Quantum Information Science In High Energy Physics

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Outline

- Motivations for Quantum Technologies
- Sensors
- Communications
- Quantum Computation
- Quantum / Machine Learning
- Summary and outlook

Impossible to do full justice to the topic in the allocated time.

*Thanks to **Heather Gray**, **Cristian Pena**, **Gabriel Perdue**, **Koji Terashi**, **Sofia Vallecorsa**, **Si Xie** for material and input.*

Why go Quantum

Scientific reasons:

- Classical computers are deterministic, quantum systems are probabilistic in nature.
- Quantum systems have rich evolution dynamics.
- Operating sensors at the highest level of precision possible.
- Quantum systems are fragile, cannot be tempered with, without information loss.

Sociological reasons:

- Quantum technologies are expanding fast.
- Outcomes with tremendous impact in industry.
- Funding for quantum technologies R&D.
- Forging the quantum minds.

Range of Applications

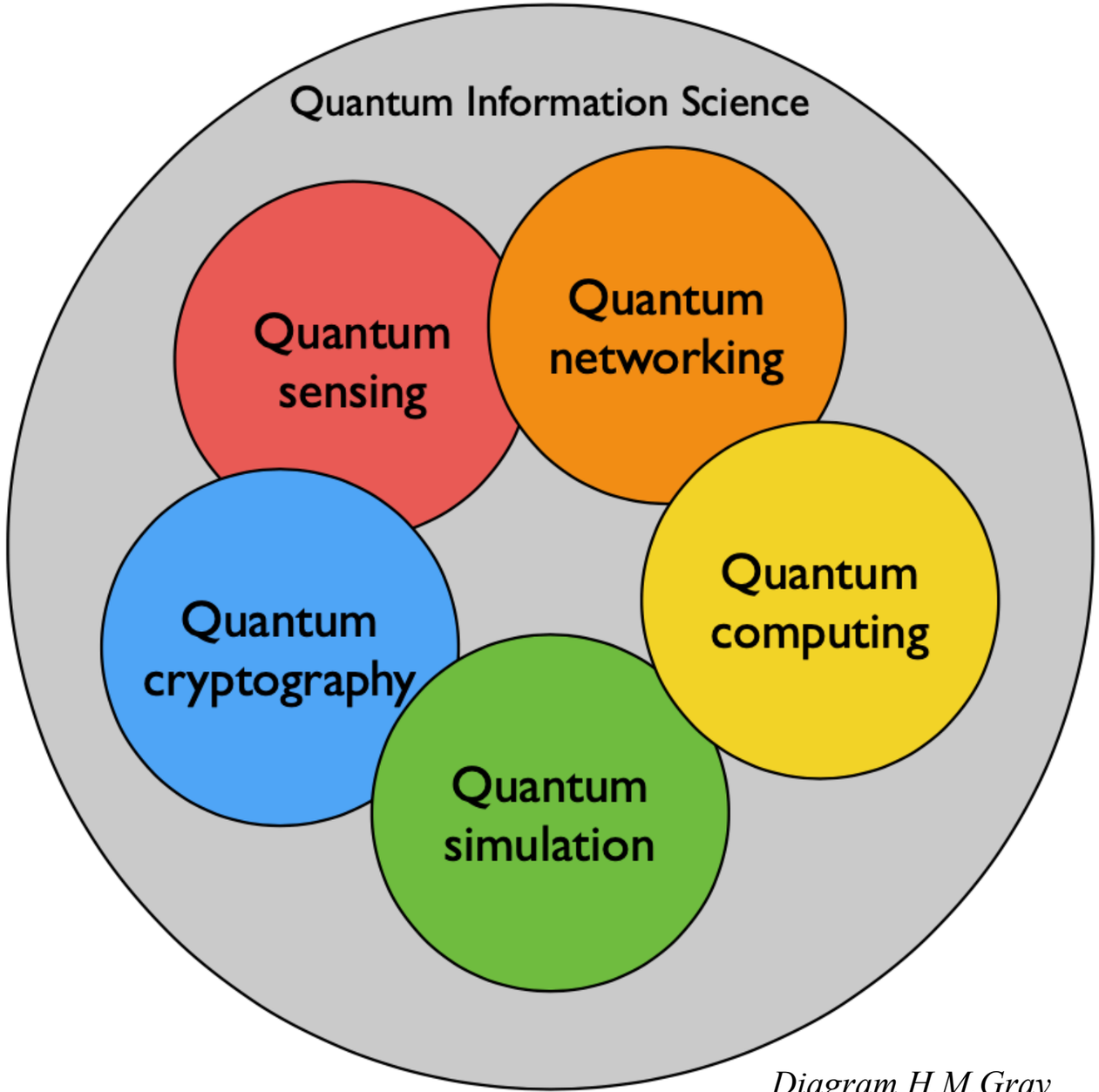
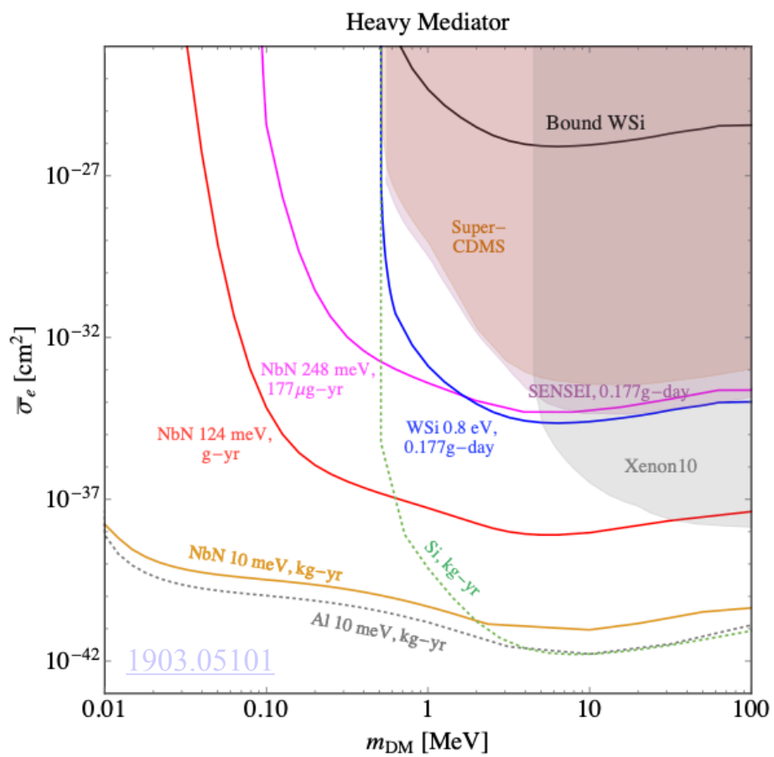
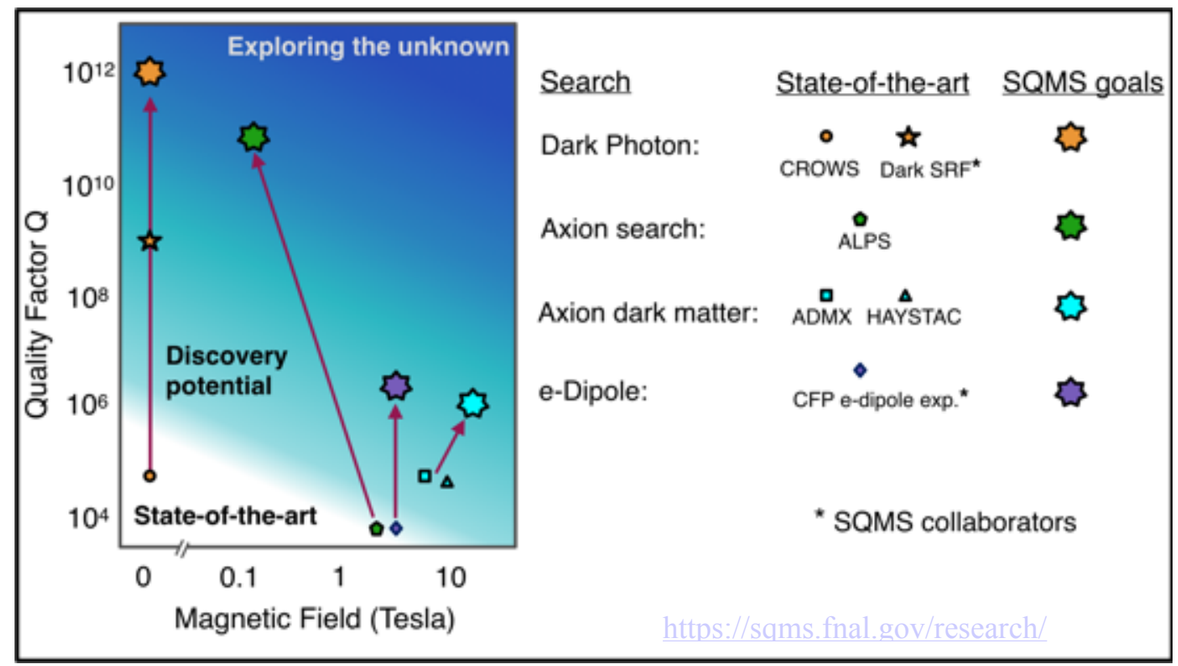


Diagram H.M.Gray

Quantum Sensors

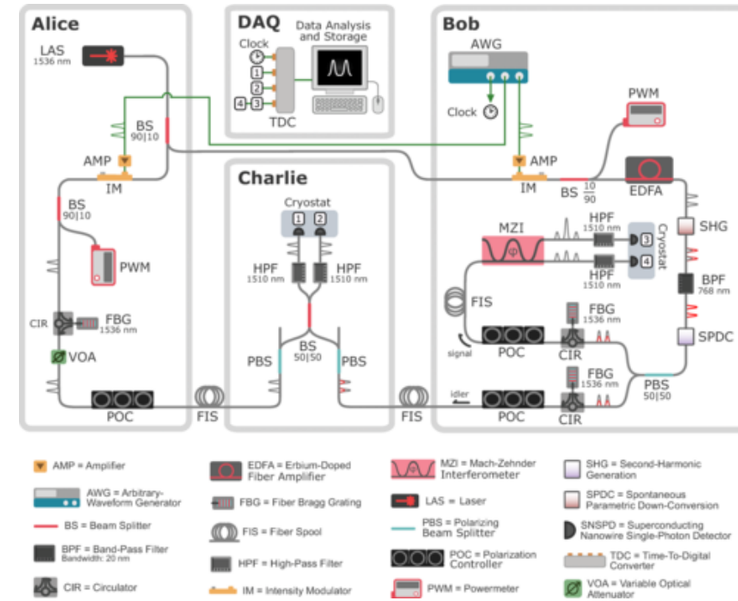
- Quantum systems are highly sensitive systems.
- Superconducting Radio-Frequency (SRF)cavities, superconducting nanowire single photon detectors (SNSPD), superconducting qubits,… operating in quantum regime can provide sensitive complementary to other experiments.
- Synergy with high precision readout R&D in quantum telecommunication.



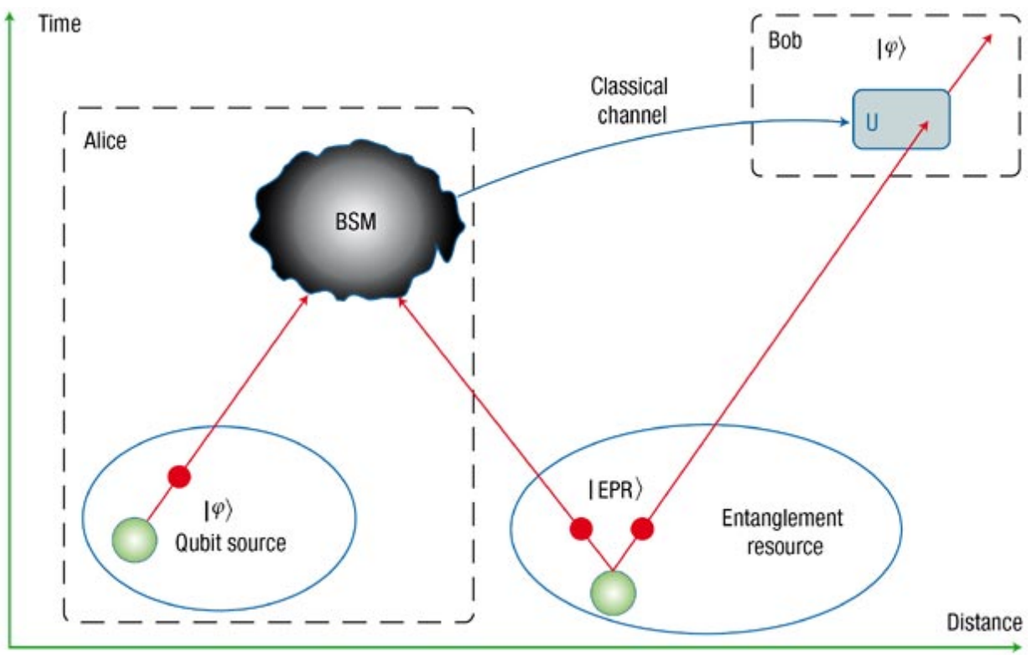


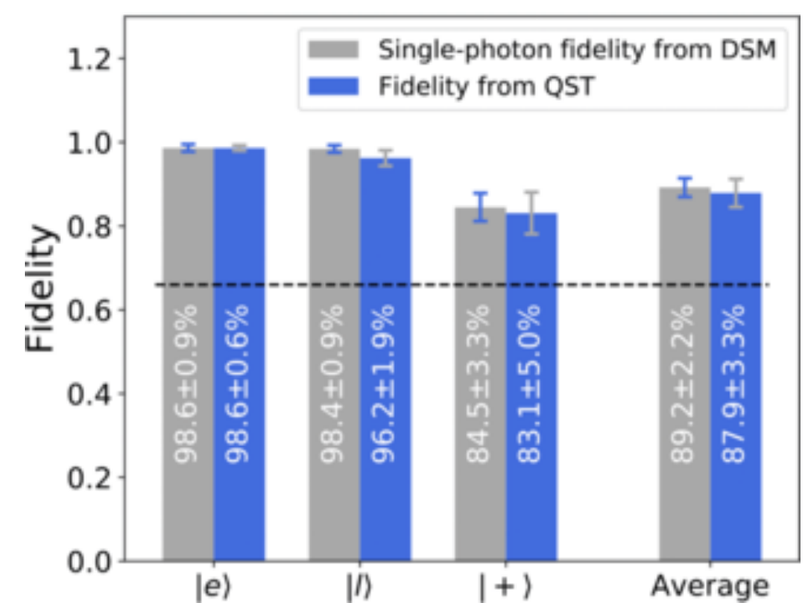
Quantum Communications

- Secure communications, connect quantum devices, …
- Based on quantum teleportation protocole.
- No “faster than the speed of light” communication.
- Destructive eavesdropping mechanism.

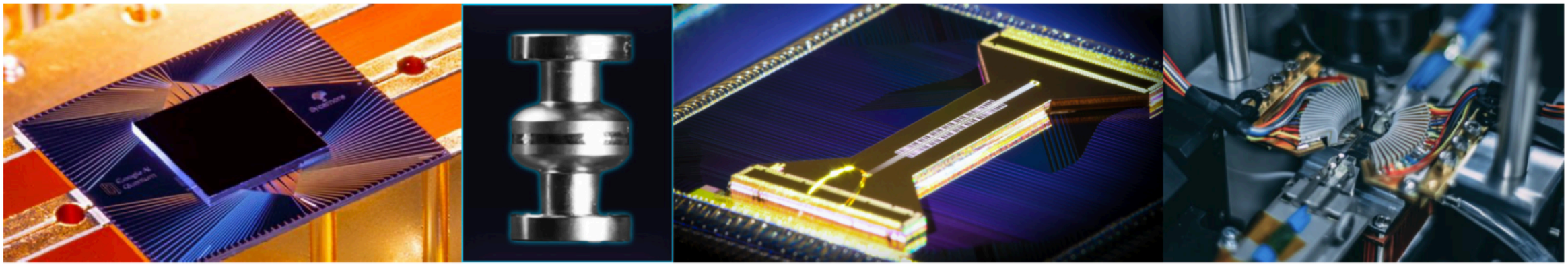


doi:10.1103/PRXQuantum.1.020317



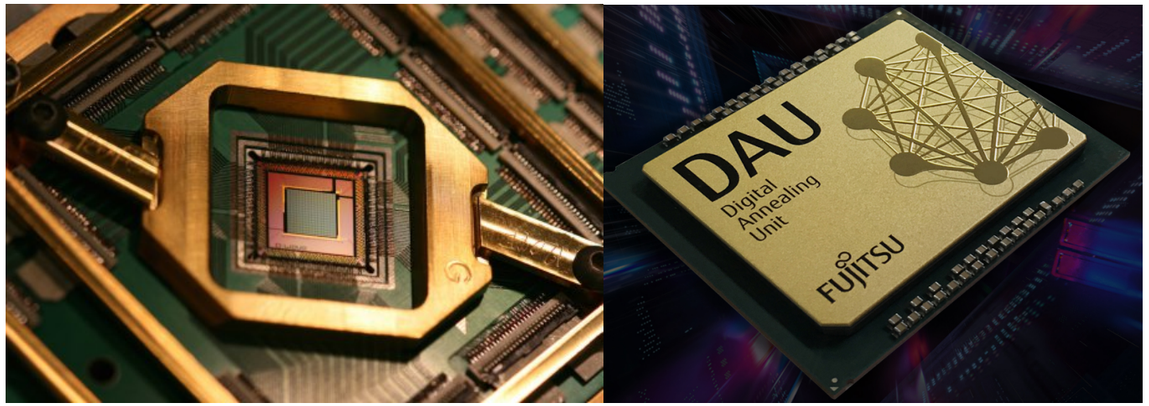


Quantum Computing Devices



https://ai.googleblog.com/2019/10/quantum-supremacy-using-programmable.html, https://sqms.fnal.gov/research/, https://www.honeywell.com/us/en/company/quantum, https://www.xanadu.ai/hardware

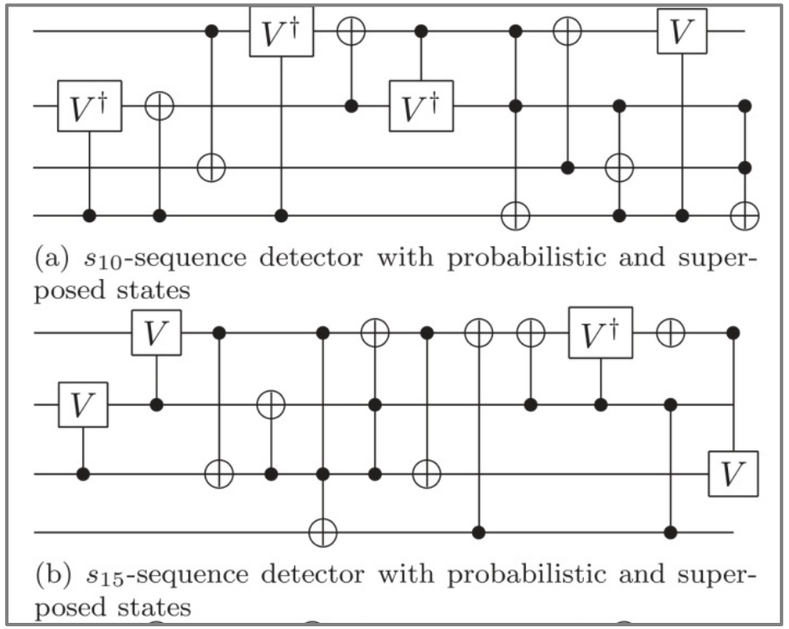
Multiple platform to implement quantum circuits available.
Multiple types of quantum substrates: superconducting qubits, ion-trap, photonics, …
System size still somehow limited, evolving fast.
Quantum Volume is the metric for comparison (4M for IonQ)



https://www.dwavesys.com/quantum-computing, https://techcommunity.ts.fujitsu.com/en/solutions-2/d/uid-70883304-f3b9-3a9f-7dba-0c65cc986bdb.html

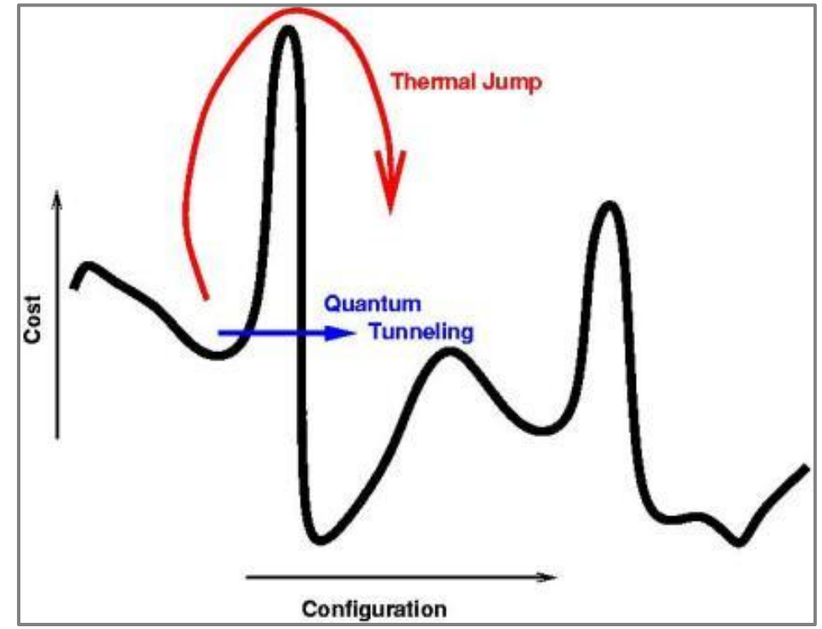
Quantum annealing device by D-Wave, digital annealer by Fujistu.
Thousands+ qubits available.

qubit and qubit



(a) s_{10}-sequence detector with probabilistic and superposed states

(b) s_{15}-sequence detector with probabilistic and superposed states



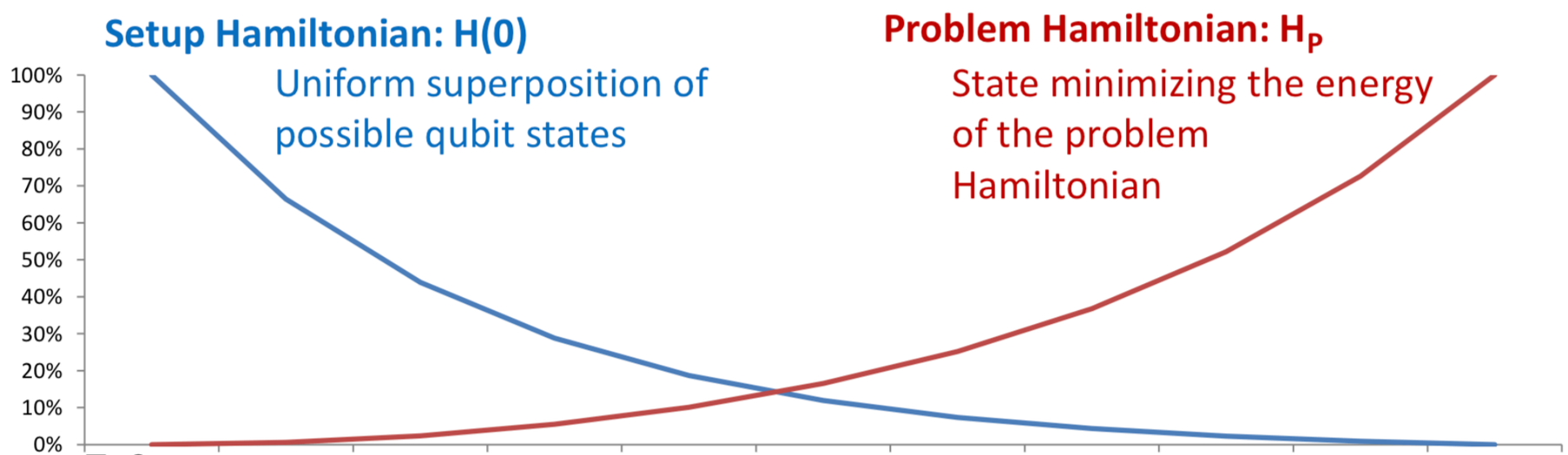
<u>Quantum Circuits</u>
Series of quantum gates operating on a set of quantum states.

<u>Quantum Annealing</u>
Evolution of a quantum system to a low T Gibbs state

Limited to a small phase of all possible algorithms.
Not a generic computer.
Only tackle problems that can be cast in the system specific formulation.

Adiabatic Quantum Annealing

- System setup with trivial Hamiltonian H(0) and ground state
- Evolve adiabatically the Hamiltonian towards the desired Hamiltonian H_p
- **Adiabatic theorem** : with a slow evolution of the system, the state stays in the ground state.



$$H(t) = A(t)H(0) + B(t)H_P$$

arxiv:0001106, arxiv:0104129

Quantum Circuit

qubits two states quantum system (qutrits, etc possible).
Quantum gates are the elementary operations on set of qubits.
Quantum circuits are composed of gates, forming a unitary transformation.

Many quantum algorithms proposed with a provable advantage over classical counterpart:

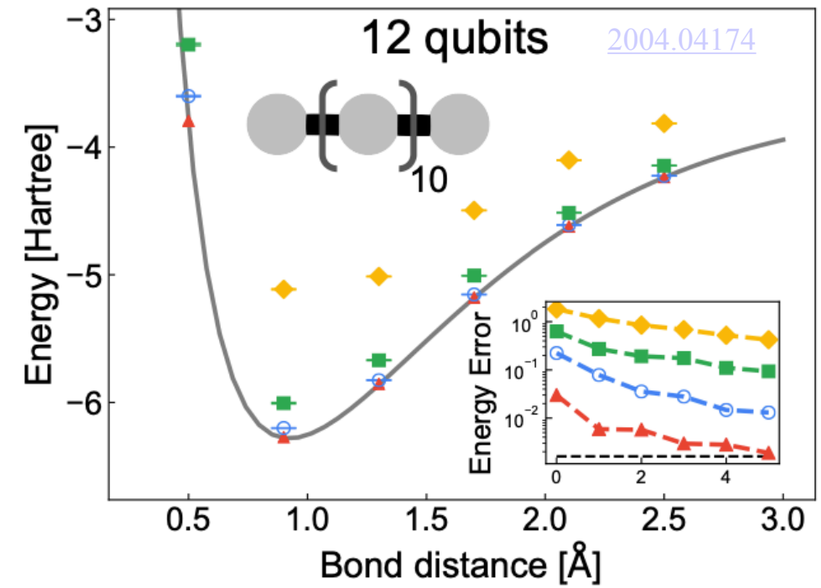
- Prime factorization (Shore's algorithm) : arxiv:9508027
- Database search (Grover's algorithm) : doi:10.1145/237814.237866
- Fast Fourier transform (qFFT) : arxiv:0201067
- Linear system solver (HHL) : arxiv:0811.3171
- …

Advantage of implementation in Noisy Intermediate-Scale Quantum (NISQ) Computing still limited by hardware arxiv:1801.00862 .

Applications to the simulation of quantum system is the most promising to date : arxiv:1512.06860 , arxiv:1704.05018 , arxiv:1902.10171 , arxiv:2004.04174, …

Software and Toolkit available : qiskit , cirq , quil , xacc

Operator	Gate(s)		Matrix
Pauli-X (X)	X	$\oplus$	$\begin{bmatrix} 0 & 1 \\ 1 & 0 \end{bmatrix}$
Pauli-Y (Y)	Y		$\begin{bmatrix} 0 & -i \\ i & 0 \end{bmatrix}$
Pauli-Z (Z)	Z		$\begin{bmatrix} 1 & 0 \\ 0 & -1 \end{bmatrix}$
Hadamard (H)	H		$\frac{1}{\sqrt{2}}\begin{bmatrix} 1 & 1 \\ 1 & -1 \end{bmatrix}$
Phase (S, P)	S		$\begin{bmatrix} 1 & 0 \\ 0 & i \end{bmatrix}$
$\pi/8$ (T)	T		$\begin{bmatrix} 1 & 0 \\ 0 & e^{i\pi/4} \end{bmatrix}$
Controlled Not (CNOT, CX)	$\bullet$ / $\oplus$		$\begin{bmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{bmatrix}$



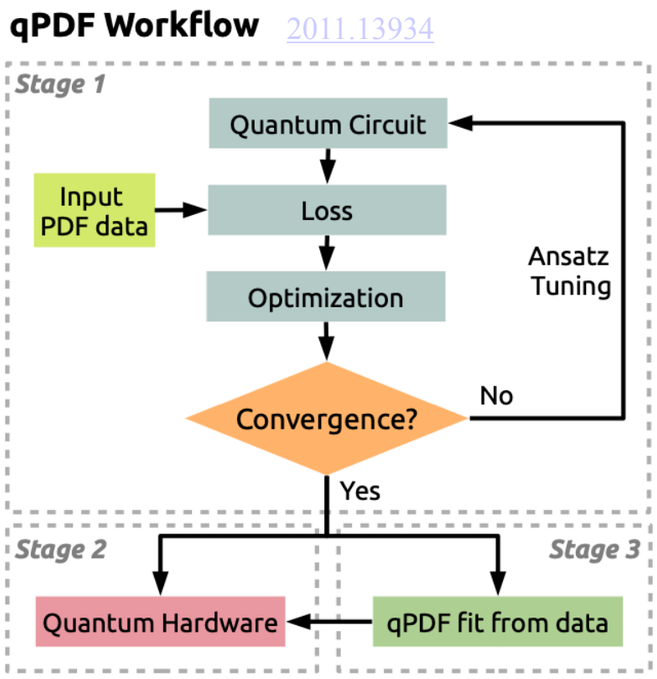
QC in HEP

- (re)cast combinatorial problems in a quantum formulation
  - ➡Pattern recognition, tracking : arxiv:1902.08324, arxiv:1902.00498, arxiv:1908.04475, arxiv:2104.11583, …
  - ➡Vertexing : arxiv:1903.08879, …
  - ➡Jet clustering : arxiv:1908.08949, arxiv:2012.14514, arxiv:2101.05618, …
- Using the probabilistic character of quantum device
  - ➡Simulation of quantum effects : arxiv:1811.10085, arxiv:1904.03196, arxiv:1904.10559, arxiv:2010.00046, arxiv:2010.06458, arxiv:2011.13934, arxiv:2105.04765, arxiv:2105.08703, …
  - ➡Unfolding : arxiv:1908.08519, …

The multi-jet QUBO objective function is

$$O_{\mathrm{QUBO}}(\{x_{ij}\}) = \sum_{r=1}^{M} \sum_{i,j=1}^{N} \left(\frac{\vec{p}_i \cdot \vec{p}_j - E_i E_j \cos R}{1 - \cos R} \right) x_{ir}\, x_{jr} + \Lambda^2 \sum_{i=1}^{N} \left(1 - \sum_{r=0}^{M} x_{ir} \right)^2 .$$

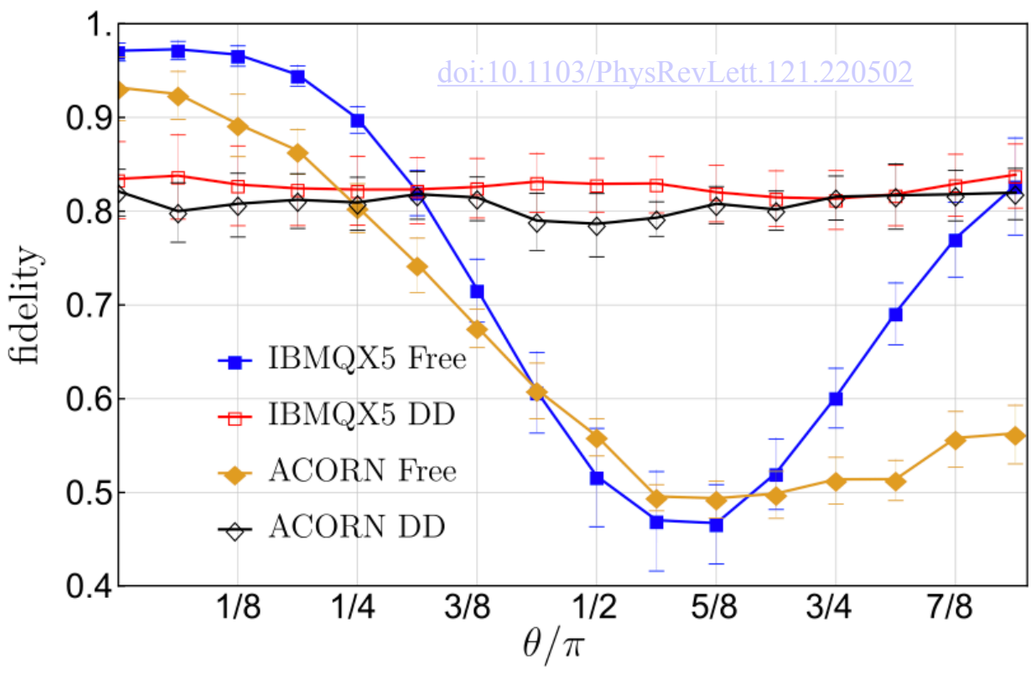
1908.08949

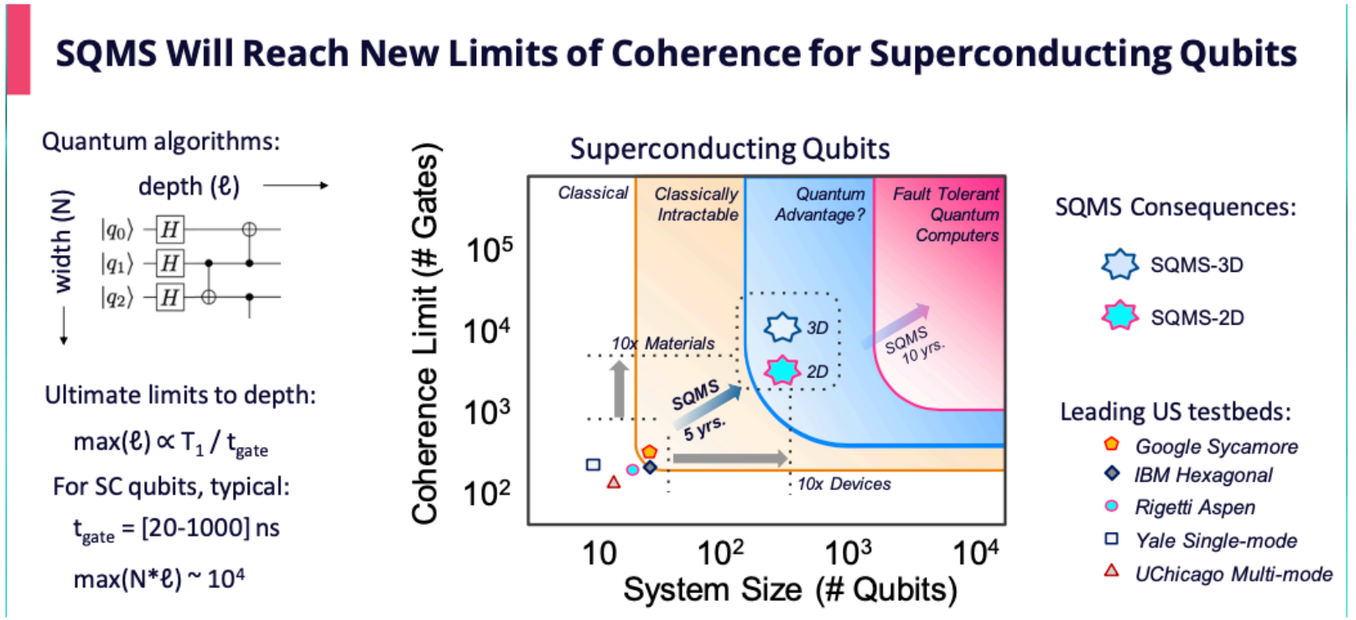


Experimental Limitations

Several aspects of current quantum circuit devices are limiting

- **Decoherence**: noise and imperfect isolation of the quantum state perturbs the computation.
  ➡Mitigated in better devices, and error correction mechanism.
- **Connectivity**: most formulation would require full connectivity, while most device only implement limited qubit neighborhood
  ➡Mitigated in newer devices, and embedding or using qubit replica.
- **System size**: casting of computationally challenging problems often requires large number of qubits. Most device can still be simulated on classical computers.
  ➡Mitigated in newer devices.





Slide by Chad Rigetti, CEO Rigetti Computing

Quantum Machine Learning

Deep learning is computing intensive, and de-facto enabled by use of GPU. People are looking for ways to leverage possible quantum advantage to accelerate machine learning techniques.

Main algorithms used in recent studies

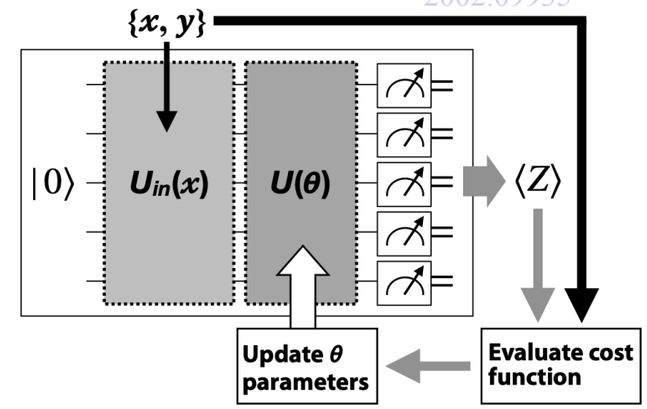
- ➡Variational Quantum Circuits (VQC)
- ➡Quantum Support Vector Machine (QSVM)
- ➡Quantum Restricted Bolztman Machine (QRBM)
- ➡Quantum Adiabatic Machine Learning (QAML)
- ➡Quantum Generative Adversarial Network (QGAN)
- ➡…

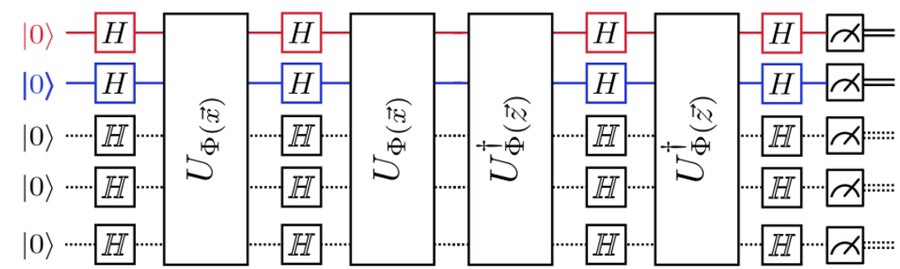
Field in constant evolution. Embedding is crucial.

Deep implications of kernel methods.

Software and toolkit available pennylane , tf-quantum

2002.09935

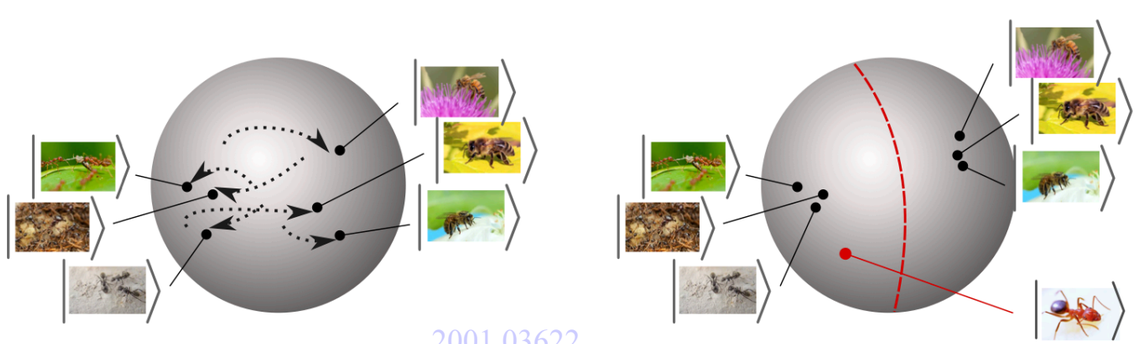




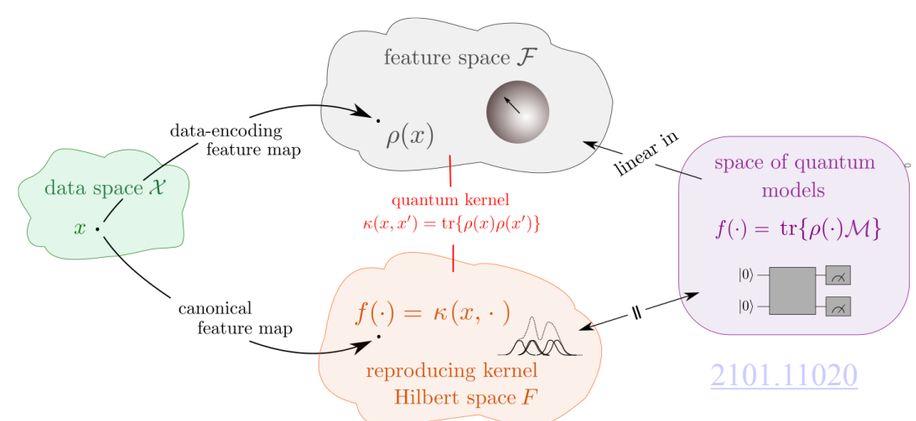
1804.11326

a. Training the embedding

b. Classification



2001.03622

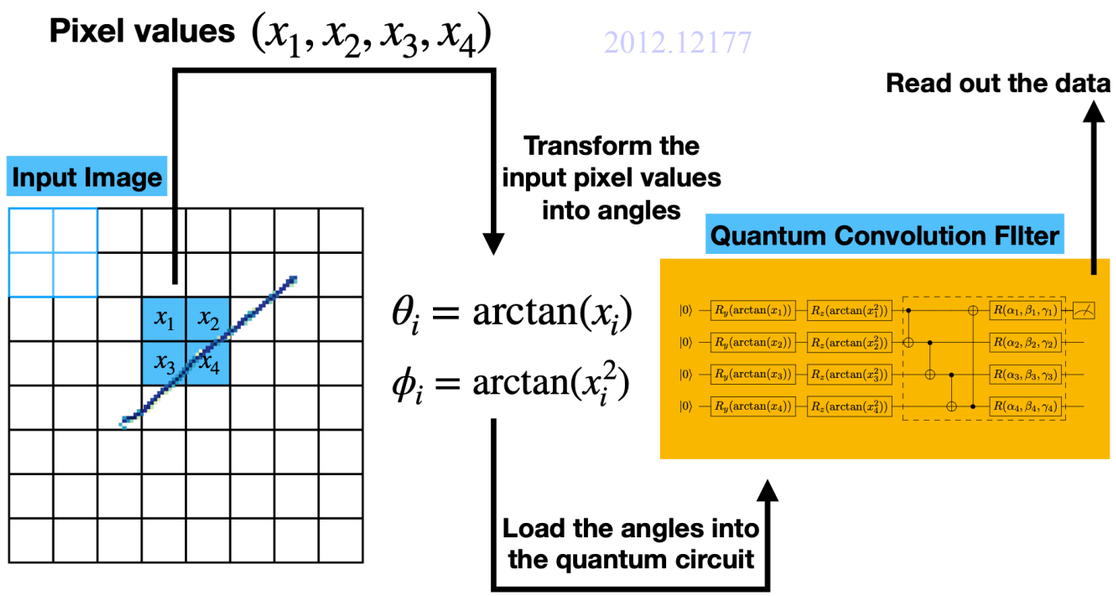


2101.11020

QML in HEP

Applied where "classical machine learning" has already been applied

- Event reconstruction
  - ➡Pattern recognition, tracking : arxiv:2003.08126, arxiv:2007.06868, arxiv:2012.01379, …
- Classification:
  - ➡arxiv:1908.04480, arxiv:2002.09935, arxiv:2010.07335, arxiv:2012.11560, arxiv:2012.12177, arxiv:2103.12257, arxiv:2103.03897, arxiv:2104.07692, …



➡Quantum Support Vector Machine with a rich space of kernels.

➡No hard evidence that QML > ML though (people keep looking).

➡Not much littérature on "quantum generative models for HEP" yet.

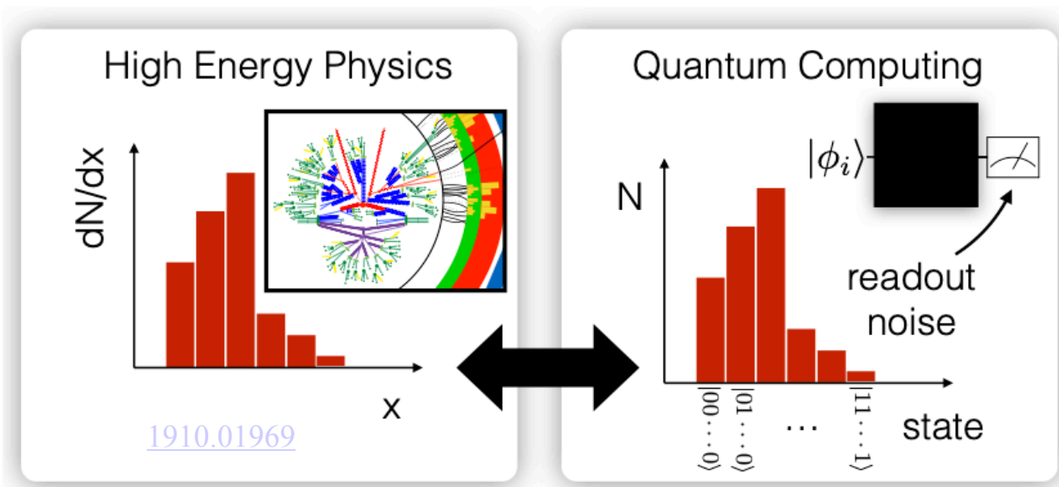
➡There might be advantages in doing QML on Quantum data.

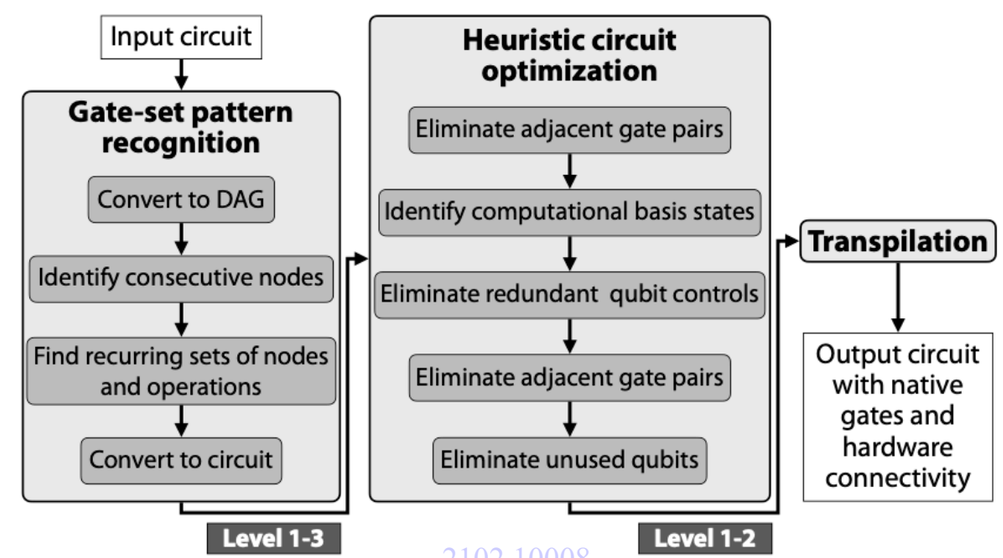
Improving the Quantum Experience

Quantum computing, quantum algorithms, quantum machine learning are evolving fast. Several aspects are key to experimentation

- **Noise correction**: finding a way to mitigate the effect of decoherence and experimental noise in evaluating the quantum circuits.
- **Circuit optimization**: finding circuit layout that go beyond the arbitrary circuit Ansatz that most proposed algorithms make use of.
- **Circuit compression**: compiling a circuit of logical gates into an optimal hardware efficient physical operators. As short as possible due to decoherence.

Applicable methods do not necessarily involved machine learning.





Summary

- Quantum sensors/devices offer novel detection capabilities.
- Quantum communication is becoming reality.
- Quantum computers hold a great deal of potential.
- Devices are getting to useful size.
- Too early for practical usage of quantum computing in HEP ; and yet a promising place for studying innovative ways of doing scientific computation.

References

Initiatives:

- Fermilab Superconducting Quantum Materials and Systems Center : https://sqms.fnal.gov
- Fermilab Quantum Institute : https://quantum.fnal.gov
- NSF QLCI : https://hqan.illinois.edu/about, https://www.colorado.edu/research/qsense/
- Alliance for Quantum Technologies : https://inqnet.caltech.edu
- CERN Quantum Technology Initiative : https://quantum.cern
- Quantum Flagship : https://qt.eu

Lectures:

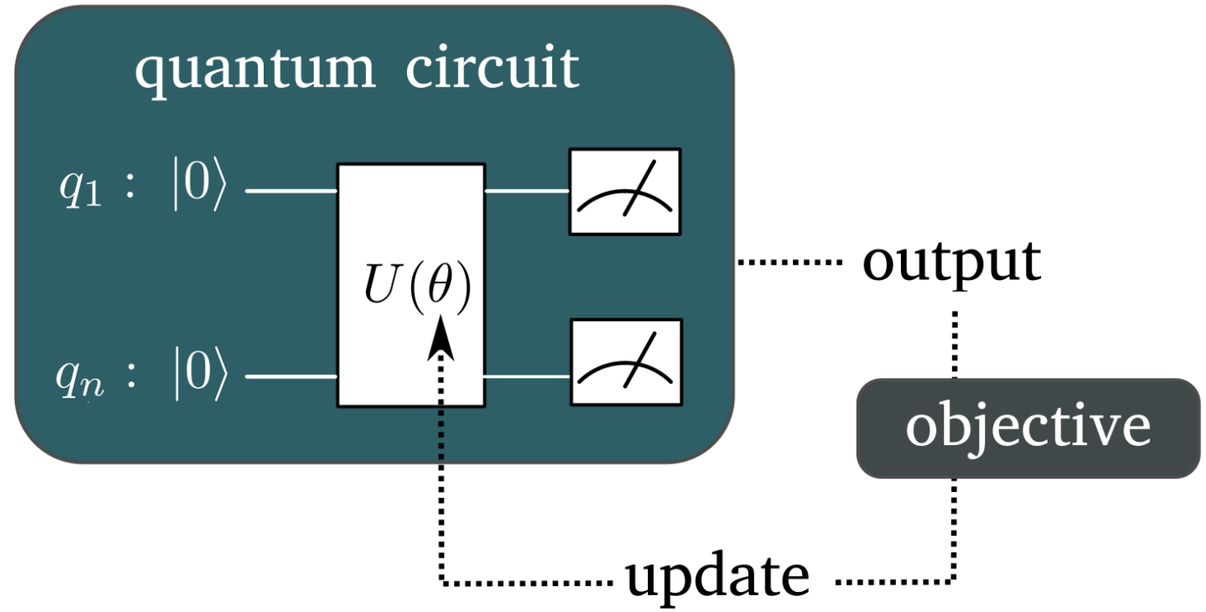
- Elias Fernandex-Combarro alvarez : https://indico.cern.ch/event/970903/
- Maria Schuld : https://indico.cern.ch/event/975609/
- Heather Gray : https://indico.cern.ch/event/870515/

Reviews:

- QML in HEP : https://doi.org/10.1088/2632-2153/abc17d
- Q-GAN : http://doi.org/10.32604/cmc.2020.010551

Quantum Derivatives

https://www.ibm.com/quantum-computing/



Objective based on quantum measurement.
Parameters of a quantum circuits as weights.
Trainable circuits for quantum machine learning.

Quantum Machine Learning [1611.09347]
Quantum Machine Learning in High Energy Physics [2005.08582]
Quantum Machine Learning Models are Kernel Methods [2101.11020]

Outlook

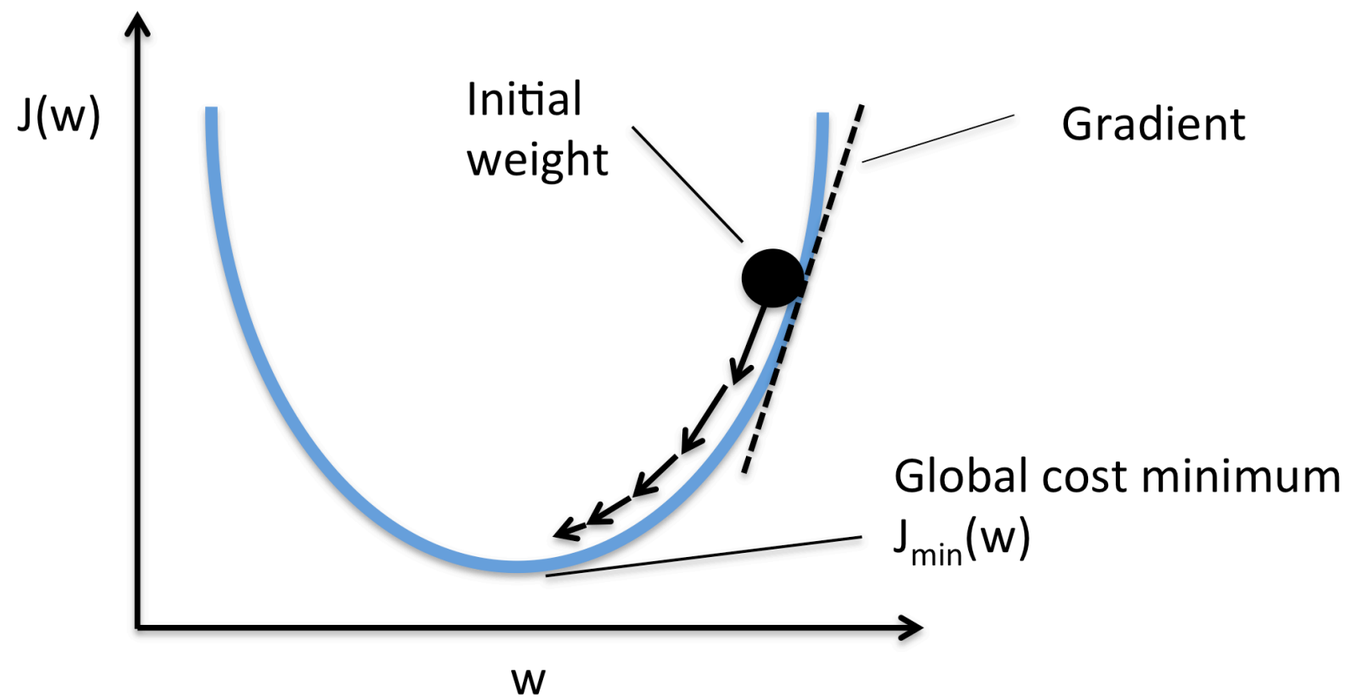
https://www.jpl.nasa.gov/news/testing-proves-its-worth-with-successful-mars-parachute-deployment

Stochastic Gradient Descent

- Application of one gradient descent is expensive. Can be prohibitive with large datasets
- Following the gradient update from each and every sample of a dataset leads to tensions
    - In binary classification, samples from opposite categories would have “opposite gradients”
- Gradients over multiple samples are independent, and can be computationally parallelyzed
- → Estimate the effective gradient over a batch of samples

$$\nabla_{eff} f(x) = \frac{1}{N} \sum_{i \in batch} \nabla_i f(x)$$

Gradient Descent Optimization



- For a differentiable loss function f, the first Taylor expansion gives

$$f(x+\varepsilon) = f(x) + \varepsilon \nabla f(x)$$

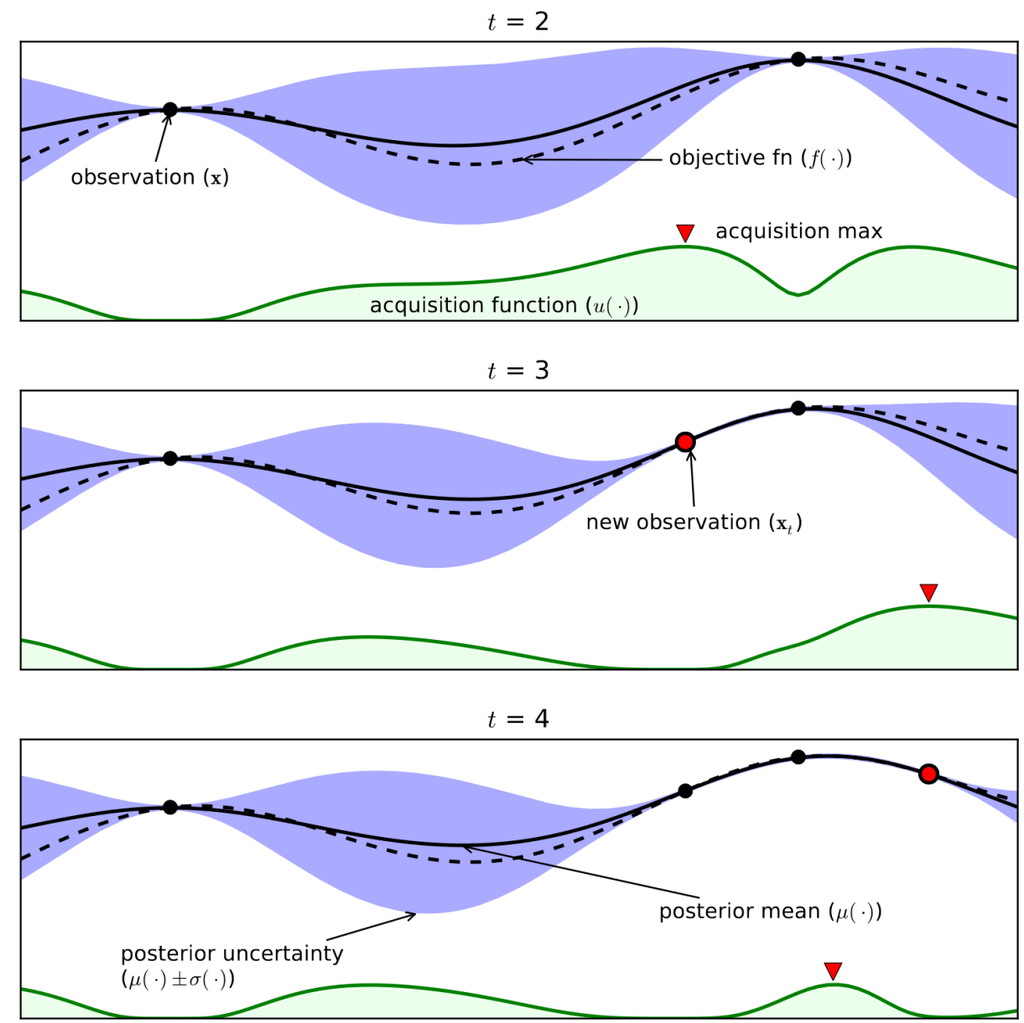
- The direction to locally maximally decrease the function value is anti-collinear to the gradient

$$\varepsilon = -\gamma \nabla f(x)$$

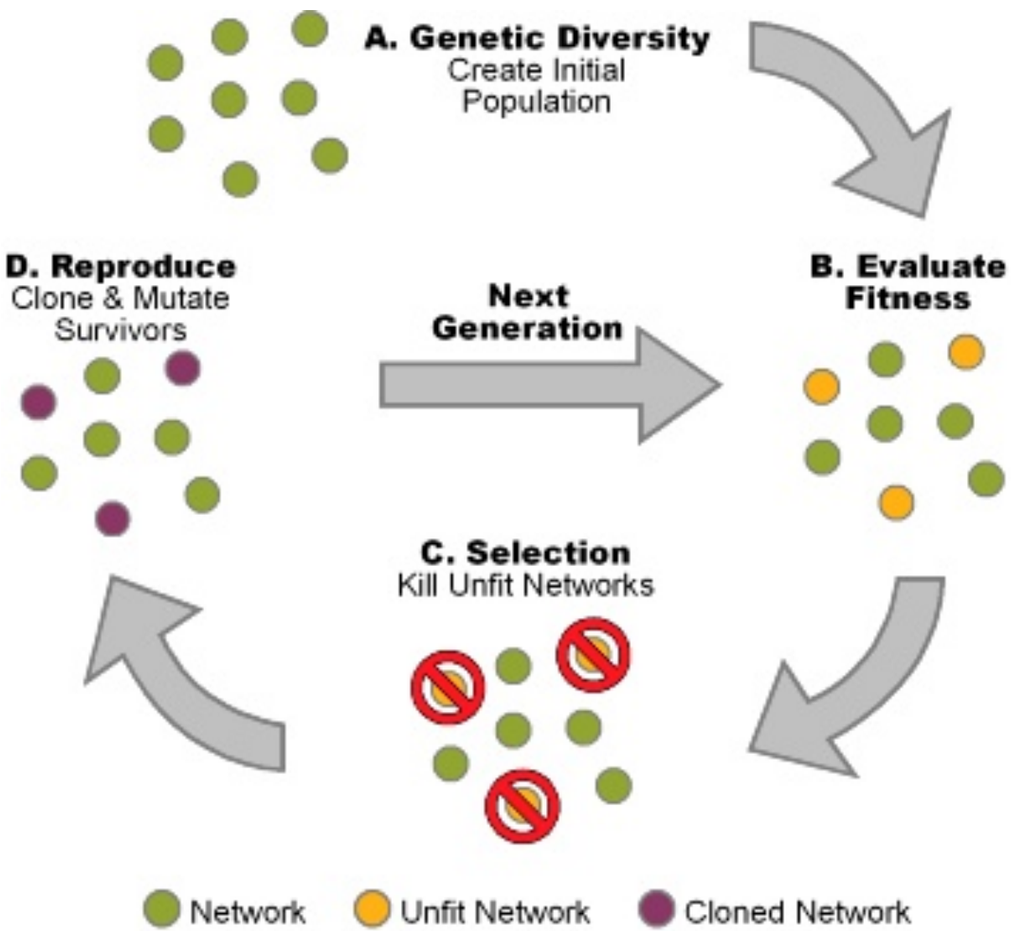
- Amplitude of the step γ to be taken with care to prevent overshooting

Bayesian Optimization

- Applicable to optimize function **without close form** and that are **expensive to call** (numerical gradient impractical)
- Approximate the objective function with **Gaussian processes** (GP)
- Start at random points, then sample according to optimized acquisition function
  - Expected improvement
    - $EI(x) = -E(f_{GP}(x) - f(x_{best}))$
  - Lower confidence bound
    $LCB(x) = \mu_{GP}(x) + \kappa\sigma_{GP}(x)$
  - Probability of improvement
    - $PI(x) = -P(f_{GP}(x) \geq f(x_{best}) + \kappa)$



Evolutionary Algorithms

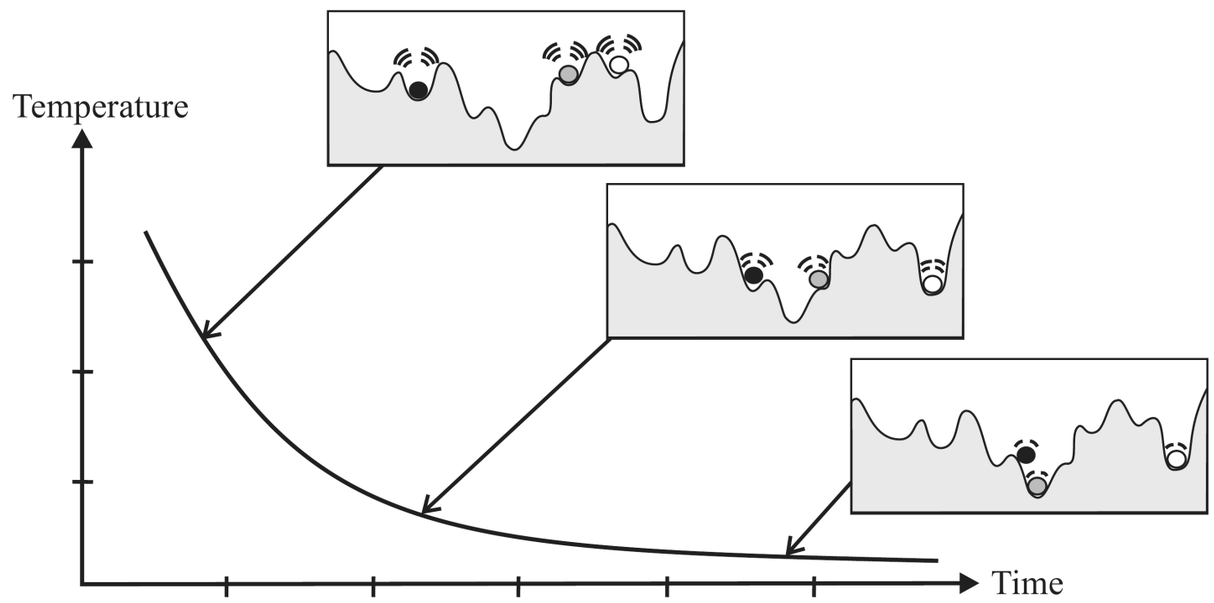


- Applicable to function in high dimensions, with a non regular landscape
- Start from random population
- Estimate fittest fraction of individuals
- Bread and mutate individuals

- Direction of optimization is given by the cross-over and mutation definition
- Multiple over algorithms : particle swarn, ...

Simulated Annealing

- Monte-Carlo based method to find ground state of energy functions
- Random walk across phase space
  - accepting descent
  - accepting ascent with probability $e^{-\Delta E/kT}$
- Decrease T with time



Non Analytical SGD

- Some valuable loss function might not be analytical and their gradients cannot be derived
- Used finite element method to estimate the gradient numerically

$$\nabla f(x) = \frac{f(x+\varepsilon) - f(x)}{\varepsilon}$$

- Method can be extended to using more sampling and better precision
- Quite expensive computationally in number of function calls and impractical in large dimension
- Robust methods available in most program library

Second Order Methods

- Newton-Raphson method defines a recursive procedure to find the root of a function, using its gradient.
- Finding optimum is equivalent to finding roots of the gradient, hence applying NR method to the gradient using the Hessian

$$f(x+\varepsilon) = f(x) + \varepsilon \nabla f(x) + \frac{1}{2}\varepsilon^T H(x)\varepsilon$$

$$\varepsilon \sim -H(x)^{-1}\nabla f(x)$$

- Convergence guaranteed in certain conditions
- Alternative numerical methods tackle the escape of saddle points and computation issue with inverting the Hessian
- In deep learning “hessian-free” methods are prohibitive computationally wise

How could quantum computing help with ML?

- Data
  - speed up sampling from data distributions
  - use fewer data samples (e.g., Arunachalam 1701.06806)
- Optimisation
  - speed up optimisation (Wiebe et al. 1204.5242, Rebentrost et al. 1307.0471, Denil & Freitas ~ 2012 `cs.ubc.ca/~nando/`)
  - find better solutions
- Model
  - speed up existing models (Pararo et al. 1401.4997, Low et al. 1402.7359, Allcock et al. 1812.03089)
  - design better models (Amin et al. 1601.02036, Benedetti et al. 1906.07682)

https://indico.cern.ch/event/975609/