Machine learning puts a new spin on spin models

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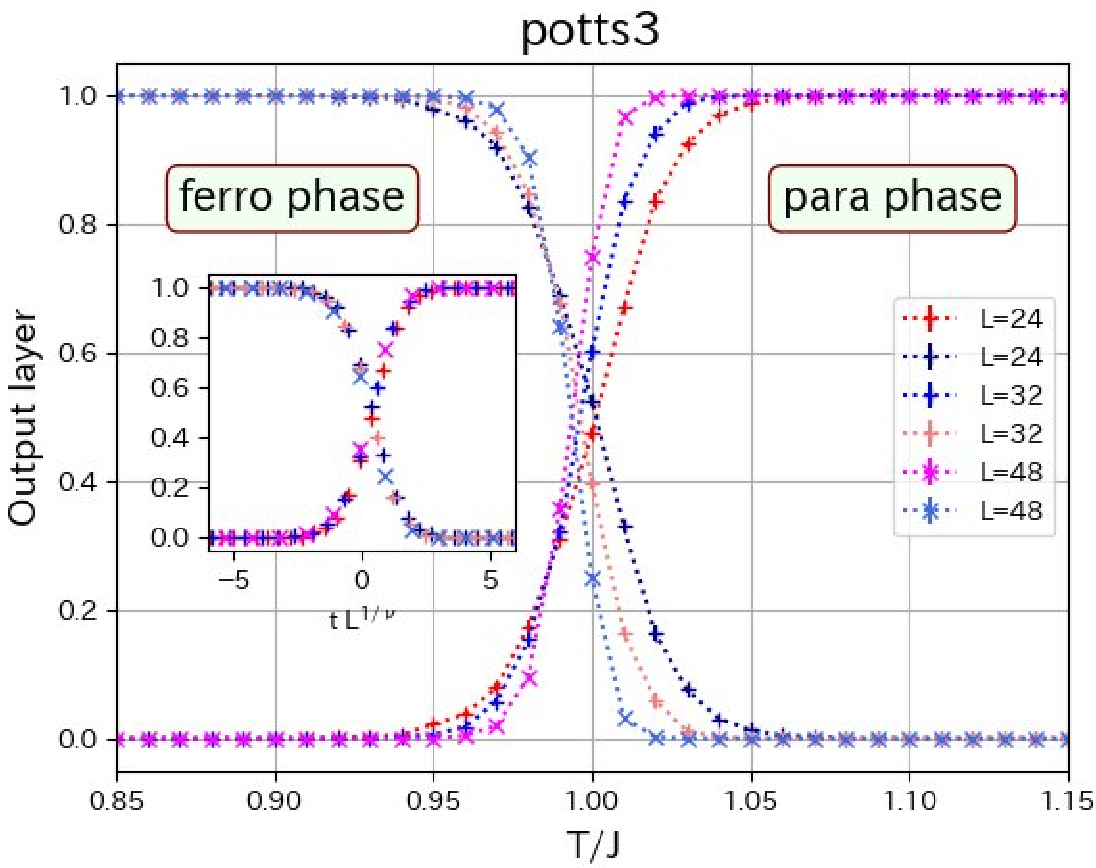
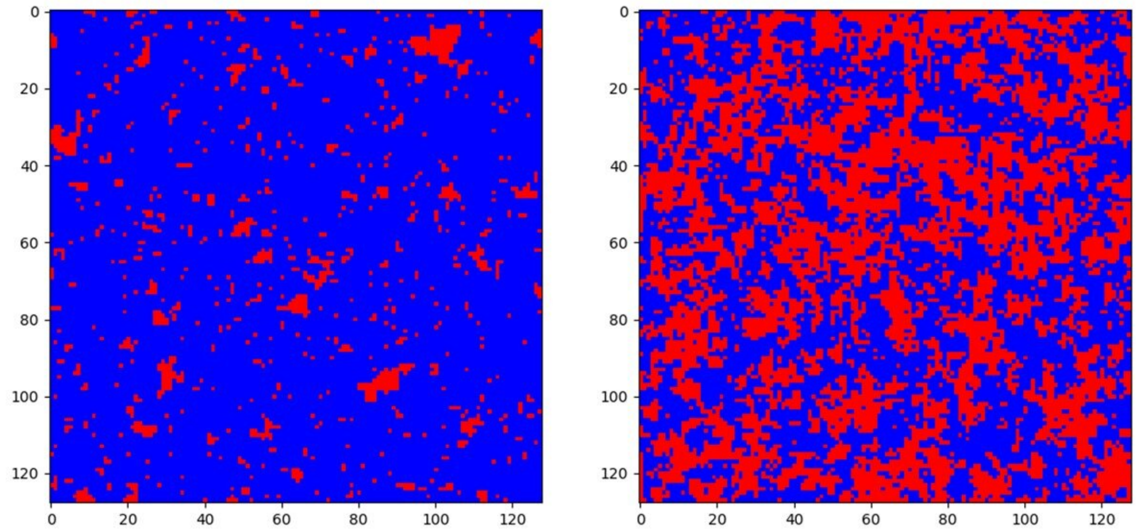


The low and high temperature phases are found in the right proportions at different temperatures relative to the transition point for different sizes of lattice. (inset) The size of the lattice may be accounted for to give a single master curve. Credit: Tokyo Metropolitan University

Researchers from Tokyo Metropolitan University have used machine learning to analyze spin models, which are used in physics to study phase transitions. Previous work showed that an image/handwriting classification model could be applied to distinguish states in the simplest models. The team showed the approach is applicable to more complex models and found that an AI trained on one model and applied to another could reveal key similarities between distinct phases in different systems.

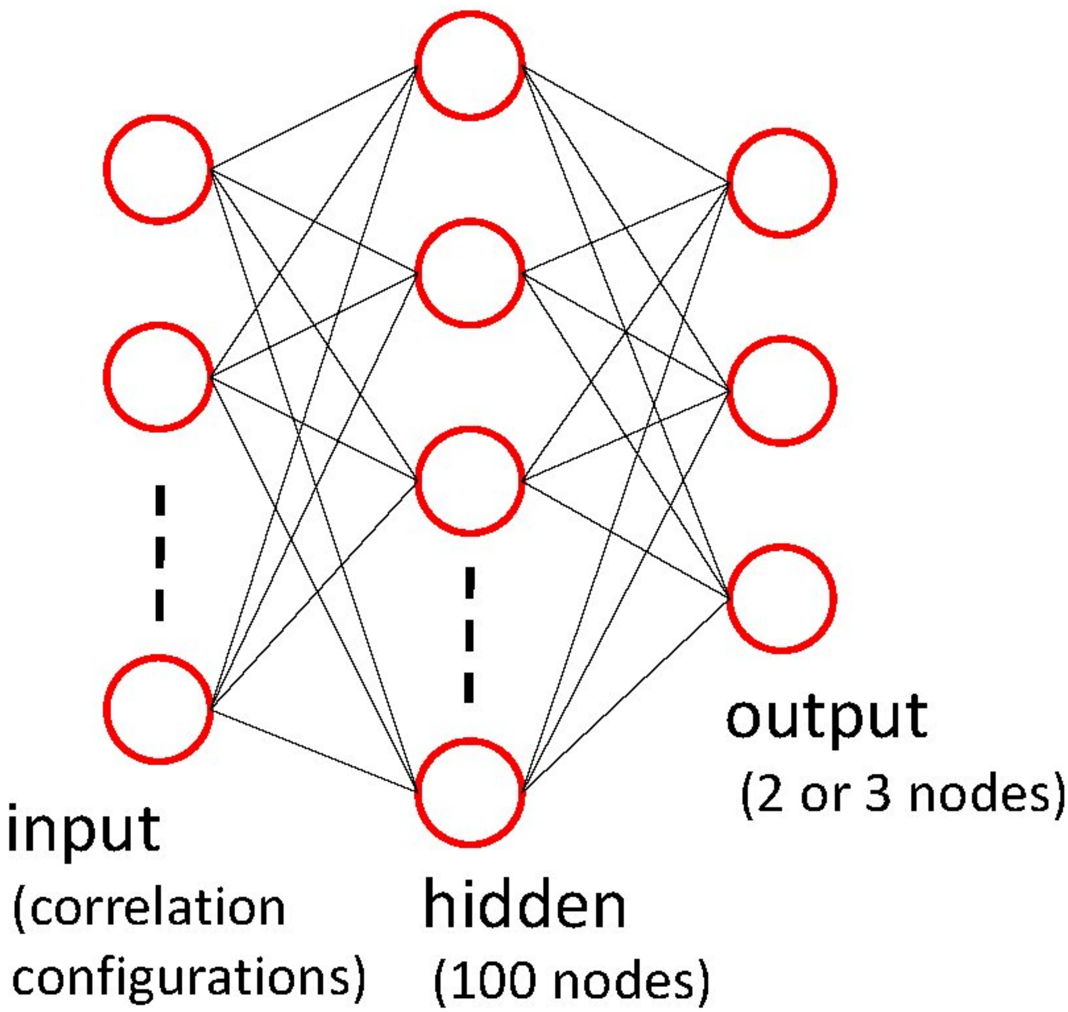
Machine learning and artificial intelligence (AI) are revolutionizing how we live, work, play, and drive. Self-driving cars, the algorithm that beat a Go grandmaster and advances in finance are just the tip of the iceberg of a wide range of applications now having a significant impact on society. AI is also making waves in scientific research. A key attraction of these algorithms is that they can be trained with pre-classified data (e.g., images of handwritten letters) and be applied to classify a much wider range of data.

In the field of condensed matter physics, recent work by Carrasquilla and Melko (*Nature Physics* (2017) 13, 431-434) has shown that neural networks, the same kind of AI used to interpret handwriting, could be used to distinguish different phases of matter (e.g., gas, liquid and solids) in simple physical models. They studied the Ising model, the simplest model for the emergence of magnetism in materials. A lattice of atoms with a spin (up or down) has an energy that depends on the relative alignment of adjacent spins. Depending on the conditions, these spins can line up into a ferromagnetic phase (like iron) or assume random directions in a paramagnetic phase. Usually, studies of this kind of system involve analyzing some averaged quantity (e.g., the sum of all the spins). The fact that an entire microscopic configuration can be used to classify a phase presented a genuine paradigm shift.



Simulated low temperature (left) and high temperature (right) phase of a 2D Ising model, where blue points are spins pointing up, and the red points are spins pointing down. Notice that the spins in the low temperature phase are mostly in the same direction. This is called a ferromagnetic phase. On the other hand, at high temperature, the ratio of up to down spins is closer to 50:50. This is called a paramagnetic phase. Credit: Tokyo Metropolitan University

Now, a team led by Professors Hiroyuki Mori and Yutaka Okabe of Tokyo Metropolitan University are collaborating with the Bioinformatics Institute in Singapore to take this approach to the next level. In its existing form, the method of Carrasquilla and Melko cannot be applied to more complex models than the Ising model. For instance, take the q-state Potts model, where atoms can take one of q states instead of just "up" or "down." Though it also has a phase transition, telling the phases apart is not trivial. In fact, in the case of a five-state model, there are 120 states that are physically equivalent. To help an AI tell the phases apart, the team gave it more microscopic information, specifically, how the state of a particular atom relates to the state of another atom some distance away, or how the spins correlate over separation. Having trained the AI with many of these correlation configurations for three- and five-state Potts models, they found that it could correctly classify phases and identify the temperature where the transition took place. The researchers could also correctly account for the number of points in their lattice, the finite-size effect.



The input (correlation configurations) is fed into a system of interconnected nodes known as a *neural network*, giving a series of outputs telling us which phase the configuration belongs to. During training, the algorithm is told whether the outputs are right or wrong, and the network is adjusted over and over again to get better agreement i.e. it *learns*. Credit: Tokyo Meropolitan University

Having demonstrated that their method works, they tried the same approach on a q-state clock model, where spins adopt one of q orientations on a circle. When q is greater than or equal to five, there are three phases that the system can take: an ordered low-temperature phase, a high-temperature phase, and a phase in between known as the Berezinskii-Kosterlitz-Thouless (BKT) phase, the investigation of which won John M. Kosterlitz, David J. Thouless and Duncan Haldane the 2016 Nobel Prize for Physics. They successfully trained an AI to tell the three phases apart with a six-state clock model. When they applied it to configurations from a four-state clock model, in which only two phases are expected, they discovered that the algorithm could classify the system as being in a BKT phase near the phase transition. This demonstrates that there is a deep connection between the BKT phase and the critical phase arising at the smooth 'second-order' phase transition point in the four-state system.

The method presented by the team is generally applicable to a wide range of scientific problems. A key part of physics is universality, identifying traits in seemingly unrelated systems or phenomena that give rise to unified behavior. Machine learning is uniquely suited to tease these features out of the most complex models and systems, letting scientists take a peek at the deep connections that govern nature and our universe.

More information: Kenta Shiina et al, Machine-Learning Studies on Spin Models, *Scientific Reports* (2020). DOI:

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