Learning Quantum State Properties with Quantum and Classical Neural Networks

Arthur Pesah
KTH

Peter Wittek
University of Toronto

Nathan Killoran
Xanadu

Overview

Goal

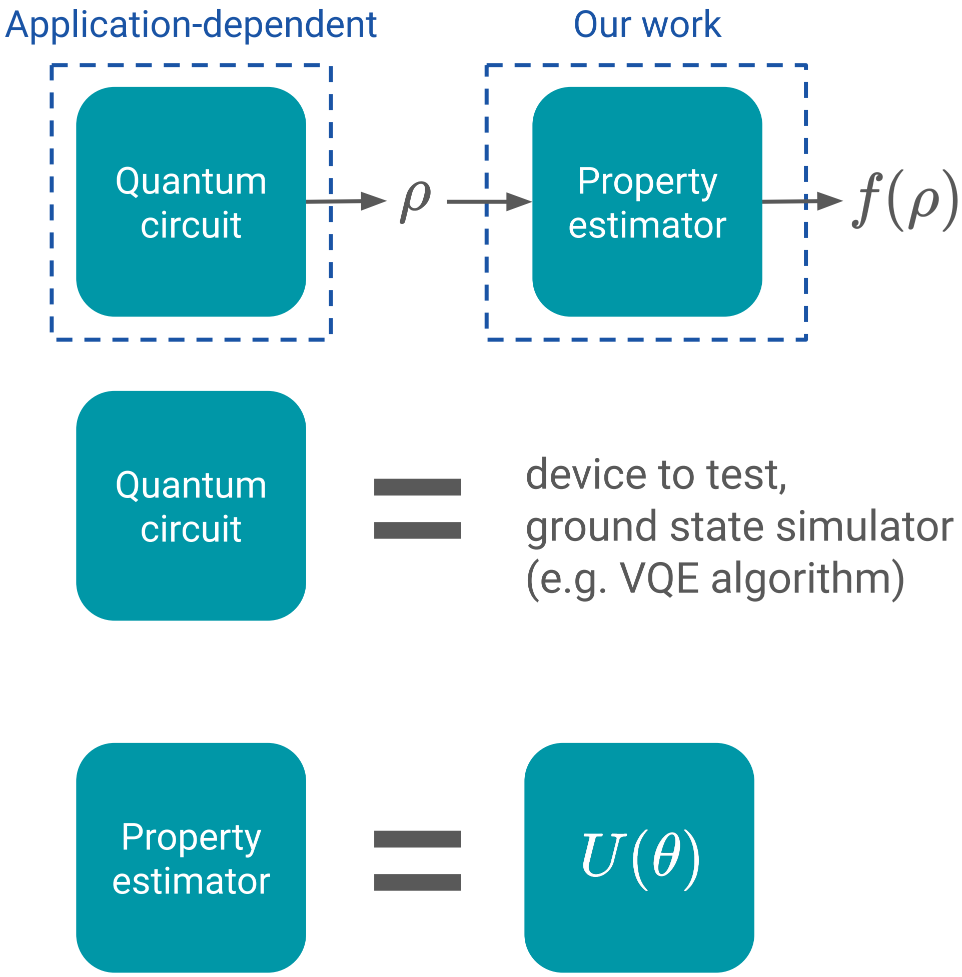
Estimating a property $f(\rho)$ of a quantum state ρ (density matrix), given as the output of a quantum circuit

Applications

- Quantum simulation: computing chemical properties of the ground state of a molecule
- Testing a device: checking if the output of a device has the desired properties

How to do that?

- Usually: quantum state tomography (requires a lot of measurements)
- Our work: quantum circuit, and in particular quantum neural net (QNN)



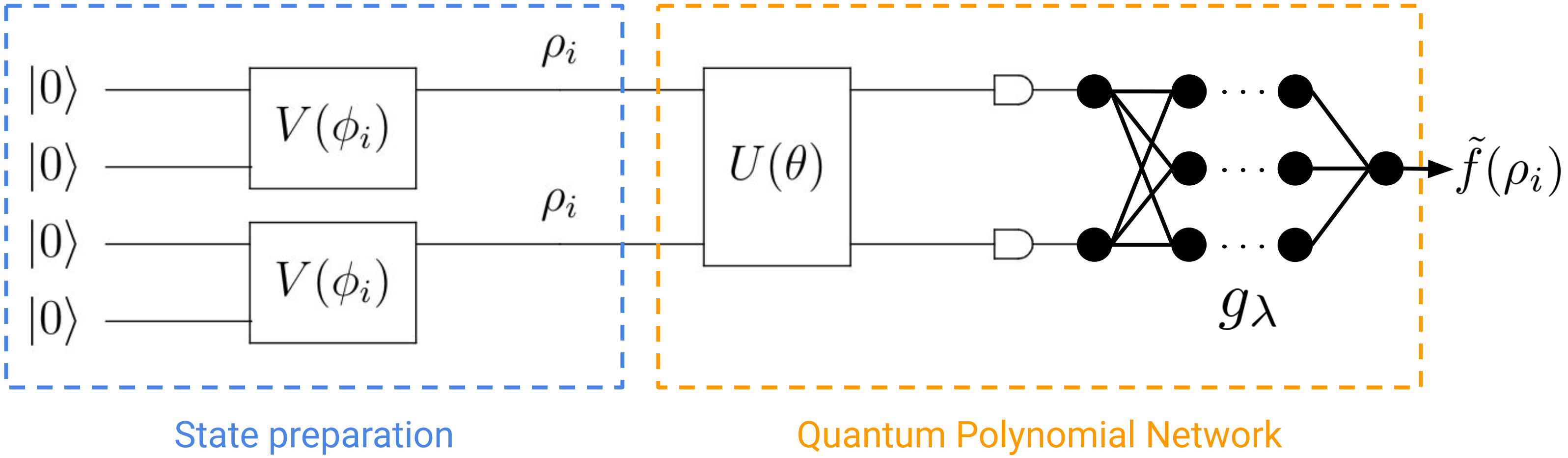
Contribution

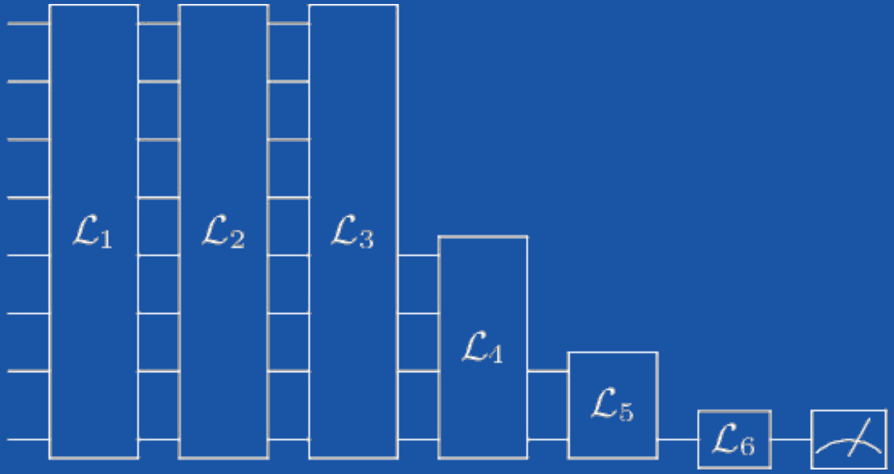
Theoretical

- Proposed 3 architectures of QNN and classical NN to learn a given polynomial property
- Studied their universality theoretically
- Proposed a protocol for arbitrary mixed state preparation

Numerical

- Tested and compared those architectures to compute the purity and the Von Neumann entropy of one-qubit (or one-qumode) states
- Tested the state preparation protocol





Quantum Neural Networks

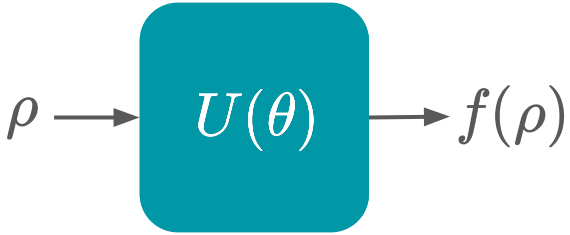
Quantum neural networks: overview

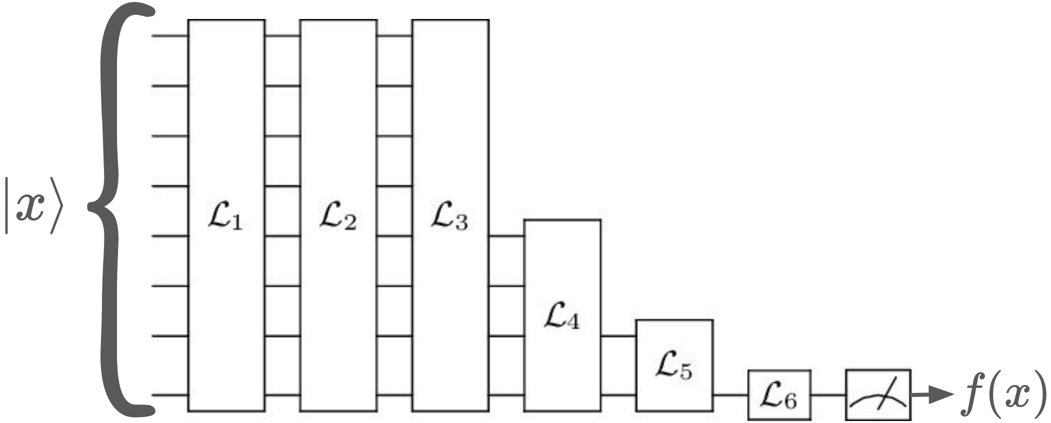
Definition

- Circuit depending on a set of parameters that can be trained to **approximate quantum functions**
- Often made of several layers
- Alternate names: *variational circuit*, *parametrized circuit*

Applications

- Classical machine learning tasks: classification, regression, etc.
- Quantum machine learning tasks: classifying quantum phase of matter
- Quantum algorithm learning: Variational Quantum Eigensolver, Variational Quantum Factoring, etc.





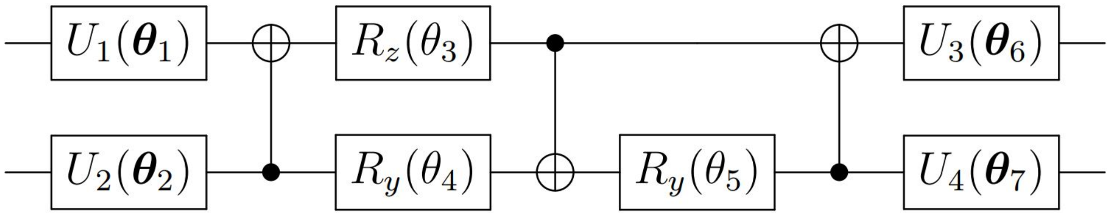
Discrete and continuous-variable (CV) quantum computing

In my thesis: QNN applied on either discrete or CV states

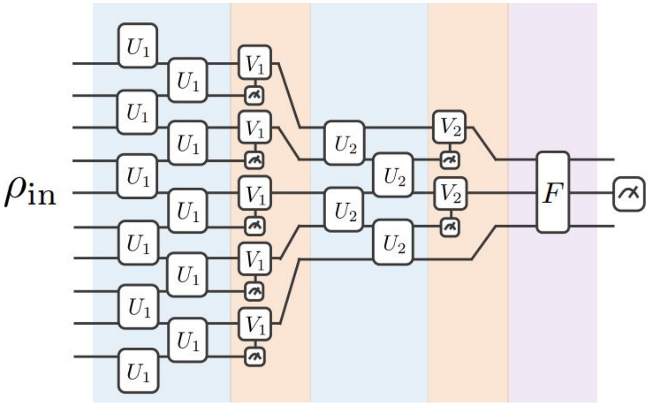
	Discrete quantum computing	**CV quantum computing**
Unit of information	Qubit or qudit: d-level system	Qumode: photonic state (harmonic oscillator)
Common gates	Hadamard, Rotations, CNOT	Beam splitter, Displacement, Squeezing, Rotations, Kerr
Measurement	Pauli basis	Homodyne, Heterodyne, Photon counting
Graphical representation	Bloch sphere	Wigner representation

Quantum neural networks: discrete ansatz

Example of two-qubit universal ansatz

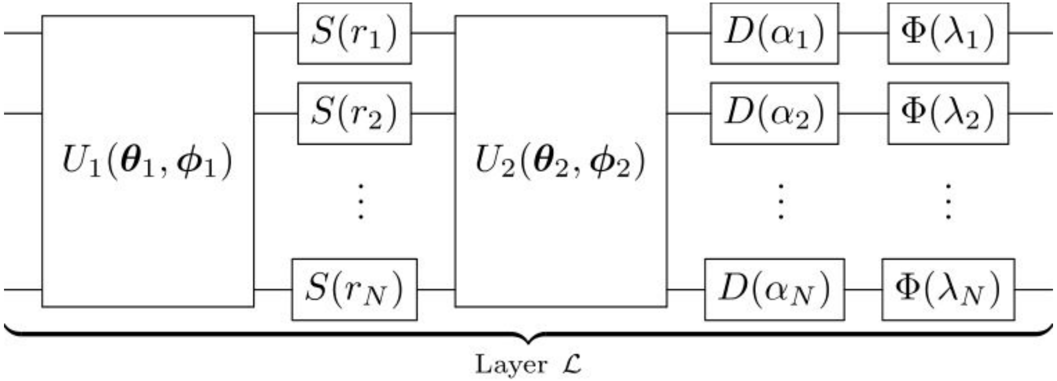


Example of n-qubit non-universal ansatz: Quantum Convolutional Neural Network

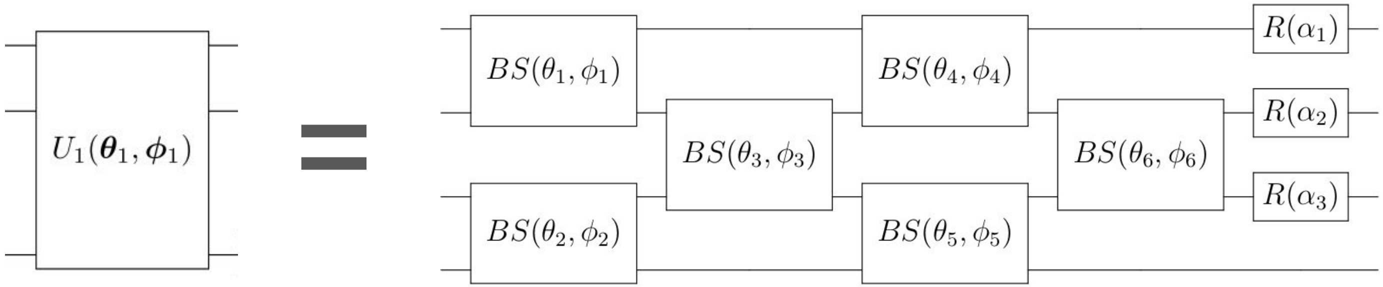


Quantum neural networks: CV ansatz

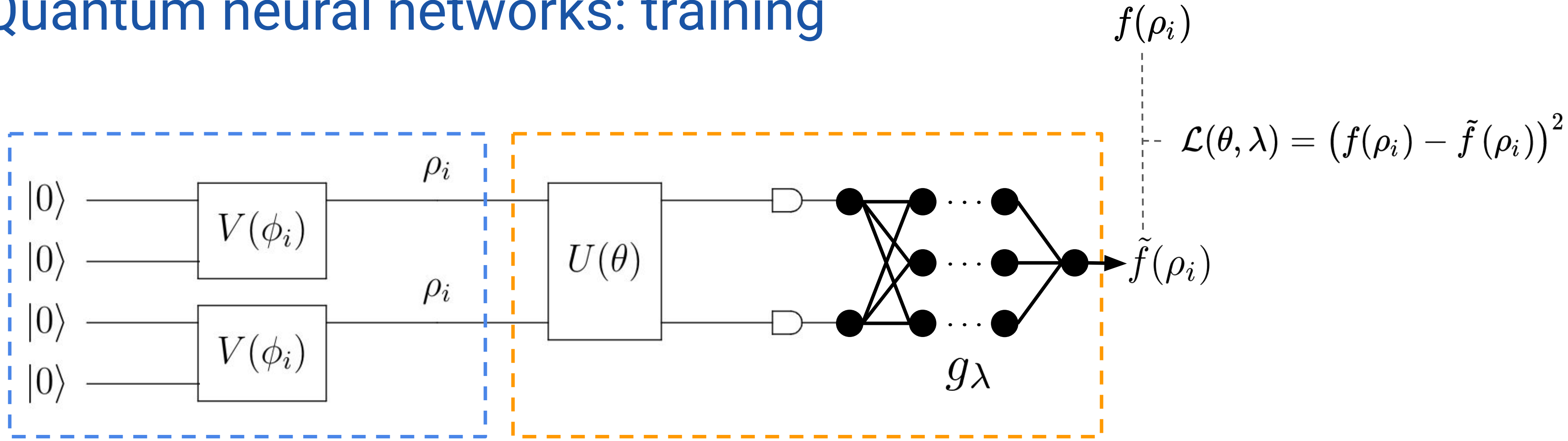
Continuous-variable Quantum Neural Network



where



Quantum neural networks: training

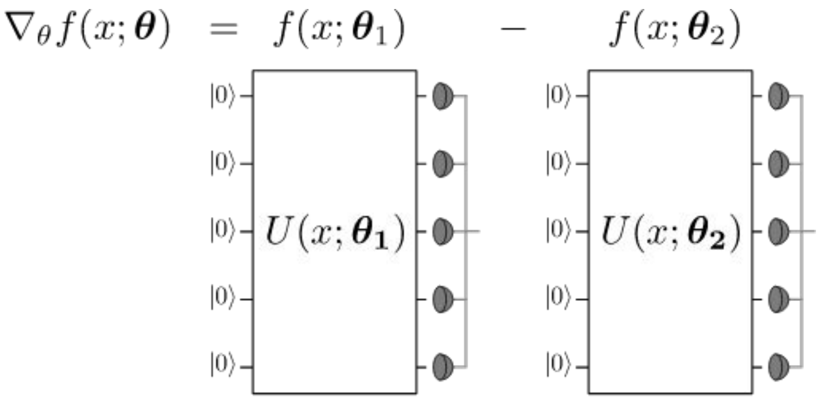


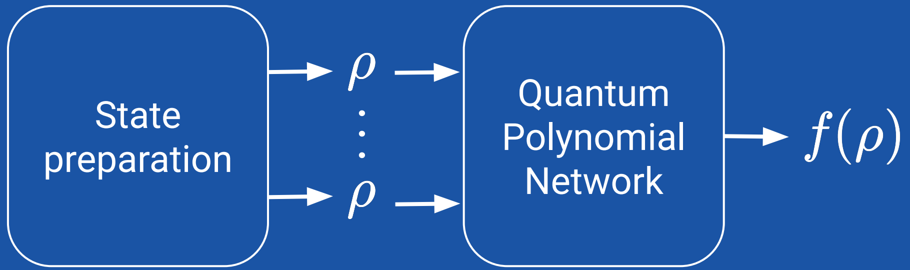
State preparation

Quantum and classical NN

Non-differentiable optimization
Numerical estimation of the gradient on the CPU

Differentiable optimization
Exact expression of the gradient using a quantum circuit (recent method)

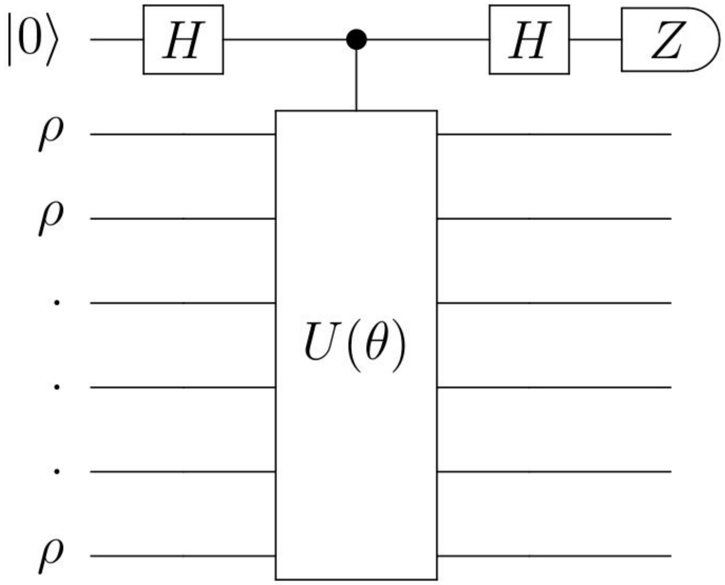




Quantum Polynomial Network

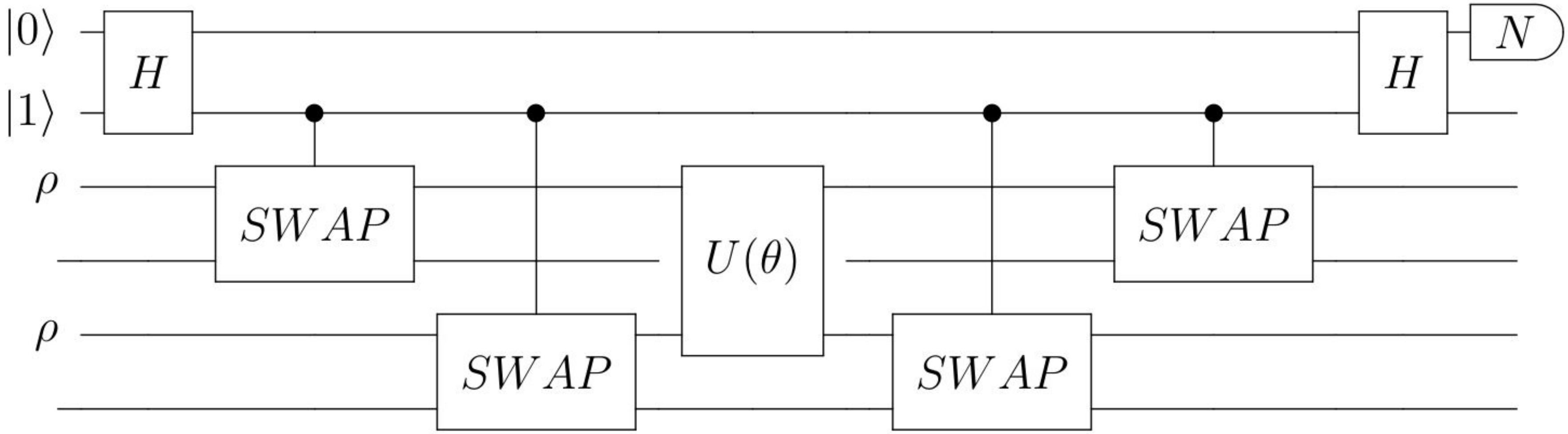
Quantum Polynomial Network with Ancilla

Discrete architecture



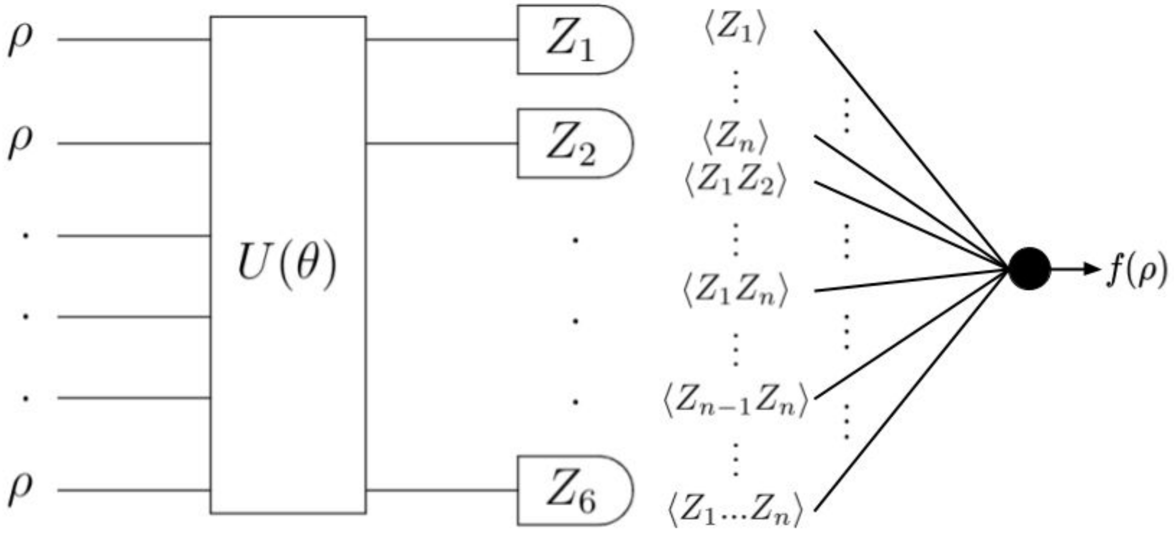
Quantum Polynomial Network with Ancilla

Photonic architecture



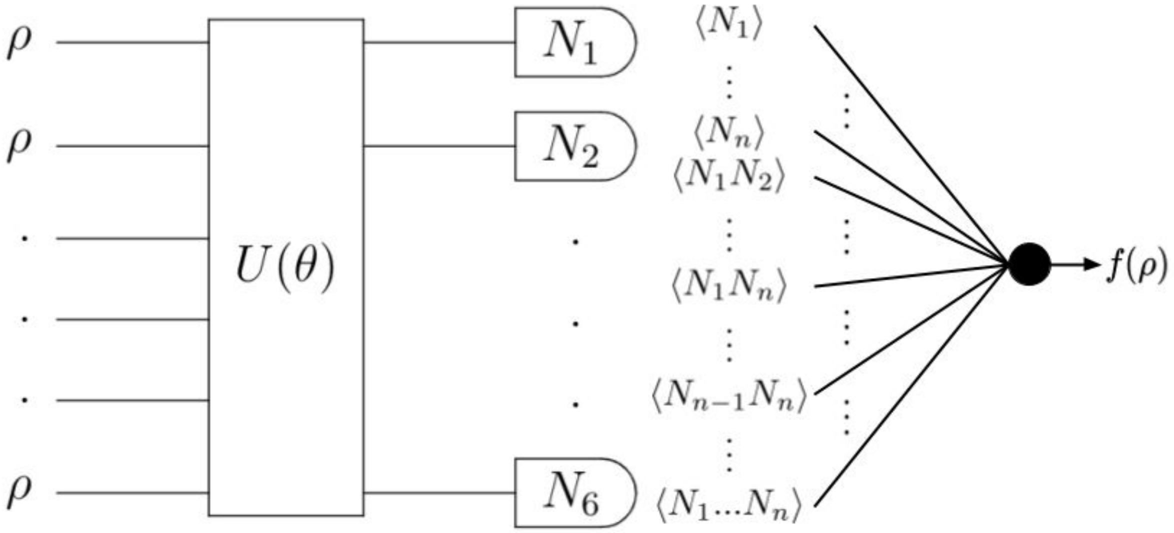
Quantum Polynomial Network with Correlations

Discrete architecture



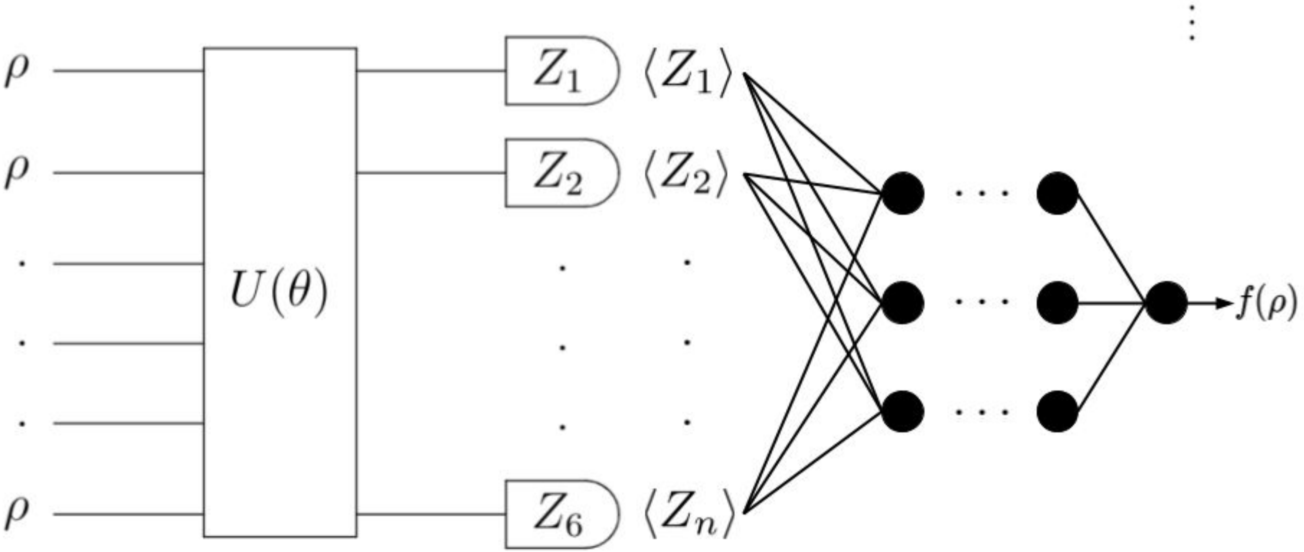
Quantum Polynomial Network with Correlations

Photonic architecture



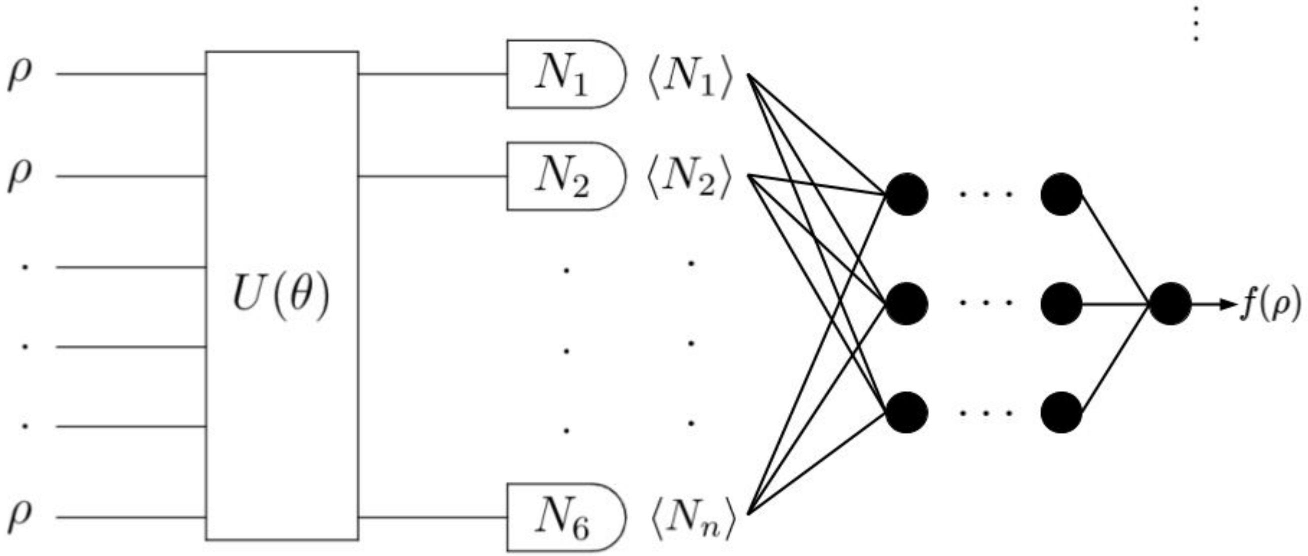
Quantum Polynomial Network with Averages

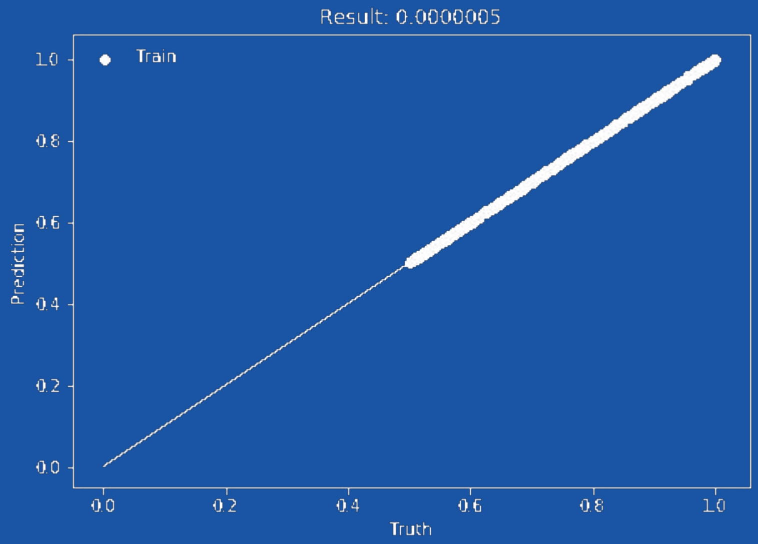
Discrete architecture



Quantum Polynomial Network with Averages

Photonic architecture





Numerical Results

Numerical results: experimental setting

States

- 1 qubit/qumode
- CV: cutoff 3
- 300 training samples
- 100 test samples

Properties to learn

- Purity:

$$f(\rho) = \mathrm{tr}\left[\rho^2\right]$$

- Entropy:

$$f(\rho) = \mathrm{tr}\left[\rho \log \rho\right]$$

Polynomial Networks

- 2 copies of ρ
- Universal ansatz for discrete
- Xanadu antatz for CV

Libraries

PYQUIL

STRAWBERRY FIELDS

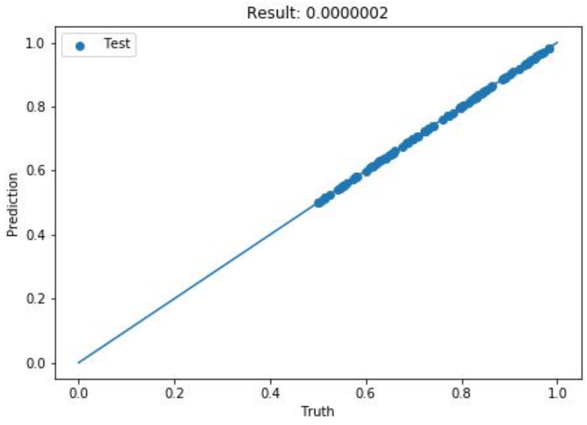
PENNY LANE

Numerical results: discrete case – purity learning

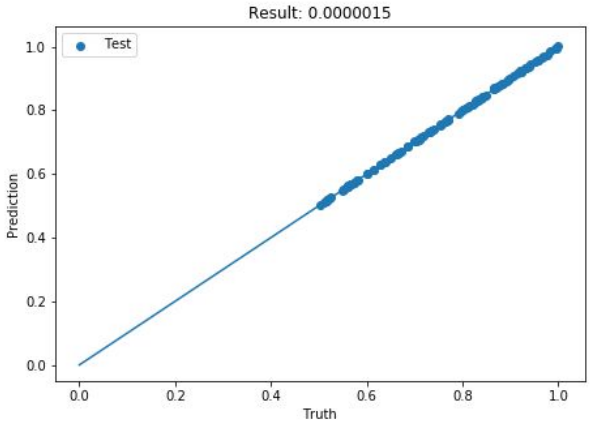
Conclusions:

- Overall good results
- Ancilla Net and Correlation Net > Average Net : theoretically expected

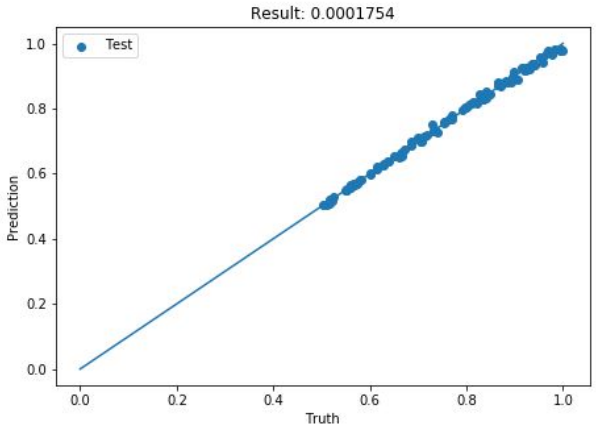
Ancilla Net



Correlation Net



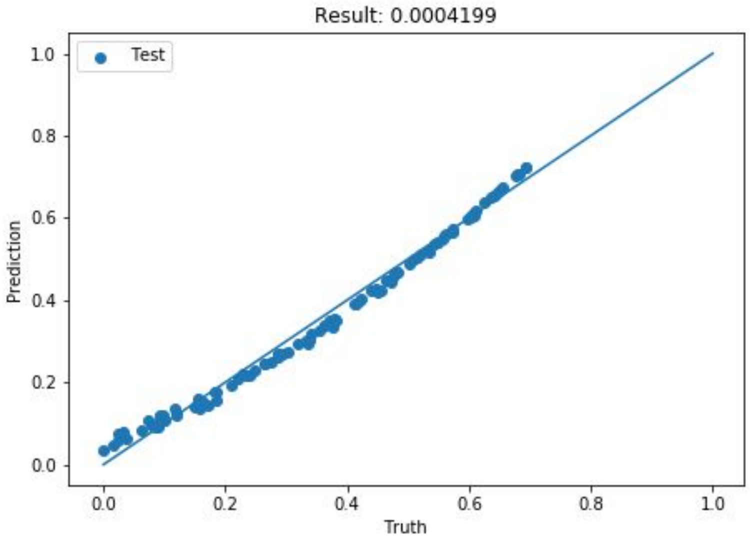
Average Net



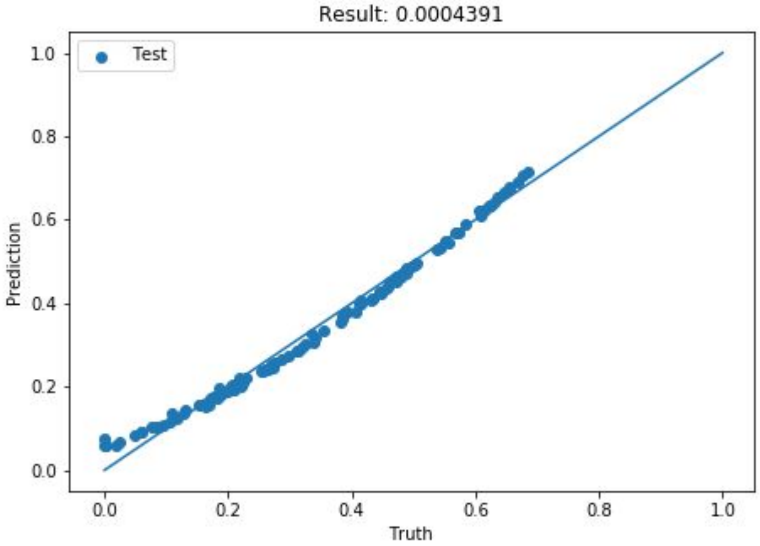
Numerical results: discrete case – entropy learning

Conclusion:
Rather good results given that entropy is not quadratic

Ancilla Net



Correlation Net

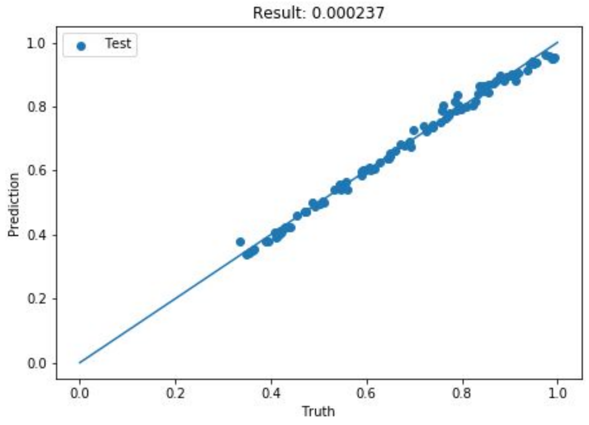


Numerical results: CV case – purity learning

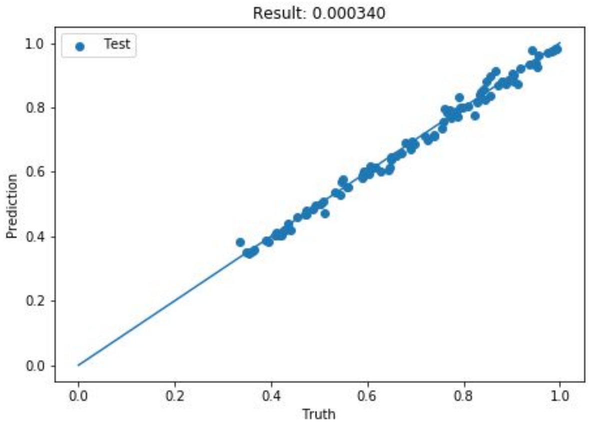
Conclusions:

- Worst results than for the discrete case: expected (no universality)
- The fact that it's not too bad is probably due to the cutoff
- Future work: test Ancilla Net (which should be universal)

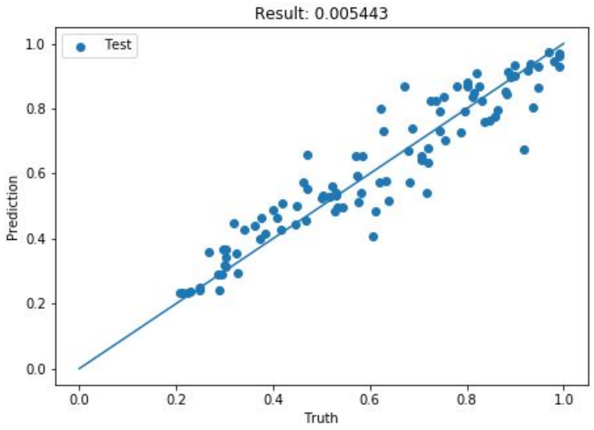
Correlation Net



Average Net, cutoff 3



Average Net, cutoff 5



Discussion

Conclusion

- Very encouraging results in the discrete case: theory and simulation in agreement
- Possibility to approximate nonlinear functionals with polynomial architectures
- No-go results in the CV case, but also an architecture idea (Ancilla Net) left to test

Future work

- Test CV Ancilla Net
- Test the architectures with more properties, more qubits
- Study the complexity of the algorithm in terms of #measurements, compare with state tomography
- Perform real experiments on real devices?

Thanks for your attention