Deep Learning Insights into Many-Body Physics

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Introduction

- Phases of Matter: Broken Symmetries

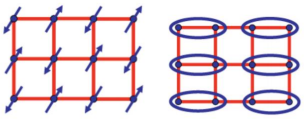

Figure: (Left) An anti-ferromagnetic phase (AF). (Right) A Valence Bond Solid (VBS) state.

- Quantum Monte Carlo samples: complex-valued matrices.

Data

- AF-to-VBS Transition.

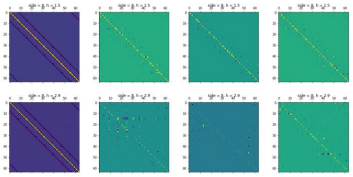

Figure: Data examples. Top four: VBS ($h = 1.5$), bottom four: AF ($h = 2.9$). For each row, leftmost: average over Monte Carlo samples (augmented), right three: individual samples.

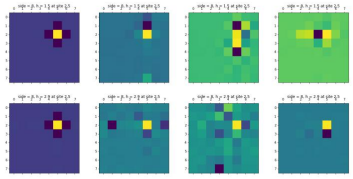

Figure: Data examples. Same dataset as above. Reshaped back into real-space 8-by-8 square lattice, look at correlations of all sites with site (2,5).

Training

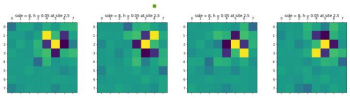

Figure: Data augmentation by rotation in real space. Here rotate about site (2, 5).

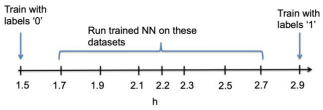

Figure: We expect a phase transition at an intermediate value of h. Method: [1]

Architectures

- Logistic Regression
- Convolutional Neural Network (filters=5, size=5)
- Tensor Train [2]

$$\mathcal{W}_{i_1 \cdots i_d} = G_1[i_1] \cdots G_d[i_d] \tag{1}$$

$$\hat{y}(\mathbf{x}) = \sum_{i_1=0}^{1} \cdots \sum_{i_d=0}^{1} \mathcal{W}_{i_1 \cdots i_d} \prod_{k=1}^{d} x_k^{i_k} \tag{2}$$

- For example

$$\hat{y}(\mathbf{x}) = \mathcal{W}_{000} + \mathcal{W}_{100}x_1 + \mathcal{W}_{010}x_2 + \mathcal{W}_{001}x_3 + \mathcal{W}_{110}x_1x_2 + \mathcal{W}_{101}x_1x_3 + \mathcal{W}_{011}x_2x_3 + \mathcal{W}_{111}x_1x_2x_3 \tag{3}$$

- Binary Cross Entropy Loss for all architectures

Results for AF-to-VBS Transition

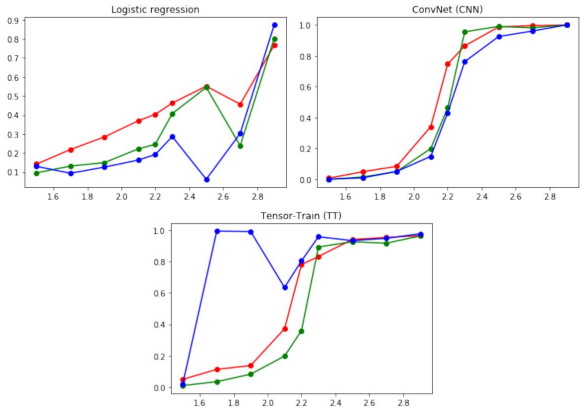

Figure: Results, x-axis is h, y-axis is average predicted label. Colors: Lattice size 8 (red), size 10 (green), size 12 (blue).

Results for QSL-to-AF Transition

- Phase recognition task fails for all three architectures.
- Likely reason: QSL is a subtle topological phase with no local correlations, but strong global correlations.

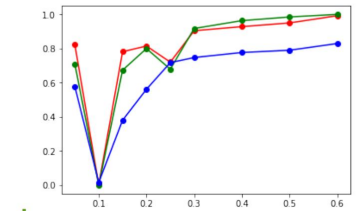

Figure: Results, x-axis is h, y-axis is average predicted label. (red) Logistic regression, (green) CNN, (blue) TT.

Future

- For Tensor-Train: Should employ parameter sharing to exploit all symmetries.
- Identification of topological features remains an open research question in machine learning physics.

References

[1] Peter Broecker, Juan Carrasquilla, Roger G Melko, and Simon Trebst.
Machine learning quantum phases of matter beyond the fermion sign problem.
Scientific reports, 7(1):8823, 2017.

[2] Alexander Novikov, Mikhail Trofimov, and Ivan Oseledets.
Exponential machines.
arXiv preprint arXiv:1605.03795, 2016.