the text mentions that there are few notable differences when compared to Experiment 1 but does not list them. On p. 68, it is not clearly distinguished what values were considered high and what intermediate.

Despite the above comments, the submitted thesis fulfills its original objective. The student was able to apprehend relevant concepts from the machine learning and data analysis disciplines, and he demonstrated the capacity to solve innovatively a relatively demanding task from an interdisciplinary area. A discussion of related issues concerning the explanation of the involved data representations, the analysis of the underlying energy landscapes, and phase boundary identification using loss heatmaps signify the author's good orientation within the field. He proved his competence in scrutinizing the gained experience and results objectively. For the discussion, I have the following questions to consider:

1) Author's contribution to the presented approach:
   What was the author's own contribution to collecting the data used for phase diagrams and its preprocessing? Can the author at least briefly demonstrate the overall functionality of the software he implemented and utilized in the experiments?

2) Evaluation and reproducibility of the experiments:
   Explain, e.g., how the experiment involving the modern Hopfield network was run and evaluated (training and validation set size, the used network architecture, confidence intervals, time costs, …). How well does the constructed phase diagram correspond to the real one? Would including available real data be possible, and would it improve the final phase diagram?

3) Scalability of the discussed approach:
   The experiments documented in the thesis (see, e.g., Figure 6.1) seem to have considered just a single material type (yet it is not clear for what material) and a 2-dimensional phase diagram. How well is the discussed technique applicable to constructing other, possibly even 3-dimensional materials' phase diagrams?

Recommendation for the defense:

Based on the above reasons, **I recommend admitting this diploma thesis for the defense, and I agree to award Elguja Archemashvili the Master's degree after a successful defense**.

I suggest not considering the thesis for the annual award.

In Prague, 2. 6. 2025

doc. RNDr. Iveta Mrázová, CSc.