The Meta-Variational Quantum Eigensolver

Alba Cervera-Lierta, Jakob S. Kottmann, Alán Aspuru-Guzik

Machine Learning for Quantum X

July 5th, 2021

the matter lab

Outlook

1. Variational Quantum Algorithms (VQA)
2. VQA for Quantum Machine Learning (QML)
3. The Meta-VQE: a QML algorithm for Hamiltonian simulation

Variational Quantum Algorithms

[Submitted on 21 Jan 2021]

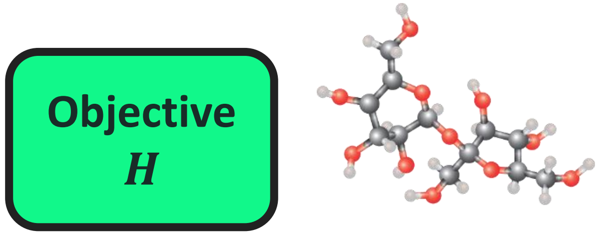
Noisy intermediate-scale quantum (NISQ) algorithms

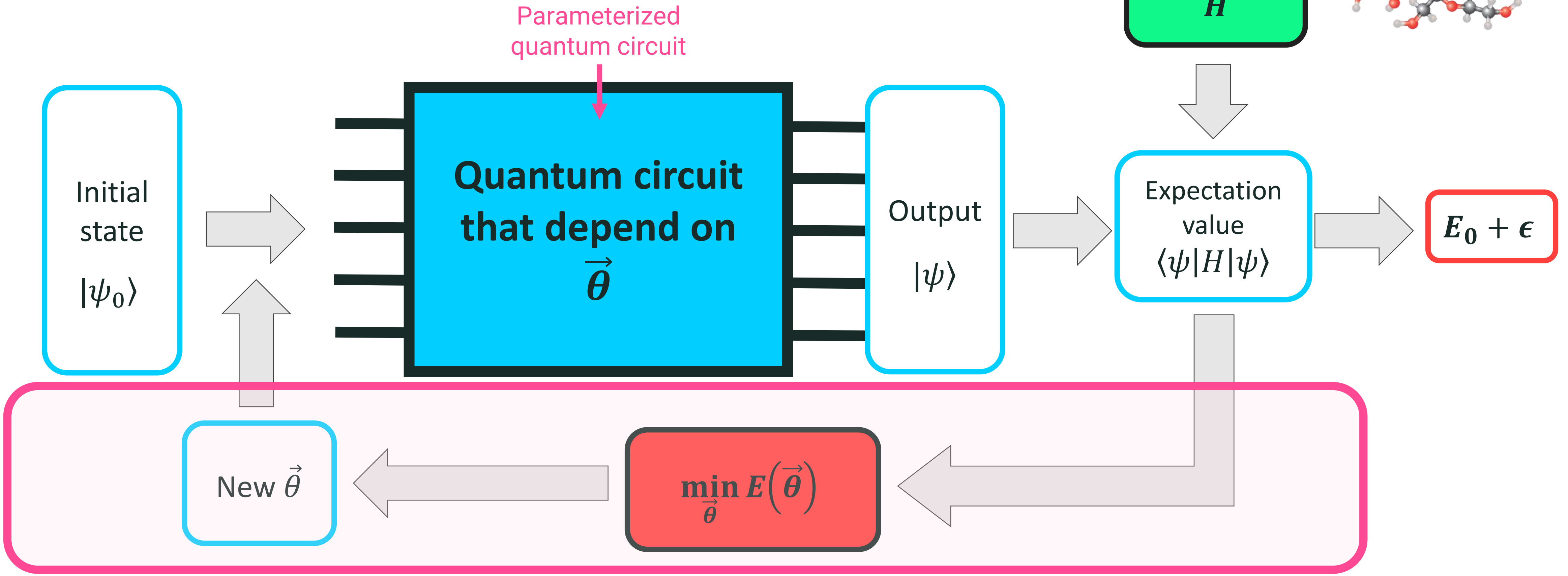
Kishor Bharti, Alba Cervera-Lierta, Thi Ha Kyaw, Tobias Haug, Sumner Alperin-Lea, Abhinav Anand, Matthias Degroote, Hermanni Heimonen, Jakob S. Kottmann, Tim Menke, Wai-Keong Mok, Sukin Sim, Leong-Chuan Kwek, Alán Aspuru-Guzik

Comments:	Review article, 82 pages, 7 figures, comments welcome
Subjects:	**Quantum Physics (quant-ph)**; Statistical Mechanics (cond-mat.stat-mech); Artificial Intelligence (cs.AI); Machine Learning (cs.LG)
Cite as:	arXiv:2101.08448 **[quant-ph]**

Variational Quantum Algorithms

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

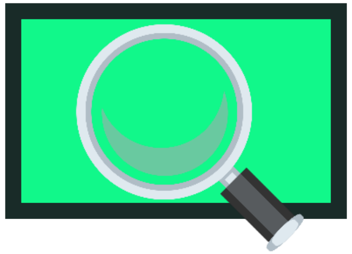




Classical optimization

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.

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

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

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

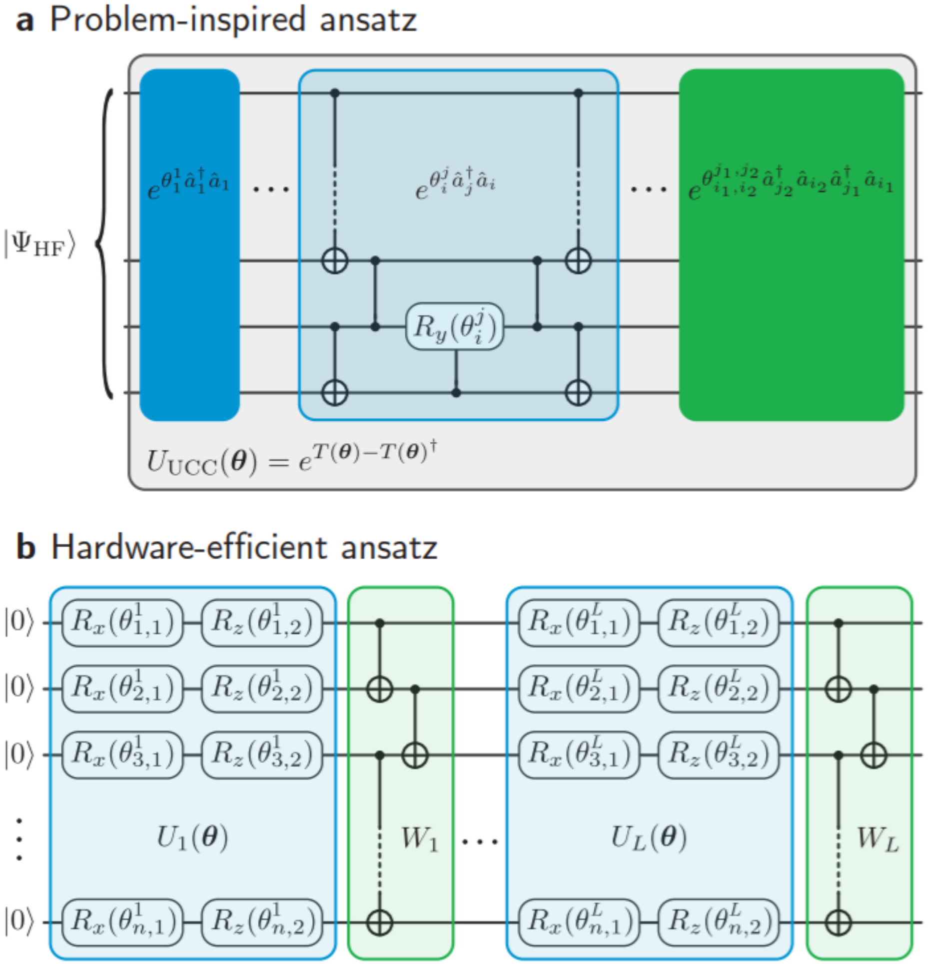
Noisy Intermediate-Scale Quantum (NISQ) algorithms, K. Bharti, ACL, T.H. Kyaw, et. al., arXiv:2101.08448 (2021)

Parameterized quantum circuits

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

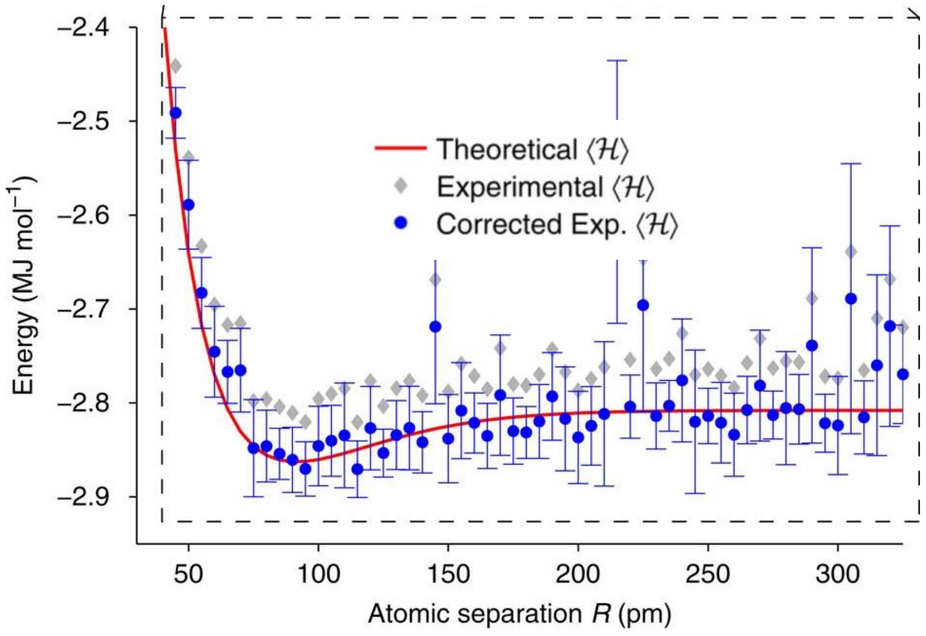
It depends on a series of parameters that have to be finetunned to minimize the objective

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).



Example: the Variational Quantum Eigensolver

Bond dissociation curve of the He–H⁺ molecule.



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

Electronic structure Hamiltonian decomposed into Pauli strings

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

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

Unitary operation (Cluster operator)

Hartree-Fock

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

Excitations Hartree-Fock orbitals

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

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

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

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

A. Peruzzo, J. McClean, P. Shadbolt, M.-H.Yung, X.-Q. Zhou, P. J. Love, A. Aspuru-Guzik , J. L. O'Brien, Nature Comm. 5, 4213 (2014)

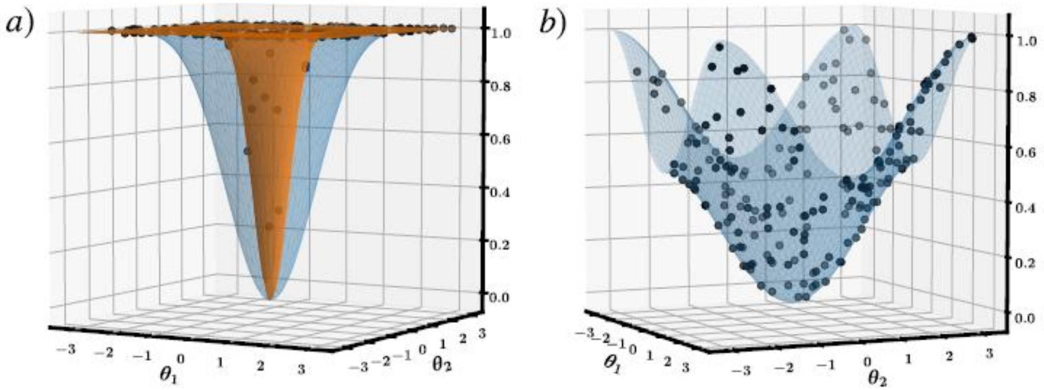
The *barren-plateaux* problem

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.

Global cost function

Local cost function



Consequence: *barren-plateaux*

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

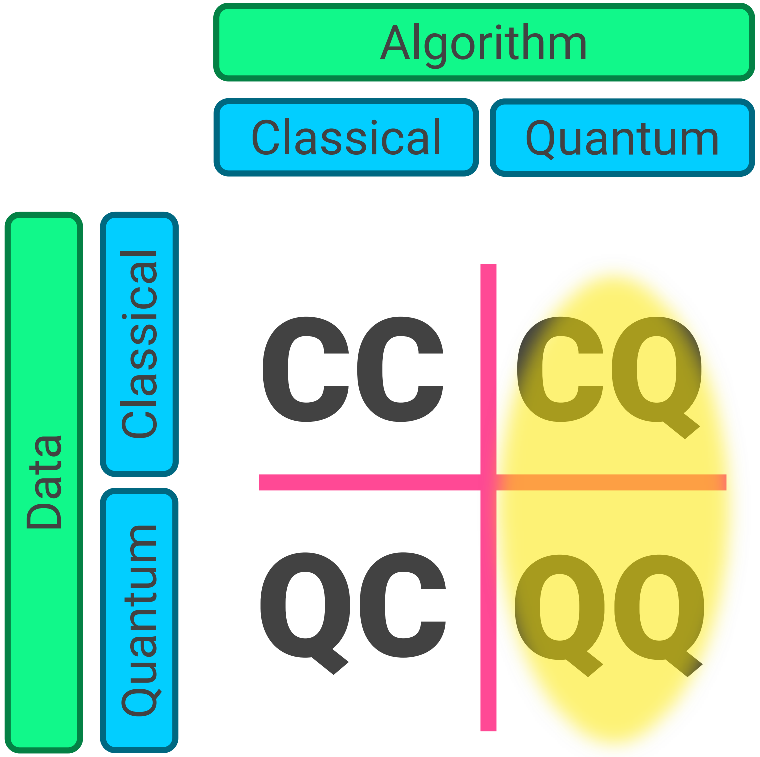
Solutions

- 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]

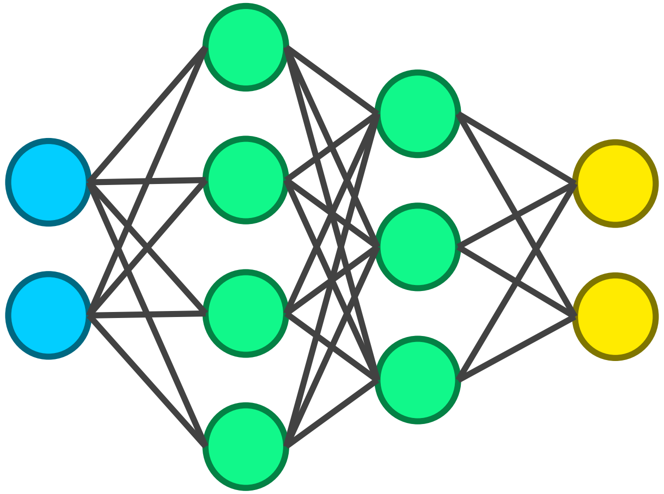
- McClean, J.R., Boixo, S., Smelyanskiy, V.N. et al. Nat Commun 9, 4812 (2018)

VQA for Quantum Machine Learning

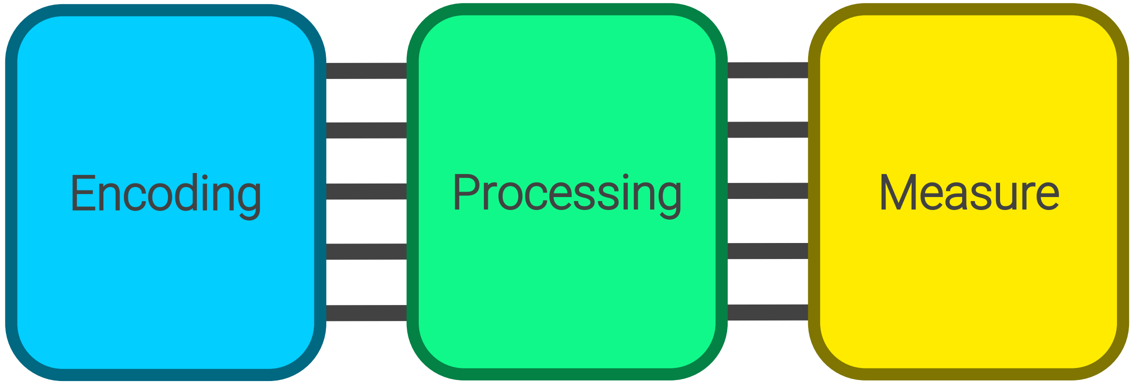


From classical to quantum NN

Classical



Quantum
(circuit centric)

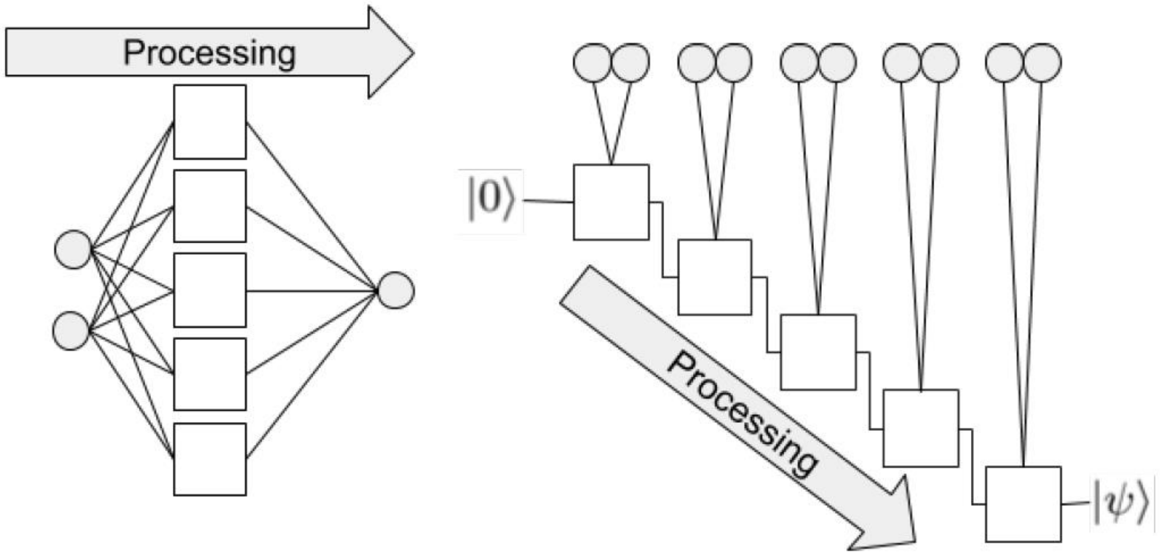


K Mitarai, M Negoro, M Kitagawa, K Fujii Phys. Revs A 98 (3), 032309 (2018)
E. Farhi and H.Neven, arXiv:1802.06002 (2018)
M. Schuld and N. Killoran, Phys. Rev. Lett. 122, 040504 (2019)
M. Schuld, A. Bocharov, K. M. Svore, and N. Wiebe, Phys. Rev. A 101, 032308 (2020)

The minimal QNN

What is the most simple (but universal) NN? → Single hidden layer NN

What is the most simple (but universal) QNN? → Single-qubit QNN



(a) Neural network (b) Quantum classifier

Encoding the data

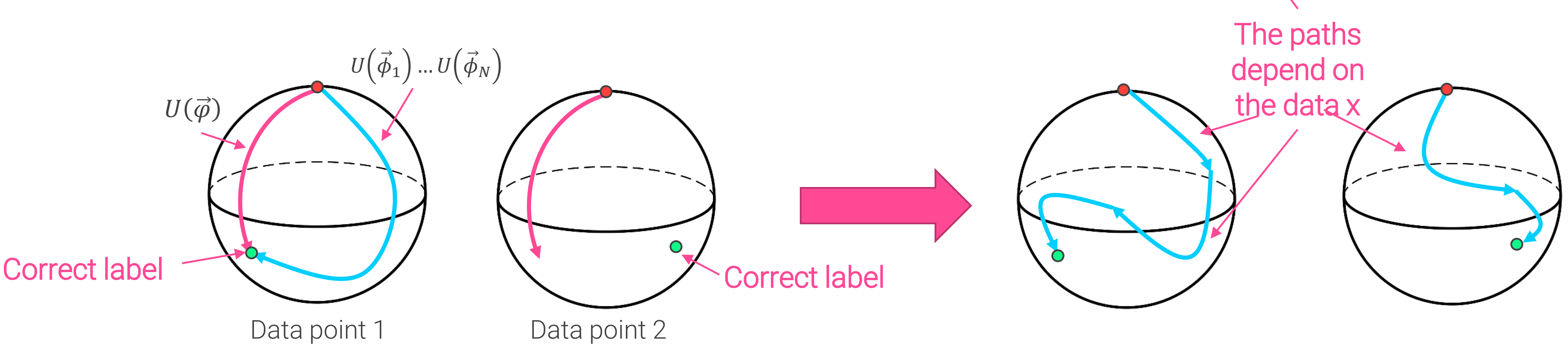
A product of unitaries can be written with a single unitary

$$U(\vec{\phi}_1) \dots U(\vec{\phi}_N) \equiv U(\vec{\varphi})$$

Data re-uploading

If we add some fixed parameter dependency (the data), the operation becomes flexible and data-depedent.

$$\mathcal{U}(\vec{\phi}, \vec{x}) \equiv U(\vec{\phi}_N)U(\vec{x}) \dots U(\vec{\phi}_1)U(\vec{x})$$



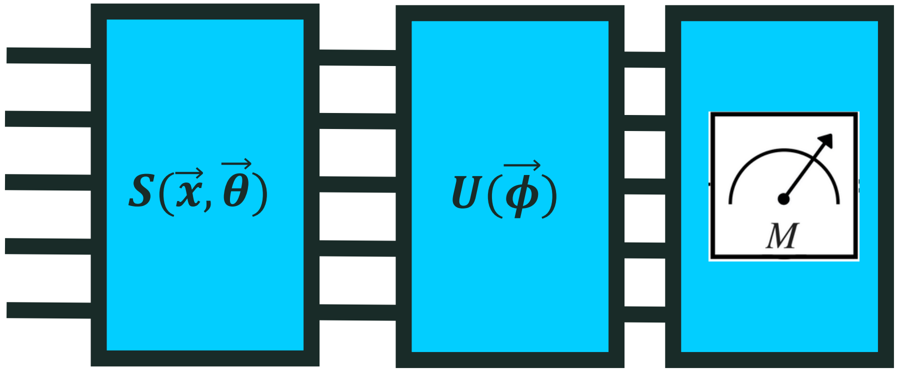
Quantum Feature Maps

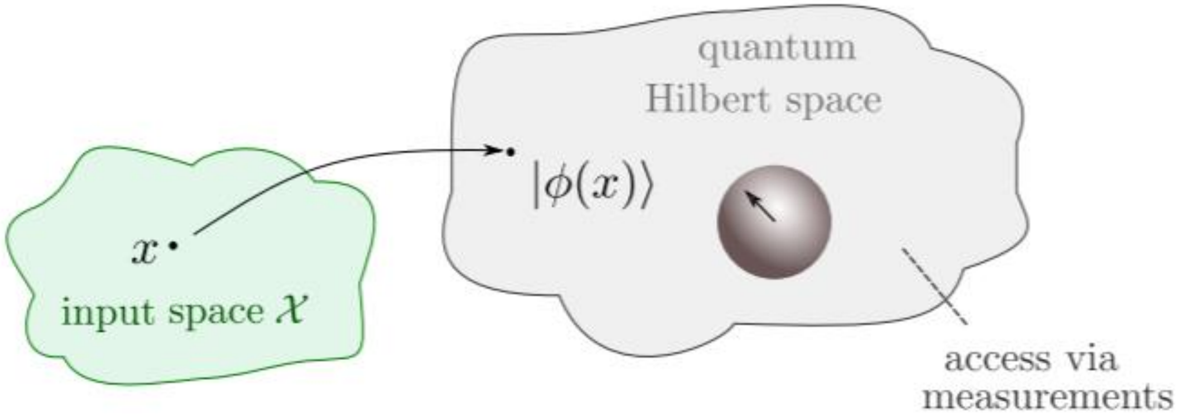
$$|\psi_0\rangle \to |\psi(\vec{x},\vec{\theta})\rangle \to |\psi(\vec{x},\vec{\theta},\vec{\phi})\rangle \to |gs\,(\vec{x})\rangle$$

Encode the data (quantum feature space)

Rotate to the correct measurement basis

Find the parameters that minimze the objective (measured in the computational basis)





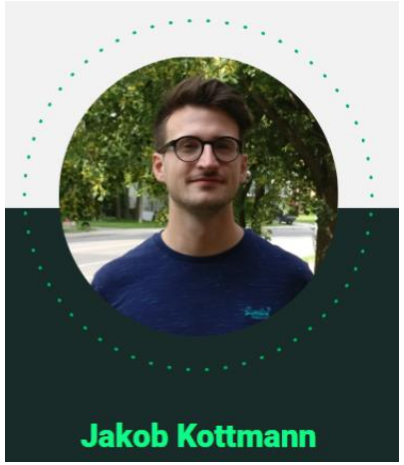
M. Schuld, arXiv:2101.11020 [quant-ph]

The Meta-Variational Quantum Eigensolver

Meta-Variational Quantum Eigensolver: Learning Energy Profiles of Parameterized Hamiltonians for Quantum Simulation

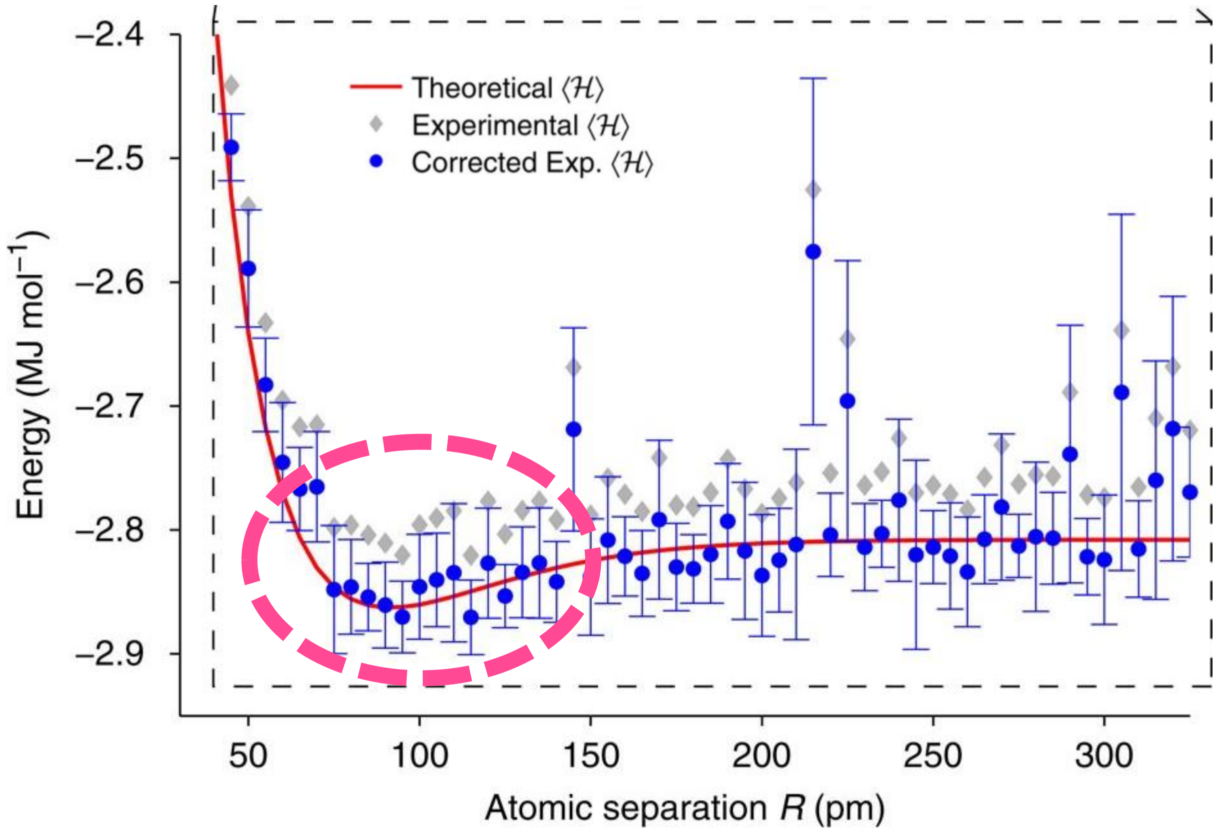
Alba Cervera-Lierta, Jakob S. Kottmann, and Alán Aspuru-Guzik

PRX Quantum **2**, 020329 – Published 28 May 2021



What's the true goal of VQE?

Bond dissociation curve of the He–H$^+$ molecule.



GOAL: find $|\psi\rangle$ that minimizes $\frac{\langle\psi|\mathcal{H}|\psi\rangle}{\langle\psi|\psi\rangle}$.

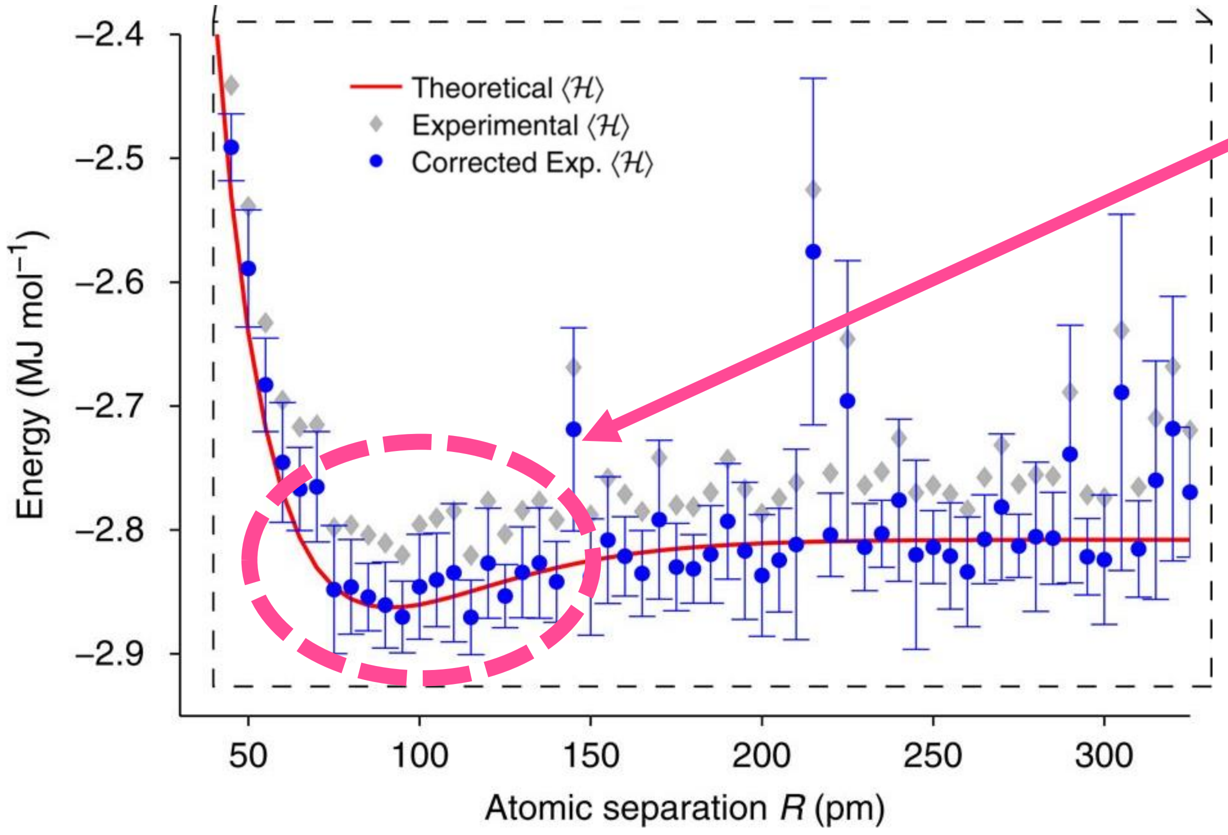
Find the atomic separation that minimizes the energy

$$\min\langle H(R)\rangle$$

A. Peruzzo, J. McClean, P. Shadbolt, M.-H.Yung, X.-Q. Zhou, P. J. Love, A. Aspuru-Guzik , J. L. O'Brien, Nature Comm. 5, 4213 (2014)

What's the true goal of VQE?

Bond dissociation curve of the He–H⁺ molecule.



To obtain this you need to scan from 0 to 300.

Each blue point is a VQE, that is, you have to **prepare, run and optimize** the quantum circuit.

Can we avoid to compute the uninteresting points?

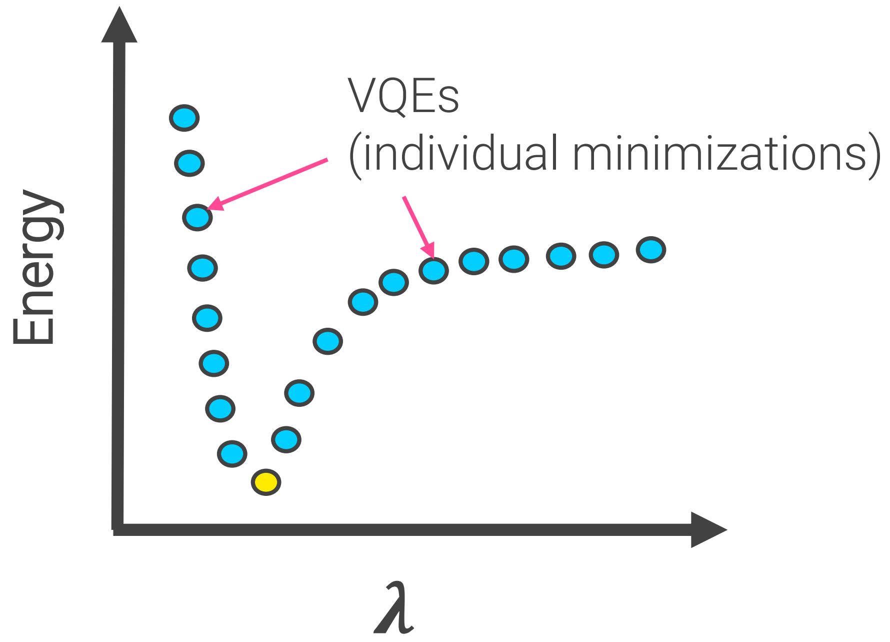
A. Peruzzo, J. McClean, P. Shadbolt, M.-H.Yung, X.-Q. Zhou, P. J. Love, A. Aspuru-Guzik , J. L. O'Brien, Nature Comm. **5**, 4213 (2014)

Meta-VQE outlook

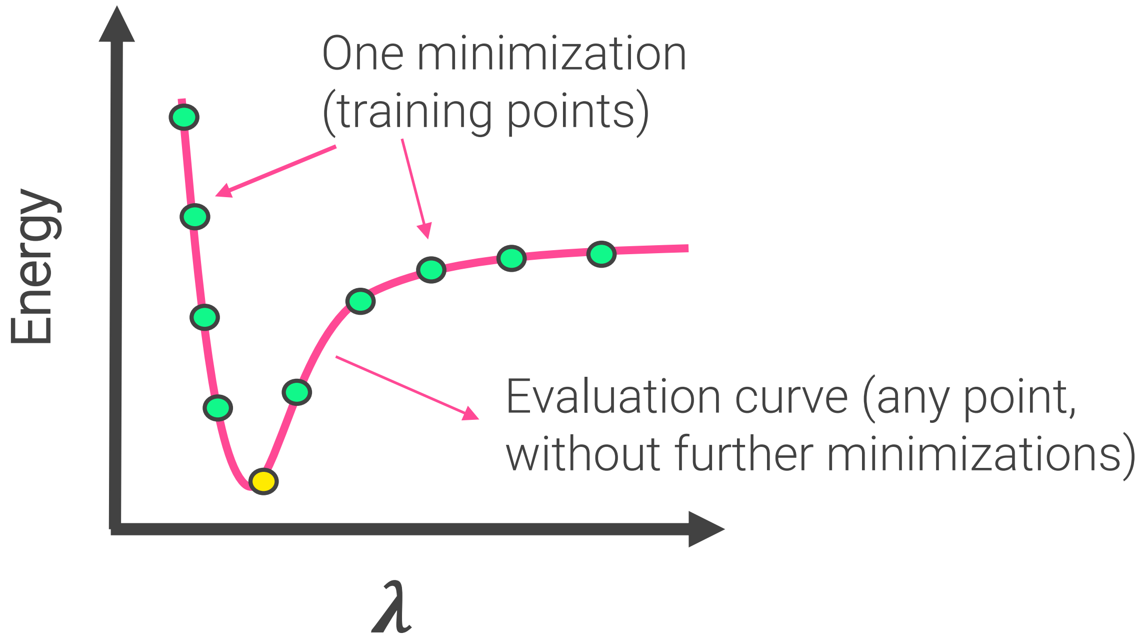
Parameterized Hamiltonian $H\left(\vec{\lambda}\right)$

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

Standard VQE



Meta-VQE



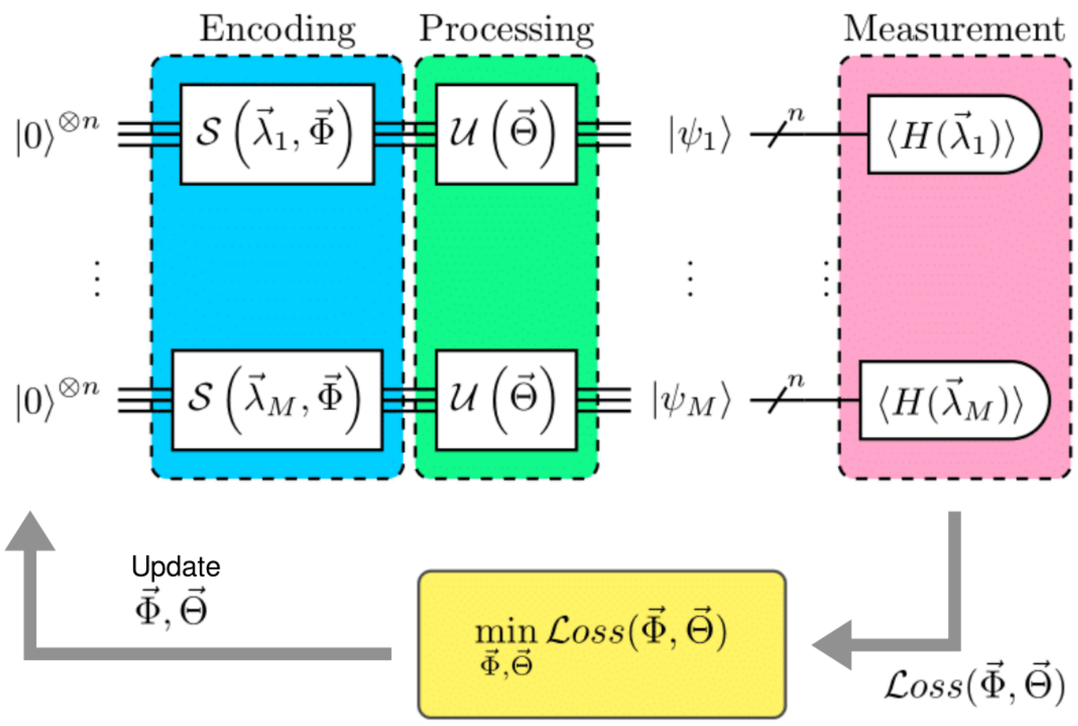
See also: K. Mitarai, T. Yan, K. Fujii, Phys. Rev. Applied **11**, 044087 (2019)

The Meta-VQE

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

Training points: $\vec{\lambda}_i$ for $i = 1, \ldots, M$

Loss function with all $\left\langle H(\vec{\lambda}_i)\right\rangle$



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

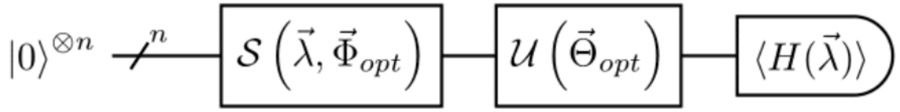
Output: $\vec{\Phi}_{opt}$ and $\vec{\Theta}_{opt}$

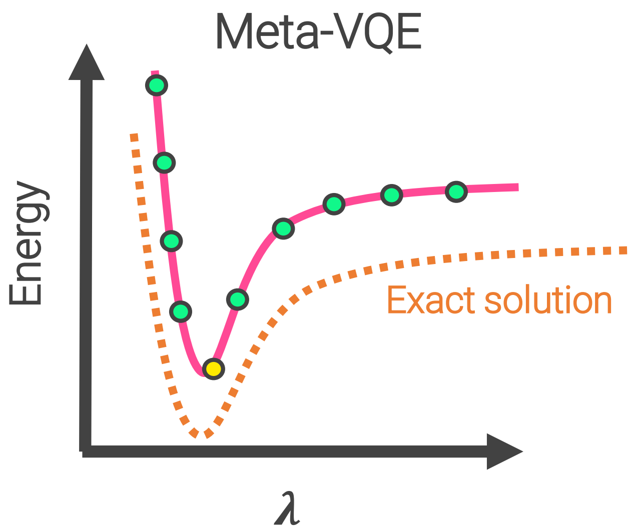
See also: K. Mitarai, T. Yan, K. Fujii, Phys. Rev. Applied **11**, 044087 (2019)

The Meta-VQE output

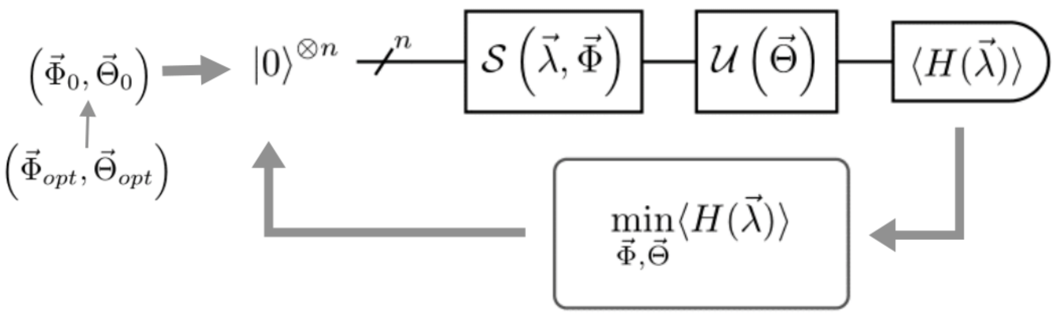
Output: $\vec{\Phi}_{opt}$ and $\vec{\Theta}_{opt}$

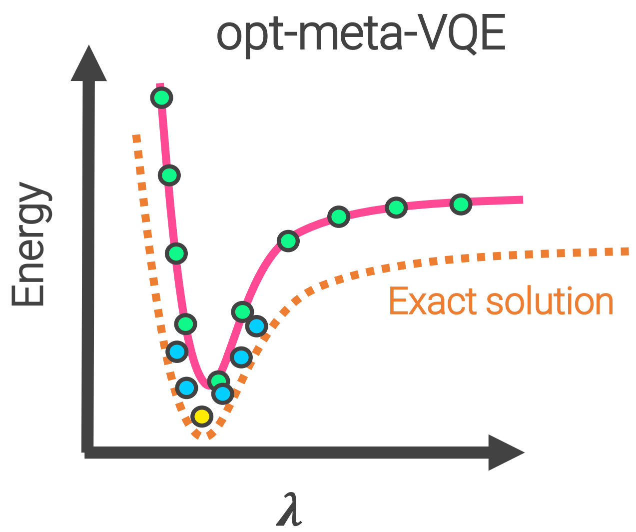
Option 1: run the circuit with test $\vec{\lambda}$ and obtain the g.s. energy profile.





Option 2: use $\vec{\Phi}_{opt}$ and $\vec{\Theta}_{opt}$ as starting point of a standard VQE optimization (*opt-meta-VQE*)





ACL, J. Kottmann, A. Aspuru-Guzik, PRX Quantum 2, 020329 (2021)

1D XXZ spin chain

$$H = \sum_{i=1}^{n} \sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \Delta \sigma_i^z \sigma_{i+1}^z + \lambda \sigma_i^z$$

For $\lambda = 0$, two QPT: $\Delta = -1$, $\Delta = 1$

Analytical solution of the model: using the Bethe ansatz (no known quantum circuit)

Good worse-case-scenario model

- We do not know which circuit ansatz will work
- The ground state is highly entangled (that's why we need quantum computers!)
- The energy profile is not trivial: it presents a peak in the region $\Delta > -1$

1D XXZ spin chain

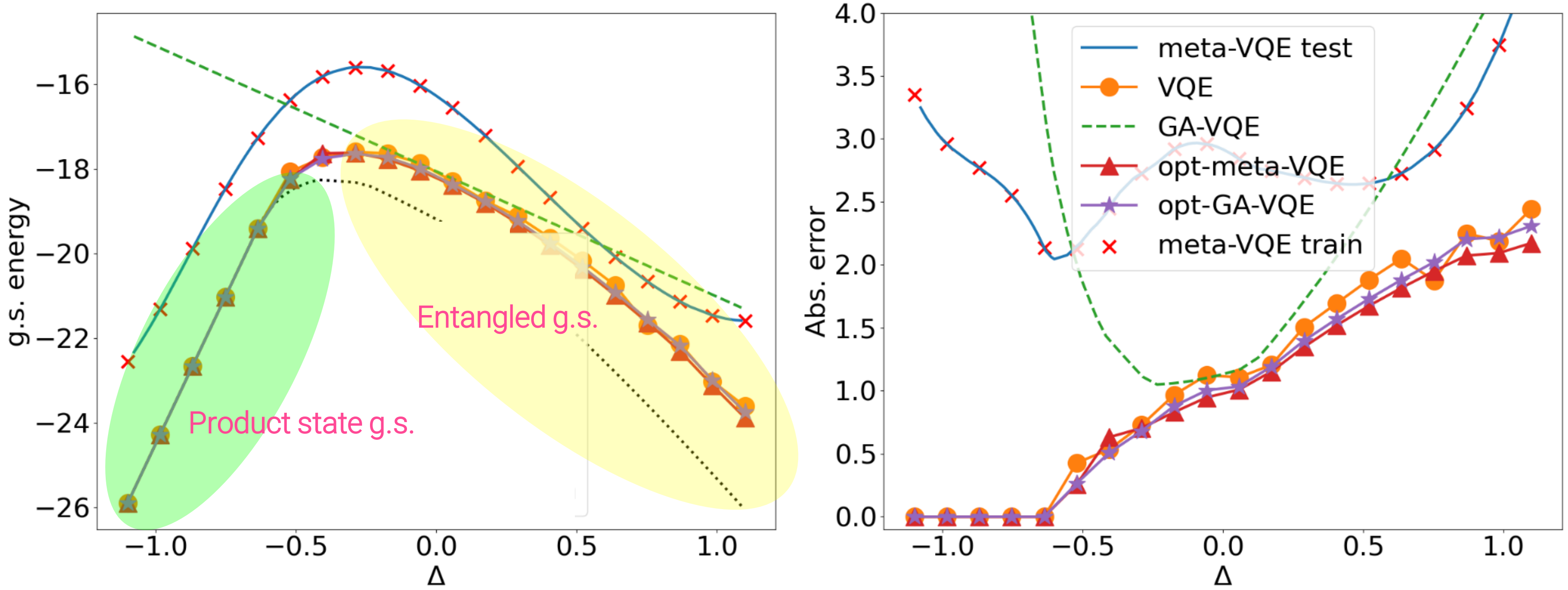
14 qubits simulation, $\lambda = 0.75$

Linear encoding: $R_z(w_1\Delta + \phi_1)R_y(w_2\Delta + \phi_2)\otimes$ Alternating CNOT

Processing layer: $R_z(\theta_1)R_y(\theta_2)\otimes$ Alternating CNOT

Results 2 encoding + 2 processing layers

$$H = \sum_{i=1}^{n} \sigma_i^x \sigma_{i+1}^x + \sigma_i^y \sigma_{i+1}^y + \Delta\sigma_i^z \sigma_{i+1}^z + \lambda\sigma_i^z$$



H_4 molecule

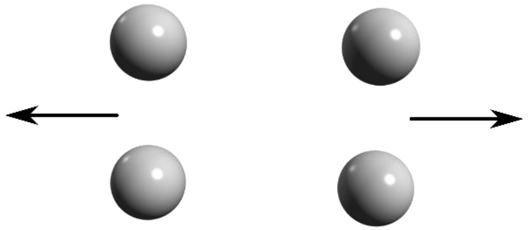
H_4 molecule in 8 spin-orbitals (STO-3G basis set)

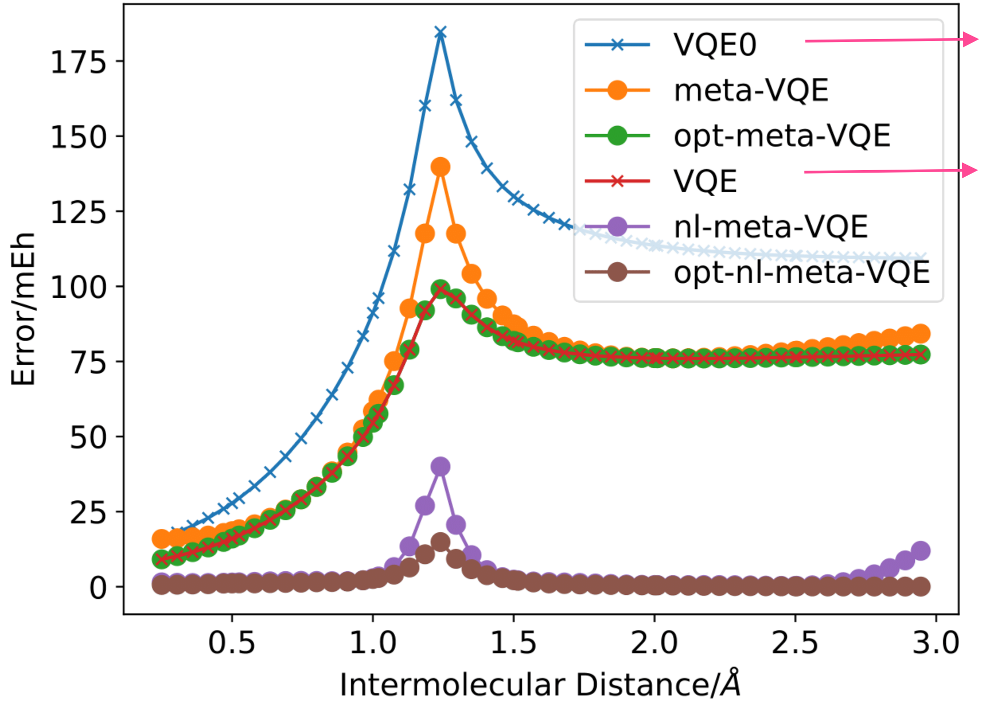
Ansatz: k-UpCCGSD (k=2 for these results)

Hamiltonian Parameter
(intermolecular distance)

Linear encoding: $\theta = \alpha + d\beta$

Non-linear encoding: $\theta = \alpha e^{\beta(\gamma - d)} + \delta$ (floating Gaussians)





Initial state: |0>

Initial state: |HF>

ACL, J. Kottmann, A. Aspuru-Guzik, PRX Quantum 2, 020329 (2021)

Single transmon

Single transmon simulation using QCAD mapping

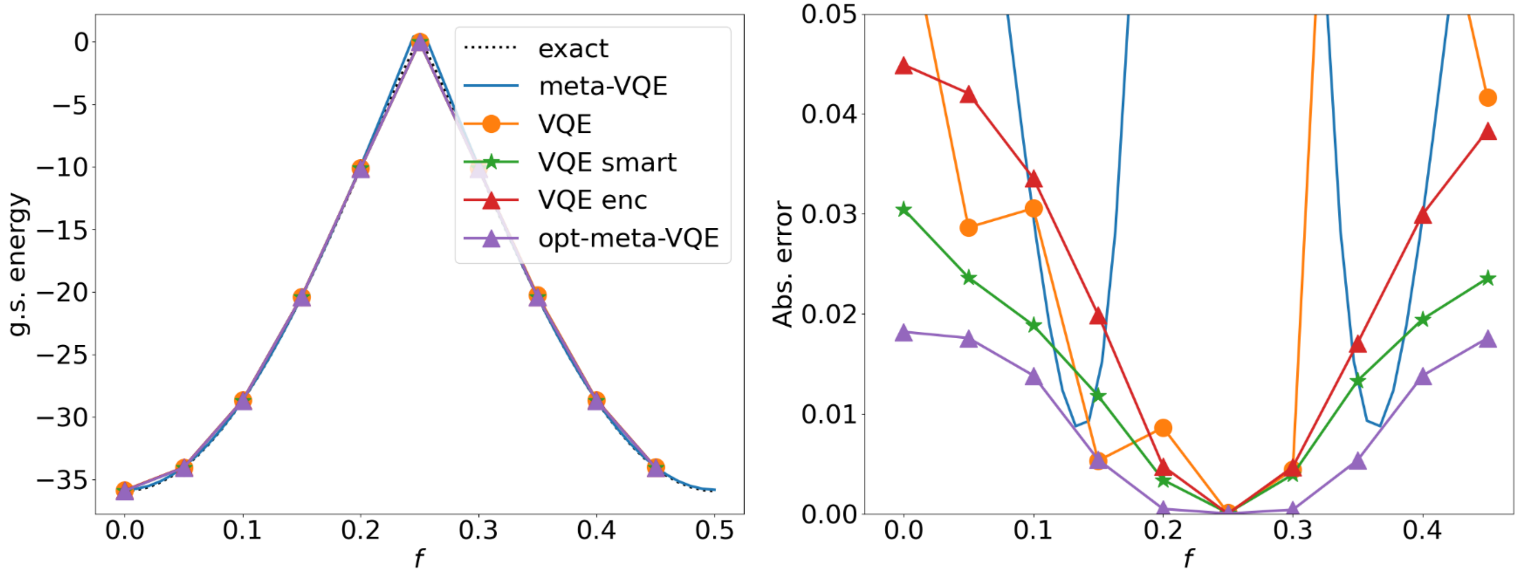
Ansatz: 1 encoding + 1 processing layers + 1 final layer of $R_x R_z$

Layer: $R_x R_z$+ all connected XX gates

Parameters of XX gates are the same in all layers (same entanglement gate)

Linear encoding: $R_x(w_1 \boldsymbol{f} + \phi_1) R_z(w_2 \boldsymbol{f} + \phi_2)$

Hamiltonian Parameter (flux)



Kyaw, Menke, Sim, Sawaya, Oliver, Guerreschi, Aspuru-Guzik, arXiV:2006.03070 (2020)

Conclusions

- Meta-VQE can be used to scan over Hamiltonian parameteres to find the interesting energy regions.

  ➡ Reduction in the total computatational cost (less number of objective evaluations)

- We can use its parameter solution to run a more precise minimization (opt-meta-VQE)

  ➡ Faster convergence, potentially avoiding barren plateaus and local minima

- The encoding strategy in VQE-type algorithms might be useful to guide the optimization towards the solution.

  ➡ Avoiding barren plateaus (T. Volkoff, P. J. Coles, Quantum Sci. Technol. **6**, 025008 (2021))

Code and demo (notebooks)

https://github.com/aspuru-guzik-group/Meta-VQE

Using Tequila quantum package

https://github.com/aspuru-guzik-group/tequila

Alán Aspuru-Guzik

Jakob Kottmann

the matter lab

VECTOR INSTITUTE | INSTITUT VECTEUR

CIFAR

Questions?