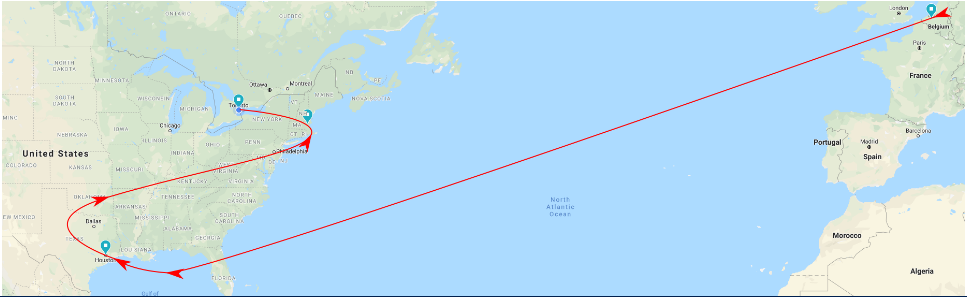
Quantum Computing and Data Science

Matthias Degroote

DSPEast Quantum Computing Meetup
19/03/2020

About me

2008-2014	Ghent University	• Electronic Structure • Tensor Networks
2014-2017	Rice University	• Electronic Structure
2018-2020	Harvard University University of Toronto	• Quantum Computing

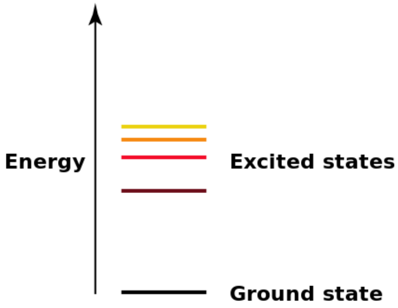


What (not) to Expect

- 👎 A sales pitch telling everyone to switch to quantum
- 👎 A full explanation of how quantum computing works
- 👍 An overview of the areas where data science and quantum computing touch
- 👍 A chance to talk about opportunities both ways

What is Quantum Mechanics?

The physical theory for what happens at very small length scales and very low temperatures

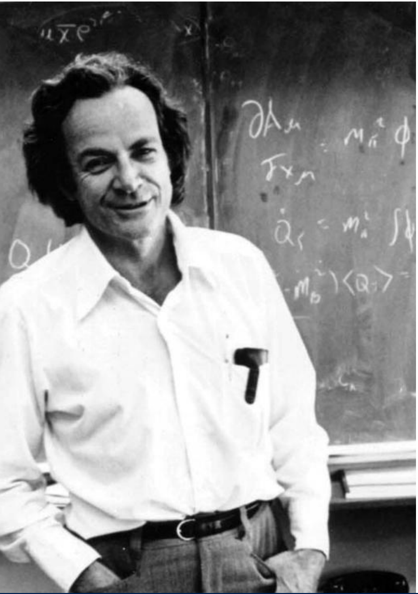


Governed by Scrödinger equation
$i\hbar\frac{\partial}{\partial t}\left|\psi(x,t)\right\rangle = H\left|\psi(x,t)\right\rangle$

Normalized under 2-norm
$\int \left|\psi(x,t)\right|^2 \mathrm{d}x = 1$

Computations with wave functions become exponentially harder when the number of particles goes up

Feynman's Vision



Richard Feynman
Physicist, annoyed at slow computers

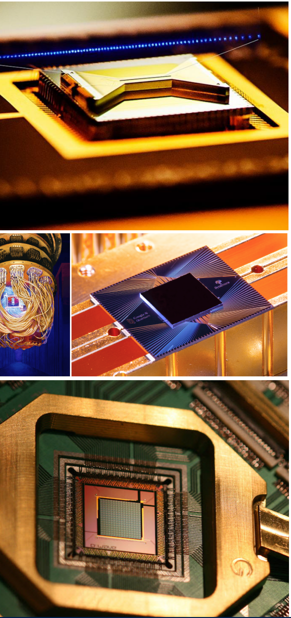
Realized Turing machines could never beat the exponential wall

Theorized about quantum matter simulating quantum matter

What about doing more than just simulating physics?

$\Rightarrow$ Need controllable quantum systems

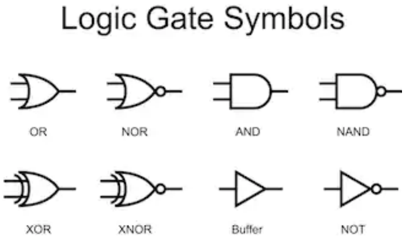
Controlled Quantum Systems

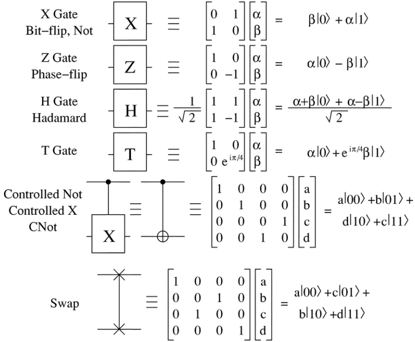


DiVicenzo Criteria

1. Scalable physical system with well-characterized qubit
2. The ability to initialize the state of the qubits to simple fiducial state
3. Long decoherence times
4. A universal set of gates
   - Single-qubit operations
     $\Rightarrow$ superposition
   - Two-qubit operations
     $\Rightarrow$ entanglement
5. Qubit-specific measurment capability

To store data in wave functions and manipulate to do computation

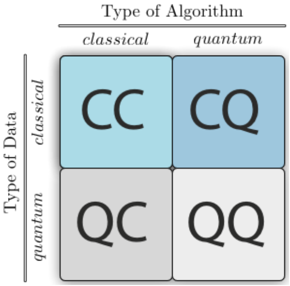




Main topics related with data science

1. Quantum Machine Learning
2. Optimization Problems
3. Quantum Linear Algebra

Quantum Machine Learning Categories



- Algorithms based on quantum building blocks
  - Grover search
  - phase estimation
  - amplitude estimation

$\Rightarrow$ Error corrected devices

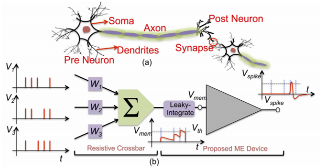
- Algorithms mimimicking classical ML
  - quantum neurons
  - quantum boltzmann machines
  - quantum convolutional networks
  - quantum variational autoencoder
  - quantum generative adversarial network

$\Rightarrow$ Noisy Intermediate Scale Quantum (NISQ) Devices

Artificial Spiking Quantum Neuron

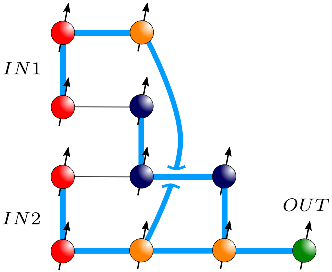
Power Consumption

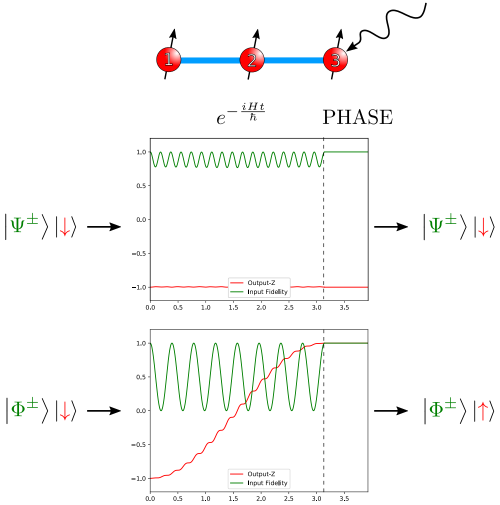
Game	Computer	Human
Chess	900W	20W
Go	1000W	20W
StarCraft II	2000W	20W



- sparse connectivity
- info transfer through spikes
- thresholding
- temporal character (firing rate, relative timing)

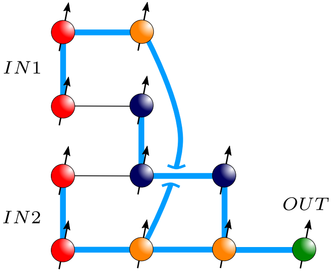
Artificial Spiking Quantum Neuron

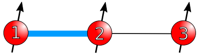




Counts excitations

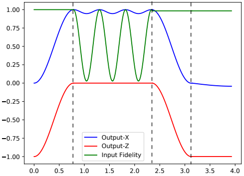
Artificial Spiking Quantum Neuron





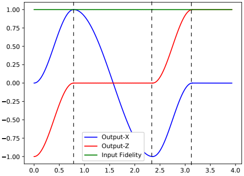
$H \quad e^{-\frac{iHt}{\hbar}} \quad H \quad \text{PHASE}$

$|\Phi^+\rangle|\downarrow\rangle$
$|\Psi^+\rangle|\downarrow\rangle$ $\longrightarrow$



$\longrightarrow$ $|\Phi^+\rangle|\downarrow\rangle$
$|\Psi^+\rangle|\downarrow\rangle$

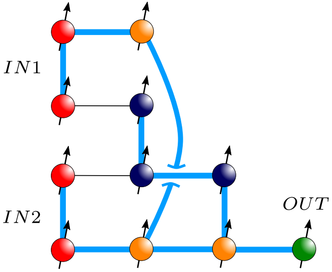
$|\Phi^-\rangle|\downarrow\rangle$
$|\Psi^-\rangle|\downarrow\rangle$ $\longrightarrow$



$\longrightarrow$ $|\Phi^-\rangle|\uparrow\rangle$
$|\Psi^-\rangle|\uparrow\rangle$

Finds phase difference

Artificial Spiking Quantum Neuron

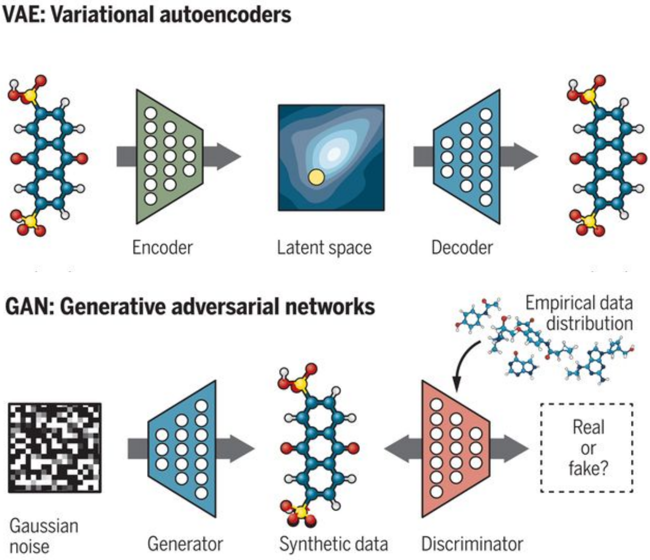


Characteristics

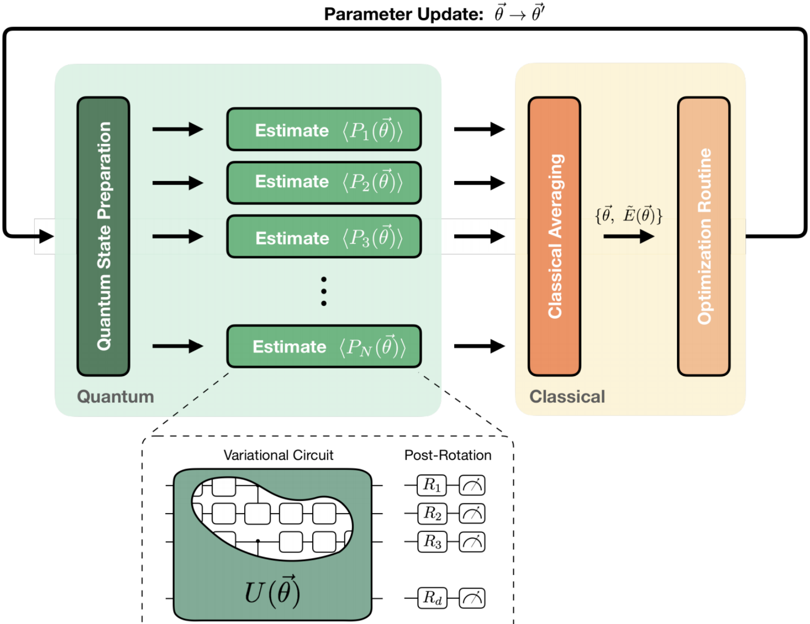
- Thresholding
- Feedforward
- Measurement backaction
- Defines expected likelihood kernel used in pattern analysis
- Nothing to optimize, topology defines function

Further reading:
L.-B. Kristensen, M. Degroote, P. Wittek, A. Aspuru-Guzik
`https://arxiv.org/abs/1907.06269`

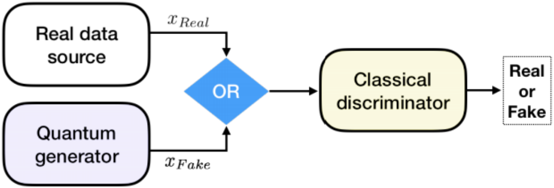
Classical Machine Learning for Chemistry

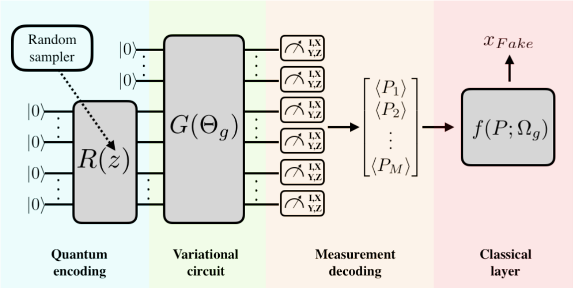


Hybrid Quantum-Classical approaches

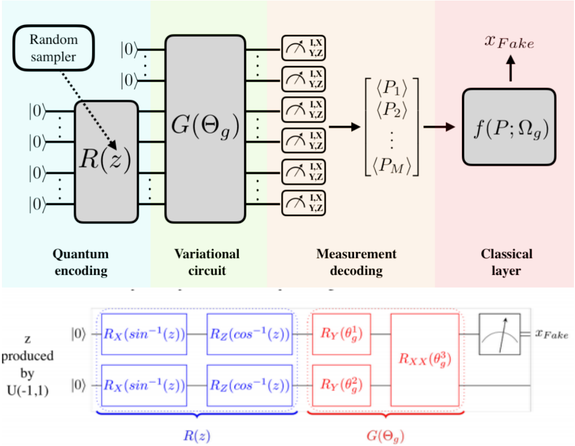


Quantum Generative Adversarial Network



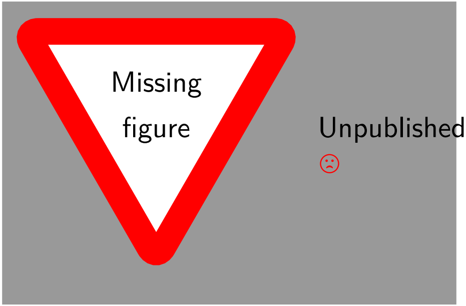


Quantum Generative Adversarial Network



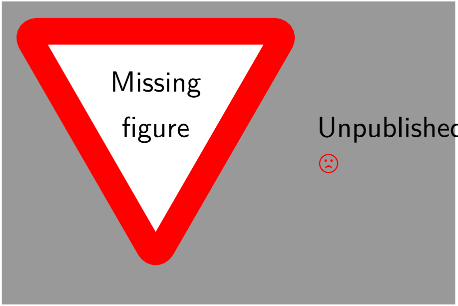
Further reading:
J. Romero, A. Aspuru-Guzik
arXiv:1901.00848

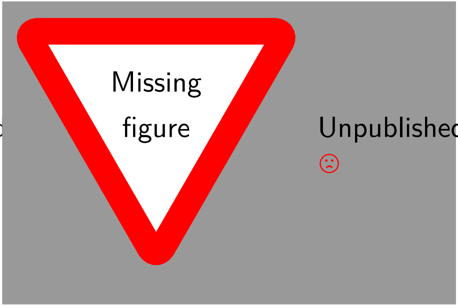
Influence of noise models, simulations



Quantum Generative Adversarial Network

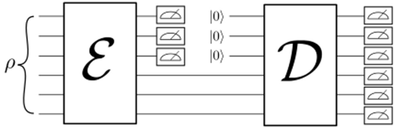
Experimental data, upcoming publication with Abhinav Anand

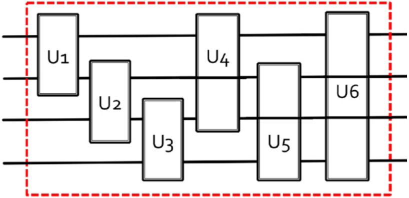


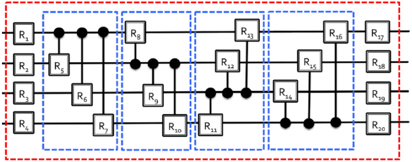


- Learning on real hardware
- Reduced number of samples
- Noise does not affect result

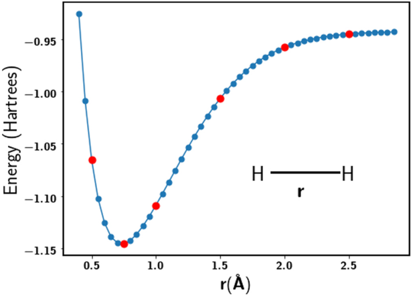
Variational Quantum Autoencoder





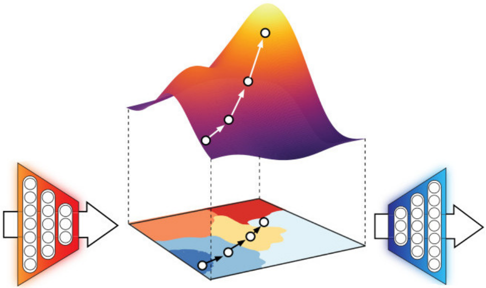


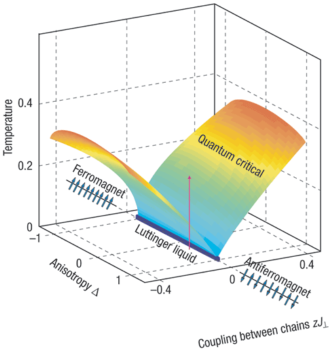
H_2 molecule



Further reading:
J. Romero, J. Olsen, A. Aspuru-Guzik
10.1088/2058-9565/aa8072

Variational Quantum Autoencoder

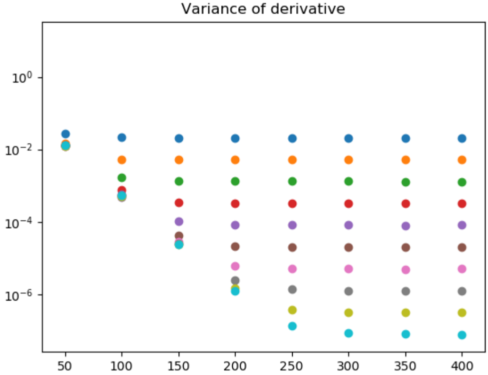




Ongoing project with Douglas Mendoza on phase transition in XXZ model

- exact wave functions
- some symmetry present
- move in the latent space

Barren Plateaus



- similar to machine learning
- dropout
- sparsification

$\Rightarrow$ work in progress...

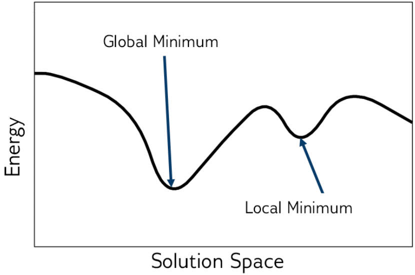
Quadratic Unconstrained Optimization Problems (QUBO)

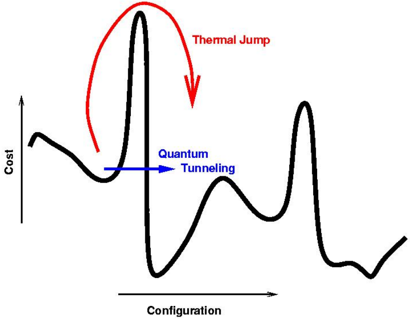
$$\mathcal{L}(x) = \sum_i Q_{ii} x_i + \sum_{i<j} Q_{ij} x_i x_j$$

Examples

- SAT problems
- Max-Cut problems
- Max-Clique problems
- Multiple Knapsack Problems
- many, many more

⇒ All very hard

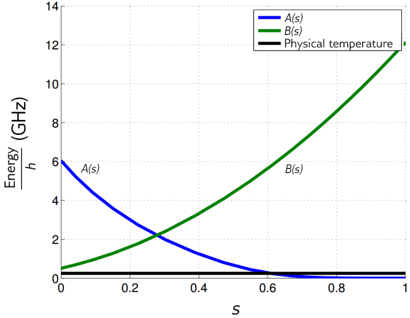


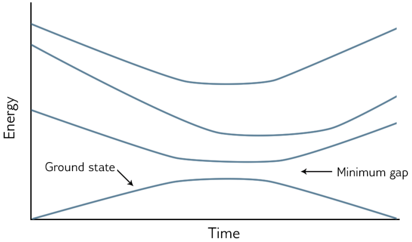


Quantum Annealing

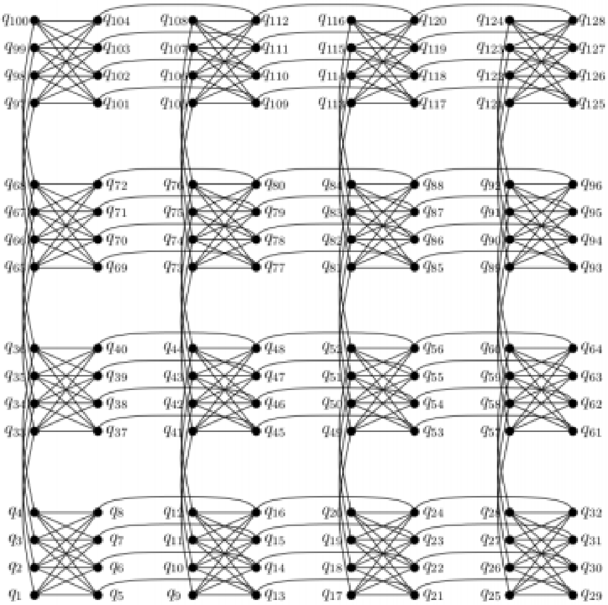
$$\mathcal{H}(\sigma) = -\frac{A(s)}{2}\sum_i \sigma_x^i + \frac{B(s)}{2}\left[\sum_i h_i\sigma_z^i + \sum_{i<j} J_{ij}\sigma_z^i\sigma_z^j\right]$$

Evolve from $s = 0$ to $s = 1$





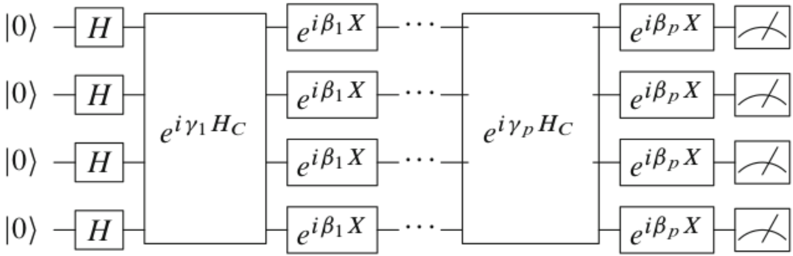
Quantum Annealing



Quantum Approximate Optimization Ansatz

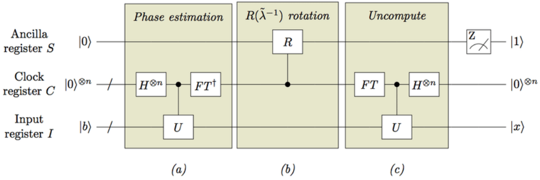
$$\begin{aligned}\mathcal{H}(\sigma) &= \sum_i \sigma_x^i + \left[\sum_i h_i \sigma_z^i + \sum_{i<j} J_{ij}\sigma_z^i \sigma_z^j\right] \\ &= H_B + H_C\end{aligned}$$

Optimize $< \psi | H_C | \psi >$ over p and β,γ



Harrow Hassidim Lloyd (HHL) Algorithm

$$A|x\rangle = |b\rangle$$



- uses QPE as subroutine
- severe limitations

$\Rightarrow$ Not really near-term

- Limitations on A
  - A is Hermitian
  - A has eigenvalues needs to be in $[0,1)$
  - oracle for $\exp(iAt)$
- Limitations on $|b\rangle$
  - $|b\rangle$ can be implemented easily

  $\Rightarrow$ QRAM
- Limitations on $|x\rangle$
  - $|x\rangle$ cannot be fully recovered

The end

Thank you for your attention!

Questions are most welcome

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