Hybrid algorithms II: quantum advantages for optimisation, convex and non-convex

Scientific applications of quantum computing

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Almost any problem can be cast as optimisation

- ‘Traditional’ NP-hard problems: travelling sales person, routing, scheduling etc...

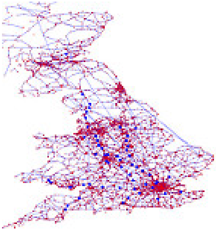


Image: public domain taken from wikimedia commons

- Chemistry: minimise energy to find ground state
  excited states are constrained minimisation
- Factoring/cryptography: construct logical operations (multiplication, stream cypher, etc...) fix outputs and minimize number of logically incorrect
- Error correction/ fault diagnosis: penalize errors and minimize number subject to observations
- Machine learning: optimise correlations to learn pattern

The basic ingredients of optimisation algorithms

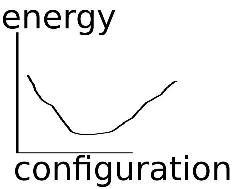
1. Evaluate fitness (energy) of candidate solution(s)
2. Propose new candidate solution(s) based on previous fitness values

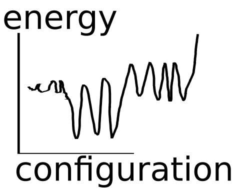
Examples:

- Monte Carlo: [1] Energy difference between new and proposed state calculated. [2] Change 'accepted' based on difference.
- Gradient descent: [1] Energy of nearby solutions calculated. [2] Used to find 'downhill' direction.
- Evolutionary algorithms: [1] Fitness evaluated. [2] Less fit die, more fit get to breed.

Same basic ingredients in quantum optimisation

Convex versus non-convex





Convex optimisation

- Only a single global energy minimum
- Can always be solved by continually 'going downhill'
- Still need to evaluate energy to solve
- Only resource intensive if evaluating energy is difficult

Non-Convex optimisation

- Many local energy minima
- Will get stuck if just trying to go downhill
- Need clever algorithms to get out of local minima
- Can be difficult even if energy evaluation is efficient

Early quantum opportunities

Early quantum computers...

- ...will be expensive → need high value problems which classical computers don't solve efficiently
- ...will be small and imperfect → need hybrid quantum/classical algorithms

Convex optimisation

- Cases where evaluating the energy itself is hard
- Chemistry and materials → energy requires QM to calculate
- Variational algorithms: QC only used to create state and calculate energy

Non-Convex optimisation

- Use QM to explore energy landscape
- Tunnelling and interference could allow faster than classical search
- Are ubiquitous: protein folding, logistics, communication, design...

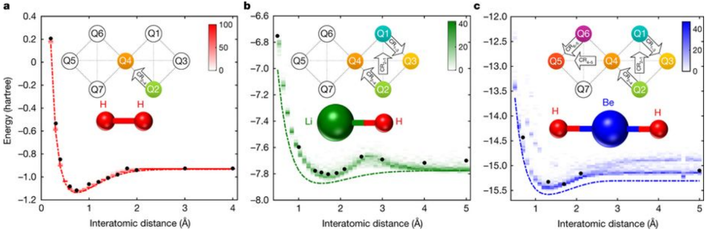
QC=quantum computer; QM=quantum mechanics

Convex: Variational quantum eigensolver (VQE)

Hybrid quantum/classical algorithm

1. QC prepares state characterized by a set of parameters
2. Quantum measurements calculate energies of ‘nearby’ states
3. Calculate update parameters to improve energies
4. Iterate until suitably converged

Applied by IBM as demonstration of early quantum computer ⋆:

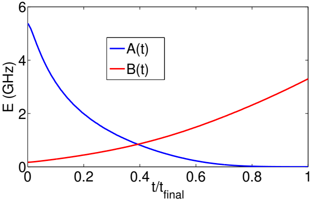


⋆A. Kandala et. al. Nature 549, 242–246 (2017).

Non-convex: Quantum annealing family of meta-heuristics

Large 'family' of meta-heuristics*: common element is superposition of a driver Hamiltonian which mixes between states and a problem Hamiltonian which defines problem through phases

$$\mathrm{H}(t) = A(t)\mathrm{H}_{\mathrm{driver}} + B(t)\mathrm{H}_{\mathrm{problem}}$$



Largest scale (dissipative) implementation is devices by D-Wave systems Inc.

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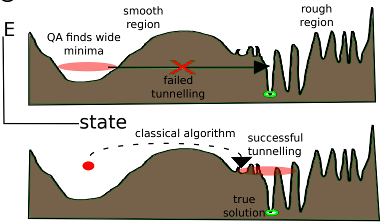
*adiabatic quantum computing, quantum annealing, continuous time quantum walk, and quantum approximate optimisation algorithm Warning! the terminology around adiabatic and quantum annealing is not standardized

Hybrid algorithms using annealing family of meta-heuristics

Build subroutine which searches based on initial solution candidate, methods known for coherent adiabatic algorithms⋆ and dissipative quantum annealing †

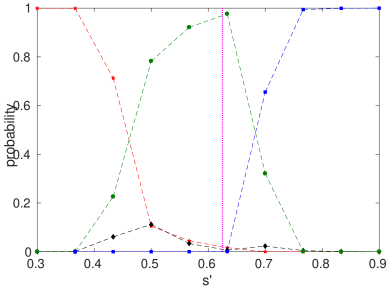


Use quantum subroutine call only for the features it handles well
→ narrow features where tunnelling can search effectively

⋆A. Perdomo-Ortiz, S. E. Venegas-Andraca, & A. Aspuru-Guzik, Quantum Inf. Process 10: 33 (2011).

†N. Chancellor, New Journal of Physics 19, 2, 023024 (2017).

Real world example: reverse annealing



- Uses dissipation on real D-Wave quantum annealer to search locally, smaller s' $\rightarrow$ broader search
- Experimental test shows that device searches locally in solution space

NQIT industrial partnership with D-Wave Systems Inc.

D-Wave The Quantum Computing Company™ NQIT Networked Quantum Information Technologies

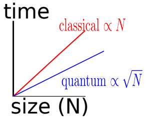
A huge number of possible reverse annealing algorithms

1. Simple version 1: search locally around best classical solution
   - Any improvement is an immediate win
   - But only likely to find solutions 'near' best classical
2. Simple version 2: search locally around randomly chosen state
   - May avoid a broad false minima
3. Monte Carlo like algorithms (see NJP 19, 2, 023024 (2017))
   - Transverse field parameter s' controls tradeoff between exploration and exploitation
     –similar to temperature in Monte Carlo
   - Quantum analogues of many known classical algorithms
4. Genetic algorithms (see arχiv:1609.05875)
   - Compose guess from two or more known solutions
   - Most general version requires more controls than currently available

What does an early quantum advantage look like?

Old way of thinking:

Algorithm with known best classical scaling $\rightarrow$ QC performs better



- Not amenable to hybrid algorithms
- Scaling not known for important real world problems, we haven't even proven that $P \neq NP$!

More realistic:

Meaningful improvement *in practice* by...

- finding more optimal solution than classical finds by itself,
- solving problem faster or using less energy,
- better sampling of a distribution,
- finding solutions which are better in some other way...

Take away messages

Image: wikimedia commons, photo taken by user: Thomas Yuan

- Many problems can be cast as optimisation
  - Convex $\rightarrow$ one global minimum
  - Non-convex $\rightarrow$ many local minima
- Quantum can be useful for both
  - Convex $\rightarrow$ useful if optimality hard to evaluate
  - Non-convex $\rightarrow$ useful for exploring solution space
- Many hybrid quantum/classical tools in both cases
- Early QCs will be small, imperfect, and expensive, need to find appropriate problems and algorithms
- Quantum advantage can come in many forms $\rightarrow$ not simple to quantify in all cases