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A machine-learning algorithm that can infer the direction of the thermodynamic arrow of time

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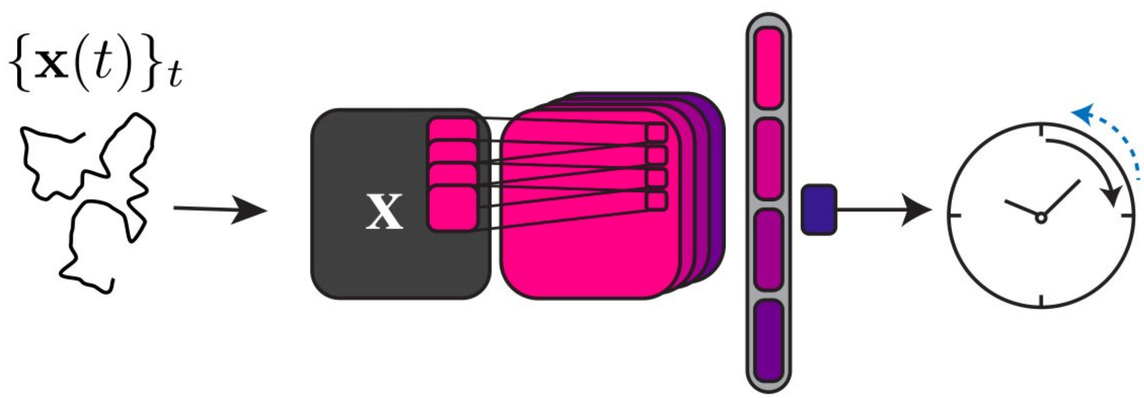

A trajectory (movie) is represented by a matrix X. This matrix is the input to a neural network, which detects the direction of time's arrow. Credit: Seif, Hafezi & Jarzynski.

The second law of thermodynamics delineates an asymmetry in how physical systems evolve over time, known as the arrow of time. In macroscopic systems, this asymmetry has a clear direction (e.g., one can easily notice if a video showing a system's evolution over time is being played normally or backward).

In the microscopic world, however, this direction is not always apparent. In fact, fluctuations in microscopic systems can lead to clear violations of the second law of thermodynamics, causing the arrow of time to become blurry and less defined. As a result, when watching a video of a microscopic process, it can be difficult, if not impossible, to determine whether it is being played normally or backwards.

Researchers at University of Maryland developed a machine learning algorithm that can infer the direction of the thermodynamic arrow of time in both macroscopic and microscopic processes. This algorithm, presented in a paper published in *Nature Physics*, could ultimately help to uncover new physical principles related to thermodynamics.

"I learned about thermodynamics at small scales when I took a course on non-equilibrium statistical mechanics taught by Prof. Jarzysnki," Alireza Seif, one of the researchers who carried out the study, told Phys.org. "At the same time, I was exploring applications of machine learning in physics, which have attracted a lot of interest in recent years. One example of machine learning applications is classifying images and the same tools have been used to classify phases of matter in physics."

As he was pursuing his studies, Seif realized that the quest of trying to determine the direction of the arrow of time could also be framed as a classification problem. He thus started exploring the possibility of developing a machine learning algorithm that can determine this direction and discussed this idea with his colleagues Mohammad Hafezi and with Christopher Jarzynski. The three researchers decided to collaborate. After the success of an initial experiment, they started studying various cases in which their neural network could provide new valuable insight.

"We used supervised learning and trained a neural network to detect the direction of the arrow of time based on a set of simulated movies of physical processes with corresponding labels indicating backward/forward," Seif explained. "Our neural network outputs a number between 0 and 1, which depends on the input (the movie), and the network's parameters (weights and biases). We then look for those parameter values that minimizes difference between the output of the neural network and the true labels (direction of time's arrow)."

When they used their neural network to analyze videos of physical processes, they found that it could successfully predict the direction of time's arrow with excellent accuracy. In addition, the algorithm's analyses revealed that dissipated work is the proper quantity to use when trying to determine this direction.

In their study, the researchers also used a technique known as inceptionism, introduced by a team of software engineers at Google. This technique allowed them to investigate what goes on inside their neural network, identifying the most representative forward and backward trajectories.

For instance, to uncover a representative forward trajectory, the team took a random input with an unknown direction (i.e., forward or backward) and changed it in such a way that the network output classified it as forward. They then showed that the representative trajectories they uncovered actually matched theoretical predictions.

"The physics of time's arrow in the context of nonequilibrium statistical physics was quantified in recent decades," Seif said. "It is interesting that a well-known algorithm (logistic regression) that existed decades before these theorems leads to the same results. It is conceivable that, with such numerical experiments, one could come up with the theoretical formulation of the solution before its discovery from physical principles."

Seif and his colleagues found that their machine learning algorithm both solved a basic physics problem and identified the most important physical parameters for effectively tackling this problem. The team also showed that the direction of time's arrow can be inferred without the need to specify what exact physical process is taking place, which is very challenging to achieve manually or analytically. In the future, the team plans to continue exploring the potential of using machine learning algorithms to conduct physics research and make new scientific discoveries.

"The physics of systems that are out-of-equilibrium is a particular area of interest for us, as it has unsolved questions that could be answered by studying the dynamics of the systems with machine learning algorithms," Seif said. "To build the toolbox to answer these questions, we have to start with concrete examples that we know how to solve as a testbed. Currently, we are looking at problems in statistical physics, both in the quantum and classical domain, and trying to understand what machine learning tools can learn from experimental observations."

More information: Alireza Seif et al. Machine learning the thermodynamic arrow of time, *Nature Physics* (2020). DOI: 10.1038/s41567-020-1018-2

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