Unsupervised detection of quantum phases and their order parameters from projective measurements

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1. Abstract

Recently, machine learning has become a powerful tool for detecting quantum phases. While the information about the presence of transition is useful by itself, the lack of interpretability prevents this tool from becoming a customary element of a physicist's toolbox. Here, we report designing a special convolutional neural network with adaptive kernels, which allows for fully interpretable detection of local order parameters out of spin configurations measured in arbitrary bases. With the proposed architecture, we detect relevant and simplest order parameters for the one-dimensional transverse-field Ising model from any combination of projective measurements in the x, y, or z basis. We also present tentative preliminary results for the bilinear-biquadratic spin-1 Heisenberg model and discuss how to extend the proposed approach to detecting topological order parameters.

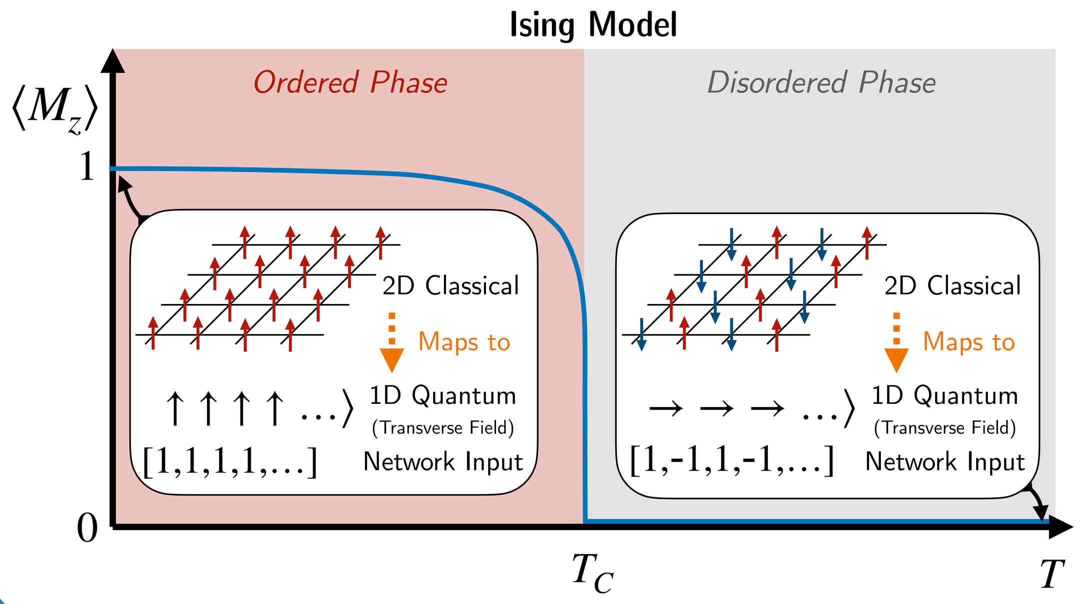
2. What is an order parameter in Physics?

Order parameter:

- **Definition**: An order parameter is like a thermometer for understanding when a system changes from chaos to order.
- **Role**: It helps scientists identify different states of matter and how they transform from disorder to organization.

Example: Ising model (Think of magnets!):

- **Ising Model**: Imagine a group of tiny magnets σ_i that can either point up or down. (spins-$\frac{1}{2}$)
- **Order Parameter**: In this case, how many magnets end up pointing in the same direction (magnetization) is the order parameter.
- **Explanation**: When we heat the magnets, they jiggle around randomly (disorder). As we cool them down, they start lining up in one direction (order).
- **Significance**: The order parameter (magnetization) helps us see when the magnets stop being chaotic and start behaving in an organized manner, which is crucial for understanding many natural processes.

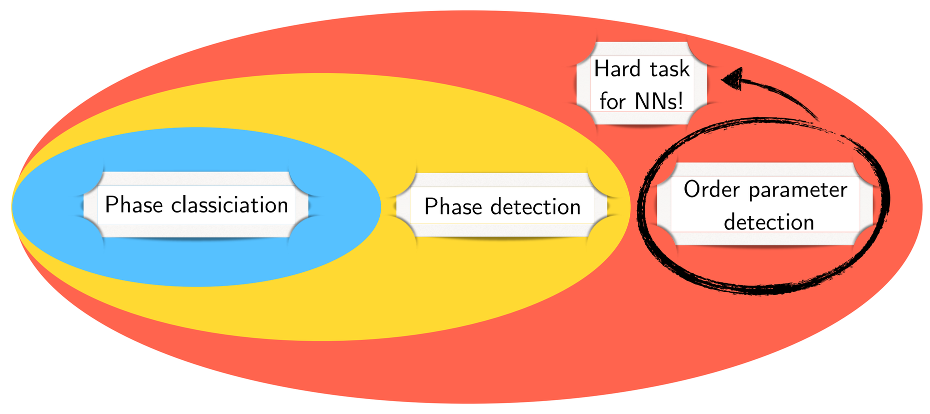


3. Automated phase detection

Why is it needed?

- In theoretical models and experiments, it can be hard to distinguish ordered and disordered phases.
- Identifying the right order parameter is crucial but can be challenging.
- Neural networks (NNs) can provide guidance to theory in finding these parameters.
- Order parameters vary, including single-body (e.g., magnetization) and more complex correlators.
- Automated phase detection can aid in analyzing new quantum systems and validating experimental data.

Order parameter detection is hard for NNs!
How does it relate to phase detection and classification?



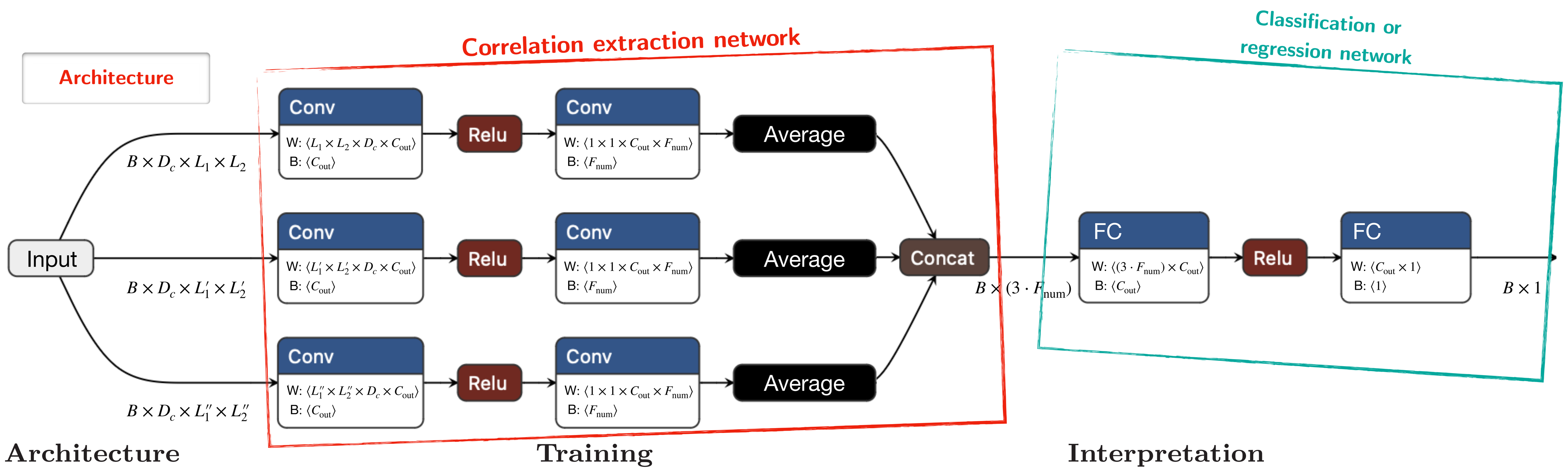
Features we add to state-of-the-art solutions [2], [3]:

- Automated detection of multi-site correlators.
- Identifying multiple phases accurately.
- Recognizing phases from snapshots taken in different measurement bases.
- Our tool is both interpretable and unsupervised.

7. Possible extensions

1. Design of special kernels to detect string-type order parameters
2. 2D systems: symmetric and non-symmetric gapped convolutions; data with topological order (e.g. Ising gauge theory); different lattice geometries.
3. Combine with Siamese NNs
4. Adaptive convolution kernels [7]

4. Tetris CNN



Architecture

- *Subnetworks*: Correlation extraction and classification.
- *Each filter size*: Dedicated branch in extraction network.
- *1x1 Convolution*: Enhances nonlinearity in each branch.
- *Bottleneck*: Combines activations for classification.
- *Phase Detection*: Can be unsupervised using regression. [1]

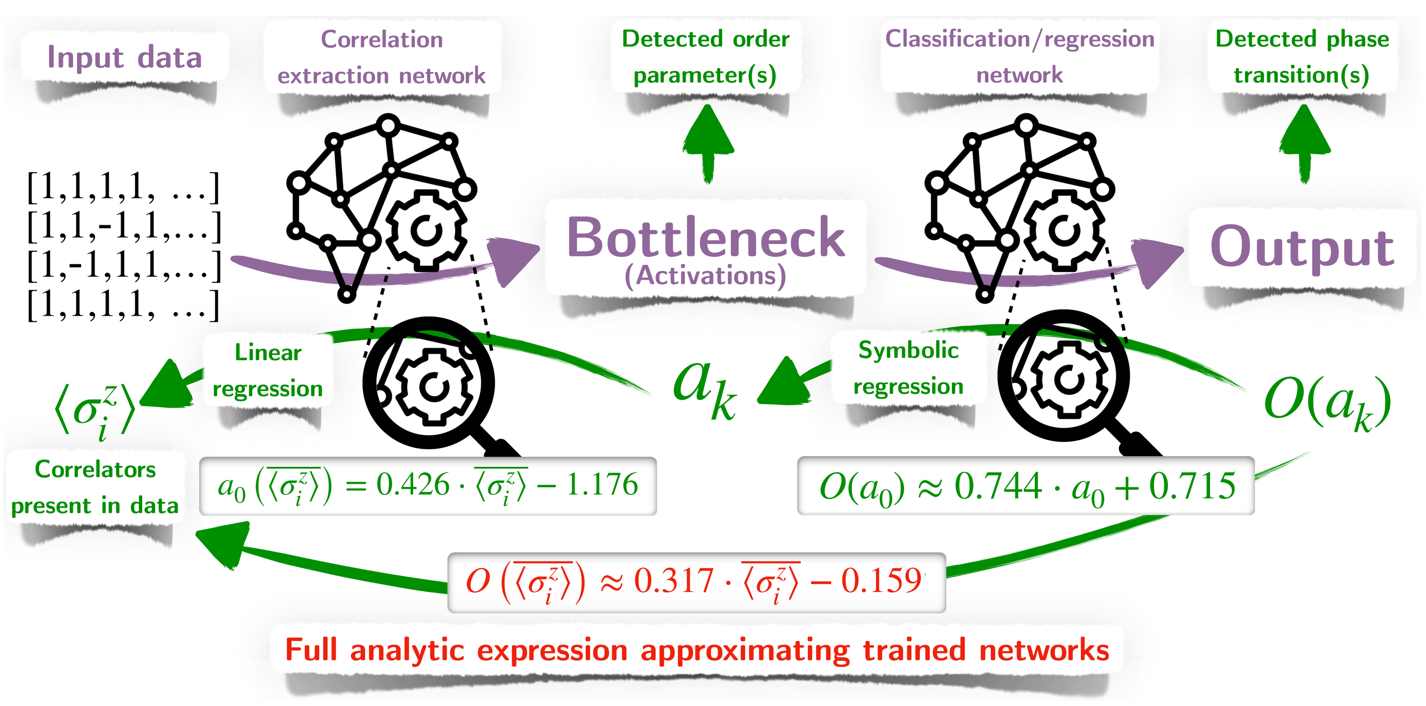
Training

- *Simultaneous Training*: Both networks are trained together.
- *Constraints*: L2 regularization on weights, penalties for complex kernels, and L1 regularization on activations.
- *Result*: The network learns to use and highlights the simplest usable correlator in input data.

Interpretation

- *Focus*: Prioritizes interpretability.
- *Bottleneck activations*: Linear combination of input correlators.
- *Input-bottleneck relationships*: Discovered through linear or symbolic regression.
- *Interpretation outcome*: Analytic expression approximating the trained neural network.

5. Network Interpretation



The architecture is **fully interpretable** by design. **Correlation extraction network:**

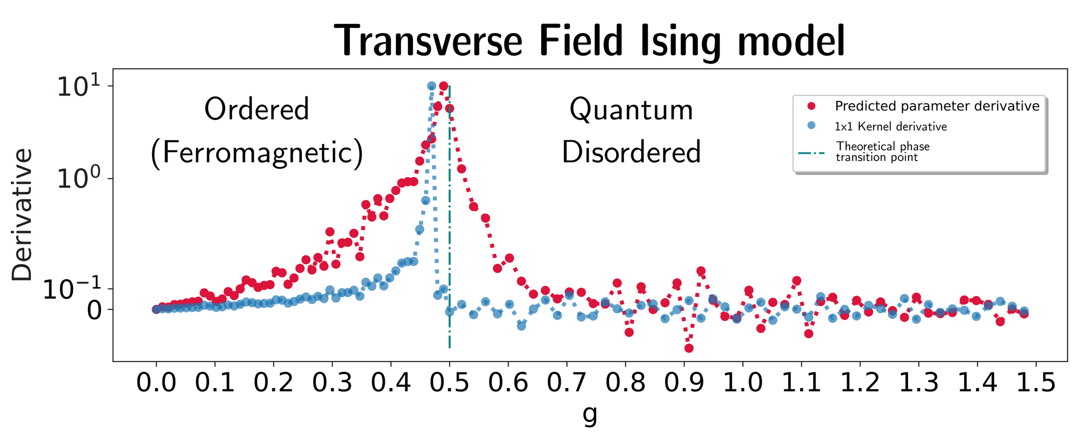
- An activation $a_k = a_k(\overline{\langle \sigma_i^z \rangle})$ - a function of a correlator present in data
- When Taylor expanded to 1[st] (2[nd]) order for spin-$\frac{1}{2}$ (spin-1) system, this relation is an exact linear combination.
- Its coefficients can be found with linear regression.

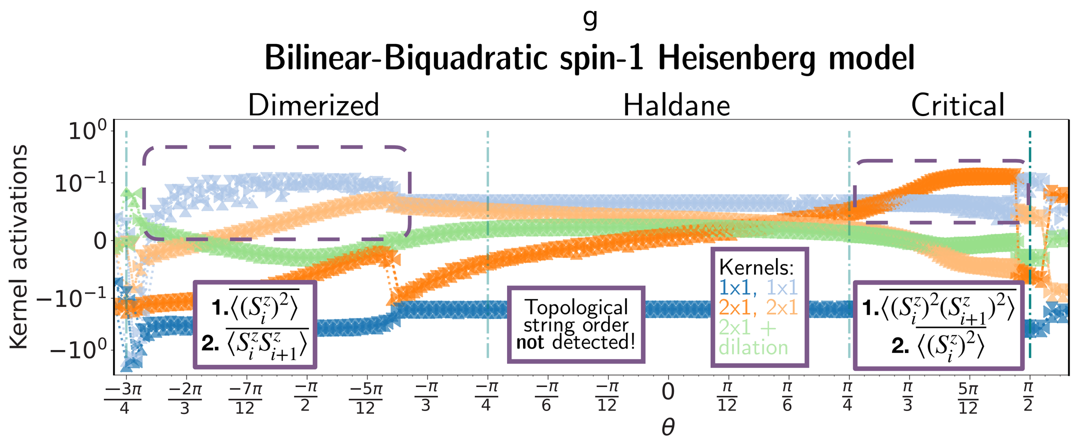
Classification/regression network:

- The mapping from output to bottleneck activations is approximated with **symbolic regression.**

From the two combined parts of this interpretation loop **we get a full analytic expression** approximating the trained neural networks. **All this, while** achieving the main goal of **finding the local order parameters and phase transition** points from the projective measurements we provide.

6. Results





1D Transverse field Ising model

- Our architecture has successfully learned the phase transition point. Input data was obtained using DMRG [4].
- To determine this, **we don't need labels** - just the *derivative* of predicted parameter [1].
- We detected the correct local order parameter and dominant correlators:
  - z basis - $\langle \sigma_i^z \rangle$ (Magnetization)
  - x basis - $\langle \sigma_i^x \rangle$
  - y basis - $\langle \sigma_i^y \sigma_{i+1}^y \rangle$
- In our architecture, **the same effect** can be achieved by inspecting **derivative of the dominant kernel.**

1D Bilinear-biquadratic spin-1 Heisenberg model

- More challenging problem with multiple phases. [5]
- Spin-1 system → Input spins $\sigma_i \in \{-1, 0, 1\}$
- **Success**: The dominant local **order parameters** our machine detected for two phases **match the theory** [6].
- Disclaimer: These results are **preliminary**, because the simulation data we use still needs refining.

References

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