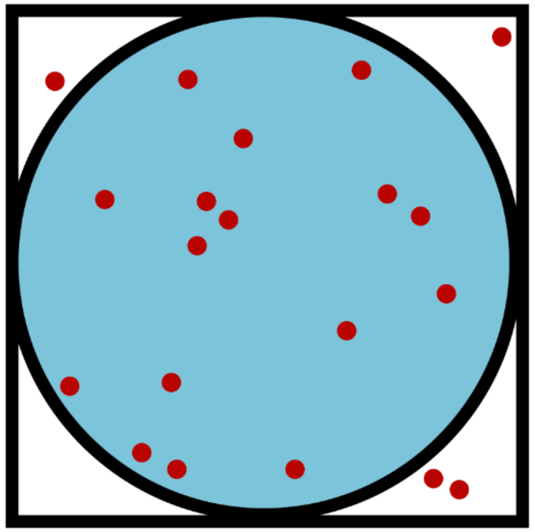
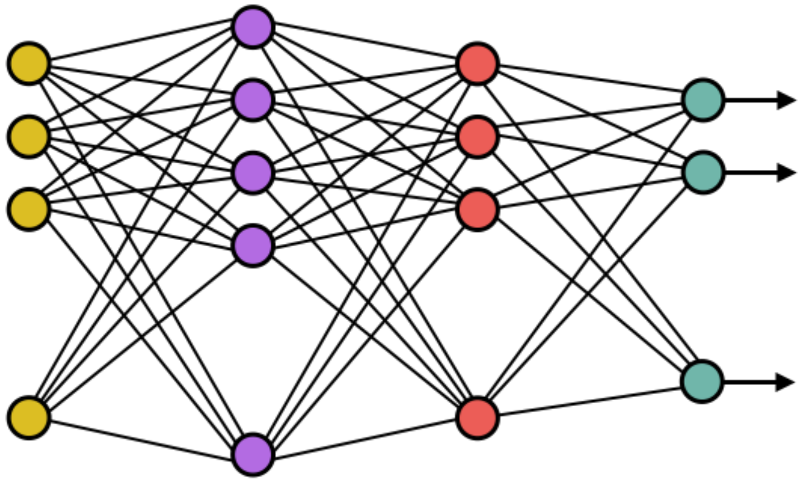
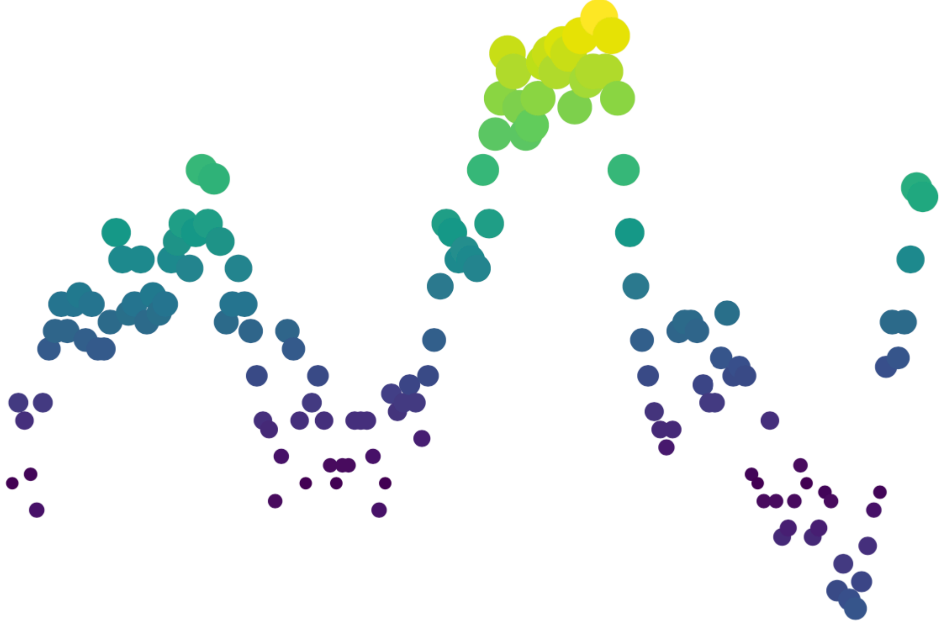
Numerical Methods

Lauren Hayward
PSI Start Online School







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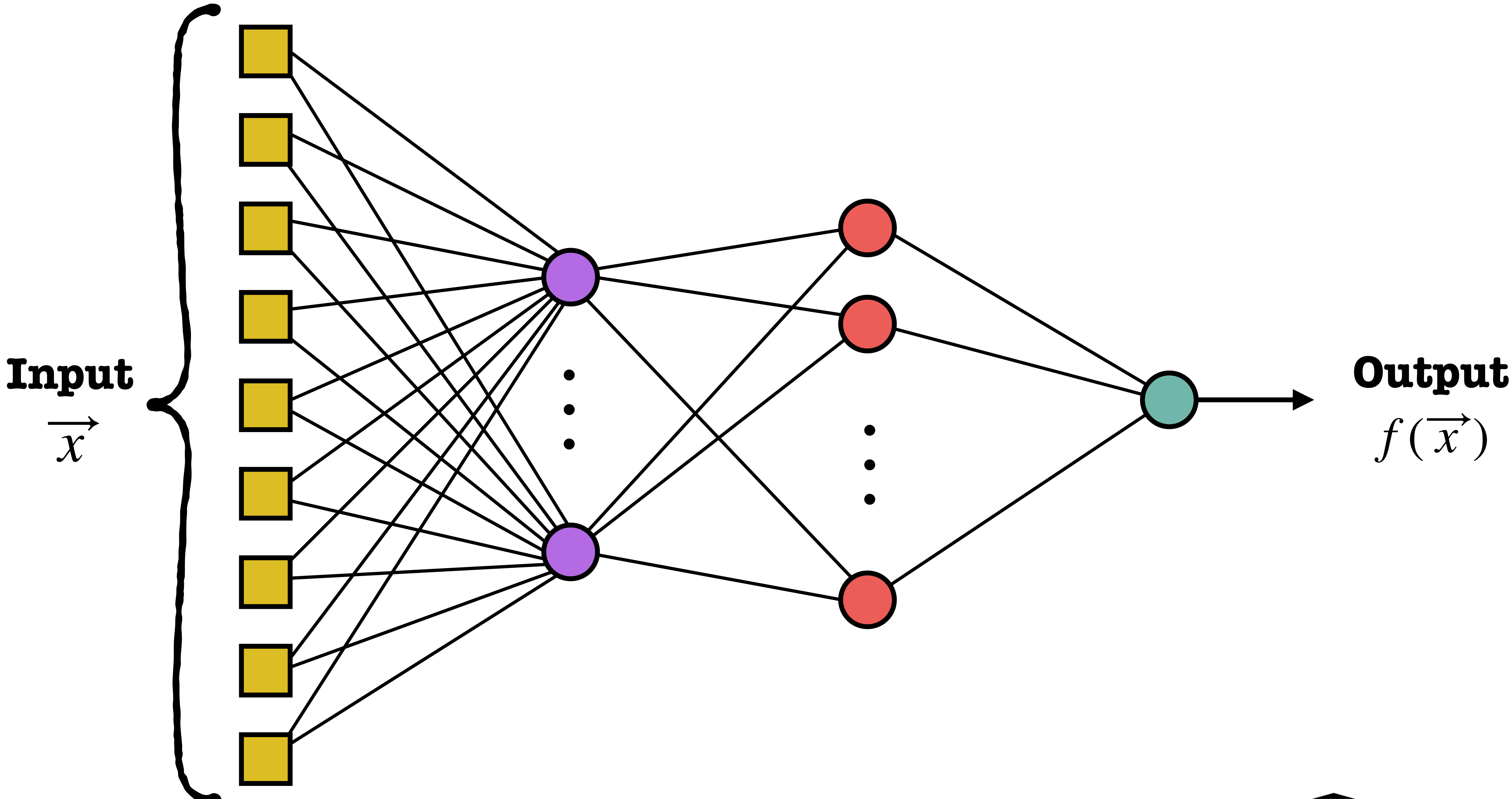
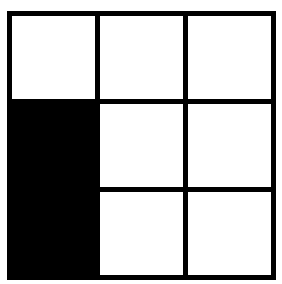
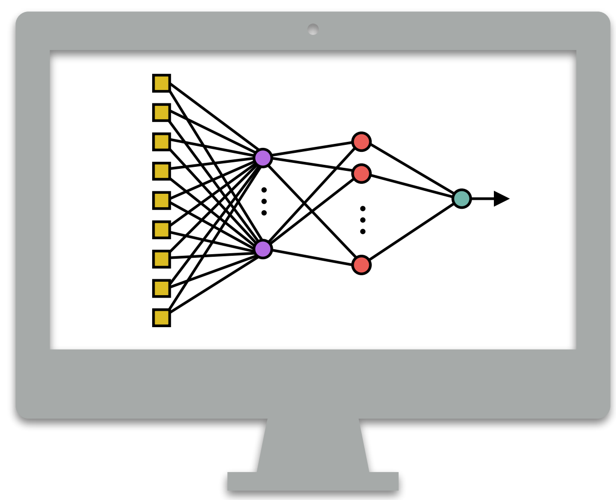
Last lecture: Feedforward neural networks



Last lecture: Neural network output

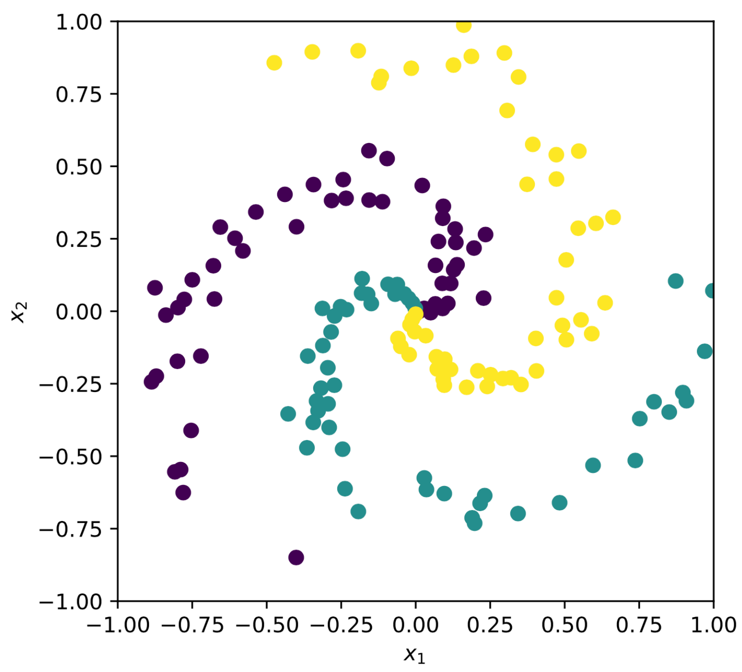
Our network might give the output:

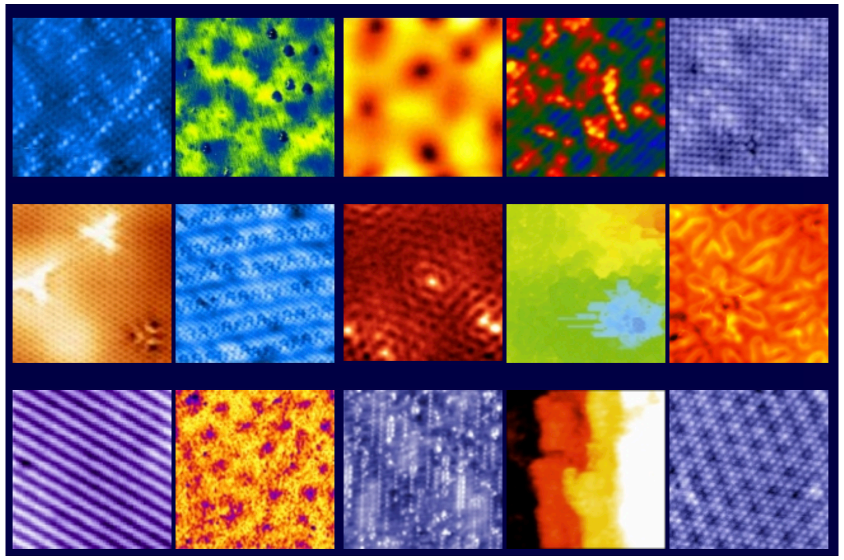
$\vec{x} =$  $\longrightarrow$  $\longrightarrow$ $f(\vec{x}) = 0.89$

While the true answer should be: $y_{\text{true}}(x) = 1$

We would like to choose the weights W and biases b such that the difference between $f(x)$ and $y_{\text{true}}(x)$ is as small as possible.

Outline for today





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Training feedforward neural networks

- Cost functions, learning algorithms, hyperparameters
- Training feedforward neural networks in PyTorch
- Applications in many-body physics

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Cost function

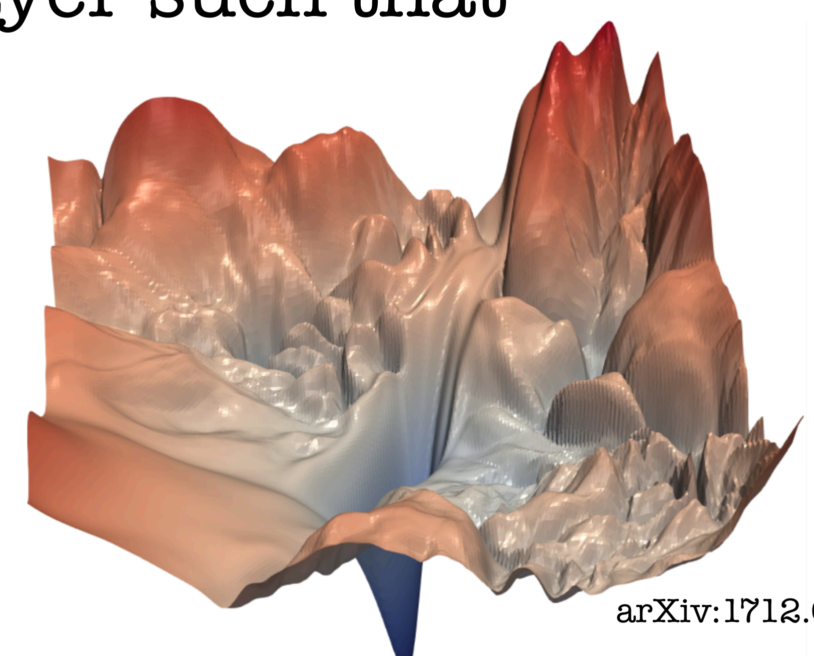
We measure how well our network is doing by calculating a cost function, such as

$$C(W,b) = \sum_{\text{inputs } x} \left[f(x) - y_{\text{true}}(x)\right]^2.$$

For a perfect classifier, $C(W,b) = 0.$

We would like to minimize the cost function over all possible weights and biases in each layer such that

$$\left.\begin{aligned} \frac{\partial C}{\partial W_{ij}^{(\ell)}} &= 0 \\ \frac{\partial C}{\partial b_j^{(\ell)}} &= 0 \end{aligned}\right\} \text{For all } i, j, \ell$$



arXiv:1712.09913

Learning algorithm

The weights and biases are adjusted as the network **learns**.

We use the cost function to modify the weights and biases with a learning algorithm such as gradient descent:

$$W_{ij}^{(\ell)} \to W_{ij}^{(\ell)} - \boxed{R} \times \frac{\partial C}{\partial W_{ij}^{(\ell)}}$$

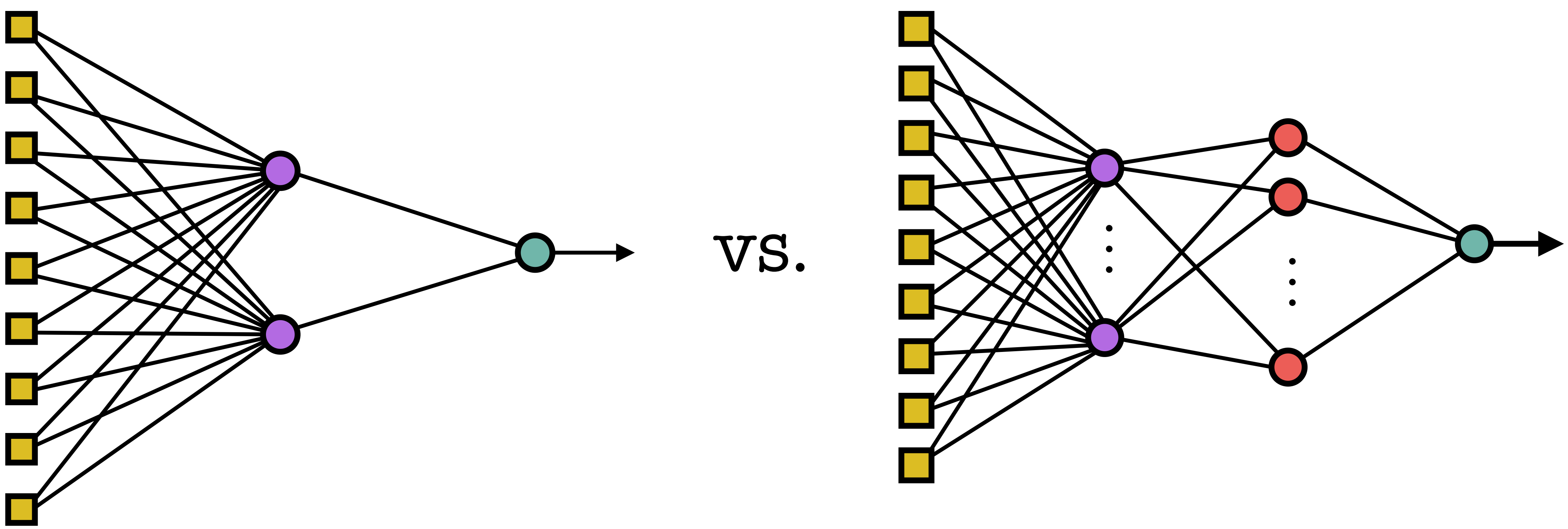
$$b_i^{(\ell)} \to b_i^{(\ell)} - \boxed{R} \times \frac{\partial C}{\partial b_i^{(\ell)}}$$

R : **learning rate**

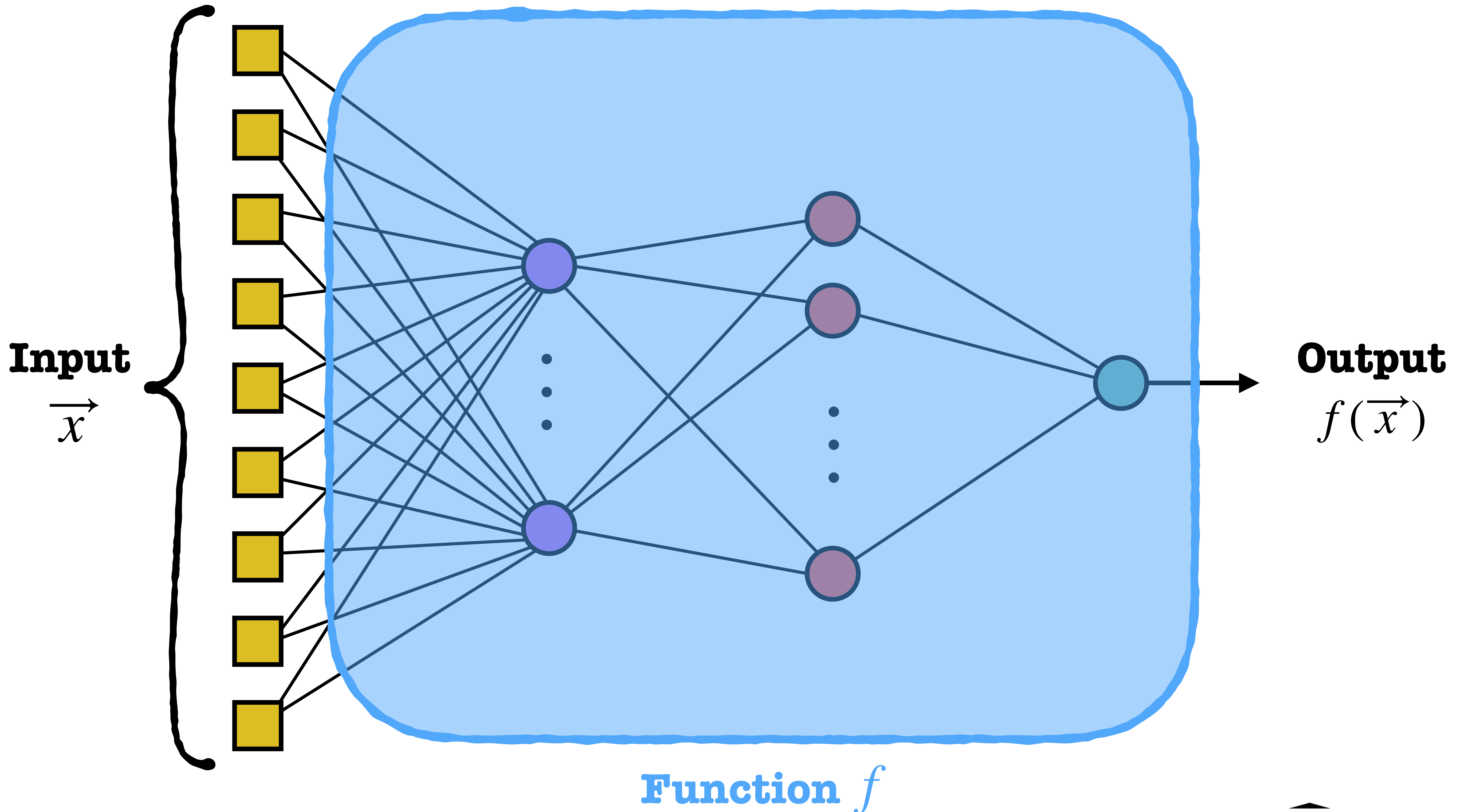
Hyperparameters

There are many hyperparameters we can adjust that affect the performance of a neural network:

- Number of hidden layers
- Number of neurons in each hidden layer
- Learning rate
- Activation function on each layer
- Cost function
- Learning algorithm



Summary of neural networks



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Machine learning algorithms

ML: Training computers to detect and characterize features from data

Categories of algorithms:

1. **Supervised learning (SL)**

   Given a dataset $\mathscr{D} = \{\vec{x}, \vec{y}\}$ of data points $\vec{x}$ and labels $\vec{y}$, fit a function $\vec{f}(\vec{x})$ to $\vec{y}$.

2. **Unsupervised learning (UL)**

   Given an dataset $\mathscr{D} = \{\vec{x}\}$ without labels, efficiently represent the data's underlying probability distribution $p(\vec{x})$.

3. **Reinforcement learning (RL)**

   Taking actions in an environment to maximize a reward.

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SO FAR: SL using neural networks

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Other supervised learning algorithms

✦k-Nearest Neighbours

✦Decision trees

✦Random forests

✦Linear regression

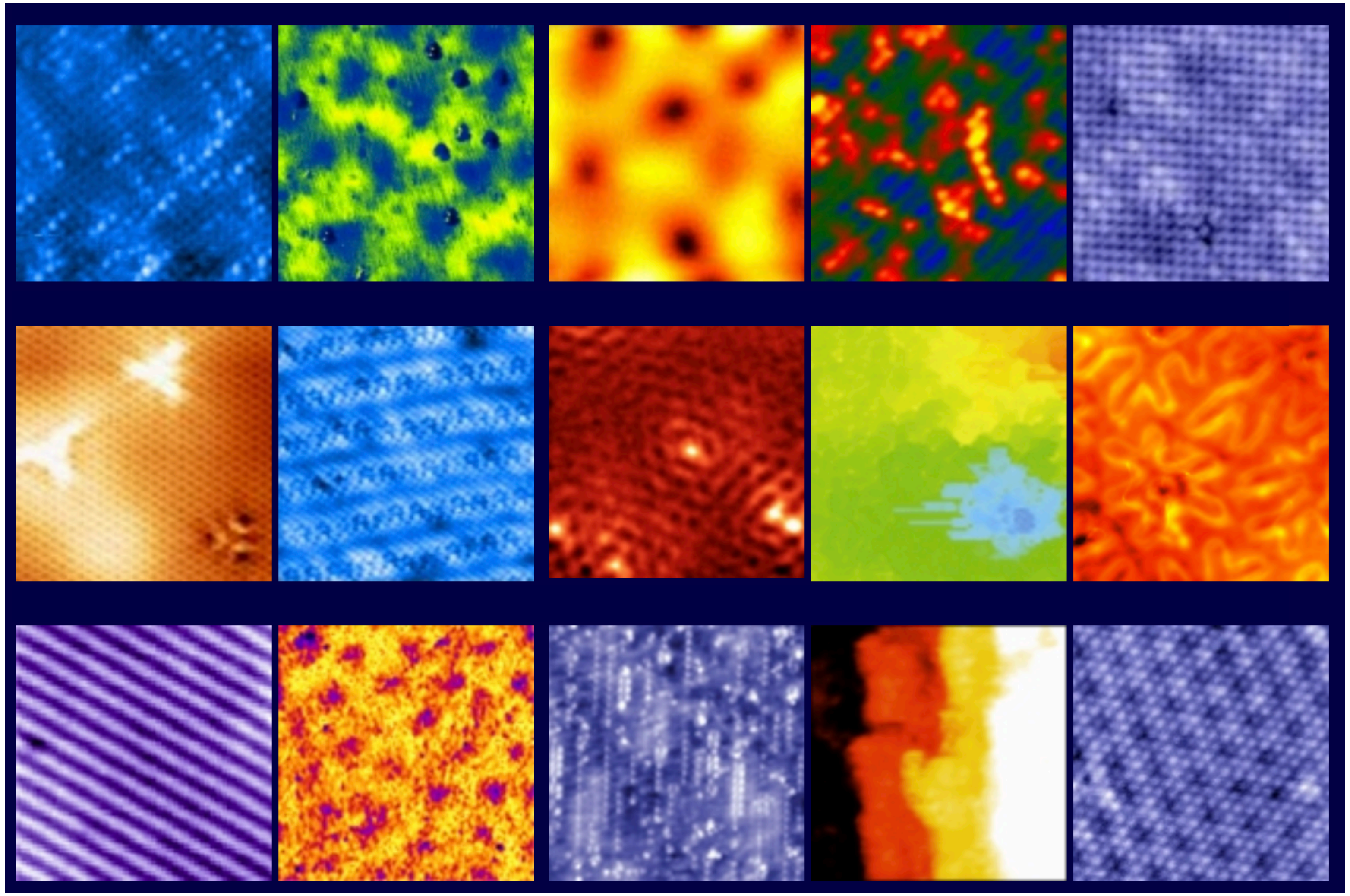
✦Logistic regression

✦Support vector machines

⋮

Applications in the physical sciences

Many of the inputs are also images:



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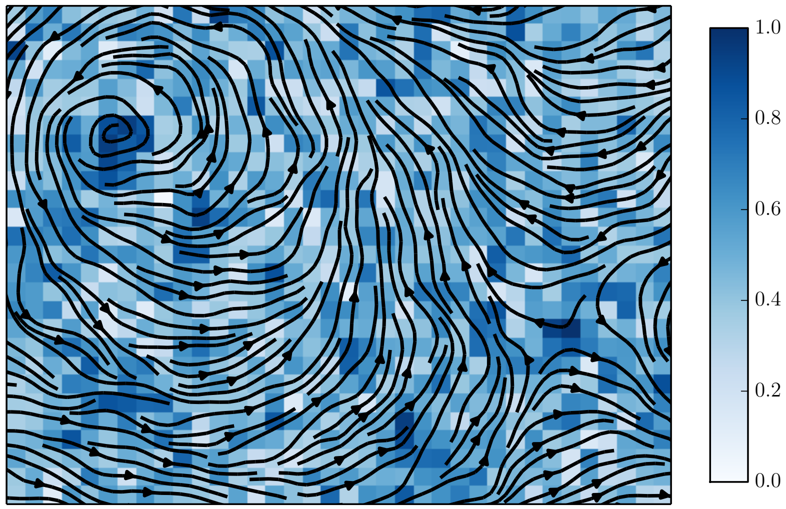
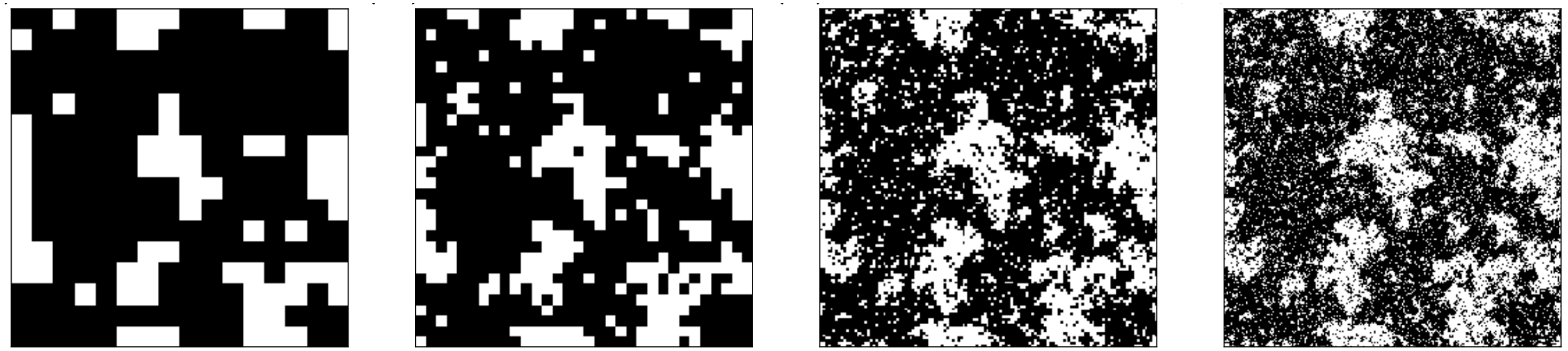


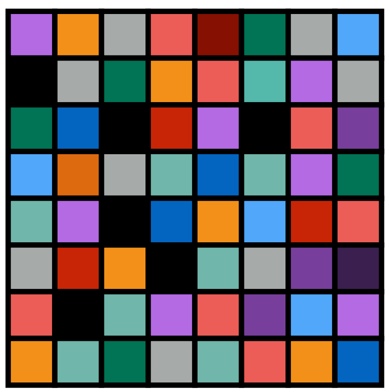
arXiv:1406.2694



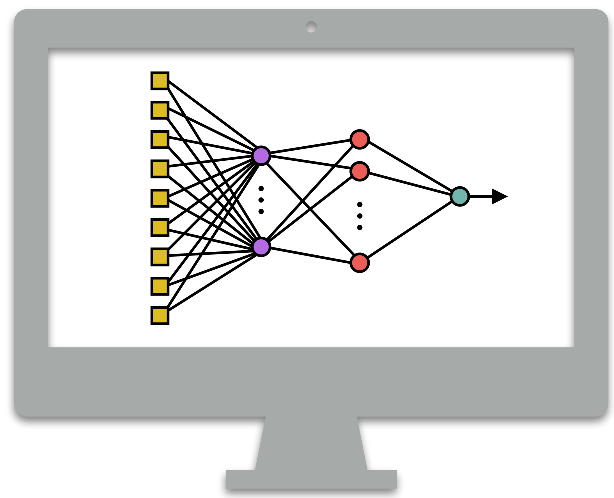
arXiv:1810.02372

Classifying phases of matter

When classifying images:



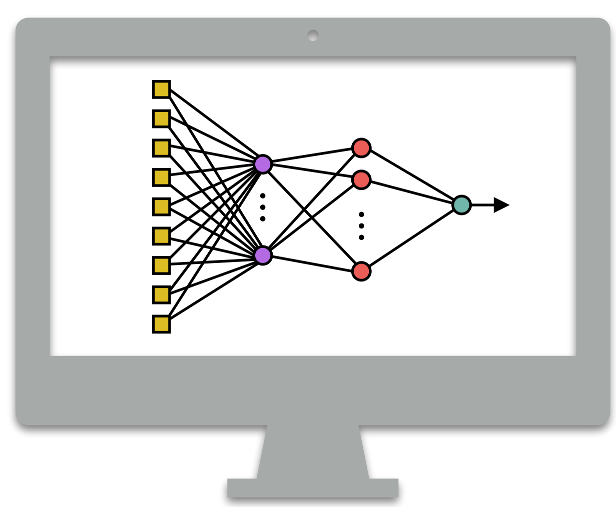
Input: an image



Output: some description of the image

To classify phases of matter:

Input: an image describing the state of a material



Output: the phase of matter that the material is in

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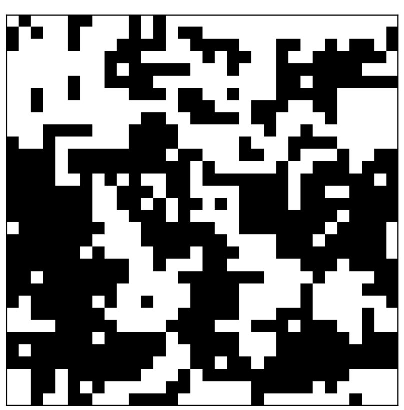
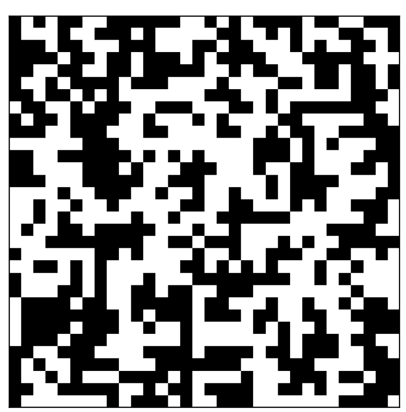
Classifying phases of matter

Two-dimensional Ising model:

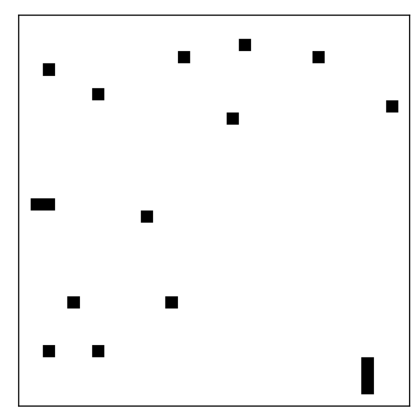
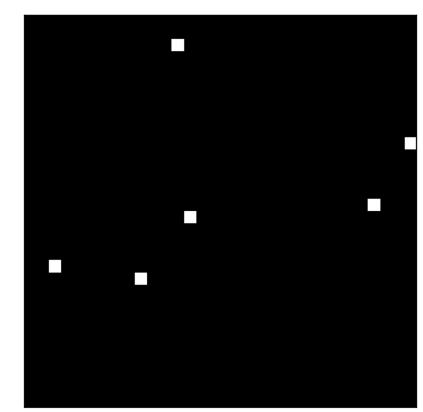
$$H = -J \sum_{\langle ij \rangle} s_i \, s_j$$

At high temperatures:

Paramagnetic phase

At low temperatures:

Ferromagnetic phase

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Classifying phases of matter

nature physics

Letter | Published: 13 February 2017

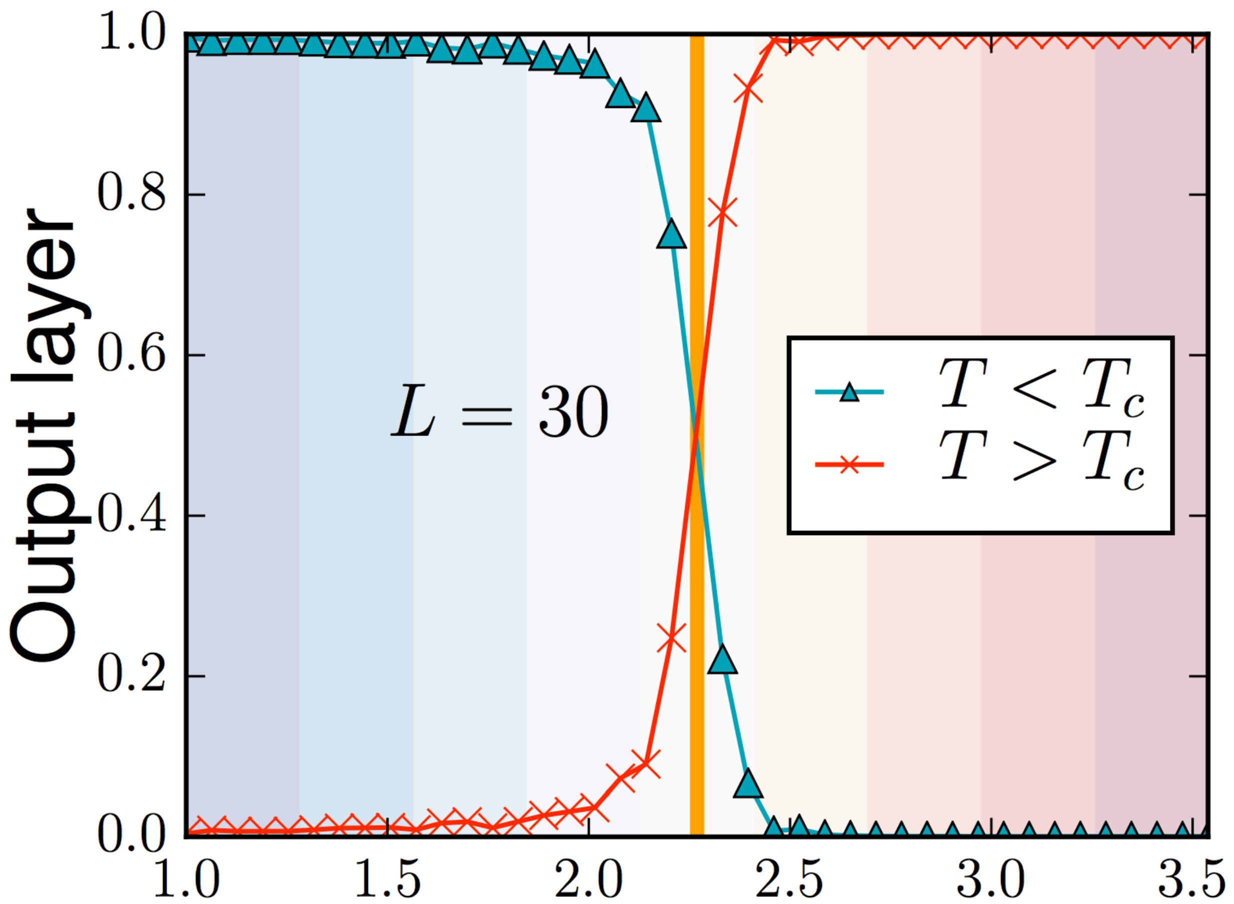
Machine learning phases of matter

Juan Carrasquilla & Roger G. Melko

Nature Physics **13**, 431–434 (2017)

Abstract

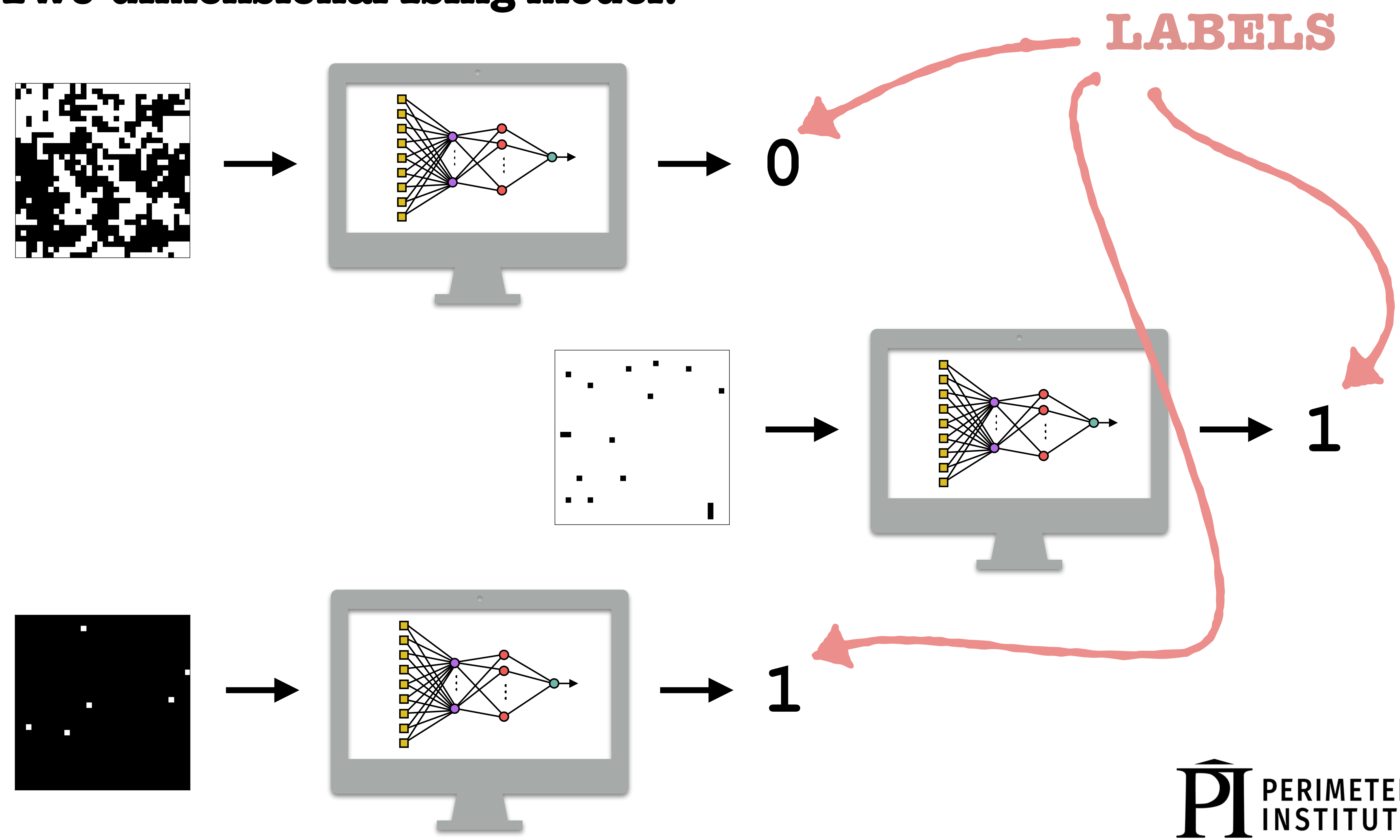
Condensed-matter physics is the study of the collective behaviour of infinitely complex assemblies of electrons, nuclei, magnetic moments, atoms or qubits[1]. This complexity is reflected in the size of the state space, which grows exponentially with the number of particles, reminiscent of the 'curse of dimensionality' commonly encountered in machine learning[2]. Despite this curse, the machine learning community has developed techniques with remarkable abilities to recognize, classify, and characterize complex sets of data. Here, we show that modern machine learning architectures, such as fully connected and convolutional neural networks[3], can identify phases and phase transitions in a variety of condensed-matter Hamiltonians. Readily programmable through modern software libraries[4,5], neural networks can be trained to detect multiple types of order parameter, as well as highly non-trivial states with no conventional order, directly from raw state configurations sampled with Monte Carlo[6,7].



2016

Classifying phases of matter

Two-dimensional Ising model:



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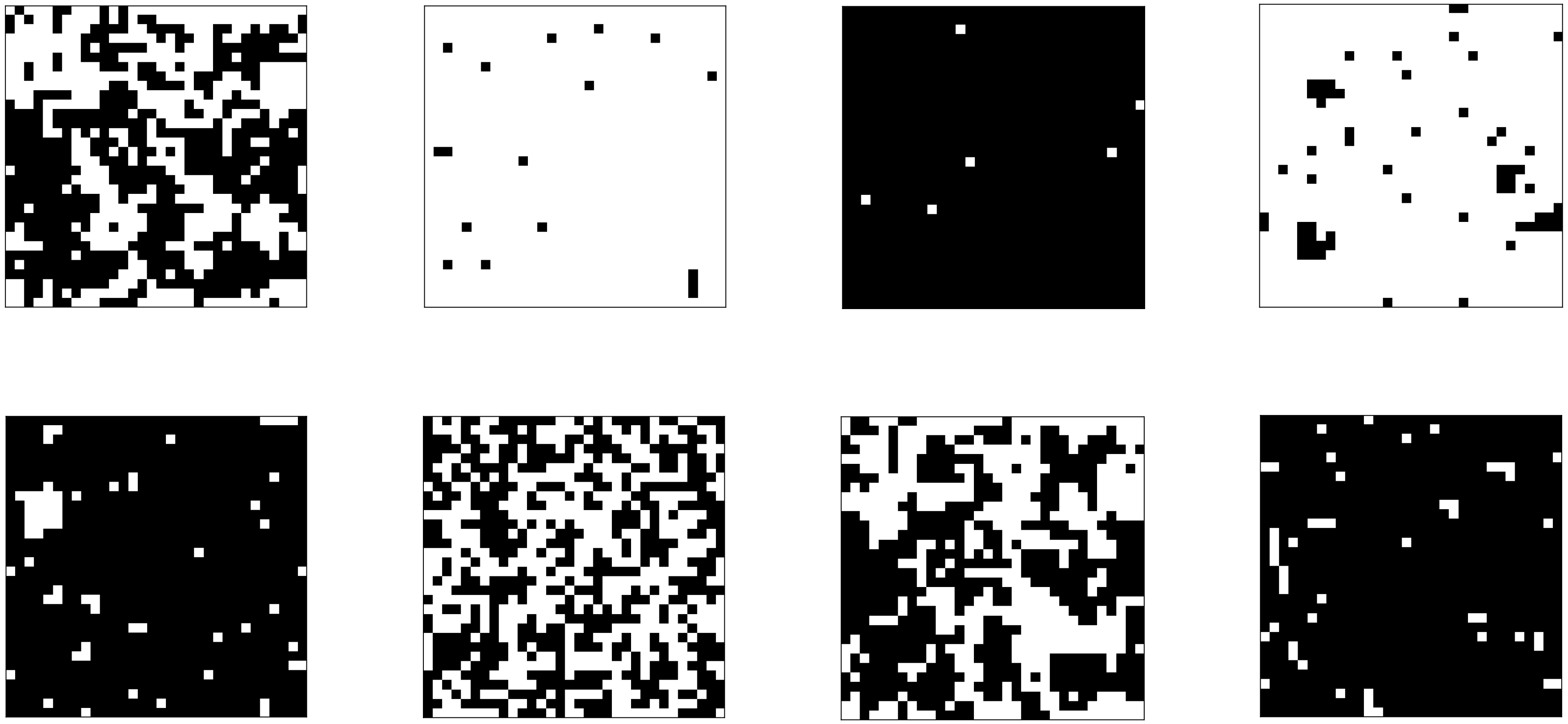
Identifying phases of matter without labels

Two-dimensional Ising model:



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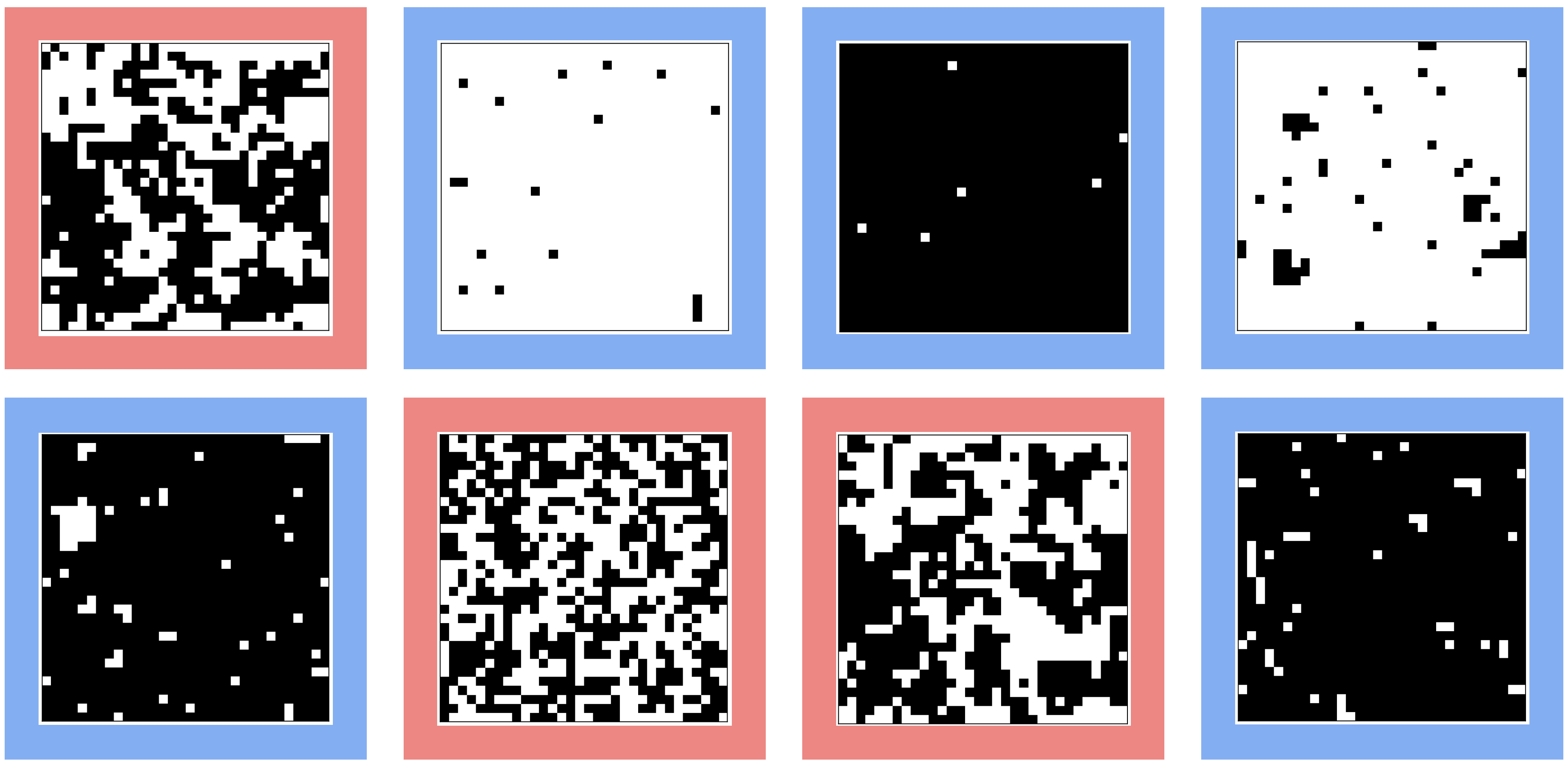
Identifying phases of matter without labels

Two-dimensional Ising model:



Group #1

Group #2

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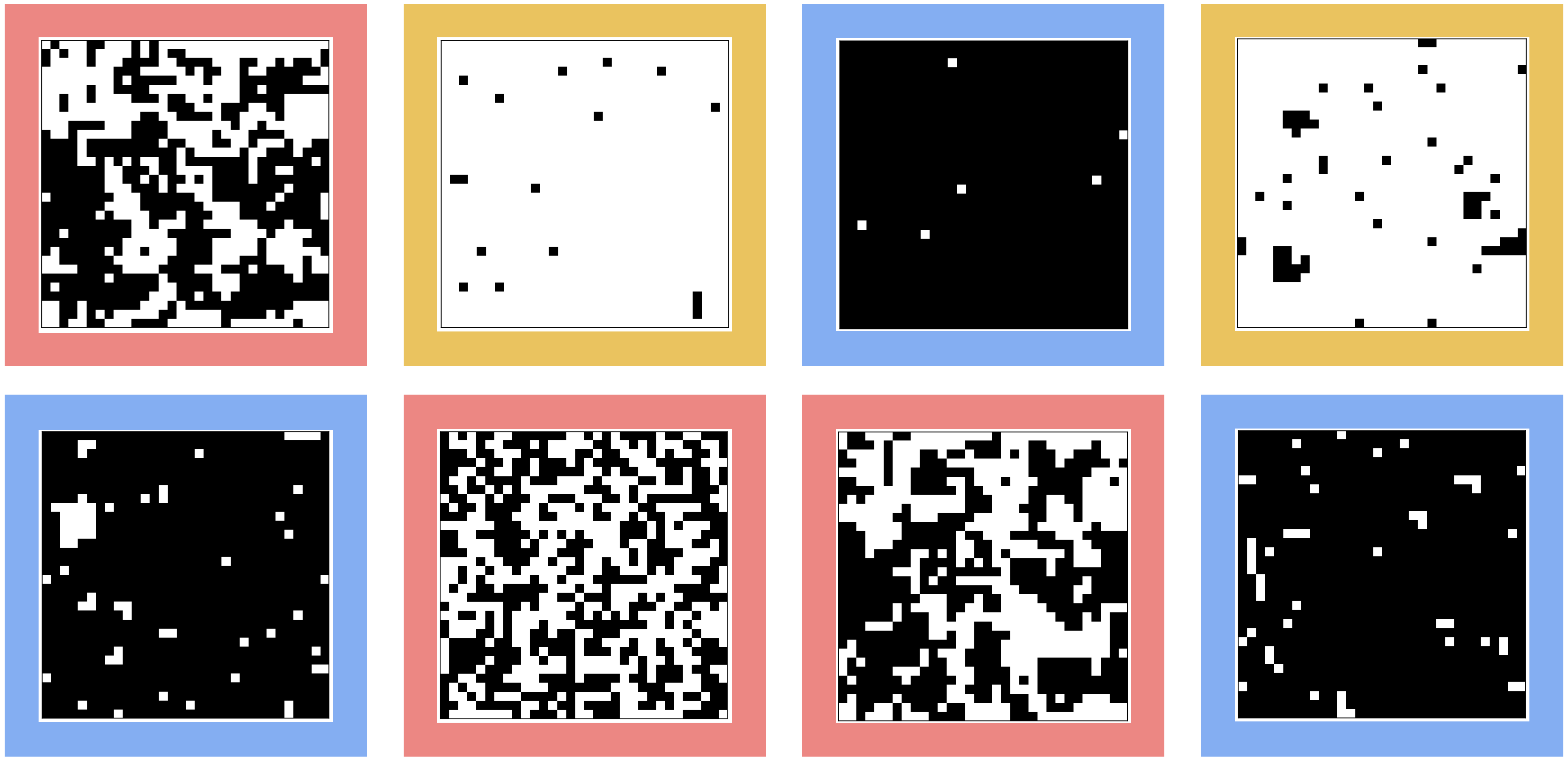
Identifying phases of matter without labels

Two-dimensional Ising model:



Group #1 Group #2 Group #3

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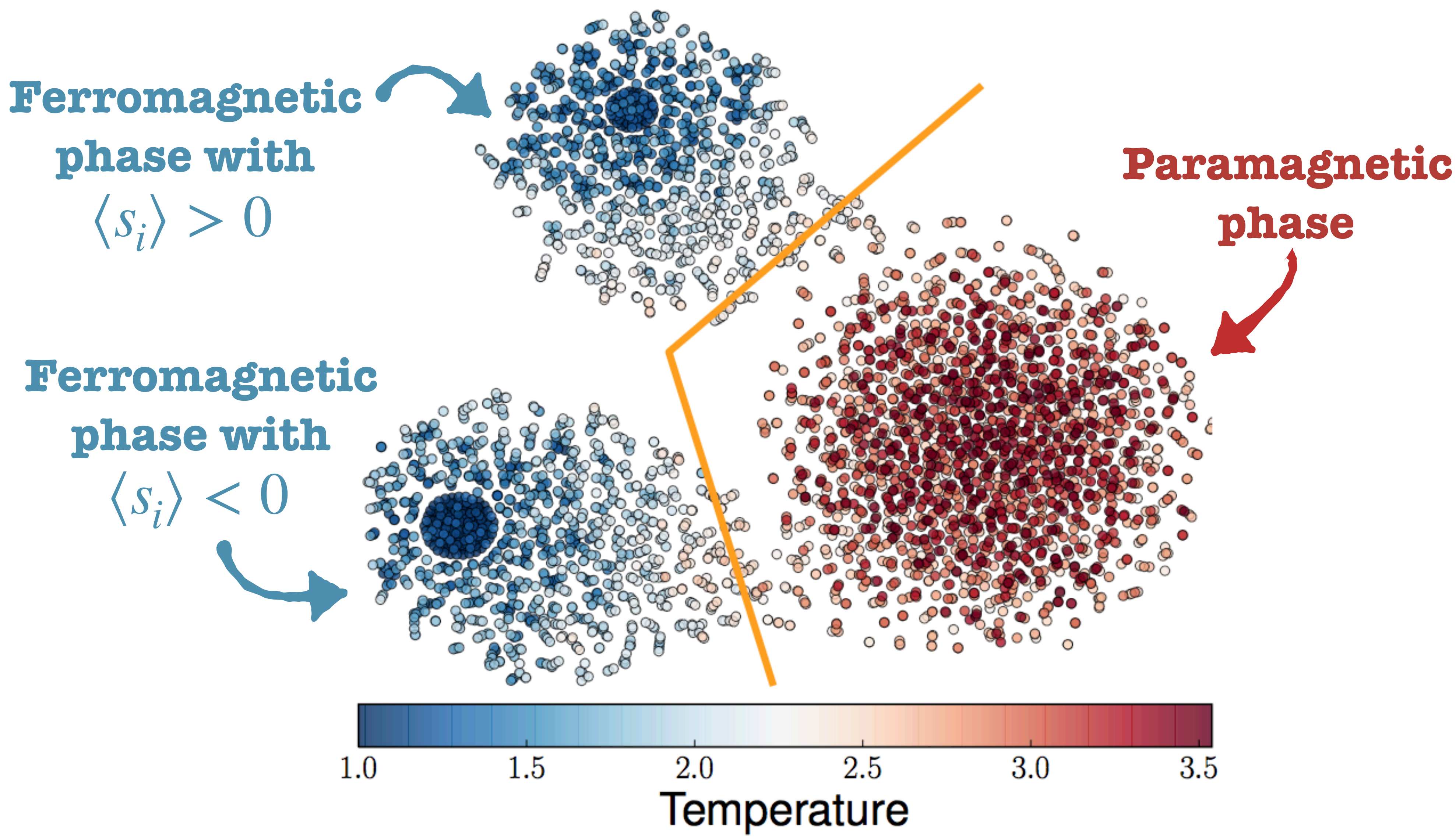
Identifying phases of matter without labels



Carrasquilla and Melko, Nature Physics **13**, 431 (2017)

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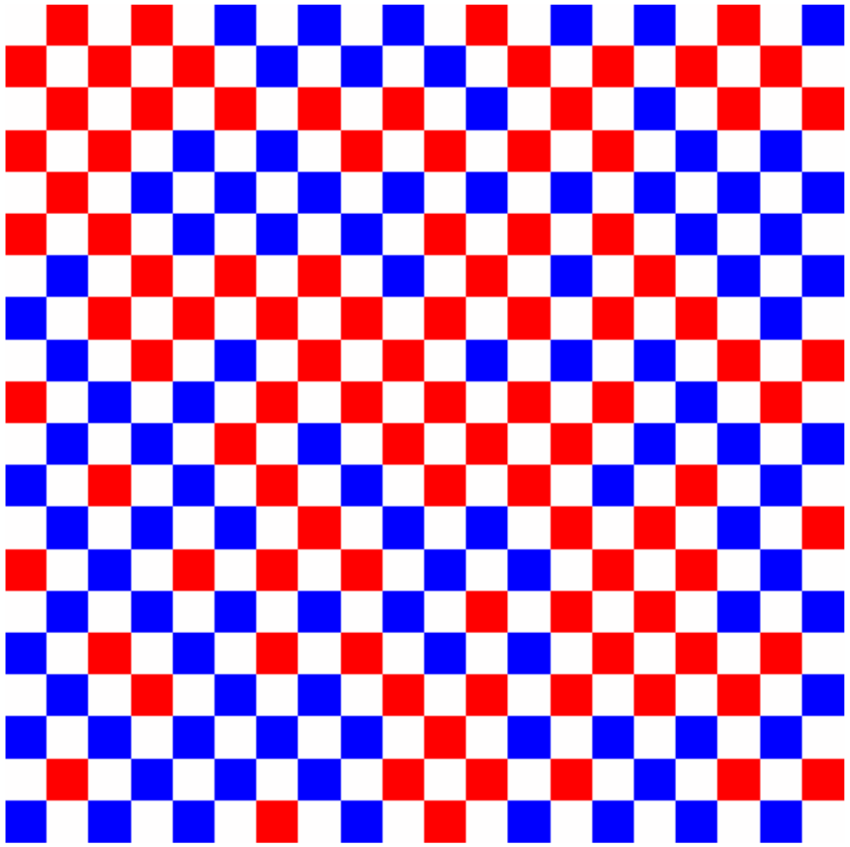
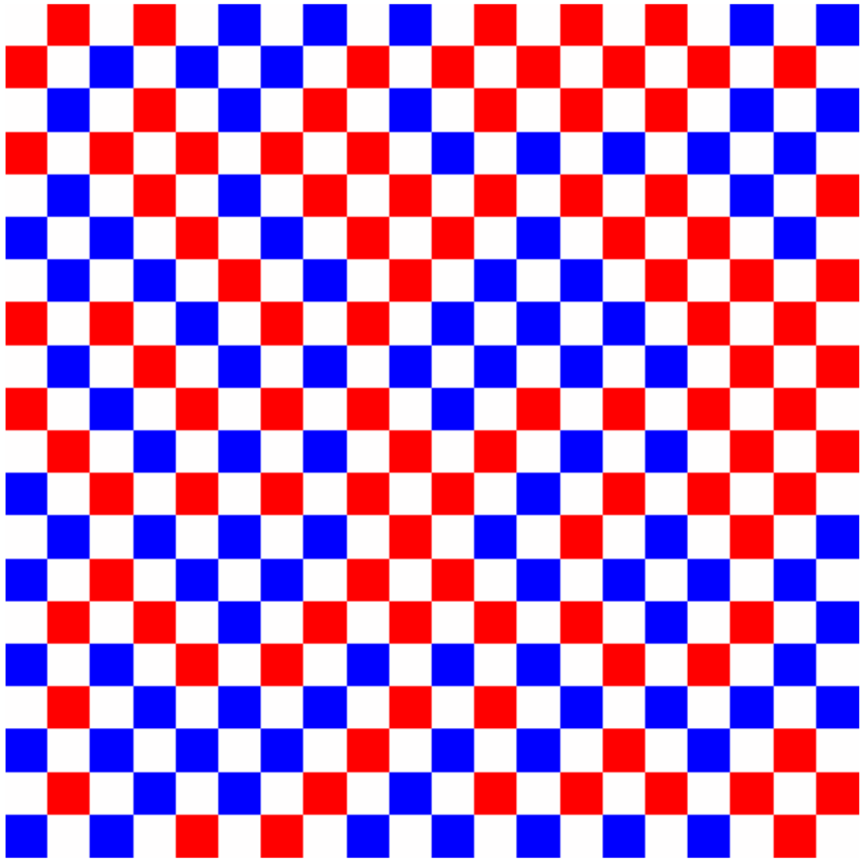
Identifying topological order without labels

Two-dimensional $\mathbb{Z}_2$ lattice gauge theory:

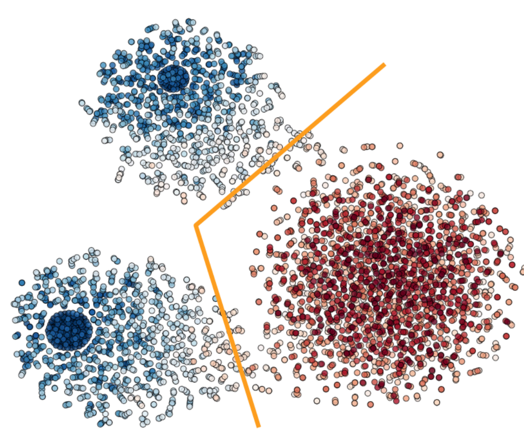




Machine learning for many-body physics

- We can classify images using **supervised** machine learning and neural networks:

- When we don't have labels, we can identify features of images using **unsupervised** machine learning:



Ising model

More to come during Mohamed's guest lecture!

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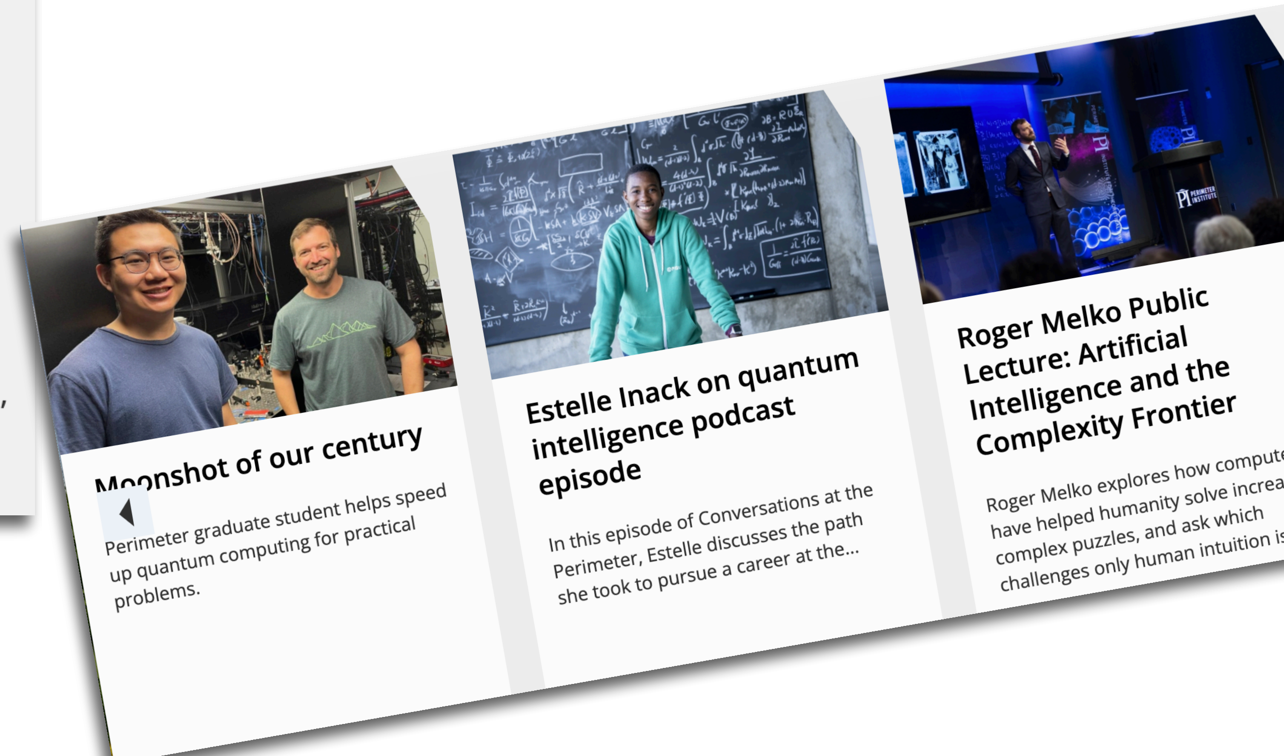
QUANTUM INTELLIGENCE LAB

Perimeter Institute Quantum Intelligence Lab (PIQuIL)

The combined powers of quantum computing and artificial intelligence are sparking breakthroughs and breakout technologies at the Perimeter Institute Quantum Intelligence Lab (PIQuIL).

PIQuIL is a first-of-its kind meeting place for entrepreneurial leaders from fundamental research, education, and high-tech industry -- people who understand the vast potential of quantum intelligence.



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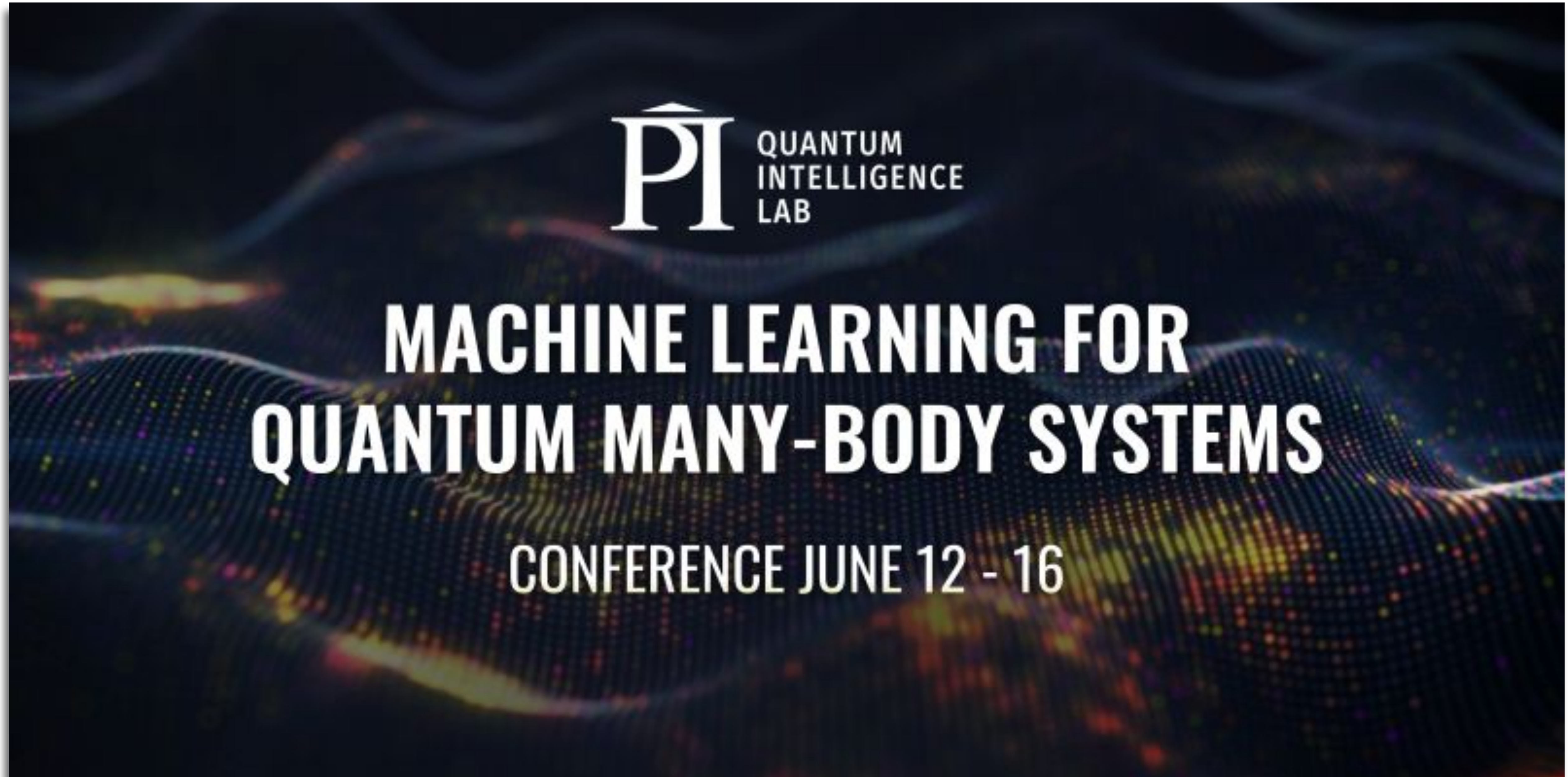

https://hubs.ly/Q01T8FTt0

See recordings from this conference and other Perimeter events at pirsa.org

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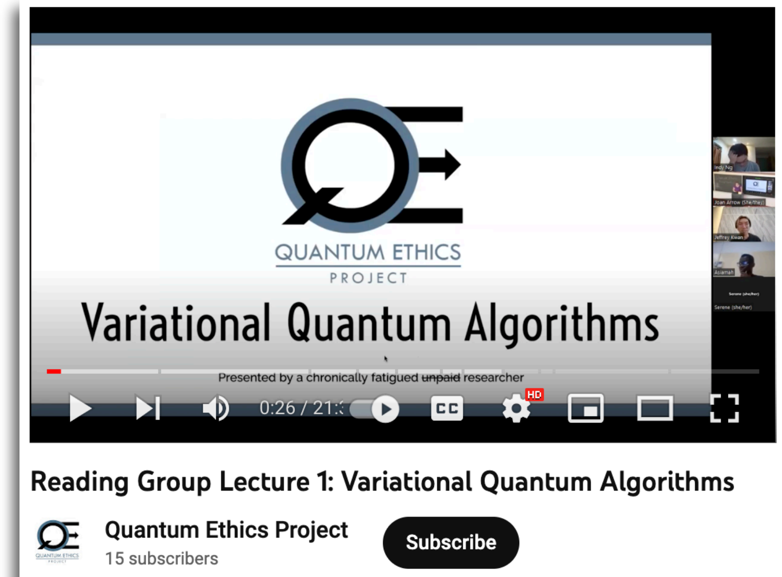
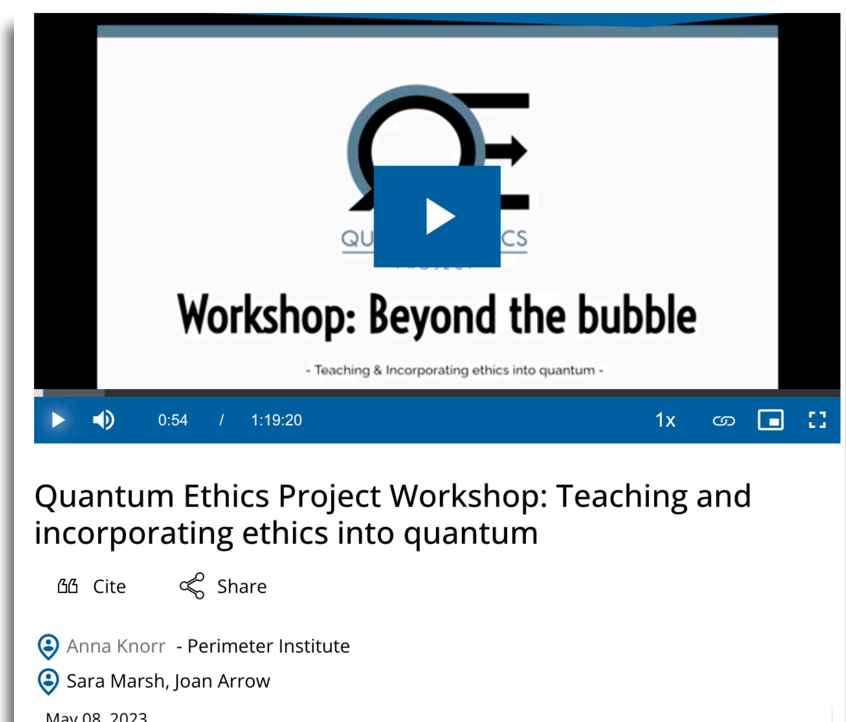
The ethics of quantum and AI

https://www.quantumethicsproject.org

https://pirsa.org/23030041



https://www.youtube.com/watch?v=p63osrbIFxY



https://pirsa.org/23050104

https://youtu.be/-VOdm2smZDc

Discussion session and talk by Gus Skorburg on June 14
https://hubs.ly/Q01T8FTt0

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Machine learning for physicists: resources

- Nielsen, "Neural networks and deep learning", **neuralnetworksanddeeplearning.com**
- Goodfellow, Bengio, and Courville, "Deep learning", MIT Press (2016), **deeplearningbook.org**
- A. Farahmand, J. Carrasquilla, and R. Grosse, "Machine Learning and Data Mining" lectures at University of Toronto, **http://www.cs.toronto.edu/~rgrosse/courses/csc411_f18**
- Carleo, Cirac, Cranmer, Daudet, Schuld, Tishby, Vogt-Maranto, and Zdeborová, "Machine learning and the physical sciences", **arXiv:1903.10563**
- Liu, Li and Wang, "Lecture note on deep learning and quantum many-body computation", **http://wangleiphy.github.io/lectures/DL.pdf**
- Mehta, Bukov, Wang, Day, Richardson, Fisher, and Schwab, "A high-bias, low-variance introduction to machine learning for physicists", **arXiv:1803.08823**
- **LEH**, M. Hibat Allah, J. Carrasquilla, J. Arrow, S. Marsh, and R. Melko, "Machine learning for many-body physics" lecture series at Perimeter Institute, **https://pirsa.org/C23011**

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Next lecture: Guest lectures

Taillte May

Mohamed Hibat Allah

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