Q for Q and Q for Q

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Support and Environment

- EPSRC grant on Distributed Quantum Computing and Applications
- EPSRC New Horizon Grant on Quantum algorithms for turbulent flows

- Imperial College QuEST Centre (Maths, Computing, Physics, Aeronautics, EEE), focusing on
  - Materials for Quantum Technologies
  - Quantum Internet
  - Applications of Quantum Computing
What this talk is NOT about

- Q advantage and Q supremacy – I am not a Sales guy
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**Goal:** Convince you that we, as (...applied...) Mathematicians have a role to play in the evolution of Q computing (in Finance).
Q mechanics or Q computing?

Q mechanics is a framework for the development of Physics theories, as originally proposed mid-1920s by N. Bohr, L. de Broglie, M. Born, W. Heisenberg, W. Pauli, E. Schrödinger, P. Dirac. The mathematics of Q mechanics allow for more general computation:

- more general definition of the memory state compared to classical computing;
- wider range of transformations / evolution of memory states.
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Why haven't we used this computation framework until now?

To perform Q computation efficiently we need actual Q mechanical systems, only proposed in the 1980s by P. Benioff, R. Feynman, Y. Manin.

Q algorithms can be run on classical computers, but require enormous amount of memory, so that exponential gains in computing power are offset by exponential memory requirements.
Q Computing
Q Machine Learning
Q optimisation
Q Monte Carlo
Q for PDEs

Postulate 1 – Statics
Postulate 2 – Dynamics
Postulate 3 – Measurement
Postulate 4 – Composite systems

Q formalism
Q formalism

- State space: complex Hilbert space $\mathcal{H} = \mathbb{C}^N$. for $u, v \in \mathcal{H}$, ($\ast$: complex conjugacy)

  $|v\rangle := \begin{bmatrix} v_1 \\ \vdots \\ v_N \end{bmatrix} \in \mathcal{H}$,  
  $\langle u | := (u_1^*, \ldots, u_N^*) \in \mathcal{H}^*$,  

  $\langle u | v \rangle := \sum_{i=1}^{N} u_i^* v_i \in \mathbb{C}$.
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• 1-qubit quantum state: $|\psi\rangle = \alpha |0\rangle + \beta |1\rangle$, for $\alpha, \beta \in \mathbb{C}$ such that $|\alpha|^2 + |\beta|^2 = 1$.

• Given $\mathcal{H}_N$ and $\mathcal{H}_M$, tensor product $\mathcal{H} := \mathcal{H}_N \otimes \mathcal{H}_M$ is the $NM$-dimensional Hilbert space spanned by $\{|i\otimes |j\rangle : i = 0, \ldots, N - 1, j = 0, \ldots, M - 1\}$. 

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- For a 2-qubit system,

  $\{|0\otimes|0\rangle , |0\otimes|1\rangle , |1\otimes|0\rangle , |1\otimes|1\rangle \} = \{|00\rangle , |01\rangle , |10\rangle , |11\rangle \} =: \{|0\rangle , |1\rangle , |2\rangle , |3\rangle \}$.
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• For a 2-qubit system,

  $$\{|0\rangle\otimes|0\rangle, |0\rangle\otimes|1\rangle, |1\rangle\otimes|0\rangle, |1\rangle\otimes|1\rangle\} = \{|00\rangle, |01\rangle, |10\rangle, |11\rangle\} =: \{|0\rangle, |1\rangle, |2\rangle, |3\rangle\}.$$  

• n-qubit quantum state: vector in $\mathbb{C}^{2^n}$ (with basis $\{|0\rangle, \ldots, |2^n-1\rangle\}$), such that

  $$|\psi\rangle = \sum_{i=0}^{2^n-1} \alpha_i |i\rangle, \quad \text{for} \ (\alpha_0, \ldots, \alpha_{2^n-1}) \in \mathbb{C}^{2^n}, \text{ such that } \sum_{i=0}^{2^n-1} |\alpha_i|^2 = 1.$$
Let $N = 2^n - 1$. The family $(|i\rangle)_{i=0,...,N}$ is an orthonormal basis of $\mathbb{R}^{2^n}$.

- $n = 1$; $|0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix}$, $|1\rangle = \begin{bmatrix} 0 \\ 1 \end{bmatrix}$;
- $n = 2$;

\[
|00\rangle = |0\rangle \otimes |0\rangle = \begin{bmatrix} 1 \\ 0 \end{bmatrix} \otimes \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 1 & 0 \\ 0 & 1 \end{bmatrix} = \begin{bmatrix} 1 \\ 0 \\ 0 \\ 0 \end{bmatrix},
|01\rangle = \begin{bmatrix} 0 \\ 1 \\ 0 \\ 0 \end{bmatrix},
|10\rangle = \begin{bmatrix} 0 \\ 0 \\ 1 \\ 0 \end{bmatrix}, \ldots
\]
- $n \in \mathbb{N}$;

\[
|0 \cdots 0\rangle = \begin{bmatrix} 1 \\ 0 \\ \vdots \\ 0 \end{bmatrix}, \ldots
|1 \cdots 1\rangle = \begin{bmatrix} 0 \\ 0 \\ \vdots \\ 1 \end{bmatrix}.
\]
Q operations

- Q Gate: reversible quantum circuit (unitary matrix: \( UU^* = U^*U = I \)).
- Standard gates:

\[
X = \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}, \quad Y = \begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}, \quad H = \frac{1}{\sqrt{2}} \begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}, \quad R_y(\theta) = \begin{bmatrix} \cos \left( \frac{\theta}{2} \right) & -\sin \left( \frac{\theta}{2} \right) \\ \sin \left( \frac{\theta}{2} \right) & \cos \left( \frac{\theta}{2} \right) \end{bmatrix}
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  \]

- **Examples**:

\[
\begin{array}{c|c}
X |0\rangle &= \begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix} \begin{bmatrix} 1 \\ 0 \end{bmatrix} = \begin{bmatrix} 0 \\ 1 \end{bmatrix} = |1\rangle. \\
H |0\rangle &= \frac{|0\rangle + |1\rangle}{\sqrt{2}} = |+\rangle \quad \text{and} \quad H |1\rangle = \frac{|0\rangle - |1\rangle}{\sqrt{2}} = |--\rangle \\
H^\otimes 2 |00\rangle &= (H |0\rangle) \otimes (H |0\rangle) = \frac{|00\rangle + |01\rangle + |11\rangle + |11\rangle}{2} \\
cX(H \otimes I) |00\rangle &= cX \left( \frac{|0\rangle + |1\rangle}{\sqrt{2}} \otimes |0\rangle \right) \\
&= \frac{|0\rangle |0\rangle + |1\rangle X |0\rangle}{\sqrt{2}} = \frac{|00\rangle + |11\rangle}{\sqrt{2}} \quad \text{(EPR)}
\end{array}
\]
Example of a Q circuit
Exciting example: Generating a uniform distribution

- 1 qubit, i.e. 2 values (discrete distribution over 2 points):

\[ H |0\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}} \]
**Exciting** example: Generating a uniform distribution

- 1 qubit, i.e. 2 values (discrete distribution over 2 points):

\[
\mathbb{H} |0\rangle = \frac{|0\rangle + |1\rangle}{\sqrt{2}}
\]

- \(n\) qubits, i.e. \(2^n\) values (discrete distribution over \(2^n\) points):

\[
\mathbb{H}^{\otimes n} |0\rangle^{\otimes n} = \left(\mathbb{H} |0\rangle\right)^{\otimes \cdots^{\otimes \left(\mathbb{H} |0\rangle\right)}}
= \left(\frac{|0\rangle + |1\rangle}{\sqrt{2}}\right)^{\otimes \cdots{\otimes \left(\frac{|0\rangle + |1\rangle}{\sqrt{2}}\right)}}
= \frac{1}{2^{n/2}} \left( |0\rangle + |1\rangle \right)^{\otimes \cdots{\otimes \left( |0\rangle + |1\rangle \right)}}
= \frac{1}{2^{n/2}} \left( |0\cdots0\rangle + |0\cdots01\rangle + \cdots + |1\cdots10\rangle + |1\cdots1\rangle \right)
= \frac{1}{2^{n/2}} \sum_{i=0}^{2^n-1} |\hat{i}\rangle.
\]
Possible to code things up:

- Simulated quantum computer
- Actual (small-size) quantum computer

from qiskit import QuantumCircuit, Aer, execute
from qiskit.visualization import plot_histogram

Running a quantum circuit on a simulator
```python
[15]:
qc = QuantumCircuit(1)
quc.h(0)
qc.measure_all()
qc.draw('mpl')
[15]:
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Postulate 1 – Statics
Postulate 2 – Dynamics
Postulate 3 – Measurement
Postulate 4 – Composite systems

6 qubits

```
[10]: n = 6
    qc = QuantumCircuit(n)
    for i in range(n):
        qc.h(i)
    qc.measure_all()
    qc.draw('mpl')

[11]: backend = Aer.get_backend('qasm_simulator')
        shots = 50000
        results = execute(qc, backend=backend, shots=shots).result()
        plot_histogram(results.get_counts())
```
Is there any sense of reality here?

Two competing technologies:

- **Superconducting qubits**: each qubit can interact with its nearest neighbour, limited decoherence time, needs super-cooling; IBM, Google, AWS, Alibaba, Rigetti, Intel, D-Wave.

- **Ion trapped**: ions trapped in electric fields, that can be *perturbed* by laser beams. Quantinuum, IonQ, Quantum Factory, Alpine Quantum Technologies, eleQtron, Oxford Ionics.
Q Tech: interesting graph theoretic problems
Postulate 1 – Statics

Associated to any physical system is a complex inner product space (Hilbert space) known as the state space of the system. The system is completely described at any given point in time by its state vector, which is a unit vector in its state space.
Postulate 2 – Dynamics

The evolution of the closed Q system is described by the Schrödinger equation

\[ i\hbar \partial_t \psi(t) = \mathcal{H} \psi(t), \]

where \( \hbar \) is Planck’s constant and \( \mathcal{H} \) is a time-independent Hermitian operator (Hamiltonian of the system).

Note that, for any \( 0 \leq t_1 \leq t_2 \), Schrödinger’s equation gives us

\[ |\psi(t_2)\rangle = \mathcal{U}(t_1, t_2) |\psi(t_1)\rangle, \quad \mathcal{U}(t_1, t_2) = \exp \left\{ \frac{-i\mathcal{H}(t_2 - t_1)}{\hbar} \right\}. \]

**Lemma:** if \( \mathcal{H} \) is Hermitian (\( \mathcal{H}^\dagger := (\mathcal{H}^*)^T = \mathcal{H} \)) and \( \alpha \in \mathbb{R} \), then \( \exp\{i\alpha\mathcal{H}\} \) is unitary.
Unitary operators – Q logic gates

Unitary operators preserve the inner product and hence norms: given $|u\rangle$ and $|v\rangle$, and a unitary operator $U$, then

$$(|Uu\rangle)^\dagger \cdot |Uv\rangle = \langle uU^\dagger | \cdot |Uv\rangle = \langle u|U^\dagger U|v\rangle = \langle u|v\rangle.$$ 

In Q mechanics, all physical transformations (rotations, translations, time evolution) correspond to (unitary) maps from Q states to Q states.

Unitary operators can then be viewed as Q logic gates implementing Q computations.

Since unitary operators are invertible ($U^{-1} = U^\dagger$), then Q computing is reversible.
Quantum logic gates

A quantum logic gate allows to transform a qubit, i.e. to rotate it on the unit sphere. It generalises classical operations. It can be represented as a unitary matrix in $\mathbb{C}^2$ ($G^\dagger G = GG^\dagger = I$).

**Example:** There is no Boolean function $\varphi$ such that applied twice to a classical bit would result in a NOT gate: $\varphi(\phi(0)) = 1$ and $\varphi(\phi(1)) = 0$. In Q computing, let

$$G := \frac{1}{2} \begin{pmatrix} 1 + i & 1 - i \\ 1 - i & 1 + i \end{pmatrix},$$

Then

$$G^2 = \frac{1}{4} \begin{pmatrix} (1 + i)^2 + (1 - i)^2 & 2(1 + i)(1 - i) \\ 2(1 + i)(1 - i) & (1 + i)^2 + (1 - i)^2 \end{pmatrix} = \begin{pmatrix} 0 & 1 \\ 1 & 0 \end{pmatrix},$$

so that

$$G^2 |0\rangle = G^2 \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} 0 \\ 1 \end{pmatrix} = |1\rangle \quad \text{and} \quad G^2 |1\rangle = G^2 \begin{pmatrix} 0 \\ 1 \end{pmatrix} = \begin{pmatrix} 1 \\ 0 \end{pmatrix} = |0\rangle.$$
The Spectral Theorem

The eigenfunctions of an Hermitian operator form a complete set of basis functions.

Spectral Theorem: *If $A$ is Hermitian, there exists an orthonormal basis consisting of eigenvectors of $A$. Each eigenvalue is real.*

Therefore the state $|\Psi\rangle$ of the system can be written as a superposition of eigenfunctions $\{|\psi_i\rangle\}$ of $A$:

$$|\Psi\rangle = \sum_i \alpha_i |\psi_i\rangle,$$

where again the coefficients $\{\alpha_i\}$ are complex *probability amplitudes* with $\sum_i |\alpha_i|^2 = 1$. 

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Postulate 3 – Measurement

If we measure the Hermitian operator $\mathcal{A}$ in the state $|\Psi\rangle$, the possible outcomes are the eigenvalues $\{\lambda_i\}$ of $\mathcal{A}$. The probability $p_i$ to measure $\lambda_i$ is given by

$$p_i = |\alpha_i|^2.$$  

After the outcome $\lambda_i$, the state of the system becomes

$$|\Psi\rangle = |\psi_i\rangle.$$  

This can be understood as a projection onto the eigenstate $|\psi_i\rangle$: define $\Pi_i := |\psi_i\rangle \langle \psi_i|$, then the state evolves from $|\Psi\rangle$ to $\Pi_i |\Psi\rangle$, with

$$\Pi_i |\Psi\rangle = |\psi_i\rangle \langle \psi_i| |\Psi\rangle = |\psi_i\rangle \langle \psi_i| \left( \sum_j \alpha_j |\psi_j\rangle \right) = \sum_j \alpha_j |\psi_i\rangle \langle \psi_i| |\psi_j\rangle = \alpha_i |\psi_i\rangle.$$  

We this need to perform measurement on the same state many times to generate sufficient statistics (akin to Monte Carlo).
Postulate 4 – Composite Systems

The state space of a composite physical system is the tensor product of the state spaces of the individual component physical systems.

If one component physical system is in state $|\psi_1\rangle$ and a second component physical system is in state $|\psi_2\rangle$, then the state of the combined system is

$$|\psi_1\rangle \otimes |\psi_2\rangle.$$

Not all combined systems can be split into a tensor product of states of individual components. When this is not the case, the components are called entangled.
The power of entanglement

Consider an $n$-qubit system, where (recall) an individual qubit can be found, after measurement, in $|0\rangle$ or $|1\rangle$, i.e. we need to specify 2 probability amplitudes to describe the state of the qubit.

If all the qubits are independent, the quantum state can be represented as

$$|\psi\rangle = |\psi_1\rangle \otimes |\psi_2\rangle \otimes \ldots \otimes |\psi_n\rangle,$$

and we need to specify $2n$ probability amplitudes.

If all individual qubits are entangled (hence, there is no tensor product representation), we need to specify $2^n$ probability amplitudes.
Quantum Machine Learning
A generator and a discriminator compete against each other to improve themselves:

- the generator improves by becoming better at generating good samples (i.e. close to real data) from random noise
- the discriminator improves by being able to recognise real data from ‘fake’ (namely generated) data.
- Both are built as neural networks with hyperparameters over which to optimise.

Given a generator $G(\cdot, \theta^G) : \mathcal{X} \to (0, 1)$ and a discriminator $D(\cdot, \theta^D) : \mathcal{X} \to (0, 1)$ ($\theta^G, \theta^D$: hyperparameters), the goal is

$$\min_{\theta^G} \max_{\theta^D} \left\{ \mathbb{E}_{x \sim P_{data}} \left[ \log(D(x; \theta^D)) \right] + \mathbb{E}_{z \sim P_{G(\cdot, \theta^G)}} \left[ \log \left( 1 - D(G(z; \theta^G); \theta^D) \right) \right] \right\},$$

where $x \sim P_{data}$ means some sample $x$ generated from the original, ‘true’ data, whereas $z \sim P_{G}$ refers to sample generated from the generator $G$. 
Q GAN

- Data represented by a density operator (positive semi-definite, Hermitian matrix of trace one) \( \sigma = |\psi\rangle \langle \psi| \);
Q GAN

- Data represented by a density operator (positive semi-definite, Hermitian matrix of trace one) $\sigma = |\psi\rangle \langle \psi|$
- Generator $G$ generates some output density matrix $\rho$
- Discriminator: tries to identify the true data from the fake one, i.e. it makes a positive operator-valued measurement with outcomes $T$ (True) or $F$ (False).
Data represented by a density operator (positive semi-definite, Hermitian matrix of trace one) \( \sigma = |\psi\rangle \langle \psi| \);

Generator \( G \) generates some output density matrix \( \rho \);

Discriminator: tries to identify the true data from the fake one, i.e. it makes a positive operator-valued measurement with outcomes \( T \) (True) or \( F \) (False).

Probability that the measurement yields a positive answer given the true data:

\[
P(T|\sigma) = \text{Tr}(T\sigma),
\]

Probability that the measurement yields a positive answer given generated data:

\[
P(T|G) = \text{Tr}(T\rho).
\]
**Q GAN**

- Data represented by a density operator (positive semi-definite, Hermitian matrix of trace one) $\sigma = |\psi\rangle \langle \psi|$;
- Generator $G$ generates some output density matrix $\rho$;
- Discriminator: tries to identify the true data from the fake one, i.e. it makes a positive operator-valued measurement with outcomes $T$ (True) or $F$ (False).

Probability that the measurement yields a positive answer given the true data:

$$P(T|\sigma) = \text{Tr}(T\sigma),$$

Probability that the measurement yields a positive answer given generated data:

$$P(T|\Phi) = \text{Tr}(T\rho).$$

Adversarial game:

$$\min_{\Phi} \max_T \left\{ \text{Tr}(T\rho) - \text{Tr}(T\sigma) \right\}.$$

*Note: Both the set of positive measurement operators $T$ (with 1-norm less than one) and the set of density matrices $\rho$ are convex.*
Variational circuit representations

- Both generator and discriminator represented as variational quantum circuits parameterised by a vector of parameters (e.g. rotation angles of all the gates);

- Optimisation performed by gradient-descent method.
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• Optimisation performed by gradient-descent method.

Questions:

• Optimal architecture of variational quantum circuit?

• Computing the gradient?
Architecture of the Q Generator

\[ G |0\rangle^{\otimes n} := \prod_{l=1}^{L} U_l(\theta_l). \]  

(1)

For each layer \( l \in \{1, \ldots, L\} \), \( U_l(\theta_l) \) acts on all \( n \) qubits, and \( \theta_l \in [0, 2\pi)^M \);
- Entanglement: pairwise controlled unitary gates;
Architecture of the Q Generator

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- Entanglement: pairwise controlled unitary gates; \( U_l \): 1- or 2-qubit gates only;
- Any 1-qubit gate can be decomposed into a sequence of \( R_Z \), \( R_X \) and \( R_Y \);
Architecture of the Q Generator

\[ G |0\rangle^{\otimes n} := \prod_{l=L}^{1} U_l(\theta_l). \]  \hspace{1cm} (1)

For each layer \( l \in \{1, \ldots, L\} \), \( U_l(\theta_l) \) acts on all \( n \) qubits, and \( \theta_l \in [0, 2\pi)^M \); 
- Entanglement: pairwise controlled unitary gates; \( U_l \): 1- or 2-qubit gates only; 
- Any 1-qubit gate can be decomposed into a sequence of \( R_Z \), \( R_X \) and \( R_Y \); 
- Imprimitive 2-qubit gates with 1-qubit gates ensure quantum universality;
Architecture of the Q Generator

\[ G |0\rangle^{\otimes n} := \prod_{l=1}^{L} U_l(\theta_l). \tag{1} \]

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- Any 1-qubit gate can be decomposed into a sequence of \( R_Z, R_X \) and \( R_Y \);
- *Imprimitive* 2-qubit gates with 1-qubit gates ensure quantum universality;

*In particular the decomposition \( R_X(\theta)Q(\phi) \) is universal, for \( \theta, \phi \in [0, 2\pi) \), where*

\[ Q(\phi) := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 1 & 0 \\ 0 & 0 & 0 & e^{i\phi} \end{pmatrix}. \]
Architecture of the Q Generator

$$\mathcal{G} |0\rangle^{\otimes n} := \prod_{l=L}^{1} U_l(\theta_l).$$  \hfill (1)

For each layer \( l \in \{1, \ldots, L\} \), \( U_l(\theta_l) \) acts on all \( n \) qubits, and \( \theta_l \in [0, 2\pi)^M \);
- Entanglement: pairwise controlled unitary gates; \( U_l \): 1- or 2-qubit gates only;
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- Imprimitive 2-qubit gates with 1-qubit gates ensure quantum universality;

In particular the decomposition \( R_X(\theta)Q(\phi) \) is universal, for \( \theta, \phi \in [0, 2\pi) \), where

$$Q(\phi) := \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 1 & 0 & 0 \\
0 & 0 & 1 & 0 \\
0 & 0 & 0 & e^{i\phi}
\end{pmatrix}.$$ 

General form of the \( L \)-layer neural network is (1), where, for each \( l \in \{1, \ldots, L\} \),

$$U_l(\theta_l) = \left\{ \bigotimes_{i=1}^{n} Q^{1+(i \mod n)}(\theta_i^{\text{imp}})R_X(\theta_i^{\text{ex}}) \right\} \left\{ \bigotimes_{i=1}^{n} R_Z(\theta_i^{Z,l}) \bigotimes_{i=1}^{n} R_X(\theta_i^{X,l}) \bigotimes_{i=1}^{n} R_Y(\theta_i^{Y,l}) \right\} ,$$

where \( Q^i \) means that qubit \( i \) is the control qubit and the gate acts on qubit \((i + 1)\).

Note that \( 1 + (i \mod n) = 1 + i \) when \( i \in \{1, \ldots, n - 1\} \) and is equal to 1 when \( i = n \). The total number of hyperparameters is therefore \( 5n \) per layer, thus \( 5nL \) in total.
Quantum ‘advantage’?

- Non-linearities?
Quantum ‘advantage’?

- Non-linearities?
- Universal approximation theorem?
Quantum ‘advantage’?

- Non-linearities?
- Universal approximation theorem?
- Conjecture: higher expressive power, only limited results so far.
Encoding classical data into quantum states. For $x_j \in [0, 1]$ and $p \in \mathbb{N}$,

$$\frac{x_{j,1}}{2} + \frac{x_{j,2}}{2^2} + \ldots + \frac{x_{j,p}}{2^p}$$  \hspace{1cm} (p-binary approximation of $x_j$),

where $x_{j,k} \in \{0, 1\}$, for $k \in \{1, 2, \ldots, p\}$.

- **Q code for $x_j$:**

  $$|x_j\rangle := |x_{j,1}\rangle \otimes |x_{j,2}\rangle \otimes \ldots \otimes |x_{j,p}\rangle = |x_{j,1}x_{j,2} \ldots x_{j,p}\rangle,$$

- **Encoding $x \in [0, 1]^n$:**

  $$|x\rangle := |x_0x_0,2 \ldots x_0,p\rangle \otimes \ldots \otimes |x_{n-1,1} \ldots x_{n-1,p}\rangle.$$

- Not so convenient.....
Simple example: Q Classifier

- Data: \((x^i := (x_{1}^{i}, x_{2}^{i}, x_{3}^{i}))_{i=1,...,N}\)
Simple example: Q Classifier

- Data: \((x^i := (x_1^i, x_2^i, x_3^i))_{i=1,...,N}\)
- For each data point \(x^i\), create a QNN:

\[
\begin{align*}
|0\rangle & \rightarrow R(x_1^i, x_2^i) R_{\theta_1} \cdots R_{\theta_p} y^i(\theta^i) = \\
\end{align*}
\]
Simple example: Q Classifier

- Data: \((x^i := (x^i_1, x^i_2, x^i_3))_{i=1,...,N}\);
- For each data point \(x^i\), create a QNN:

\[
|0\rangle - R_{(x^i_1, x^i_2)} - R_{\theta^i_1} - \cdots - R_{\theta^i_p} - y^i(\theta^i) =
\]

- Compute the loss function \(L^i := \|y^i(\theta^i) - x^i_3\|^2\)
Simple example: Q Classifier

- Data: \((x^i := (x^i_1, x^i_2, x^i_3))_{i=1,\ldots,N}\)
- For each data point \(x^i\), create a QNN:

\[
|0\rangle \rightarrow \underbrace{R_{(x^i_1, x^i_2)}}_{\cdot} \overbrace{R_{\theta_1} \ldots R_{\theta_p}}^{\cdot} \overbrace{\cdots}^{\cdot} \overbrace{y^i(\theta^i)}^{\cdot} = \]

- Compute the loss function \(L_i := \|y^i(\theta^i) - x^i_3\|^2\)
- Objective:

\[
\min_{\theta=(\theta^1, \ldots, \theta^N)} \sum_{i=1}^{N} L_i(\theta^i). \]
Simple example: Q Classifier

- Data: \((x^i := (x^i_1, x^i_2, x^i_3))_{i=1,...,N}\);
- For each data point \(x^i\), create a QNN:
  \[
  |0\rangle \rightarrow R_{(x^i_1, x^i_2)} \rightarrow R_{\theta^i_1} \rightarrow \cdots \rightarrow R_{\theta^i_p} \rightarrow y^i(\theta^i)
  \]
- Compute the loss function \(L_i := \|y^i(\theta^i) - x^i_3\|^2\);
- Objective:
  \[
  \min_{\theta=(\theta^1,...,\theta^N)} \sum_{i=1}^{N} L_i(\theta^i).
  \]

Comments:
- Very similar to a classical NN;
- No activation function;
- No weights;
- No entanglement;
- Simple encoding of classical data into quantum states.
Simple example: Q Classifier

- Data: \((x^i := (x^i_1, x^i_2, x^i_3))_{i=1,...,N}\);
- For each data point \(x^i\), create a QNN:

\[
|0\rangle - R_{(x^i_1, x^i_2)} - R_{\theta^i_1} - \cdots - R_{\theta^i_p} = y^i(\theta^i) = \ 
\]

- Compute the loss function \(L_i := \|y^i(\theta^i) - x^i_3\|^2\)
- Objective:

\[
\min_{\theta = (\theta_1, ..., \theta_N)} \sum_{i=1}^{N} L_i(\theta^i). 
\]

Comments:
- Very similar to a classical NN;
- No activation function;
- No weights;
- No entanglement;
- Simple encoding of classical data into quantum states.

Inner product? Construct \(U_w\) such that
\[
U_w \left( H^\otimes m |0\rangle^\otimes m |x\rangle \right) = \left[ \sum_{j=0}^{2^m - 1} e^{2i\pi j x^T w} |j\rangle \right] \otimes |x\rangle \rightarrow \text{inverse Q Fourier transform.} 
\]

Activation function? Build \(U\) such that \(U |x\rangle = e^{2i\pi \sigma(x)} |x\rangle \rightarrow \text{Q Phase estimation} \).
Application: Generating SVI

\[ p_T(k) = \left( \frac{\partial^2 C_{BS}(k, T, \sigma_{\text{imp}}(k, T))}{\partial K^2} \right)_{K=S_0e^k} \]

SVI parameterisation proposed by Gatheral:

\[ w_{SVI}(k, T) = \sigma_{\text{imp}}^2(k, T) T = a + b \left( k - m + \rho \sqrt{(k - m)^2 + \xi^2} \right), \quad \text{for any } k \in \mathbb{R}, \]

with the parameters \( \rho \in [-1, 1], a, b, \xi \geq 0 \) and \( m \in \mathbb{R} \).

SVI Density:

\[ p_T(k) = \frac{g_{SVI}(k, T)}{\sqrt{2\pi w_{SVI}(k, T)}} \exp \left\{ -\frac{d_-(k, w_{SVI}(k, T))^2}{2} \right\}, \]

with (all derivatives with respect to \( k \)).

\[ g_{SVI}(k, T) := \left( 1 - \frac{kw'_{SVI}(k, T)}{2w_{SVI}(k, T)} \right)^2 - \frac{w'_{SVI}(k, T)^2}{4} \left( \frac{1}{4} + \frac{1}{w_{SVI}(k, T)} \right) + \frac{w''_{SVI}(k, T)}{2}, \]
SVI Example

**Figure:** Density of $\log(S_T)$ in SVI

**Figure:** Discretised distribution of $\log(S_T)$ on $[-1, 1]$ with $2^{14}$ points

Antoine (Jack) Jacquier
Target wave function:

$$|\psi_{\text{target}}\rangle = \sum_{i=0}^{2^n-1} \sqrt{p_i} |i\rangle,$$

where, for each \( i \in \{0, \ldots, 2^n - 1\} \), \( p_i = \mathbb{P} \left( \log(S_T) \in \left[ -1 + \frac{2i}{2^n}, -1 + \frac{2(i + 1)}{2^n} \right] \right) \).

**Figure:** Comparison between the target and the generated distributions at the end of the training.
• Barren plateaux?
  • Consider a Q circuit \( U(\theta) = \prod_{l=1}^{L} U_l(\theta_l) \), with \( U_l(\theta_l) = e^{-i\theta_l V_l} \).
  • Objective function of a variational problem: \( \mathcal{E}(\theta) := \langle 0 | U(\theta)^\dagger A U(\theta) | 0 \rangle \).
  • We can show that 
    \[
    \nabla \mathcal{E}(\theta) = \cdots \frac{\cdots}{N^2 - 1}.
    \]
Q Food for thought

• Barren plateaux?
  • Consider a Q circuit $U(\theta) = \prod_{l=L}^{1} U_l(\theta_l)$, with $U_l(\theta_l) = e^{-i\theta_l V_l}$.
  • Objective function of a variational problem: $\mathcal{E}(\theta) := \langle 0 | U(\theta)^\dagger A U(\theta) | 0 \rangle$.
  • We can show that

$$\nabla \mathcal{E}(\theta) = \frac{\cdots}{N^2 - 1}.$$ 

• Q Wasserstein GAN
• Barren plateaux?
  • Consider a quantum circuit $U(\theta) = \prod_{l=1}^{L} U_l(\theta_l)$, with $U_l(\theta_l) = e^{-i\theta_l V_l}$.
  • Objective function of a variational problem: $\mathcal{E}(\theta) := \langle 0 | U(\theta)^\dagger A U(\theta) | 0 \rangle$.
  • We can show that
    \[ \nabla [\nabla \mathcal{E}(\theta)] = \frac{\cdots}{N^2 - 1}. \]

• Q Wasserstein GAN
• Other types of NN?
Quantum Wasserstein GAN

- Classical Wasserstein distance:

\[
\min_{\pi \in \Pi(p,q)} \int_X \int_Y \pi(x, y)c(x, y)dxdy
\]
Quantum Wasserstein GAN

• Classical Wasserstein distance:

$$\min_{\pi \in \Pi(p, q)} \int_X \int_Y \pi(x, y)c(x, y)dx\,dy$$

• Encode the (discretised) classical distribution $p$ into a mixed quantum state

$$\rho^p := \sum p_i |\psi_i\rangle \langle \psi_i|, \quad \text{for some basis } \{|\psi_i\rangle\}_i.$$
Quantum Wasserstein GAN

• Classical Wasserstein distance:

\[
\min_{\pi \in \Pi(p, q)} \int_{\mathcal{X}} \int_{\mathcal{Y}} \pi(x, y)c(x, y)dxdy
\]

• Encode the (discretised) classical distribution \( p \) into a mixed quantum state

\[
\rho^p := \sum p_i |\psi_i\rangle \langle \psi_i|, \quad \text{for some basis } \{|\psi_i\rangle\}_i.
\]

• \( Q \) Wasserstein distance:

\[
\min_{\pi \in \Pi(P, Q)} \text{Tr}\left(\pi^\top C\right),
\]

subject to \( \text{Tr}(P_Y\pi) = \text{Diag}(p(x))_{x \in \mathcal{X}}, \quad \text{Tr}(P_X\pi) = \text{Diag}(q(y))_{y \in \mathcal{Y}} \)

where \( C = \text{Diag}(c(x, y)_{x, y \in \mathcal{X} \times \mathcal{Y}}) \)
Quantum Wasserstein GAN

- Classical Wasserstein distance:

$$\min_{\pi \in \Pi(p, q)} \int_{\mathcal{X}} \int_{\mathcal{Y}} \pi(x, y) c(x, y) dx dy$$

- Encode the (discretised) classical distribution $p$ into a mixed quantum state

$$\rho^p := \sum p_i |\psi_i\rangle \langle \psi_i|, \text{ for some basis } \{|\psi_i\rangle\}_i.$$  

- Q Wasserstein distance:

$$\min_{\pi \in \Pi(P, Q)} \text{Tr} \left( \pi^\top C \right),$$

subject to $\text{Tr}(P_Y \pi) = \text{Diag}(p(x))_{x \in \mathcal{X}}, \quad \text{Tr}(P_X \pi) = \text{Diag}(q(y))_{y \in \mathcal{Y}}$

where $C = \text{Diag}(c(x, y))_{x, y \in \mathcal{X} \times \mathcal{Y}}$

- This is only a semi-metric (no triangle inequality)
Optimisation, Q annealing, Hamiltonians, noise...
An optimisation problem

**Problem:** Given $f: \{0, 1\}^n \to \mathbb{R}$, \( \min_{z \in \{0,1\}^n} f(z) \). \( (2) \)

- Hamiltonian formulation: \( \mathcal{H}_F := \sum_{z \in \{0,1\}^n} f(z) |z\rangle \langle z| \).

- If \( |z_i\rangle \) are eigenvectors of \( \mathcal{H}_F \), then

\[
\mathcal{H} |z_i\rangle = \left( \sum_{z \in \{0,1\}^n} f(z) |z\rangle \langle z| \right) |z_i\rangle
\]
\[
= \left( \sum_{z \in \{0,1\}^n \setminus \{z_i\}} f(z) |z\rangle \langle z| \right) |z_i\rangle + \left( f(z_i) |z_i\rangle \langle z_i| \right) |z_i\rangle
\]
\[
= 0 + f(z_i) |z_i\rangle \langle z_i|z_i\rangle
\]
\[
= f(z_i) |z_i\rangle,
\]

so that \( (f(z_i)) \) are eigenvalues of \( \mathcal{H}_F \).

- Solving (2) amounts to finding the smallest eigenvalues (minimum energy) of \( \mathcal{H}_F \).
- Problem: it is often difficult to find them.
Constant Hamiltonian simulation

Schrödinger equation (normalised with $\hbar = 1$):

$$i\hbar \frac{d|\psi(t)\rangle}{dt} = \mathcal{H} |\psi(t)\rangle \quad \text{(Schrödinger equation)}.$$ 

is solved as

$$|\psi(t)\rangle = e^{-i\mathcal{H}t} |\psi(0)\rangle$$

at time $t \geq 0$. If $\mathcal{H} |\psi_0\rangle = \lambda_0 |\psi_0\rangle$, then

$$|\psi(t)\rangle = e^{-i\mathcal{H}t} |\psi_0\rangle = e^{-i\lambda_0 t} |\psi_0\rangle,$$

i.e. no transition over time between different eigenstates!!
Time-dependent Hamiltonian simulation $\mathcal{H}(\cdot)$

Schrödinger equation over $[0, \tau]$; time change $t(\cdot)$ with $t(0) = 1$ and $t(1) = \tau$:

$$i \frac{d |\psi(s)\rangle}{ds} = t'(s) \mathcal{H}(s) |\psi(s)\rangle, \quad \text{on } [0, 1].$$

(3)

Consider $\mathcal{H}(s) = r(s) \mathcal{H}_0 + (1 - r(s)) \mathcal{H}_F$, for two Hamiltonians $\mathcal{H}_0$ and $\mathcal{H}_F$, where $r(\cdot)$ is a continuous adiabatic evolution path decreasing from $r(0) = 1$ to $r(1) = 0$. Let $|\psi(\cdot)\rangle$ be the solution to the Schrödinger equation, so that

$$|\psi(s)\rangle = \mathcal{U}(s) |\psi(0)\rangle, \quad \text{for some unitary operator } \mathcal{U}.$$ 

Consider (3) with $t(s) = s\tau$, hence

$$i \frac{d |\psi(t)\rangle}{dt} = \tau \mathcal{H}(t) |\psi(t)\rangle, \quad \text{on } [0, 1].$$
Let $|\phi(t)\rangle$ be the ground state of $\mathcal{H}_t$ and the adiabatic schedule $r(s) = 1 - s$, so that

$$\mathcal{H}(s) = (1 - s)\mathcal{H}_0 + s\mathcal{H}_F.$$ 

**Theorem[...].** If there exists $\delta > 0$ such that

$$\tau \geq \frac{2}{\delta} \left\{ c_0 \frac{\|\mathcal{H}_F - \mathcal{H}_0\|}{\bar{\Delta}^2} + \left(3c_1^2 + c_1 + c_3\right) \frac{\|\mathcal{H}_F - \mathcal{H}_0\|^2}{\bar{\Delta}^3} \right\},$$

with $\bar{\Delta} := \min_{s \in [0,1]} \Delta_s$, then, starting the system in the state $|\psi(0)\rangle = |\phi(0)\rangle$, the Schrödinger evolution yields at time 1 a state $|\psi(1)\rangle$ satisfying $\|\|\phi(1)\rangle - |\psi(1)\rangle\| \leq \delta$. 
The 1-bit Disagree problem

The 1-bit Disagree problem reads

\[ f(z) := \begin{cases} 1, & \text{if } z = 1, \\ 0, & \text{if } z = 0. \end{cases} \]

\[ \mathcal{H}_F := \frac{1 + \sigma^z}{2} = \frac{1}{2} \left( \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = |0\rangle \langle 0|, \]

so that

\[ \mathcal{H}_F |0\rangle = |0\rangle \langle 0| |0\rangle = |0\rangle = 1 \cdot |0\rangle, \]

\[ \mathcal{H}_F |1\rangle = |0\rangle \langle 0| |1\rangle = 0 = 0 \cdot |1\rangle, \quad \text{(ground state)}. \]
The 1-bit Disagree problem

The 1-bit Disagree problem reads

\[ f(z) := \begin{cases} 
1, & \text{if } z = 1, \\
0, & \text{if } z = 0. 
\end{cases} \]

\[ \mathcal{H}_F := \frac{1 + \sigma^z}{2} = \frac{1}{2} \left( \begin{pmatrix} 1 & 0 \\ 0 & 1 \end{pmatrix} + \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \right) = \begin{pmatrix} 1 & 0 \\ 0 & 0 \end{pmatrix} = |0\rangle \langle 0|, \]

so that

\[ \mathcal{H}_F |0\rangle = |0\rangle \langle 0| |0\rangle = |0\rangle = 1 \cdot |0\rangle, \]

\[ \mathcal{H}_F |1\rangle = |0\rangle \langle 0| |1\rangle = 0 = 0 \cdot |1\rangle, \quad \text{(ground state)} \]

Define now

\[ \mathcal{H}_0 := \frac{1 - \sigma^x}{2} = \frac{1}{2} \begin{pmatrix} 1 & -1 \\ -1 & 1 \end{pmatrix} = \frac{1}{2} \left( |0\rangle \langle 0| + |1\rangle \langle 1| - |1\rangle \langle 0| - |0\rangle \langle 1| \right). \]

One can check that

\[ \mathcal{H}_0 |+\rangle = |+\rangle = 1 \cdot |+\rangle, \]

\[ \mathcal{H}_0 |-\rangle = 0 = 0 \cdot |-\rangle, \quad \text{(ground state)}. \]
Interpolating Hamiltonian:

\[ \mathcal{H}(t) := (1 - t) \mathcal{H}_0 + t \mathcal{H}_F, \quad t \in [0, 1]. \]

Eigenvalues: \( \lambda_{\pm}(t) = \frac{1}{2} \left( 1 \pm \sqrt{1 - 2t(1-t)} \right). \)

The adiabatic theorem applies!!
The commuting issue for the 1-bit Disagree problem

Consider instead

\[ \mathcal{H}_0 := \frac{1 - \sigma^z}{2} = \frac{1}{2} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = |1\rangle \langle 1|, \]

\[ \mathcal{H}_0 |0\rangle = |1\rangle \langle 1| |0\rangle = 0 \quad \text{and} \quad \mathcal{H}_0 |1\rangle = |1\rangle \langle 1| |1\rangle = |1\rangle. \]
The commuting issue for the 1-bit Disagree problem

Consider instead

\[ \mathcal{H}_0 := \frac{1 - \sigma^z}{2} = \frac{1}{2} \begin{pmatrix} 0 & 0 \\ 0 & 1 \end{pmatrix} = |1\rangle \langle 1|, \]

\[ \mathcal{H}_0 |0\rangle = |1\rangle \langle 1| |0\rangle = 0 \quad \text{and} \quad \mathcal{H}_0 |1\rangle = |1\rangle \langle 1| |1\rangle = |1\rangle. \]

Interpolating Hamiltonian:

\[ \mathcal{H}(t) := (1 - t) \mathcal{H}_0 + t \mathcal{H}_F = \begin{pmatrix} t & 0 \\ 0 & 1 - t \end{pmatrix}, \quad \text{for } t \in [0, 1]. \]

Eigenvalues: \( \lambda(t) \in \{ t, 1 - t \} \): \( \mathcal{H}(t) |0\rangle = t |0\rangle \) and \( \mathcal{H}(t) |1\rangle = (1 - t) |1\rangle. \)

![Graph showing eigenvalues](image-url)
Adding noise.....

Consider a noisy version of the interpolating Hamiltonian:

\[ H^\varepsilon(t) := H(t) + \varepsilon \begin{pmatrix} 0 & t(1 - t) \\ t(1 - t) & 0 \end{pmatrix} = \begin{pmatrix} t & \varepsilon t(1 - t) \\ \varepsilon t(1 - t) & 1 - t \end{pmatrix}, \quad \text{for } t \in [0, 1]. \]

The two eigenvalues (say for \( \varepsilon = 0.2 \) behave as follows:

And the spectral gap is restored!
The 2-bit Disagree problem

\[ f(x) := \begin{cases} 
0, & \text{if } x_1 \neq x_2, \\
1, & \text{otherwise.} 
\end{cases} \]

\[ \mathcal{H}_F := \begin{pmatrix}
1 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 0 \\
0 & 0 & 0 & 1
\end{pmatrix} = \frac{1}{2} \{ I \otimes I + (Z \otimes I)(I \otimes I) \} \]

with \( I \) the identity matrix in \( \mathcal{M}_2(\mathbb{R}) \), \( Z = \begin{pmatrix} 1 & 0 \\ 0 & -1 \end{pmatrix} \) and \( \otimes \) the Kronecker product.

Eigenvalues:

\[ e_1^F = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix}, \quad e_2^F = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \quad e_3^F = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \quad e_4^F = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix}, \]

with eigenvalues 0, 0, 1, 1, so that the ground states are \( \{ e_1^F, e_2^F \} \).
• Initial Hamiltonian:

\[
\mathcal{H}_0 = \frac{1}{2} \left\{ (I \otimes I - X \otimes I) + (I \otimes I - I \otimes X) \right\} = \frac{1}{2} \begin{pmatrix}
2 & -1 & -1 & 0 \\
-1 & 2 & 0 & -1 \\
-1 & 0 & 2 & -1 \\
0 & -1 & -1 & 2
\end{pmatrix};
\]

• Eigenvalues \{0, 1, 1, 2\} and ground state \(e_1^0 = (1, 1, 1, 1)^\top = 2 \left| ++ \right\rangle\);
• Take \(\mathcal{H}_t := (1 - r(t))\mathcal{H}_0 + r(t)\mathcal{H}_F\);
• Apply the Q Adiabatic theorem;

Questions

• How to find \(\mathcal{H}_0\) in general? Idea: PQC.
• Reality has noise: \(\mathcal{H}_t \rightarrow \mathcal{H}_t^\varepsilon\) for all \(t \in (0, 1)\) (or noise-induced algorithm);
• Question: understand \(\mathcal{H}_t^\varepsilon\) (pathwise) as \(\varepsilon \downarrow 0\).
Quantum Monte Carlo
Classical Monte Carlo

$X$: random variable, with $\mu := \mathbb{E}[\nu(X)]$ and $\sigma^2 := \mathbb{V}[\nu(X)]$.
($\Phi$: given nice enough map, both $\mu$ and $\sigma^2$ are finite).

$$\hat{\mu}_N := \frac{1}{N} \sum_{i=1}^{N} X_i.$$  

- **Law of large numbers**: $\hat{\mu}_N$ converges to $\mu$ almost surely as $N \uparrow \infty$;
- **Central Limit Theorem**:

$$\lim_{N \uparrow \infty} \frac{\hat{\mu}_N - \mu}{\sigma/\sqrt{N}} = \mathcal{N}(0, 1) \text{ in distribution.}$$

This implies that

$$\mathbb{P} \left( |\hat{\mu}_N - \mu| \leq \varepsilon \right) = \mathbb{P} \left( \left| \frac{\hat{\mu}_N - \mu}{\sigma/\sqrt{N}} \right| \leq \frac{\varepsilon \sqrt{N}}{\sigma} \right) = \mathbb{P} \left( |\mathcal{N}(0, 1)| \leq \frac{\varepsilon \sqrt{N}}{\sigma} \right).$$

If we want $\mathbb{P}(|\mathcal{N}(0, 1)| \geq z) = 1 - \delta$, we require $z = \frac{\varepsilon \sqrt{N}}{\sigma}$, i.e. $N = \mathcal{O} \left( \frac{1}{\varepsilon^2} \right)$.

One may replace $\sigma^2$ by its unbiased estimator $s^2 := \frac{1}{N-1} \sum_{i=1}^{N} (X_i - \hat{\mu}_N)^2$. 

Antoine (Jack) Jacquier

Q for Q and Q for Q
Amplitude estimation

[Brassard, Høyer, Mosca, Tapp, 2002] and [Montanaro, 2015]

• Inputs:
  • a quantum state $|\psi\rangle$ and a projector $P$;
  • Unitary $U := 2 |\psi\rangle \langle \psi | - I$ and $V := I - 2P$;
  • $N \in \mathbb{N}$

• Output: Estimate $\hat{a}$ of $a = \langle \psi | P | \psi \rangle$ such that

$$|\hat{a} - \langle \psi | P | \psi \rangle| \leq 2\pi \frac{\sqrt{a(1 - a)}}{N} + \frac{\pi^2}{N^2},$$

with probability at least $\frac{8}{\pi^2}$, using $U$ and $V$, $N$ times each.

Note: the probability can be improved to $1 - \delta$ (for any $\delta > 0$) using the Powering Lemma, at the cost of a $O(\log(1/\delta))$ multiplicative factor.

Fix $\varepsilon > 0$ and let $N := \frac{2\pi}{\varepsilon \sqrt{a}}$. Then (for $|a| < 1$)

$$|\hat{a} - \langle \psi | P | \psi \rangle| \leq a \sqrt{1 - a \varepsilon} + \frac{a}{4} \varepsilon^2 \leq \varepsilon a,$$
Powering Lemma

[Jerrum, Valiant, Vazirani, 1986]
Let $\mathcal{A}$ be a (quantum or classical) algorithm aiming at estimating $\mu$ and whose output satisfies

$$|\hat{\mu} - \mu| \leq \varepsilon,$$

except with probability less than $\frac{1}{2}$. Then, for any $\delta > 0$, it suffices to repeat $\mathcal{A}$ $\log(1/\delta)$ times and take the median to obtain $\hat{\mu}$ with

$$|\hat{\mu} - \mu| < \varepsilon,$$

with probability at least $1 - \delta$. 
Quantum Monte Carlo [Montanaro, 2015]

Algorithm

- **Inputs:**
  - Algorithm $\mathcal{A}$ with random output $\nu(\mathcal{A}) \in [0, 1]$; $N \in \mathbb{N}$; $\delta > 0$; $n$ qubits;
  - $k < n$ qubits are measured. The outcome of the measurement of $x \in \{0, 1\}^k$ is mapped into $\nu(x) \in [0, 1]$;
  - $\mathcal{W} |x\rangle_k |0\rangle := |x\rangle_k \left( \sqrt{1 - \nu(x)} |0\rangle + \sqrt{\nu(x)} |1\rangle \right)$;

- **Steps:**
  - Apply $N$ iterations of Amplitude Estimation with
    \[
    |\psi\rangle := (I \otimes \mathcal{W})(\mathcal{A} \otimes I) |0\rangle^{\otimes(n+1)} \quad \text{and} \quad P := I \otimes |1\rangle \langle 1|.
    \]
  - Repeat (4) $\mathcal{O}(\log(1/\delta))$ times and output the median.

Theorem

The algorithm outputs $\tilde{\mu}$ such that, with probability at least $1 - \delta$, \[
|\tilde{\mu} - \mathbb{E}[\nu(\mathcal{A})]| \leq C \left( \frac{\sqrt{\mathbb{E}[\nu(\mathcal{A})]}}{N} + \frac{1}{N^2} \right),
\]

To get $|\tilde{\mu} - \mathbb{E}[\nu(\mathcal{A})]| \leq \varepsilon$, one then needs $N = \mathcal{O}(1/\varepsilon)$
Cost of the QMC algorithm

- The circuit $U$ is used $O(N \log(1/\delta))$ times:
  - $N$ times for Quantum Amplitude Estimation;
  - $\log(1/\delta)$ times for the Powering Lemma;

Refinements:
- output bounded in $l^2$ [Montanaro, 2015];
- output with bounded variance;
- multilevel....
- variance reduction....
Application to option pricing

**Goal:** $\Pi := \mathbb{E}[\nu(W_T)]$, for some Brownian motion $W$.

- Discretise (*quantisation*) the support $\mathbb{R} \to [\underline{w}, \overline{w}]$ with $2^n$ points, and assume that

$$A |0\rangle \otimes^n = \sum_{j=0}^{2^n-1} \sqrt{p_j} |j\rangle,$$

with $p_j := \frac{\mathbb{P}(w_j)}{\sum_k \mathbb{P}(w_k)}$,

and we identify $w_j$ with $|j\rangle$.

- In particular, take $\nu(w) = \left(S_0 \exp \left\{ \sigma w - \frac{\sigma^2 T}{2} \right\} - K \right)_+$

$$B : |j\rangle |0\rangle \mapsto |j\rangle |\tilde{\nu}_j\rangle,$$

$\tilde{\nu}_j :$ binary approximation of $\nu(w_j)$.

- $W |j\rangle |\tilde{\nu}_j\rangle \mapsto |j\rangle |\tilde{\nu}_j\rangle (\sqrt{1 - \tilde{\nu}_j} |0\rangle + \sqrt{\tilde{\nu}_j} |1\rangle)$ (as in QMC)

- Inverting $B$ yields $|j\rangle |0\rangle \otimes^n (\sqrt{1 - \tilde{\nu}_j} |0\rangle + \sqrt{\tilde{\nu}_j} |1\rangle)$.

- Ignoring $|0\rangle \otimes^n$, we can now use QMC to obtain an estimate of $\mathbb{E}[\nu(W_T)]$. 

Antoine (Jack) Jacquier
Quantum simulation (different...)

Schrödinger: the evolution of a quantum system satisfies (ignoring Planck):

$$i \partial_t |\psi(t)\rangle = \mathcal{H} |\psi(t)\rangle, \quad |\psi(0)\rangle \in \ldots$$

with solution $|\psi(t)\rangle = e^{-i\mathcal{H}t} |\psi(0)\rangle$. The Hamiltonian $\mathcal{H}$ is usually large and $e^{-i\mathcal{H}t}$ is hard to compute. First-order approximation $e^{-i\mathcal{H}t} \approx 1 - i\mathcal{H}t$ unsatisfactory.

**Assumptions**

- $\mathcal{H} = \sum_{l=1}^{L} \mathcal{H}_l$, where each $\mathcal{H}_l$ acts on a ‘small’ subsystem (such that $e^{-i\mathcal{H}_lt}$ is easy to compute); note that $\mathcal{H}_l$ and $\mathcal{H}_k$ do not commute, but $e^{-i\mathcal{H}t}$ can be approximated with the Suzuki-Lie-Trotter formula.

- $T = m\delta$ ($m$ represents the number of time steps in the Suzuki-Lie-Trotter discretisation);

- Measurement operator $\mathcal{M}$ and $\mu := \mathbb{E}[\mathcal{M}] = \text{Tr}(\mathcal{M}\rho)$, with $\rho = |\psi\rangle \langle \psi|$;

- $\hat{\mu} := \frac{1}{N} \sum_{j=1}^{N} X_j$;

**Theorem** [Wang, 2011] There exist $C_1, C_2 > 0$ such that, for all $n, m$,

$$\mathbb{E} \left[ (\hat{\mu} - \mu)^2 \right] \leq \frac{C_1}{N} + \frac{C_2}{m^4}.$$
Q for PDEs
Option Pricing in the Black-Scholes model

- **Black-Scholes SDE:**
  \[
  \frac{dS_t}{S_t} = r dt + \sigma dW_t, \quad \text{for } t \geq 0.
  \]

- **European Call option with payoff** \(V(T, S_T) = \max(S_T - K, 0)\)

- **Feynman-Kac:**
  \[
  \left( \partial_t + \frac{\sigma^2 S^2}{2} \partial_{ss} + rS \partial_s - r \right) V(t, s) = 0, \quad \text{for } s > 0, \ t \in [0, T),
  \]
  with terminal condition \(V(T, s)\). This is equivalent to the heat equation
  \[
  \partial_{\tau} u(\tau, x) = \frac{1}{2} \partial_{xx} u(\tau, x),
  \]
  where the boundary condition is now at time zero \((\tau = \sigma^2 (T - t))\).
From Black-Scholes to Schrödinger

- The Wick rotation $\xi = -i\tau$ turns the heat PDE into 
  $$-i\partial_\xi u(\xi, x) = \frac{\partial_{xx} u(\xi, x)}{2},$$
  or
  $$-i\partial_\xi |\psi\rangle = \mathcal{H} |\psi\rangle \quad \text{(Schrödinger equation)},$$
  where $|\psi\rangle$ plays the role of the $u(\cdot, \cdot)$, and $\mathcal{H} = \frac{1}{2} \partial_{xx}$.

- **Explicit solution:**
  $$|\psi(\xi)\rangle = e^{i\mathcal{H}\xi} |\psi(0)\rangle,$$
  where $e^{i\mathcal{H}\xi}$ is the time evolution operator and $|\psi(0)\rangle$ an initial state with
  $$\langle \psi(0)|\psi(0)\rangle = 1.$$

**Possible algorithms:**
- HHL algorithm: to solve (high-dimensional) linear systems;
- Variational algorithms: Zhao, Sun, Cohen, Stokes, Veerapaneni [2022], Fontanela, Jacquier, Oumgari [2021]
A hybrid quantum algorithm

- Problem: normalised imaginary time evolution

\[ |\psi(\tau)\rangle = \gamma(\tau) \ e^{-\mathcal{H} \tau} \ |\psi(0)\rangle. \]

- Approximate \( |\psi(\tau)\rangle \) by a Q circuit composed of parameterised gates such that \( |\psi(\tau)\rangle \approx |\phi(\theta_{\tau})\rangle \), for some time-dependent parameters \( \theta_{\tau} = (\theta_{1\tau}, \ldots, \theta_{N\tau}) \in \mathbb{R}^N \).

- Assuming an initial state \( |\psi_0\rangle \), so that the ansatz is \( |\phi(\tau)\rangle = \Phi(\theta_{\tau}) \ |\psi_0\rangle \) at time \( \tau \), where \( \Phi(\theta_{\tau}) \) is sequence of unitary gates
\[ \Phi(\theta_{\tau}) = S \ (U_N(\theta^N_{\tau}), \ldots, U_k(\theta^k_{\tau}), \ldots, U_1(\theta^1_{\tau})). \]

\[ \theta^*_\tau := \arg\min_{\theta \in \mathbb{R}^N} \| |\psi(\tau)\rangle - \Phi(\theta_{\tau}) \ |\psi_0\rangle \|. \]
At time $\tau$

The optimisation problem reduces to the system of ODEs

$$A(\tau)\dot{\theta}_\tau = C(\tau),$$

for all $\tau$, where $\dot{\theta}_\tau := \partial_\tau \theta_\tau$, and

$$A(\tau) = \left(\Re \left( \frac{\partial \langle \phi(\tau) | \partial \phi(\tau) \rangle}{\partial \theta^i} \right) \right)_{i,j=1,\ldots,N}, \quad C(\tau) = \left(\Re \left( \frac{\partial \langle \phi(\tau) | \mathcal{H} | \phi(\tau) \rangle}{\partial \theta^i} \right) \right)_{i=1,\ldots,N}.$$

In this setting, both $A$ and $C$ can be measured efficiently using a quantum computer. In order to build the hybrid classical-quantum scheme, we assume:

1. Every unitary gate in the algorithm depends on a single parameter.
2. $\mathcal{H} = \sum_{i=1}^{N} \lambda_i h_i$, for $\lambda \in \mathbb{R}^N$ and tensor products $h_i$ of Pauli matrices.
Simulation from $\tau$ to $\Delta_\tau$

- Once $A(\tau)$ and $C(\tau)$ are obtained, the time evolution can be computed numerically using a classical computer.

- Euler scheme:

  $$\theta_{\tau+\Delta_\tau} = \theta_\tau + \Delta_\tau \dot{\theta}_\tau = \theta_\tau + \Delta_\tau A(\tau)^{-1} C(\tau),$$  

  for some small time step $\Delta_\tau$.

- ... and so on until time $\tau = T$. 
European Call option

- **Model:** Black-Scholes $dS_t = \sigma S_t dW_t$, with $\sigma = 20\%$, $S_0 = K = 100$, $T = 1$.
- **Goal:** Compute $\mathbb{E}[\max(S_T - K, 0)]$.
- Discretise the state space on logarithmic scale on an equidistant grid $[S_{\text{min}}, S_{\text{max}}] = [50, 150]$.
- With four qubits, the discretisation represents $|\psi\rangle$ using $2^4 = 16$ points, where $|\psi_F\rangle = |0000\rangle$ and $|\psi_F\rangle = |1111\rangle$ represent the solution at $S_{\text{min}}$ and $S_{\text{max}}$.
- The Hamiltonian $\mathcal{H} = \frac{1}{2} \partial_{xx}$ is discretised by second-order finite differences

\[
\frac{1}{2\Delta_x^2} \begin{bmatrix}
-2b\Delta_x^2 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\
1 & -2 & 1 & 0 & \cdots & 0 & 0 & 0 \\
0 & 1 & -2 & 1 & \cdots & 0 & 0 & 0 \\
\vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\
0 & 0 & 0 & 0 & \cdots & 1 & -2 & 1 \\
0 & 0 & 0 & 0 & \cdots & 0 & 0 & -2b\Delta_x^2 \\
\end{bmatrix}
\]

where $\Delta_x$ is the discretisation step in space.
- We split $[0, T]$ into $n_T$ steps.
- We compute $A$ and $C$ as above.
- The evolution of $\theta_T$ is obtained from the Euler scheme.
Figure: Top: European prices (left) and errors (right) \[ \| |\psi(\tau)\rangle - |\phi(\theta_\tau)\rangle \|. \] Bottom: Comparison with closed-form formula at maturity (left) and at inception (right).
Wrapping up
IBM roadmap

Figure: Source: ibm.com
Take-away message

- Initial entering cost (new language, new culture)
- New tools and methods, to learn
- Get *inspired*
- More maths are needed: numerical analysis, stochastic
- Q hardware is advancing fast
- Future: Hybrid Q / Classical
- Q solvers for (non-)linear systems
- Q Monte Carlo
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