# Quantum-Enhanced Machine Learning in Practice

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# Landscape of commercial quantum computing

XANADU

rigetti

IONQ

D:WAVE
The Quantum Computing Company™

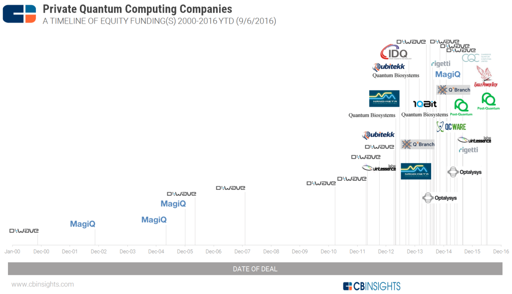
IBM

Microsoft

Google

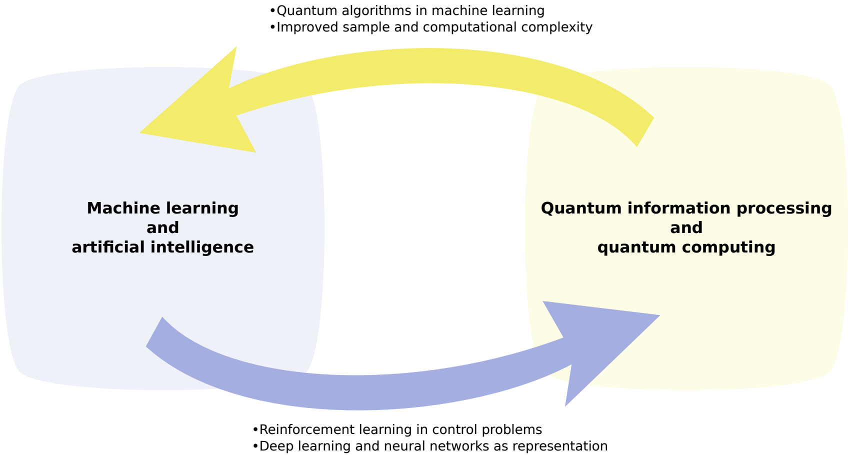
# Investments in quantum computing

Private equity funding:




- €1 billion quantum flagship by the European Union.
- September 2017: China invests $10 billion in research centre for quantum technologies.
- October 2017: Alibaba invests $15 billion in quantum computing.

# The Virtuous Cycle!

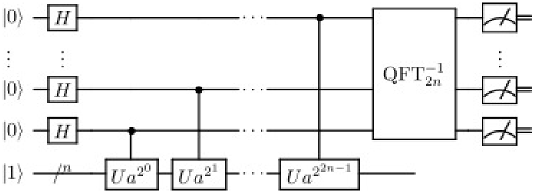


# FAQ

1. When can we start using quantum computers? Right now.
2. When can we expect any tangible advantage? 3-4 years.
3. Can we just call a Python API? $\frac{|\text{yes}\rangle + |\text{no}\rangle}{\sqrt{2}}$.

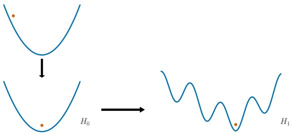
# The Holy Grail: Universal Quantum Computers

- Like in digital computers, a finite set of gates is sufficient for universality.
- This is a surprising result.
- Gate-based model.
- Quantum computation≈transformation of probability distribution.
- Notoriously hard engineering challenge.



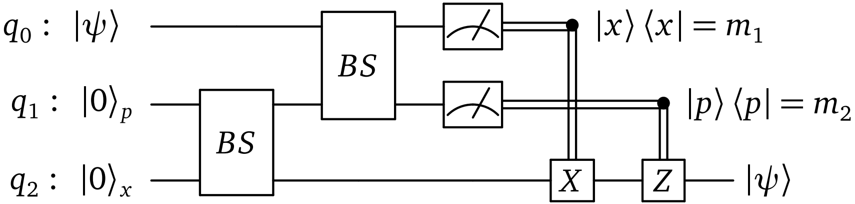
# Quantum Annealing

- An analogue paradigm with no classical equivalent.
- It essentially solves a binary optimization problems.
- Could be equivalent to a gate-based model.
- Most advanced implementation today.
    - Up to 2048 superconducting qubits.
    - It is not an ‘ideal’ quantum annealer.



# Continuous-Variable Systems

- Natural fit for simulating bosonic systems:
  - Electromagnetic fields
  - Harmonic oscillators
  - phonons
  - Bose-Einstein condensates
- Position & momentum operators.
- Room-temperature photonic implementations.



# Why Quantum-Enhanced Machine Learning?

- Intermediate step between now and perfect, scalable universal quantum computers.
  - It also provides a use case for universal quantum computers.
- It also works well for current quantum annealing technologies.
  - Which suffer from many problems: noise, finite temperature, precision of digital-analogue converters. . .
- Tangible benefits are within three to four years.

# In the Wild!

- The first-ever incubator program in the world for QML startups!
- Includes:
  - Technical training and continued support by leading scientists.
  - Business guidance and investor access.
  - Pre-seed investment up to $80k from three Silicon Valley venture capital firms.

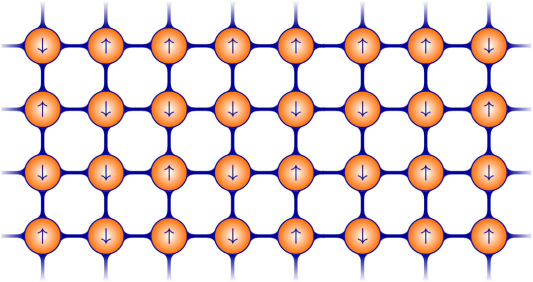
# Brave Enough Hardware Partners

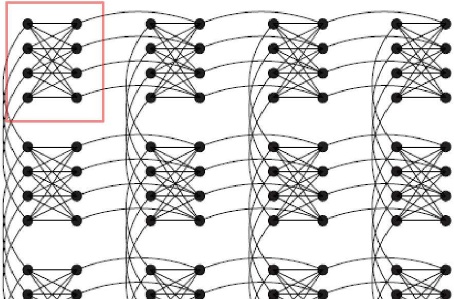
- The CDL is also host of the largest ML startup accelerator in the world.

# Optimization

# More on Adiabatic Quantum Computing

- Generic procedure: map learning problem to an Ising model.
    - $H(\sigma) = -\sum_{<ij>} J_{ij}\sigma_i\sigma_j - \mu \sum_j h_j\sigma_j$
- Current solid-state implementation:
    - Qubits have a connectivity structure.
    - Number of qubits remains limited.
    - Temperature too high, speed too fast, too much noise.
- Do we need the actual ground state?





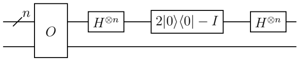
# Gate-based approach to optimization

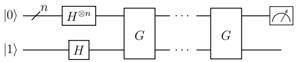
Grover's search:

- Find an element in an unordered set in $O(\sqrt{n})$ steps.
- Given: (unitary) oracle. $O|x\rangle = \begin{cases} -|\omega\rangle & \text{for } x = \omega \\ |x\rangle & \text{for } x \neq \omega \end{cases}$
- Also works for finding minimum or maximum.

Grover's search as a building block:

- Discrete search space.
- Quantum associative memories.



# Learning and Grover's search

- Without decoherence, Grover's search finds an element in an unordered set quadratically faster than the classical limit.
- Variant for finding minimum and maximum.
- It is a plug-and-play method.
- Implementations are not quite clear on actual speedup.
  - Overcooking the search.
  - Real system: decoherence.

# Gate-model search on contemporary quantum computers

Quantum approximate optimization algorithm (QAOA)

- **Designed for imperfect quantum computers.**
    - This is a whole **new trend** in quantum computing.
- Classical-quantum hybrid algorithm.
- Shallow circuit depth.
- One of the most immediate pathways to tangible quantum supremacy.

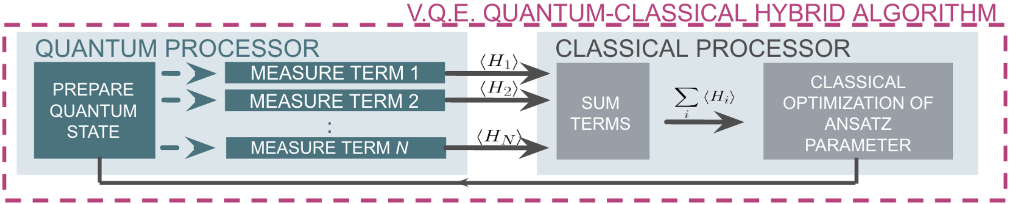
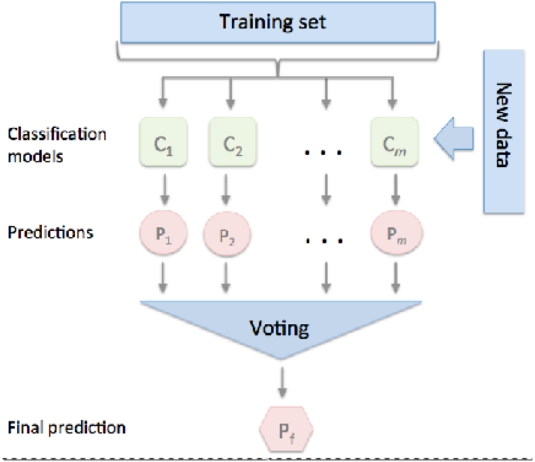
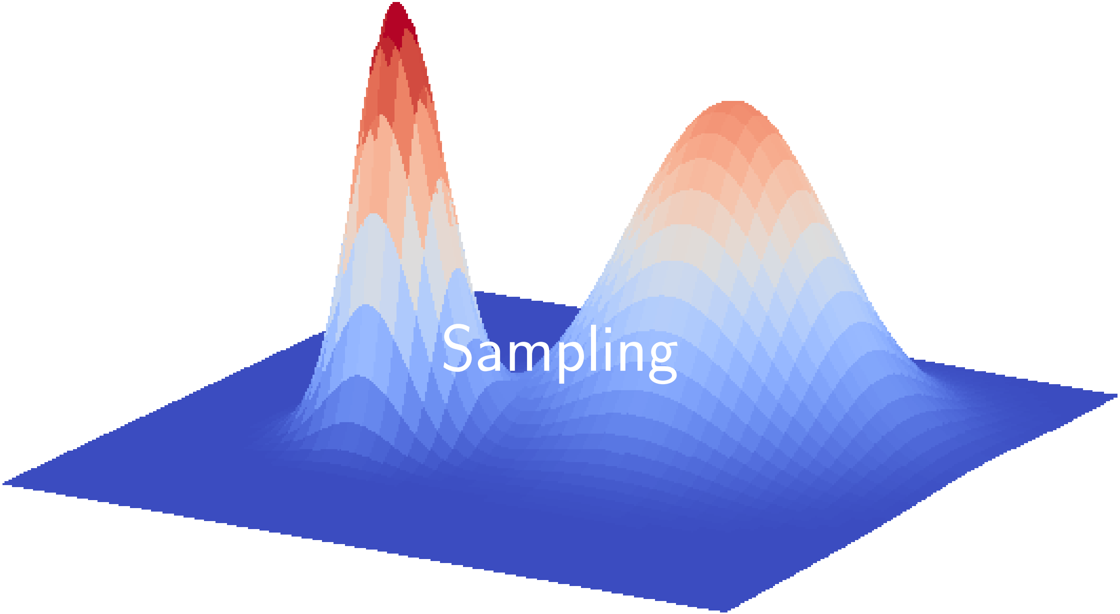



Image credit: Rigetti.

# Discrete optimization in machine learning?

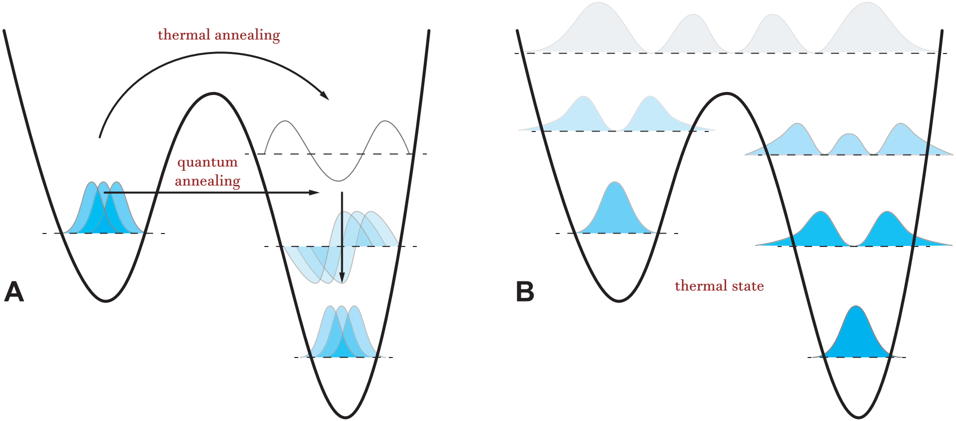
- Deep learning is out.
- Ensemble models: reduce risk by using several learning models.
- Democracy?
- ~~Democracy?~~
- Weighted average: discrete weights.




Sampling

# Quantum annealing and Gibbs sampling

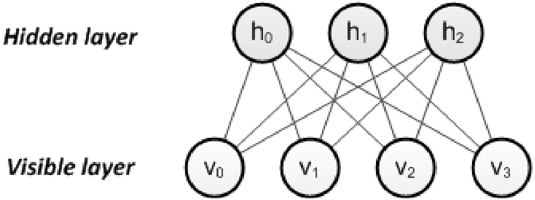
Real-world quantum annealing is noisy. So what can we do?

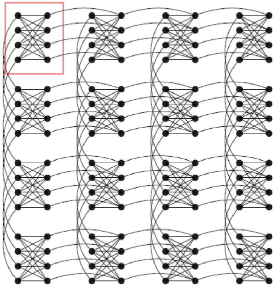



Sampling is the **most useful** quantum-enhanced routine for ML today.

# A love affair with Boltzmann machines

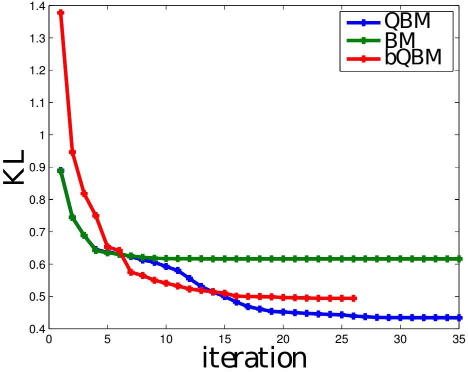
- **Generative models** are hard by backprop.
- Unsupervised feature extraction is not easy either.
- BMs are out fashion because of the limitations of contrastive divergence.
- Great advantage: perfect fit for contemporary quantum annealers.
- Replace contrastive divergence by sampling.



# Quantum Boltzmann machines

- Boltzmann machine corresponds to a classical Ising model.
- Add a noncommuting term (a transverse field) to get a quantum variant.
- Right way of thinking of quantum-enhanced learning protocols.

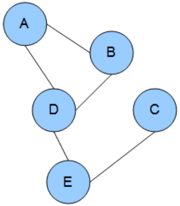


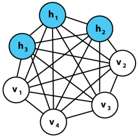
- Uncertainty (probabilities) and logical structure (independence constraints).
- Goal: compact representation of a joint probability distribution.
  - For $\{X_1, \ldots, X_N\}$ binary random variables, there are $2^N$ assignments.
- Complexity is dealt through graph theory.
- Factorization: compactness.
- Inference: reassembling factors.
- Conditional independence $(X \perp Y | W)$:

$$P(X = x, Y = y | W = w) = P(X = x | W = w) P(Y = y | W = w)$$
$$\forall x \in X, y \in Y, w \in W$$

# Markov Networks

- Aka Markov random fields
  - Direction may not be important.
  - E.g., computer vision.
  - See also pattern recognition.
- D: set of random variables. Ideally a clique in the graph.
- Factor: $\pi : Val(D) \mapsto \mathbb{R}^+$
- A distribution factorizes over $G$ if:
  - $P(X_1, \ldots, X_N) = \frac{1}{Z} P'(X_1, \ldots, X_N)$, where
  - $P'(X_1, \ldots, X_N) = \pi_1[C_1] \times \ldots \times \pi_k[C_k]$ and
  - $C_i$ is a clique in $G$.
- If all probabilities are positive: $P(\mathbf{X} = \mathbf{x}) = \frac{1}{Z} \exp(\sum_k w_j g_j(\mathbf{x}))$.
- Connection to Boltzmann machines



# Probabilistic Inference

- How to apply the learned model?
- NP-hard, in fact, it is in #P.
  - Contrast this to the cost of applying a model in other machine learning models.
- Two types of queries:
  - Conditional probability: $P(Y|E=e) = \frac{P(Y,e)}{P(e)}$.
  - Maximum a posteriori: $\mathrm{argmax}_y P(y|e) = \mathrm{argmax}_y \sum_W P(y, W|e)$.
- Inference by Markov chain Monte Carlo Gibbs sampling.

# Markov Logic Networks

- Real world can never match a KB.
- Weight each formula in a KB: high weight indicates high probability.

## Markov Logic Network

Apply a KB $\{F_i\}$ with matching weights $\{w_i\}$ to a finite set of constants $C$ to define a Markov network:

- Add a binary node for each possible grounding for each atom.
- Add a binary feature for each possible grounding of each formula $F_i$.

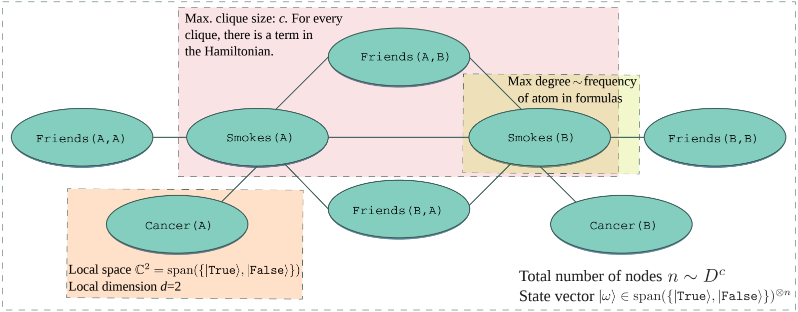
- It is like a template to generate Markov networks.

# Tons of untapped potential

This is an area where we will see a **constant-time speedup in five years with the highest probability**.
Look for learning algorithms and probabilistic methods where sampling helps.

| Formula | Weight |
|---|---|
| ∀x `Smokes(x)`⇒`Cancer(x)` | $w_1$ |
| ∀x,y `Friends(x,y)`⇒(`Smokes(x)` ⇔ `Smokes(y)`) | $w_2$ |

Domain: {`A`,`B`}
Domain size: D = |{A,B}| =2
Inverse temperature: $\beta := \max_j |w_j|$




arXiv:1611.08104

# Quantum Data & Control

# When You Have Coherent Quantum Data

Exponential speedup:

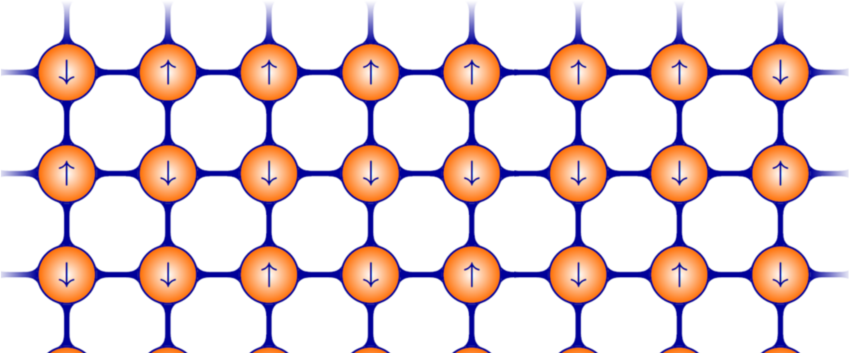
- Quantum principal component analysis and quantum singular value decomposition.
- Quantum support vector machines: sparsity lost.
- Topological data analysis.
- Quantum anomaly detection.

Core idea: do **linear algebra** exponentially faster.

- Quantum matrix inversion is fast: HHL algorithm.

# Where Do You Get Quantum Data From?

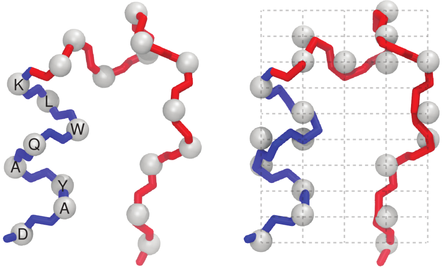
- State preparation from classical data.
  - **Reverse is hard**: state tomography.
  - This is why exponential speedup claims have to be taken with a pinch of salt.
- **Quantum simulations**.
  - For example, drive the design of new materials based on quantum mechanical properties.
- **Internal working of a quantum computer**.



# So What Do QML Startup Companies Do?

# ProteinQure

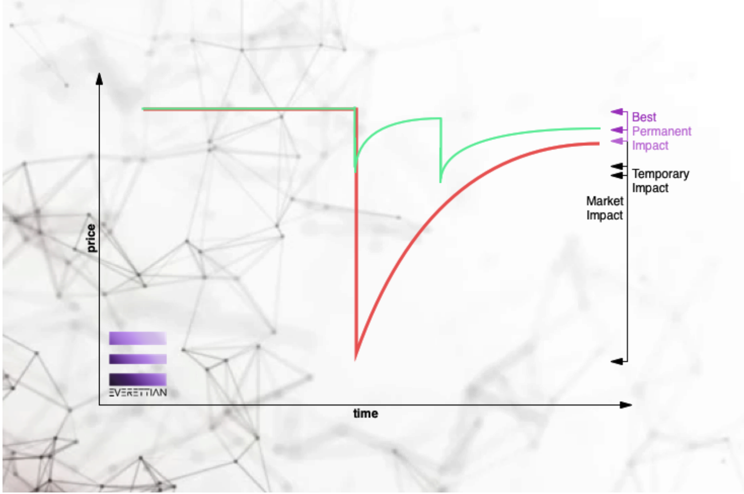
ProteinQure




DAYAQWLKDGGPSSGRPPPS

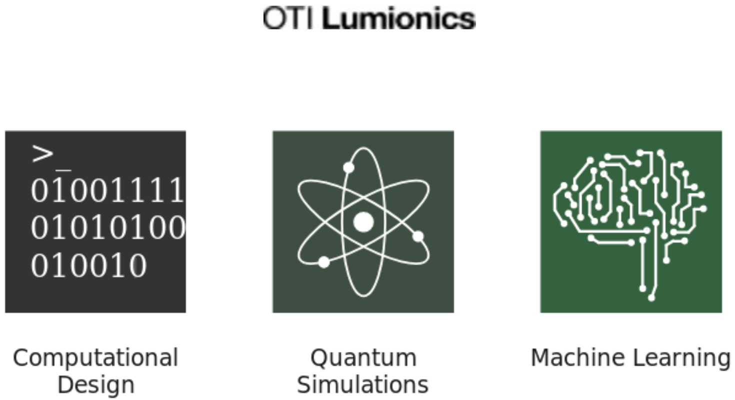
Lattice-based protein folding with quantum annealing and reinforcement learning.

# Everettian




Reduce variance on estimations of financial assets by hybrid quantum algorithms.

# OTI Luminoics




Massive reduction of computational time in material design by quantum simulations.

# How Can I Get Started?

- Keep an eye on the ICFO QML reading group: `https://github.com/peterwittek/qml-rg`
- Keep another eye on the PhysicsML page: `https://physicsml.github.io/`.
- Check out open source software related to quantum computing: `https://github.com/markf94/os_quantum_software`
- Join the QML group on LinkedIn: `https://www.linkedin.com/groups/8592758`

# Take-Home Message

- First application area of imperfect quantum computers is machine learning with **hybrid classical-quantum algorithms**.
- Whatever happens today in QML is **80-90 % classical**.
- Target: constant-times speedup in **three-four years**.
- **Complementary** to current state-of-the-art machine learning.
- Recruitment of second QML cohort in the Creative Destruction Lab:
  - Deadline: May 30.
  - Start: June 25.
  - Both individuals and startups are welcome.
  - https://creativedestructionlab.com/quantum
- QML Workshop at KDD-18:
  - Submissions: May 8.
  - Notifications: June 8.
  - Workshop: August 19.
  - https://www.quantummachinelearning.org/qmlkdd2018.html