Posudek práce

předložené na Matematicko-fyzikální fakultě
Univerzity Karlovy

❑ posudek vedoucího ☒ posudek oponenta
☒ bakalářské práce ❑ diplomové práce

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Název práce:	Reconstruction of magnetic configurations using machine learning approaches
Studijní program a obor:	Fyzika / Fyzika
Rok odevzdání:	2022

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Odborná úroveň práce:
❑ vynikající ☒ velmi dobrá ❑ průměrná ❑ podprůměrná ❑ nevyhovující

Věcné chyby:
❑ téměř žádné ☒ vzhledem k rozsahu přiměřený počet ❑ méně podstatné četné ❑ závažné

Výsledky:
☒ originální ❑ původní i převzaté ❑ netriviální kompilace ❑ citované z literatury ❑ opsané

Rozsah práce:
❑ veliký ☒ standardní ❑ dostatečný ❑ nedostatečný

Grafická, jazyková a formální úroveň:
❑ vynikající ☒ velmi dobrá ❑ průměrná ❑ podprůměrná ❑ nevyhovující

Tiskové chyby:
❑ téměř žádné ☒ vzhledem k rozsahu a tématu přiměřený počet ❑ četné

Celková úroveň práce:
❑ vynikající ☒ velmi dobrá ❑ průměrná ❑ podprůměrná ❑ nevyhovující

Slovní vyjádření, komentáře a připomínky oponenta:

Tatiana Vargincová analyzes in her bachelor thesis the usage of various autoencoders for reconstructing complex magnetic orderings. Autoencoders are a type of artificial neural network that is trained to reconstruct the input data on its output. In principle it consists of two parts. The first one encodes, i.e., compresses the complex structure to a layer which has much less degrees of freedom than the original data. The second part of the autoencoder then decompresses this layer. The aim is to train a network where the input and the output are as close to each other as possible. In physics, this has many potential applications. For example, if the autoencoder is trained for some typical ordering, it can detect an outlier in the data simply by failing to reproduce it. Analogous strategy can be used for unsupervised phase classification and automatic construction of order parameters of complex phases. However, as discussed and illustrated in the thesis there is a fundamental problem. When the input is a physical state, for example a configuration of classical Heisenberg spins on a lattice, the reconstructed state might be close geometrically yet still extremely far physically. Meaning, that it can contain excitations that would never be realized physically because the final state would have a very high energy. The thesis analyzes a potential remedy for this problem. Namely, an extended loss function. Besides a measure of the geometric difference between the states it also considers the energy of the state via the Hamiltonian of the system. Several versions of such loss functions were carefully studied, including function which relies on the absolute value of the output-state energy, function that uses the difference between input and output energy and finally one that relies on local energy differences. According to the thesis, the last one proved to be the best.

The work is clearly motivated, presents a very thorough analysis of the problem, and gives some clear conclusions. I would especially like to highlight the graphics. The work contains the most beautiful figures and illustrations I have ever seen in a thesis.

Unfortunately, there are also problems.

The work would have benefited from careful proofreading. There are some "autocorrect" types of mistakes like "From the expression (6) we see KNOW, that to …", or "we can derive a PHONOLOGICAL explanation". Less amusing are the inconsistencies in referencing formulas and figures. For example, in the first chapter the figures are labeled as 1.1, 1.2 etcetera but referred to in the text first by (1), (2) later by the whole form 1.2. There are two formulas labeled as (1.1). The first one is on page 5, the second on page 13. Similar inconsistencies are in referencing the figures. On page 37 the text points the reader to figures (42) and (43) where they should have been (4.21) and (4.22) I suppose. Caption of figure 4.8 discusses five columns, but there are only four columns plotted there. Figure 2.1 is a beautiful illustration of filters; however, I have checked the highlighted values in matrix E and two of them are wrong. References to older work also show some problems. For example, the journals from APS do not have the last letter (e.g., there is several times Phys. Rev. instead of Phys. Rev. B) and I have noticed a misspelled name namely Iakolev instead of Iakovlev.

More serious is the problem with the formulas. Not a single sum has the subscript that would give an information through which indices we should sum it. That this is a real problem can be illustrated by the formula (1.2). The formula after the sum should refer to the surface of a specific spherical triangle with vertices determined by three-unit spin vectors S_i, S_j and S_k. Therefore, the sum should run over these triangles. This cannot be deduced from the formula stated in the thesis or from the accompanied text.

Considering science, I have several questions.

1. The phase diagram in Fig. 3.3 is divided into 11 phases, which are then also used in the analysis of the autoencoder results. I am a bit confused by the number and the character of the phases or, better to say, distinct regions. For example, why is it necessary to distinguish skyrmions with few bimerons, some bimerons and many bimerons? What is the quantitative criterion used to draw the boundaries between these regions? It seems to me that this is a bit counterproductive, as it lowers the number of samples in each phase.

2. How was the formula (3.1) derived? When should it work? Naively, if I assume just 4 skyrmions I would expect dc to be approximately 100, but according to the formula it is around 400.

3. The section Minimal Energy was very confusing to me. Could the author explain what was meant by this statement: “Nevertheless, the minimum energy state might not necessarily represent the thermodynamically most favored state, not even if one approaches absolute zero temperature.”

4. I was wondering about the loss function (4.4), here besides the standard difference between the spin configurations also the difference in their energies is considered. I understand that both parts are unitless, however, are they of the same order?

5. What would happen if you suppressed the MSE-spin and fed the network with random configurations? Would the MSE-H be enough for the network to find some approximation of the ground-state?

6. Figures 4.19,21,22 contain these nice cookies, but I do not understand how the contribution of distinct phases to the MSE is calculated. Is this adjusted to the fact that distinct phases are represented by different numbers of samples? Could you explain in detail what is meant by this and what are the implications for some applications? E.g., phase classification, or detection of an outlier configuration.

7. Finally, at figures 4.24 and 4.25 the MSE of spirals is significantly smaller than the similar spirals with merons. Why is that the case?

To sum it up. The bachelor thesis shows some formal problems, sometimes it feels a bit drowned in unnecessary details and several points should be clarified during the defense. However, it also presents a very thorough analysis of the stated problem. The investigated refinements for the autoencoder are physically motivated and can lead to a physically more meaningful reconstruction of complex magnetic configurations. As such the work is motivated by very recent progress in the field and the obtained results are potentially useful for setting future architectures suitable for analysis of magnetic structures. Or at least it can be used as a good starting point. Therefore, and despite all the mentioned problems, I am grading the thesis by mark “výborně”.

Práci
☒ doporučuji
☐ nedoporučuji
uznat jako ~~diplomovou~~/bakalářskou.

Navrhuji hodnocení stupněm:
☒ výborně ☐ velmi dobře ☐ dobře ☐ neprospěl/a

Místo, datum a podpis vedoucího/oponenta:

V Praze,
2. 09. 2022
RNDr. Martin Žonda, Ph.D.