Quantum annealing and Quantum Monte Carlo

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Overview

Q annealing, Hamiltonians and noise...

Simulated annealing

SA: metaheuristic inspired by thermal annealing. Goal: $\min_{D \subset \mathbb{R}^n} f(\mathrm{x})$.

1. Start with an initial value $\mathrm{x} \in D$ and compute $f(\mathrm{x})$;
2. Randomly choose a neighbour y of x and evaluate $f(\mathrm{y})$;
3. If $f(\mathrm{y}) < f(\mathrm{x})$, then set $\mathrm{x} := \mathrm{y}$,
4. else, either keep x as is or set $\mathrm{x} := \mathrm{y}$;
5. Repeat until an end criterion is attained.

Crucial step: Step 4, to avoid being stuck in a local minimum and favouring, at least at the beginning of the algorithm, exploration rather than exploitation.

If $f(\mathrm{y}) \geq f(\mathrm{x})$, we switch $\mathrm{y} \mapsto \mathrm{x}$ with the probability

$$\mathbb{P}(\text{switch}) = \exp\left\{-\frac{f(\mathrm{y}) - f(\mathrm{x})}{\tau}\right\},$$

where τ plays the role of the thermal annealing temperature: when the system is hot, particles move (exploration), and cools down when refinement (exploitation) is required.

An optimisation problem

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

- Hamiltonian formulation: $\mathcal{H} := \sum_{z \in \{0,1\}^n} f(z) \left|z\right\rangle \left\langle z\right|$.
- If $(\left|z_i\right\rangle)$ are eigenvectors of $\mathcal{H}$, then

$$\begin{aligned}
\mathcal{H}_F \left|z_i\right\rangle &= \left(\sum_{z \in \{0,1\}^n} f(z) \left|z\right\rangle \left\langle z\right| \right) \left|z_i\right\rangle \\
&= \left(\sum_{z \in \{0,1\}^n \setminus \{z_i\}} f(z) \left|z\right\rangle \left\langle z\right| \right) \left|z_i\right\rangle \quad + \left(f(z_i) \left|z_i\right\rangle \left\langle z_i\right| \right) \left|z_i\right\rangle \\
&= 0 \qquad\qquad\qquad\qquad\qquad\qquad + f(z_i) \left|z_i\right\rangle \left\langle z_i | z_i\right\rangle \\
&= f(z_i) \left|z_i\right\rangle ,
\end{aligned}$$

  so that $(f(z_i))$ are eigenvalues of $\mathcal{H}$.
- Solving (1) amounts to finding the smallest eigenvalues (minimum energy) of $\mathcal{H}$.
- Problem: it is often difficult to find them.

Constant Hamiltonian simulation

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

$$\mathrm{i}\hbar \frac{\mathrm{d}\,|\psi(t)\rangle}{\mathrm{d}t} = \mathcal{H}\,|\psi(t)\rangle\,, \quad t \in [0,\tau] \qquad \text{(Schrödinger equation)}.$$

is solved as

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

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

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

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 $t(1) = \tau$:

$$\mathrm{i}\frac{\mathrm{d}\,|\psi(s)\rangle}{\mathrm{d}s} = t'(s)\mathcal{H}(s)\,|\psi(s)\rangle\,, \qquad \text{on } [0,1]. \tag{2}$$

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

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

Consider (2) with $t(s) = s\tau$, hence

$$\mathrm{i}\frac{\mathrm{d}\,|\psi(s)\rangle}{\mathrm{d}s} = \tau\mathcal{H}(s)\,|\psi(s)\rangle\,, \qquad \text{on } [0,1].$$

Q Adiabatic Theorem

Let $|\phi(s)\rangle$ be the ground state of $\mathcal{H}(s)$ and the adiabatic schedule $r(s) = 1 - s$:

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

Theorem. Assume that $\mathcal{H}_0$ and $\mathcal{H}_F$ do not commute and that there is no spectral gap. If there exists $\delta > 0$ such that

$$\tau \geq \frac{2}{\delta}\left\{C_0 \frac{\|\mathcal{H}_F - \mathcal{H}_0\|}{\overline{\Delta}^2} + C_1 \frac{\|\mathcal{H}_F - \mathcal{H}_0\|^2}{\overline{\Delta}^3}\right\},$$

with $\overline{\Delta} := \min_{s\in[0,1]} \Delta_s$, 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

$$\begin{aligned} \mathcal{H}_F |0\rangle &= |0\rangle\langle 0|\,|0\rangle = |0\rangle = 1 \cdot |0\rangle, \\ \mathcal{H}_F |1\rangle &= |0\rangle\langle 0|\,|1\rangle = 0 = 0 \cdot |1\rangle, \qquad \text{(ground state)}. \end{aligned}$$

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so that

$$\begin{aligned} \mathcal{H}_F|0\rangle &= |0\rangle\langle 0|0\rangle = |0\rangle = 1\cdot|0\rangle, \\ \mathcal{H}_F|1\rangle &= |0\rangle\langle 0|1\rangle = 0 = 0\cdot|1\rangle, \qquad \text{(ground state)}. \end{aligned}$$

Define now

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

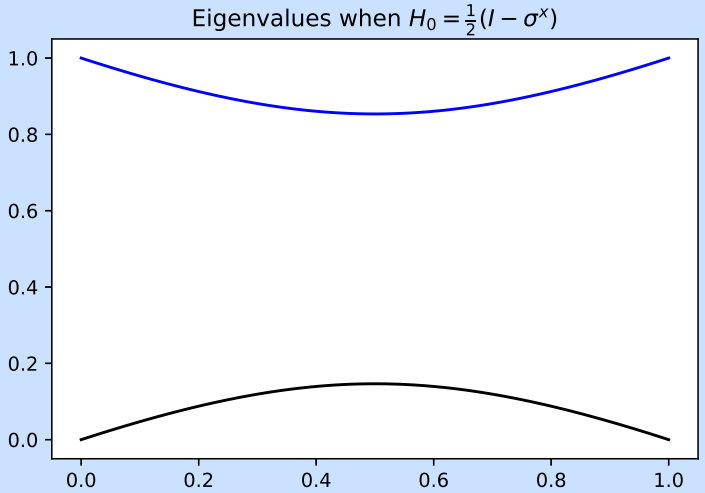
One can check that

$$\begin{aligned} \mathcal{H}_0|+\rangle &= |+\rangle = 1\cdot|+\rangle, \\ \mathcal{H}_0|-\rangle &= 0 = 0\cdot|-\rangle, \qquad \text{(ground state)}. \end{aligned}$$

Interpolating Hamiltonian:

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

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



The Q adiabatic theorem applies!!

The commuting issue for the 1-bit Disagree problem

Consider instead

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

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One can check that

$$\mathcal{H}_0 |0\rangle = |1\rangle\langle 1|0\rangle = 0, \qquad \text{(ground state)}$$
$$\mathcal{H}_0 |1\rangle = |1\rangle\langle 1|1\rangle = |1\rangle .$$

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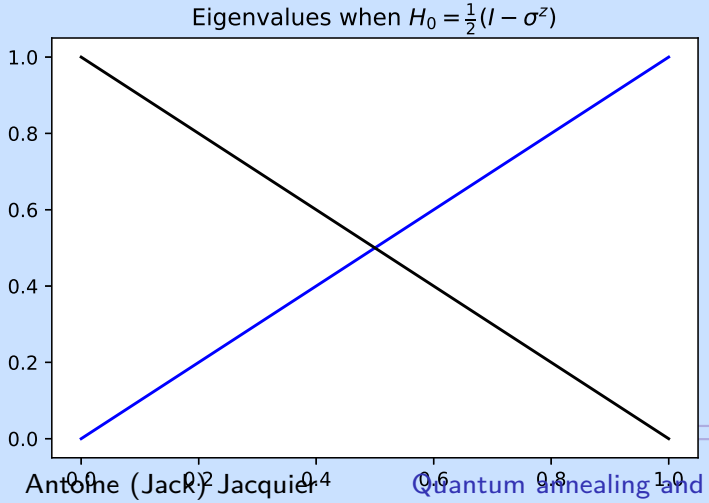
Interpolating Hamiltonian:

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

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

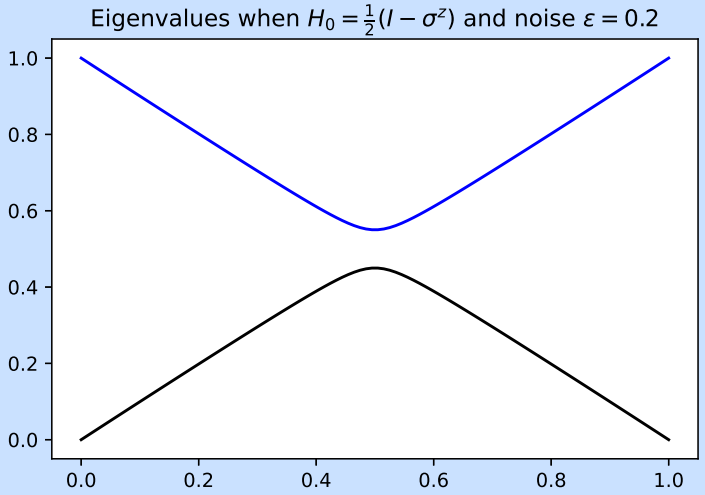


Adding noise.....

Consider a noisy version of the interpolating Hamiltonian:

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

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



And the spectral gap is restored!

The 2-bit Disagree problem

The 2-bit Disagree problem reads

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

$$\mathcal{H}_F := \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 0 \\ 0 & 0 & 0 & 1 \end{pmatrix} = \frac{1}{2}\left\{\mathtt{I}\otimes\mathtt{I} + (\mathtt{Z}\otimes\mathtt{I})(\mathtt{I}\otimes\mathtt{Z})\right\} = \frac{1+\sigma_1^z\sigma_2^z}{2},$$

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

Eigenvalues:

$$e_1^F = \begin{pmatrix} 0 \\ 1 \\ 0 \\ 1 \end{pmatrix}, \qquad e_2^F = \begin{pmatrix} 0 \\ 0 \\ 1 \\ 0 \end{pmatrix}, \qquad e_3^F = \begin{pmatrix} 1 \\ 0 \\ 0 \\ 0 \end{pmatrix}, \qquad e_4^F = \begin{pmatrix} 0 \\ 0 \\ 0 \\ 1 \end{pmatrix},$$

with eigenvalues $0, 0, 1, 1$, so that the ground states are $\{e_1^F, e_2^F\}$.

- Initial Hamiltonian:

$$\mathcal{H}_0 = \frac{1}{2}\sum_{i=1}^{2}(1-\sigma_i^x) = \frac{1}{2}\left\{(\mathtt{I}\otimes\mathtt{I}-\mathtt{X}\otimes\mathtt{I})+(\mathtt{I}\otimes\mathtt{I}-\mathtt{I}\otimes\mathtt{X})\right\}$$
$$= \frac{1}{2}\begin{pmatrix} 2 & -1 & -1 & 0 \\ -1 & 2 & 0 & -1 \\ -1 & 0 & 2 & -1 \\ 0 & -1 & -1 & 2 \end{pmatrix};$$

- Eigenvalues $\{0,1,1,2\}$ and ground state $e_1^0 = (1,1,1,1)^\top = 2\,|{+}{+}\rangle$;
- 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: $\mathcal{H}_t \longrightarrow \mathcal{H}_t^\varepsilon$ for all $t \in (0,1)$ (or noise-induced algorithm);
- Question: understand $\mathcal{H}^\varepsilon$ as $\varepsilon \downarrow 0$.

Monte Carlo simulations

Classical Monte Carlo

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

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

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

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

This implies that

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

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 σ^2 by its unbiased estimator $s^2 := \frac{1}{N-1} \sum_{i=1}^{N} (X_i - \widehat{\mu}_N)^2$.

Amplitude estimation

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

- Inputs:
  - a quantum state $|\psi\rangle$ and a projector $\mathtt{P}$;
  - Unitary $\mathtt{U} := 2\,|\psi\rangle\langle\psi| - \mathtt{I}$ and $\mathtt{V} := \mathtt{I} - 2\mathtt{P}$;
  - $\mathtt{N} \in \mathbb{N}$
- Output: Estimate $\widehat{\mu}$ of $\mu = \langle\psi|\mathtt{P}|\psi\rangle$ such that

$$|\widehat{\mu} - \mu| \leq 2\pi \frac{\sqrt{\mu(1-\mu)}}{\mathtt{N}} + \frac{\pi^2}{\mathtt{N}^2},$$

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

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

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

$$|\widehat{\mu} - \mu| \leq \mu\sqrt{1-\mu}\varepsilon + \frac{\mu}{4}\varepsilon^2 \leq \varepsilon\mu,$$

Powering Lemma

[Jerrum, Valiant, Vazirani, 1986]

Let $\mathcal{A}$ be a (quantum or classical) algorithm estimating μ and whose output satisfies

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

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 $\widehat{\mu}$ with

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

with probability at least $1 - \delta$.

Quantum Monte Carlo [Montanaro, 2015]

Algorithm

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

$$\left|\psi\right\rangle := (\mathtt{I}\otimes\mathtt{W})(\mathcal{A}\otimes\mathtt{I})\left|0\right\rangle^{\otimes(n+1)} \qquad \text{and} \qquad \mathtt{P} := \mathtt{I}\otimes\left|1\right\rangle\left\langle 1\right| . \tag{3}$$

  - Repeat (3) $\mathcal{O}(\log(1/\delta))$ times and output the median.

Theorem (let $\mu := \mathbb{E}[\nu(\mathcal{A})]$)

The algorithm outputs $\widehat{\mu}$ such that, with probability at least $1-\delta$,

$$|\widehat{\mu} - \mu| \leq C\left(\frac{\sqrt{\mu}}{\mathtt{N}} + \frac{1}{\mathtt{N}^2}\right),$$

To get $|\widetilde{\mu} - \mu| \leq \varepsilon$, one then needs $\mathtt{N} = \mathcal{O}(1/\varepsilon)$

Cost of the QMC algorithm

- The circuit $\mathtt{U}$ is used $\mathcal{O}(\mathtt{N}\log(1/\delta))$ times:
  - $\mathtt{N}$ 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;

Proof of the theorem

We have

$$\mathcal{A}\left|0\right\rangle^{\otimes n} = \sum_x \alpha_x \left|\psi_x\right\rangle_{n-k} \left|x\right\rangle_k .$$

Therefore

$$\begin{aligned}
\left|\psi\right\rangle &= (\mathtt{I}\otimes\mathtt{W})(\mathcal{A}\otimes\mathtt{I})\left|0\right\rangle^{\otimes n}\left|0\right\rangle = (\mathtt{I}\otimes\mathtt{W})\sum_x \alpha_x \left|\psi_x\right\rangle_{n-k}\left|x\right\rangle_k\left|0\right\rangle \\
&= \sum_x \alpha_x \left|\psi_x\right\rangle_{n-k} \mathtt{W}\left|x\right\rangle_k \left|0\right\rangle \\
&= \sum_x \alpha_x \left|\psi_x\right\rangle_{n-k}\left|x\right\rangle_k \left(\sqrt{1-\nu(x)}\left|0\right\rangle + \sqrt{\nu(x)}\left|1\right\rangle\right) \\
&= \underbrace{\sum_x \alpha_x \left|\psi_x\right\rangle_{n-k}\left|x\right\rangle_k \sqrt{1-\nu(x)}\left|0\right\rangle}_{\left|\Psi_{Bad}\right\rangle} + \underbrace{\sum_x \alpha_x \left|\psi_x\right\rangle_{n-k}\left|x\right\rangle_k \sqrt{\nu(x)}\left|1\right\rangle}_{\left|\Psi_{Good}\right\rangle} .
\end{aligned}$$

Clearly $\langle\Psi_{Bad}|\Psi_{Good}\rangle = 0$. Now, project $|\psi\rangle$ onto the Good subspace, i.e. using the projective measurement $\mathtt{P}_1 := \mathtt{I}^{\otimes n} \otimes |1\rangle\langle 1|$, so that

$$\begin{aligned}
\langle\psi|\mathtt{P}_1|\psi\rangle &= \left(\langle\Psi_G| + \langle\Psi_B|\right)\mathtt{P}_1\left(|\Psi_G\rangle + |\Psi_B\rangle\right) \\
&= \langle\Psi_G|\mathtt{P}_1|\Psi_G\rangle + \langle\Psi_G|\mathtt{P}_1|\Psi_B\rangle + \langle\Psi_B|\mathtt{P}_1|\Psi_G\rangle + \langle\Psi_B|\mathtt{P}_1|\Psi_B\rangle .
\end{aligned}$$

$$\begin{aligned}
\langle \Psi_G | \mathrm{P}_1 | \Psi_G \rangle &= \left(\sum_x \alpha_x \left| \psi_x \right\rangle_{n-k} \left| x \right\rangle \sqrt{\nu(x)} \left| 1 \right\rangle \right)^\dagger \mathrm{P} \left(\sum_x \alpha_x \left| \psi_x \right\rangle_{n-k} \left| x \right\rangle \sqrt{\nu(x)} \left| 1 \right\rangle \right) \\
&= \left(\sum_x \alpha_x^* \sqrt{\nu(x)}^* \left\langle 1 \right| \left\langle x \right| \left\langle \psi_x \right|_{n-k} \right) \mathrm{I}^{\otimes n} \otimes \left| 1 \right\rangle \left\langle 1 \right| \left(\sum_x \alpha_x \left| \psi_x \right\rangle_{n-k} \left| x \right\rangle \sqrt{\nu(x)} \left| 1 \right\rangle \right) \\
&= \left(\sum_x \alpha_x^* \sqrt{\nu(x)}^* \left\langle 1 \right| \left\langle x \right| \left\langle \psi_x \right|_{n-k} \right) \sum_x \alpha_x \left| \psi_x \right\rangle_{n-k} \left| x \right\rangle \sqrt{\nu(x)} \left| 1 \right\rangle \\
&= \sum_x |\alpha_x|^2 \left| \sqrt{\nu(x)} \right|^2 = \sum_x |\alpha_x|^2 |\nu(x)| = \mathbb{E}[\nu(\mathcal{A})].
\end{aligned}$$

Since $\langle \Psi_G | \mathrm{P}_1 | \Psi_B \rangle = \langle \Psi_B | \mathrm{P}_1 | \Psi_G \rangle = \langle \Psi_B | \mathrm{P}_1 | \Psi_B \rangle = 0$, then

$$\langle \psi | \mathrm{P}_1 | \psi \rangle = \sum_x |\alpha_x|^2 \nu(x) = \mathbb{E}[\nu(\mathcal{A})].$$

We then apply Amplitude Estimation and the Powering Lemma.

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

$$\mathcal{A}\,|0\rangle^{\otimes n} = \sum_{j=0}^{2^n-1} \sqrt{p_j}\,|j\rangle\,, \qquad \text{with } p_j := \frac{\mathbb{P}(w_j)}{\sum_k \mathbb{P}(w_k)},$$

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

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

$$\mathtt{B} : |j\rangle\,|0\rangle \mapsto |j\rangle\,|\widehat{\nu}_j\rangle\,, \qquad \widehat{\nu}_j : \text{binary approximation of } \nu(w_j).$$

- $\mathtt{W}\,|j\rangle\,|\widehat{\nu}_j\rangle \mapsto |j\rangle\,|\widehat{\nu}_j\rangle\left(\sqrt{1-\widehat{\nu}_j}\,|0\rangle + \sqrt{\widehat{\nu}_j}\,|1\rangle\right)$ (as in QMC)
- Inverting $\mathtt{B}$ yields $|j\rangle\,|0\rangle^{\otimes n}\left(\sqrt{1-\widehat{\nu}_j}\,|0\rangle + \sqrt{\widehat{\nu}_j}\,|1\rangle\right)$.
- Ignoring $|0\rangle^{\otimes n}$, we can now use QMC to obtain an estimate of $\mathbb{E}[\nu(W_T)]$.

Quantum simulation (different...)

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

$$\mathrm{i}\partial_t \left|\psi(t)\right\rangle = \mathcal{H}\left|\psi(t)\right\rangle, \qquad \left|\psi(0)\right\rangle \in \dots$$

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

Assumptions

- $\mathcal{H} = \sum_{l=1}^{L} \mathcal{H}_l$, where each $\mathcal{H}_l$ acts on a 'small' subsystem (such that $\mathrm{e}^{-\mathrm{i}\mathcal{H}_l t}$ is easy to compute); note that $\mathcal{H}_l$ and $\mathcal{H}_k$ do not commute, but $\mathrm{e}^{-\mathrm{i}\mathcal{H}t}$ 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 $\mathtt{M}$ and $\mu := \mathbb{E}[\mathtt{M}] = \mathrm{Tr}(\mathtt{M}\rho)$, with $\rho = \left|\psi\right\rangle\left\langle\psi\right|$;
- $\widehat{\mu} := \frac{1}{\mathtt{N}} \sum_{j=1}^{\mathtt{N}} X_j$;

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

$$\mathbb{E}\left[(\widehat{\mu} - \mu)^2\right] \leq \frac{C_1}{\mathtt{N}} + \frac{C_2}{m^4}.$$

Option Pricing in the Black-Scholes model

- Black-Scholes SDE:

$$\frac{\mathrm{d}S_t}{S_t} = r\,\mathrm{d}t + \sigma\,\mathrm{d}W_t, \qquad \text{for } t \geq 0.$$

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

- Feynman-Kac:

$$\left(\partial_t + \frac{\sigma^2 s^2}{2}\partial_{ss} + rS\partial_s - r\right) V(t, s) = 0, \qquad \text{for } s > 0,\ t \in [0, T),$$

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 $\xi = -\mathrm{i}\tau$ turns the heat PDE into $-\mathrm{i}\partial_\xi u(\xi, x) = \frac{\partial_{xx} u(\xi,x)}{2}$, or

$$-\mathrm{i}\partial_\xi |\psi\rangle = \widehat{\mathcal{H}} |\psi\rangle \qquad \text{(Schrödinger equation)},$$

  where $|\psi\rangle$ plays the role of the $u(\cdot,\cdot)$, and $\widehat{\mathcal{H}} = \frac{1}{2}\partial_{xx}$.

- Explicit solution:

$$|\psi(\xi)\rangle = \exp\left\{\mathrm{i}\widehat{\mathcal{H}}\xi\right\} |\psi(0)\rangle\,,$$

  where $\exp\left\{\mathrm{i}\widehat{\mathcal{H}}\xi\right\}$ is the time evolution operator and $|\psi(0)\rangle$ a normalised initial state with $\langle\psi(0)|\psi(0)\rangle = 1$.

A hybrid quantum algorithm

- Problem: normalised imaginary time evolution

$$|\psi(\tau)\rangle = \gamma(\tau)\, \mathrm{e}^{-\widehat{\mathcal{H}}\tau}\, |\psi(0)\rangle\,.$$

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

- Assuming an initial state $|\psi_0\rangle$, so that the ansatz is $|\phi(\tau)\rangle = \Phi(\boldsymbol{\theta}_\tau)\,|\psi_0\rangle$ at time τ, where $\Phi(\boldsymbol{\theta}_\tau)$ is sequence of unitary gates $\Phi(\boldsymbol{\theta}_\tau) = \mathcal{S}\left(\mathrm{U}_N(\theta_\tau^N), \ldots, \mathrm{U}_k(\theta_\tau^k), \ldots, \mathrm{U}_1(\theta_\tau^1)\right)$.

$$\boldsymbol{\theta}_\tau^* := \underset{\boldsymbol{\theta}\in\mathbb{R}^N}{\arg\min} \left\| |\psi(\tau)\rangle - \Phi(\boldsymbol{\theta}_\tau)\,|\psi_0\rangle \right\|.$$

At time τ

The optimisation problem reduces to the system of ODEs

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

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

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

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:

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

Simulation from τ to Δ_τ

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

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

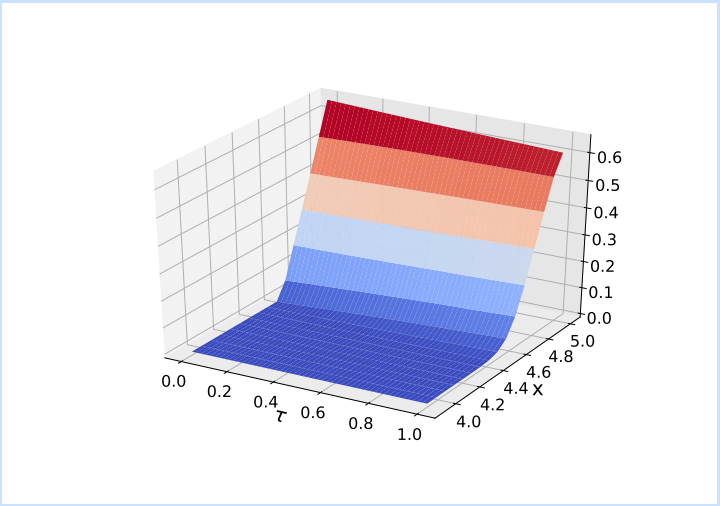
  for some small time step Δ_τ.
- ... and so on until time $\tau = T$.

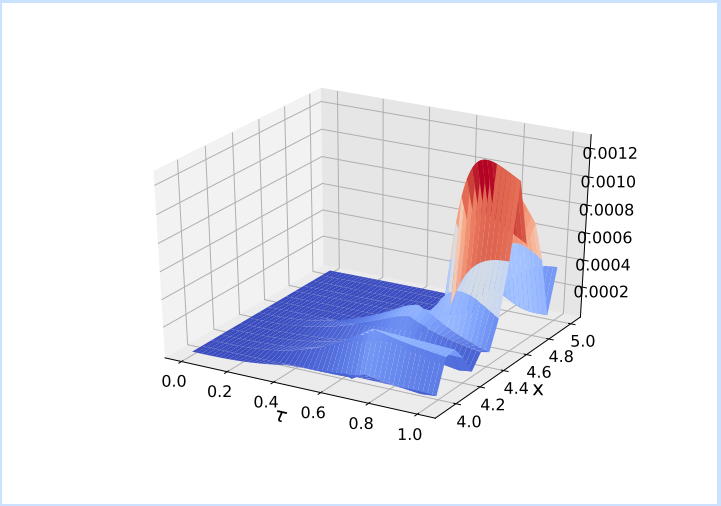
European Call option

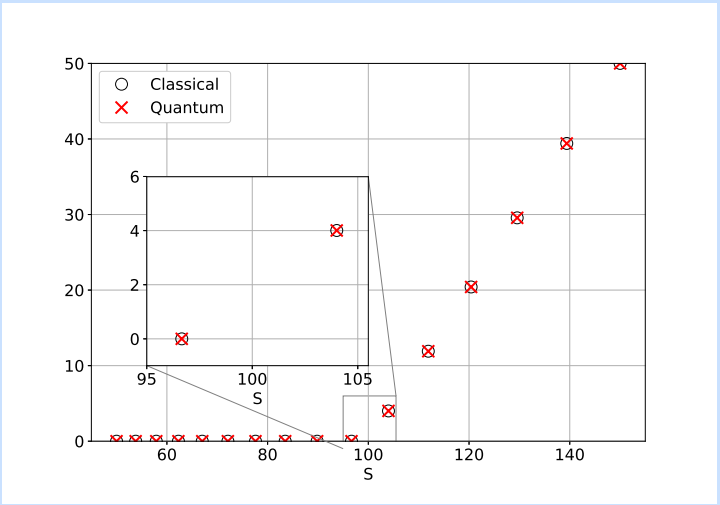
- **Model:** Black-Scholes $\mathrm{d}S_t = \sigma S_t \mathrm{d}W_t$, with $\sigma = 20\%$, $S_0 = K = 100$, $T = 1$.
- **Goal:** Compute $\mathbb{E}[\max(S_T - K, 0)]$.
- Discretise the state space on logarithmic scale on an equidistant grid $[S_{\min}, S_{\max}] = [50, 150]$.
- With four qubits, the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

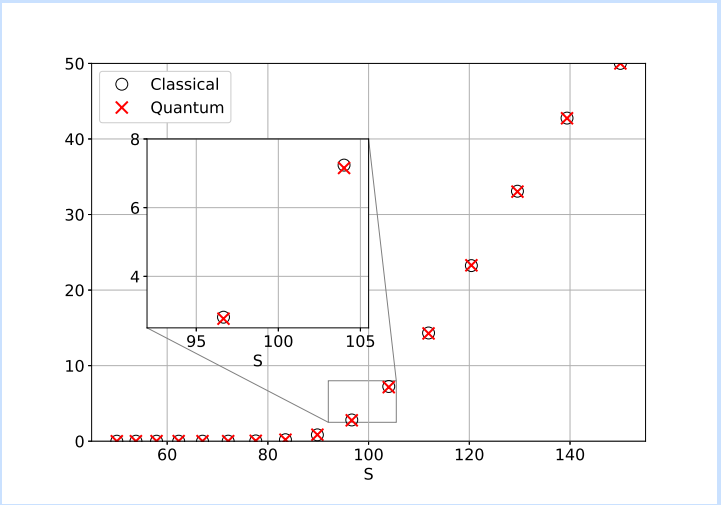
$$\frac{1}{2\Delta_x^2}\begin{bmatrix} -2b\Delta_x^2 & 0 & 0 & 0 & \cdots & 0 & 0 & 0 \\ 1 & -2 & 1 & 0 & \cdots & 0 & 0 & 0 \\ 0 & 1 & -2 & 1 & \cdots & 0 & 0 & 0 \\ \vdots & \vdots & \vdots & \vdots & \ddots & \vdots & \vdots & \vdots \\ 0 & 0 & 0 & 0 & \cdots & 1 & -2 & 1 \\ 0 & 0 & 0 & 0 & \cdots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

  where Δ_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 $\boldsymbol{\theta}_\tau$ is obtained from the Euler scheme.









Top: European prices (left) and errors (right) $\| |\psi(\tau)\rangle - |\phi(\boldsymbol{\theta}_\tau)\rangle \|$. Bottom: Comparison with closed-form formula at maturity (left) and at inception (right).

Wrapping up...

Applications of QC

- Optimisation
- Simulation
- Machine Learning

Future of QC (for Finance)

- Clear realisation from the (Finance) industry that 'it may work'...
- Parallel development of hardware and software.
- Problem-specific algorithms.
- Hybrid Quantum-Classical algorithms.