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

Speakers:

Collection: Machine Learning for Quantum Many-Body Systems

Date: June 14, 2023 - 2:00 PM

URL: https://pirsa.org/23060038

Abstract: Recently, machine learning has become a powerful tool for detecting quantum phases. While the sole information about the presence of transition is valuable, the lack of interpretability and knowledge on the detected order parameter 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 and unsupervised 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. Moreover, we successfully tackle the bilinear-biquadratic spin-1 model with a nontrivial nematic order. We also consider extending the proposed approach to detecting topological order parameters. This work can lead to integrating machine learning methods with quantum simulators studying new exotic phases of matter.

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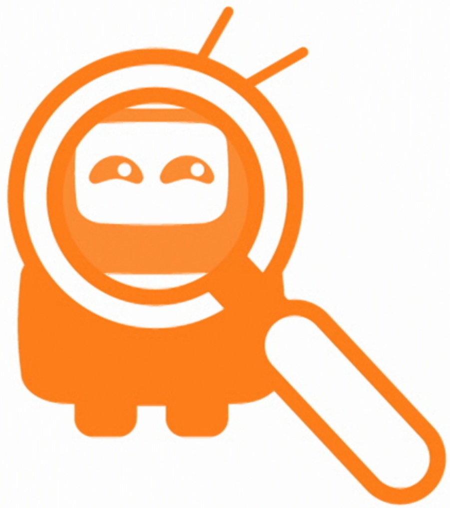
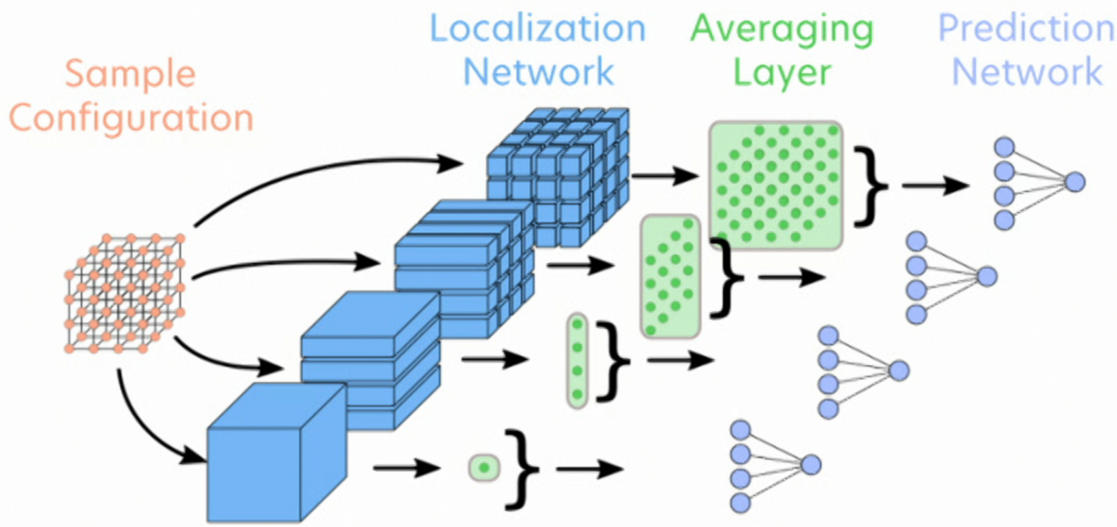
Unsupervised detection of quantum phases and their order parameters from projective measurements



ANNA DAWID
ML for QMBP at Perimeter Institute
June 14, 2023

Interpretation Net

S. Wetzel *et al.*



Receptive Field Size	Train Loss	Validation Loss
28×28	$6.1588e-04$	0.0232
1 × 2	**1.2559e-04**	**1.2105e-07**
1 × 1	**0.2015**	**0.1886**
baseline	0.6931	0.6931

} separate trainings

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Phys. Rev. B 96, 184410 (2017)

Interpretation Net

S. Wetzel *et al.*

1x1

$$f(s_i) = f_0 + f_1\ s_i + f_2\ \underbrace{s_i^2}_{1} + f_3\ \underbrace{s_i^3}_{s_i} + \dots$$

$$F\left(\frac{1}{N}\sum_i f(s_i)\right)$$

1x2

$$f(s_i, s_j) = f_{0,0} + f_{1,0}\, s_i + f_{0,1}\, s_j + f_{2,0}\, s_i^2 + f_{1,1}\, s_i\, s_j + f_{0,2}\, s_j^2 + \dots,$$

$$F\left(\frac{1}{N}\sum_{<i,j>_T} s_i s_j\right)$$

Receptive Field Size	Train Loss	Validation Loss
28×28	$6.1588e-04$	0.0232
1×2	**1.2559e-04**	**1.2105e-07**
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separate trainings

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Interpretation Net

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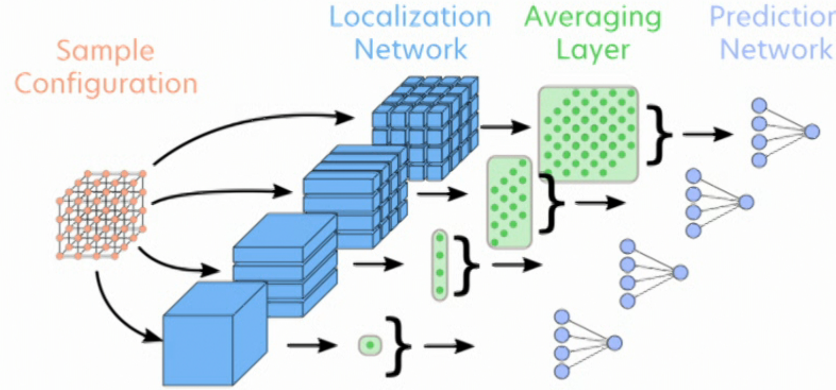

- It requires multiple training runs
  The more complex correlators you consider, the larger number of training runs.

- Multi-class problems are challenging to implement
  What if one phase is driven by one-body and another by two-body correlators?

Receptive Field Size	Train Loss	Validation Loss
28×28	$6.1588e-04$	0.0232
1×2	**1.2559e-04**	**1.2105e-07**
1×1	**0.2015**	**0.1886**
baseline	0.6931	0.6931

separate trainings (rows 28×28, 1×2, 1×1)

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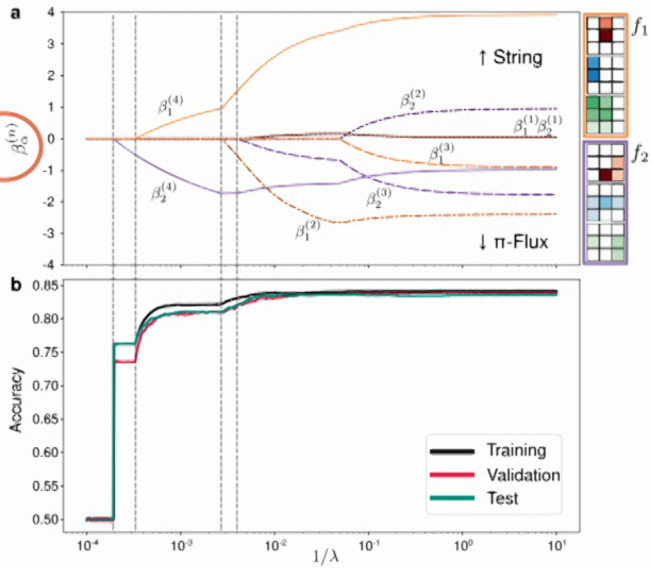
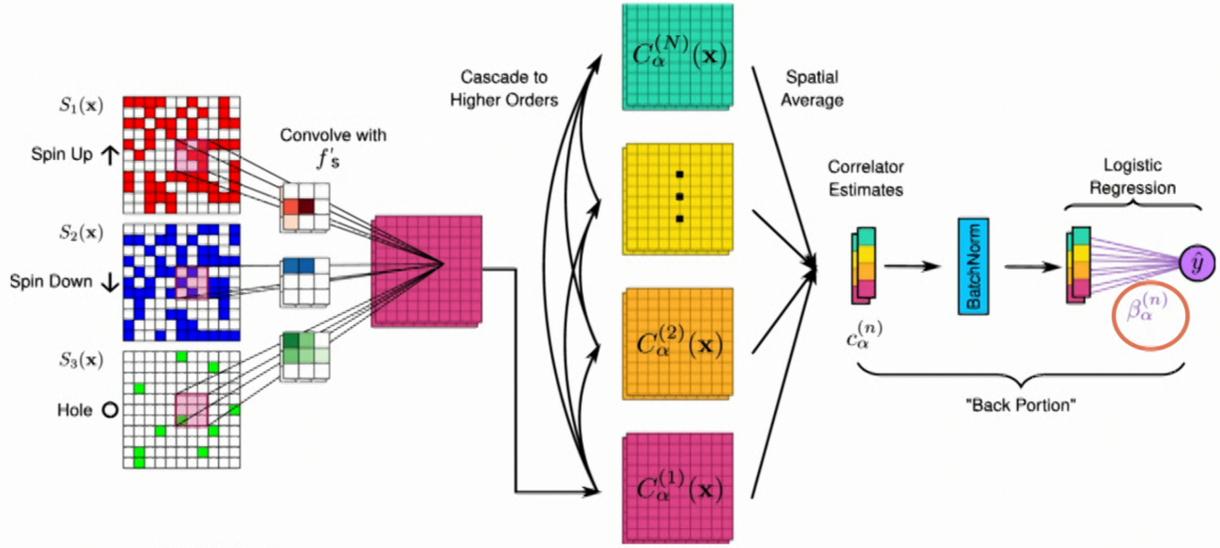
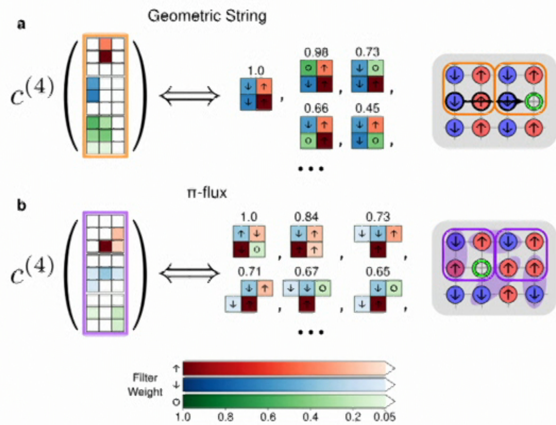
Phys. Rev. B 96, 184410 (2017)

Correlator CNN

C. Miles, A. Bohrdt,
E.-A. Kim *et al.*







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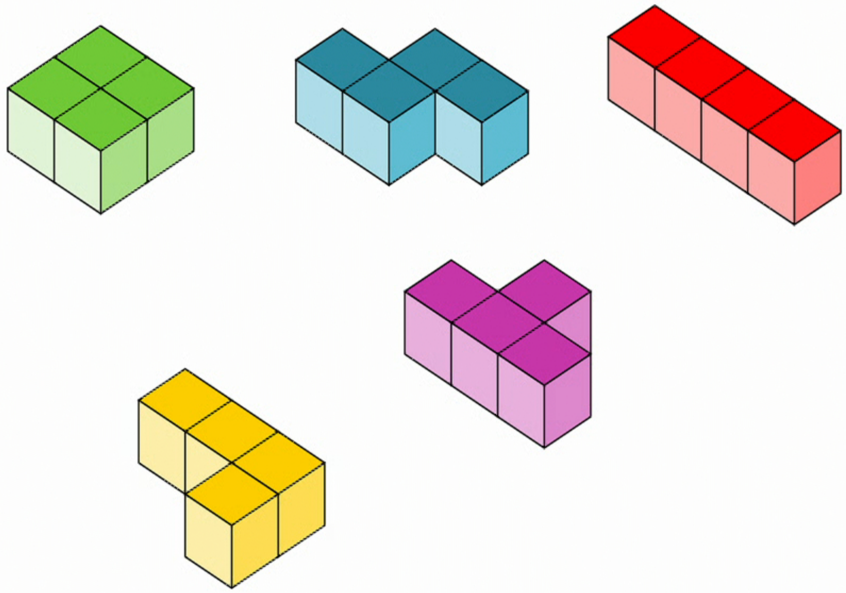
Tetris

~~Adaptive~~ CNN



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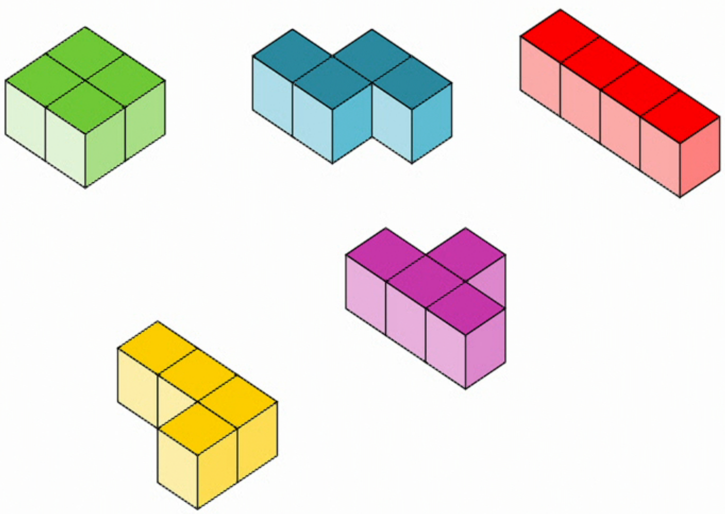
Tetris
~~Adaptive~~ CNN



+

Loss function promoting the use of:

1. simple kernels (correlators)
2. the smallest number of kernels (correlators)

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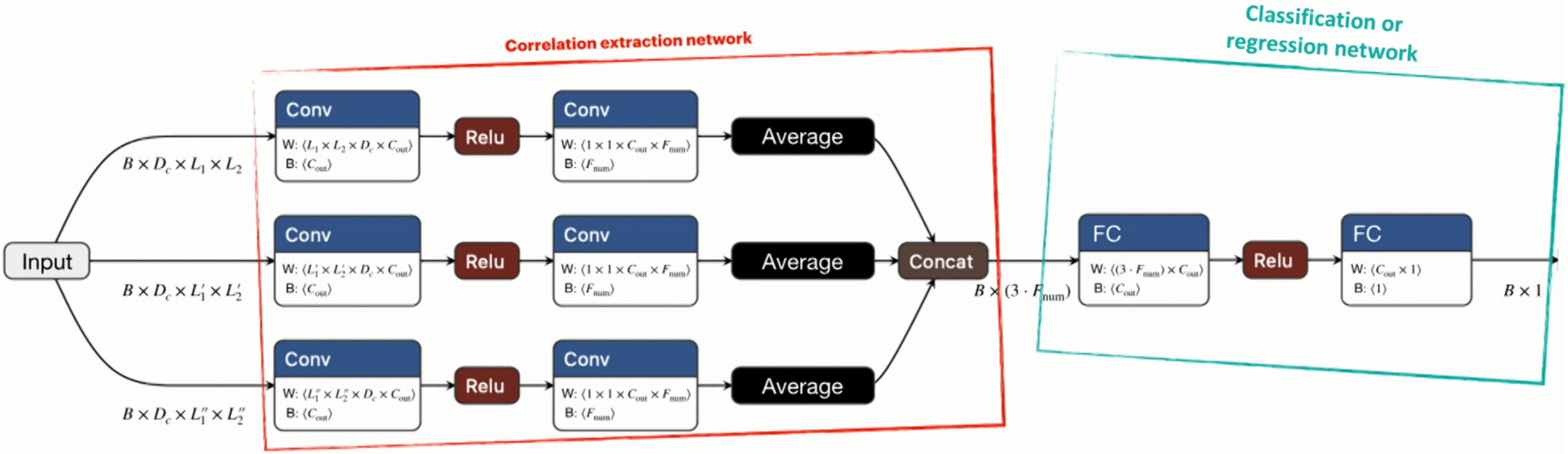
Adaptive CNN
for order parameter detection



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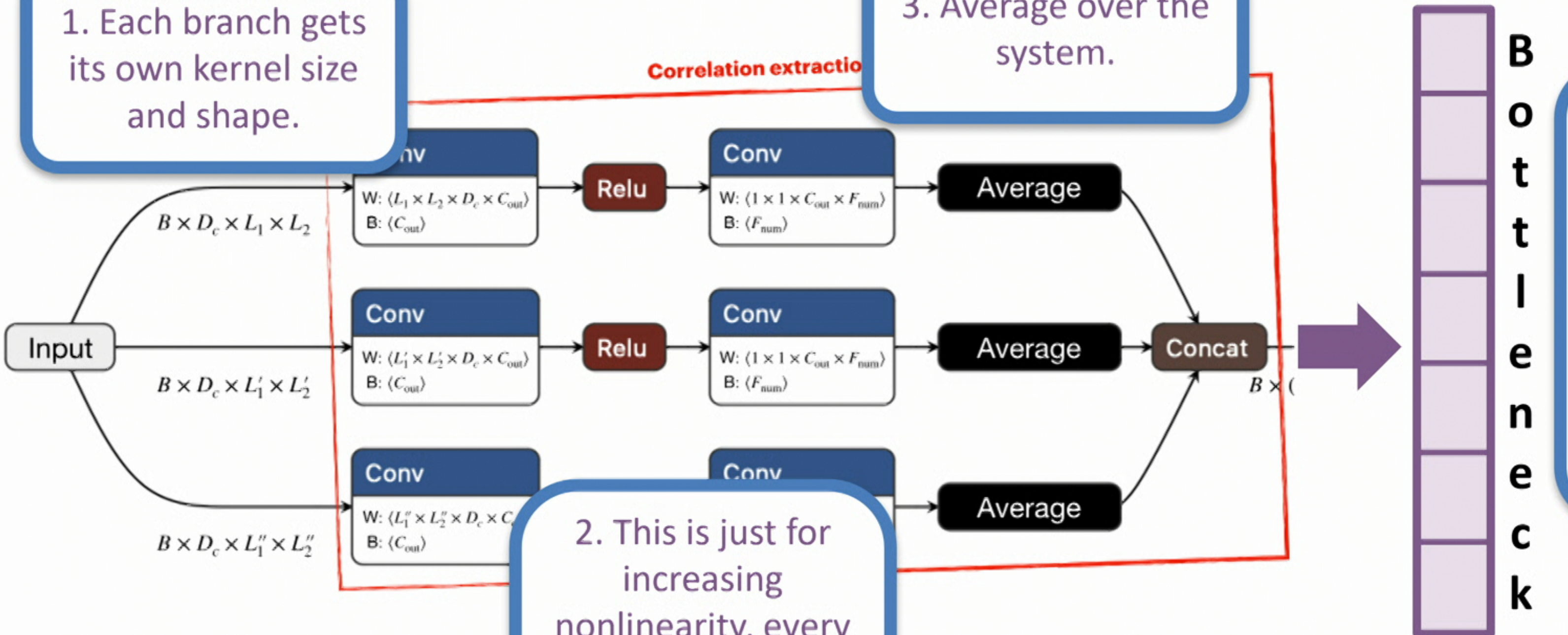
Cybiński, Dawid, et al. (2023) in preparation

Adaptive CNN
for order parameter detection



1. Each branch gets its own kernel size and shape.

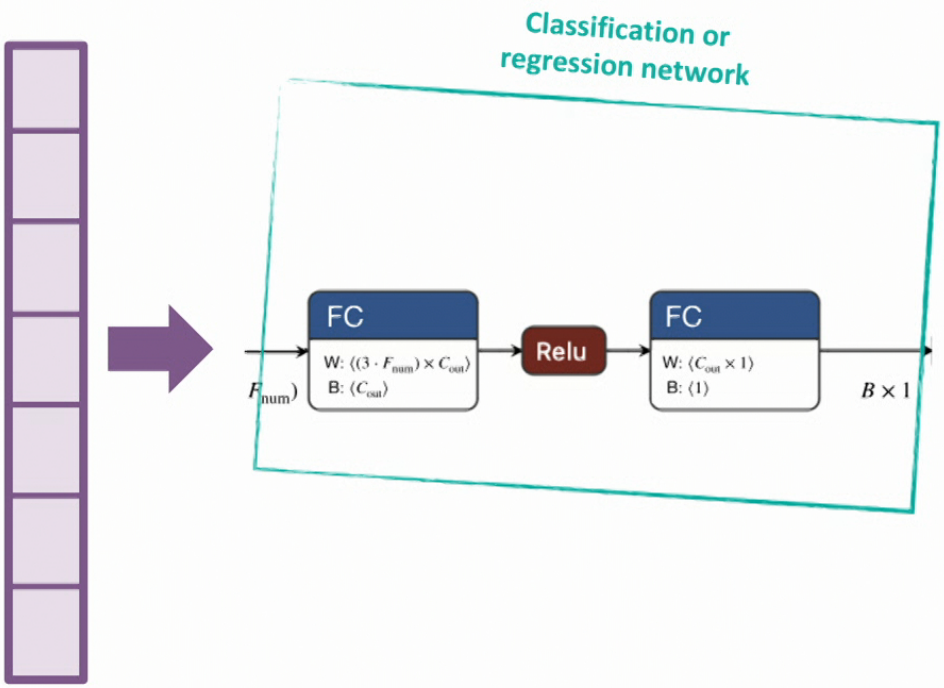
2. This is just for increasing nonlinearity, every branch has here kernel 1x1 – no new correlations can be picked up.

3. Average over the system.

4. Activations coming from each branch – each kernel and corresponding correlator.

Adaptive CNN
for order parameter detection

4. Activations coming from each branch – each kernel and corresponding correlator.



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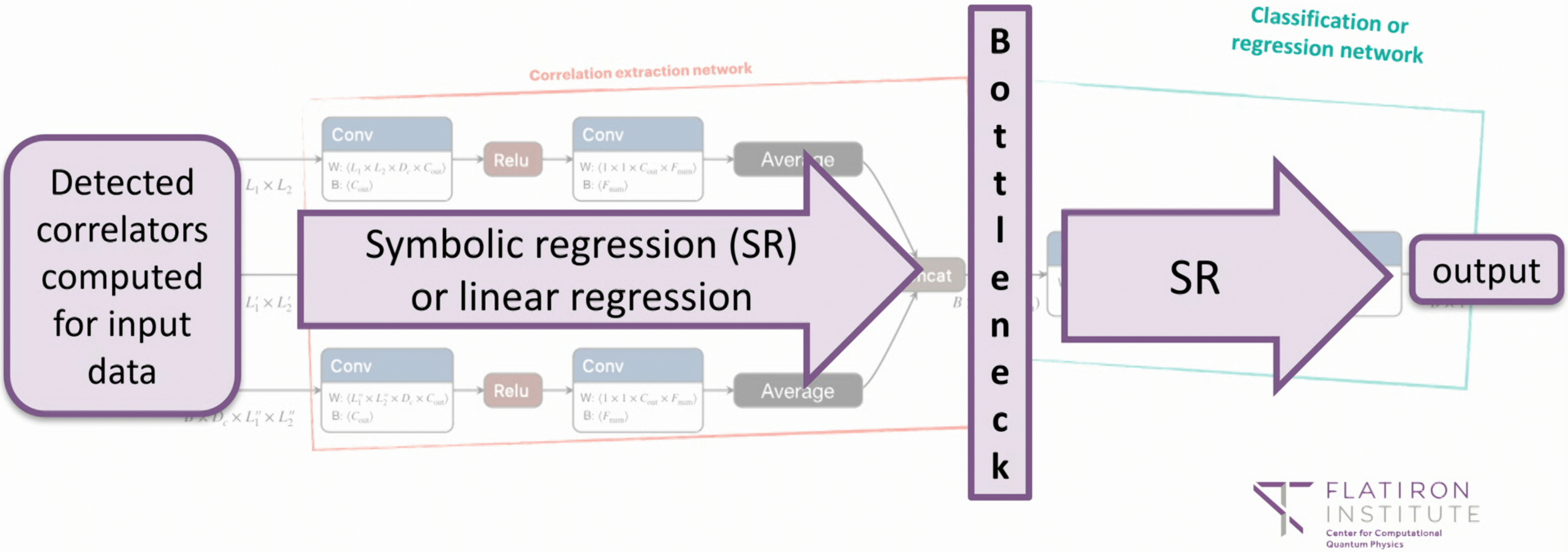
Adaptive CNN
for order parameter detection



Outline

State-of-the-art of order parameter detection

Adaptive CNN

Preliminary results

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1D transverse-field Ising

$$\hat{H} = -J\left(\sum_{\langle i,j\rangle} \hat{S}_i^z \hat{S}_j^z + g\sum_j \hat{S}_j^x\right)$$

Two setups:

1. supervised classification: training data far from the transition
2. unsupervised analysis with regression (task: predict *g*)

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DMRG using ITensors.jl library in Julia

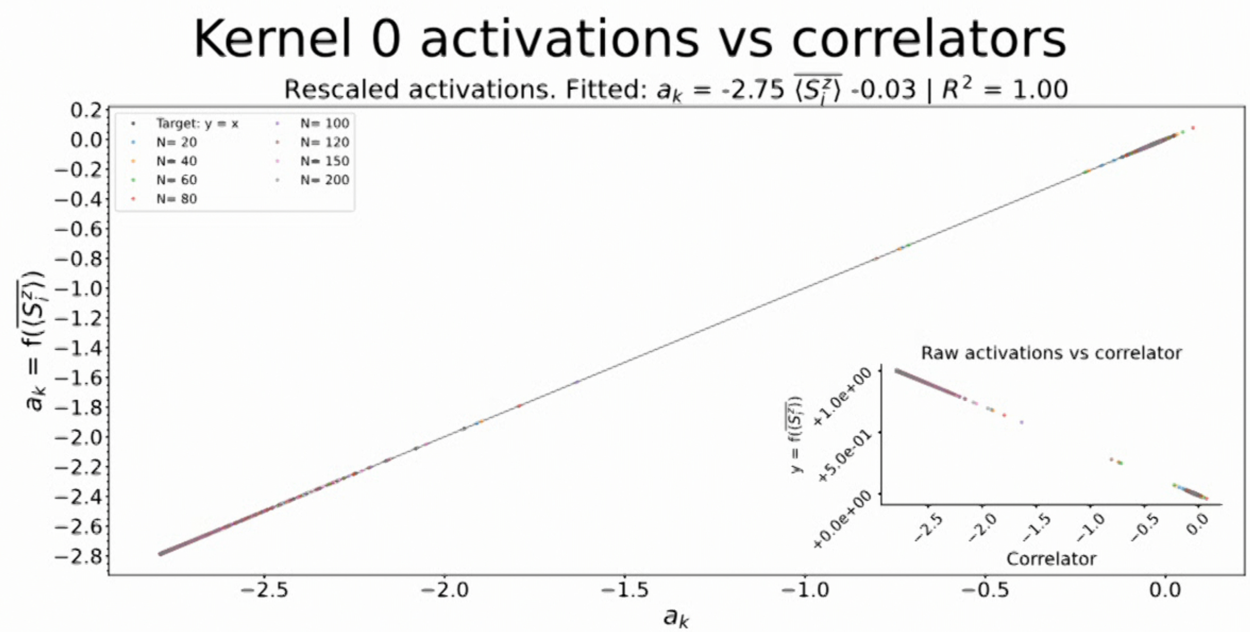
1D transverse-field Ising

Data in *z* basis

Detected correlators computed for input data

SR / lin reg

Bottleneck



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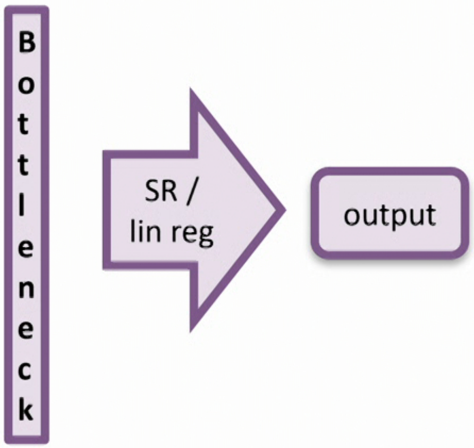
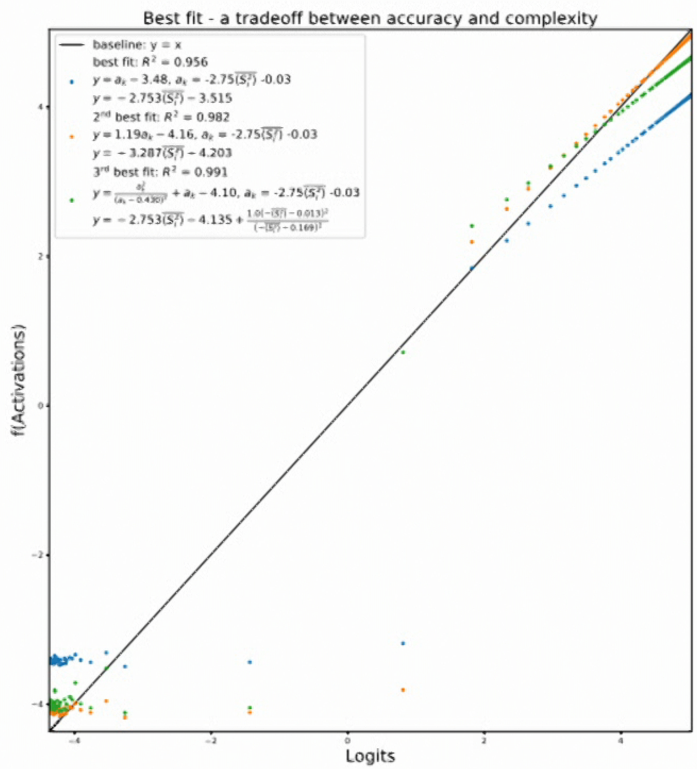
1D transverse-field Ising

Data in z basis





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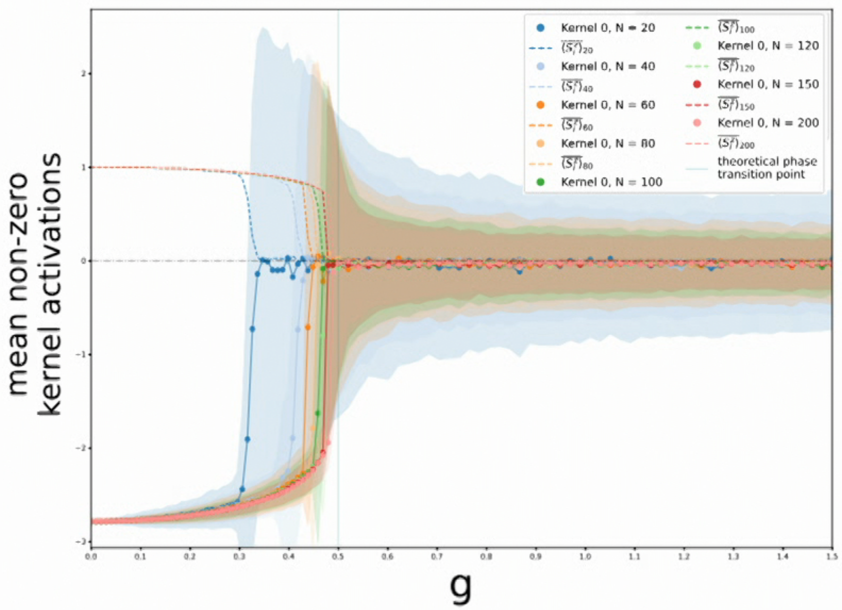
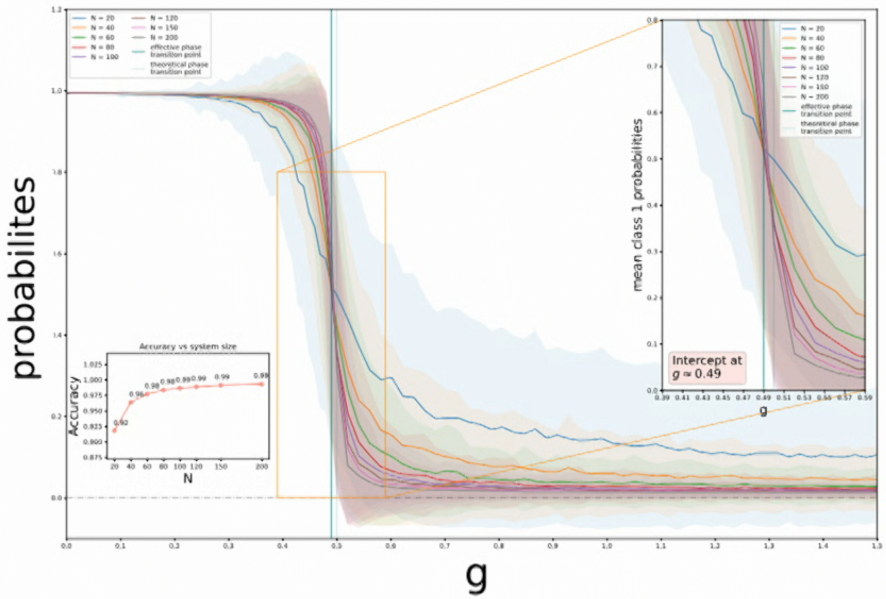
1D transverse-field Ising

Data in *z* basis





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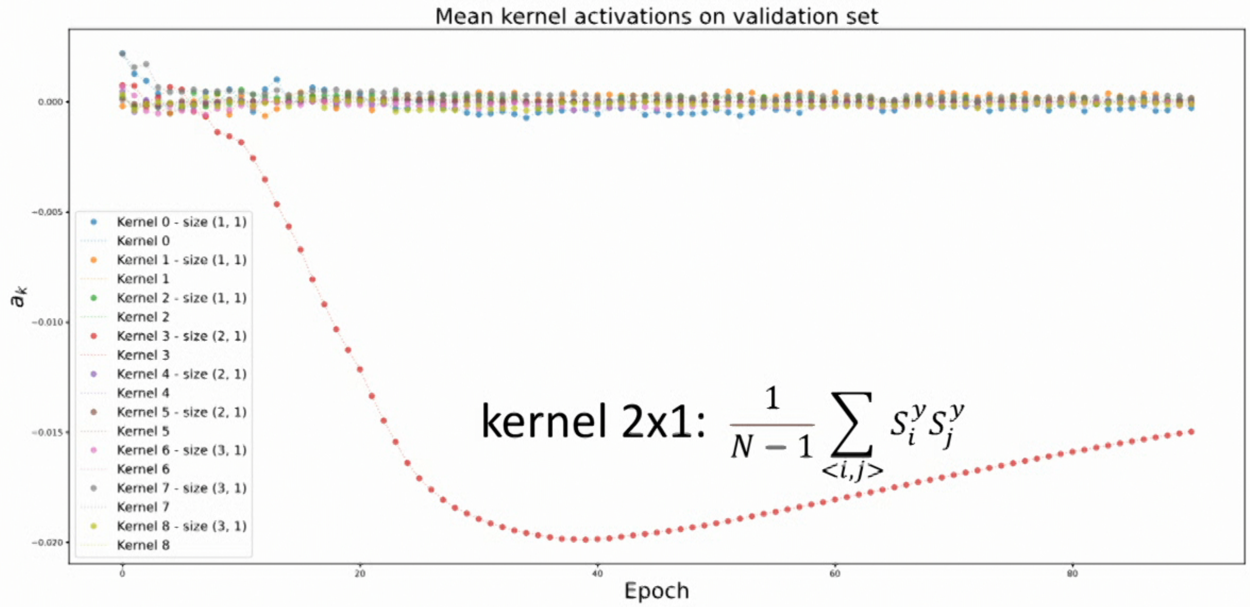
1D transverse-field Ising

Data in *y* basis



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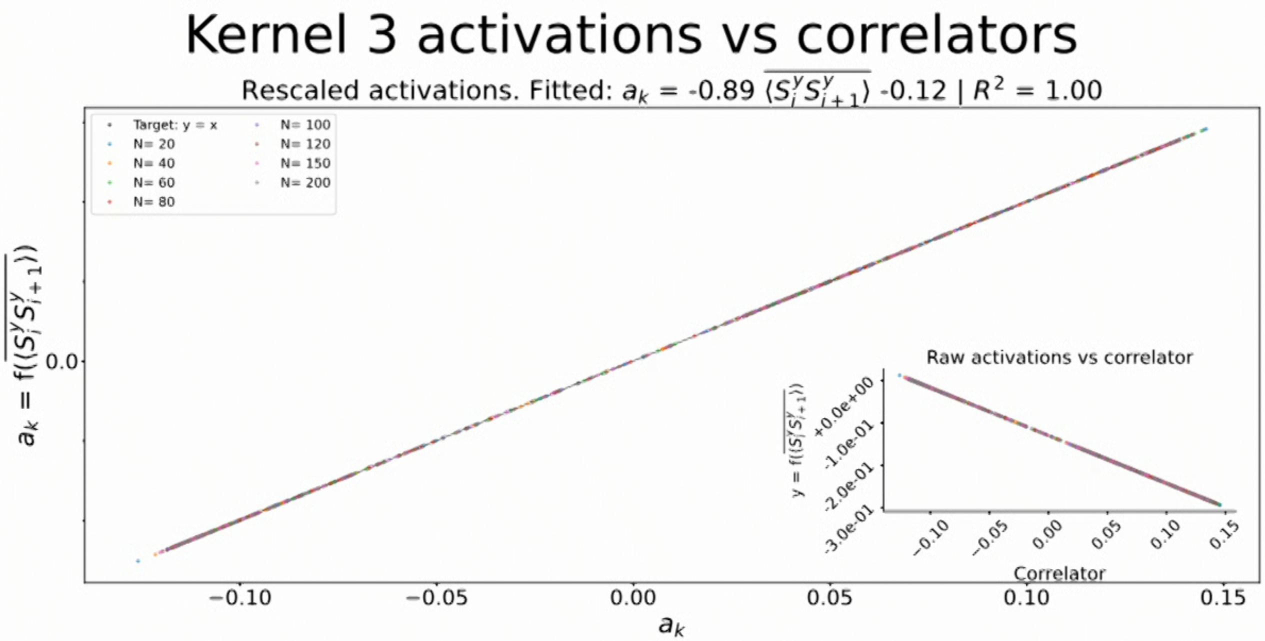
1D transverse-field Ising

Data in *y* basis



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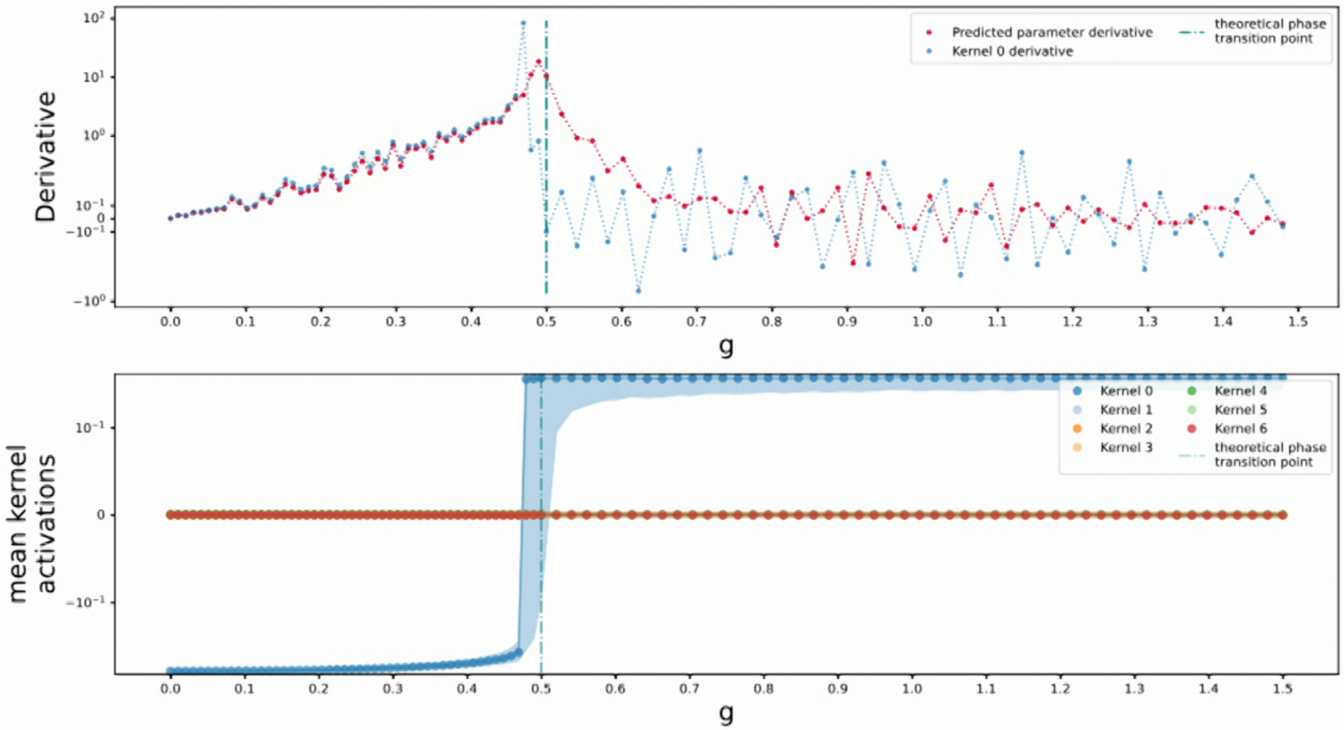
How to make it unsupervised?

Prediction-based method by Eliška *et al*!



$y = -1.176\overline{\langle S_i^z \rangle} + 0.426$

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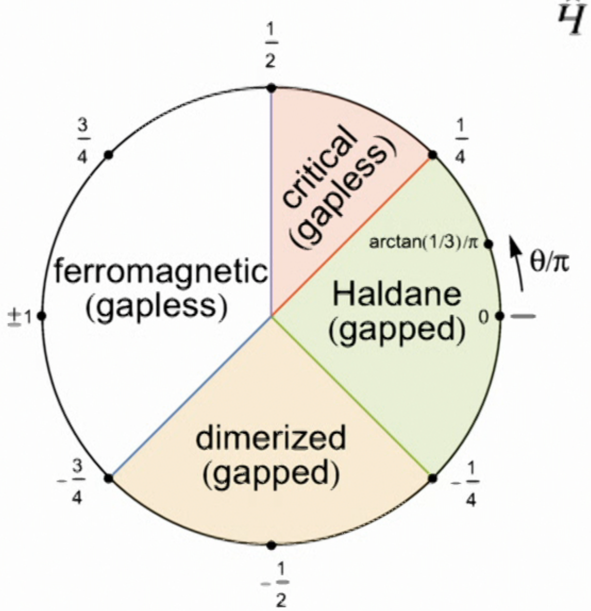
1D bilinear-biquadratic **spin-1** Heisenberg model

$$\hat{\mathcal{H}} = \sum_{i=1}^{N} \cos(\theta)\left(\vec{S}_i \otimes \vec{S}_{i+1}\right) + \sin(\theta)\left(\vec{S}_i \otimes \vec{S}_{i+1}\right)^2$$



M. V. Rakov & M. Weyrauch (2022)
Phys. Rev. B 105, 024424

$(S_i^d)^2 \in \{0,1\}$

$$(S_i^d)^p = \begin{cases} (S_i^d)^2 & \text{if } p \text{ is even} \\ S_i^d & \text{if } p \text{ is odd} \end{cases} \Longrightarrow$$

$S_i^d \in \{-1,0,1\}$

We need to modify our Taylor expansion (spin-1!)

$$f\left(S_i^z, S_{i+1}^z\right) = C_1 + C_2 S_i^z + C_3 S_{i+1}^z + C_4 S_i^z S_{i+1}^z + C_5 \left(S_i^z\right)^2$$
$$+ C_6 \left(S_{i+1}^z\right)^2 + C_7 \left(S_i^z\right)^2 S_{i+1}^z + C_8 S_i^z \left(S_{i+1}^z\right)^2 + C_9 \left(S_i^z S_{i+1}^z\right)^2$$

DMRG using ITensors.jl library in Julia

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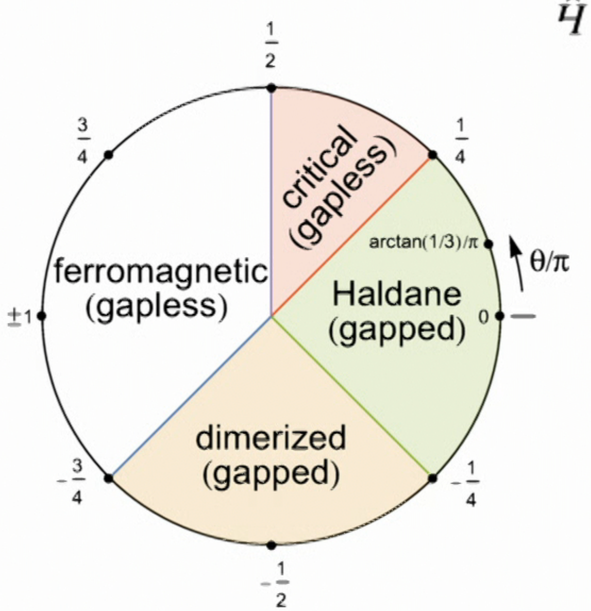
1D bilinear-biquadratic **spin-1** Heisenberg model

$$\hat{\mathcal{H}} = \sum_{i=1}^{N} \cos(\theta)\left(\vec{S}_i \otimes \vec{S}_{i+1}\right) + \sin(\theta)\left(\vec{S}_i \otimes \vec{S}_{i+1}\right)^2$$



M. V. Rakov & M. Weyrauch (2022)
Phys. Rev. B 105, 024424

Preliminary!!

- Because our DMRG-generated data is suboptimal
- Because we need to regularize the CNN more

DMRG using ITensors.jl library in Julia

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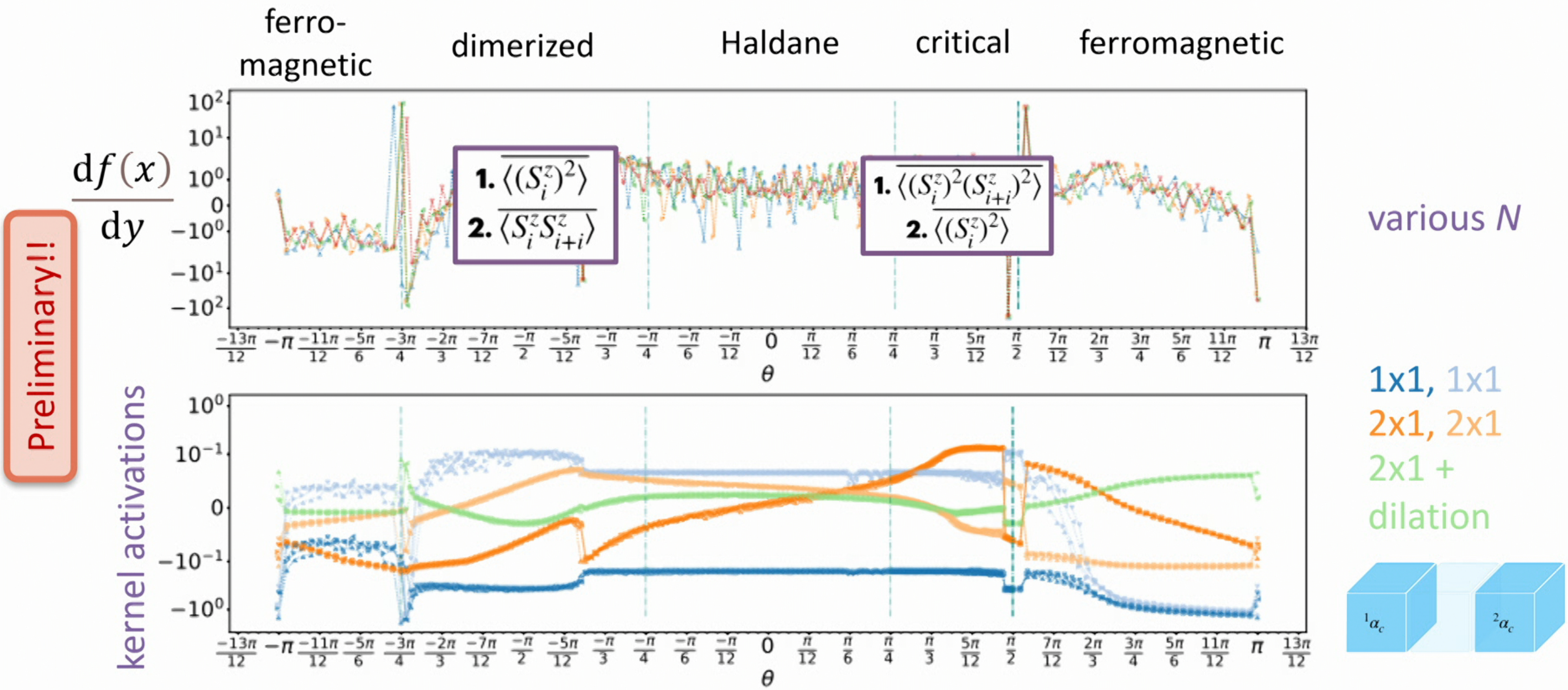
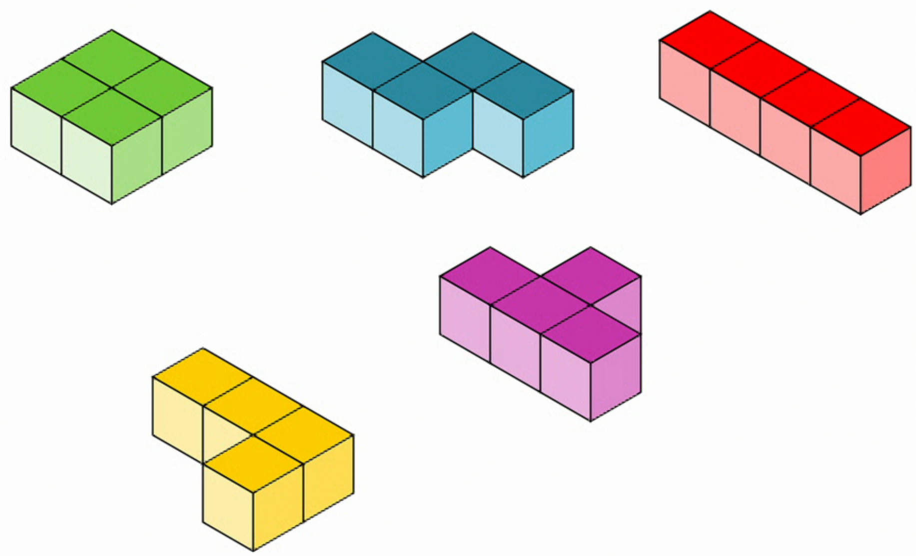
1D bilinear-biquadratic spin-1 Heisenberg model



Läuchli et al. (2006) Phys. Rev. B 74, 144426

Extensions

1. Design special kernels to detect string-type order parameters
2. Apply to 2D: symmetric and non-symmetric gapped convolutions
3. Apply to 2D with topological order (Ising gauge theory-ready!)
4. Combine with Siamese NNs
5. Adaptive convolution kernels, *arXiv:2009.06385*



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Take-home message

Force your NN to speak the language you know!

Beware! Limits expressivity!

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