Generative deep neural networks for topological defects and their microstructure reconstruction in two-dimensional spin systems

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Topological defects and their interactions are highly relevant for many physics fields, especially in spin physics. While being a stable local perturbation of an underlying field, on larger length scales topological defects can be described as point-like particles characterised by their winding number. The range of the associated deformation field around each of their core is very large. One consequence of this is, e.g., the existence of a phase transition induced by topological defects, the so called Berezinskii-Kosterlitz-Thouless phase transition [1]. Due to the multiscale character of topological defect structures and their long range correlation, numerically simulating a large number of them in full microscopic detail is computationally extremely demanding. As a possible solution for this problem, we propose to use generative neural networks to bridge between the macroscopic description of a model with topological defects and its underlying microscopic field. With data from a spin dynamic simulated microscopic model, we train our physics induced conditional generative adversarial network system [2] with a loss-function based on the Wasserstein-metric [3,4] (WGAN) to generate realistic spin configurations from given defect configuration inputs. The training process of the WGAN is split into two steps. An initial pretraining process and a global training with customisable physical constraints as additional input, such that the trained WGAN can generate full physically realistic spin fields from given defect position configurations. The resulting neural network backmapping tool provides the opportunity to construct representative sets of microscopic spin configurations of magnetic materials from topological defect distributions and other input parameters, such as temperature and magnetisation. Possible applications include the enhancement of large and complex simulations as well as the more in-depth analysis of experimental data.

References

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