Machine Learning Phases of Matter

Daniel Kirchhoff

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Ising Model

Ising Model

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \sigma_i \sigma_j \text{ with } \sigma_k = \pm 1$$

$$m = \frac{1}{N} \sum \sigma_i \quad \text{magnetization}$$

Ising Model

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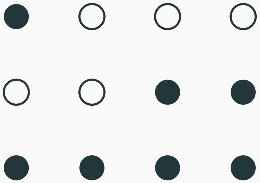
$$m = \frac{1}{N} \sum \sigma_i \quad \text{magnetization}$$

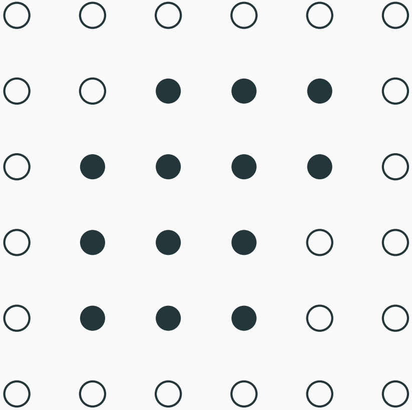
We are interested in the 2 dimensional case on a square lattice with periodic boundary conditions and $J > 0$:



$J > 0$ ferromagnetic $\leftrightarrow$ $J < 0$ antiferromagnetic

Phase Transition in the Ising Model

Look at free energy needed to create an island of $+1$ in a sea of -1 with boundary length L ("Peierls Argument"):



$$\Delta E \approx 2JL$$
$$\Delta S \approx \ln 3^L$$
$$\Rightarrow \Delta F \approx L\,(2J - T\ln 3) < 0$$

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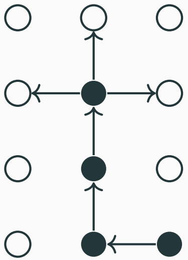

$$\begin{aligned} \Delta E &\approx 2JL \\ \Delta S &\approx \ln 3^L \\ \Rightarrow \Delta F &\approx L\,(2J - T\ln 3) < 0 \end{aligned}$$

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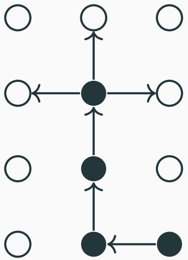


$$\Delta E \approx 2JL$$
$$\Delta S \approx \ln 3^L$$
$$\Rightarrow \Delta F \approx L\,(2J - T\ln 3) < 0$$
$$\Leftrightarrow T > T_C = \frac{2}{\ln 3} J \approx 1.8J$$

Qualitatively different behaviour at different temperatures

Phase Transition of the Ising Model

Phase Transition (Ehrenfest (1933)):

n-th order phase transition has a discontinuity at any n-th partial derivative of the free energy F.

Phase Transition of the Ising Model

Exact solution in the thermodynamic limit (Onsager (1944)):

$$-\beta f = \ln 2 + \frac{1}{8\pi} \int_0^{2\pi} \mathrm{d}\,\phi\,\mathrm{d}\,\theta \ln\left[\cosh^2 2\beta J - \sinh 2\beta J \left(\cos\phi + cos\theta\right)\right]$$

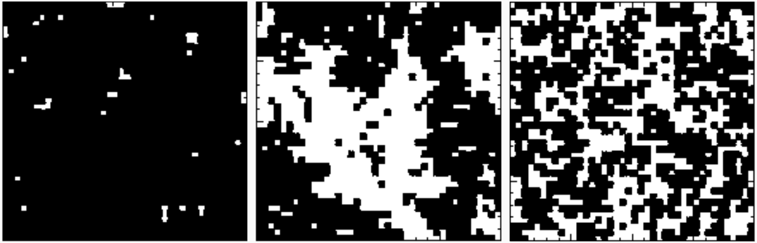
Heat capacity $c = -\beta^2 \partial_\beta^2 f$ has a log-divergence at the critical temperature

$$T_C = \frac{2}{\ln\left(1+\sqrt{2}\right)} J \approx 2.27J$$

Easy to determine from magnetization:

$$m = \begin{cases} \left[1 - \left(\sinh 2\beta J\right)^4\right]^{\frac{1}{8}}, & T < T_C \\ 0, & T > T_C \end{cases}$$

Phase Transition in the Ising Model



(a) $T = 1.8J$ **(b)** $T = 2.32J$ **(c)** $T = 5J$

Source: `http://farside.ph.utexas.edu/teaching/329/lectures/node110.html`

Machine Learning Phases of Matter (2017)

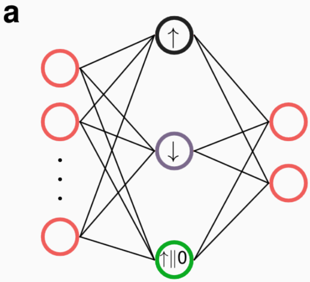
Machine Learning Phases of Matter (2017)

Published on 13 February 2017 by Carrasquilla and Melko

Try to find critical temperature of a ferromagnetic (square) Ising model with supervised machine learning

Machine Learning Phases of Matter (2017)

Analytical toy model with free parameter ϵ:



Input layer is $\sigma_i = \pm 1$

Machine Learning Phases of Matter (2017)

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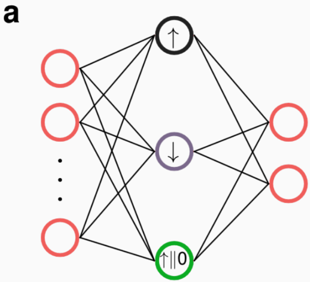


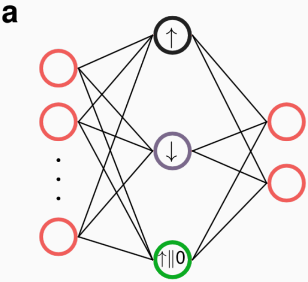
$$W = \frac{1}{N(1+\epsilon)} \begin{pmatrix} 1 & 1 & \cdots & 1 \\ -1 & -1 & \cdots & -1 \\ 1 & 1 & \cdots & 1 \end{pmatrix} \quad b = \frac{\epsilon}{(1+\epsilon)} \begin{pmatrix} -1 \\ -1 \\ 1 \end{pmatrix}$$

Input layer is $\sigma_i = \pm 1$

Hidden layer consists of perceptrons (Heaviside)

Machine Learning Phases of Matter (2017)

Analytical toy model with free parameter ϵ:



$$Wx + b = \frac{1}{(1+\epsilon)} \begin{pmatrix} m(x) - \epsilon \\ -m(x) - \epsilon \\ m(x) + \epsilon \end{pmatrix}$$

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Machine Learning Phases of Matter (2017)

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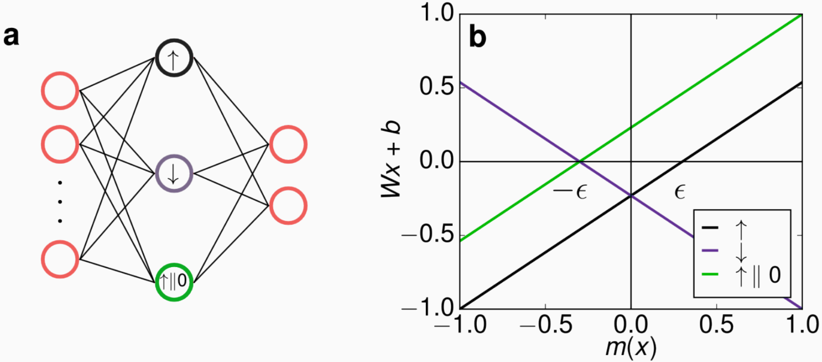

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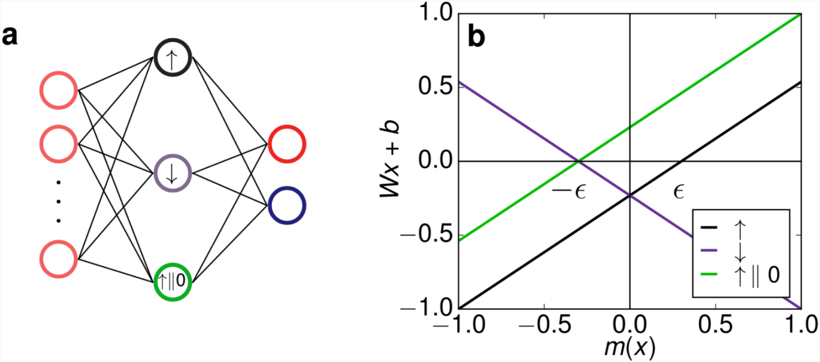


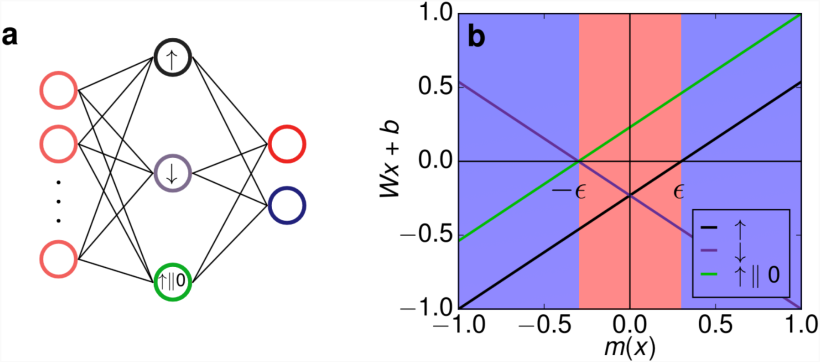
Input layer is $\sigma_i = \pm 1$

Hidden layer consists of perceptrons (Heaviside)

Output layer consists of sigmoids

Machine Learning Phases of Matter (2017)

Analytical toy model with free parameter ϵ:



Input layer is $\sigma_i = \pm 1$

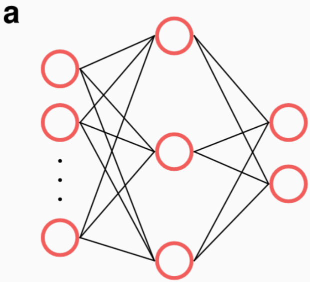
Hidden layer consists of perceptrons (Heaviside)

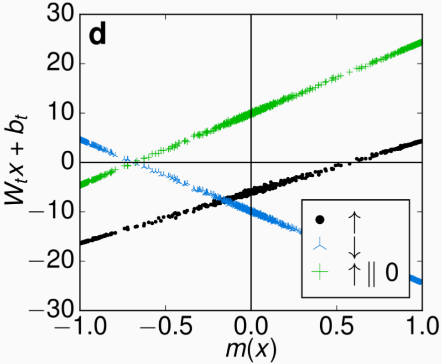
Output layer consists of sigmoids

Machine Learning Phases of Matter (2017)

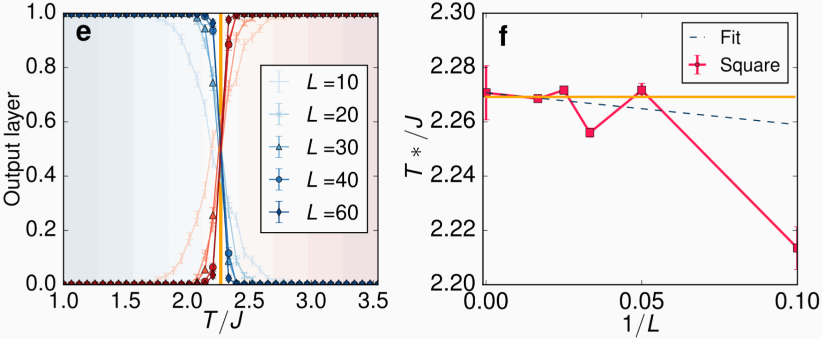
Learning toy model:

Train same network with arbitrary weights far from T_C



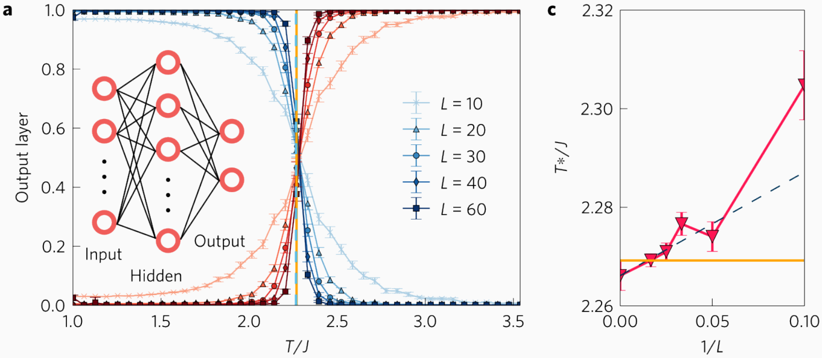


Machine Learning Phases of Matter (2017)



Machine Learning Phases of Matter (2017)

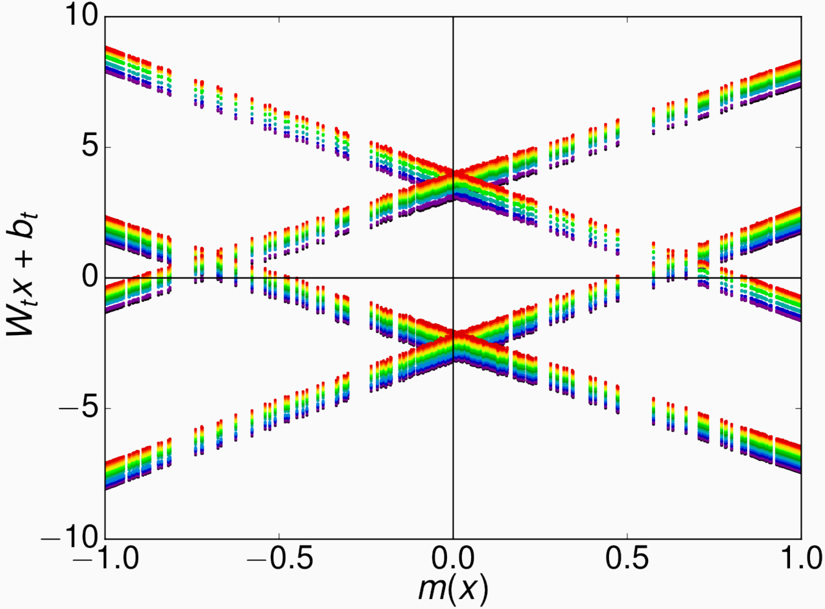
Fully connected network with single hidden layer consisting of 100 sigmoid neurons



$\rightarrow T_C = (2.266 \pm 0.002)J$

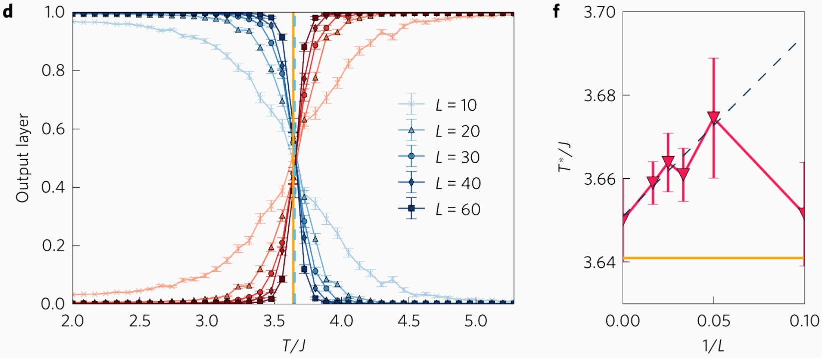
Literature: $T_C = 2.2692J$

Machine Learning Phases of Matter (2017)



Machine Learning Phases of Matter (2017)

Use same network without retraining on a triangular Ising model



$\rightarrow T_C = (3.65 \pm 0.01)J$

Literature: $T_C = 3.641J$

Fermion Sign Problem

Quantum Monte Carlo

Heisenberg model for spin 1/2-particles:

$$\mathcal{H} = -J \sum_{\langle i,j \rangle} \vec{S}_i \vec{S}_j$$

Two particle Hamiltonian $H = -J\vec{S}_1\vec{S}_2$ has eigenbasis

$$|\uparrow\uparrow\rangle\,,\ |\downarrow\downarrow\rangle\,,\ \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle - |\downarrow\uparrow\rangle\right),\ \frac{1}{\sqrt{2}}\left(|\uparrow\downarrow\rangle + |\downarrow\uparrow\rangle\right)$$

Entangled eigenstates!

Quantum Monte Carlo

1d-Chain with periodic boundary conditions:

$$\mathcal{H} = -J\sum_{i} \vec{S}_i \vec{S}_{i+1} = \sum_{i} H_i = \sum_{\text{even } i} H_i + \sum_{\text{odd } i} H_i = \mathcal{H}_e + \mathcal{H}_o$$

Quantum Monte Carlo

1d-Chain with periodic boundary conditions:

$$\mathcal{H} = -J \sum_i \vec{S}_i \vec{S}_{i+1} = \sum_i H_i = \sum_{\text{even } i} H_i + \sum_{\text{odd } i} H_i = \mathcal{H}_e + \mathcal{H}_o$$

Try to get the partition function numerically:

$$Z = \operatorname{Tr} e^{-\beta \mathcal{H}} = \operatorname{Tr} \left(e^{-\Delta\tau \mathcal{H}} \right)^m = \operatorname{Tr} \left[\left(e^{-\Delta\tau \mathcal{H}_e} e^{-\Delta\tau \mathcal{H}_o} \right)^m \right] + \mathcal{O}(\Delta\tau^2)$$

$$= \sum_{\substack{|\sigma_1\rangle, \dots, |\sigma_{2m}\rangle \\ \{|\sigma_i\rangle\} \text{ Basis } \forall i}} \langle \sigma_1 | e^{-\Delta\tau \mathcal{H}_e} | \sigma_{2m} \rangle \langle \sigma_{2m} | e^{-\Delta\tau \mathcal{H}_o} | \sigma_{2m-1} \rangle \dots \langle \sigma_2 | e^{-\Delta\tau \mathcal{H}_o} | \sigma_1 \rangle$$

$$+ \mathcal{O}(\Delta\tau^2) = \sum_\omega p(\omega)$$

$\rightarrow$ Is $p(\omega) \geq 0$?

Sign Problem

$$Z = \sum_{\substack{|\sigma_1\rangle,\ldots,|\sigma_{2m}\rangle \\ \{|\sigma_i\rangle\}\text{ Basis }\forall i}} \langle\sigma_1| e^{-\Delta\tau\mathcal{H}_e} |\sigma_{2m}\rangle \langle\sigma_{2m}| e^{-\Delta\tau\mathcal{H}_o} |\sigma_{2m-1}\rangle \ldots \langle\sigma_2| e^{-\Delta\tau\mathcal{H}_o} |\sigma_1\rangle$$

Look at "spin flip" term:

$$\langle\uparrow\downarrow| e^{-\Delta\tau\vec{S}_1\vec{S}_2} |\downarrow\uparrow\rangle = e^{-\Delta\tau J/4}\sinh\frac{\Delta\tau J}{4} < 0 \text{ if } J < 0$$

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Two particle system (m=1 for simplicity):

$$Z = \dots + \langle\uparrow\downarrow| e^{-\Delta\tau\vec{S}_1\vec{S}_2} |\downarrow\uparrow\rangle \langle\downarrow\uparrow| e^{-\Delta\tau\vec{S}_2\vec{S}_1} |\uparrow\downarrow\rangle + \dots$$

$\rightarrow p \geq 0$

Sign Problem

Three particles: $\mathcal{H} = -J\left(\vec{S}_1\vec{S}_2 + \vec{S}_2\vec{S}_3 + \vec{S}_3\vec{S}_1\right)$:

$$Z = \sum \langle\sigma_1| \, e^{-\Delta\tau\vec{S}_1\vec{S}_2} \, |\sigma_3\rangle \, \langle\sigma_3| \, e^{-\Delta\tau\vec{S}_2\vec{S}_3} \, |\sigma_2\rangle \, \langle\sigma_2| \, e^{-\Delta\tau\vec{S}_3\vec{S}_1} \, |\sigma_1\rangle$$

One can create a configuration similar to before which generates negative probabilites:

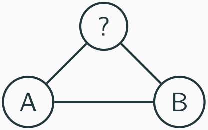
$$|\downarrow\uparrow\uparrow\rangle, |\uparrow\downarrow\uparrow\rangle, |\uparrow\uparrow\downarrow\rangle$$

$\rightarrow$ "frustrated antiferromagnet"

Sign Problem

Ingredients for trouble:

- fermions
- negative couplings
- non bipartite lattice



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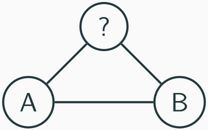

theoretical fix: always work in hamiltonian eigenbasis!

Sign Problem

Ingredients for trouble:

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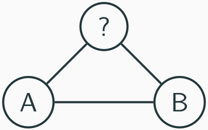
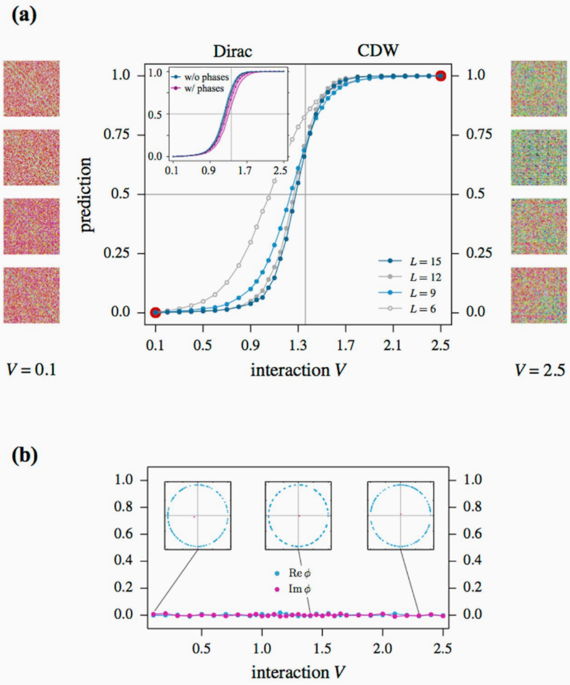


theoretical fix: always work in hamiltonian eigenbasis!

but diagonalization scales exponentially $\rightarrow$ NP-complete problems

Machine learning quantum phases of matter beyond the fermion sign problem (2017)

Also treat sign-problematic models with machine learning (Hubbard model)



(a)
Dirac
CDW
prediction
interaction V
V = 0.1
V = 2.5
w/o phases
w/ phases
L = 15
L = 12
L = 9
L = 6
(b)
Re ϕ
Im ϕ
interaction V

Learning phase transitions by confusion (2017)

Learning phase transitions by confusion (2017)

Published on 13 February 2017 by van Nieuwenburg, Liu and Huber

Try to find an unknown critical point of a system with pseudo-supervised machine learning

Learning phase transitions by confusion (2017)

Suppose a model which depends on a parameter T and there exists some critical value T_C in the interval (T_a, T_b) which yields differently structured output above and below T_C.

Learning phase transitions by confusion (2017)

General Strategy to find the critical point T_C:

- Propose some critical point T_C'
- Generate configurations far from T_C' and train the network with it
- Generate more configurations and record the performance of the trained network

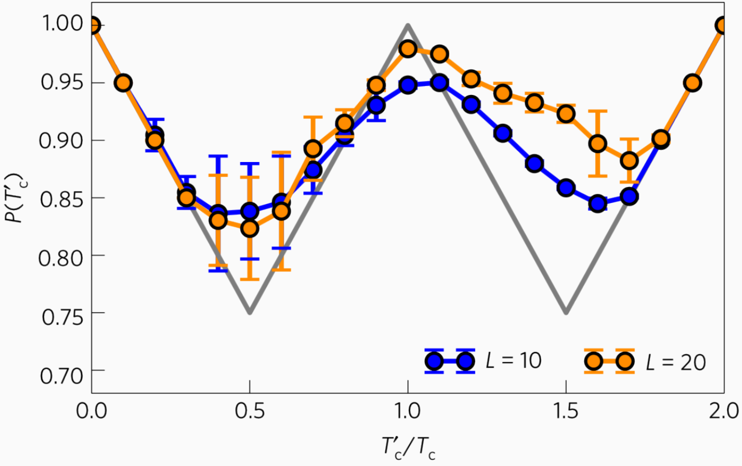
Do the above for all $T_C' \in (T_a, T_b)$.

Learning phase transitions by confusion (2017)

The performance $P(T_C')$ should be maximal for $T_C' = T_a, T_C, T_b$ as it is easier to distinguish between differently structured configurations which should be separated by T_C:

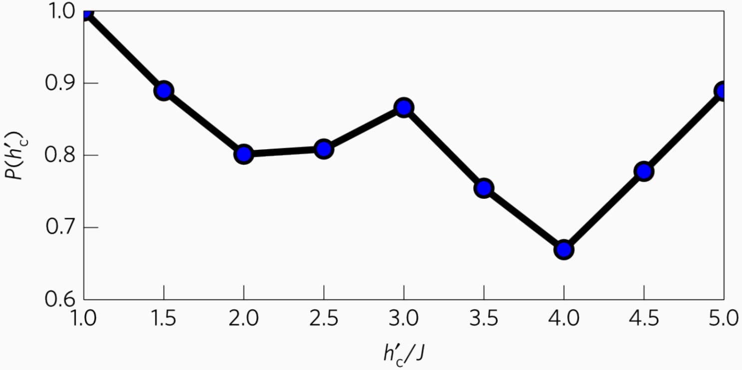
$$P(T_C') \propto 1 - \frac{\min\{|T_C' - T_a|, |T_C' - T_C|, |T_C' - T_b|\}}{T_b - T_a}$$

Learning phase transitions by confusion (2017)



Ising model with T_C being the on at the thermodynamic limit

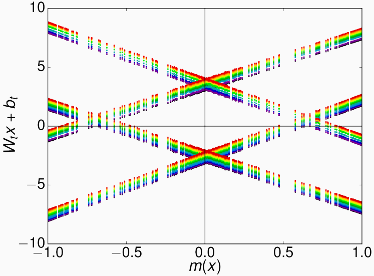
Learning phase transitions by confusion (2017)



Heisenberg model with external field; $T_C = 3J$ being the literature value

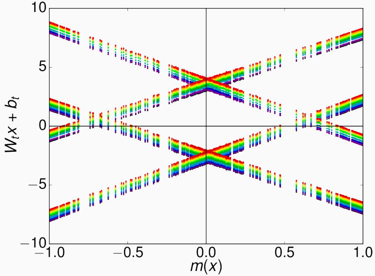
Summary

Neural networks can be trained to distinguish different phases



Summary

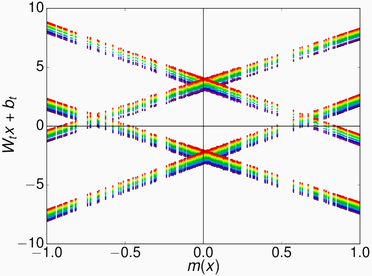
Neural networks can be trained to distinguish different phases but choosing the correct approach and network may be difficult.

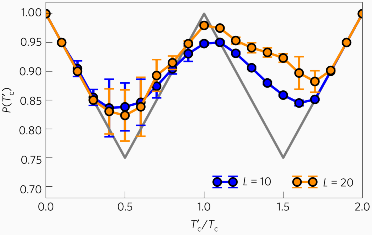


Summary

Neural networks can be trained to distinguish different phases but choosing the correct approach and network may be difficult.

Neural networks can find unkown phase transitions on their own

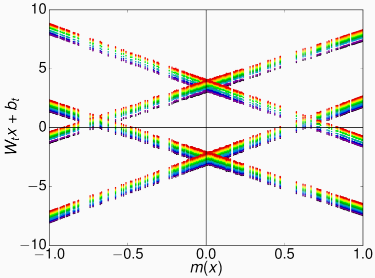


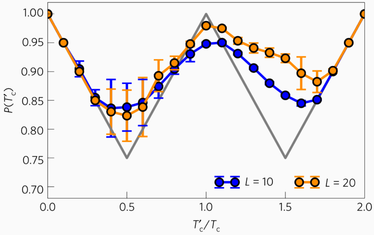


Summary

Neural networks can be trained to distinguish different phases but choosing the correct approach and network may be difficult.

Neural networks can find unkown phase transitions on their own but that doesn't have to be a phase transition.





Further Reading

Ising model and statistical physics
Schwarz: Statistical Physics
`https://www.thphys.uni-heidelberg.de/~biophys/PDF/Skripte/StatPhys.pdf`

Quantum monte carlo
Assaad and Evertz: World line and determinantal Quantum Monte Carlo methods for spins, phonons, and electrons.
`https://pawn.physik.uni-wuerzburg.de/~assaad/Reprints/assaad_evertz.pdf`

Paper
Machine learning phases of matter `DOI:10.1038/nphys4035`
Machine learning quantum phases of matter beyond the fermion sign problem `DOI:10.1038/s41598-017-09098-0`
Learning phase transitions by confusion `DOI: 10.1038/nphys4037`