Capacity Measures of Parameterised Quantum Circuits

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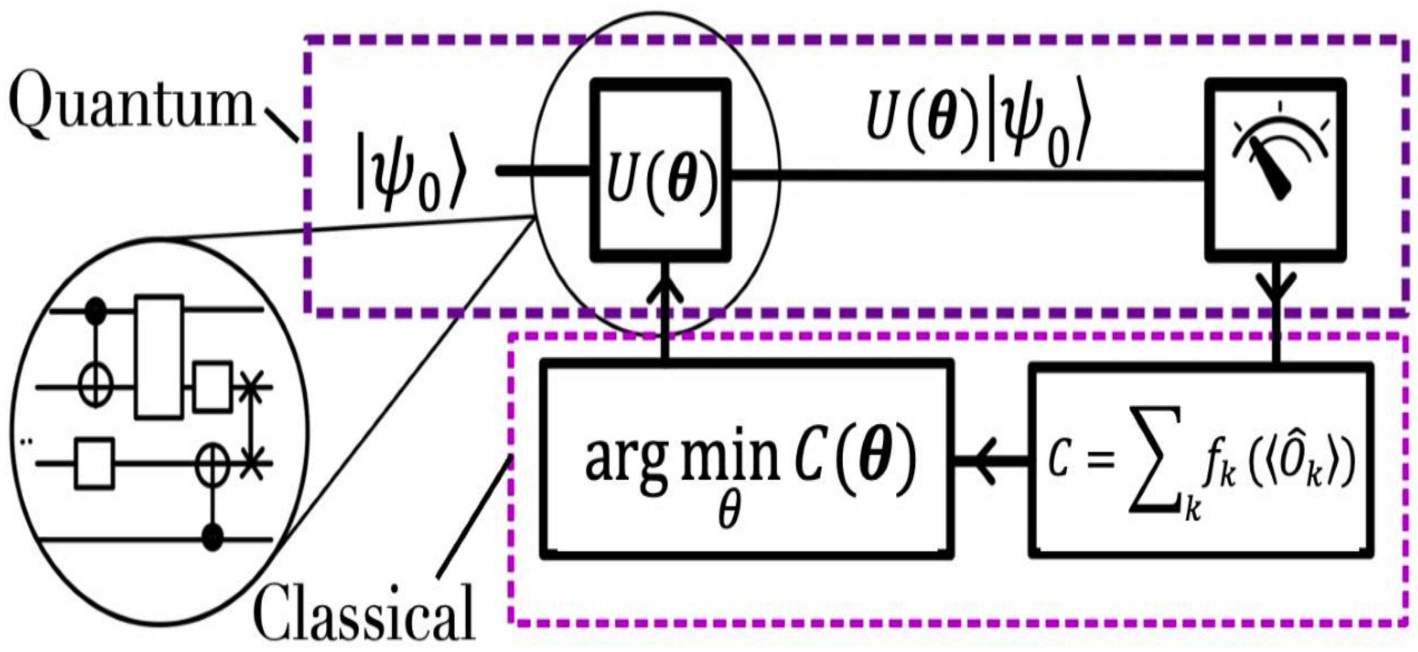
1. Variational Quantum Algorithms

- Current quantum computers limited to tens to hundreds of qubits and shallow circuit depth



- Variational Quantum Algorithms (VQAs) [1]:
  - Designed to run on current hardware
  - A 'hybrid quantum-classical loop' where parameters iteratively updated with classical optimiser to minimise cost function
  - Run on Parameterised Quantum Circuits (PQCs)
  - Have applications in quantum chemistry and combinatorial optimisation
- Studying what makes a PQC architecture effective for VQAs is highly desirable

2. Circuit Design and Capacity Measures

- Many possible circuit designs:
  - Hardware Efficient (HE) circuits are generalisable but difficult to train
  - Problem-Inspired (PI) circuits designed to solve one problem: trainable but specific
  - Some circuits based on preserving symmetries
- Various possible capacity measures [1]:
  - **Entanglement** via Meyer-Wallach measure
  - **Expressibility**: how well can circuit generate states representative of the N qubit Hilbert space?

$$\text{Expr} = D_{KL}(\hat{P}_{PQC}(F;\boldsymbol{\theta}) \,||\, P_{\text{Haar}}(F))$$

  - **Réyni Entropy of Magic**: how far away is a state from the Clifford group of classically simulatable states? [2]

$$\mathcal{M}_2(|\psi\rangle) = -\log \mathbf{d}\|\Xi(|\psi\rangle)\|_2^2$$

  - **Quantum Fisher Information Matrix (QFIM)**: metric that expresses how variation in circuit parameter changes quantum state

$$\mathcal{F}_{ij} = \Re(\langle\partial_i\psi(\boldsymbol{\theta})|\partial_j\psi(\boldsymbol{\theta})\rangle - \langle\partial_i\psi(\boldsymbol{\theta})|\psi(\boldsymbol{\theta})\rangle\langle\psi(\boldsymbol{\theta})|\partial_j\psi(\boldsymbol{\theta})\rangle)$$

  - **Effective Quantum Dimension**: rank of the QFIM, or the number of independent directions in state space accessible by infinitesimal parameter change [3]

3. Computational Method

- Developed Python module based on QuTip [4] library to create, train and measure PQCs

```python
import PQC_lib as pqc
"""Define a 4-qubit, 6-layer PQC with X
   rotations on each qubit and a chain
   of CNOT gates as entanglers"""
N = 4
rotations = [pqc.R_x(i, N) for i in range(N)]
entanglers = [pqc.CHAIN(pqc.CNOT, N)]
layer = rotations + entanglers
circuit = pqc.PQC(N)
circuit.add_layer(layer, n=6)
```

```python
import measurement as msr
"""Make various capacity measurements
   of the circuit, and train it using
   BFGS method."""
capacity = msr.Measurements(circuit)
expr = capacity.expressibility()
eom = capacity.entropy_of_magic()
capacity.train(method="BFGS")
# Maximise magic:
capacity.train(method="BFGS", magic=True)
```

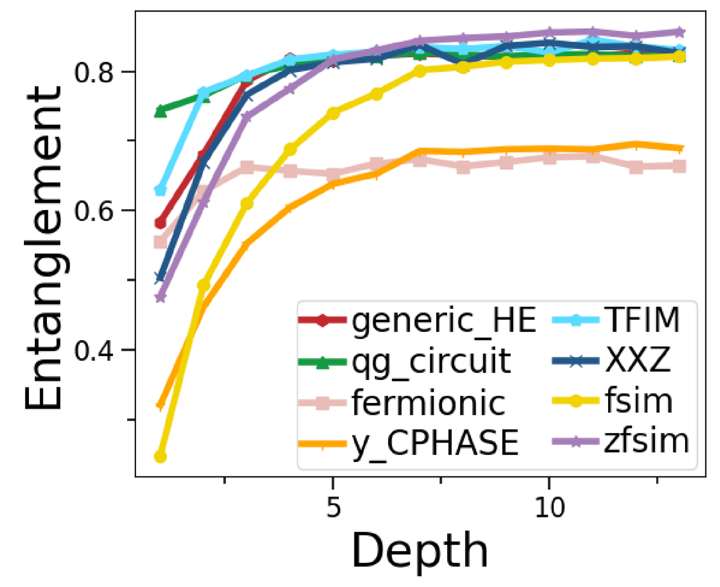
- Validated with known test cases: Clifford circuits, product states, analytic single-qubit expressions, circuits with known QFIMs or ground states
- Implemented different circuits (TFIM, XXZ, Fermionic, etc.) and made capacity measurements for varying qubit number and layer depth

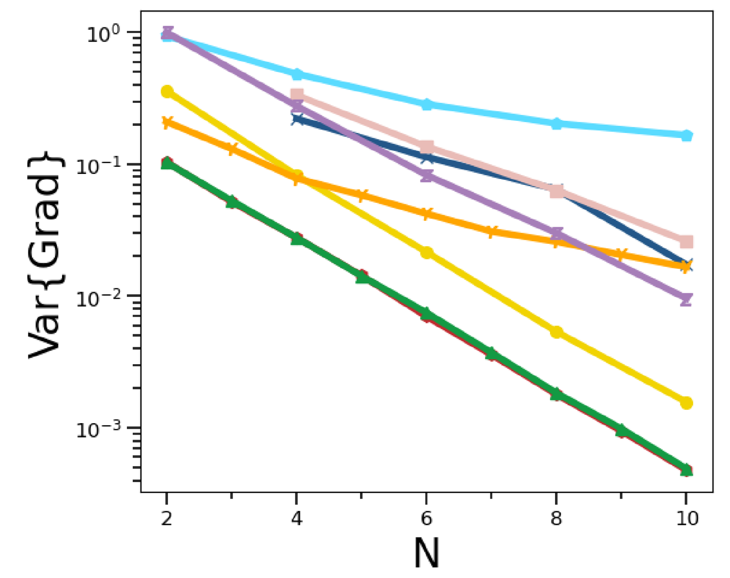
4. Results

- Single codebase for capacity measures and PQC architectures a useful tool for quantum computing

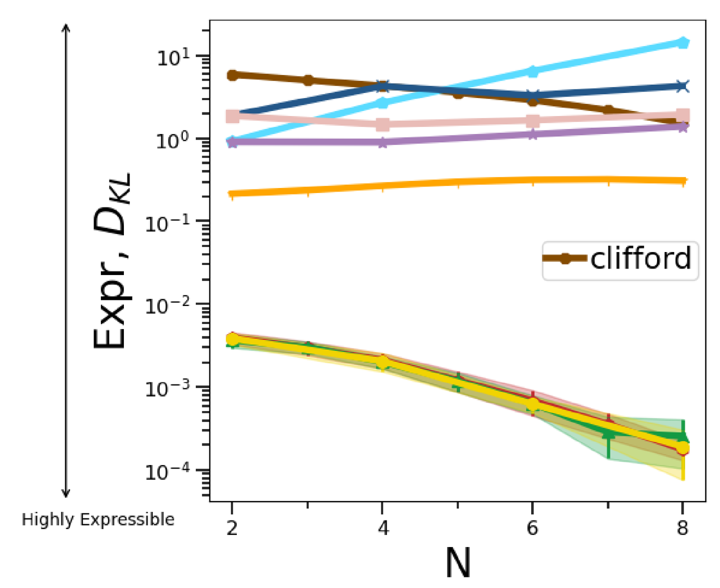
4a. Capacity

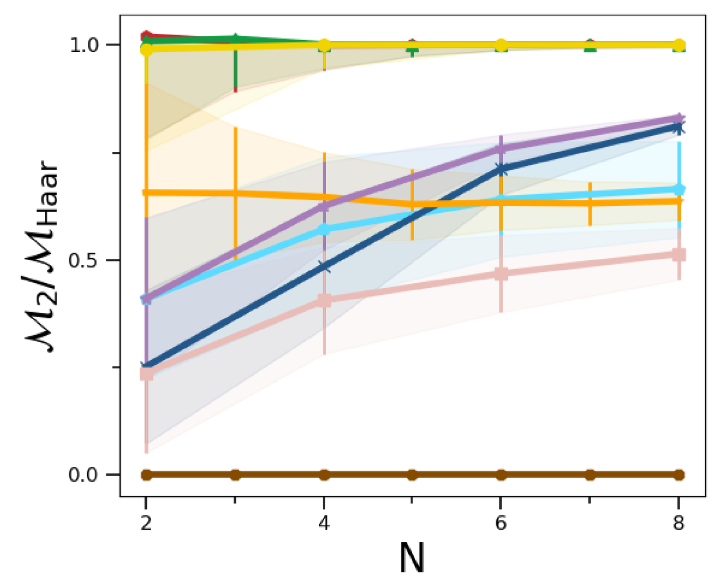
- Recorded capacity measures against layer depth and qubit number for various circuits:





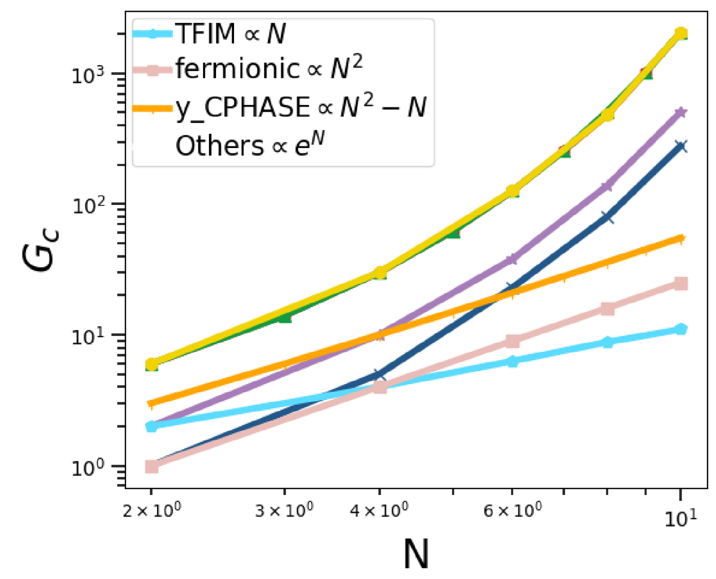
- Entanglement saturates at 0.8 for most circuits at high depth
- Variance of gradient vanishes exponentially for HE, fSim and XXZ circuits – these 'barren plateaus' make training difficult



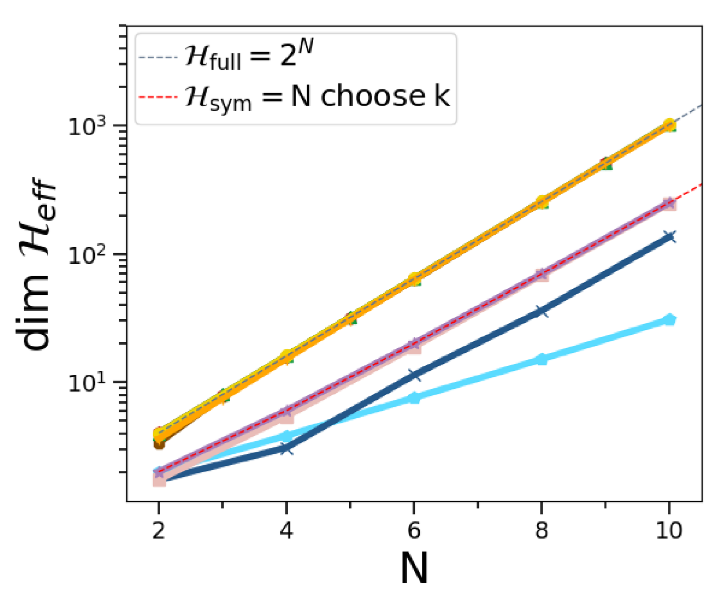


- HE circuits highly expressible & tend to Haar-random Reyni Magic**,** PI circuits less expressible and less Magic
- Clifford circuit has a reasonable expressibility, but no Magic (so no quantum advantage) - highlights importance of characterising using multiple measures

4b. Dimensionality



- Effective quantum dimension of HE, XXZ and fSim circuits scales exponentially with N ⟹ reaches more states
- TFIM has linear scaling, fermionic and y-CPHASE quadratic
- We introduce a **new measure** based on finding the Hilbert space that minimises the expressibility
- Describes the subspace the PQC operates in, and even what symmetries it possesses!
- Evaluates the scaling of expressibility with qubit number relative to space circuit is designed for



5. Conclusion

- Integrated PQC construction and measurement into a cohesive package
- Evaluated PQC performance over multiple capacity measures as functions of depth and qubit number
- Derived new insights into circuit performance and defined new measure based on a circuit's expressibility relative to its subspace

References:
[1] K. Bharti *et al.*, "Noisy intermediate-scale quantum algorithms", *Reviews of Modern Physics*, vol. 94, no. 1, 2022.
[2] L. Leone, S. Oliviero and A. Hamma, "Stabilizer Rényi Entropy", *Physical Review Letters*, vol. 128, no. 5, 2022.
[3] T. Haug, K. Bharti, and M. S. Kim, "Capacity and quantum geometry of parametrized quantum circuits," 2021. [Online]. Available: https://arxiv.org/abs/2102.01659.
[4] J. R. Johansson, P. D. Nation and F. Nori: "QuTiP 2: A Python framework for the dynamics of open quantum systems.", *Comp. Phys. Comm.* vol. 184, no. 1234, 2013.