MACHINE LEARNING PHASES OF MATTER

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THANKS TO MY PHYSICS/ML FRIENDS FOR DISCUSSIONS AND COLLABORATIONS
CONTENTS

➢ Introduction: ML and condensed matter, phases, phase transitions.
➢ What we mean by learning phases of matter
➢ Ising model and conventional phases of matter
➢ Square ice, Ising gauge theory
➢ Sign problem
➢ Conclusions and outlook
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PHASES, PHASE TRANSITIONS, AND THE ORDER PARAMETER

Ising ferromagnet in two dimensions

\[ H = -J \sum_{\langle ij \rangle} \sigma_i^z \sigma_j^z \]

Ferromagnet

Paramagnet

Temperature

Lars Onsager Phys. Rev. 65, 117
PHASES, PHASE TRANSITIONS, AND THE ORDER PARAMETER

Ferromagnetic transition: order parameter

\[ M = \frac{1}{N} \sum_i \langle \sigma_i \rangle, \quad \sigma_i = \pm 1 \]

Ferromagnet \( M > 0 \)

Paramagnet \( M = 0 \)

It is a measure of the degree of order in the system

\[ T \]

Lars Onsager Phys. Rev. 65, 117
INSPIRATION: FLUCTUATIONS HANDWRITTEN DIGITS (MNIST)

ML community has developed powerful *supervised* learning algorithms

\[ \sum = 5 \text{ Fluctuations} \]

**FM phase**

**High T phase**

gray = spin up

white = spin down

FM (0)  

PM (1)

1605.01735
COLLECTING THE TRAINING/TESTING DATA:
MC SAMPLING ISING MODEL AND LABELS
COLLECTING THE TRAINING/TESTING DATA: MC SAMPLING ISING MODEL AND LABELS

2D Ising model in the ordered phase

2D Ising model in the disordered phase

Training/testing data is drawn from the Boltzmann distribution

\[ p(\sigma_1, \sigma_2, \ldots, \sigma_N) = \frac{e^{-\beta E(\sigma_1, \sigma_2, \ldots, \sigma_N)}}{Z(\beta)} \]
COLLECTING THE TRAINING/TESTING DATA: MC **SAMPLING** ISING MODEL AND **LABELS**

2D Ising model in the **ordered phase**

2D Ising model in the **disordered phase**

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COLLECTING THE TRAINING/TESTING DATA: MC **SAMPLING** ISING MODEL AND **LABELS**

2D Ising model in the **ordered phase**

2D Ising model in the **disordered phase**

Successful training amounts to finding functions

\[ F_{\text{High}}(\sigma_1, \ldots, \sigma_N) \quad F_{\text{Low}}(\sigma_1, \ldots, \sigma_N) \]

![Graph showing phase transition and t-SNE visualization](image)
RESULTS: SQUARE LATTICE ISING MODEL (TEST SETS)

2D Ising model in the ordered phase

2D Ising model in the disordered phase

20K samples below $T_c$  20K samples above $T_c$

$T_c/J = 2/\ln(1 + \sqrt{2})$

Critical

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DO THE RESULTS EXTEND TO OTHER INTERESTING CASES?

Yes. We can obtain $T_c$ in the triangular lattice from numerically trained model on the square lattice!

$T_c/J = 4/\ln 3$

$T_c$ within $<1\%$!
Toy model: only three analytically "trained" perceptrons with precise functions: quantifying the magnetization of each configuration

In general the hidden layer discovers the order parameter of the phase during the training

\[ \Rightarrow \text{Works for AF Ising model} \]
ANALYTICAL UNDERSTANDING

Investigating the argument of the hidden layer during the training

\[ W = \frac{1}{N(1+\epsilon)} \begin{pmatrix} 1 & 1 & \cdots & 1 \\ -1 & -1 & \cdots & -1 \\ 1 & 1 & \cdots & 1 \end{pmatrix} \quad \text{and} \quad b = \frac{\epsilon}{(1+\epsilon)} \begin{pmatrix} -1 \\ -1 \\ 1 \end{pmatrix} \quad \text{and} \quad Wx + b = \frac{1}{(1+\epsilon)} \begin{pmatrix} m(x) - \epsilon \\ -m(x) - \epsilon \\ m(x) + \epsilon \end{pmatrix} \]

\[ x = [\sigma_1 \sigma_2, \ldots, \sigma_N]^T \quad m(x) = \frac{1}{N} \sum_{i=1}^{N} \sigma_i \]

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\[ x = [\sigma_1 \sigma_2, \ldots, \sigma_N]^T \quad m(x) = \frac{1}{N} \sum_{i=1}^{N} \sigma_i \]

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The neural net discovers the order parameter and uses it to perform the classification task.

\[
W = \frac{1}{N(1+\epsilon)} \begin{pmatrix} -1 & -1 & \cdots & -1 \\ 1 & 1 & \cdots & 1 \\ 1 & 1 & \cdots & 1 \end{pmatrix}, \quad b = \frac{\epsilon}{(1+\epsilon)} \begin{pmatrix} -1 \\ 1 \end{pmatrix}, \quad Wx + b = \frac{1}{(1+\epsilon)} \begin{pmatrix} -m(x) - \epsilon \\ m(x) + \epsilon \end{pmatrix},
\]

\[
x = [\sigma_1 \sigma_2, \ldots, \sigma_N]^T \quad m(x) = \frac{1}{N} \sum_{i=1}^{N} \sigma_i
\]
SQUARE ICE, ISING GAUGE THEORY AND TOPOLOGICAL PHASES OF MATTER
PHASES OF MATTER **WITHOUT AN ORDER PARAMETER AT T=0**

- **Topological phases of matter.** Examples: Fractional quantum hall effect. Potential applications in topological quantum computing.

- **Coulomb phases** = Highly correlated “spin liquids” described by electrodynamics. Examples: Common water ice and spin ice materials (Ho$_2$Ti$_2$O$_7$ and Dy$_2$Ti$_2$O$_7$)

*ST Bramwell, MJP Gingras* *Science* 294 (5546), 1495-1501
PHASES OF MATTER WITHOUT AN ORDER PARAMETER AT T=0

- Defy the Landau symmetry breaking classification. Neural nets *capture* the subtle differences between low- and high-temperature states successfully!
- Square ice: 99% accuracy
- Ising gauge theory: 50% (guessing) with a fully-connected neural net. Training fails. How to overcome this issue?
For two configurations
**ISING GAUGE THEORY**  
*(Kogut Rev. Mod. Phys. 51, 659 (1979))*

\[ H = -J \sum_p \prod_{i \in p} \sigma_i^z \]
**ISING GAUGE THEORY**  
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- 2x2 maps (64 per sublattice)
- Fully connected layer (64)
- Softmax
- 99% accuracy *easy to train*
- dropout regularization
ANALYTICAL UNDERSTANDING: WHAT DOES THE CNN USE TO MAKE PREDICTIONS?

- The convolutional neural net relies on the detection of satisfied local constraints to make accurate predictions of whether a state is drawn at low or infinite temperature.

- Based on this observation we derived the weights of a streamlined convolutional network *analytically* that works perfectly on our test sets.

100% accuracy on test sets

16 2x2 maps on each sublattice

Fully connected output layer

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## Analytical Model for the Ising Gauge Theory

### Convolutional Layer

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<td>-1 1 0 0 0</td>
<td>16</td>
<td>-1 0 -1 0 1</td>
<td>-1 0 0 0 0</td>
</tr>
</tbody>
</table>

### Output Layer

\[
W_o = \begin{pmatrix}
\underbrace{\frac{sL^2}{2}} & \underbrace{\frac{sL^2}{2}} \\
-1 & \cdots & 1 & -L^2 & \cdots & -L^2 \\
-1 & \cdots & -1 & L^2 & \cdots & L^2 \\
\end{pmatrix}, \quad \text{and} \quad b_o = \begin{pmatrix} 0 \\ 0 \end{pmatrix}
\]

\[
b_c = -(2 + \epsilon)
\begin{bmatrix}
1 \\
\vdots \\
1
\end{bmatrix}
\]
\[ H = -J_p \sum_p \prod_{i \in p} \sigma_i^z - J_v \sum_v \prod_{i \in v} \sigma_i^x \]

\[ |\Psi \rangle = \sum | \] 

Neural net represents a ground state of the toric code: equal weight superposition of closed string states

Non trivial ground states can be written as a NN

Optimize using VMC for other more challenging ground state problems (efficient sampling is possible)
Only Quantum Slide of the talk

\[ H = -J_p \sum_p \prod_{i \in p} \sigma_i^z - J_v \sum_v \prod_{i \in v} \sigma_i^x \]

\[ |\Psi\rangle = \sum |\text{State}\rangle \]

Neural net represents a ground state of the toric code: equal weight superposition of closed string states

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Optimize using VMC for other more challenging ground state problems (efficient sampling is possible)
LET’S EXPLOIT THIS MORE

Condensed matter/stat mech

Machine learning

Stoudenmire, Schwab 1605.05775

Energy-Based Models

Carleo, Troyer 1606.02318

Torlai, Melko 1606.02718
LET'S EXPLOIT THIS MORE

Condensed matter/stat mech

Carleo, Troyer 1606.02318
Torlai, Melko 1606.02718

Machine learning

Stoudenmire, Schwab 1605.05775
Energy-Based Models
CONCLUSION

➤ We encode and discriminate phases and phase transitions, both conventional and topological, using neural network technology.

➤ We have a solid understanding of what the neural nets do in those cases through controlled analytical models.

OUTLOOK

➤ We expect a rapid adoption of ML techniques as a tool in condensed matter physics.

➤ Variational interpretation of CNNs and their optimization for ground state and real-time dynamics.

➤ Attempt at circumventing the sign problem (Check Peter Broecker’s talk this afternoon)

➤ Establish a more practical connection between RG and deep learning and turn it into a useful tool.

➤ Train numerically using QMC and use machinery to analyze experimental data: 1. Phase transitions in quantum gas microscopes. 2. Measure temperature from experimental snapshots.