Machine Learning Nonequilibrium Phase Transition

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Introduction

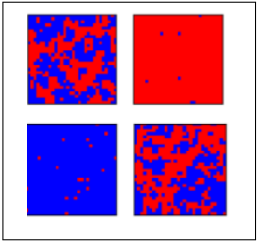
1. Introduction

Introduction

- The study applies $\underbrace{\texttt{Convolutional Neural Networks}}_{\textbf{CNN}}$ to identify and classify phase transitions in an Ising model under nonequilibrium conditions.
- Nonequilibrium systems do NOT obey the **DBC**. (−More complex compared to the equilibrium systems)
- However, advancements in ML provides a **data-driven** approach (Motivation)

Motivation

CNN can detect configurations of spin system—akin to imgs.



That is;

■ If a CNN is able to identify imgs of **cats** from that of **dogs**, it can be used to classify **d/t states** of spin confg.

∴ We aim to evaluate the generalization scope of this model.

⇒ **Train on EPT and Test on NEPT**

... Motivation: **CNN** can detect configurations

- We can use CNN to classify the **d/t states (≅phases)**. E.g: ordered and disordered states of spin configurations.

One of **previous studies** [Carrasquilla, 2017]—that inspiring:

$\boxed{\surd}$ It was studed that CNN can recognize phases and phase transision of equilibrium Ising model.

Contribution of the present study:

$\boxed{?}$ Can CNN recognize nonequilibrium phase transition?

Method: MC+Supervised ML (≅Modified Metropolis + **CNN**)

Supervised ML —*learns a function that maps the input to the output by learning how inputs correlate to outputs.*

Description of the Ising Model ($\mathscr{B} = 0$)

- Define model of the ferromagnet by Hamiltonian

$$\mathscr{H} = -J \sum_{\langle i,j \rangle} s_i s_j, \quad \texttt{where } s_i = \pm 1(\textit{up or down}) \qquad (1)$$

- The system undergoes a second order PT at critical T_c.
- ▷ For $T < T_c$, the system is in ordered(FM) state.
- ▷ For $T > T_c$, the system is in disordered(PM) state.
- ◀ **Recall: CNN** classifies d/t states–"**FM**" & "**PM**" here.
- For an infinite 2D lattice T_c was derived [Onsager, 1944]

$$T_c = 2/\ln(1+\sqrt{2}) \approx \underline{\underline{2.2692}}, \texttt{in units}[J/K_B], \qquad (2)$$

and ML was studied [Carrasquilla, 2017]

☐ Set $k_B = 1$, $\implies T$ in J, & T/J is dimensionless.

Equilibrium vs Nonquilibrium Ising Model

- System in contact with hb−generates *stochastic* spin flips.

▶ **The Modified Metropolis:** $\boxed{\mathbb{M} = \mathtt{MIN}\left[1, e^{-\beta\Delta E_{\mathtt{eff}}}\right]}$,

✓ $\mathbb{M} =$ Modified rate of transition from **old** to a **new** state,

✓ $\beta = 1/T$,

✓ $\boxed{\Delta E_{\mathtt{eff}} = \Delta E + \varepsilon}$ $\equiv$ **Effective Energy change**[This work],

✓ $\underbrace{\Delta E = \{-8,-4,0,4,8\} \equiv \textbf{Known Energy change [Litrature]}, \; \textit{Varepsilon}[-8 \le \varepsilon \le 8] \equiv \textbf{Non-zero parameter} \texttt{ to break DB.}}$

Equilibrium vs Nonquilibrium Ising Model (this study context)

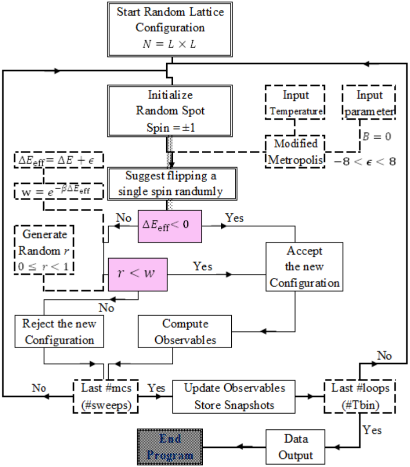
Equilibrium (with DB)	**Nonquilibrium** (without DB)
▶ Obeys DB condition($\varepsilon = 0$) $\Delta E_{\mathtt{eff}} = \Delta E$	▶ Violates DB condition($\varepsilon \neq 0$) $\Delta E_{\mathtt{eff}} \neq \Delta E$ e.g. $\varepsilon = \pm 2$ and $\Delta E_{\mathtt{eff}} = \Delta E \pm 2$

Method

2. Method

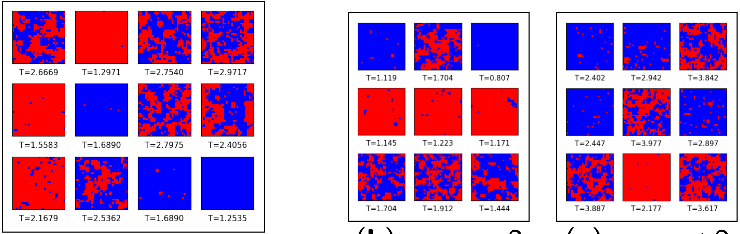
MC Generate 200,000 Image Snapshots (Imgs)

- We perform MC simulation of Ising model using the MMA.



Square lattice of
$L = \{10, 20, 40, 60\}$
$N = L \times L$.
MC sweeps $= 10N$
Start: Thigh $= 4.5$
End: Tlow $= 0.5$
Tbin $= 200$ data points
Ensemble of 800 samples
$\therefore$ 160kimgs
16k is for validation.
More 40k test dataset

Samples of Imgs

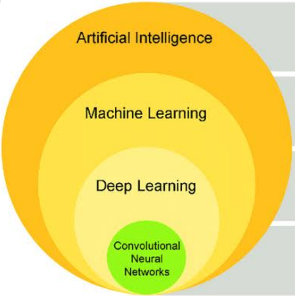


(**a**) $\varepsilon = 0$ (**b**) $\varepsilon = -2$ (**c**) $\varepsilon = +2$

Equilibrium (Train Dataset) Nonequilibrium Representative (Test Datasets)

Reptv. (40×40) configurations: Training(**a**), & Test(**b**,**c**) datasets. The low temperature ($T < T_c(\varepsilon)$) configurations tend to be predominately aligned in either "up" / "down".

CNN-is a DL algorithm



AI cloud team at IBM explains

$\underbrace{\textbf{AI, ML, ANN, DL}}_{\texttt{computer science terms}}$

as a series of AI system

$\boxed{\mathtt{DL} \longrightarrow \mathtt{ANN} \longrightarrow \mathtt{ML} \longrightarrow \mathtt{AI}}$

each encompassing the next.

- **CNN** is a DL algorithm—used for the image type data.
- In our case, we use imgs of Ising spin configurations.

ANN – *a subset of ML and the backbone of DL.*
– called "neural" b/c mimic how neurons in brain.

TenserFlow integrated with Keras API

Build & train a CNN using TensorFlow Keras sequential model.

Optimization = **Adam**,
Loss function = **categorical cross-entropy**,
Activation function = **ReLU**,
Final Dense = 2 nodes,
Activation function= **Softmax**.

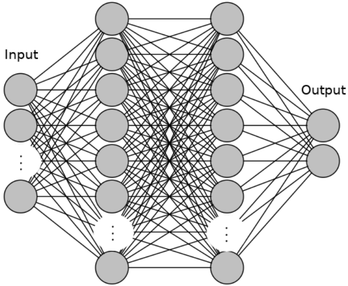
- The first part of model consists of two conv. layers.
  Each of these layers has 64 output filters of kernel size 3×3.
- The data are flattened & passed to Dense layer, +ReLU.
- Apply Softmax on last Dense layer so that the output for each sample is a probability distribution over the outputs.

Results

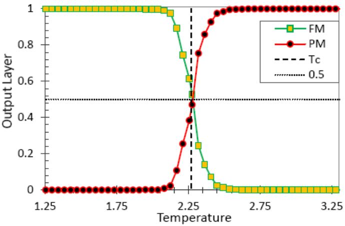
3. Results

Result: Training—& Validation ($\varepsilon = 0$), $L = 40$

- Plot shows the average output layer vs temperatures



Fully connected layer



Plot of output layer

- Crossing point refers point of maximal (POM) confusion
- Critical T at POM confusion is almost $\cong$ to analytical T_c.

ML the equilibrium model: $L = \{10, 20, 40, 60\}$.

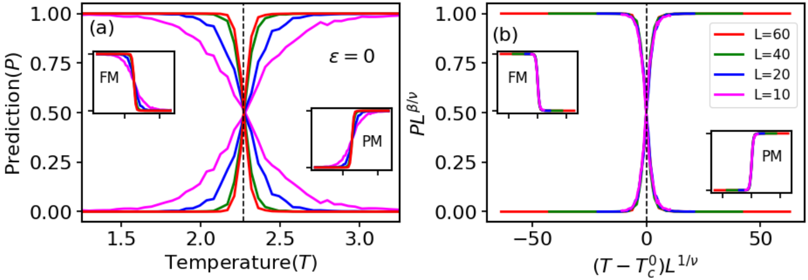


Figure: (a) Output layer prediction as a function of T ($\varepsilon = 0$). The vertical dashed line signals $T_c^0 \approx 2.267$.
(b) Plot showing FSS of the av. output layer versus $(T - T_c)L^{1/\nu}$.
Note: The prediction is indpendent of L at POM confusion —consistent with TD response function.

ML Nonequilibrium Model: $L = \{10, 20, 40, 60\}$

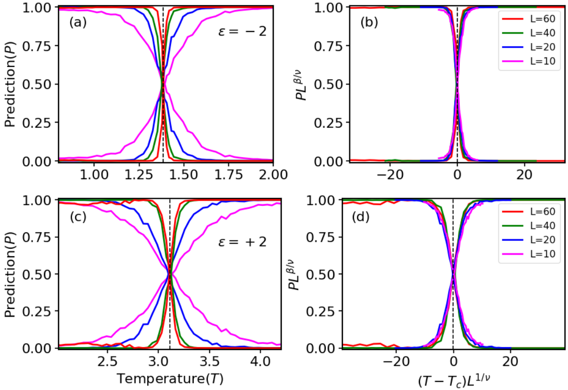
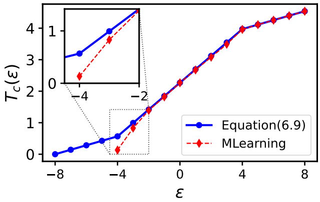
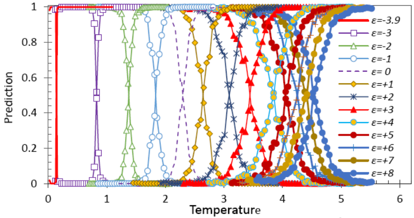


Figure: Output layer prediction vs T for ($\varepsilon = \pm 2$). The vertical dashed line signals (a & b) $T_c(\varepsilon = -2) \approx 1.385$, and (c & d) $T_c(\varepsilon = +2) \approx 3.106$

Key Findings

- The CNN successfully identifies the critical temperature.
- Furthermore, a disagreement b/n CNN and graphical calculation has been observed for $\varepsilon < -2$.





- The figure shows that the variant becomes **bolder** for $\varepsilon < -2$, and even CNN totally fails for $\varepsilon \leq -4$.
- This discrepancy has been resolved by introducing the effective parameter $|h| \leq 1$.

Conclusions

4. Conclusions

Summary

- For $\varepsilon = \pm 2$: ML(**this**) and MC(Literature) are almost in agrement

ML(**This Work**)		
ε	Analytical	$T_c(\varepsilon)^{\mathtt{ML}}$ in $[J]$
-2	$5/4\ln(1+\sqrt{2}) \approx 1.4182$	1.3769(87)
$+2$	$11/4\ln(1+\sqrt{2}) \approx 3.1201$	3.1071(175)

MC (Literature)
$T_c(\varepsilon)^{\mathtt{MC}}$ in $[J]$
1.3604(3)
3.1267(4)

Testing: $L = \{10, 20, 40, 60\}$

Conclusions

- By using supervised ML, we have studied nonequilibrium phase transitions in a 2D Ising model on square lattice.
  - ▷ Result shows that CNN can identify nonequilibrium phase transitions. [More Information:] `https://doi.org/10.3390/condmat8030083`

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T H A N K Y O U

[1]Promoting basic sciences in LDC since 1961 (http://www.isp.uu.se/)