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WHAT IS MY QUANTUM COMPUTER GOOD FOR? QUANTUM CAPABILITY LEARNING WITH PHYSICS-AWARE NEURAL NETWORKS

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Abstract:

Quantum computers have the potential to revolutionize diverse fields, including quantum chemistry, materials science, and machine learning. However, contemporary quantum computers experience errors that often cause quantum programs run on them to fail. Until quantum computers can reliably execute large quantum programs, stakeholders will need fast and reliable methods for assessing a quantum computer's capability-i.e., the programs it can run and how well it can run them. Previously, off-the-shelf neural network architectures have been used to model quantum computers' capabilities, but with limited success, because these networks fail to learn the complex quantum physics that determines real quantum computers' errors. We address this shortcoming with a new quantum-physics-aware neural network architecture for learning capability models. Our architecture combines aspects of graph neural networks with efficient approximations to the physics of errors in quantum programs. This approach achieves up to ~50% reductions in mean absolute error on both experimental and simulated data, over state-of-the-art models based on convolutional neural networks.

Capability Models

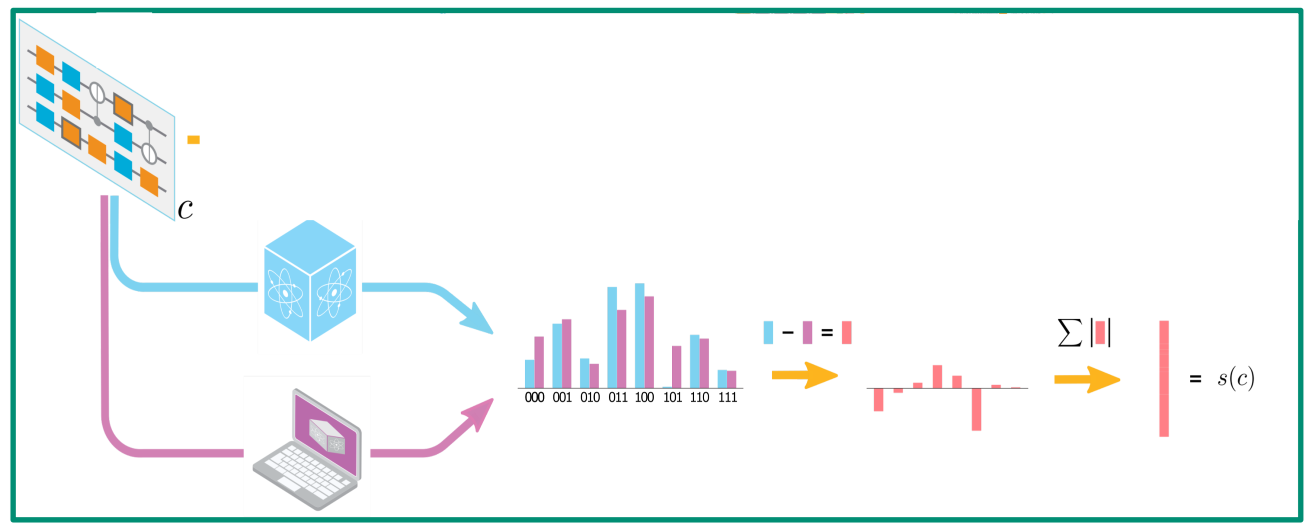

Fig. 1: Modelling capability. Capability models are predictive parametrized models of a quantum computers *capability*---i.e., a quantum computer's ability to run circuits. Formally a quantum computer's capability is defined by a *capability function*:

$$s(c) = \varepsilon(\text{ideal implementation of } c, \text{actual implementation of } c),$$

where $\varepsilon(\cdot,\cdot)$ is some quality metric (e.g., total variational distance, process fidelity, diamond distance).

Modelling Errors

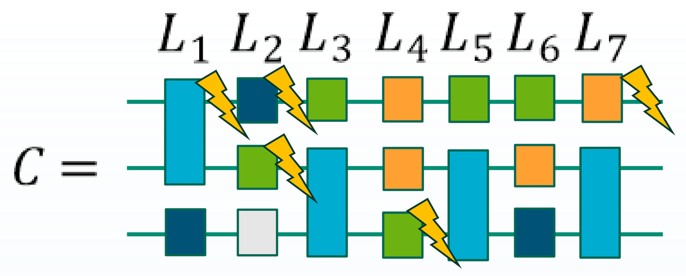

Fig. 2: Errors in quantum computers. A quantum circuit C is an instruction to perform a big unitary operation $U(C)$ on the qubits in a quantum computer. Typically, we break a circuit up into layers:

$$U(C) = U(L_m)\cdots U(L_2)U(L_1).$$

Noisy quantum circuits are modelled as sequences of noisy circuit layers, i.e., an error channel proceeding the ideal unitary operation, or as an end-or-circuit error channel following the ideal circuit unitary:

$$\tilde{U}(C) = \Lambda_m \circ U(L_m) \circ \cdots \circ \Lambda_2 \circ U(L_2) \circ \Lambda_1 \circ U(L_1),$$
$$\tilde{U}(C) = \Lambda(C) \circ U(C).$$

Many capability functions can be approximated if you know $\Lambda(C)$.

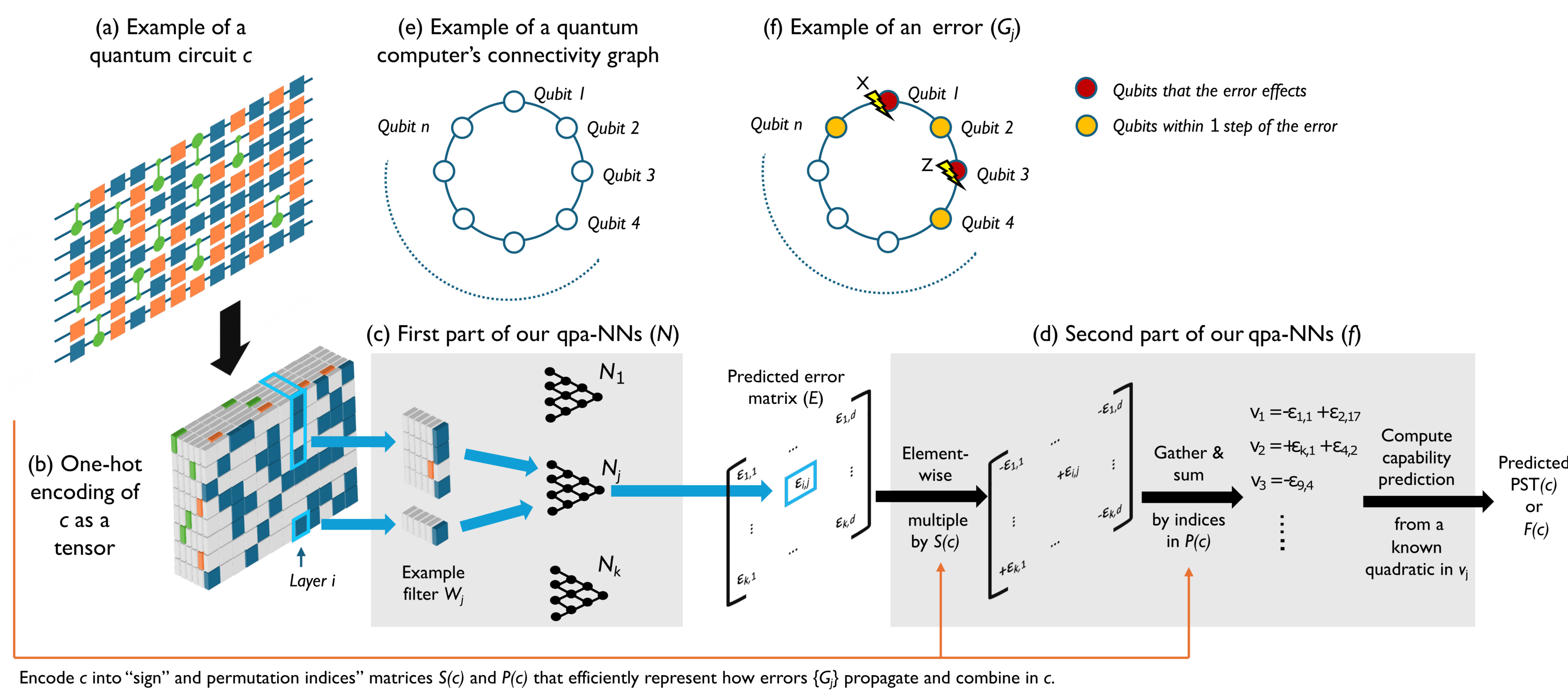

Fig. 3: Quantum-physics aware neural networks. (a-b) circuits are one-hot encoded as 3D tensors; (c) multi-layered perceptrons predict the strengths of individual errors in each layer using space-time slices of the circuit around (e-f) where each error occurs; (d) these error rates are used to estimate the end-of-circuit error channel $\Lambda(C)$, which is then used to estimate $s(c)$.

Motivation

Can we build accurate, interpretable, and fast-to-query digital twins of a quantum computer to help us evaluate and improve the quantum computer's performance?

Experimental Results

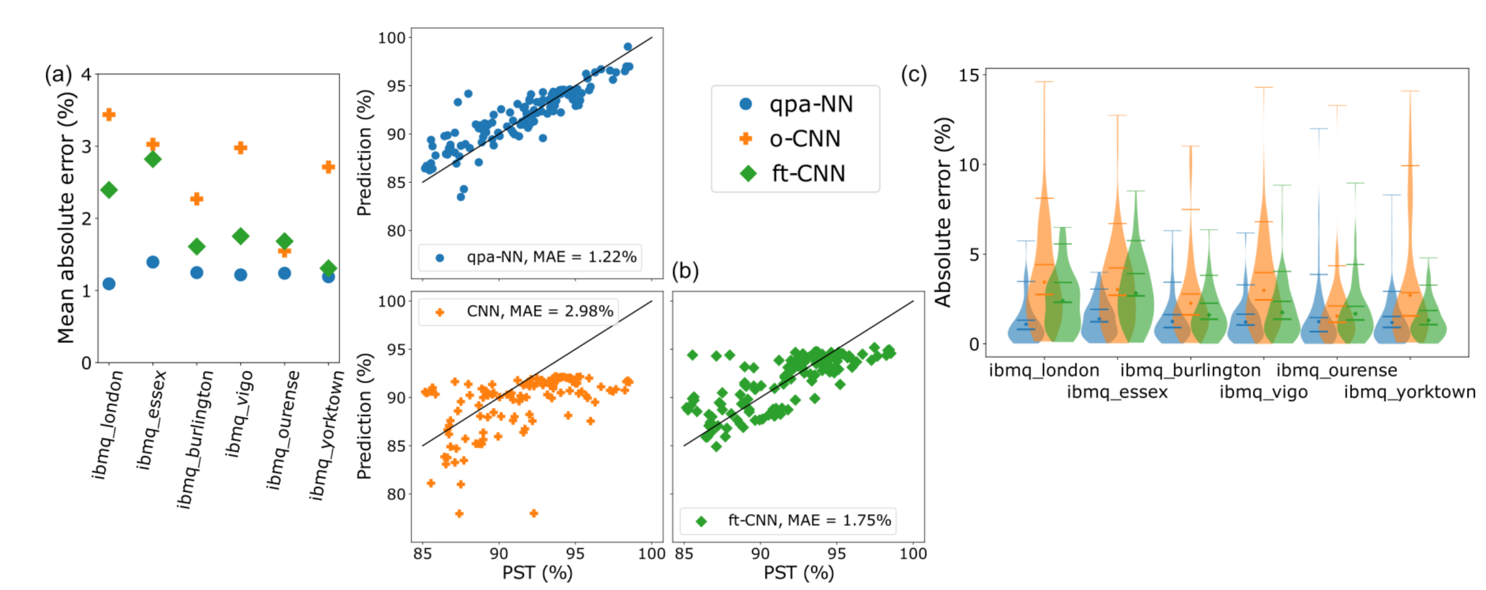

Fig. 5: Prediction accuracy on real quantum computers. (a) The mean absolute error of our qpa-NNs (•), the CNNs from Hothem et al. [2023c] (o-CNN, +), and fine-tuned CNNs (ft-CNN, ◆) on the test data. **(b)** The predictions of the three models for ibmq_vigo on the test data, and **(c)** the distribution of each model's absolute error on the test data, including the 50th, 75th, 95th and 100th percentiles (lines) and the means (points)

Simulated Results

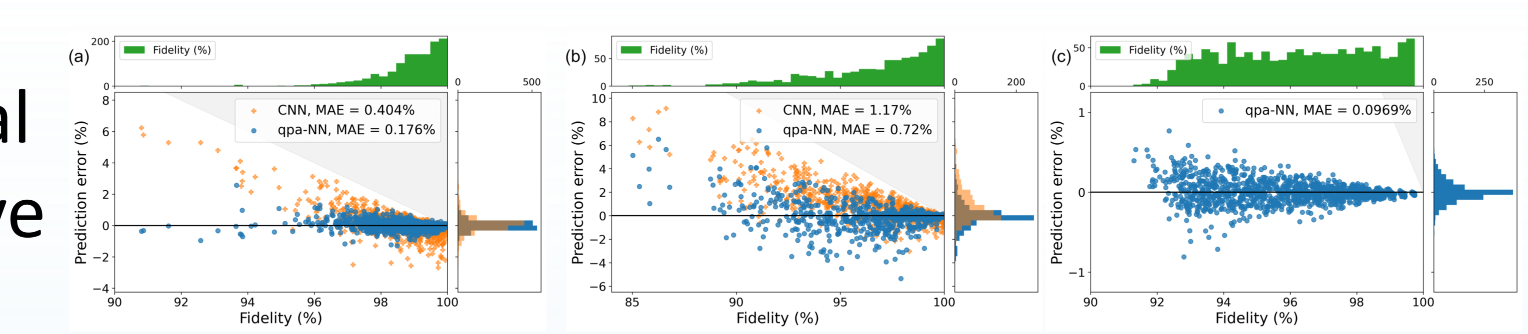

Fig. 6: Demonstrating our qpa-NNs' accuracy for hard-to-model coherent errors and at scale. (a) Scatter plot of the prediction errors on test data of a qpa-NN (•) and CNN (•) trained to predict the fidelity F (c) of random circuits run on a hypothetical 4-qubit quantum computer. The qpa-NN significantly outperforms the CNN. **(b)** Prediction errors on out-of-distribution test data from random mirror circuits.. **(c)** Prediction errors on the 100-qubit test data, demonstrating that our qpa-NN approach can accurately predict F (c) for circuits run on large-scale quantum computers.

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