Equivariant Quantum Graph Circuits

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Challenges of quantum ML

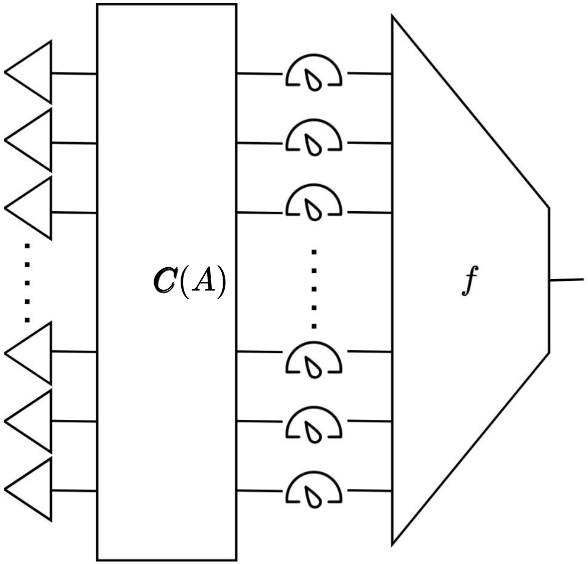
- Quantum ML: an emerging field
- Current hardware limits to **tiny experiments**, so how do you do ML?
  → Focus on **theory**
- We build on established literature on GNN model expressivity and ask similar questions about quantum models

Contributions

- Our framework for quantum methods on graphs:
  Equivariant Quantum Graph Circuits (EQGC)
  - Formalize what properties a *parameterized quantum circuit* should satisfy for graph ML
  - Explore design space, propose subclasses, relate to prior work
  - Plenty of further open questions
- Prove universal approximation of functions over bounded-size graphs
  - Shown for a certain EQGC subclass, *EDU-QGCs*
  - Quantum circuits are probabilistic – needed size depends on confidence parameter
- This exceeds the expressivity of popular classical GNNs called Message-Passing Neural Networks (MPNNs), and matches that of randomized MPNNs

A broad class of quantum methods

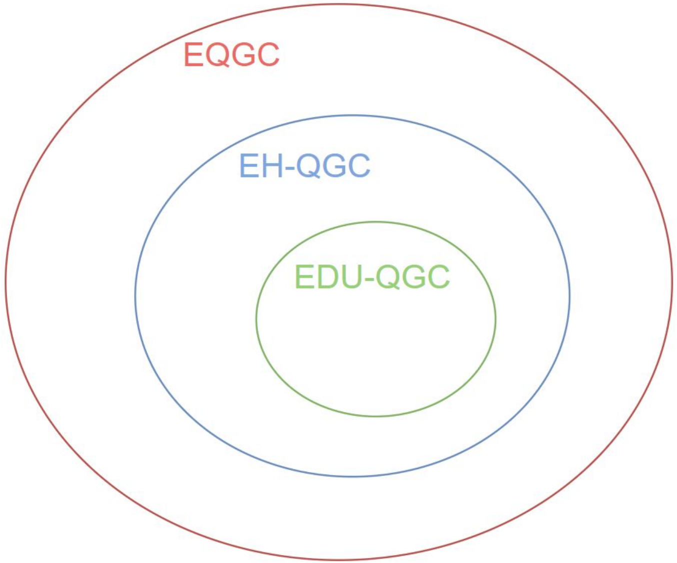
- We investigate a broad class of architectures with the following structure:



- Reordering input should change output appropriately:
  Equivariant Quantum Graph Circuits (EQGC)

Subclasses of EQGCs

- We consider parameterizations of EQGCs, via one- and two-node Hamiltonians and unitary operators ⇒ more practical subclasses



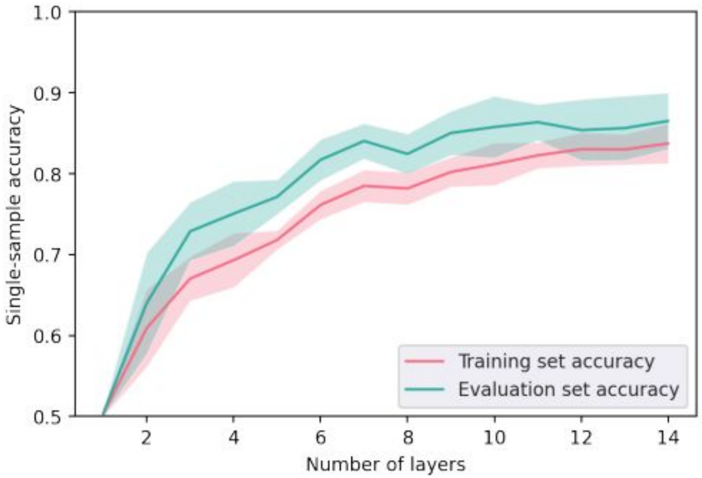
Achieving universality

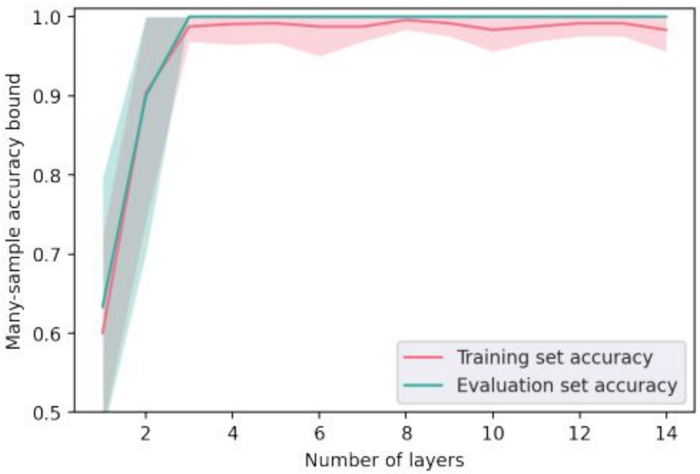
- Step 1: a sufficiently large EDU-QGC can "simulate" any deterministic MPNN with sum aggregation
- Step 2: a simple quantum circuit can "simulate" classical randomization
- By similar arguments to randomized MPNNs, this gives us universality:

For any real-valued function f over graphs up to size n, a sufficiently large EDU-QGC can represent it with arbitrarily low probability of error.

Experiments

- Toy dataset challenging for MPNNs: "one cycle or two cycles", 6 to 10 nodes
- Separate 8-node graphs as test set
- EDU-QGC models with one qubit per node, different depths
- Training in classical simulation with Adam optimizer
- Success, scales well to many layers!





Significance and limitations

- First steps in understanding the capabilities of quantum models over graphs
- Potential for plenty of further work, both theoretical and experimental
- Further work *could* show quantum advantage!
  - *More scalable ansatze:* perhaps similar results hold for less powerful EQGC models?
  - *Function classes for quantum advantage:* perhaps some class of functions can be approximated by small quantum models, but would need huge randomised MPNNs?

Thank you for listening!

Any questions?

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