Towards Quantum Machine Learning

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Introduction

NISQ era

$\Rightarrow$ **We are in a Noisy Intermediate-Scale Quantum era** $\Leftarrow$

How can we contribute?

- Develop new algorithms
  $\Rightarrow$ using classical simulation of quantum algorithms
- Adapt problems and strategies for current hardware
  $\Rightarrow$ hybrid classical-quantum computation

Quantum Algorithms

There are three families of algorithms:

Gate Circuits

- Search (Grover)
- QFT (Shor)
- Deutsch

Variational (AI inspired)

- Autoencoders
- Eigensolvers
- Classifiers

Annealing

- Direct Annealing
- Adiabatic Evolution
- QAOA

Variational Quantum Circuits

Getting inspiration from **AI**:

- Supervised Learning $\Rightarrow$ Regression and classification
- Unsupervised Learning $\Rightarrow$ Generative models, autoencoders
- Reinforcement Learning $\Rightarrow$ Quantum RL / Q-learning

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Define new parametric model architectures for quantum hardware:

$\Rightarrow$ **Variational Quantum Circuits**

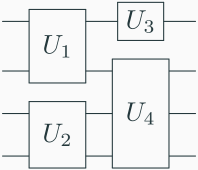
Rational

Rational for Variational Quantum Circuits

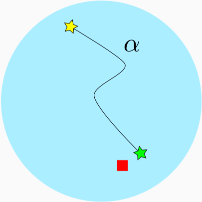
Rational:

Deliver variational quantum states $\rightarrow$ explore a large Hilbert space.

$$U(\vec{\alpha}) = U_n \dots U_2 U_1$$



Near optimal solution



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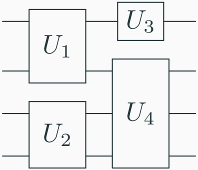

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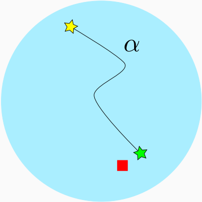


Idea:

Quantum Computer is a machine that generates variational states.

$\Rightarrow$ **Variational Quantum Computer!**

Solovay-Kitaev Theorem

Let $\{U_i\}$ be a dense set of unitaries.
Define a circuit approximation to V:

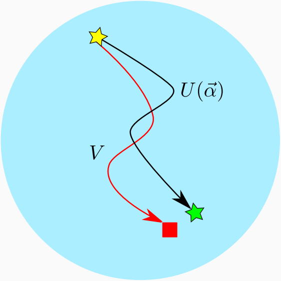
$$|U_k \ldots U_2 U_1 - V| < \delta$$

Scaling to best approximation

$$k \sim \mathcal{O}\left(\log^c \frac{1}{\delta}\right)$$

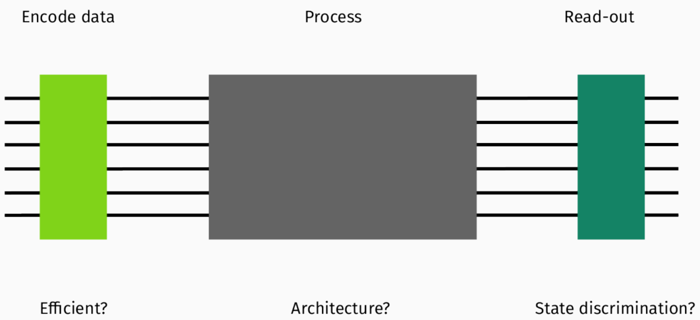
where $c < 4$.

Optimal solution



$\Rightarrow$ The approximation is efficient and requires a finite number of gates.

Many unexplored options



Add data in the course of computation?

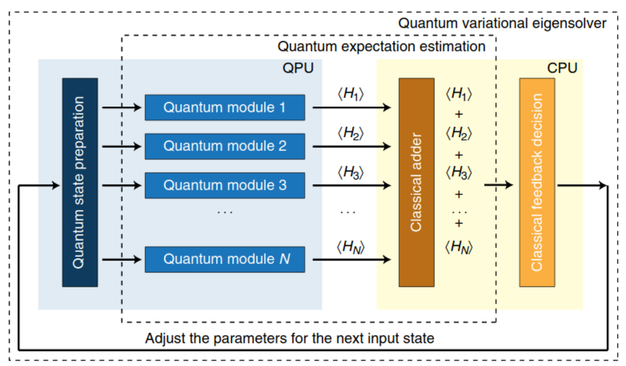
Example 1: VQE

Variational Quantum Eigensolvers (VQE)

Aspuru-Guzik et al., IBM, Zapata, Blatt.

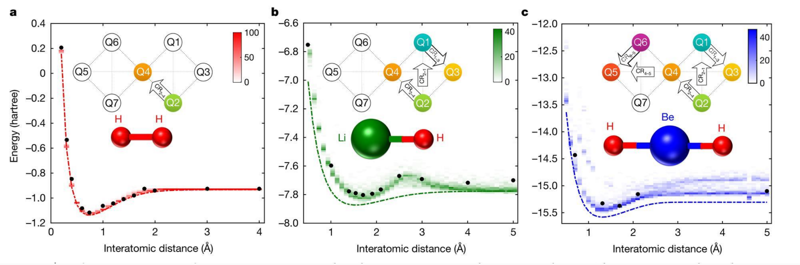
VQE is hybrid classical-quantum algorithm.

1. Define an optimization problem, e.g. energy, correlations, etc.
2. Apply "machine learning" on circuit design.



Variational Quantum Eigensolvers (VQE)

First successful applications in quantum chemistry:

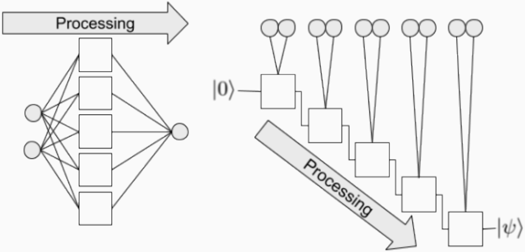


Example 2: Quantum Classifier

Data re-uploading strategy

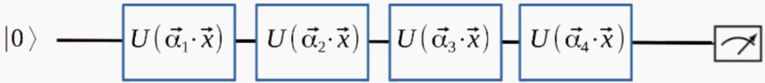
Pérez-Salinas et al. [arXiv:1907.02085]

Encode data directly "inside" circuit parameters:

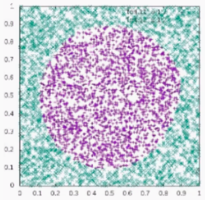


(a) Neural network (b) Quantum classifier

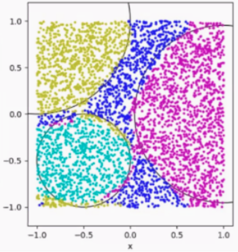
Data re-uploading strategy



D dimensional via re-uploading
K categories via final measurement



Layers	2 classes			4 classes	
	Circle	Sphere	Hypersphere	Wavy-lines	3-circles
1	75.2%	70.2%	68.0%	70.4%	74.5%
2	89.7%	75.0%	72.6%	88.2%	83.0%
6	92.8%	86.5%	93.2%	89.8%	83.8%
10	96.1%	91.7%	85.5%	90.0%	91.6%
20	96.9%	93.0%	89.2%	89.4%	92.3%



Data re-uploading strategy

Problem	Classical classifiers		Quantum classifier	
	NN	SVC	χ_f^2	χ_{wf}^2
Circle	0.96	0.97	0.96	0.97
3 circles	0.88	0.66	0.91	0.91
Hypersphere	0.98	0.95	0.91	0.98
Annulus	0.96	0.77	0.93	0.97
Non-Convex	0.99	0.77	0.96	0.98
Binary annulus	0.94	0.79	0.95	0.97
Sphere	0.97	0.95	0.93	0.96
Squares	0.98	0.96	0.99	0.95
Wavy Lines	0.95	0.82	0.93	0.94

Table 5: Comparison between single-qubit quantum classifier and two well-known classical classification techniques: a neural network (NN) with a single hidden layer composed of 100 neurons and a support vector classifier (SVC), both with the default parameters as defined in `scikit-learn` python package. We analyze nine problems: the first four are presented in Section 6 and the remaining five in Appendix B. Results of the single-qubit quantum classifier are obtained with the fidelity and weighted fidelity cost functions, χ_f^2 and χ_{wf}^2 defined in Eq. (7) and Eq. (9) respectively. This table shows the best success rate, being 1 the perfect classification, obtained after running ten times the NN and SVC algorithms and the best results obtained with single-qubit classifiers up to 10 layers.

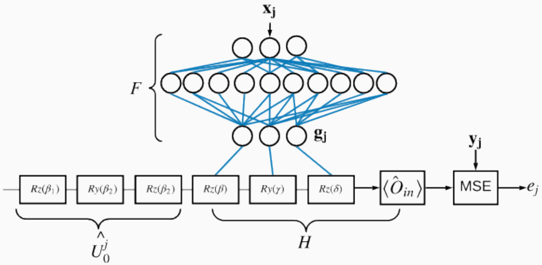
Example 3: ML to Quantum

VQE with reinforcement learning

A. Garcia-Saez, J. Riu [arXiv:1911.09682], Google [arXiv:2003:02989]

Strategies:

- Use Reinforcement Learning to tune VQE circuits.
- Use DL for variational circuit tune and data pre-post processing.



Code tutorials

Qibo applications and tutorial

- **VQE-like examples:**
  - Scaling of VQE for condensed matter systems
  - Variational Quantum Classifier
  - Data reuploading for a universal quantum classifier
  - Quantum autoencoder for data compression
  - Measuring the tangle of three-qubit states
  - Quantum autoencoders with enhanced data encoding (**New!**)

See: `https://qibo.readthedocs.io/en/latest/applications.html`

Thank you for your attention.