Title: Machine Learning (2021/2022)

Speakers: Lauren Hayward

Collection: Machine Learning (2021/2022)

Date: May 05, 2022 - 11:30 AM

URL: https://pirsa.org/22050011

Abstract: This course is designed to introduce modern machine learning techniques for studying classical and quantum many-body problems encountered in condensed matter, quantum information, and related fields of physics. Lectures will focus on introducing machine learning algorithms and discussing how they can be applied to solve problem in statistical physics. Tutorials and homework assignments will concentrate on developing programming skills to study the problems presented in lecture.

Machine Learning for Many-Body Physics
Lecture #15

Roger Melko

UNIVERSITY OF WATERLOO

PI QUANTUM INTELLIGENCE LAB

Outline

- A cherrypicked history of ML in physics
- Research by Perimeter students
    - Supervised & unsupervised learning in physics
    - The role of industry connections in research
- The frontier of quantum + machine learning

Condensed matter physics and (machine) learning

Philip W. Anderson

Nobel Prize 1977
(Semiconductors, superconductivity, magnetism)

Harvard, Bell Labs, Cambridge, Princeton

The ability to reduce everything to simple fundamental laws does not imply the ability to start from those laws and reconstruct the universe

The constructionist hypothesis breaks down when confronted with the twin difficulties of scale and complexity.

Condensed matter physics and (machine) learning

In Phil's thinking, `consciousness' was an emergent property of inanimate matter.

Around 1985, while discussing this issue at Princeton we had a bet. He said, in about 30 years from now our friends will build machines (artificial intelligence) which will possess, what you call `consciousness'. I said it will not happen. We had a bet.

. . .

Phil and Baskaran

Condensed matter physics and (machine) learning

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. . .

One day we were both traveling in a train, from Princeton junction to NY city… It was around early 1987…

As usual we had discussion on a variety of topics and turned into issue of `consciousness'. I told him, `Phil, I can understand, using laws of quantum mechanics etc., rigidity of solids, magnetism, superconductivity and so on. With no stretch of my imagination I can comprehend the possibility of emergence of self, self awareness, consciousness etc. ..'

Phil smiled and said, `Yes, things do become thorny'.

Then his attention got diverted…

Phil and Baskaran

Condensed matter physics and (machine) learning

John Hopfield

Buckley Prize, 1968

"For their joint work combining theory and experiment which has advanced the understanding of the interaction of light with solids"

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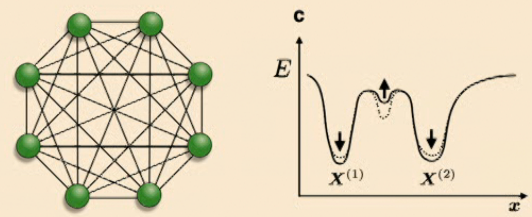


G. Torlai, PhD Thesis
https://uwspace.uwaterloo.ca/handle/10012/14196

“Over time, his research meandered from hard physics to neuroscience, where he applied his knowhow from the former to construct an artificial neural network capable of modeling certain functions of the human brain.

Decades later, these fundamental concepts have helped to unleash the tide of “deep learning” technologies that allow machines to observe, remember, and learn on their own.”

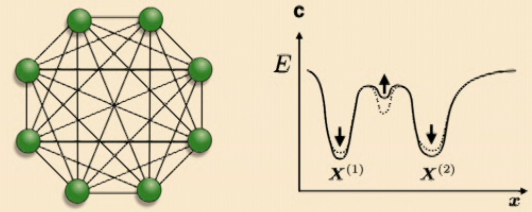
“The Hopfield neural net was not only an intriguing demonstration of possibility and a proof by demonstration of the information-handling capabilities of neural nets, but also was an enormous stimulant in reviving the perceptron and other machine-learning programs.”

Condensed matter physics and (machine) learning

John Hopfield

Buckley Prize, 1968

"For their joint work combining theory and experiment which has advanced the understanding of the interaction of light with solids"



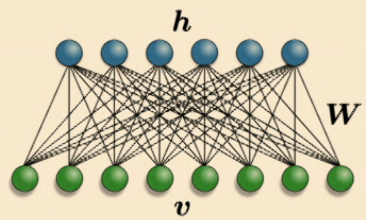
G. Torlai, PhD Thesis
https://uwspace.uwaterloo.ca/handle/10012/14196

2020 Nicholas Metropolis Award for Outstanding Doctoral Thesis Work in Computational Physics Recipient

Giacomo Torlai

Citation:

"*For pioneering achievements in adopting machine learning technology, especially restricted Boltzmann Machines, into the field of condensed matter and quantum information physics.*"



$$p_{\boldsymbol{\lambda}}(\boldsymbol{v}) = \mathrm{Tr}_{\boldsymbol{h}}\left[p_{\boldsymbol{\lambda}}(\boldsymbol{v},\boldsymbol{h})\right] = Z_{\boldsymbol{\lambda}}^{-1}\sum_{\boldsymbol{h}} e^{-E_{\boldsymbol{\lambda}}(\boldsymbol{v},\boldsymbol{h})}$$

$$E_{\boldsymbol{\lambda}}(\boldsymbol{v},\boldsymbol{h}) = -\sum_{j=1}^{N}\sum_{i=1}^{n_h} W_{ij}h_iv_j - \sum_{j=1}^{N} b_jv_j - \sum_{i=1}^{n_h} c_ih_i$$

Outline

- A cherrypicked history of ML in physics
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Quantum Physics

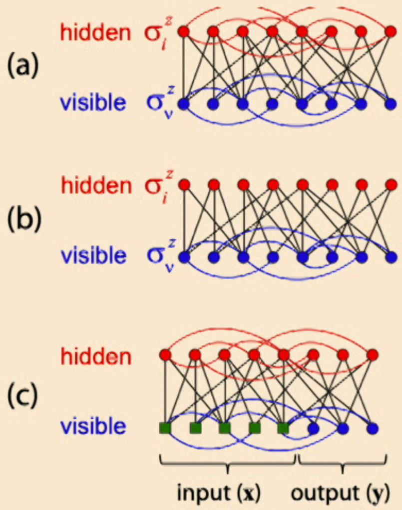
[Submitted on 8 Jan 2016]

Quantum Boltzmann Machine

Mohammad H. Amin, Evgeny Andriyash, Jason Rolfe, Bohdan Kulchytskyy, Roger Melko

Inspired by the success of Boltzmann Machines based on classical Boltzmann distribution, we propose a new machine learning approach based on quantum Boltzmann distribution of a transverse-field Ising Hamiltonian. Due to the non-commutative nature of quantum mechanics, the training process of the Quantum Boltzmann Machine (QBM) can become nontrivial. We circumvent the problem by introducing bounds on the quantum probabilities. This allows us to train the QBM efficiently by sampling. We show examples of QBM training with and without the bound, using exact diagonalization, and compare the results with classical Boltzmann training. We also discuss the possibility of using quantum annealing processors like D-Wave for QBM training and application.

$$H = -\sum_a \Gamma_a \sigma_a^x - \sum_a b_a \sigma_a^z - \sum_{a,b} w_{ab} \sigma_a^z \sigma_b^z$$



arXiv > cond-mat > arXiv:1704.05848

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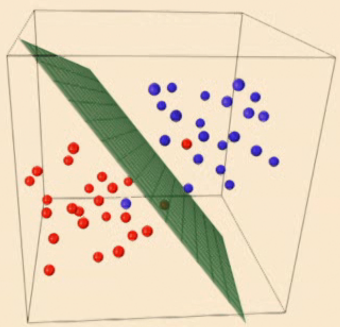
Condensed Matter > Statistical Mechanics

[Submitted on 19 Apr 2017]

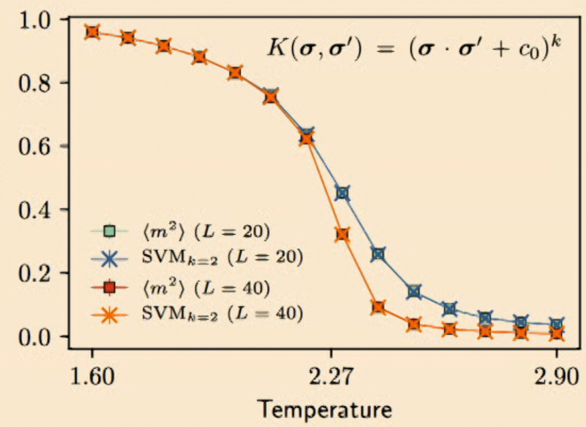
Kernel methods for interpretable machine learning of order parameters

Pedro Ponte, Roger G. Melko

Machine learning is capable of discriminating phases of matter, and finding associated phase transitions, directly from large data sets of raw state configurations. In the context of condensed matter physics, most progress in the field of supervised learning has come from employing neural networks as classifiers. Although very powerful, such algorithms suffer from a lack of interpretability, which is usually desired in scientific applications in order to associate learned features with physical phenomena. In this paper, we explore support vector machines (SVMs) which are a class of supervised kernel methods that provide interpretable decision functions. We find that SVMs can learn the mathematical form of physical discriminators, such as order parameters and Hamiltonian constraints, for a set of two-dimensional spin models: the ferromagnetic Ising model, a conserved-order-parameter Ising model, and the Ising gauge theory. The ability of SVMs to provide interpretable classification highlights their potential for automating feature detection in both synthetic and experimental data sets for condensed matter and other many-body systems.



$$d(\boldsymbol{x}) = \sum_{i=1}^{N} \alpha_i y_i K(\boldsymbol{x}^{(i)}, \boldsymbol{x}) + b,$$



– Optimal hyperplane for linearly separable patterns
– Extend to patterns that are not linearly separable by transformations of original data to map into new space – the **Kernel** function

arXiv > cond-mat > arXiv:2102.01103

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Condensed Matter > Strongly Correlated Electrons

[Submitted on 1 Feb 2021 (v1), last revised 12 Sep 2021 (this version, v2)]

Machine-Learned Phase Diagrams of Generalized Kitaev Honeycomb Magnets

Nihal Rao, Ke Liu, Marc Machaczek, Lode Pollet

We use a recently developed interpretable and unsupervised machine-learning method, the tensorial kernel support vector machine (TK-SVM), to investigate the low-temperature classical phase diagram of a generalized Heisenberg-Kitaev-Γ (J-K-Γ) model on a honeycomb lattice. Aside from reproducing phases reported by previous quantum and classical studies, our machine finds a hitherto missed nested zigzag-stripy order and establishes the robustness of a recently identified modulated $S_3 \times Z_3$ phase, which emerges through the competition between the Kitaev and Γ spin liquids, against Heisenberg interactions. The results imply that, in the restricted parameter space spanned by the three primary exchange interactions -- J, K, and Γ, the representative Kitaev material α-$RuCl_3$ lies close to the boundaries of several phases, including a simple ferromagnet, the unconventional $S_3 \times Z_3$ and nested zigzag-stripy magnets. A zigzag order is stabilized by a finite Γ' and/or J_3 term, whereas the four magnetic orders may compete in particular if Γ' is anti-ferromagnetic.

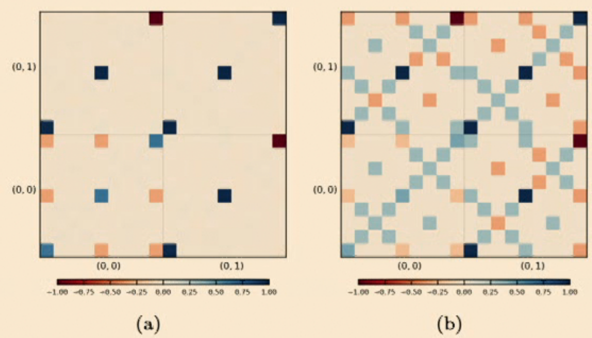


FIG. 14. Representative blocks of the $C_{\mu\nu}$ matrices of the ZZ/D_{2h} phase learned by a rank-2 TK-SVM with the eight-spin D_{2h} magnetic cell, away from (a) and at (b) the $O(3)$ point. Blocks are labeled by the spin indices (i, j). Nonvanishing entries in a block correspond to correlations between quadratic components $S_i^\alpha S_j^\beta$ and $S_{i'}^{\alpha'} S_{j'}^{\beta'}$. Negative elements in the $(0, 0)$ block reflect the spin normalization $|\vec{S}| = 1$. Nontrivial entries in (a) are the diagonal ones in each 9×9 sub-block.

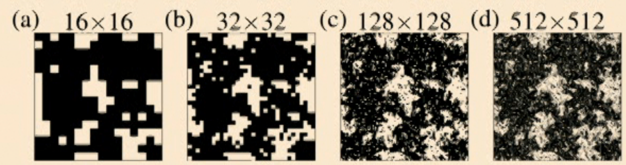
Condensed Matter > Statistical Mechanics

[Submitted on 4 Oct 2018 (v1), last revised 30 Jan 2019 (this version, v2)]

Super-resolving the Ising model with convolutional neural networks

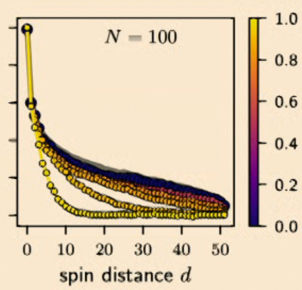
Stavros Efthymiou, Matthew J. S. Beach, Roger G. Melko

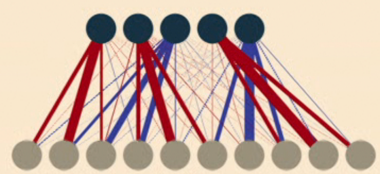
Machine learning is becoming widely used in condensed matter physics. Inspired by the concept of image super-resolution, we propose a method to increase the size of lattice spin configurations using deep convolutional neural networks. Through supervised learning on Monte Carlo (MC) generated spin configurations, we train networks that invert real-space renormalization decimations. We demonstrate that super-resolution can reproduce thermodynamic observables that agree with MC calculations for the one and two-dimensional Ising model at various temperatures. We find that it is possible to predict thermodynamic quantities for lattice sizes larger than those used in training by extrapolating the parameters of the network. We use this method to extrapolate the exponents of the 2D Ising critical point towards the thermodynamic limit, which results in good agreement with theory.



$$H = -\sum_{\langle i,j \rangle} \sigma_i \sigma_j$$

FIG. 2. Critical configurations obtained using the weight extrapolation idea presented in Section II C. We show the original Monte Carlo configuration in (a) and the results after (b) one, (c) three and (d) five consecutive super-resolutions.





A. Golubeva

Ψ

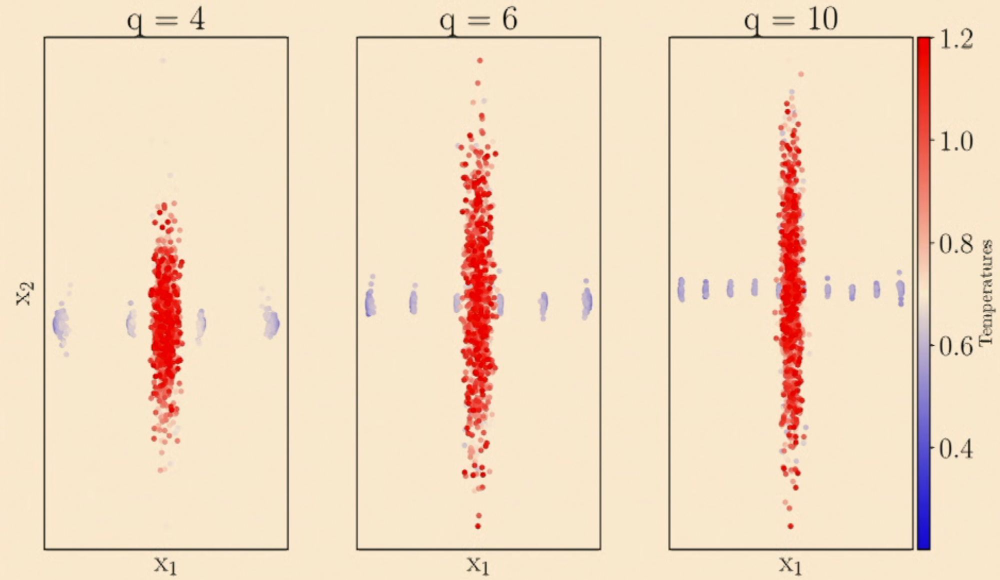
Distinguishing phases and detecting local and non-local order using t-SNE and Monte Carlo methods

Matthew Duschenes

An essay submitted for partial fulfilment of Perimeter Scholars International

June, 2018

PCA of Pott's model



$$H_{\text{Potts}} = -J \sum_{<ij>} \delta_{s_i s_j} \qquad s_i \in \{1, 2, ..., q\}$$

arXiv > cond-mat > arXiv:1710.09842

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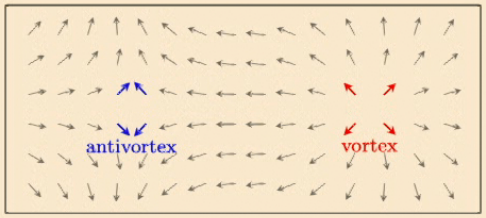
Condensed Matter > Statistical Mechanics

[Submitted on 26 Oct 2017]

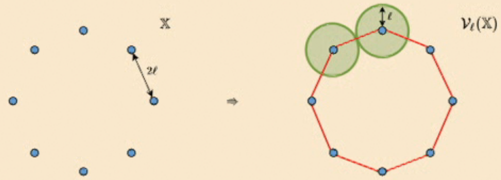
Machine learning vortices at the Kosterlitz-Thouless transition

Matthew J. S. Beach, Anna Golubeva, Roger G. Melko

Efficient and automated classification of phases from minimally processed data is one goal of machine learning in condensed matter and statistical physics. Supervised algorithms trained on raw samples of microstates can successfully detect conventional phase transitions via learning a bulk feature such as an order parameter. In this paper, we investigate whether neural networks can learn to classify phases based on topological defects. We address this question on the two-dimensional classical XY model which exhibits a Kosterlitz-Thouless transition. We find significant feature engineering of the raw spin states is required to convincingly claim that features of the vortex configurations are responsible for learning the transition temperature. We further show a single-layer network does not correctly classify the phases of the XY model, while a convolutional network easily performs classification by learning the global magnetization. Finally, we design a deep network capable of learning vortices without feature engineering. We demonstrate the detection of vortices does not necessarily result in the best classification accuracy, especially for lattices of less than approximately 1000 spins. For larger systems, it remains a difficult task to learn vortices.



$$\mathcal{H}_{XY} = -J \sum_{\langle ij \rangle} \cos(\theta_i - \theta_j)$$



Dan Sehayek

arXiv > hep-lat > arXiv:1904.12072

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High Energy Physics - Lattice

[Submitted on 26 Apr 2019 (v1), last revised 9 Sep 2019 (this version, v3)]

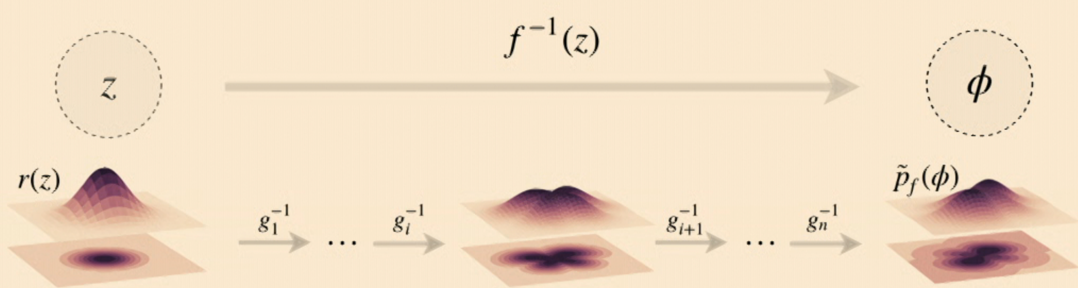
Flow-based generative models for Markov chain Monte Carlo in lattice field theory

M. S. Albergo, G. Kanwar, P. E. Shanahan

A Markov chain update scheme using a machine-learned flow-based generative model is proposed for Monte Carlo sampling in lattice field theories. The generative model may be optimized (trained) to produce samples from a distribution approximating the desired Boltzmann distribution determined by the lattice action of the theory being studied. Training the model systematically improves autocorrelation times in the Markov chain, even in regions of parameter space where standard Markov chain Monte Carlo algorithms exhibit critical slowing down in producing decorrelated updates. Moreover, the model may be trained without existing samples from the desired distribution. The algorithm is compared with HMC and local Metropolis sampling for ϕ^4 theory in two dimensions.

Comments: 13 pages, 7 figures; corrected normalization conventions in eqns. 20 and 23

Subjects: **High Energy Physics - Lattice (hep-lat)**; Disordered Systems and Neural Networks (cond-mat.dis-nn); Statistical Mechanics (cond-mat.stat-mech); Machine Learning (cs.LG)



(a) Normalizing flow between prior and output distributions arXiv > quant-ph > arXiv:2105.08086

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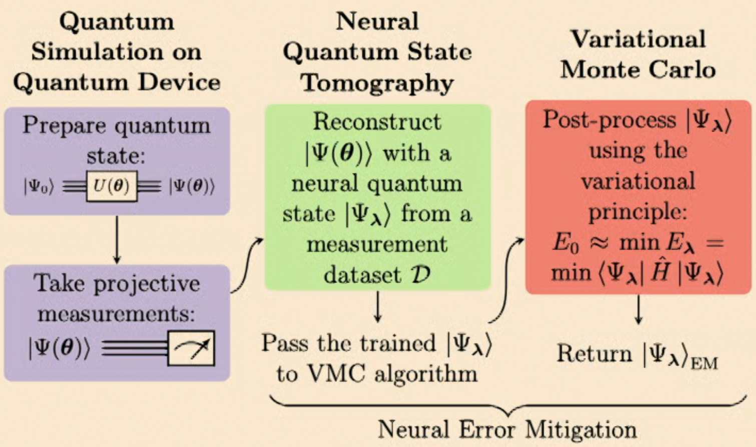
Quantum Physics

[Submitted on 17 May 2021]

Neural Error Mitigation of Near-Term Quantum Simulations

Elizabeth R. Bennewitz, Florian Hopfmueller, Bohdan Kulchytskyy, Juan Carrasquilla, Pooya Ronagh

One of the promising applications of early quantum computers is the simulation of quantum systems. Variational methods for near-term quantum computers, such as the variational quantum eigensolver (VQE), are a promising approach to finding ground states of quantum systems relevant in physics, chemistry, and materials science. These approaches, however, are constrained by the effects of noise as well as the limited quantum resources of near-term quantum hardware, motivating the need for quantum error mitigation techniques to reduce the effects of noise. Here we introduce *neural error mitigation*, a novel method that uses neural networks to improve estimates of ground states and ground-state observables obtained using VQE on near-term quantum computers. To demonstrate our method's versatility, we apply neural error mitigation to finding the ground states of H_2 and LiH molecular Hamiltonians, as well as the lattice Schwinger model. Our results show that neural error mitigation improves the numerical and experimental VQE computation to yield low-energy errors, low infidelities, and accurate estimations of more-complex observables like order parameters and entanglement entropy, without requiring additional quantum resources. Additionally, neural error mitigation is agnostic to both the quantum hardware and the particular noise channel, making it a versatile tool for quantum simulation. Applying quantum many-body machine learning techniques to error mitigation, our method is a promising strategy for extending the reach of near-term quantum computers to solve complex quantum simulation problems.

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WTF is attention
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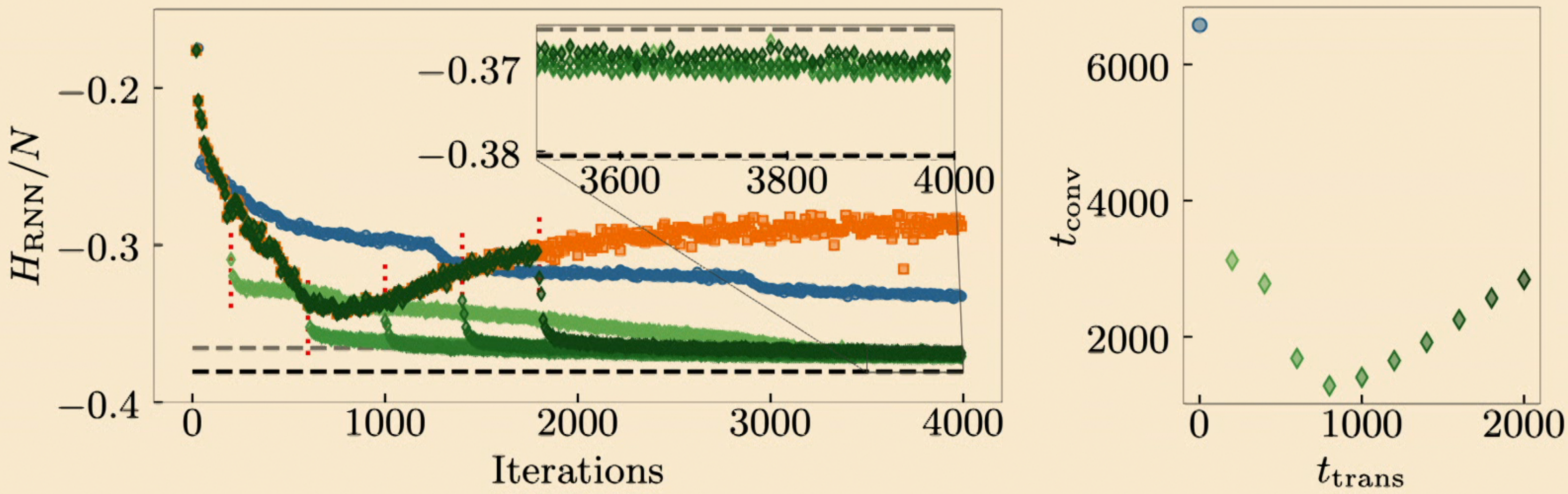
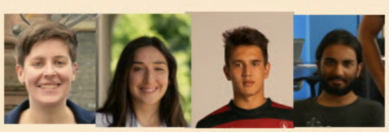
Hybrid optimization of RNN wavefunction for Rydberg arrays

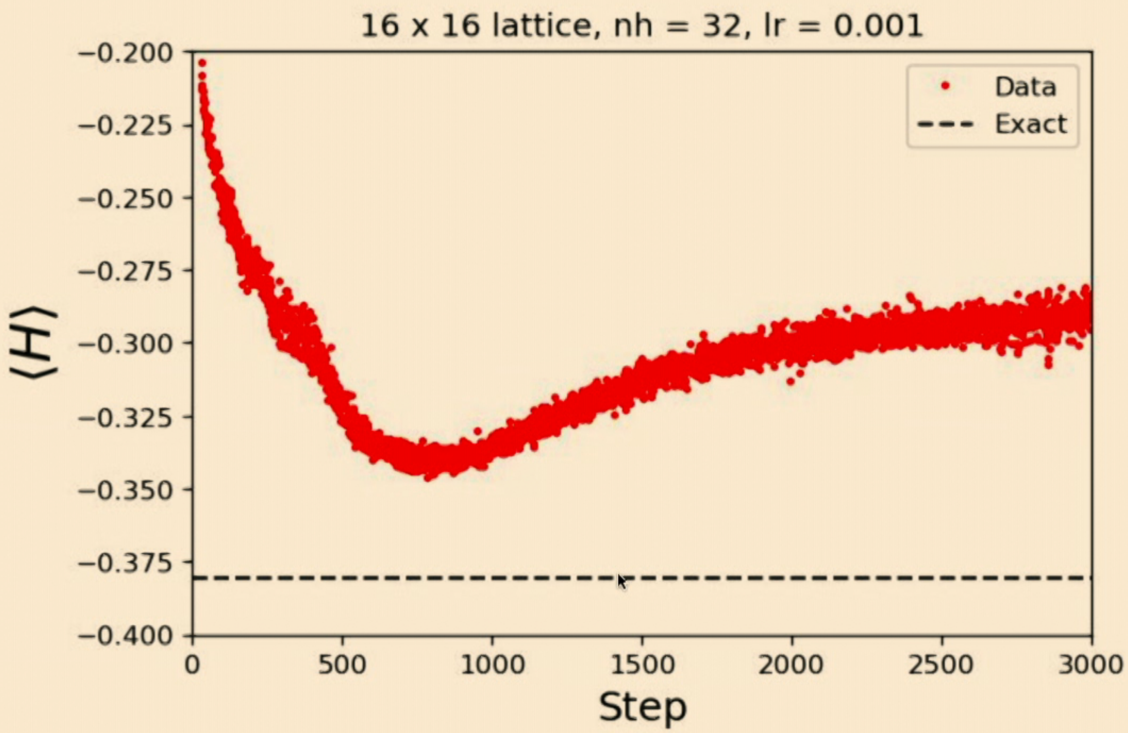


- A limited amount of data-driven pre-training can vastly improve time to solution for variational optimization

arXiv:2203.04988

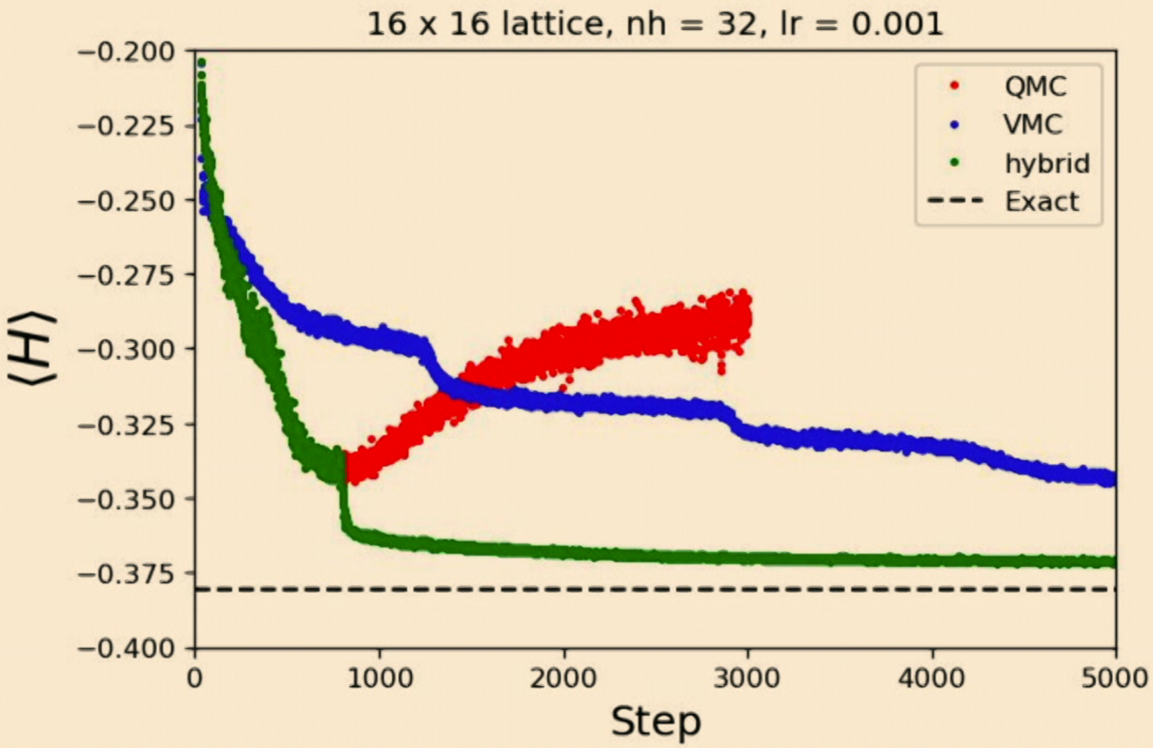


Data-driven optimization of RNN wavefunction for Rydberg arrays

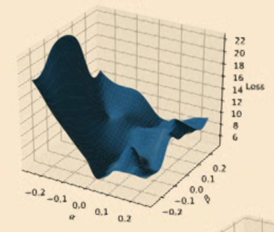


- Overfitting expected due to limited shot budgets in Rydberg experiments

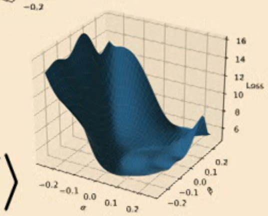
Hybrid optimization of RNN wavefunction for Rydberg arrays



Discussion



$\langle H \rangle$



- Providing measurements for pre-training could be the most exciting application of quantum computers

- The next frontier of physics is the combined fields of condensed matter, quantum information and machine learning

- Industry/academic engagement has always produced breakthroughs in fundamental physics. Startups are the new Bell Labs

- There's no better place to carry on the traditions of this field than at Perimeter

"Where in the Schrödinger equation do you put the joy of being alive?

"It's nice the know the computer understands the situation, but I would like to understand it too."
— Eugene Wigner