Unsupervised clustering of magnetisation vector fields

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Magnetic materials at the nanoscale are important for science and technology. A key aspect for their research and advancement is the understanding of the emerging magnetization vector field configurations within samples and devices. A systematic parameter space exploration—varying for example material parameters, temperature, or sample geometry—leads to the creation of many thousands of field configurations [1, 2] that need to be sighted and classified. This task is usually carried out manually, for example by looking at a visual representation of the field configurations. We find that it is possible to automate this process, using unsupervised machine learning (ML) algorithms [3]. In this study, we use a combination of convolutional auto-encoder [4] and density-based spatial clustering of applications with noise (DBSCAN) [5] algorithm for magnetic phase diagram discovery of an FeGe disc using micromagnetic simulations. Keeping the geometry of the disc constant, we obtain the equilibrium magnetisation configurations by changing the externally applied magnetic field values. Subsequently, we obtain a latent space of reduced dimensionality with the help of the convolutional auto-encoder (Fig. 1). Finally, we perform the DBSCAN clustering on the latent space to sort the configurations in different classes (Fig. 2). We find that the classification algorithm is accurate, fast, requires little human intervention, and compares well against the published results in the literature [1] on the same material geometry and range of external fields. Moreover, we were able to identify additional equilibrium magnetisation states compared to the published study owing to the difference in the initial configurations for the simulations. Our study shows that machine learning can be a powerful tool in the research of magnetic materials by automating the classification of magnetization field configurations. This work was financially supported by the EPSRC UK Skyrmion Project Grant EP/N032128/1 and the MaMMoS project (Nr. 101135546) funded by the European Union. We are grateful for useful discussions with Andreas Marek and team members from the Max Planck Compute and Data Facility.

References

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Figures

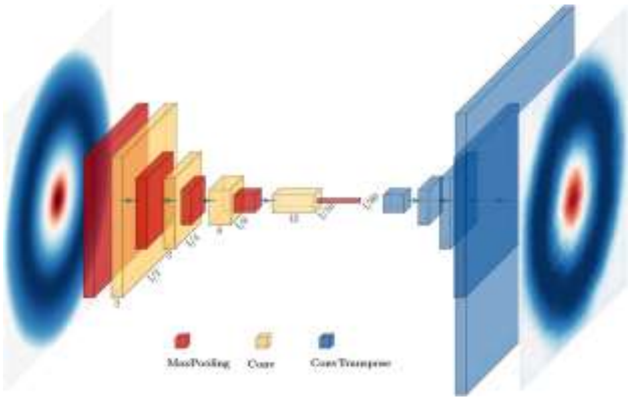

Figure 1. Convolutional auto-encoder architecture used to reduce the dimensionality of the simulation magnetization array from 19200 (80 × 80 × 3) to 12 (12 × 1).

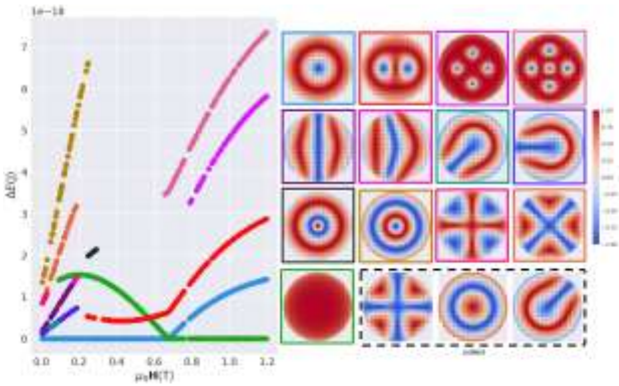

Figure 2. Magnetisation configurations of 13 different clustered classes and their distribution as a function of changing externally applied magnetic field ($\mu_0\mathbf{H}$) as obtained by the clustering algorithm. The *y* axis shows the energy difference of a given configuration with respect to the ground state at that external field. Additionally, to the clustered classes, we obtain outlier configurations, which are not part of any class. We find the results to be in a good agreement with the Fig. 3b of Ref. 1 of the published study on the same material geometry and range of external fields.