Noisy Intermediate-Scale Quantum algorithms

Alba Cervera-Lierta

Alexandria Quantum Computing Hypatia Series

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the matter lab

UNIVERSITY OF TORONTO

Outlook

1. Quantum computing in the NISQ era
2. Variational Quantum Algorithms
3. Squeezing the NISQ lemon
4. Applications
5. NISQ horizon

Quantum computing in the NISQ era

Quantum Computing in the NISQ era and beyond

John Preskill

Quantum 2, 79 (2018)

Noisy intermediate-scale quantum (NISQ) algorithms

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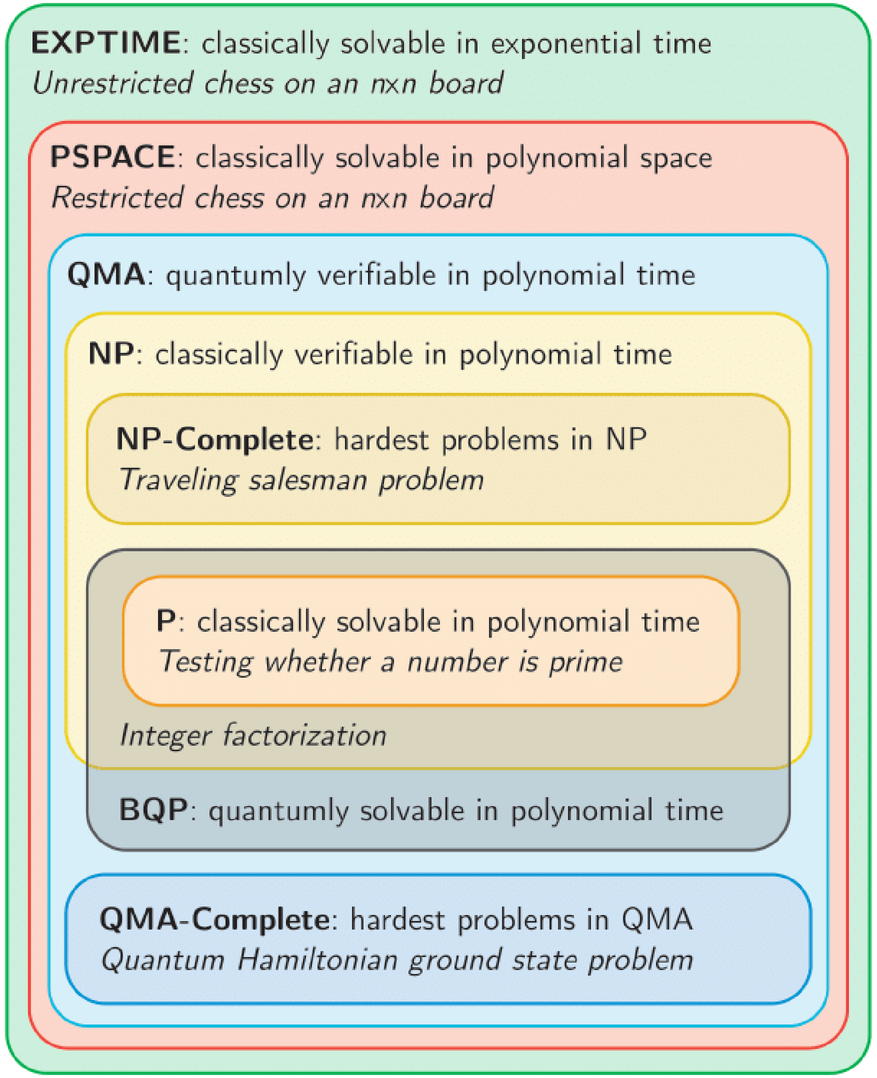
arXiv:2101.08448

The power of quantum



Why do we need a quantum computer?

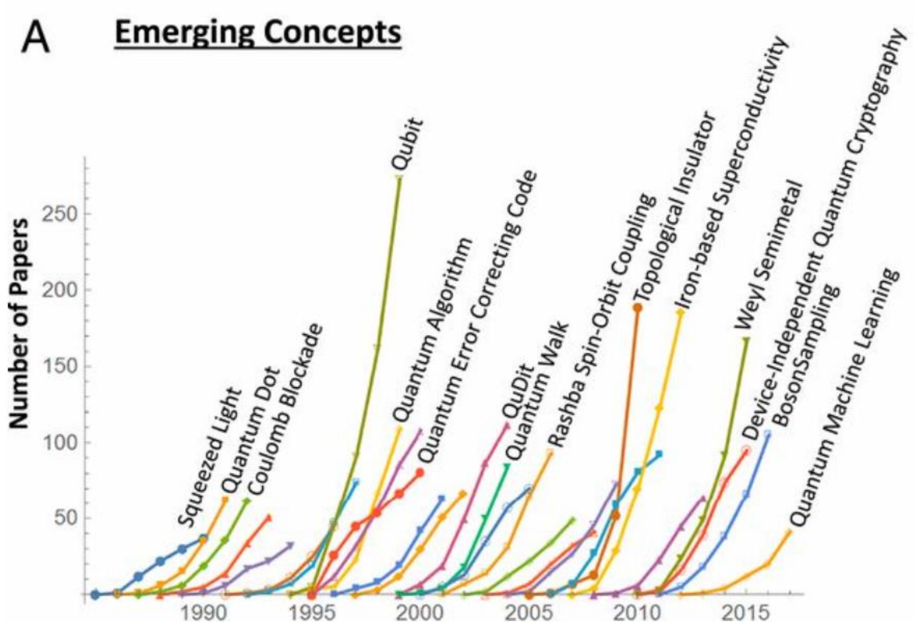
- Quantum simulation
- Solve problems beyond P and BPP

Quantum computers are powerful but not limitless

Which problems are BQP?

Approximate solutions to NP problems?

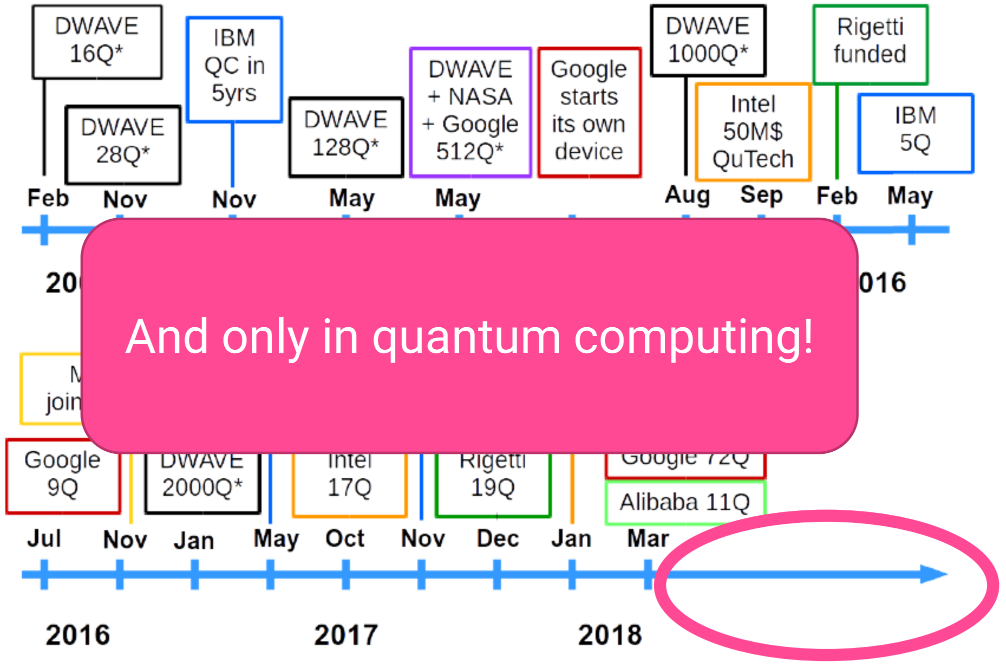
The power of quantum



qubit, April '95, Schumacher, *Quantum coding*. PRA 51, 2738–2747

Predicting research trends with semantic and neural networks with an application in quantum physics, M. Krenn, A. Zeilinger, PNAS 117 (4) 1910-1916 (2020)

From a popular science talk in 2018:



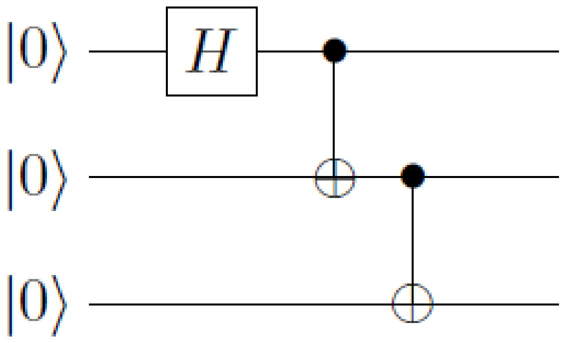
Trapped ions companies: IonQ, Honeywell, Alpine QT

Quantum supremacy using a programmable superconducting processor, Google AI, Nature 574, 505(2019).

Quantum computational advantage using photons, USTC (Chao-Yang Lu, Jian-Wei Pan's group), Science 370, 1460 (2020).

Gate-based Quantum Computing

Name	Definition	Mathematically	Diagramatically	Experimentally
Qubits	2-level quantum systems	Two-dimensional complex vector	Lines	Photons, superconducting circuits, trapped ions, …
Gates	Interactions between qubits that generate superposition and entanglement in a controlable way	SU(2^n) matrices where n is the number of qubits involved in the operation	Boxes that specify the gate and some vertical symbols that represent particular entangling gates (CNOT and SWAP)	Laser pulses (ions, photons), optical devices (SPDC, PS, …) microwave pulses
Measurement	Interaction with the individual qubits that forces its collapse to one of the two levels	Projector over the computational basis state	Box with a “meter” symbol	Coupling with a cavity, photon detectors,…



$$H = \frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}.$$

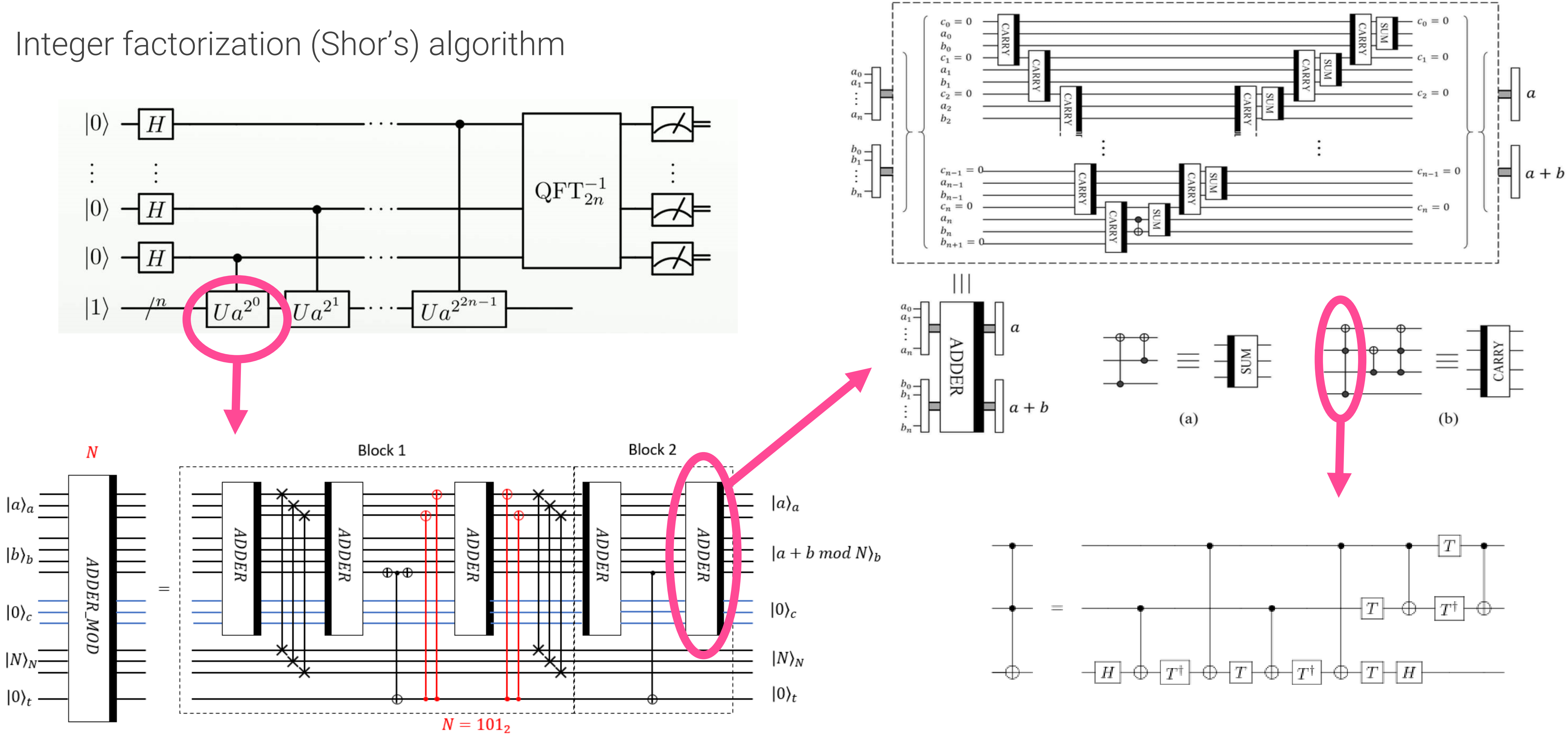
$$\mathrm{CNOT} = \mathrm{CX} = \begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}.$$

This quantum circuit generates the GHZ state

Noisy Intermediate-Scale Quantum (NISQ) algorithms, K. Bharti, ACL, T.H. Kyaw, et. al., arXiv:2101.08448 (2021)

From theory to experiment

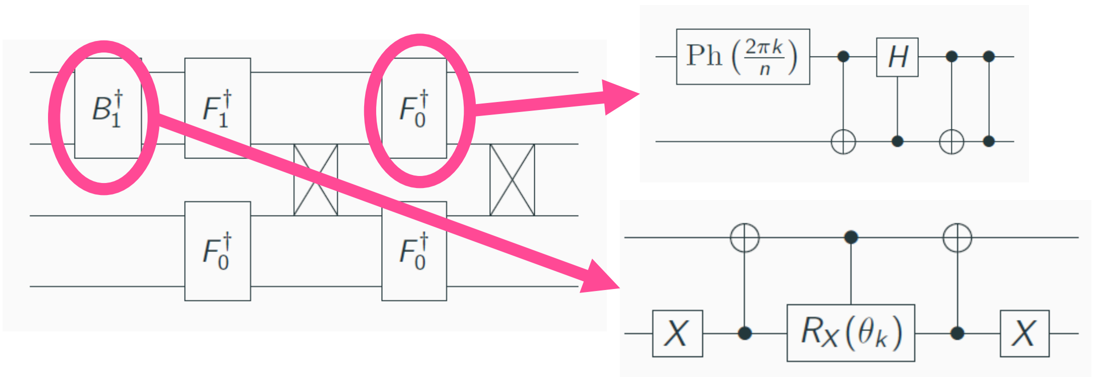
Integer factorization (Shor's) algorithm

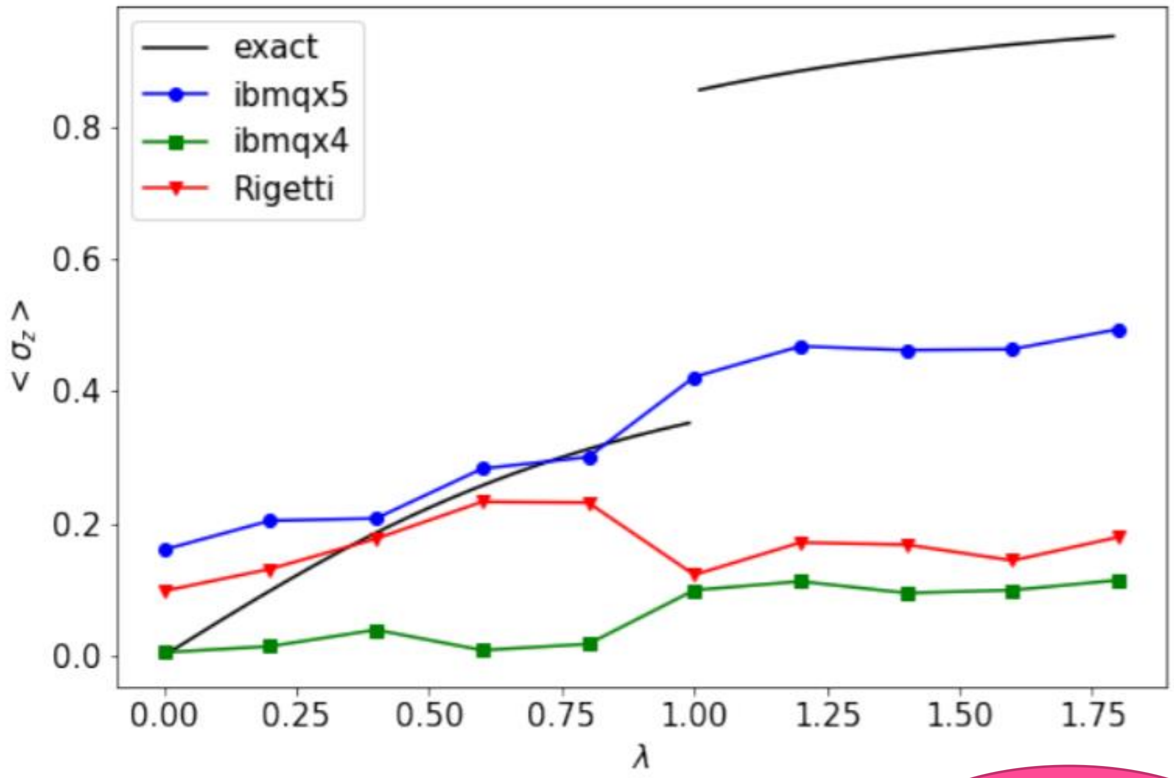


Shor, P.W. , IEEE Comput. Soc. Press: 124 (1994), A. Ekert, R. Jozsa, Rev. Mod. Phys. 68, 733 (1996)

From theory to experiment

Example: $n = 4$ Ising model simulation.





$\sim$35 gates circuit depth
$\sim$500 ns entangling gates
$\sim$100 ns single-qubit

<17500 ns = 17.5 μs

Qubits coherence time → $\sim$50 μs

March-May 2018

Errors coming from readout, cross-talk, relaxation, … are relevant and difficult to track

F. Verstraete, J. I. Cirac, J. I. Latorre, Phys. Rev. A 79 032316 (2009), ACL, Quantum 2 114 (2018)

Noisy Intermediate-Scale Quantum

Why is QC hard experimentally?

- Qubits have to interact strongly (by means of the quantum logic gates)…
- …but not with the environment…
- …except if we want to measure them.

What is the state-of-the-art in digital quantum computing?

- ~50 qubit devices
- Error rates of ~10^-3
- No Quantum Error Correction (QEC)

Noisy Intermediate-Scale Quantum (NISQ) computing

- 50-100 qubits
- Low error rates
- No QEC

What can we do in NISQ?

- Good trial field to study physics
- Possible applications?
- A step in the path towards Fault Tolerant QC

Noisy Intermediate-Scale Quantum (NISQ) algorithms, K. Bharti, ACL, T.H. Kyaw, et. al., arXiv:2101.08448 (2021)

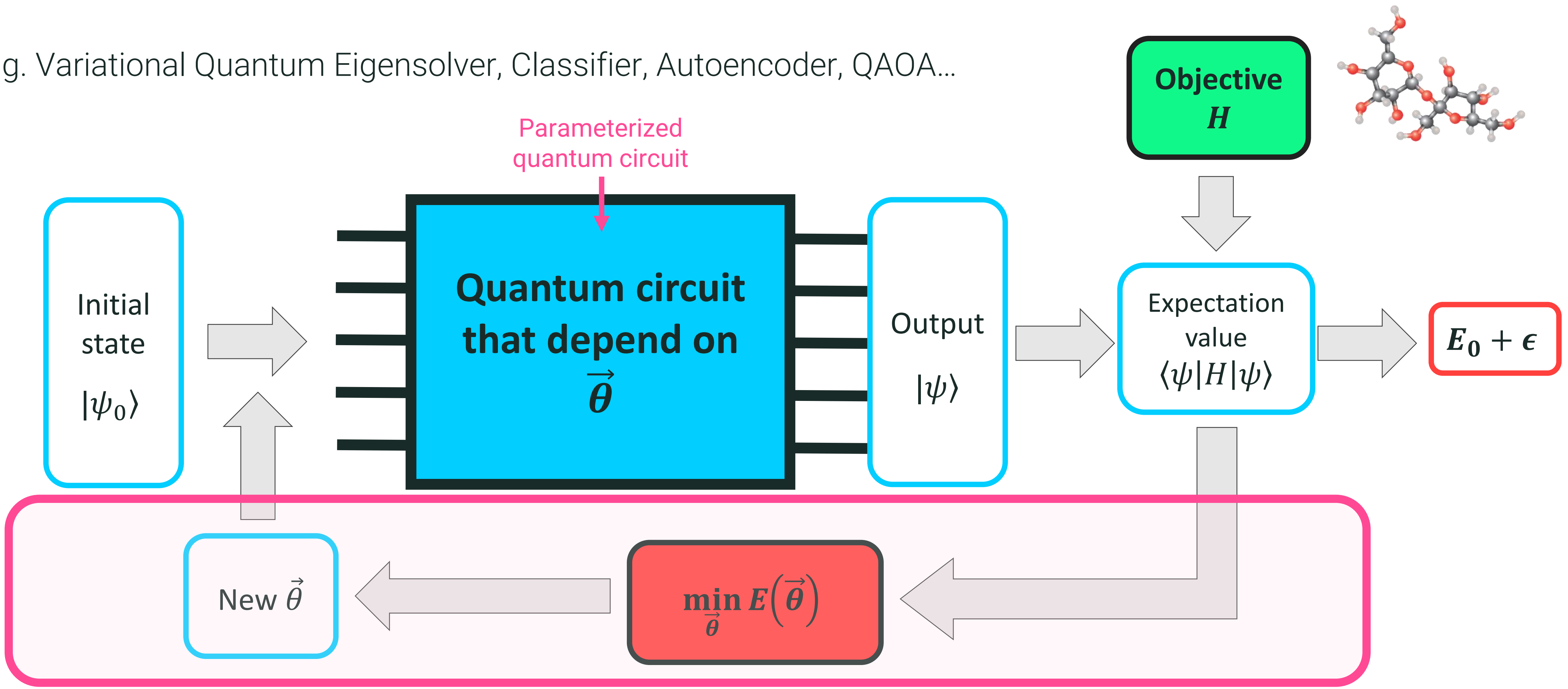
Variational Quantum Algorithms

Variational Quantum Algorithms is one of the most used NISQ paradigms, but it is not the only one

The parents of VQA are the Variational Quantum Eigensolver (VQE) and the Quantum Approximate Optimization Algorithm (QAOA).

Variational Quantum Algorithms

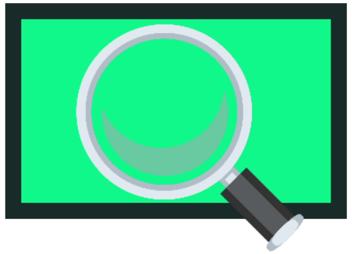
e.g. Variational Quantum Eigensolver, Classifier, Autoencoder, QAOA…



Classical optimization

Variational principle: $\mathrm{E} = \langle\psi|H|\psi\rangle \geq E_0$

Objective function



It encodes the problem in a form of a quantum operator, e.g. a Hamiltonian

$$\langle H \rangle_{\mathcal{U}(\boldsymbol{\theta})} \equiv \langle 0 | \mathcal{U}^{\dagger}(\boldsymbol{\theta}) H \mathcal{U}(\boldsymbol{\theta}) | 0 \rangle$$

The objective is decomposed into Pauli strings which expectation value can be measured with the quantum computer.

$$H = \sum_{k=1}^{M} c_k \hat{P}_k \longrightarrow \langle H \rangle_{\mathcal{U}} = \sum_{k=1}^{M} c_k \langle \hat{P}_k \rangle_{\mathcal{U}}$$

An objective can also be the fidelity w.r.t. a particular target state that we are trying to match.

$$F\left(\Psi, \Psi_{\mathcal{U}(\boldsymbol{\theta})}\right) \equiv |\langle \Psi | \Psi_{\mathcal{U}(\boldsymbol{\theta})} \rangle|^2$$

We can use projectors or SWAP test to obtain the value of that fidelity

$$\max_{\boldsymbol{\theta}} F\left(\Psi, \Psi_{U(\boldsymbol{\theta})}\right) = \min_{\boldsymbol{\theta}} \left(-\langle \hat{\Pi}_{\Psi} \rangle_{\mathcal{U}(\boldsymbol{\theta})}\right)$$

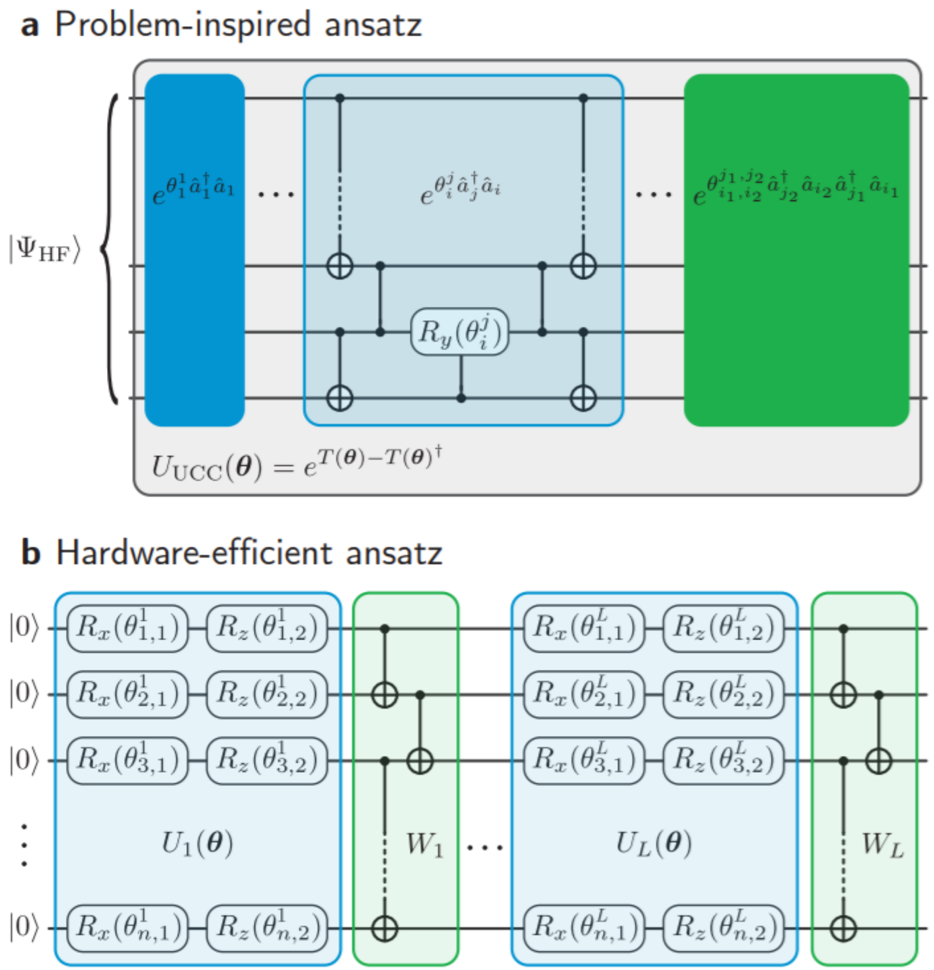
Noisy Intermediate-Scale Quantum (NISQ) algorithms, K. Bharti, ACL, T.H. Kyaw, et. al., arXiv:2101.08448 (2021)

Parameterized quantum circuits

It prepares what will eventually be the approximation of the g.s. of our Objective function.

It depends on a series of parameters that have to be finetunned to minimize the objective

They can be designed from a physical point of view (e.g. UCC, QAOA,...) or from a practical point of view (using a limited set of gates and circuit topology).



Classical optimization

We need to navigate the quantum circuit parameter space, e.g. by using gradiend based methods

$$\theta_i^{(t+1)} = \theta_i^{(t)} - \eta \, \partial_i f(\boldsymbol{\theta})$$

The gradients are expectation values of the quantum circuit derivatives w.r.t. a parameter.

Example: parameter-shift rule

$$\mathcal{U}(\boldsymbol{\theta}) = V(\boldsymbol{\theta}_{\neg i}) G(\theta_i) W(\boldsymbol{\theta}_{\neg i}) \qquad G = e^{-i\theta_i g}$$

Eigenvalues of g are $\pm\lambda$

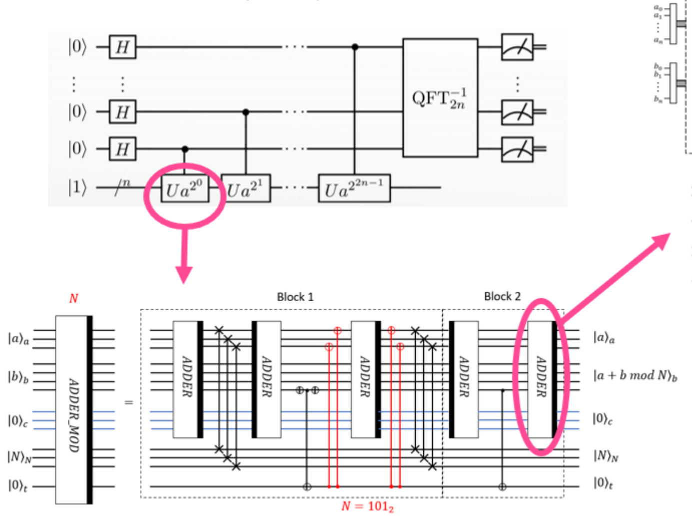
$$\partial_i \langle f(\boldsymbol{\theta}) \rangle = \lambda \left(\langle f(\boldsymbol{\theta}_+) \rangle - \langle f(\boldsymbol{\theta}_-) \rangle \right) \qquad \boldsymbol{\theta}_\pm = \boldsymbol{\theta} \pm (\pi/4\lambda) \boldsymbol{e}_i$$

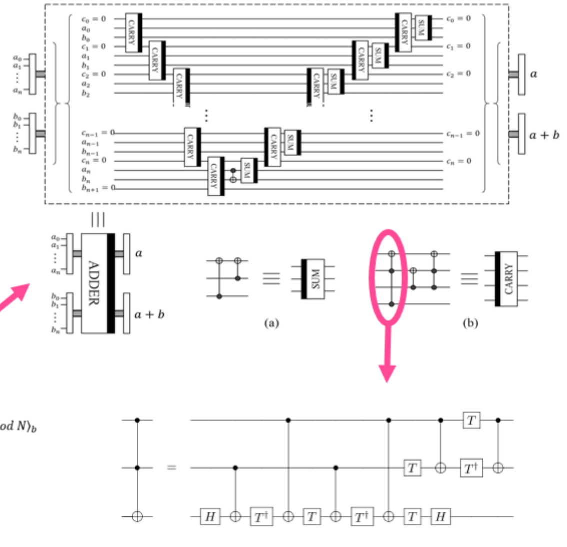
Gradient-free: genetic algorithms, reinforcement learning, …

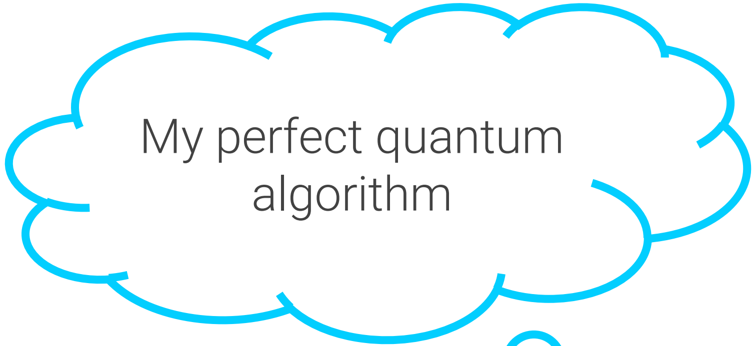
Noisy Intermediate-Scale Quantum (NISQ) algorithms, K. Bharti, ACL, T.H. Kyaw, et. al., arXiv:2101.08448 (2021)

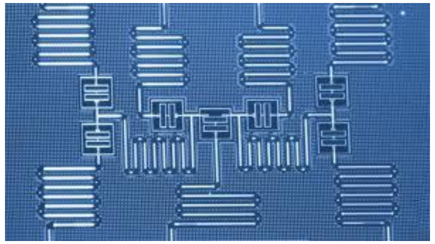
Squeezing the NISQ lemon

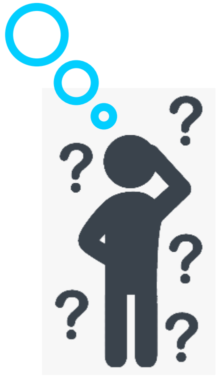
Integer factorization (Shor's) algorithm











Quantum Error Mitigation

A set of classical post-processing techniques and active operations on hardware that allow to correct or compensate the errors from a noisy quantum computer.

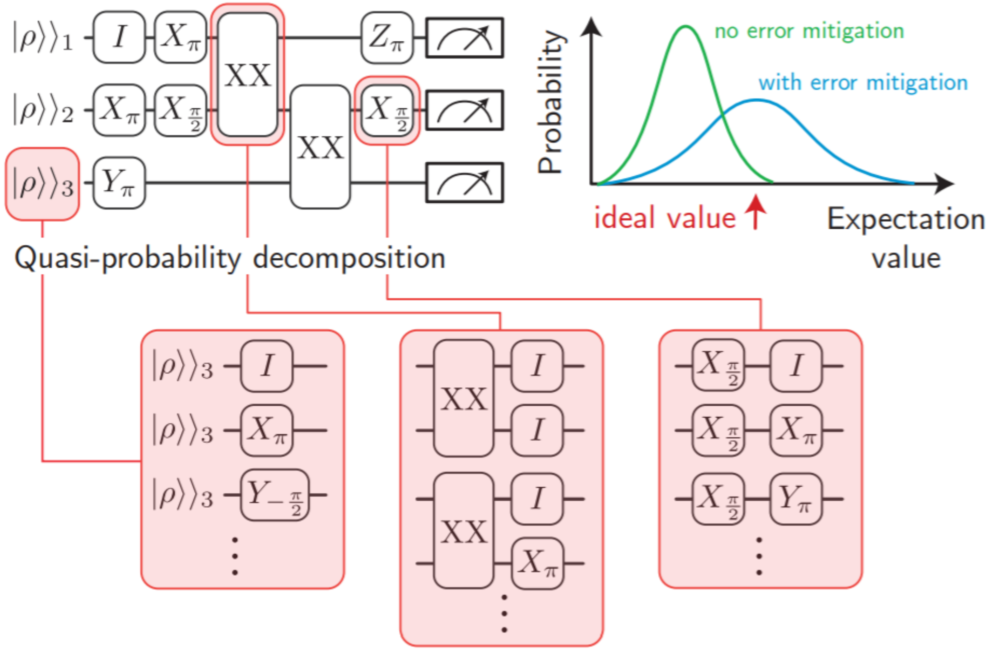
Zero-noise extrapolation

Instead of running our circuit unitary U, we run different circuits $U(UU^\dagger)^n$ (increasingly noisy). Extrapolate the result for zero-noise U

Stabilizer based approach

relies on the information associated with conserved quantities such as spin and particle number conserving ansatz. If any change in such quantities is detected, one can pinpoint an error in the circuit.

Probabilistic error cancellation



Quantum Error Mitigation

Quantum Optimal Control strategies

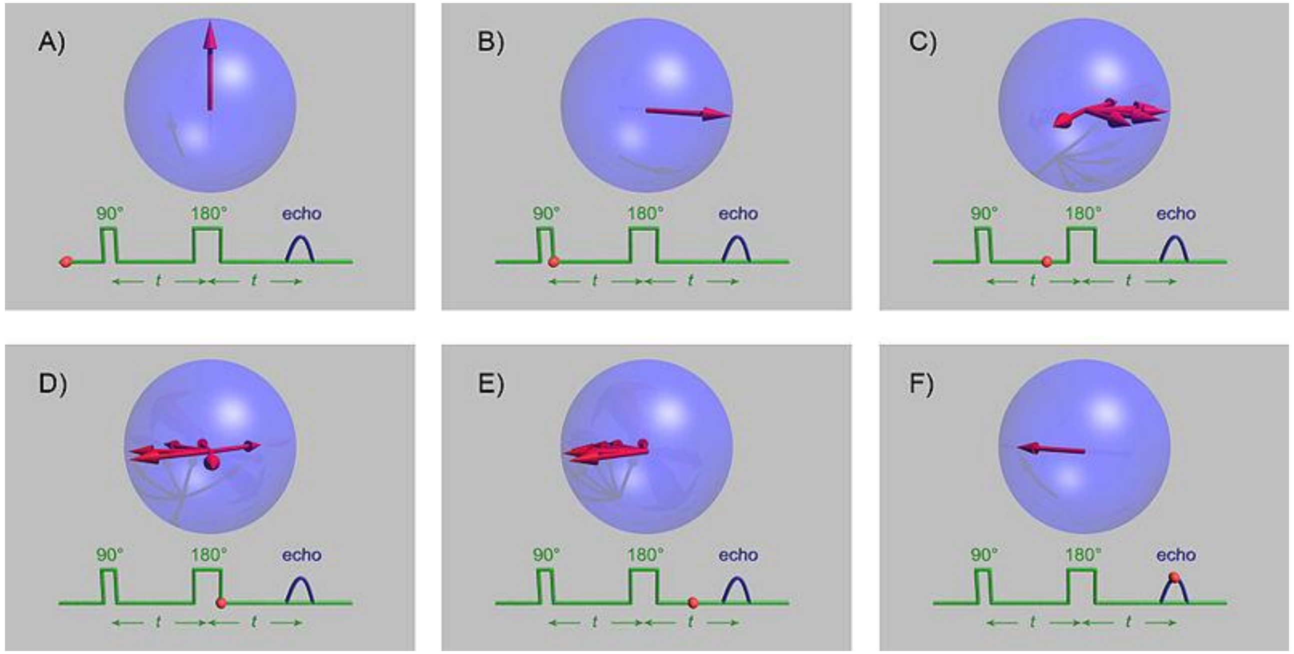
Dynamical Decoupling:

Designed to suppress decoherence via fancy pulses to the system so that it cancels the system-bath interaction to a given order in time dependent perturbation theory

Pulse shaping technique:

passive cancellation of system-bath interaction.

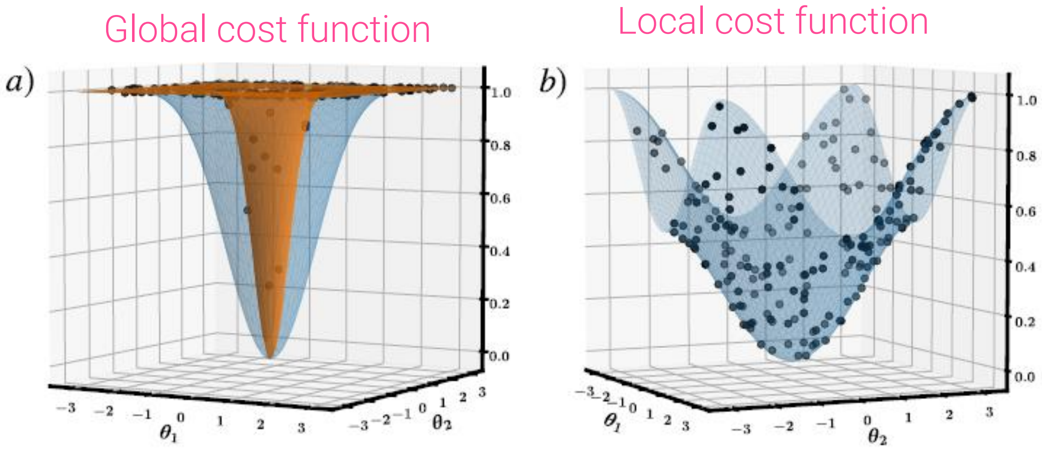
Among many others…



The *barren-plateaux* problem

Compute the gradients with the quantum circuit and use these values to run a classical minimizer, e.g. Nelder-Mead, Adam, …

With no prior knowledge about the solution, $\vec{\theta}$ parameters are initialized at random.



Consequence: *barren-plateaux*

The expected value of the gradient is zero!
The expected value of the variance is also zero!

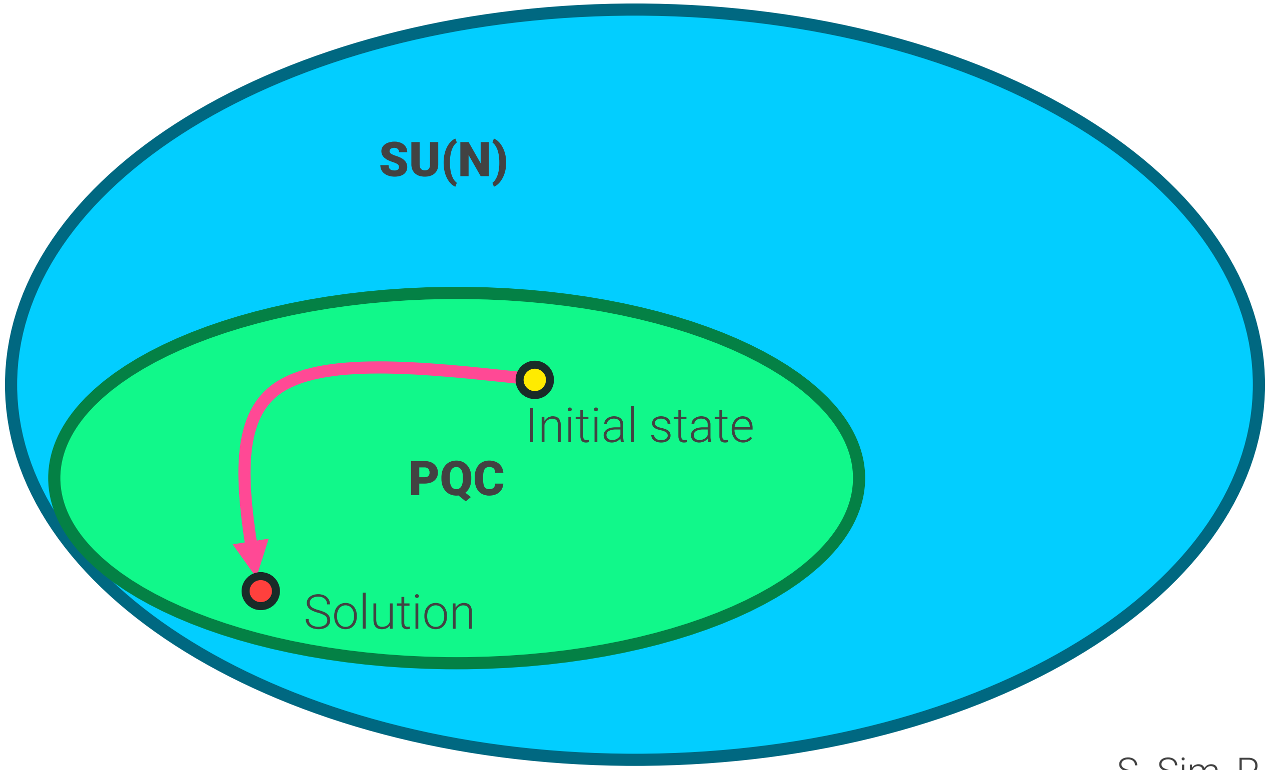
Solutions

- Use parameters close to the solution.
- Use local cost functions instead of global ones.
- Introduce correlations between parameters.

Ref.: M. Cerezo *et. al.* arXiv:2001.00550v2 [quant-ph]

Expressibility

When setting a PQC ansatz we have to be careful to not narrow the Hilbert space accesible by the PQC so we can reach a good approximation of the solution state.

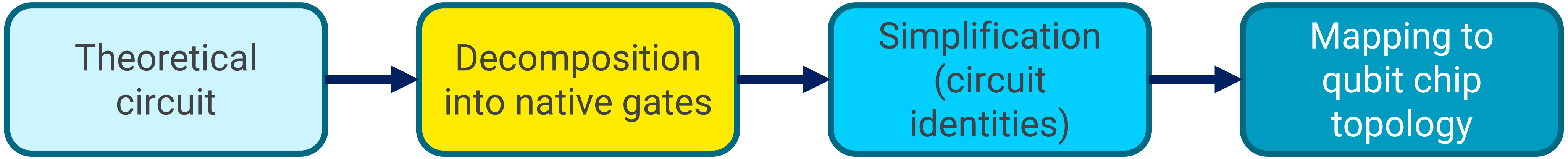


We can quantify the expressibility of a PQC by computing the distance between a Haar distribution of the states and states generated by the PQC.

$$A_U^{(t)} = \left\| \int_{\mathrm{Haar}} (|\psi\rangle\langle\psi|)^{\otimes t} d\psi - \int_{\boldsymbol{\theta}} (|\psi_{\boldsymbol{\theta}}\rangle(\langle\psi_{\boldsymbol{\theta}}|)^{\otimes t} d\psi_{\boldsymbol{\theta}} \right\|$$

S. Sim, P. D. Johnson, A. Aspuru-Guzik, Adv. Quantum Technol. 2 1900070 (2019)

Circuit compilation



Native and universal gate sets:

Solovay-Kitaev theorem: With a universal gate set we can approximate with epsilon accuracy any SU(N) with a circuit of polynomial depth.

Gottesman–Knill theorem: Circuits composed by gates from the Clifford group (Clifford circuits) can be simulated efficiently with a classical computer.

Gate sets are usually composed by Clifford gates + one non-clifford gate, e.g. {H, S, CNOT} + T

However, depending on the hardware implementation, some gates are easier to control.
e.g. CZ gates for superconducting circuits, XX gates for trapped ions.

The more native gates, the shorter and simpler the circuit

Noisy Intermediate-Scale Quantum (NISQ) algorithms, K. Bharti, ACL, T.H. Kyaw, et. al., arXiv:2101.08448 (2021)

Circuit compilation

Theoretical circuit → Decomposition into native gates → Simplification (circuit identities) → Mapping to qubit chip topology

Circuit simplification: use identities or tools like the ZX calculus (graph representation of quantum circuits)

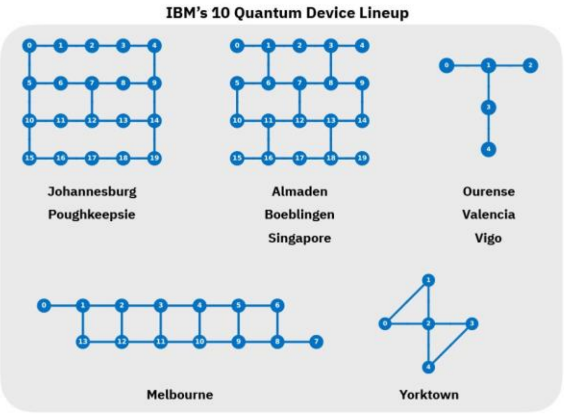
"Interacting quantum observables: categorical algebra and diagrammatics",
B. Coecke, R. Duncan, NJP 13 (4): 043016 (2011).

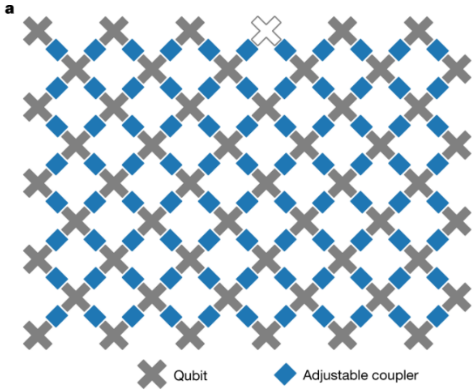
Circuit compilation

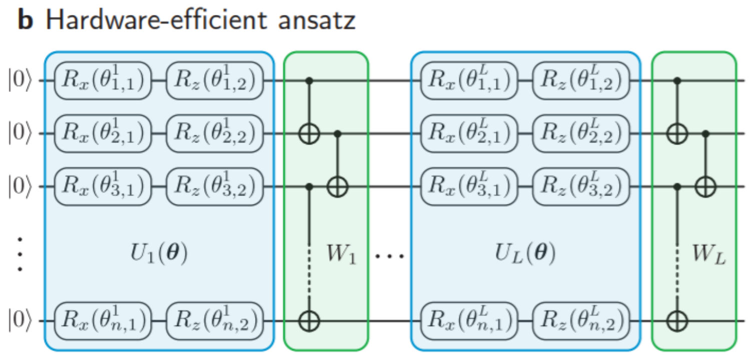
Theoretical circuit → Decomposition into native gates → Simplification (circuit identities) → Mapping to qubit chip topology

Circuit simplification: use identities or tools like the ZX calculi (graph representation of quantum circuits)

Qubits connectivity problem: not all qubits are physically connected, so we have to map our quantum circuits to the real devices.







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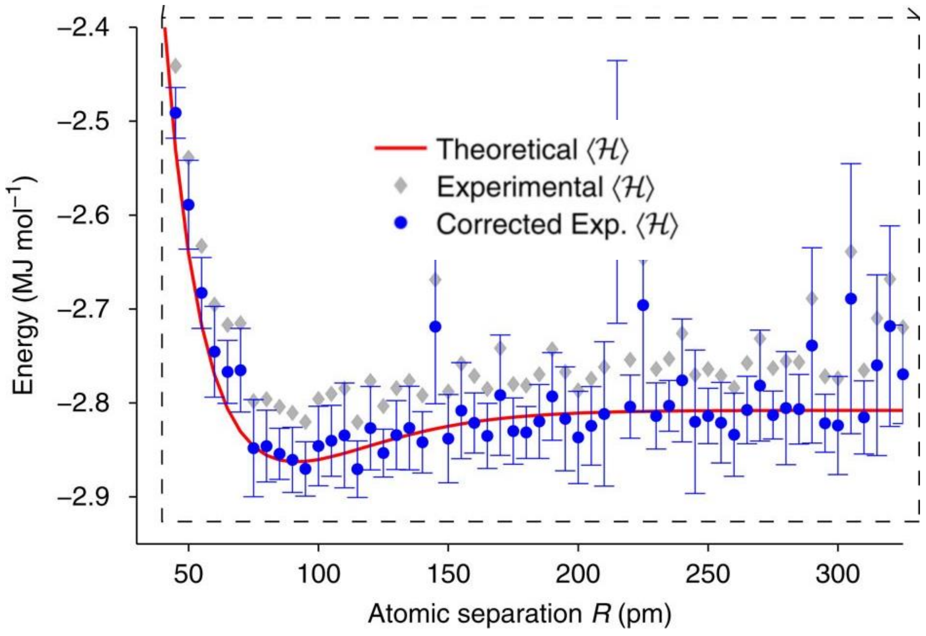
Applications

Chemistry: the Variational Quantum Eigensolver

Bond dissociation curve of the He–H⁺ molecule.



<u>GOAL</u>: find $|\psi\rangle$ that minimizes $\dfrac{\langle\psi \mid \mathcal{H} \mid \psi\rangle}{\langle\psi \mid \psi\rangle}$.

Electronic structure Hamiltonian decomposed into Pauli strings

$$\langle\mathcal{H}\rangle = \sum_{i\alpha} h^i_\alpha \langle\sigma^i_\alpha\rangle + \sum_{ij\alpha\beta} h^{ij}_{\alpha\beta}\langle\sigma^i_\alpha \sigma^j_\beta\rangle + \ \dots$$

Quantum circuit that generates the ground state of that Hamiltonian (Unitary Couple-Cluster ansatz)

Unitary operation (Cluster operator)

Hartree-Fock

Excitations Hartree-Fock orbitals

$$|\Psi(\boldsymbol{\theta})\rangle = e^{T(\boldsymbol{\theta})-T(\boldsymbol{\theta})^\dagger}\,|\Psi_{\mathrm{HF}}\rangle$$

$$T(\boldsymbol{\theta}) = T_1(\boldsymbol{\theta}) + T_2(\boldsymbol{\theta}) + \cdots$$

$$T_1(\boldsymbol{\theta}) = \sum_{\substack{i\epsilon\mathrm{occ}\\ j\epsilon\mathrm{virt}}} \theta_i^j \hat{a}_j^\dagger \hat{a}_i$$

$$T_2(\boldsymbol{\theta}) = \sum_{\substack{i_1,i_2\epsilon\mathrm{occ}\\ j_1,j_2\epsilon\mathrm{virt}}} \theta_{i_1,i_2}^{j_1,j_2} \hat{a}_{j_2}^\dagger \hat{a}_{i_2} \hat{a}_{j_1}^\dagger \hat{a}_{i_1}$$

Transform the fermionic operators to Pauli strings (e.g. Jordan Wigner) and they become the generators of the quantum gates.

Quantum Approximate Optimization Algorithm

Can be understood as an approximation of the Trotter decompositiong of adiabatic evolution.

Mixing Hamiltonian

$$H_M \equiv \sum_{i=1}^{n} \hat{\sigma}_x^i$$

Problem Hamiltonian

$$H_P \equiv \sum_{i=1}^{n} C(e_i)|e_i\rangle$$

Combinatorial optimization problem encoded in Pauli strings

$$C_\alpha(z) = \begin{cases} 1 & \text{if } z \text{ satisfies } C_\alpha(z) \\ 0 & \text{if } z \text{ does not satisfy} \end{cases}$$

$$H_P = \sum_{(i,j)\in E} \frac{1}{2}\left(I - \hat{\sigma}_z^i \otimes \hat{\sigma}_z^j\right) \equiv \sum_{(i,j)\in E} C_{ij}$$

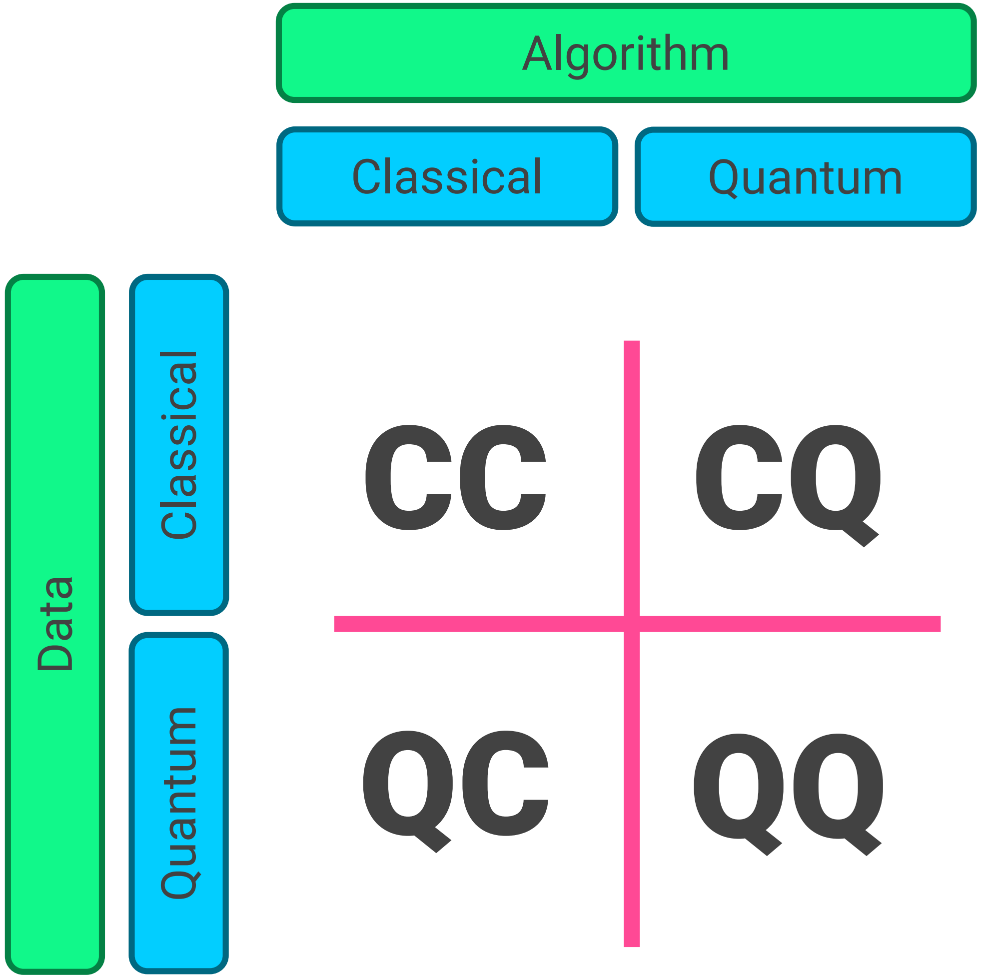
Construct the circuit ansatz by alternating the problem and mixing Hamiltonians where β and γ are the variational parameters to be optimized classically.

full superposition state

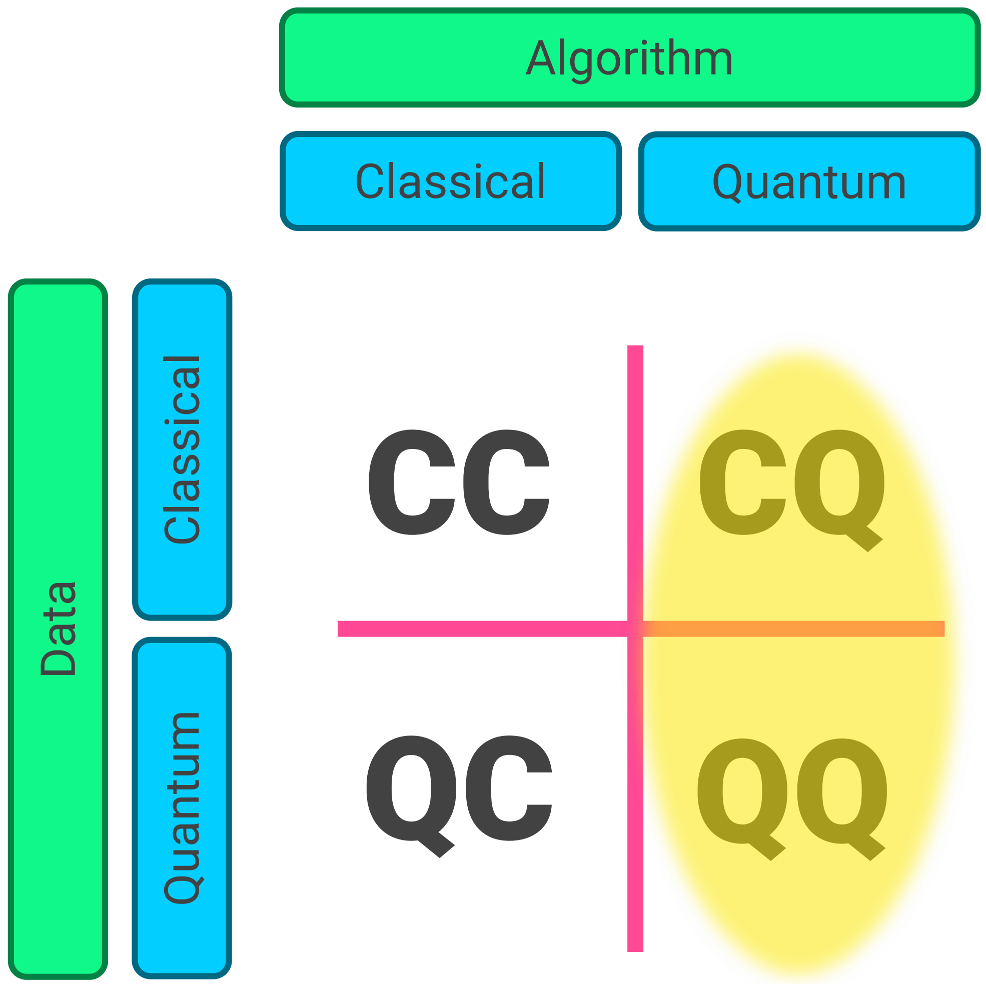
$$|\Psi(\gamma,\beta)\rangle \equiv e^{-i\beta_p H_M} e^{-i\gamma_p H_P} \cdots e^{-i\beta_1 H_M} e^{-i\gamma_1 H_P} |D\rangle$$

Objective function: $\langle\Psi(\gamma,\beta)|\, H_P(\gamma,\beta)\, |\Psi(\gamma,\beta)\rangle$

Machine Learning



Machine Learning

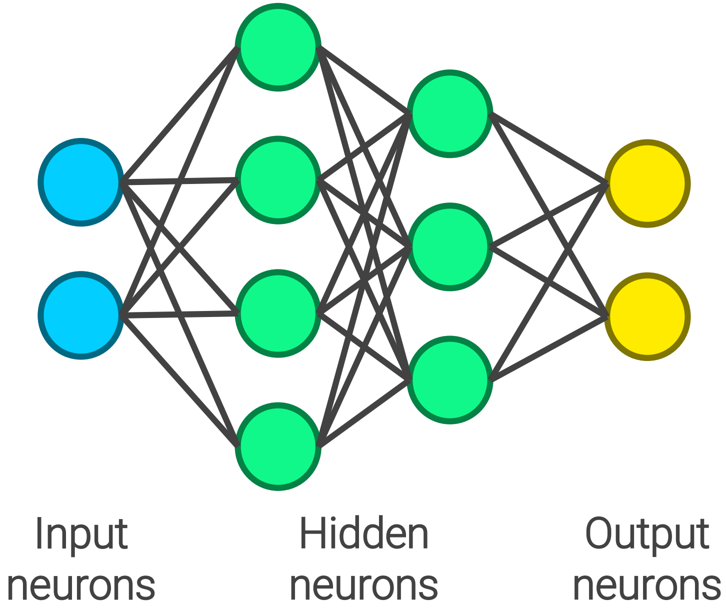


QML
Quantum algorithms feed with classical or quantum data

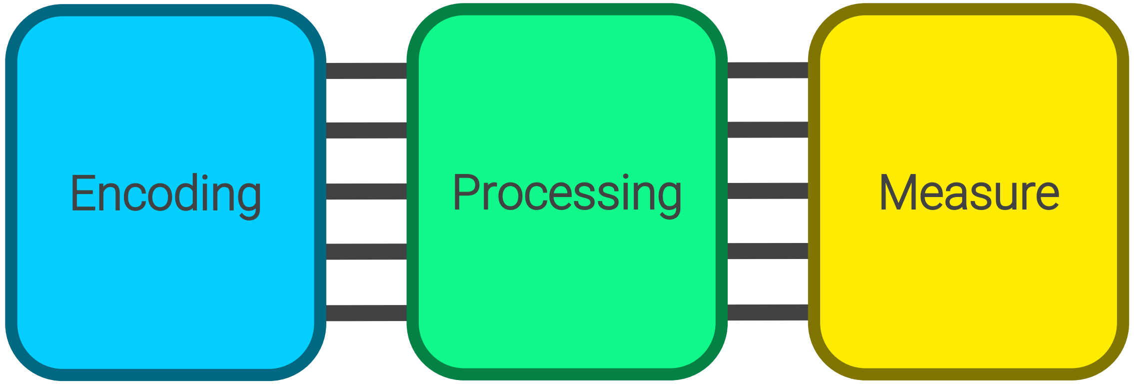
- Supervised Learning
- Unsupervised Learning
- Reinforcement Learning

From classical to quantum NN

Classical



Quantum
(circuit centric)



K Mitarai, M Negoro, M Kitagawa, K Fujii Phys. Revs A 98 (3), 032309 (2018)

E. Farhi and H.Neven, arXiv:1802.06002 (2018)

M. Schuld and N. Killoran, Phys. Rev. Lett. 122, 040504 (2019)

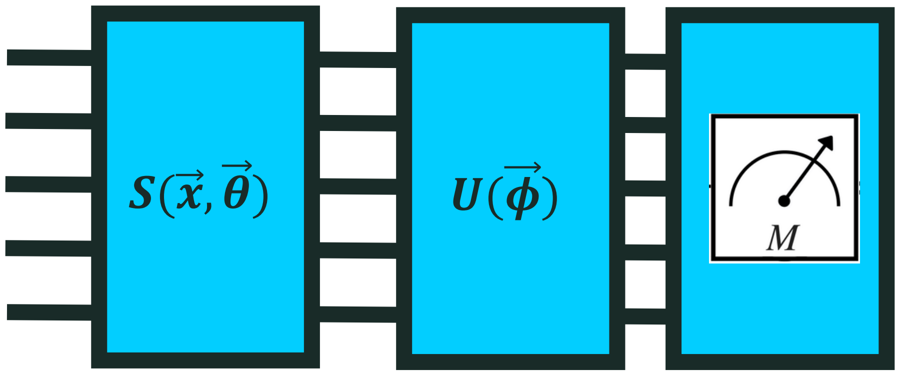
M. Schuld, A. Bocharov, K. M. Svore, and N. Wiebe, Phys. Rev. A 101, 032308 (2020)

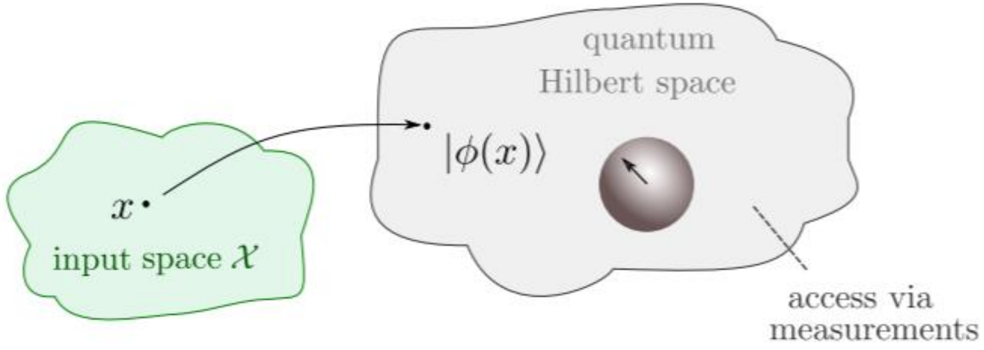
Supervised Learning

$$|\psi_0\rangle \rightarrow |\psi(\vec{x},\vec{\theta})\rangle \rightarrow |\psi(\vec{x},\vec{\theta},\vec{\phi})\rangle$$

Encode the data (quantum feature space)

Rotate to the correct measurement basis





We can then compute the Kernel

$$\kappa(\boldsymbol{x}_i,\boldsymbol{x}_j) \equiv \langle \Phi(\boldsymbol{x}_i)|\Phi(\boldsymbol{x}_j)\rangle$$

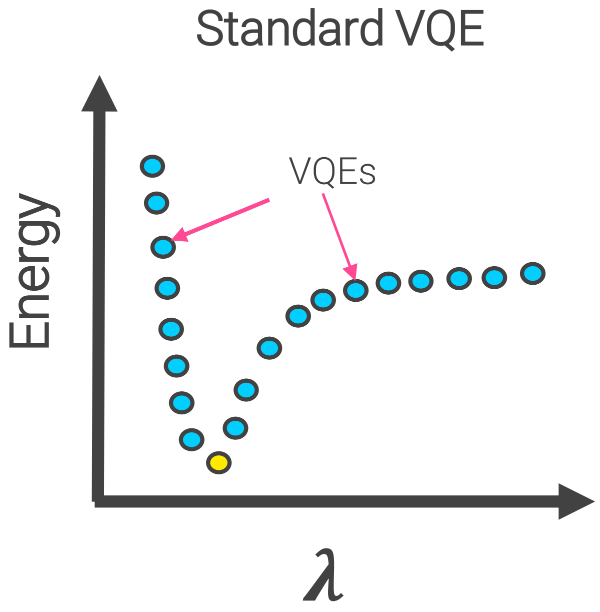
Or minimize the fidelity w.r.t. target states

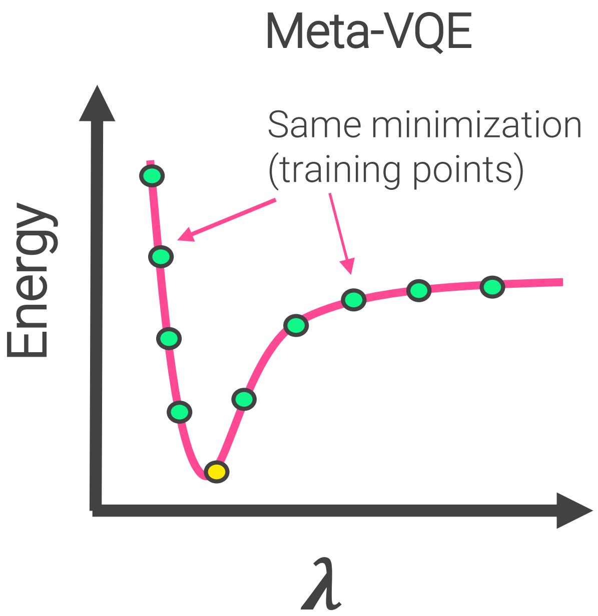
$$C(\boldsymbol{\theta}) = \sum_{i=1}^{\mathcal{D}} \left(1 - |\langle y_i|\Psi(\boldsymbol{x}_i,\boldsymbol{\theta})\rangle|^2\right)$$

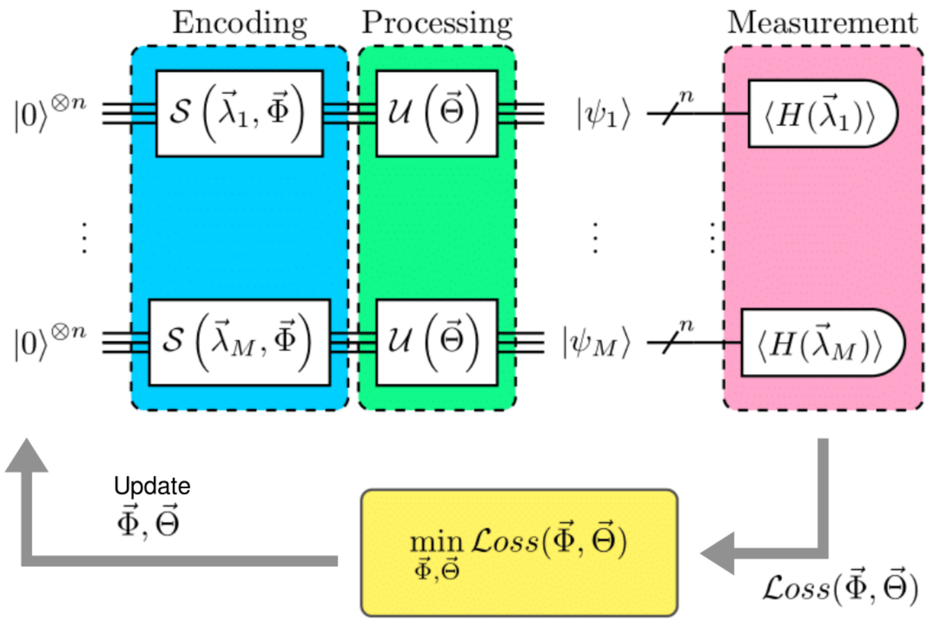
Bonus: QML applied to many-body g.s.

Parameterized Hamiltonian $H\left(\vec{\lambda}\right)$

<u>Goal:</u> to find the quantum circut that encodes the ground state of the Hamiltonian for any value of $\vec{\lambda}$





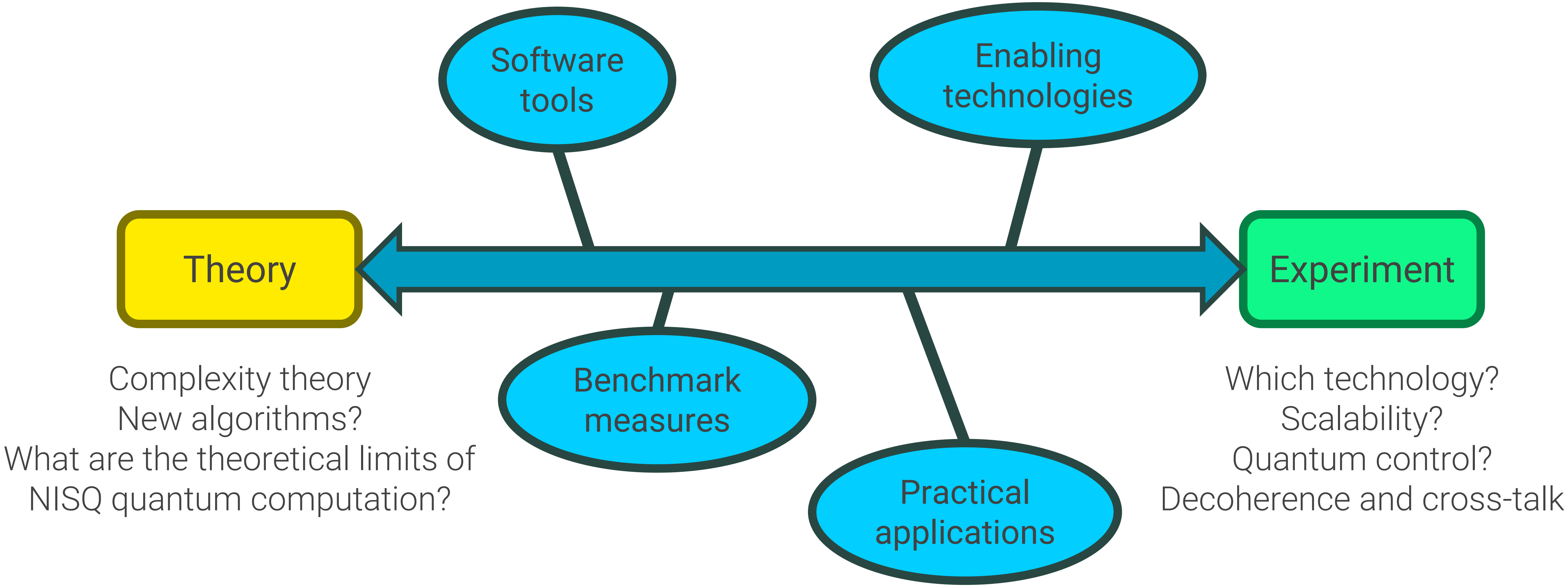


A collection of VQE with a global cost function that is used to learn the g.s. energy profile

ACL, J. S. Kottmann and A. Aspuru-Guzik, arXiv:2009.13545 [quant-ph] (2020)

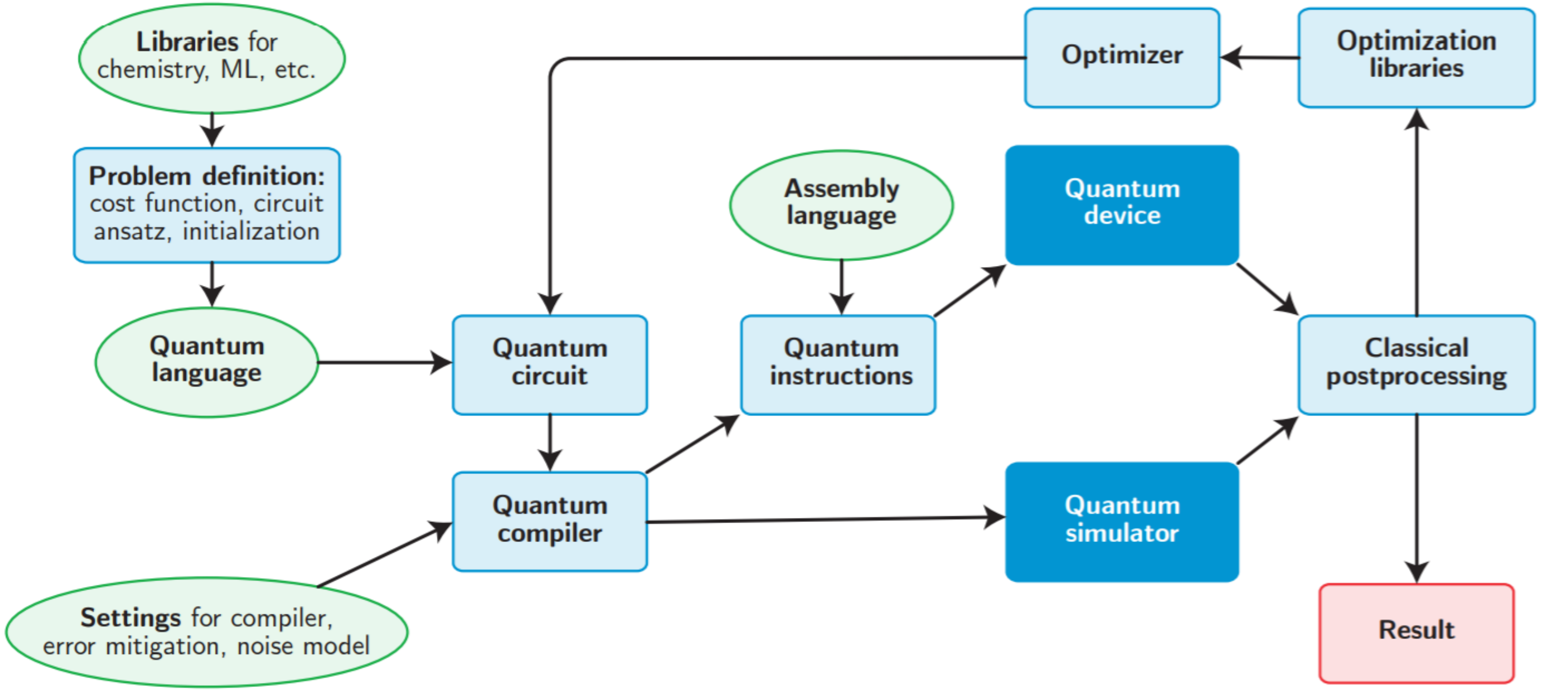
NISQ horizon

NISQ road



Noisy Intermediate-Scale Quantum (NISQ) algorithms, K. Bharti, ACL, T.H. Kyaw, et. al., arXiv:2101.08448 (2021)

How to program a NISQ algorithm



J. Kottmann, S. Alperin-Lea, T. Tamayo-Mendoza, et. al.,
Quantum Sci. Technol. 6 024009 (2021).

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Next goal: fault-tolerant quantum computing

Quantum Error Correction: protect the quantum information in a highly entangled state.

QEC comes with a big qubit overhead: thousands (posible milions) of qubits to implement a quantum advantage experiment.

That's why we have NISQ… but most of the NISQ algorithms can also be implemented in the **Fault-Tolerant era.**

Noise limits NISQ algorithms such as VQAs.

Next goal in quantum computing is Fault-tolerant quantum computation. We don't know how much will it take, but so much physics to explore along the way!

Acknowledgements

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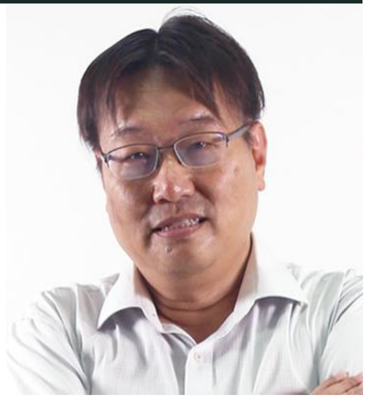

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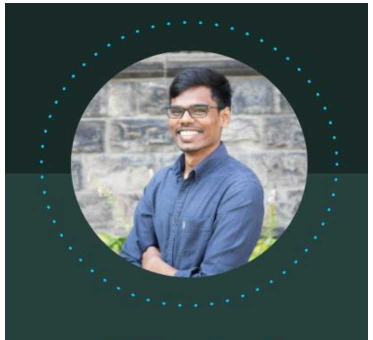

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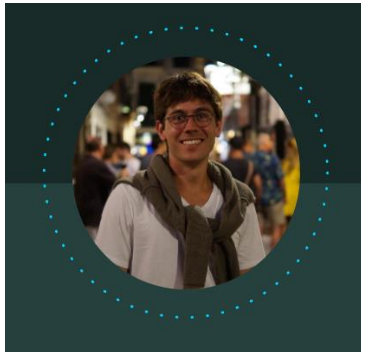

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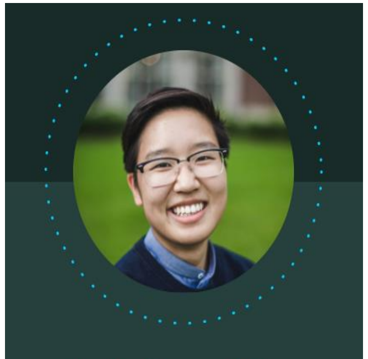

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