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PIANO NAZIONALE DI RIPRESA E RESILIENZA
NQSTI
National Quantum Science and Technology Institute

Missione 4 Istruzione e Ricerca

Quantum Computing @ INFN

29-31 October 2024

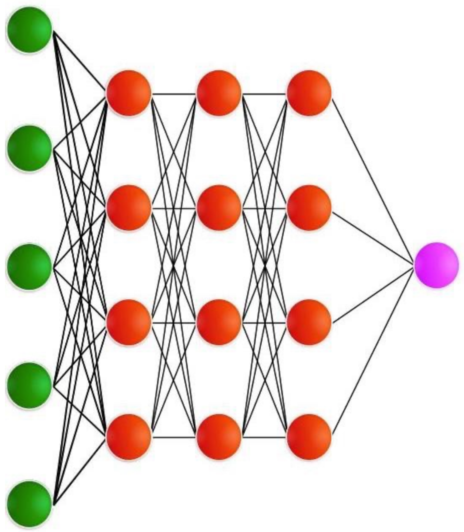
Synergy between quantum computers and classical deep learning

Sebastiano Pilati

Complex Quantum Matter, University of Camerino

IS LINCOLN @ PG

Classical deep learning



Gate-based quantum computers

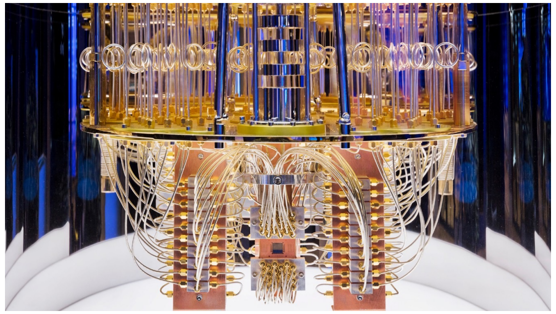


Image from:
https://www.esa.int/ESA_Multimedia/Images/2020/11/Interior_of_IBM_s_quantum_computer

Adiabatic quantum computers

Image from:
https://thequantuminsider.com/2023/05/05/d-wave-quantum-annealer-practical-usage-in-2023/

COLLABORATORS:
<u>Simone Cantori,</u> Luca Brodoloni, Andrea Mari, G. Spada, David Vitali (UniCAM)
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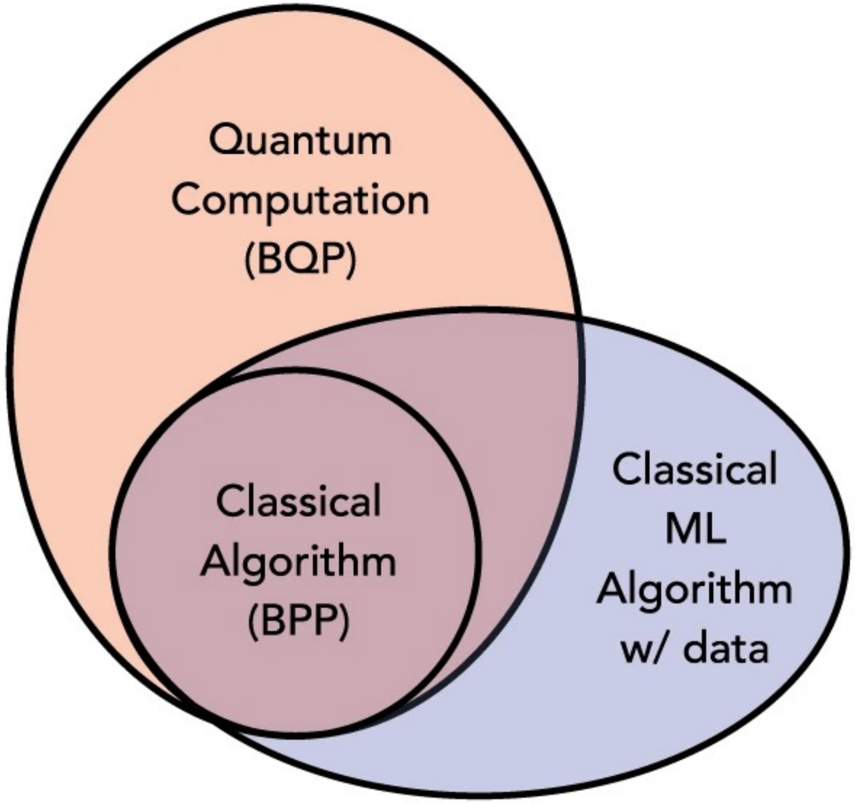
Questions:

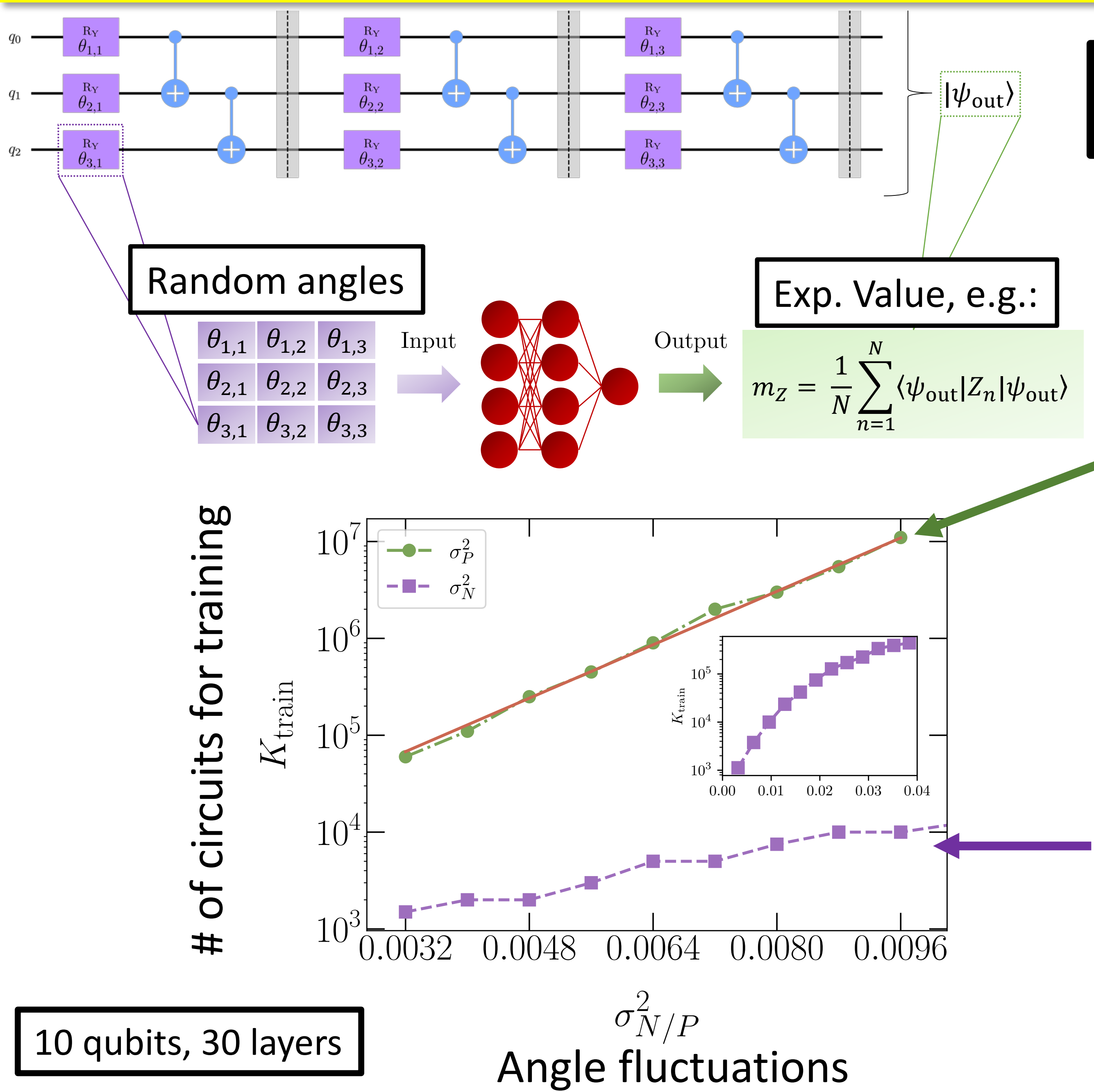
- Can quantum computers outperform classical deep learning?
- Can classical deep learning boost noisy quantum computers?
- Can quantum data boost classical deep learning?

Classical machine learning algorithm trained on (quantum) data can solve otherwise classically intractable problems.

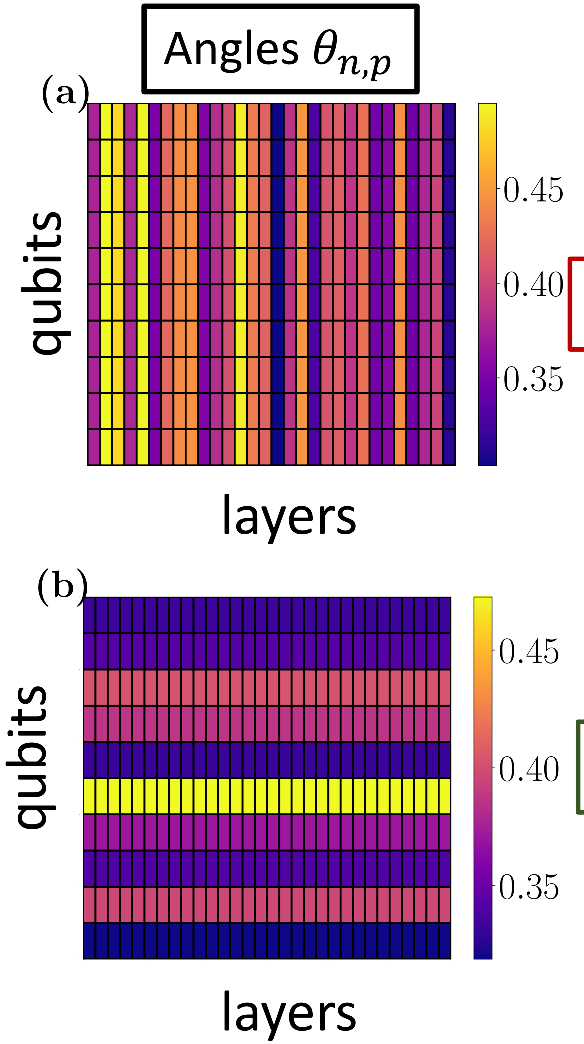


H.-Y. Huang et al, *Power of data in quantum machine learning,* Nat. Commun. **12**, 2631 (2021)
H.-Y. Huang et al., *Provably efficient machine learning for quantum many-body problems,* Science (2022)

Supervised learning of output expectation values



Relevant for VQE, cannot be simulated via Pauli propagation
See: Angrisani *et al.* 2409.01706 (2024)



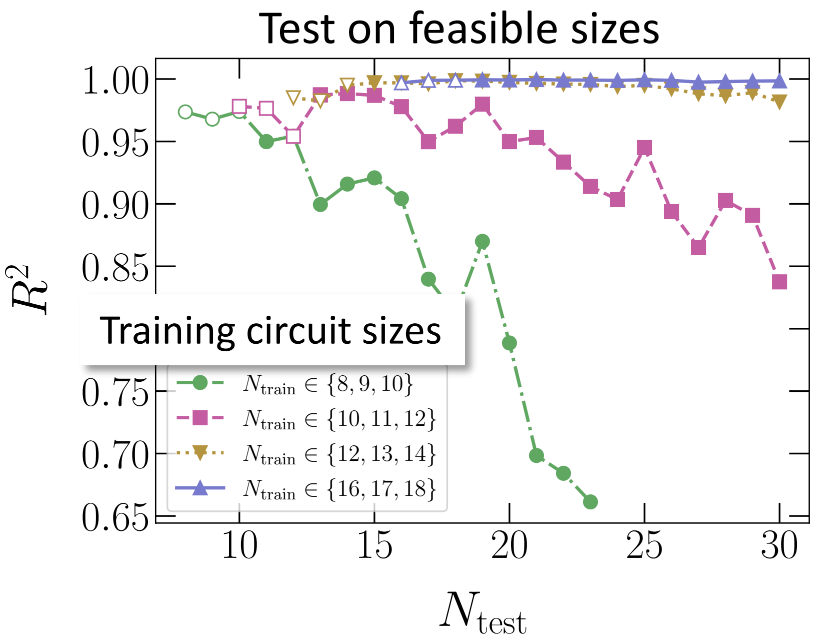
Classically unlearnable

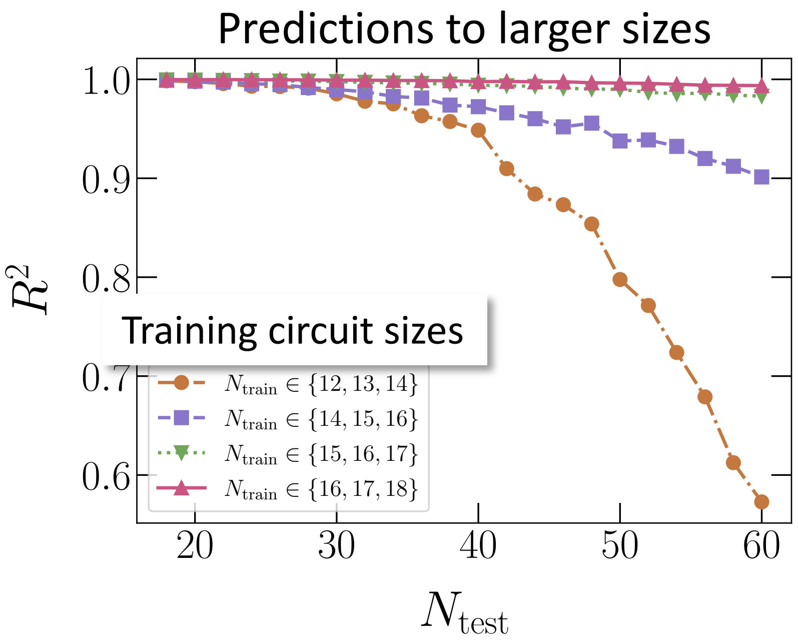
Classically learnable

10 qubits, 30 layers

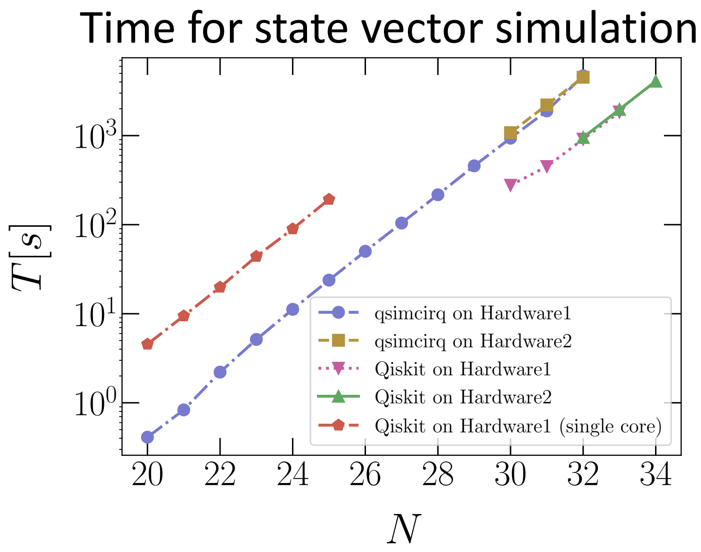
Neural extrapolations to classically intractable circuit sizes

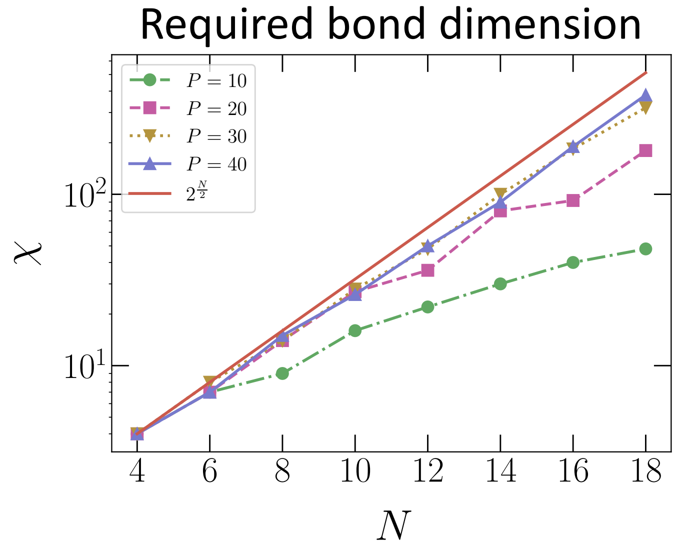
Accuracy





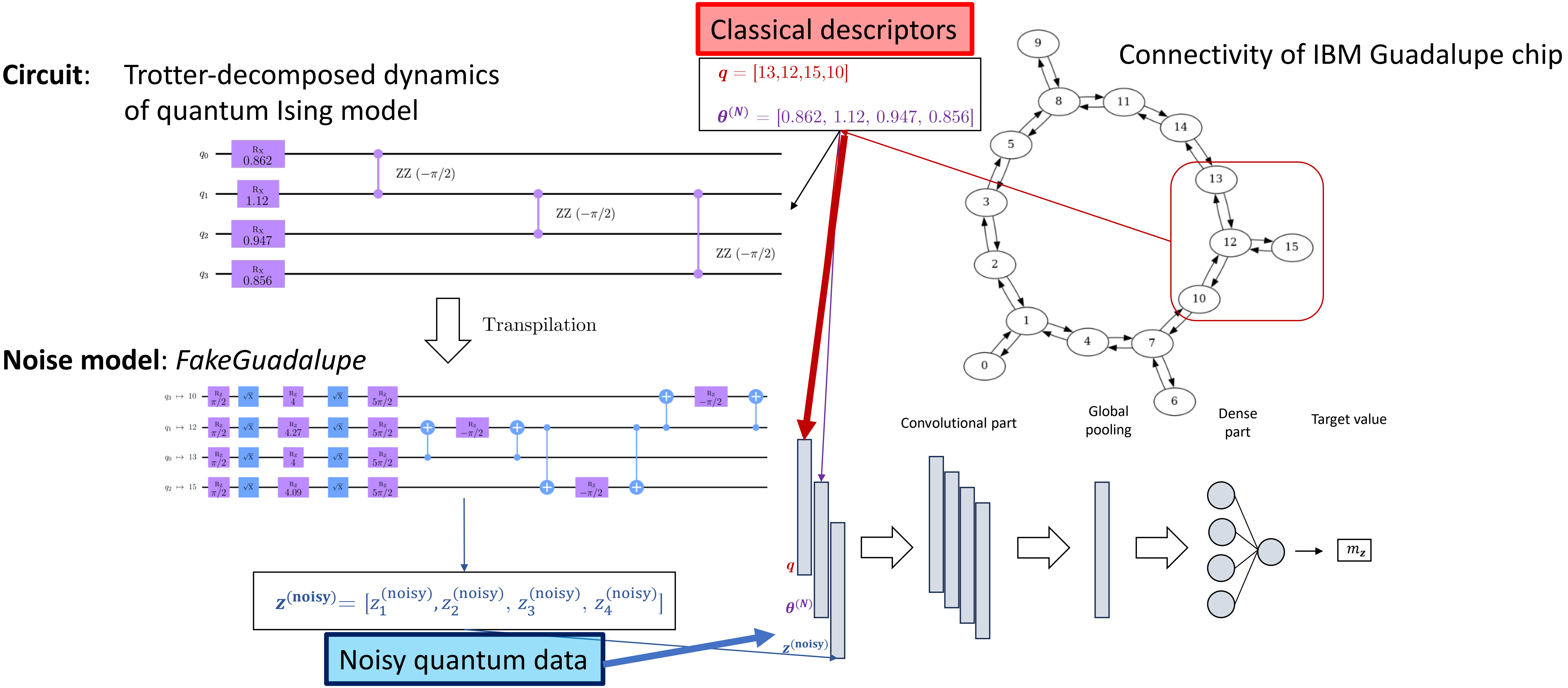
# of qubits for test



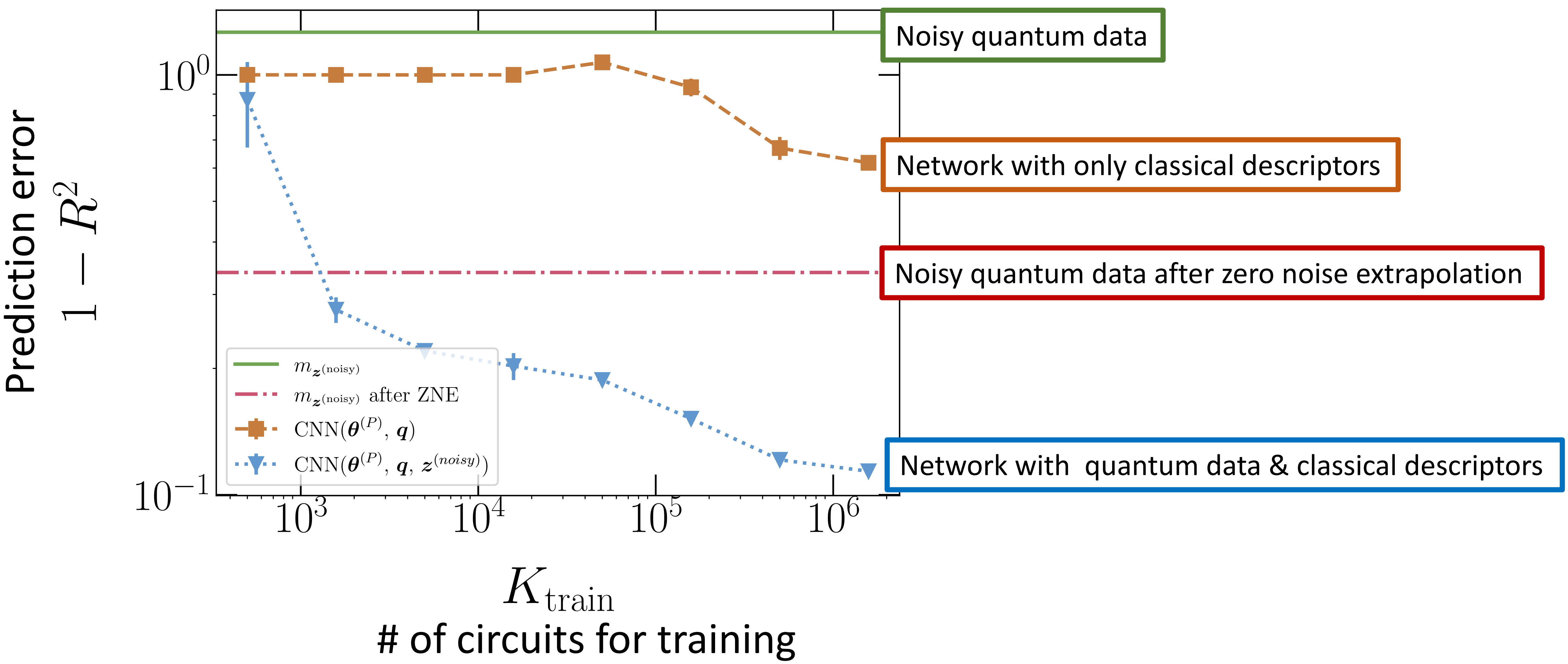


→ Classical simulation unfeasible

Combining classical descriptors and noisy quantum data



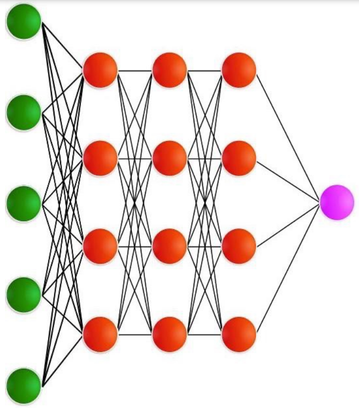
Error mitigation on larger circuits with scalable NNs



Network trained on $\boldsymbol{N \leq 10}$ qubit $P = 20$ layers, tested on $\boldsymbol{N = 16}$

Quantum annealers

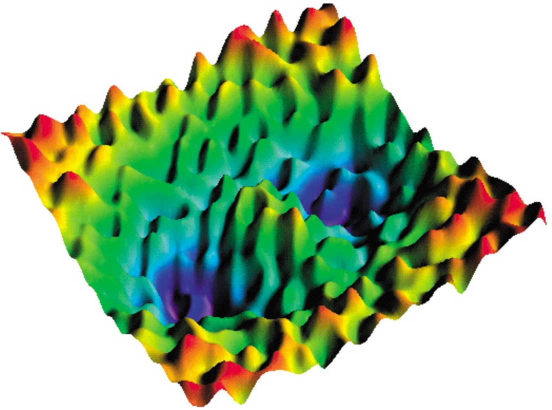
Classical deep learning

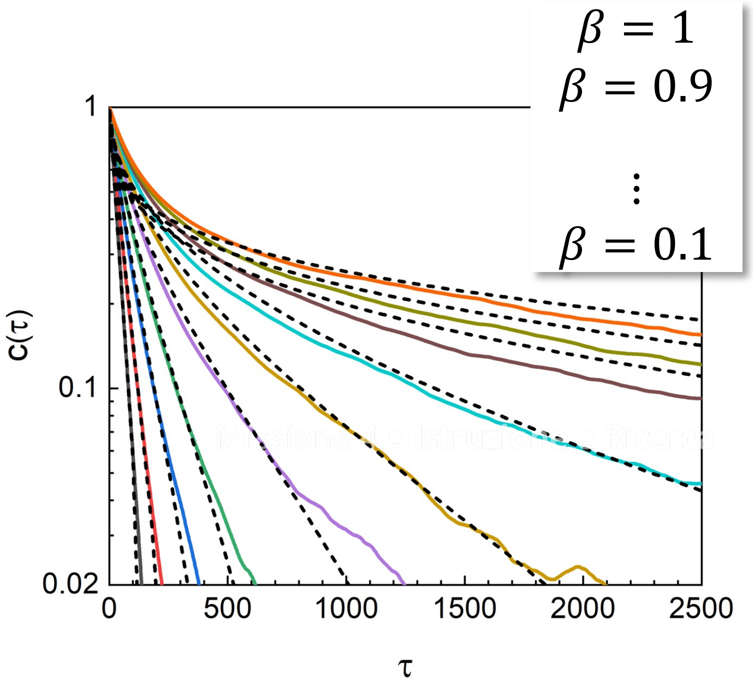


Low-T equilibrium properties of classical spin glasses

$$H = \sum_{ij} J_{ij} x_i x_j$$

Energy landscape





NEURAL CLASSICAL MONTE CARLO SIMULATIONS

Metropolis-Hastings algorithm

Acceptance probability: $A_{\mathbf{x}'\mathbf{x}} = \min\left(1, \frac{p_{\mathrm{BOLTZ}}(\mathbf{x}')w_{\mathbf{x}\mathbf{x}'}}{p_{\mathrm{BOLTZ}}(\mathbf{x})w_{\mathbf{x}'\mathbf{x}}}\right)$

McNaughton, Milošević, Perali, SP, PRE (2020)

Proposals in via NNs: $w_{\mathbf{x}'\mathbf{x}} = p_{\mathrm{NETWORK}}(\mathbf{x}')$

Autoregressive NNs → ancestral sampling

Related work:

- K. A. Nicoli et al., PRE **101**, 023304 (2020): MCMC+autoregressive n. for ferromagnetic models.
- F. Noè et al., Science **365**, 1147 (2019): normalizing flows for complex-molecule simulations.
- X. Ding et al., J. Phys. Chem. B **124**, 10166 (2020): normalizing flows for free-energy computations.
- M. Gabrié et al., arXiv:2105.12603 (2021): adaptive MCMC via normalizing flows.
- G. S. Hartnett, M. Mohseni,arXiv:2001.00585v2 (2020): spin-glass simulations via normalizing flows.

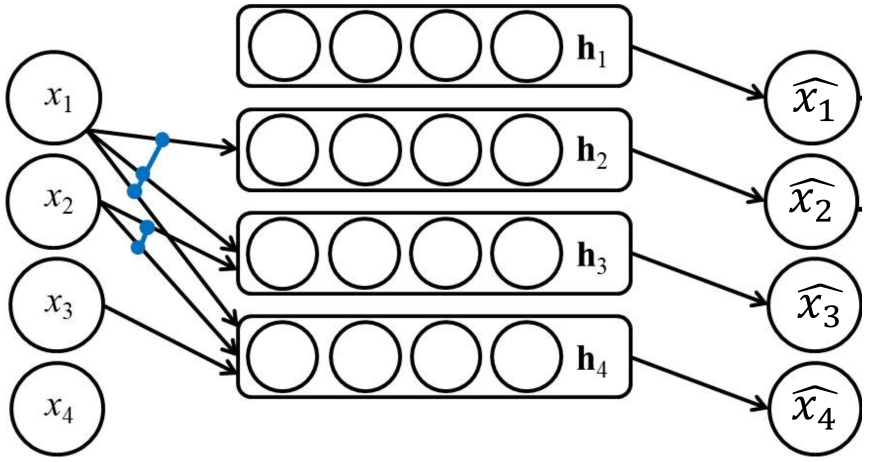
Autoregressive neural networks

Chain of conditional distributions: $p_{\text{Network}}(\mathbf{x}) = \prod_{d=1}^{N} p_d(x_d|\mathbf{x}_{<d})$

$\mathbf{x} \quad = (x_1, \dots, x_N)$
$\mathbf{x}_{<d} = (x_1, \dots, x_{d-1})$

Direct samples via ancestral sampling: given $\mathbf{x}_{<d}$, sample $x_d \backsim p_d(x_d|\mathbf{x}_{<d})$

Normalized probability distribution: $\mathrm{Z} = \sum_{\boldsymbol{x}} p_{\text{Network}}(\boldsymbol{x}) = 1$



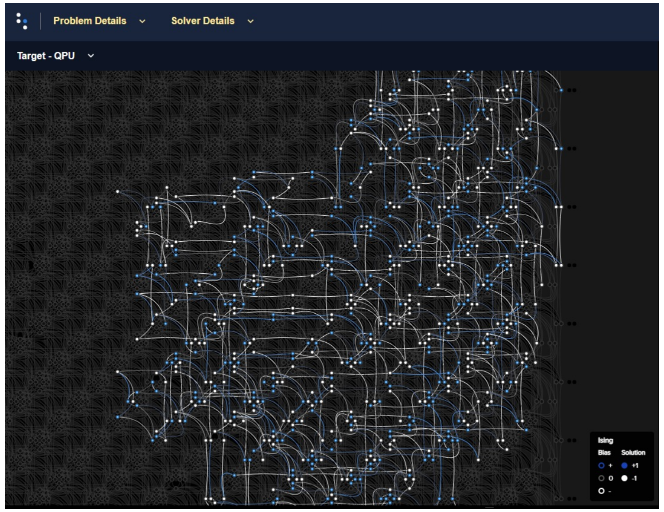
Neural autoregressive distribution estimator (NADE)
H. Larochelle, I. JMLR: W&CP 15 (2011).

Masked Autoencoder for Distribution Estimation (MADE)
M. Germain et al., PMLR 37, 2015 (2015).

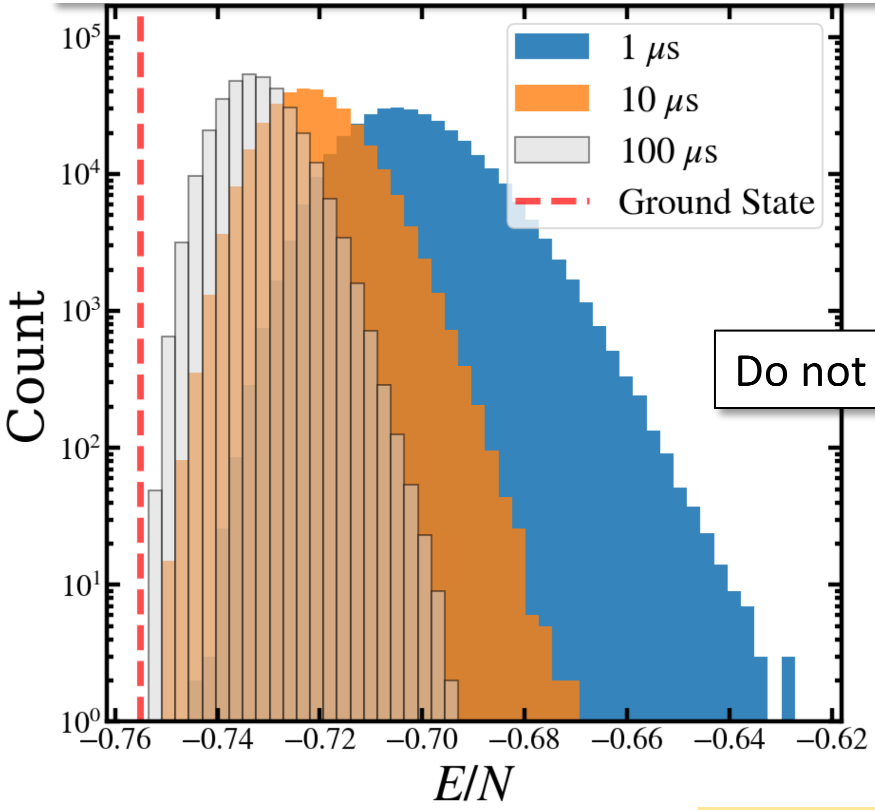
PixelCNN:
A. v. d. Oord et al., arXiv:1601.06759 (2016).

Neural MC with NN trained on D-WAVE data

Access to D-Wave QPU time via CINECA ISCRA Project



Energy histogram of D-Wave data



Do not represent Boltzmann distribution!

2D square lattice N=484
Nearest and next-nearest neighbor interaction
Uniform random couplings

Hybrid MC algorithm: Combines **neural** and **single-spin flip** updates

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Algorithm 2 Hybrid Monte Carlo

Require: τ, N, NN()

$\quad \boldsymbol{\sigma}, q(\boldsymbol{\sigma}) \leftarrow \mathrm{NN}()$

$\quad i \leftarrow 1$

$\quad$ **for** $i \leq \tau \cdot N + \tau$ **do**

$\qquad$ **if** $\mathrm{mod}\ (i, N+1) \neq 0$ **then**

$\qquad\quad k \leftarrow \mathrm{Unif}\{1, N\}$

$\qquad\quad \boldsymbol{\sigma}' \leftarrow (\sigma_1, \cdots, -\sigma_k, \cdots, \sigma_N)$

$\qquad\quad r \leftarrow h(\boldsymbol{\sigma}')/h(\boldsymbol{\sigma})$

$\qquad\quad q(\boldsymbol{\sigma}') \leftarrow \mathrm{NN}(\boldsymbol{\sigma}')$

$\qquad$ **else**

$\qquad\quad \boldsymbol{\sigma}', q(\boldsymbol{\sigma}') \leftarrow \mathrm{NN}()$

$\qquad\quad r \leftarrow \frac{h(\boldsymbol{\sigma}')}{h(\boldsymbol{\sigma})} \cdot \frac{q(\boldsymbol{\sigma})}{q(\boldsymbol{\sigma}')}$

$\qquad$ **end if**

$\qquad A \leftarrow \min(1, r)$

$\qquad$ **if** $A > \mathrm{Unif}[0, 1)$ **then**

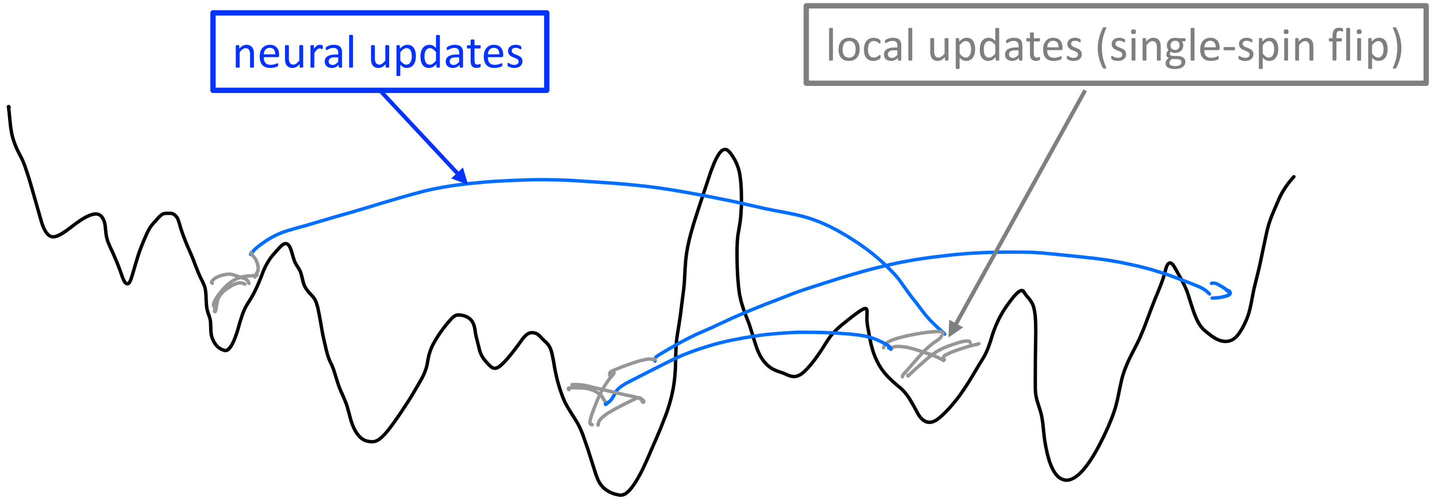
$\qquad\quad \boldsymbol{\sigma}, q(\boldsymbol{\sigma}) \leftarrow \boldsymbol{\sigma}', q(\boldsymbol{\sigma}')$

$\qquad$ **end if**

$\qquad i \leftarrow i + 1$

$\quad$ **end for**

Cartoonish representation

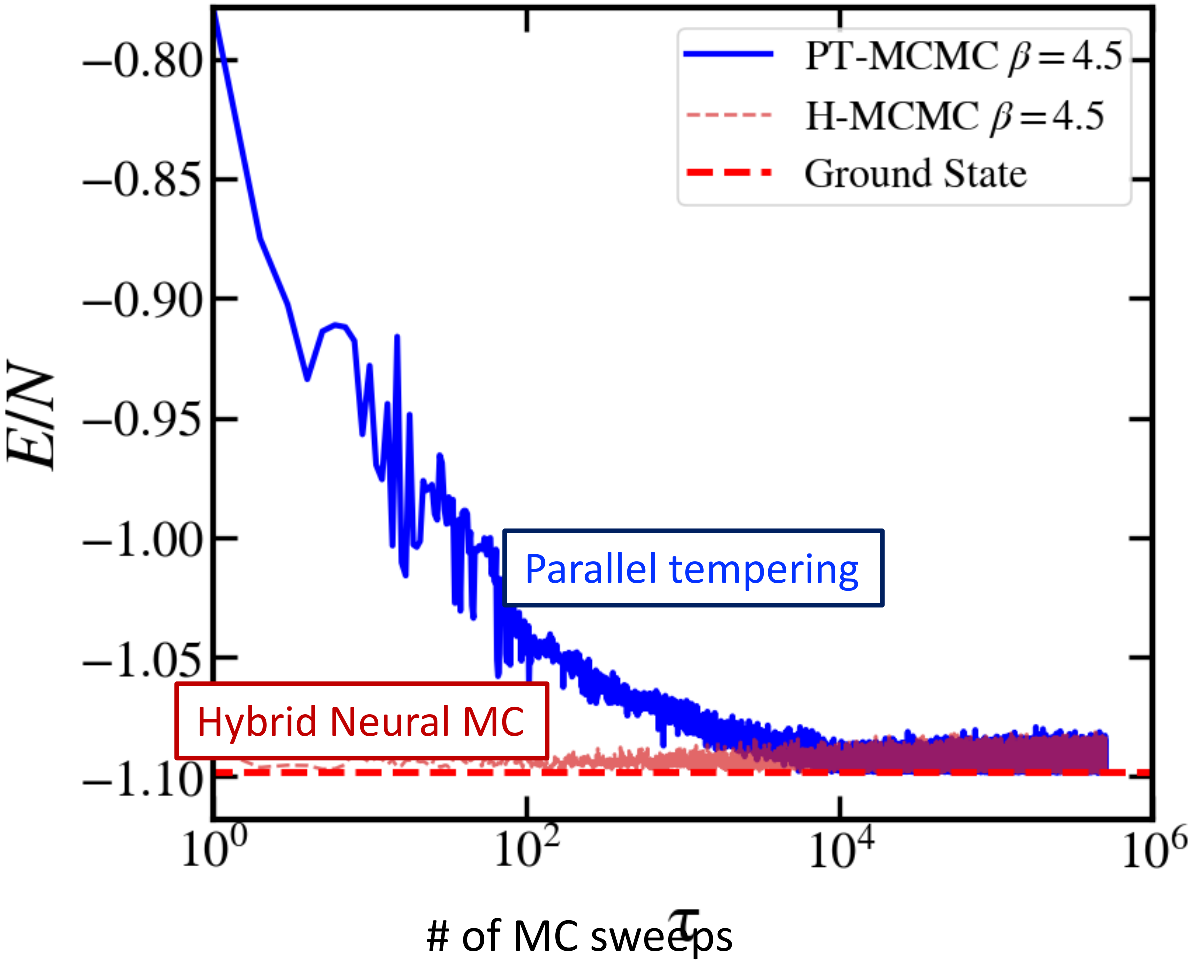


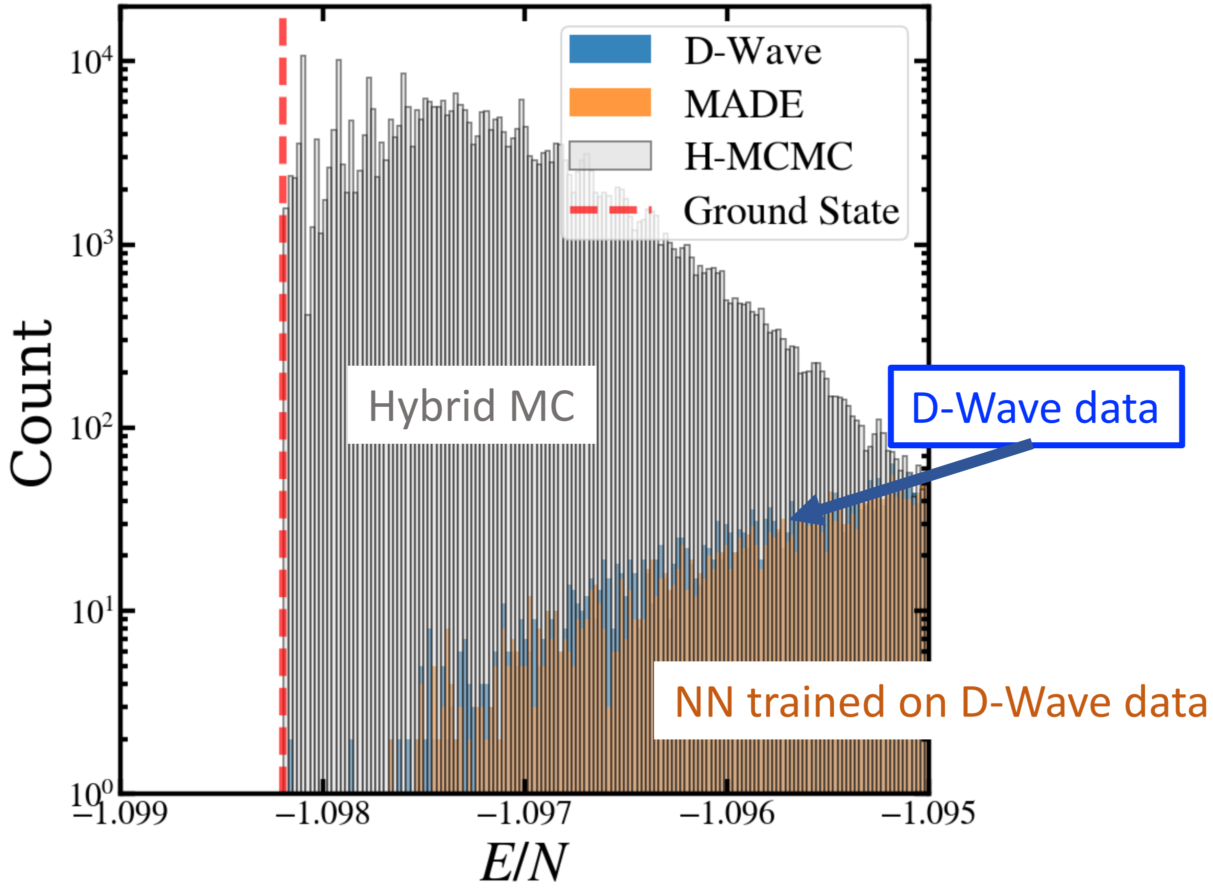
Hybrid neural simulation of a spin glass at low T

G. Scriva, E. Costa, B. McNaughton, SP, SciPost Phys. **15**, 018 (2023)

NN trained on D-WAVE data
Annealing time: 100μs

β/J = 4.5
2D square lattice N=484
Nearest and next-nearest neighbor interaction
Uniform random couplings in (-1,1)





Summary:

S. Cantori, A. Mari, D. Vitali, SP, EPJ Quantum Technology **11**, 1-13 (2024)
G. Scriva, E. Costa, B. McNaughton, SP, SciPost Phys. **15**, 018 (2023)
S. Cantori, D. Vitali, SP, Quantum Sci. Technol. **8**, 025022 (2023)

- Deep NNs sometimes fail to simulate quantum computers.
- Scalable NNs can simulate classically intractable circuits.
- Deep NNs with hybrid classical-quantum inputs perform effective error mitigation.
- Autoregressive NNs trained on data produced by quantum annealers accelerate low-T simulations of spin glasses.

Outstanding question:

- What makes a QC intractable for NNs?

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Provided access to D-Wave QA

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