Posudek diplomové práce

Matematicko-fyzikální fakulta Univerzity Karlovy

Autor práce	Elguja Archemashvili		
Název práce	Construction of phase diagrams of spin models using unsupervised machine learning		
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Studijní program	Informatika	**Studijní obor**	Umělá inteligence

Autor posudku	RNDr. dr Pavel Baláž	**Role**	Vedoucí
Pracoviště	Katedra fyziky kondenzovaných látek		

Text posudku:

The master's thesis by Elguja Archemashvili investigates the application of unsupervised machine learning (ML) techniques for constructing phase diagrams of the Falicov-Kimball model, a prominent system in condensed matter physics. The research aims to bridge theoretical physics and data-driven methods, exploring both the capabilities and limitations of ML approaches in the study of phase transitions between disordered and ordered states in solid materials.

The thesis is clearly structured. It begins with a concise introduction to the Falicov-Kimball model and its phase diagram. Section 3 describes the machine learning methods employed in the study, namely principal component analysis (PCA), t-distributed stochastic neighbor embedding (t-SNE), and artificial neural networks. Among neural network approaches, the student focuses on autoencoders and Hopfield networks. Clustering algorithms and their use for phase detection are also briefly mentioned. Section 4 reviews previous studies where unsupervised ML techniques have been applied to physical models. Section 5 presents the dataset used in the thesis in considerable detail. The original research conducted by the student is described in Section 6, followed by the concluding section.

The aims and methodology are clearly presented in the introduction. The ML techniques are described with sufficient detail in Section 3. However, the dataset description in Section 5 contains some unnecessary information, such as the names of specific files, which is not relevant at this point in the thesis. On the other hand, the section provides a valuable account of parameter grids and data preprocessing steps, which facilitates reproducibility. A notable shortcoming is the lack of a proper citation for the dataset, which has already been published online [1].

In Section 6, Elguja consistently analyzes the performance of each ML method in identifying the phase structure of the Falicov-Kimball model, with particular attention to their limitations. While a wide range of methods is employed, the interpretation of their results is somewhat superficial. The thesis does not examine how the outcomes vary with dataset size or model hyperparameters. In many cases, essential details such as the perplexity value for t-SNE or the activation functions and regularization techniques for neural networks are omitted. This omission compromises the reproducibility of the results and prevents a rigorous assessment of their reliability.

A major strength of the thesis lies in the large number of the explored methods and in the emphasis on their respective limitations. The results show that PCA and t-SNE can successfully distinguish between ordered and disordered phases, while more advanced neural network models can detect transitions between weakly localized and Anderson insulating phases.

One of the original contributions of the student is the proposal to use modern Hopfield networks for phase diagram reconstruction. Although this approach yields phase boundaries that are close to the expected ones, the lack of essential details precludes a firm evaluation of the results' validity.

Nevertheless, the thesis provides meaningful insights into the use of unsupervised machine learning models for the analysis of the Falicov-Kimball model. Some of the results are part of a recently published research article [2]. Therefore, I recommend the thesis for defense.

Minor remark

- The student uses the term “experiment” when referring to the application of ML methods. This could be confusing, especially, in the context of physics.
- In Section 6.3, PCA is incorrectly referred to as a nonlinear dimensionality reduction method.
- The thesis contains numerous grammatical errors, typos, and inconsistencies in style.

Questions

- Which dataset (d or f electrons) was used to train the Hopfield network?
- Can the capacity of the Hopfield network used in the study be estimated?
- Is the dataset size appropriate for the Hopfield network used?

References

[1] M. Žonda, P. Baláž, L. Frk, E. Archemashvili, Phases in the 2-Dimensional Falicov-Kimball Model [Data set]. Zenodo (2024). https://doi.org/10.5281/zenodo.14029088
[2] L. Frk, P. Baláž, E. Archemashvili, M. Žonda, Phys. Rev. B **111**, 205116 (2025).

Práci doporučuji k obhajobě.

Práci nenavrhuji na zvláštní ocenění.

Pokud práci navrhujete na zvláštní ocenění (cena děkana apod.), prosím uveďte zde stručné zdůvodnění (vzniklé publikace, významnost tématu, inovativnost práce apod.).

Datum 23. 05. 2025 **Podpis**