Machine learning quantum phases of matter beyond the fermion sign problem

Station Q
September 2016

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Collaborators

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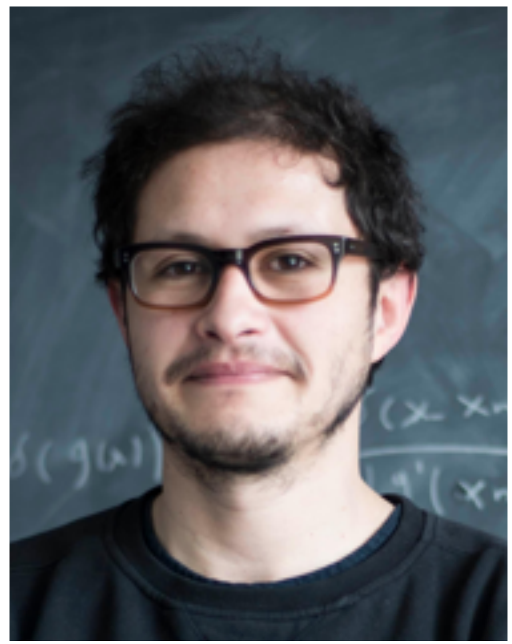
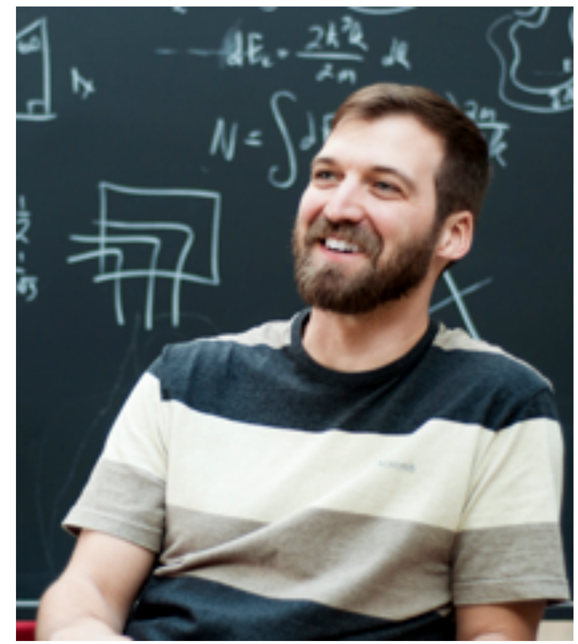


Juan Carrasquilla

Perimeter



Roger Melko

Waterloo / Perimeter

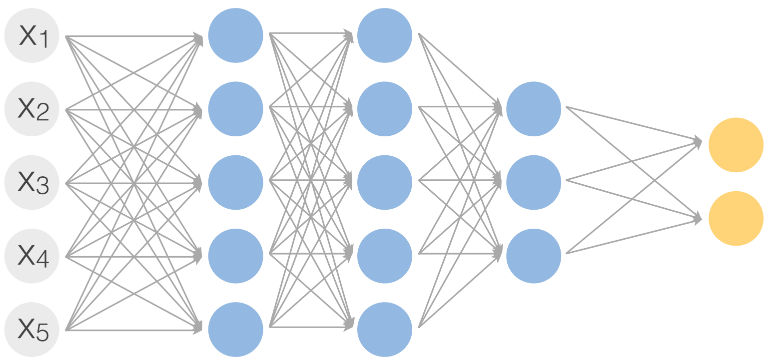
Machine learning

Machine learning 101

In computer science, machine learning is concerned with algorithms that allow for **data analytics**, most prominently **dimensional reduction** and **feature extraction**.

Examples include **spam filters**, **face** and **voice recognition**.

Implicit knowledge representation in **artificial neural networks**, which are trained in **supervised or unsupervised learning** settings.



Hierarchical neural networks gathered a lot of attention for their **“deep learning”** capabilities, e.g. playing Go.


ARTICLE

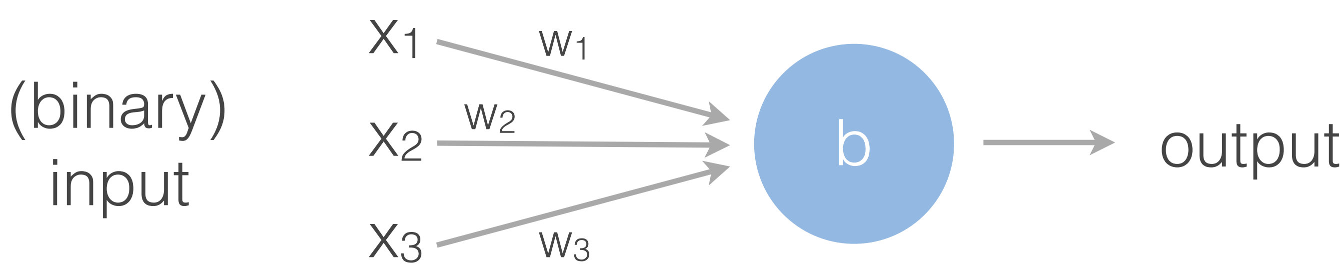
doi:10.1038/nature16961

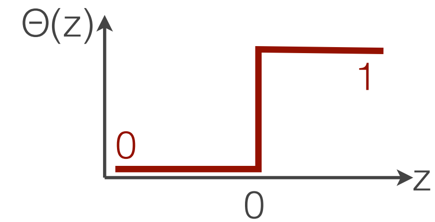
Mastering the game of Go with deep neural networks and tree search

David Silver[1]*, Aja Huang[1]*, Chris J. Maddison[1], Arthur Guez[1], Laurent Sifre[1], George van den Driessche[1], Julian Schrittwieser[1], Ioannis Antonoglou[1], Veda Panneershelvam[1], Marc Lanctot[1], Sander Dieleman[1], Dominik Grewe[1], John Nham[2], Nal Kalchbrenner[1], Ilya Sutskever[2], Timothy Lillicrap[1], Madeleine Leach[1], Koray Kavukcuoglu[1], Thore Graepel[1] & Demis Hassabis[1]

artificial neural networks

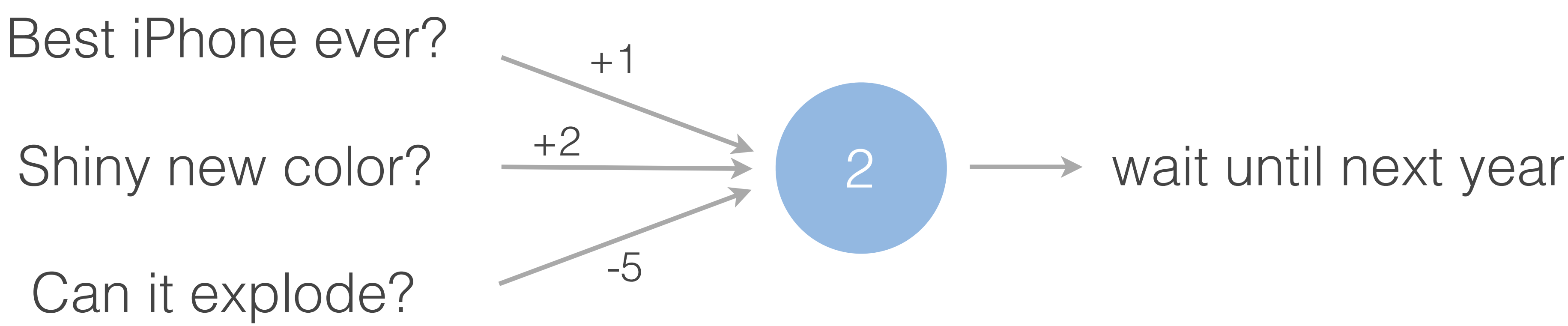
artificial neurons





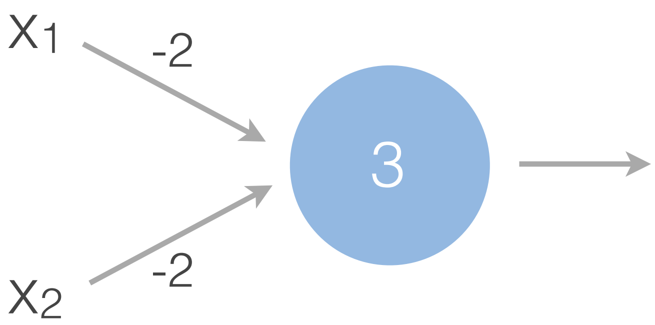
$$\Theta\left(\vec{w}\cdot\vec{x}-b\right)$$

example – Should I buy the new iPhone?



artificial neural networks

Artificial neural networks are pretty powerful.



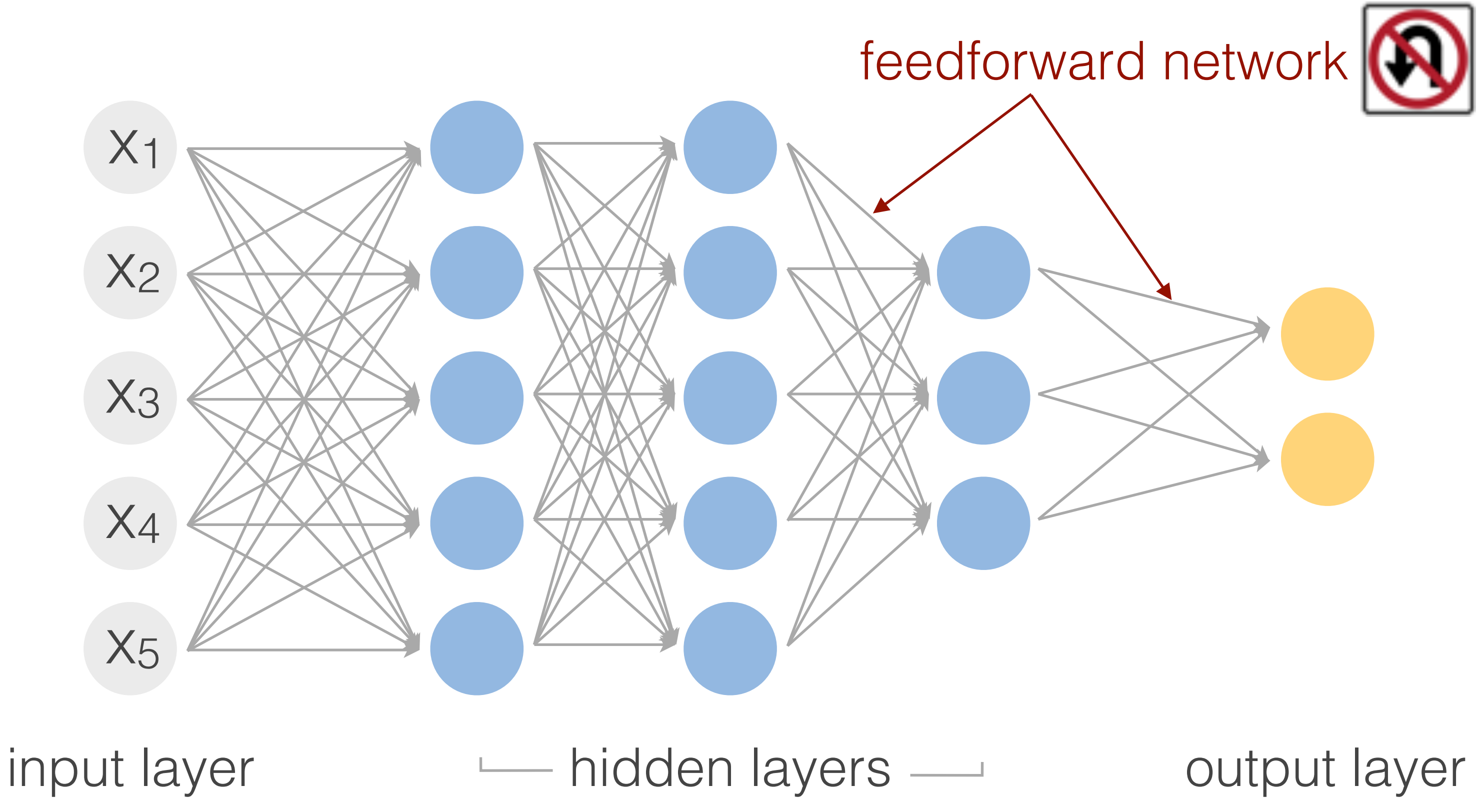
x_1	x_2	output
0	0	1
0	1	1
1	0	1
1	1	0

NAND-gate

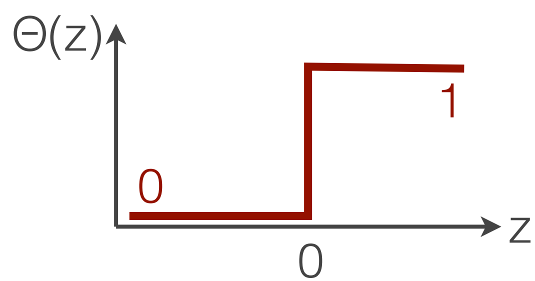
Like circuits of NAND gates artificial neural networks can encode arbitrarily complex logic functions, thus allowing for **universal computation**.

But the power of neural networks really comes about by **varying the weights** such that one obtains some desired **functionality**.

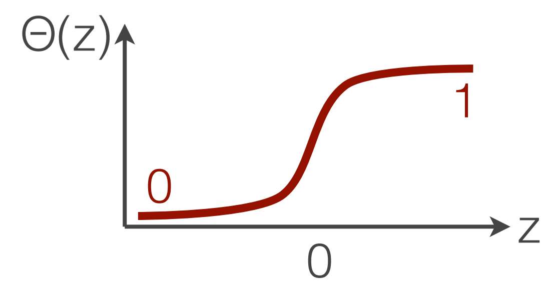
How to train a neural network?



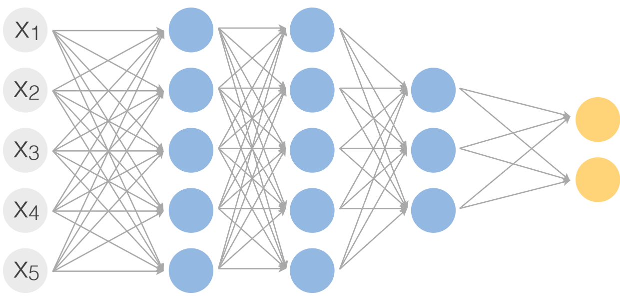
perceptrons



sigmoid neurons



How to train a neural network?

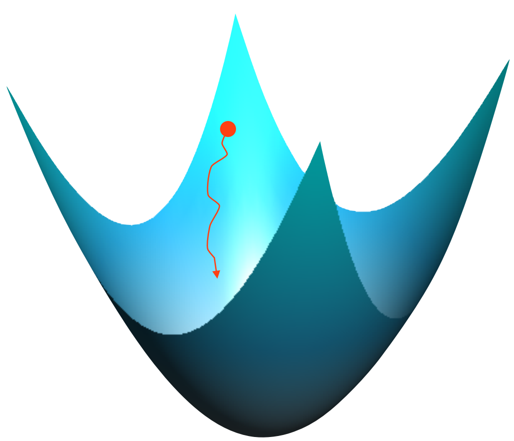


- quadratic **cost function**

$$C(\vec{w},\vec{b}) = \frac{1}{2n}\sum_x ||y(x) - a(x)||^2$$

desired output

actual output



gradient descent

- **back propagation** algorithm

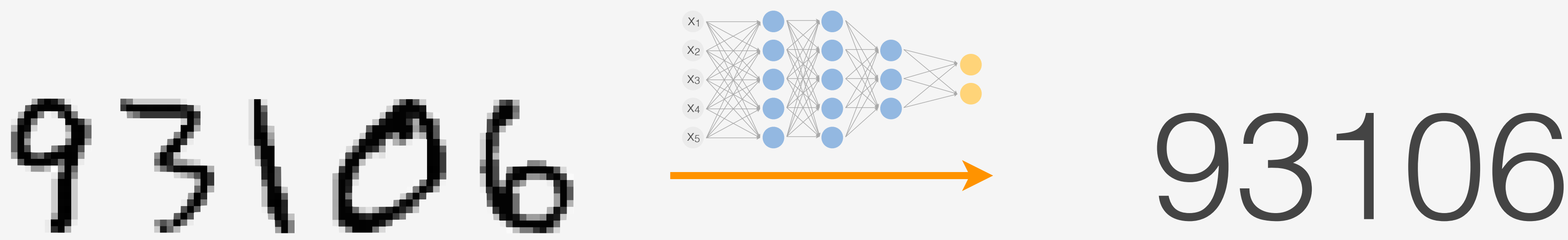
Rumelhart, Hinton & Williams, Nature (1986)

extremely efficient way to calculate *all* partial derivatives

$$\frac{\partial C}{\partial w} \qquad \frac{\partial C}{\partial b}$$

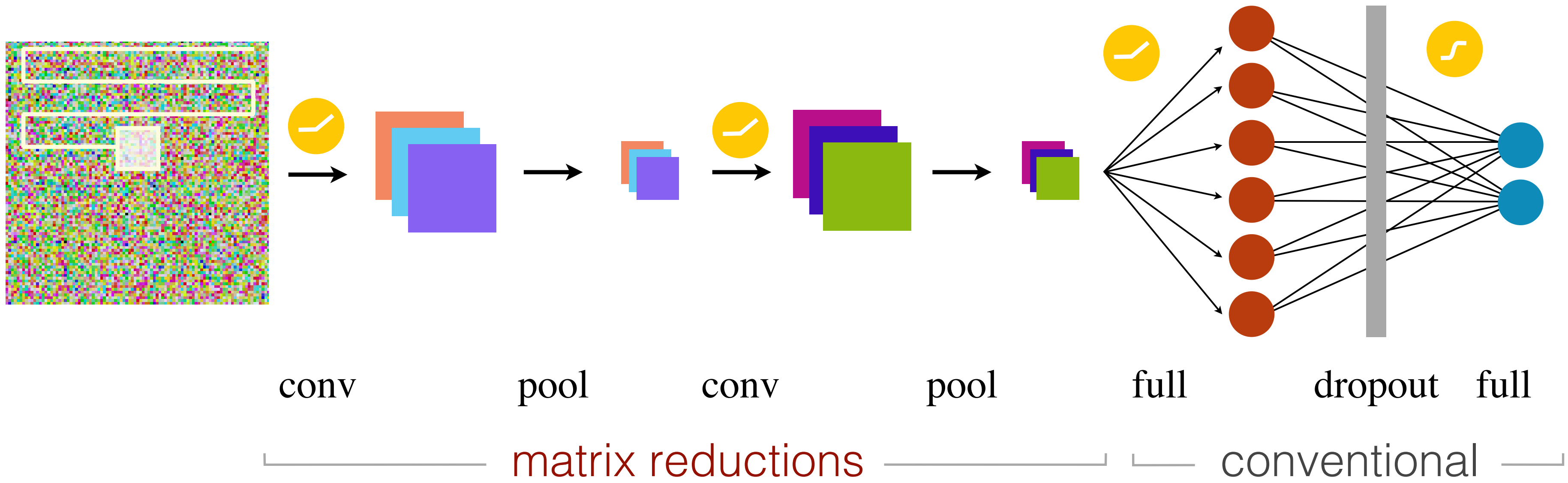
needed for a **gradient descent** optimization.

pattern recognition



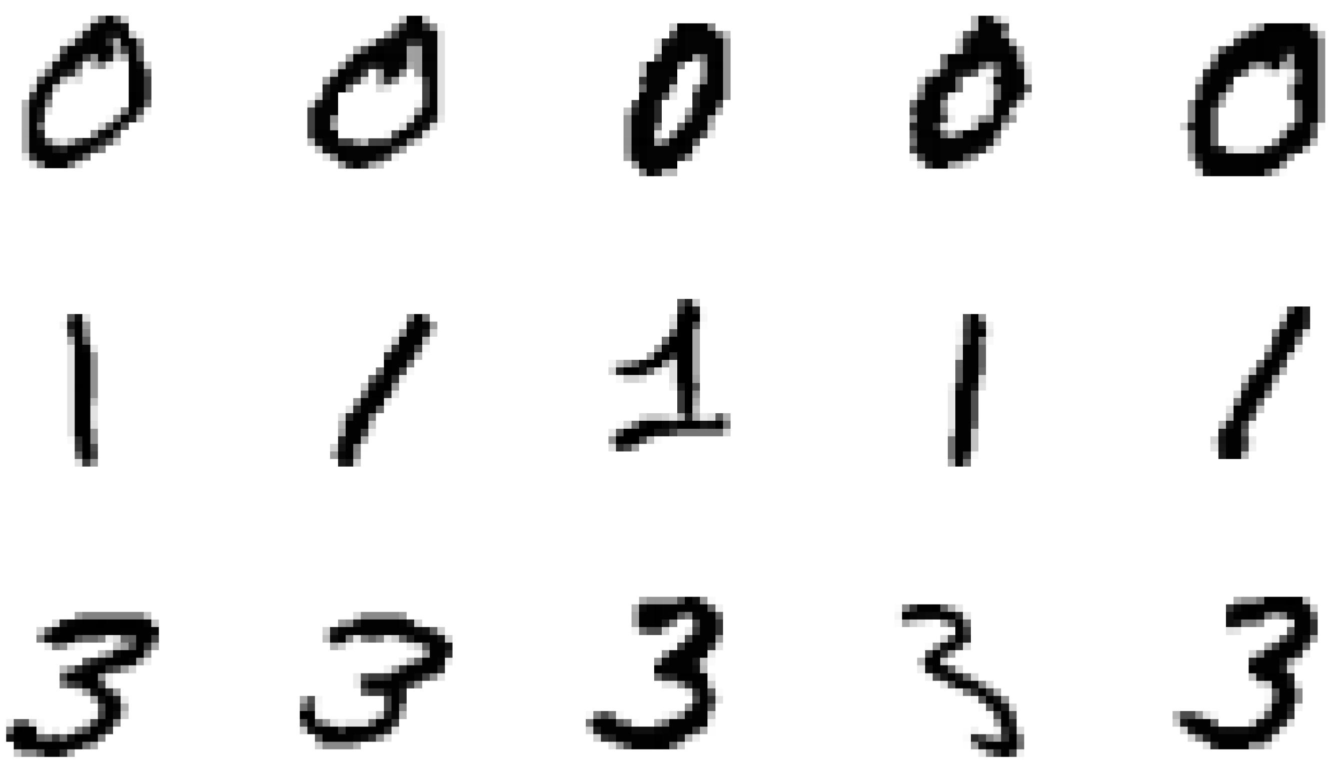
Some **60 lines of code** (Python/Julia) will do this for you with **>95% accuracy**.

Much **higher accuracy** possible for networks with additional **convolutional layers**.



convolutional neural networks

Convolutional neural networks look for **recurring patterns** using small filters.



convolutional neural networks

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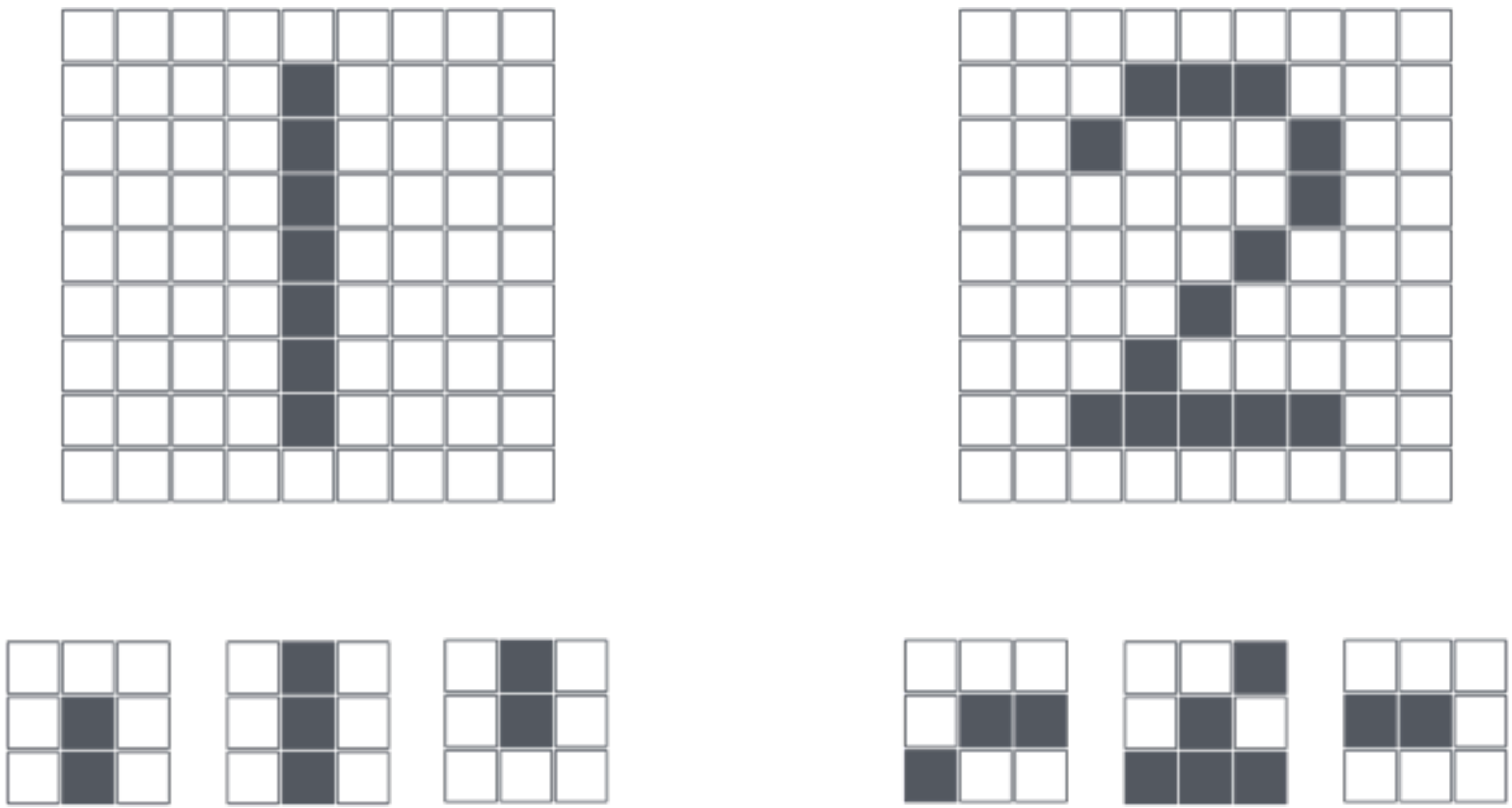

convolutional neural networks

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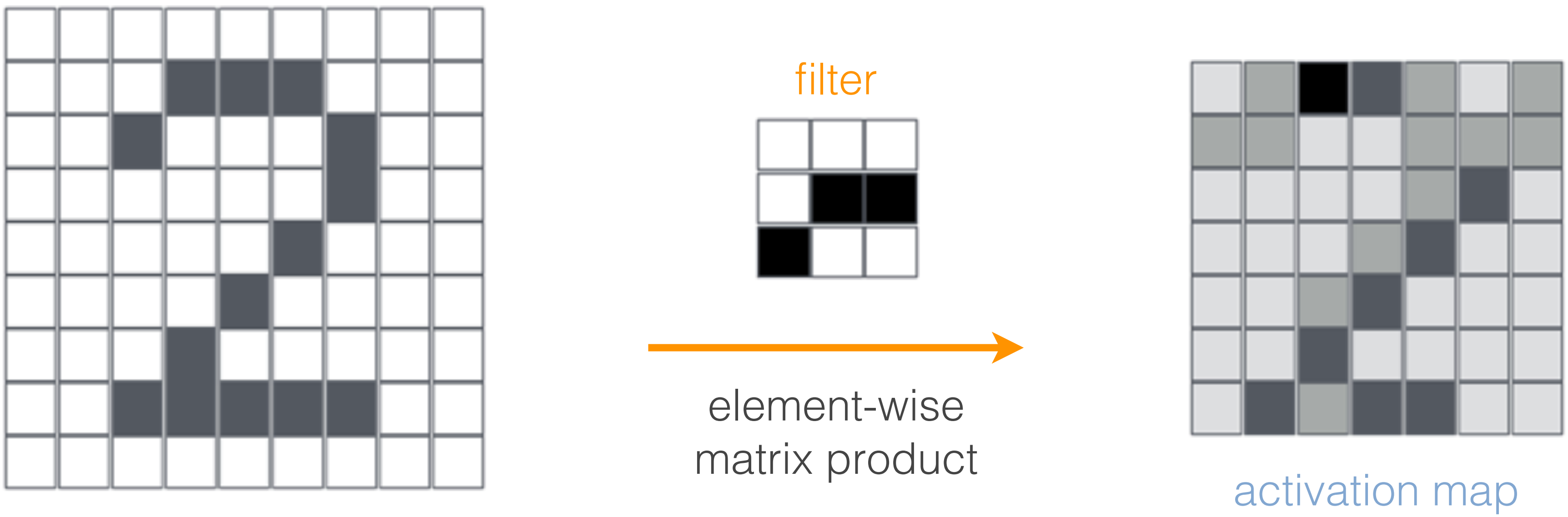
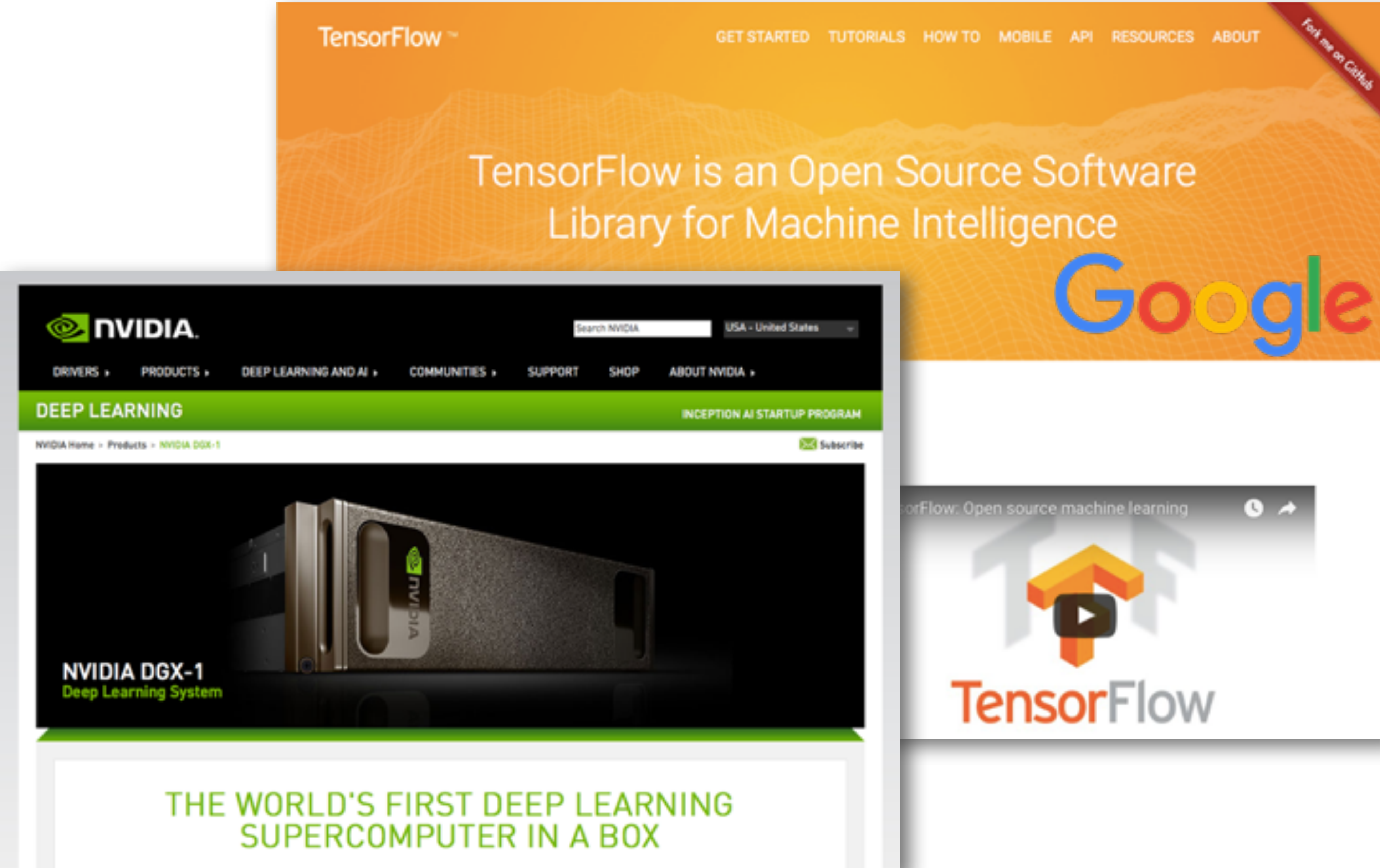


Slide filters across image and create new image based on how well they fit.

GPUs & open-source codes



Machine learning quantum phases of matter

Supervised learning approach

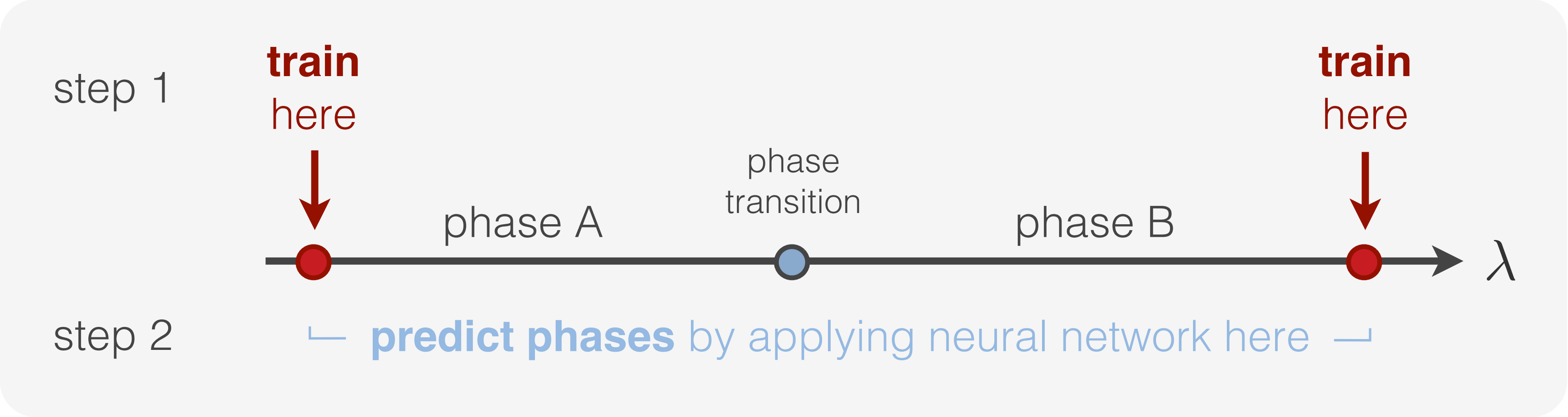
General setup

Consider some Hamiltonian, which as a function of some parameter λ exhibits a phase transition between two phases.

Supervised learning approach

1) **train** convolutional neural network on representative "images" deep within the two phases

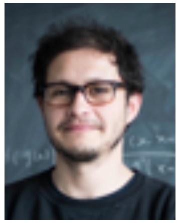
2) apply trained network to "images" sampled elsewhere to **predict phases + transition**



What are the **right images** to feed into the neural network?

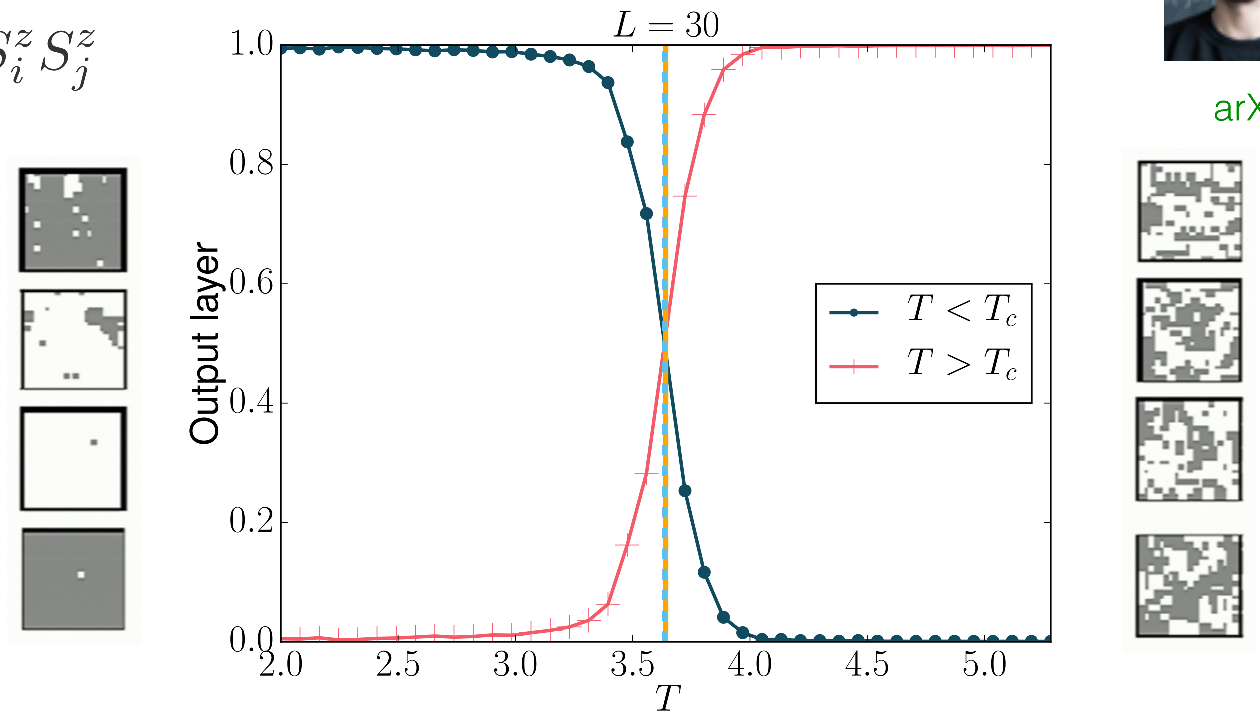
classical phases of matter

Finite-temperature transition in the Ising model

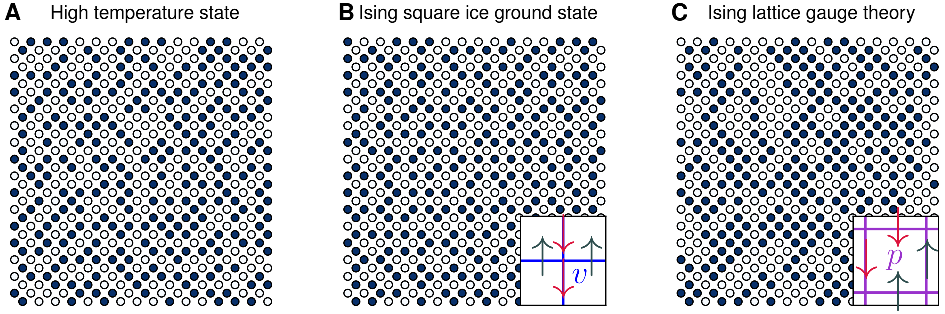


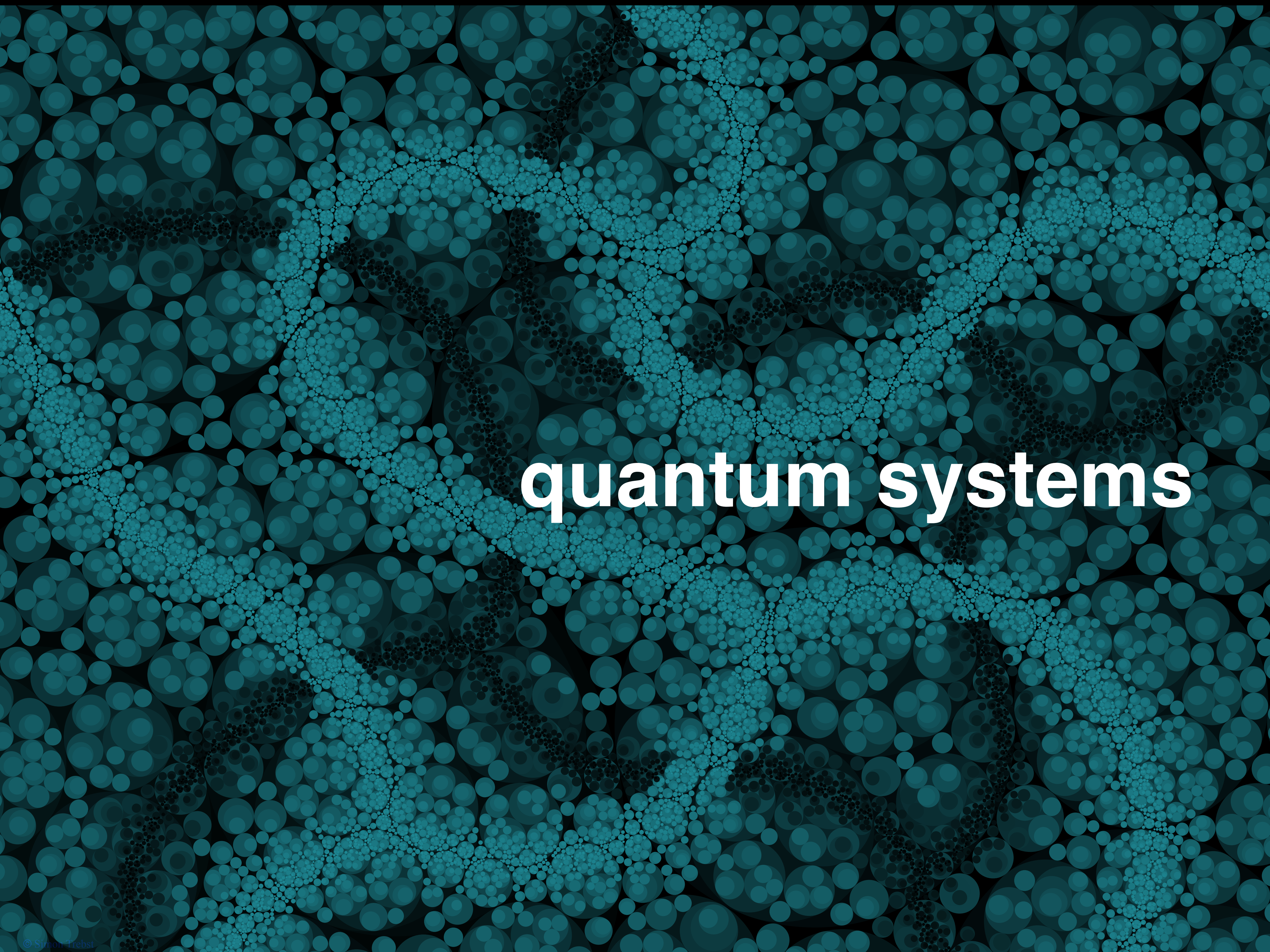

arXiv:1605.01735

$$H = -J \sum_{\langle i,j \rangle} S_i^z S_j^z$$



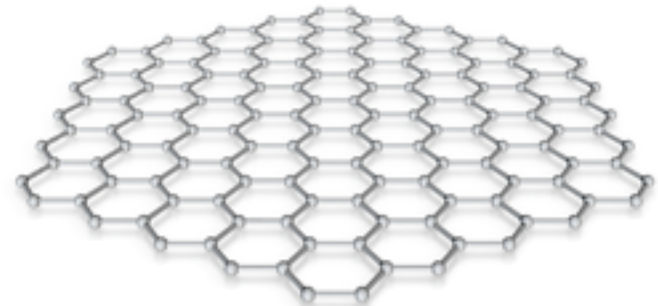
More interestingly, the convolutional neural network can also be trained to distinguish the high-T **paramagnet** from a **Coulomb phase** or **loop gas** ground state, i.e. phases without a local order parameter.




quantum systems
© Simon Trebst

Dirac fermions

Hubbard models on the honeycomb lattice



Spinful fermions

$$H = -t \sum_{\langle i,j \rangle, \sigma} c^\dagger_{i,\sigma} c_{j,\sigma} + U \sum_i n_{\uparrow,i} n_{\downarrow,i}$$

no sign problem

semi-metal — spin density wave → U/t

Gross-Neveu type
fermionic quantum phase transition

Spinless fermions

$$H = -t \sum_{\langle i,j \rangle} \left(c^\dagger_i c_j + c^\dagger_j c_i \right) + V \sum_{\langle i,j \rangle} n_i n_j$$

severe sign problem

semi-metal — charge density wave → V/t

Supervised learning approach

Supervised learning approach

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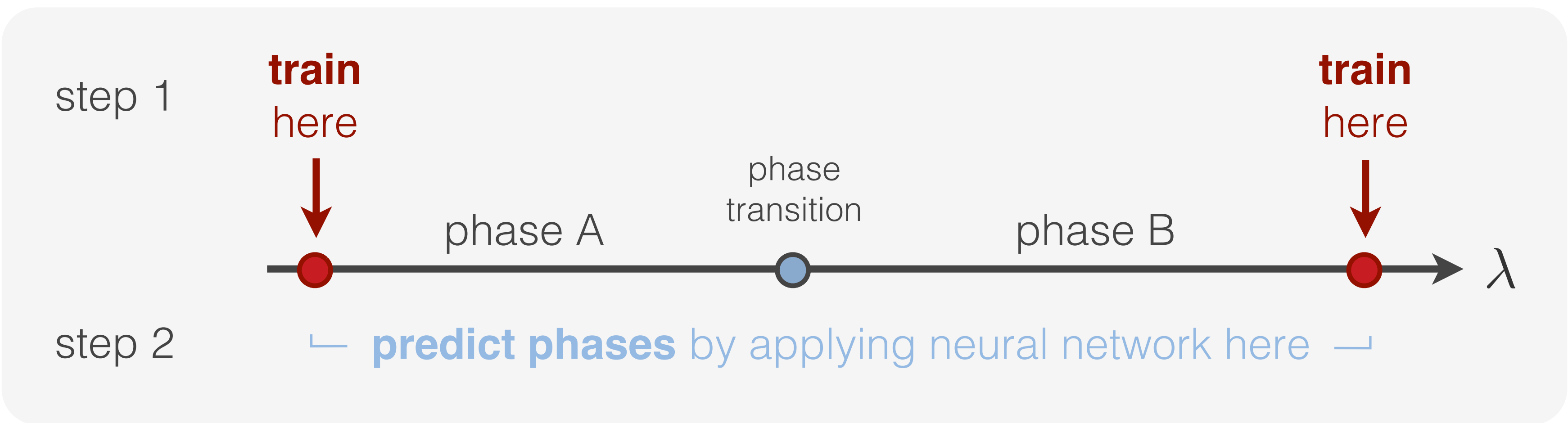


But what are the **right images** to represent a quantum state?

Monte Carlo for fermions

Determinantal (or auxiliary field) quantum Monte Carlo for unbiased studies of strongly interacting fermions

Path integral representation of partition sum

$$\mathrm{Tr}\, e^{-\beta\mathcal{H}} = \mathrm{Tr}\, \left(e^{-\Delta\tau\mathcal{H}}\right)^L \qquad \mathcal{H} = \mathcal{K} + \mathcal{V}$$

Decouple quartic interaction via **Hubbard-Stratonovich** transformation

Now integrate out **free fermions** moving in **background field**

$$\mathcal{Z} = \sum_s \det U(s)$$

sample **Hubbard-Stratonovich** field

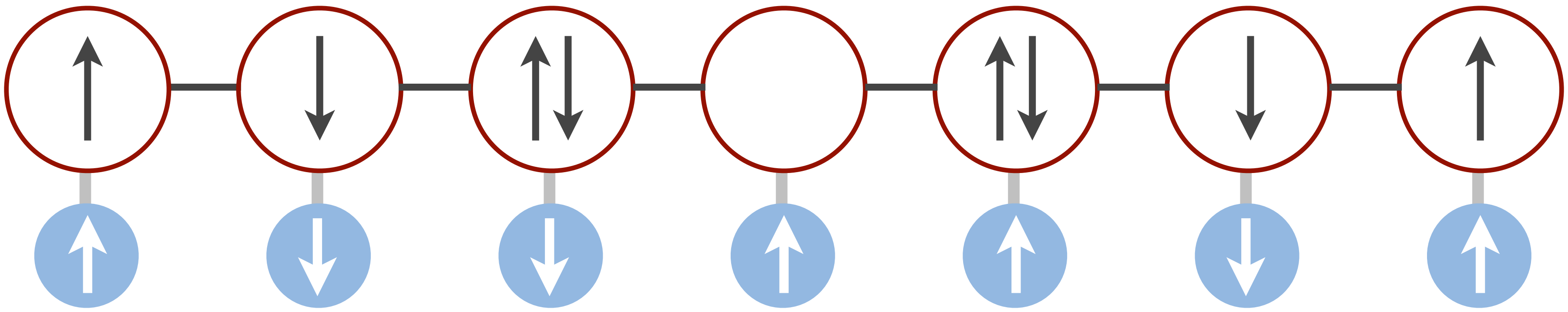
Hubbard-Stratonovich decoupling

Decoupling quartic interaction via Hubbard-Stratonovich transformation introduces an Ising-type **auxiliary field**

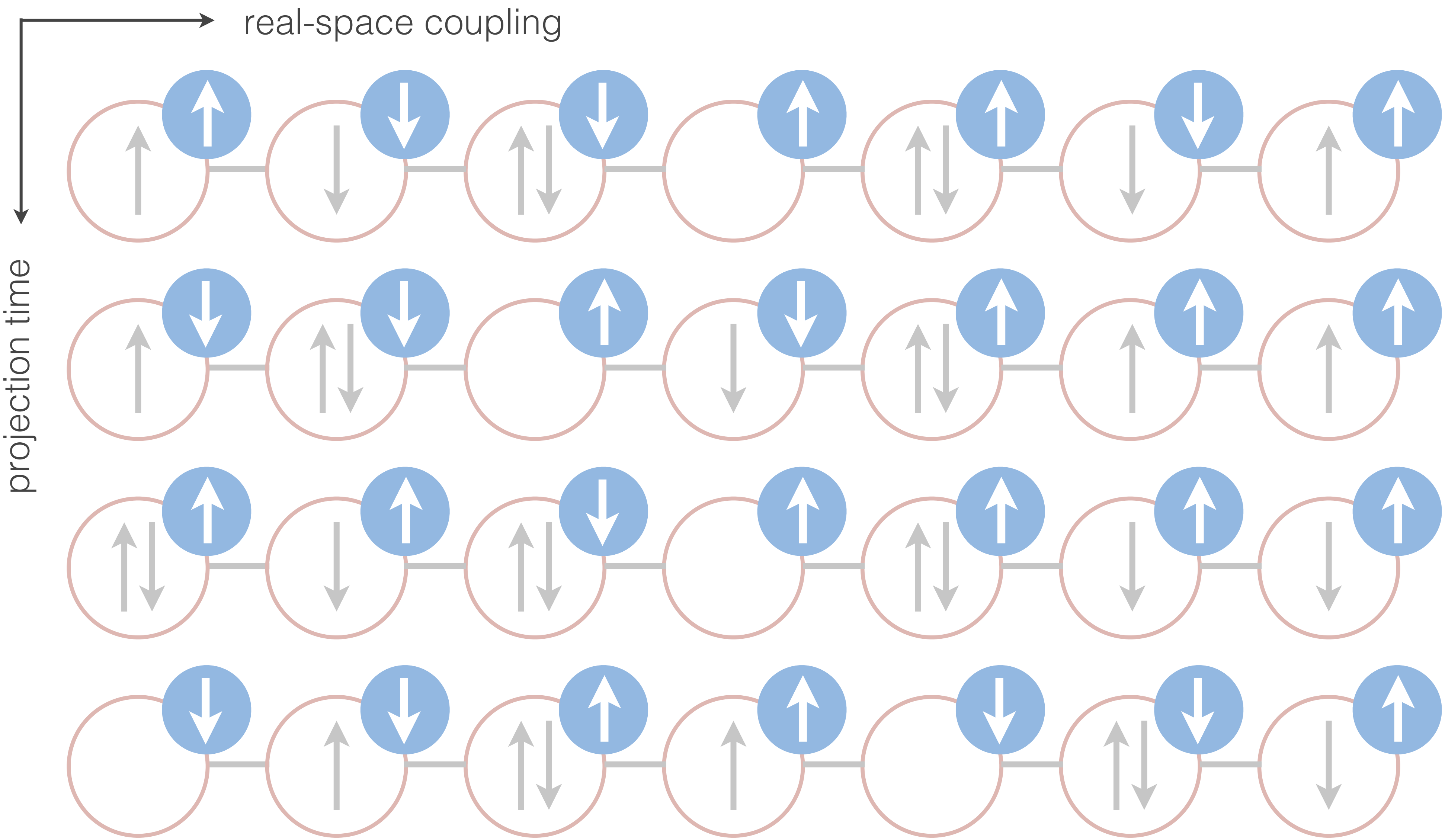
$$V_i = n_i^{\uparrow} n_i^{\downarrow} \quad \longrightarrow \quad V_i(s)$$

Hubbard-Stratonovich decoupling

$\longrightarrow$ real-space coupling

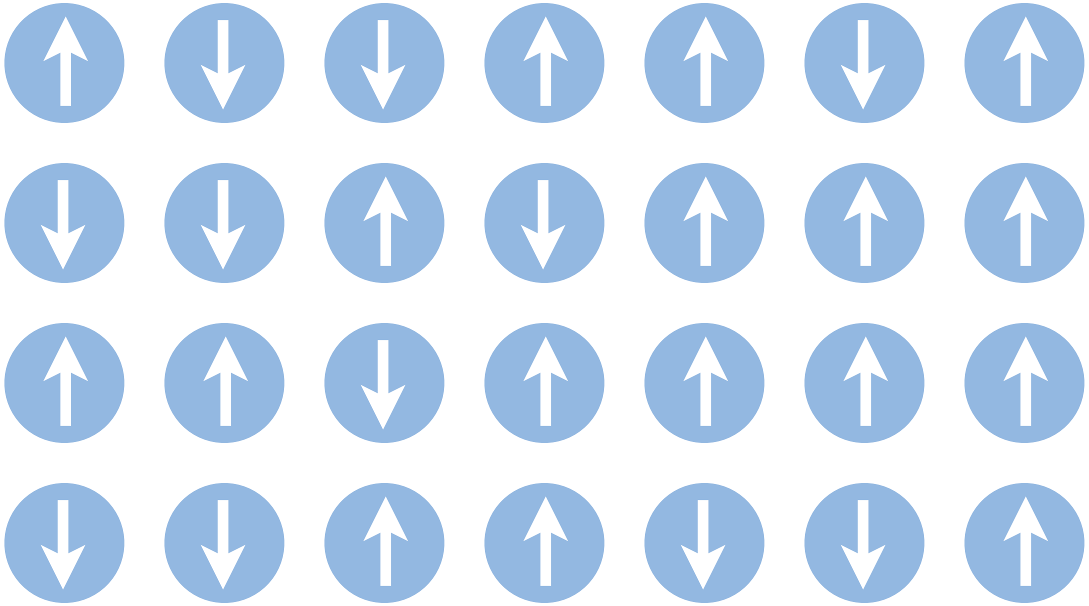


Hubbard-Stratonovich decoupling



Hubbard-Stratonovich decoupling

The auxiliary field has a natural interpretation has **“image”**.



Hubbard-Stratonovich decoupling

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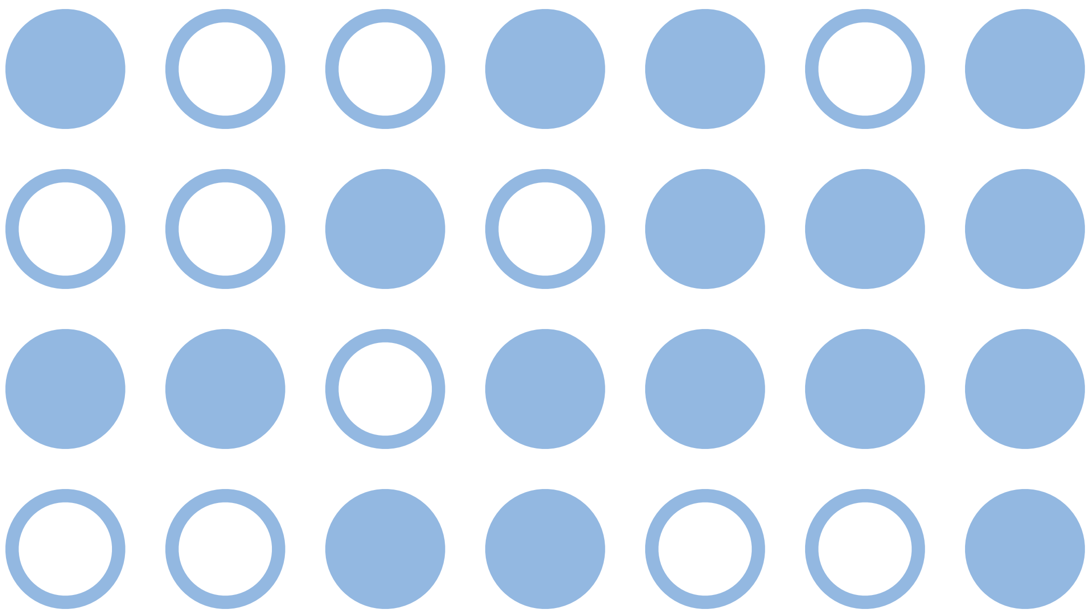


Supervised learning / auxiliary fields

Case 1 – **spinful fermions**

The choice of Hubbard-Stratonovich transformation influences image, i.e. when coupling to ...

magnetization

breaks SU(2)

semi-metal

SDW

charge

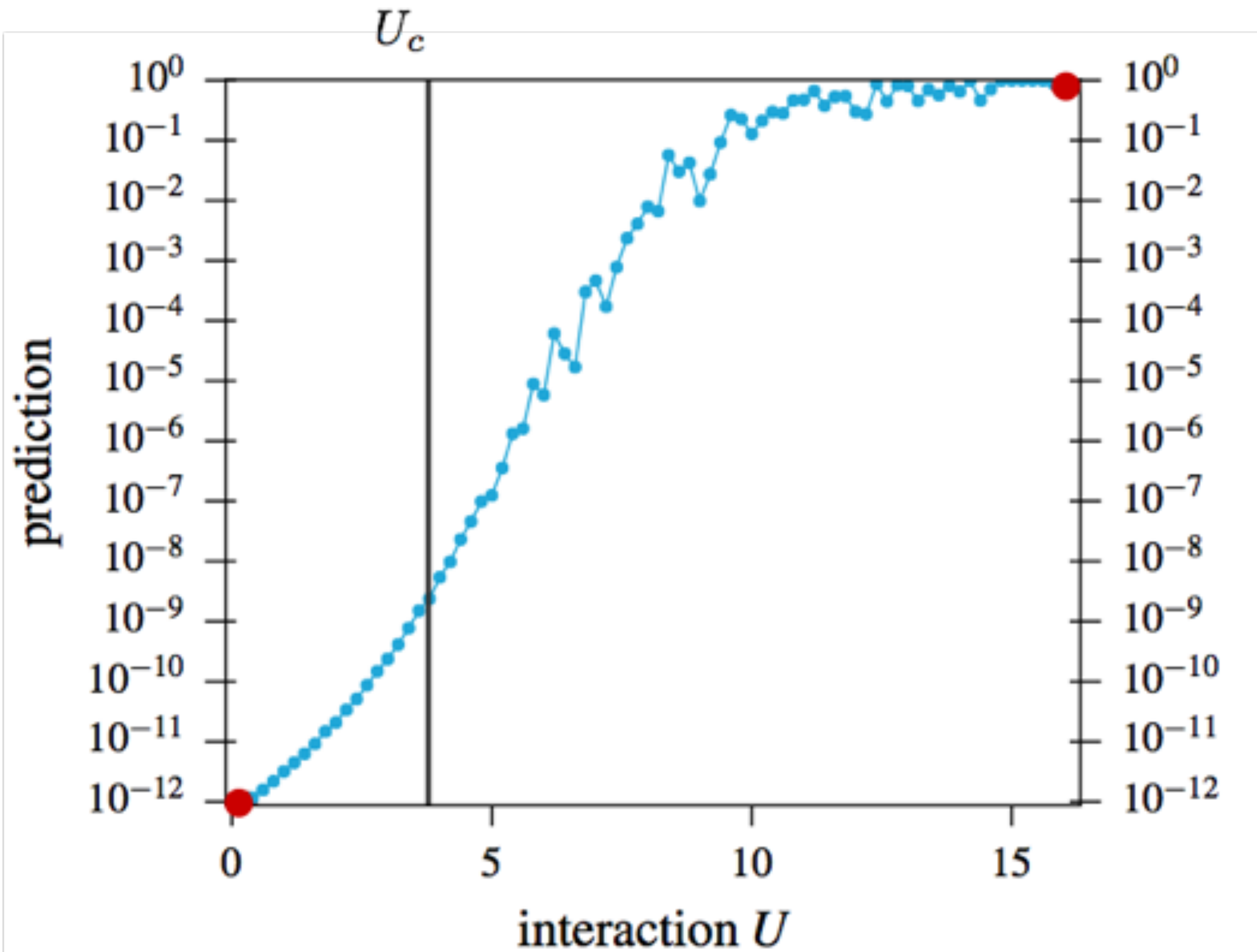
preserves SU(2)

semi-metal

SDW

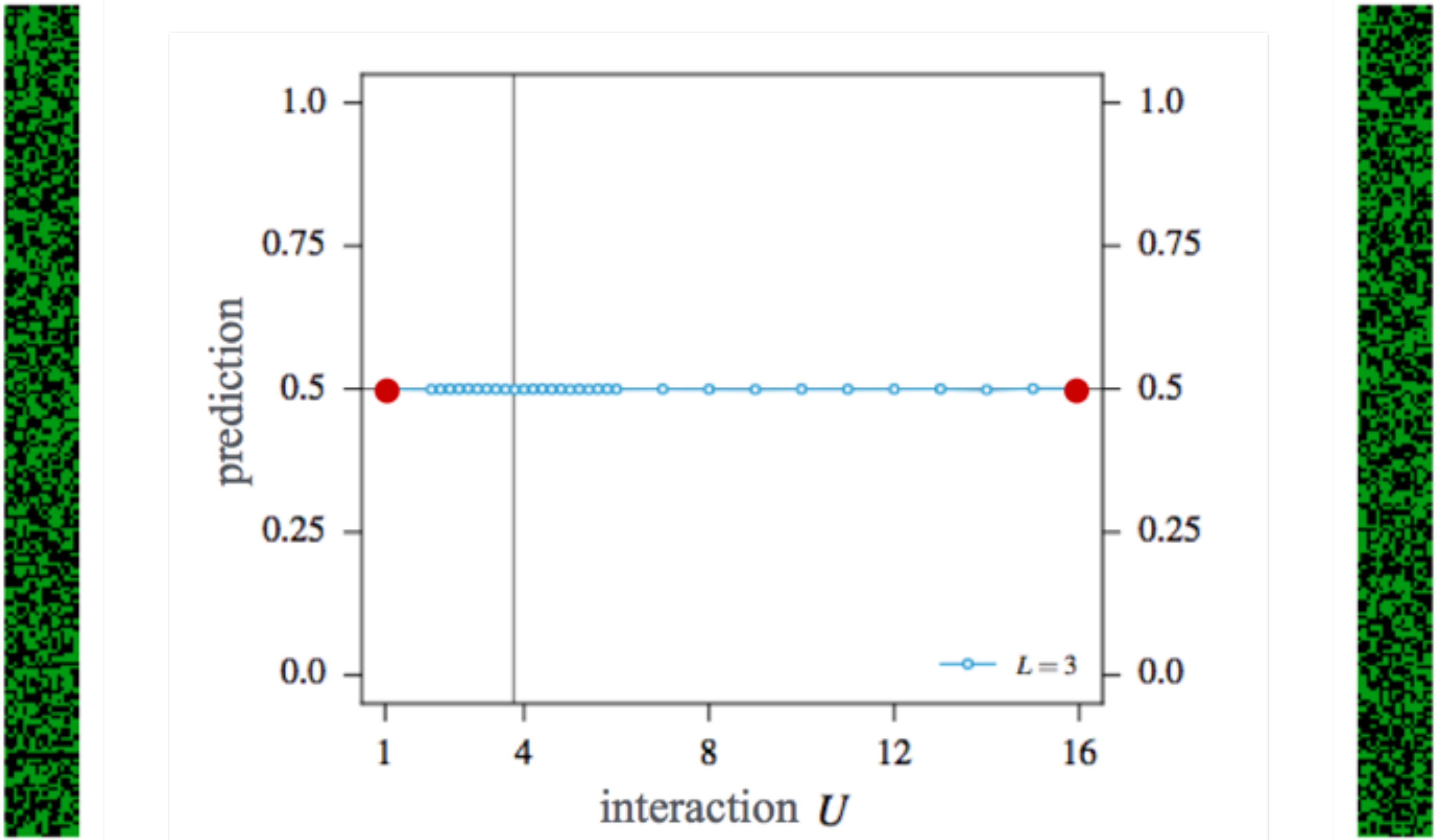
Supervised learning / auxiliary fields

coupling to **magnetization**



Supervised learning / auxiliary fields

coupling to **charge**



Supervised learning / auxiliary fields

Hubbard-Stratonovich fields might not be ideal objects/images for machine learning based discrimination of quantum phases.

general observations

- supervised learning does not work very well
- sensitive to choice of Hubbard-Stratonovich transformation

on a more technical level

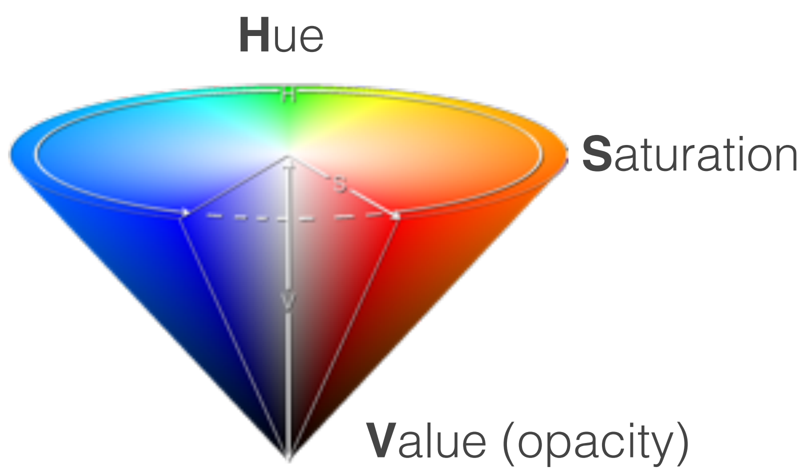
- finite temperatures require adjusting discretization step
- each coupling enlarges dataset

Alternative – **Green's functions** $G(i,j) = \langle c_i c_j^\dagger \rangle$

Supervised learning / Green's functions

Green's functions sampled as **complex valued matrices**.

Convert into color-coded image using HSV color scheme.



Our color mapping

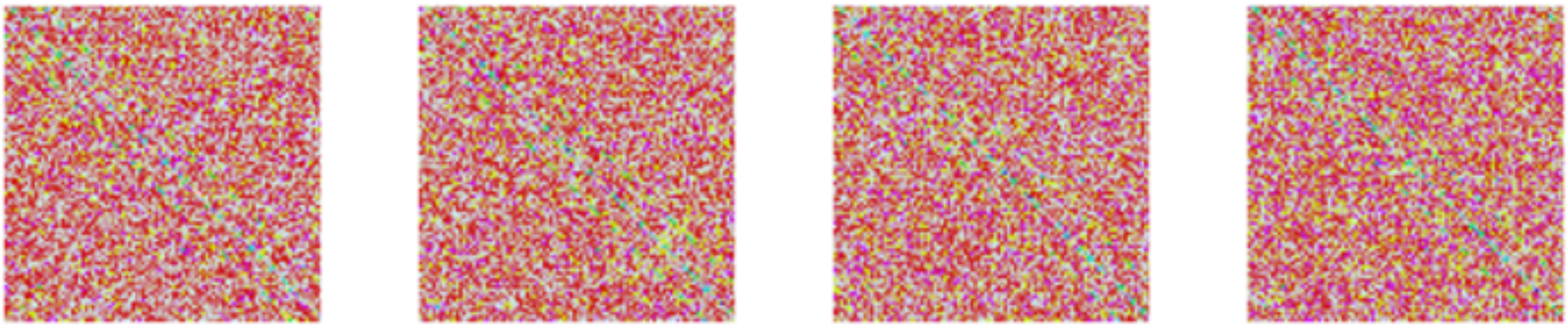
$$c = \underbrace{|c|}_{\text{hue}} \cdot e^{\overbrace{i\phi}^{\text{saturation}}}$$

Supervised learning / Green's functions

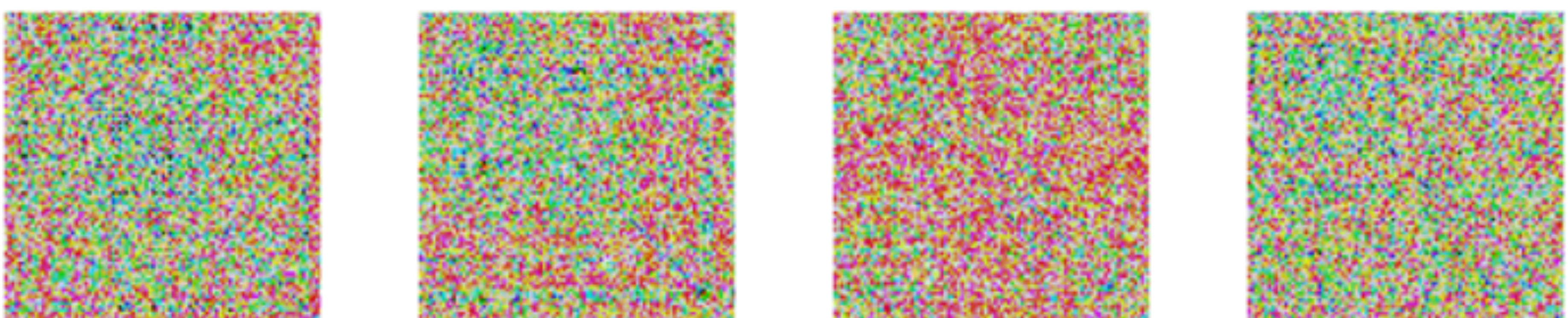
Green's functions for **spinful fermion** model

semi-metal

L = 2x9x9

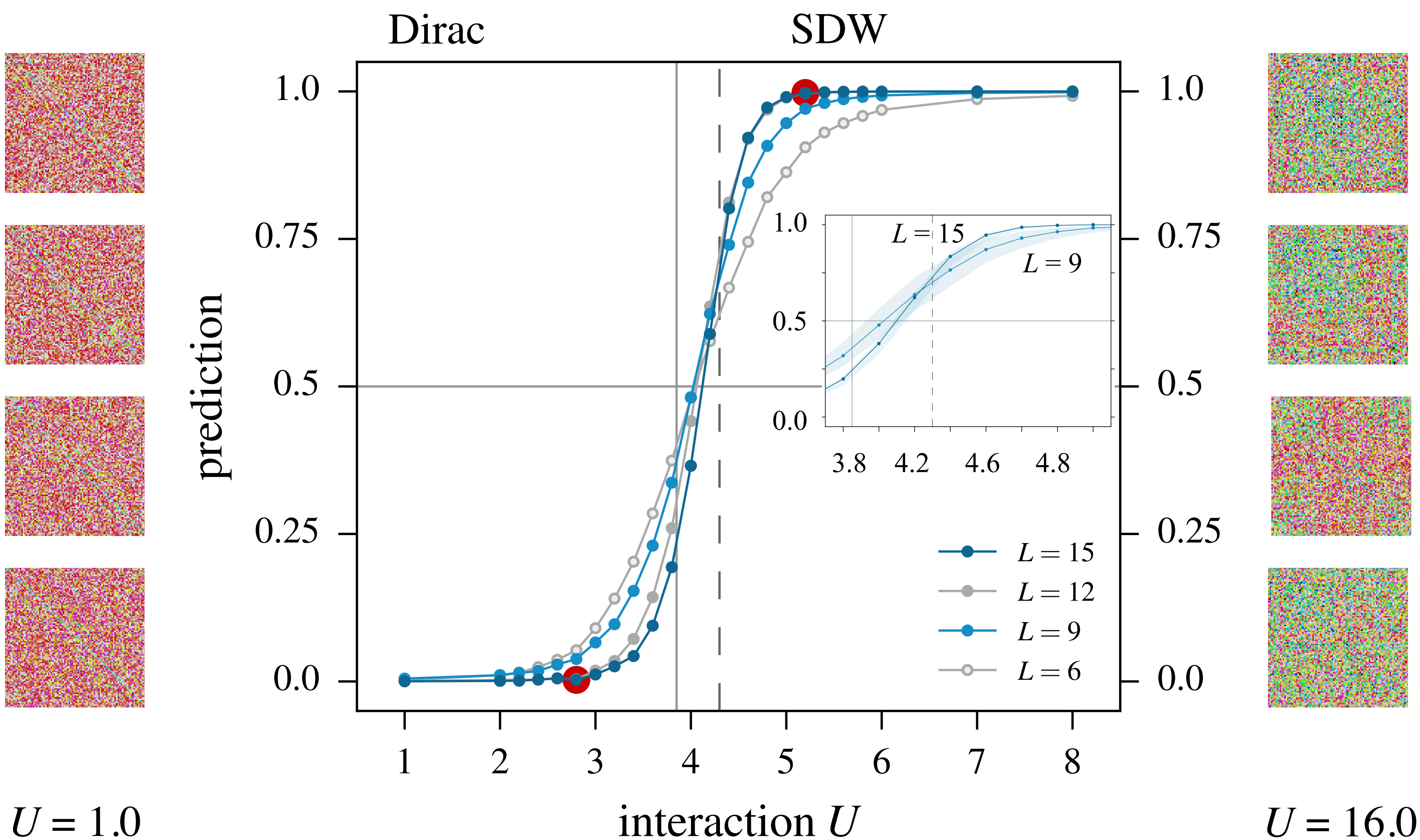


SDW



Spinful fermions

Green's functions are ideal objects/images for machine learning based discrimination of quantum phases.



Some intermediate conclusions

QMC + machine learning approach can be used to distinguish phases of interacting many-fermion systems.

Green's functions are ideal "images" for machine learning.

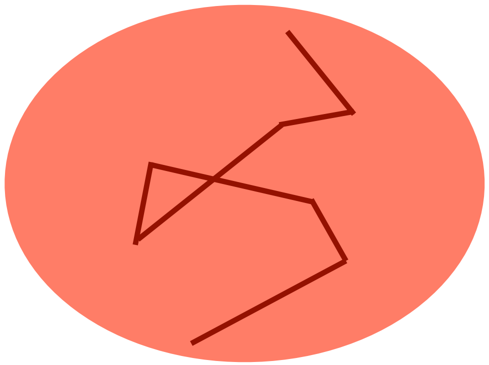
The ensemble of sampled Green's functions contains sufficient information to discriminate fermionic phases.

sign problem

Algorithmic power of Monte Carlo

Sample configurations in **high-dimensional** space

$$c_1 \rightarrow c_2 \rightarrow \ldots c_i \rightarrow c_{i+1} \rightarrow \ldots$$



Metropolis (1953): accept new configuration with probability

$$p_{\rm acc} = \min\left(1, \frac{w(c_j)}{w(c_i)}\right)$$

Simultaneously measured observables converge in **polynomial time**.

Tremendous impact across many different fields.
In hard condensed matter

- percolation
- phase transitions
- quantum magnetism
- ultracold bosons

Quantum Monte Carlo

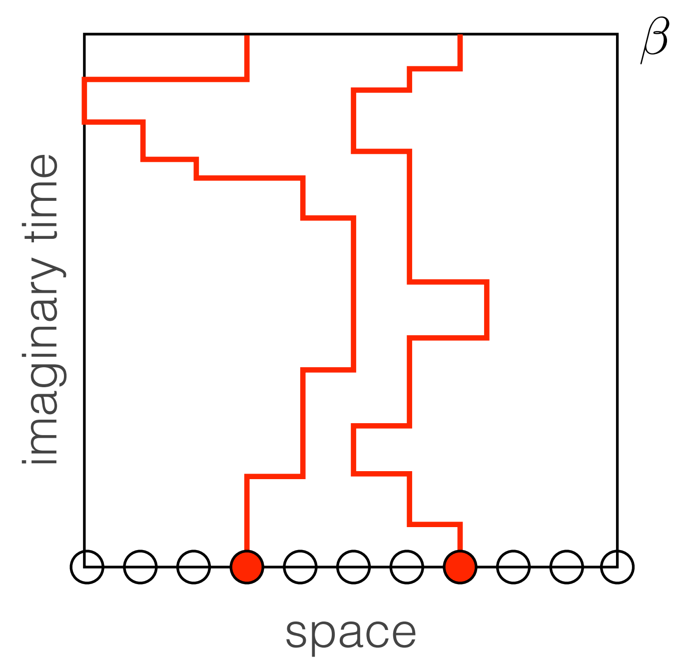
classical Monte Carlo $$\langle \mathcal{O} \rangle = \frac{\sum_{\mathcal{C}} \mathcal{O}(\mathcal{C})\, e^{-\beta E(\mathcal{C})}}{\sum_{\mathcal{C}} e^{-\beta E(\mathcal{C})}}$$

quantum Monte Carlo $$\langle \mathcal{O} \rangle = \frac{\mathrm{Tr}\, \mathcal{O} e^{-\beta \mathcal{H}}}{\mathrm{Tr}\, e^{-\beta \mathcal{H}}}$$

Map quantum to classical system $$Z = \mathrm{Tr}\, e^{-\beta \mathcal{H}} = \sum_{\mathcal{C}} p(\mathcal{C})$$

Map to “**world lines**” of the trajectories of the particles

Monte Carlo sampling of these world lines



The sign problem

Expectation value for observables

$$\langle \mathcal{O} \rangle = \frac{\sum \mathcal{O}(C) p(\mathcal{C})}{\sum p(\mathcal{C})}$$

when we **ignore the sign** of the configuration weights.

... but the **average sign decreases exponentially**

$$\langle \sigma \rangle_{\text{abs}} = \frac{\sum \sigma(C) |p(\mathcal{C})|}{\sum |p(\mathcal{C})|} = \frac{Z}{Z_{\text{abs}}} = \exp\left(-\beta N \Delta f\right)$$

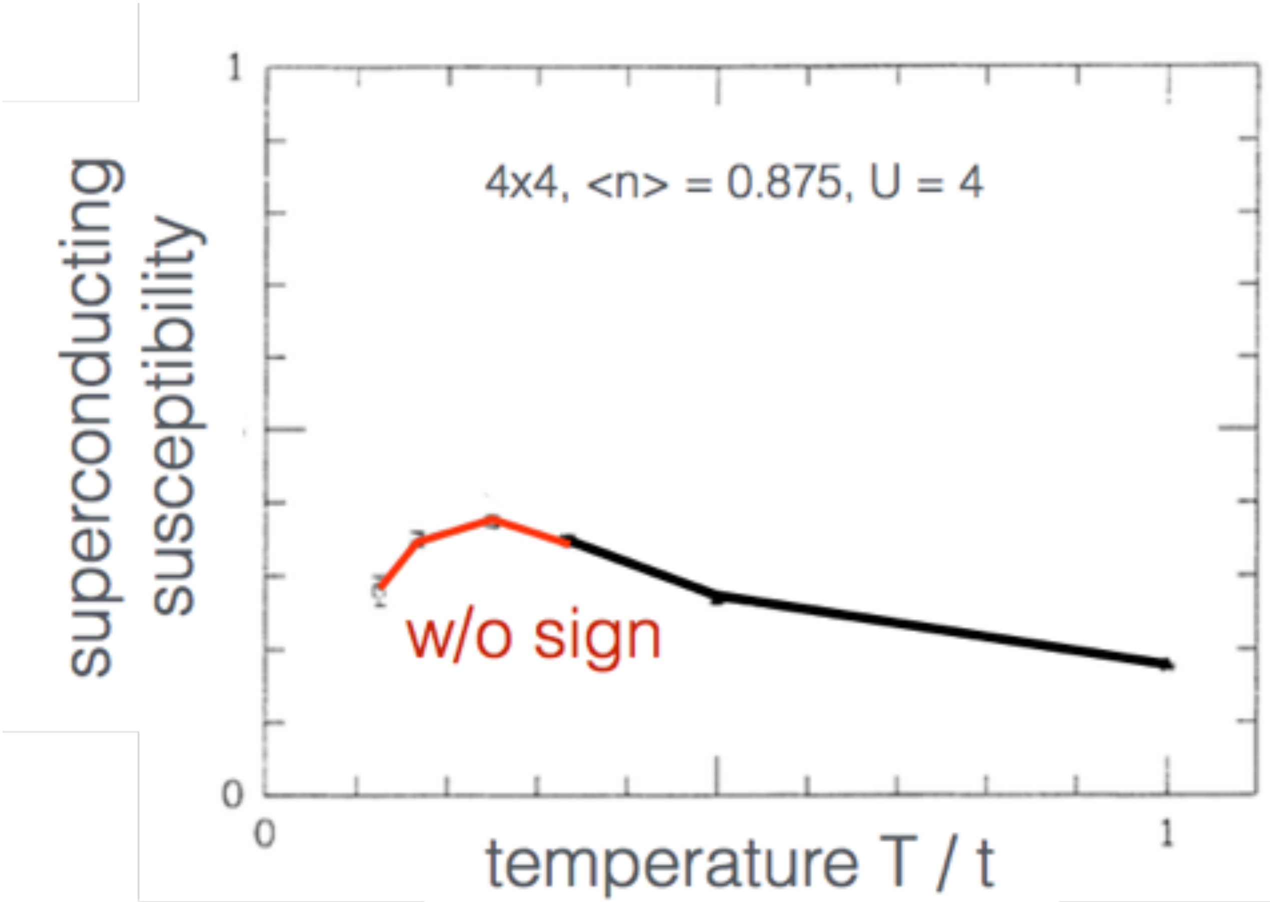
... resulting in an **exponentially slow convergence** of the statistical error

$$\frac{\Delta \sigma}{\langle \sigma \rangle} = \frac{\sqrt{\langle \sigma^2 \rangle - \langle \sigma \rangle^2}}{\sqrt{M} \langle \sigma \rangle} \approx \frac{e^{\beta N \Delta f}}{\sqrt{M}}$$

It’s a real problem ...

classic example: superconductivity in **doped Hubbard model**

Loh, Gubernatis, Scalettar, White, Scalapino and Sugar, PRB 1990



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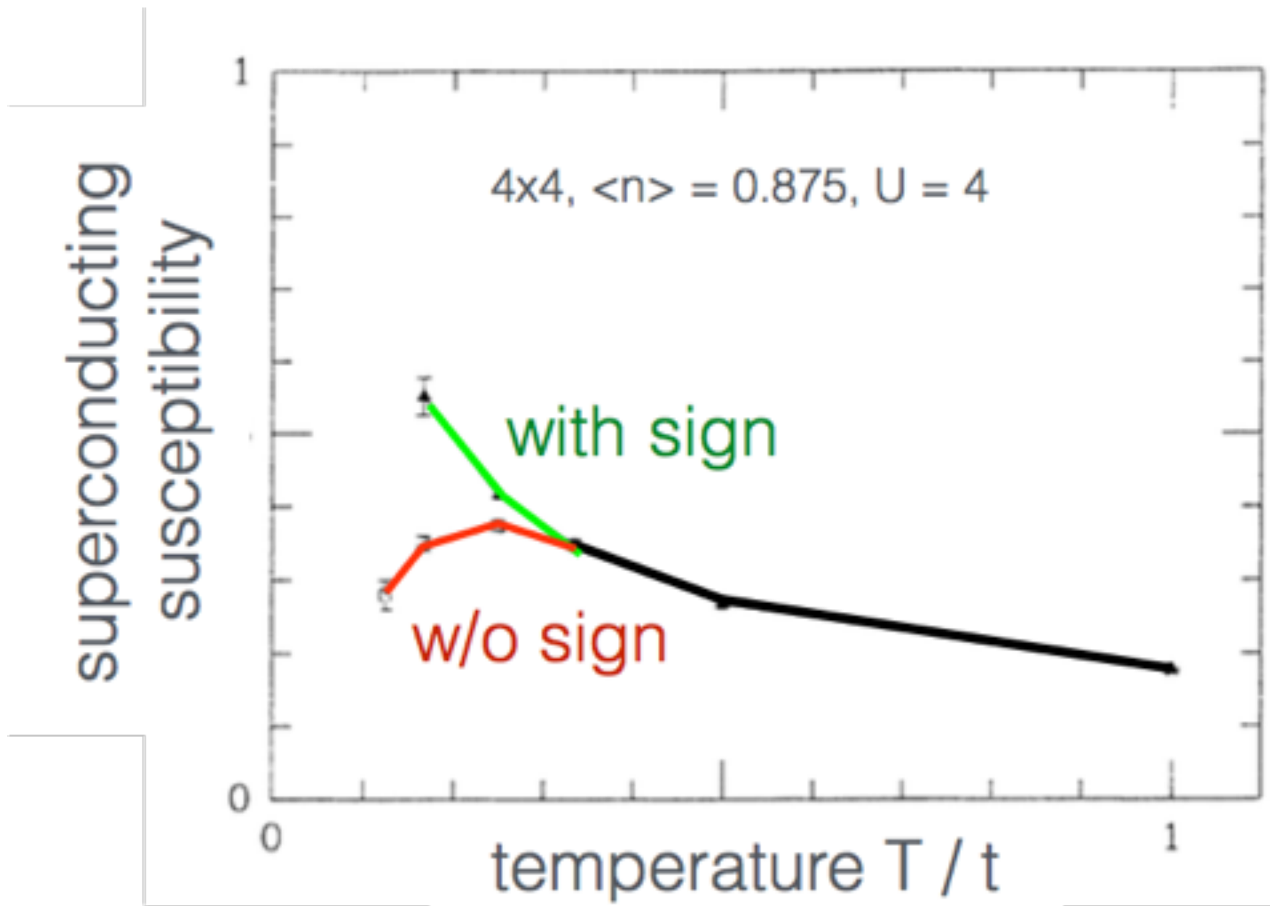


correlation functions come out wrong!

Is there a way out?

The sign problem is **basis dependent**

energy eigenbasis ⟷ simulation basis

exponentially hard

Successful **basis changes**

meron cluster — Wiese et al., PRL (1995)

fermion bag — Chandrasekharan, PRD (2009)

Majorana fermion basis — Yao et al., PRB (2015)

no general solution — Troyer and Wiese, PRL (2005) — the sign problem is **NP-hard**

Change of **perspective**

effective, sign-problem free actions — Berg, Metlitski, and Sachdev, Science (2012); Schattner, Gerlach, Trebst and Berg, PRL (2016)

entanglement entropies — Broecker and Trebst, PRB (2016)

sign problem
+ machine learning

Can we bypass the sign problem?

QMC sampling + **statistical analysis**

$$\langle \mathcal{O} \rangle = \frac{\sum \mathcal{O}(C) p(\mathcal{C})}{\sum p(\mathcal{C})} = \frac{\sum \mathcal{O}(C) \sigma(\mathcal{C}) |p(\mathcal{C})|}{\sum \sigma(\mathcal{C}) |p(\mathcal{C})|} = \frac{\langle \mathcal{O} \cdot \sigma \rangle_{\text{abs}}}{\langle \sigma \rangle_{\text{abs}}}$$

QMC sampling + **machine learning**

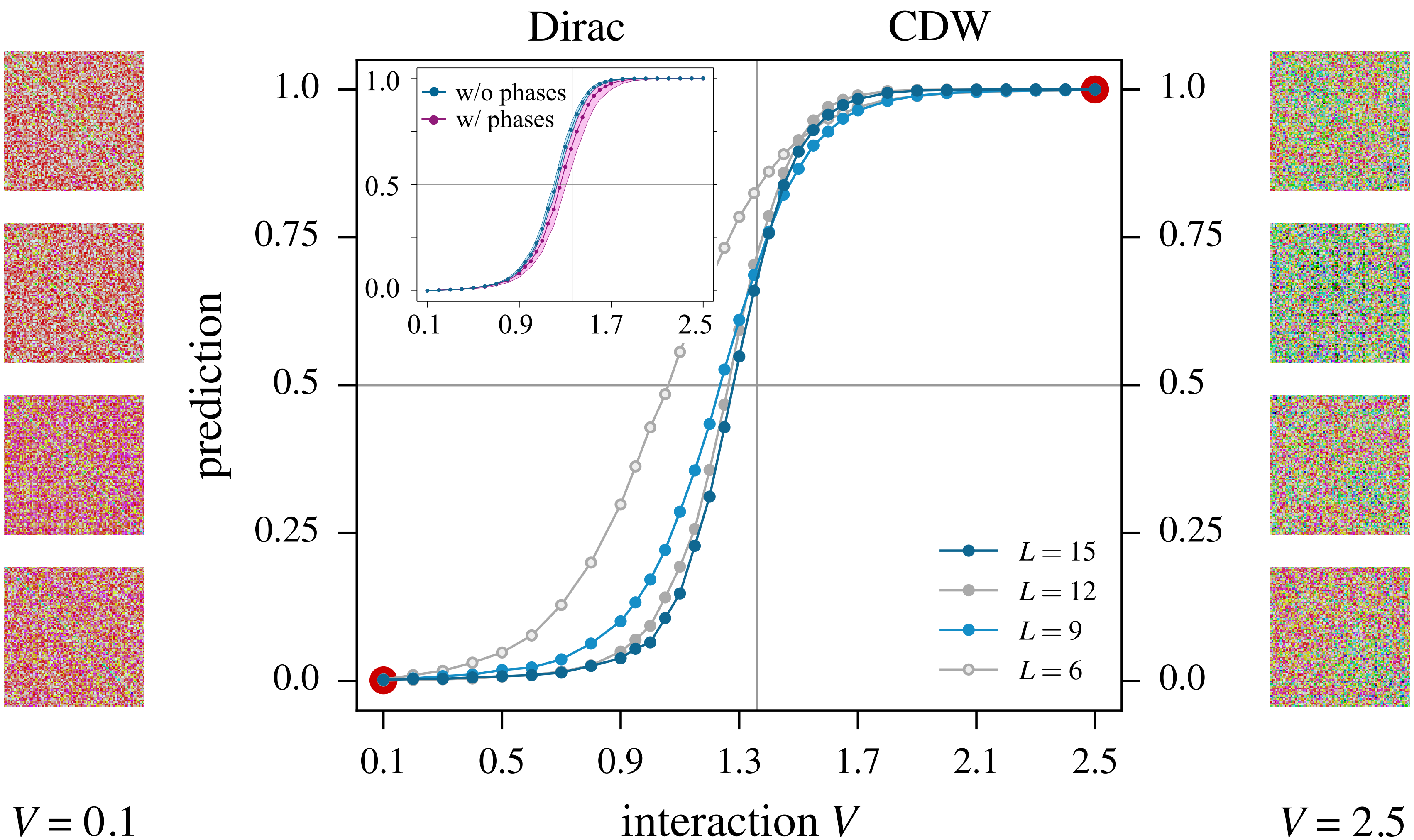
Assume there exists a "state function"

$$\langle \mathcal{F} \rangle_{\text{abs}} = \frac{\sum \mathcal{F}(C) |p(\mathcal{C})|}{\sum |p(\mathcal{C})}$$

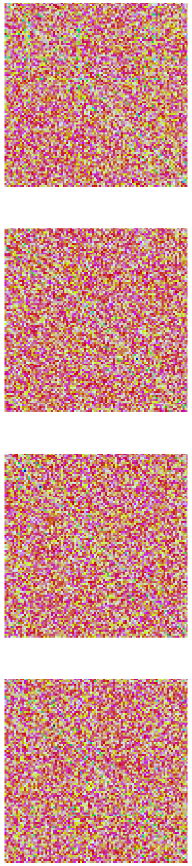
that is 0 deep in phase A and 1 deep in phase B.

Spinless fermions

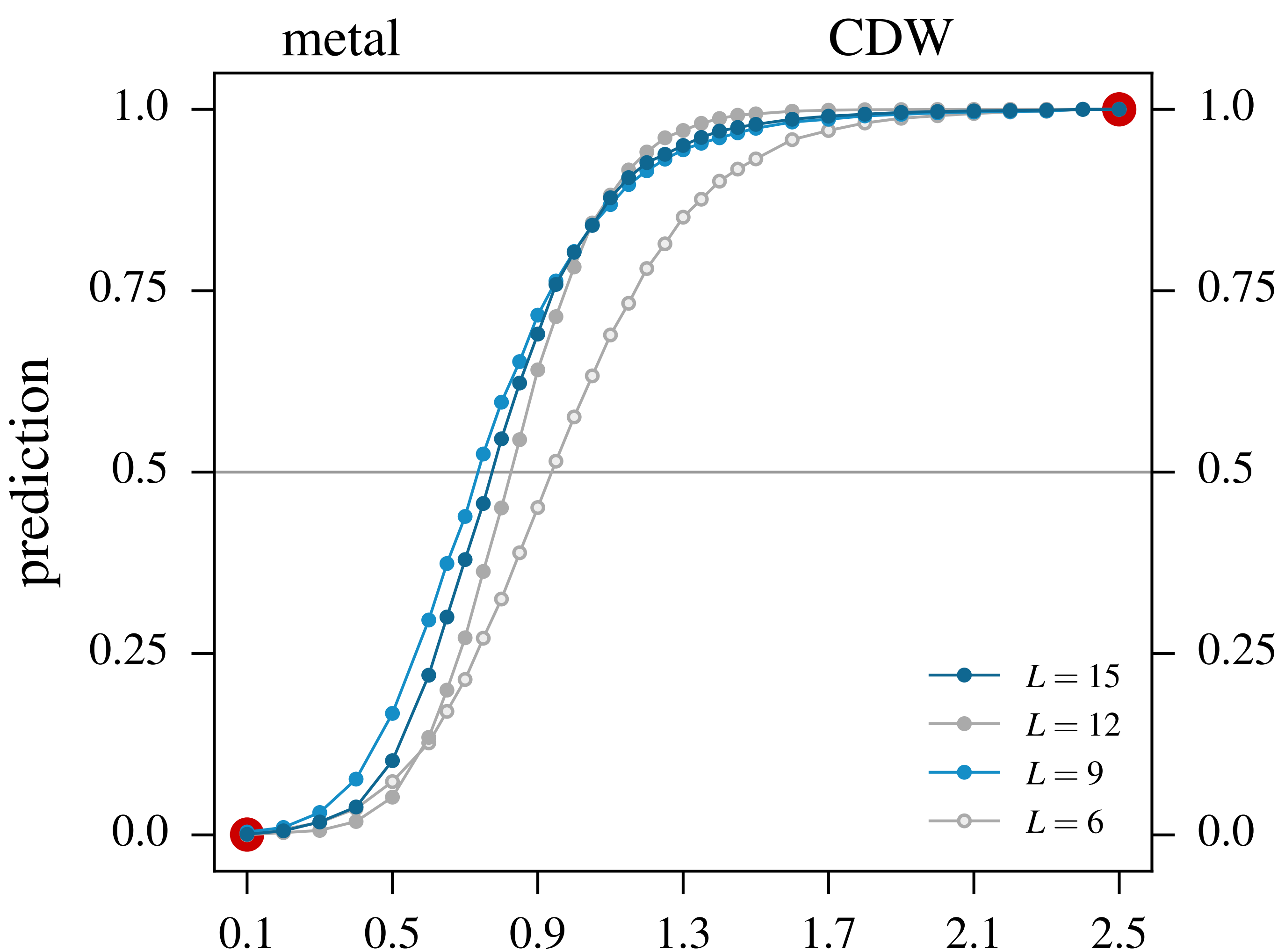
QMC + machine learning approach gives useful results even for systems with a severe sign problem.

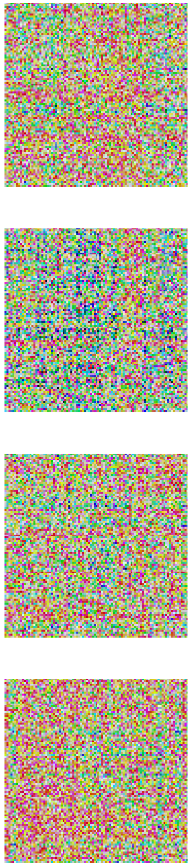


Spinless fermions @ 1/3 filling



$V = 0.1$

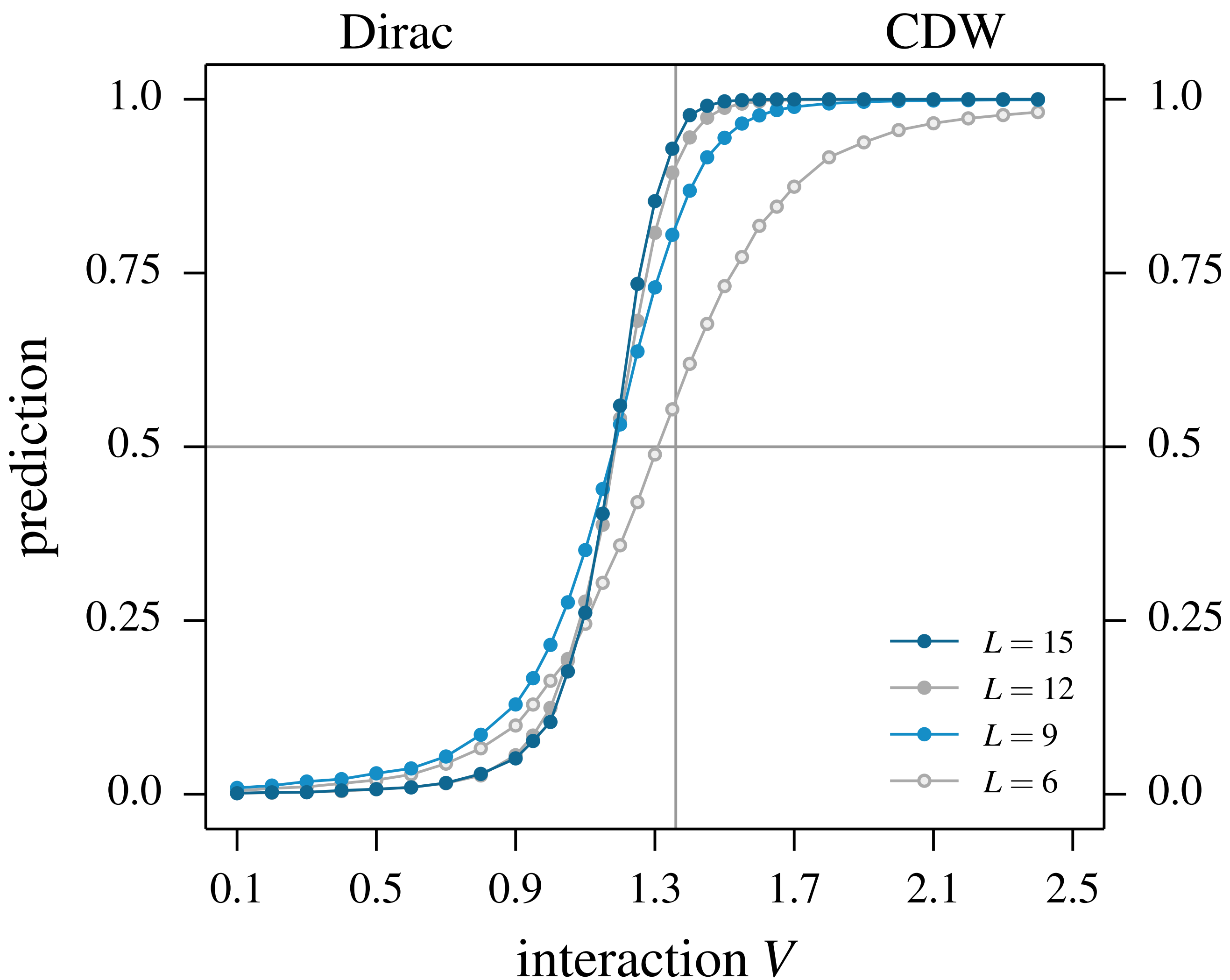




$V = 2.0$

Transfer learning

Training on spinful, sign-problem free fermion model, application to spinless, sign-problematic fermion model.



Summary

Summary

QMC + machine learning approach can be used to distinguish phases of interacting many-fermion systems even in the presence of a severe sign problem..

The ensemble of sampled Green's functions contains sufficient information to discriminate quantum phases. Accessible in most quantum Monte Carlo flavors.

The future: QMC + machine learning will become a robust tool for quickly and semi-automatically mapping out phase diagrams of quantum many-body systems.

arXiv:1608.07848