Inside the Latent Space of a Qauntum Autoencoder

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Quantum Techniques in Machine Learning 2019
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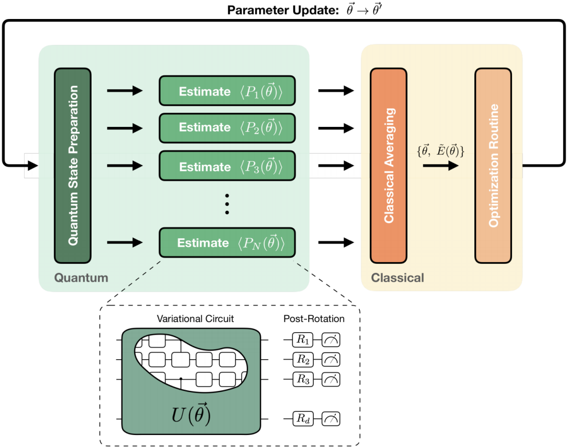
Parametrized circuits for quantum chemistry



10.1038/ncomms5213

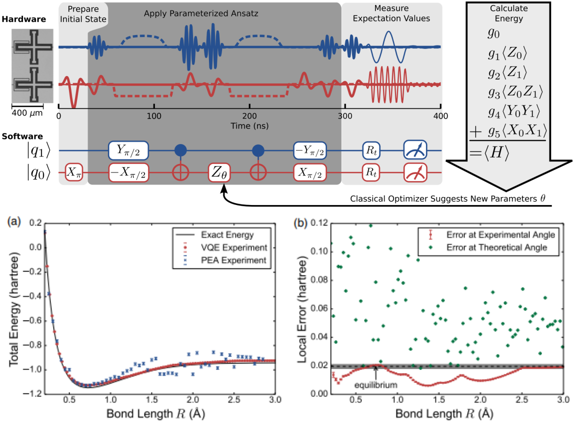
VQE

- operations
  $\Updownarrow$
  measurements
- qpu does quantum
  $\Updownarrow$
  cpu does classical

$\Rightarrow$ pragmatic near-term

VQE on real devices

PhysRevX.6.031007



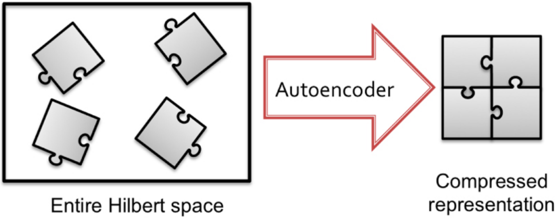
Transmon pulse diagram

H_2 PES

Scale up = end of story?

- What can you do once you have a ground state wave function?
- How large does the system have to be to be useful?
- How to find systems that are interesting?

Qubits are a scarce resource ⇒ compression



Scale up = end of story?

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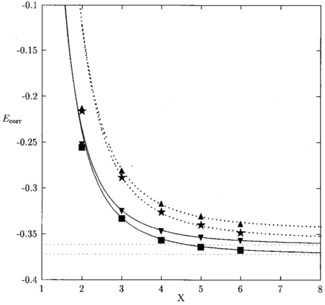
X=	2	3	4	5	6
cc-pVXZ	24	58	115	201	322
cc-pCVXZ	28	71	144	255	412



10.1063/1.473863

Scale up = end of story?

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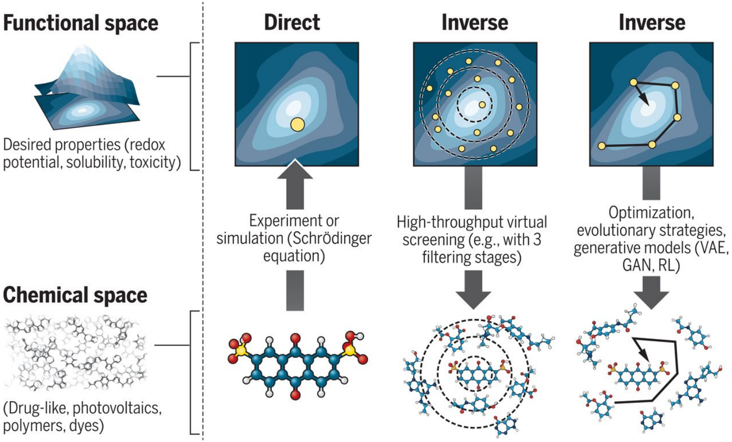
Challenge 1. The Designer Challenge. While the mission of the 20th century was related to providing answers to questions pertaining to properties of specific chemical structures, the questions of the 21st century revolve around the *inverse design* problem:[88−94] finding the best chemical structures that are associated with desired and requested properties. A potential solution for this challenge is the use of invertible models from machine learning such as generative models (GANs, autoencoders, ...)[48,89] or inverting molecules from families of Hamiltonians.[90−93]

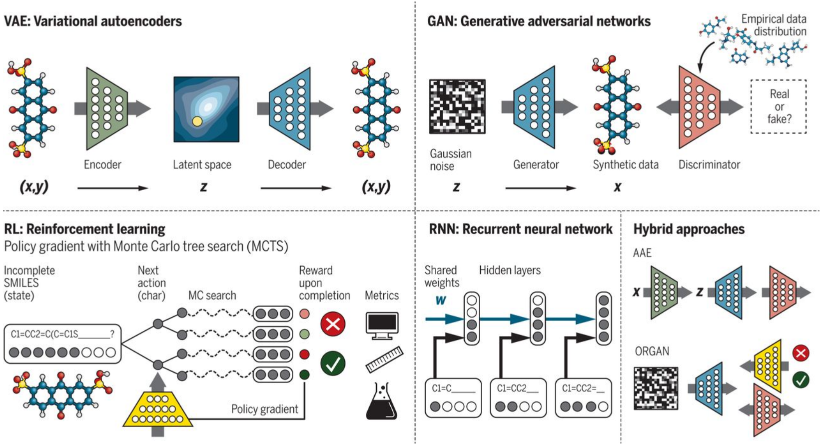
10.1021/acscentsci.7b00550

Inverse design



10.1126/science.aat2663

Classical Machine Learning for Chemistry



10.1021/acscentsci.7b00572
10.1126/science.aat2663

End of the story?

Can we reformulate this machine learning toolbox for near-term quantum devices?

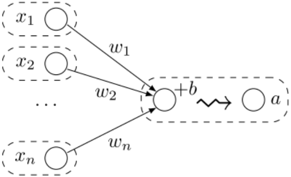
- recreate functions of classical neural nets in quantum circuits
- preferrably learn on quantum data

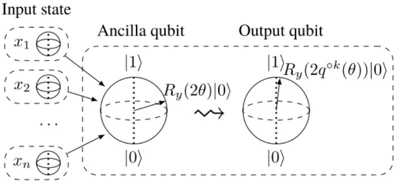
At the level of the neuron

Yudong Cao

arXiv:11711.11240

- replicate classical distribution
- repeat until success

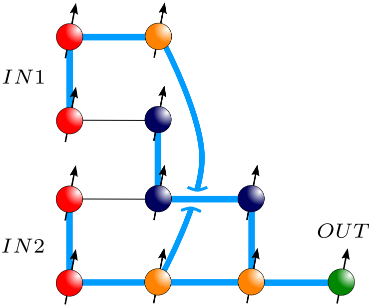




Lasse Bjørn Kristensen

Spiking quantum neuron

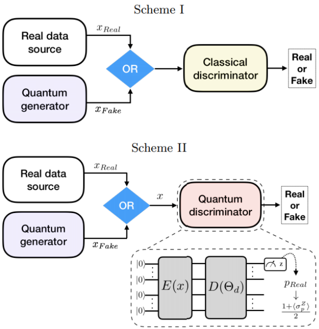
- fully quantum
- temporal character
- not gate based



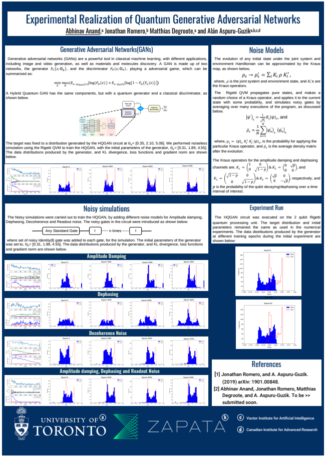
Quantum Generative Adversial Network

Jhonathan Romero
arXiv:1901.00848

- replicate classical distribution
- adversial training

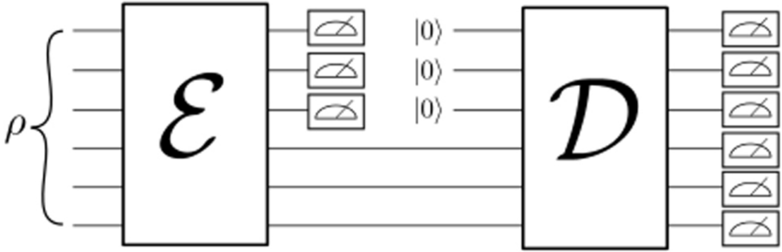


Abhinav Anand
Poster 49 about Noise Resilience

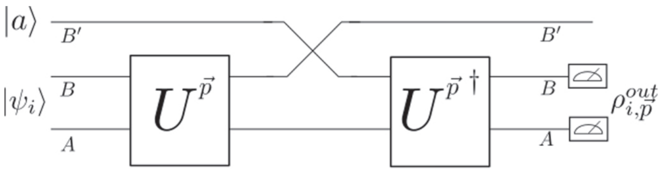


Jhonathan Romero

10.1088/2058-9565/aa8072



Cost function



Training modes:

- input - output training

$$C_1 = \sum p_i F\left(|\psi_i\rangle_{AB}, \rho^{out}_{i,\vec{p}}\right)$$

- trash training

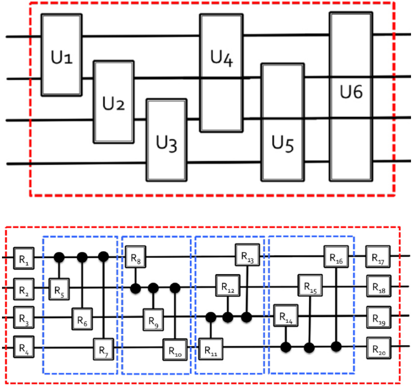
$$C_2 = \sum p_i F\left(\mathrm{Tr}_A\left[|\psi_i'\rangle\langle\psi_i'|_{AB}\right], |a\rangle_B\right)$$

  - requires less copies of original state

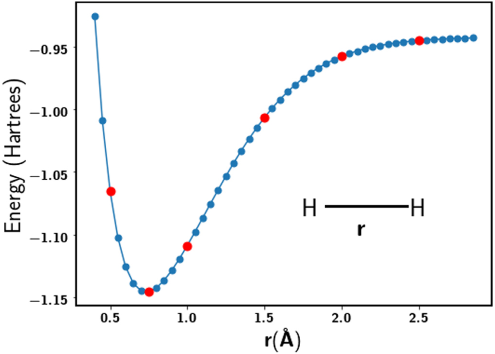
Parametrized unitaries

- sometimes compressibility is known based on symmetries
- we would like the autoencoder to figure out
- general unitary intractable
- resort to templates
  - Scheme A: $15n(n-1)/2$
  - Scheme B: $3n(n-1)+6n$

Example Circuits



Test system: H_2



$$
\begin{aligned}
|\Psi_i\rangle &= a_i\,|1100\rangle + b_i\,|0011\rangle \\
&\to a_i\,|0\rangle + b_i\,|1\rangle
\end{aligned}
$$

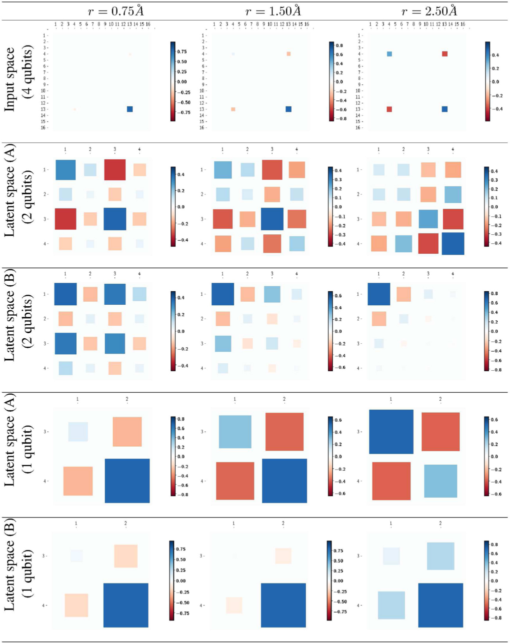
- 4 qubit system
- compressible to 1 qubit

Results: Fidelities

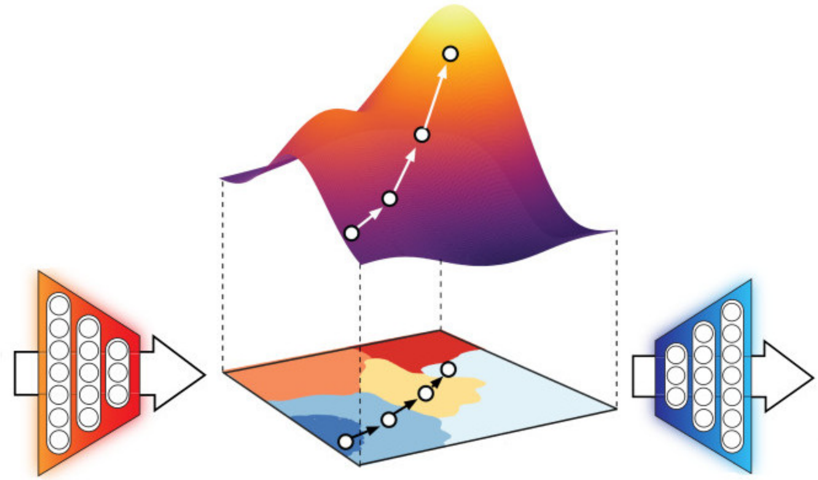
Circuit	Final size (# qubits)	Set	$-\log_{10}(1 - \mathcal{F})$ MAE[a]	$-\log_{10}$ Energy MAE[a] (Hartrees)
Model	2	Training	6.96(6.82–7.17)	6.64(6.27–7.06)
A	2	Testing	6.99(6.81–7.21)	6.76(6.18–7.10)
	1	Training	6.92(6.80–7.07)	6.60(6.23–7.05)
	1	Testing	6.96(6.77–7.08)	6.72(6.15–7.05)
Model	2	Training	6.11(5.94–6.21)	6.00(5.78–6.21)
B	2	Testing	6.07(5.91–6.21)	6.03(5.70–6.21)
	1	Training	3.95(3.53–5.24)	3.74(3.38–4.57)
	1	Testing	3.81(3.50–5.38)	3.62(3.35–4.65)

[a] MAE: Mean absolute error. Log chemical accuracy in Hartrees ≈ -2.80.

Results: Density Matrices



Goal: Explore Latent Space



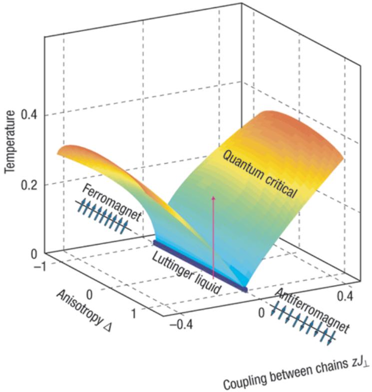
10.1021/acscentsci.7b00572

Look at phase transitions in wave functions

How does Compression affect Phase Information?

Douglas Mendoza
Phase transition in XXZ model

- exact wave functions
- some symmetry present
- look at fidelity susceptibility



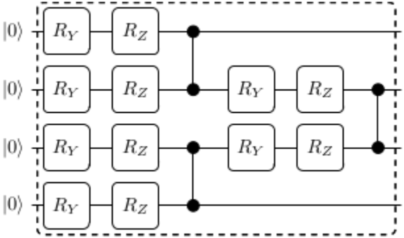
10.1038/nmat1358

Influence of expressibility

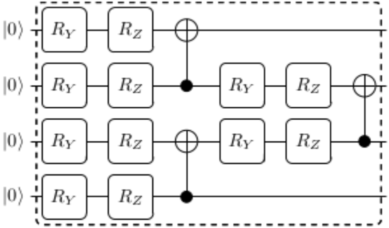
Hannah Sim

arXiv:1905.10876

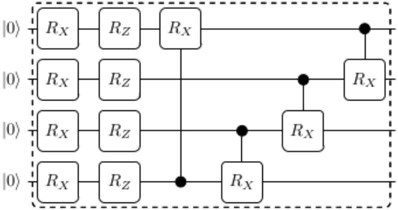
- choose circuits with different expressibilities
- study influence on conservation of information



Circuit 12



Circuit 11



Circuit 19

Conclusions

Done:

- Quantum Neurons
- Quantum Variational Autoencoder compression

Underway:

- From simulation to experimental demonstration
- Information in latent space

To Do:

- Expand machine learning functions
- Apply concepts to new problems

The end

Thank you for your attention!

Questions are welcome

Slides: `https://mfdgroot.github.io/`