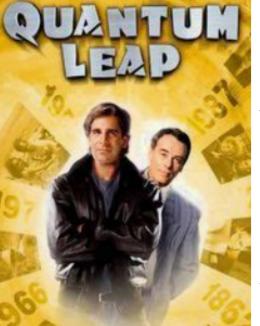


Quantum Computing for High-Energy Physics

Michael Spannowsky
with Steve Abel and Simon Williams

IPPP, Durham University

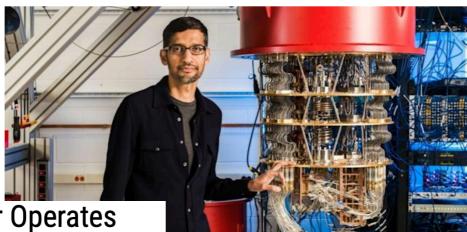


Kristen Philipkoski

The Morning After: Google claims 'quantum' supremacy'

And a controversial 'Ghost in the Shell' trailer.





First Quantum Computer Simulator Operates The Speed Of Light

Published 10 years ago: September 2, 2011 at 7:02 am - Filed to: COMPUTING V













hris Ferrie and whurley

uantum Computers Will Be Incredibly Useful For

Computers don't exist in a vacuum. They serve to solve problems, and the type of problems they can solve are influenced by their hardware. Graphics processors are specialized for rendering images; artificial intelligence processors for AI; and quantum computers designed for... what? While the power of quantum computing is impressive, it does not mean that existing ...





Master in Elektrotechnik, Informatik, Robotik, Maschinenwesen o. ä. (w/m/d)

German Aerospace Center (DLR) · Oberpfaffenhofen, Bavaria, Germany (On-site)



4 company alumni



Professor Cyber Security im Online Fernstudium (m/w/d)

IU International University of Applied Sciences · Germany (Remote)



Actively recruiting



Expertin für Post-Quanten-Kryptographie (w/m/d)

Deutsche Bahn · Frankfurt, Hesse, Germany (On-site)



Actively recruiting



Master Thesis: Design of digitally enhanced power management circuits for Future Quantum Computers

Forschungszentrum Jülich · Jülich, North Rhine-Westphalia, Germany (On-site)



1 company alum



Expertin für Quantenkommunikation (w/m/d)

Deutsche Bahn · Frankfurt, Hesse, Germany (On-site)



Actively recruiting





"Nature is quantum [...]
so if you want to
simulate it, you need a
quantum computer"
- Richard Feynman

(1982)

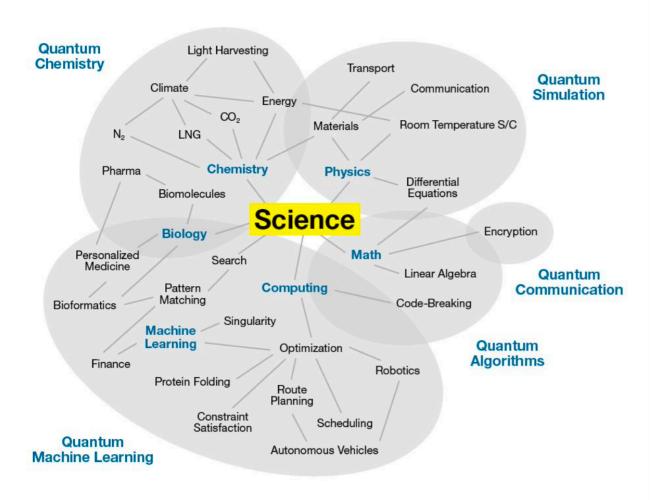


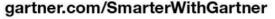
Easily said ... so how do we do that?

Beginning of a scientific journey that accelerated in recent years tremendously....

Private and Public Sector is placing big bets on Quantum Computing

Quantum Computing Use Cases

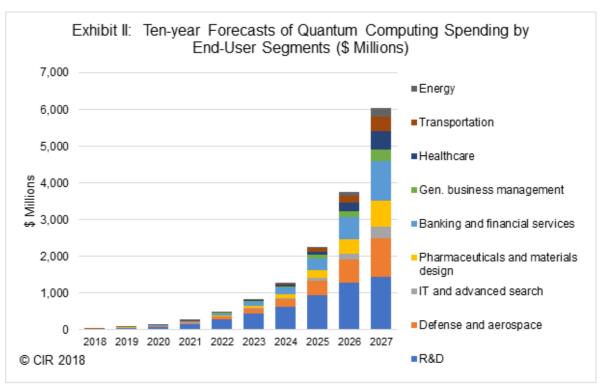




Source: Adapted from Pete Shadbolt and Jeremy O'Brien

© 2017 Gartner, Inc. and/or its affiliates. All rights reserved. Gartner is a registered trademark of Gartner, Inc. or its affiliates. PR 338248



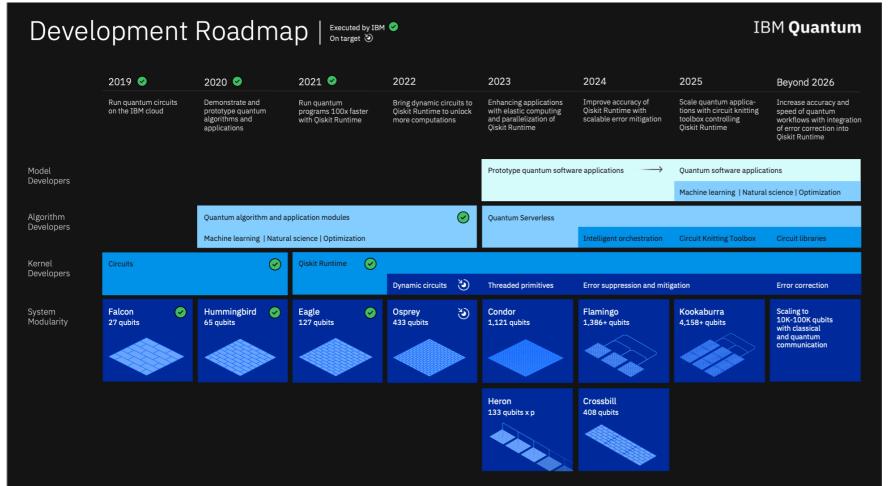


Significant financial investment expected across many sectors

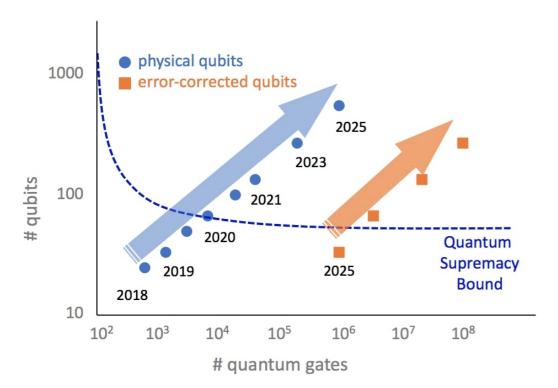
In US, already now higher financial investment from private than public sector



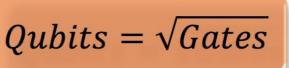
All national and international labs have QC programmes (Fermilab, BNL, LBNL, DESY, CERN, Singapur, Abu Dhabi, ...)



IonQ Roadmap into the Future









1 mio physical qubits
->
1k logical qubits
by 2029

timescales much smaller than FCC's

Popular Quantum Computing paradigms

Туре	Discrete Gate (DG)	Continuous Variable (CV)	Quantum Annealer (QA)	
Computing	Digital	Digital/Analog	Analog	
Property	Universal (any quantum algorithm can be expressed)	Universal - GBS non-Universal	Not universal — certain quantum systems	
Advantage	most algorithms and tech support	uncountable Hilbert (configuration) space	continuous time quantum process	
How?	IBM – Qiskit ~500 Qubits	Xanadu	DWave - LEAP ~7000 Qubits	
What?				
	input 0) H X H H H Iwo-qubit gate two-qubit gate	Interferometer Squeezing Interferometer Displacement Nonlinearity U_1 D Φ	E QA finds wide region region region region state	

See S. Abel

How most quantum algorithms work

operator acts on Hilbert space states

$$U|x\rangle = |\Psi_1\rangle$$

measurement of observable \hat{U} corresponds to exp. $\left\langle \hat{U}\right\rangle _{\Psi}$ value of operator U

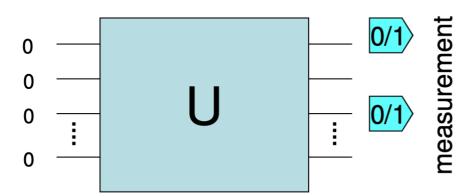
$$\left\langle \hat{U} \right\rangle_{\Psi} = \frac{\langle \Psi | U | \Psi \rangle}{\langle \Psi | \Psi \rangle}$$

Need to encode Hilbert space and operator suitable for quantum system

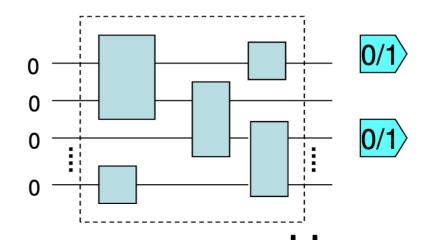


statistical statement need to evaluate often







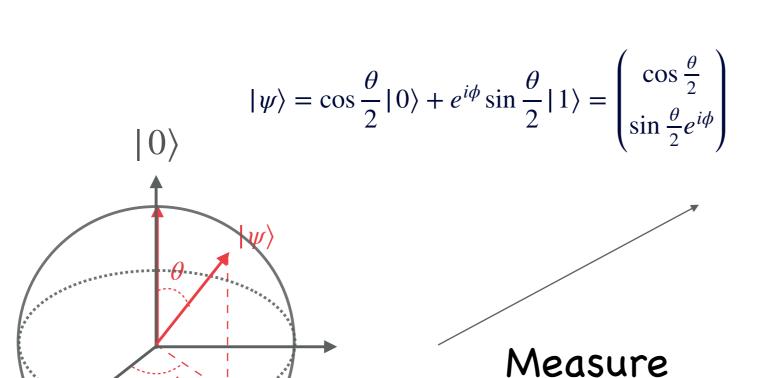


- Operator expressed in terms of individual gates
- Often 'Trotterization' (Suzuki-Trotter decomposition) needed:

For
$$H = \sum_{j=1}^m H_j$$

For
$$H=\sum_{j=1}^m H_j$$
 $e^{iHt}=\left(\prod_{j=1}^m e^{-iH_jt/r}\right)^r+\mathcal{O}(m^2t^2/r)$

Rotation about the Bloch Sphere and state parametrisation



 $|0\rangle$

$$|1\rangle \operatorname{Prob}(|1\rangle) = \left(e^{i\phi}\sin\frac{\theta}{2}\right)^2$$

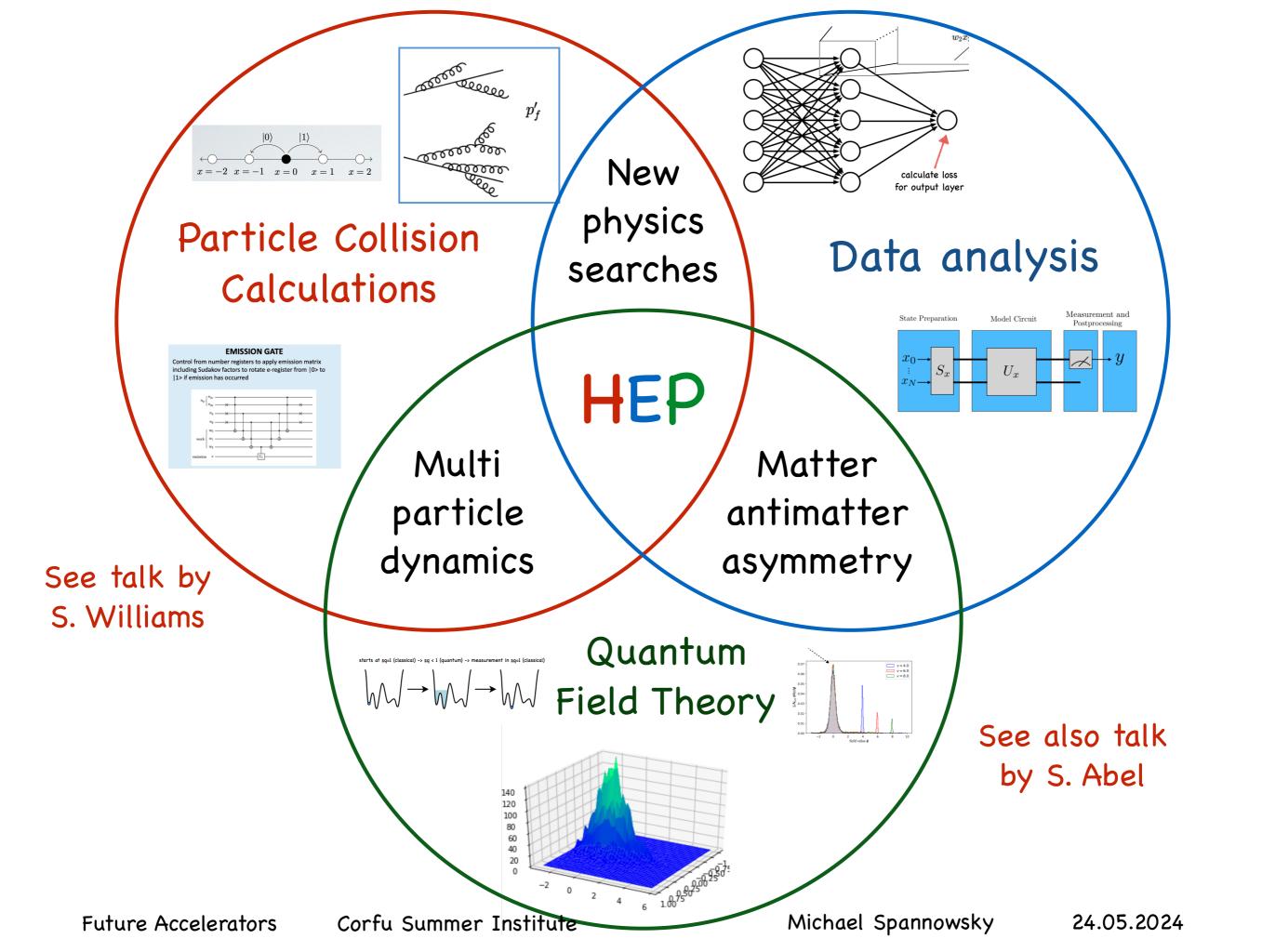
$$|0\rangle \operatorname{Prob}(|0\rangle) = \left(\cos\frac{\theta}{2}\right)^2$$

Apply Unitary rotation
$$U_3 \mid 0$$
: $U_3(\theta, \phi, \lambda) = \begin{pmatrix} \cos(\frac{\theta}{2}) & -e^{i\lambda}\sin(\frac{\theta}{2}) \\ e^{i\phi}\sin(\frac{\theta}{2}) & e^{i(\phi+\lambda)}\cos(\frac{\theta}{2}) \end{pmatrix}$

 $|1\rangle$

Extending this to a system of N qubits forms a 2^N -dimensional Hilbert Space

 $|1\rangle$



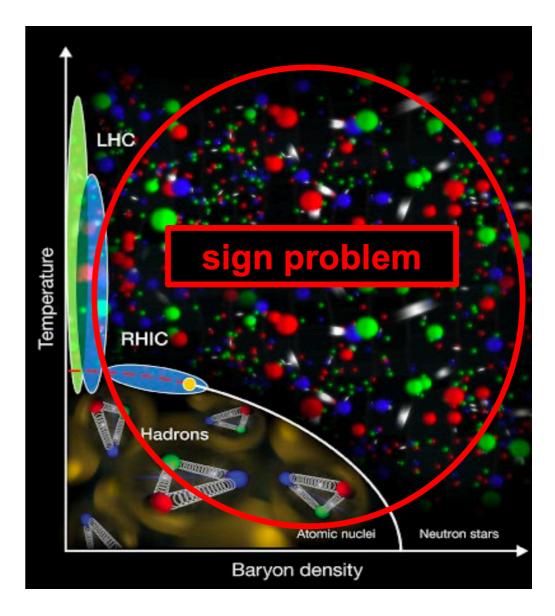
HEP application focused quantum simulation

- Sign problem profound challenge for simulation of field theories
- Can arise in presence of chemical potential, topological terms, multi-particle dynamics, ...
- ullet Example chemical potential $\muar{\psi}\gamma^0\psi$

$$Z = \int \mathcal{D}\bar{\psi}\mathcal{D}\psi\mathcal{D}A \ e^{-S[\bar{\psi},\psi,A]} \quad \text{(partition function)}$$

$$S = \int_0^{1/T} d\tau \int d^3x \left[\bar{\psi} (\gamma^{\mu} D_{\mu} + m) \psi + \frac{1}{4} F^a_{\mu\nu} F^{a\mu\nu} + \mu \bar{\psi} \gamma^0 \psi \right]$$

and integration over fermion fields and Wick rotation



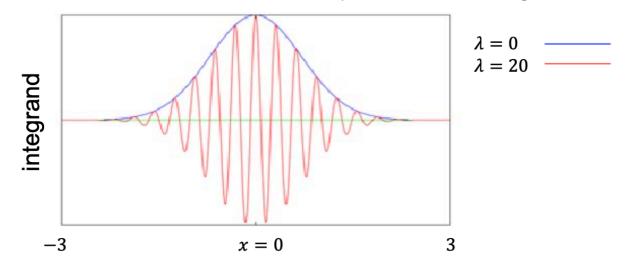
$$Z = \int \mathscr{D} A e^{-S_{\rm gauge}[A]} \cdot \det(\gamma^{\mu} D_{\mu} + m + \mu \gamma^4) \quad \longrightarrow \quad \text{For } \mu \neq 0 \text{ complex phases don't cancel}$$

HEP application focused quantum simulations

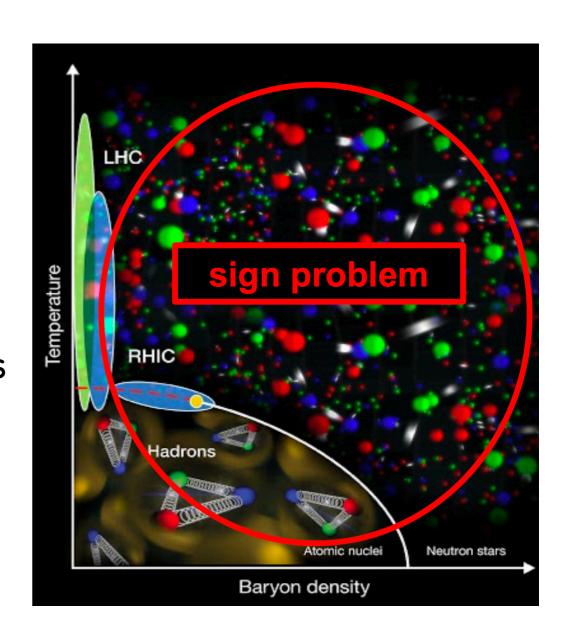
- Highly oscillatory integrands

$$\langle O \rangle = \frac{\int \mathcal{D}Ae^{-S_{\text{gauge}}} O |\det(M)| e^{i\phi}}{\int \mathcal{D}Ae^{-S_{\text{gauge}}} |\det(M)| e^{i\phi}}$$

near cancellation of pos and neg contribs



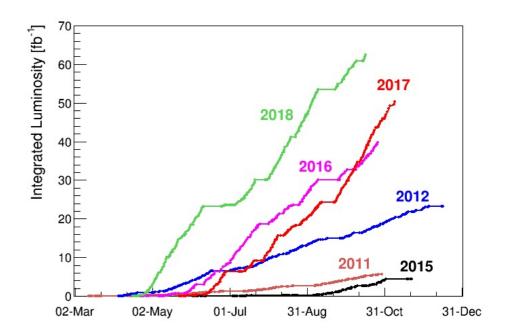
$$\int dx \exp(-x^2 + i\lambda x) \to \int dx \exp(-x^2)\cos(\lambda x)$$



[de Forcrand '10]

Big Data in HEP @ the LHC

- ATLAS/CMS 200 events/s passing triggers
- → ATLAS/CMS 2 PB/year of data



High-Energy Physics

Tremendous amount of highly complex data

However, theoretically very precise description of data



Ideal interplay

See talk by T. Golling

Machine Learning

Highly performant data analysis techniques

Often used for classification in HEP:

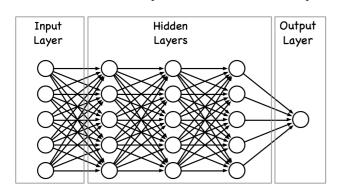
- Supervised learning
- Anomaly detection

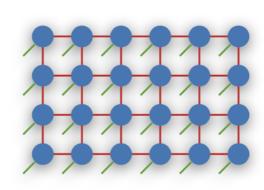
Classical ML Algorithms

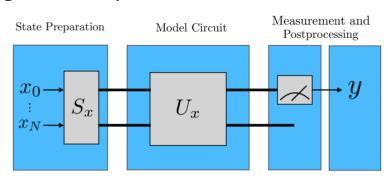
Tensor Networks

Quantum Computing

1. an adaptable complex system that allows approximating a complicated function







2. the calculation of a loss function used to define the task the method

$$E(y,y')=rac{1}{2}|y-y'|^2$$

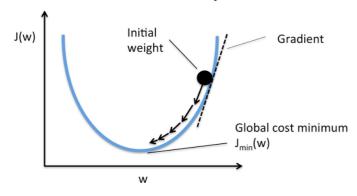
$$B_{p_1 p_2}^{s_2} \Gamma_{s_2}^{l p_1 p_2} = f^l(\mathbf{x}^{(\mathbf{n})})$$

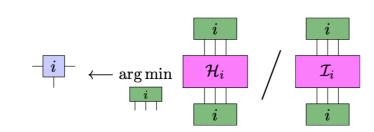
$$\mathcal{L} = L\left(p(l, \mathbf{x}), \ l^{truth}\right)$$

ground state

$$|\Gamma
angle := rg \min_{|\psi
angle \in \mathcal{D}} rac{\langle \psi | H | \psi
angle}{\langle \psi | \psi
angle}$$

3. a way to update 1. while minimising the loss function





quantum: annealing

hybrid: classical opti.

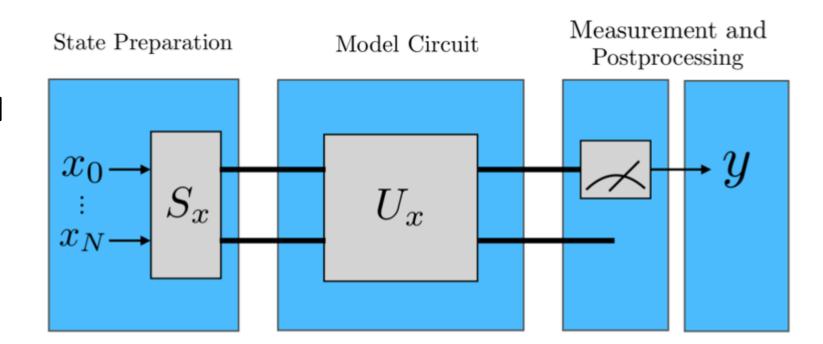


Data Analysis (Classification, anomaly, regression, fitting, ...)
Simulation of field theories (Groundstate, tunnelling, Real-time...)
Calculation of differential equations, etc etc

Quantum Machine Learning with a Variational Quantum Circuit

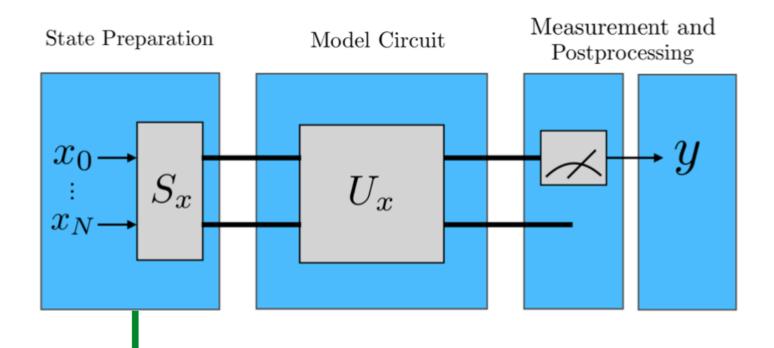
[McClean et al '16] [Farhi, Neven '18] [Schuld et al '20] [Blance, MS '20]

Future Accelerators



Michael Spannowsky

Quantum Machine Learning with a Variational Quantum Circuit



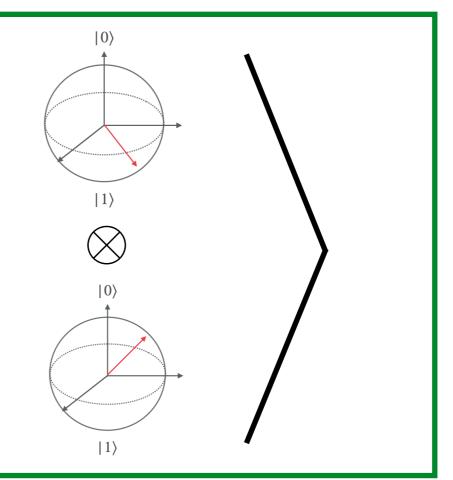
state preparation

n corresponds to # features

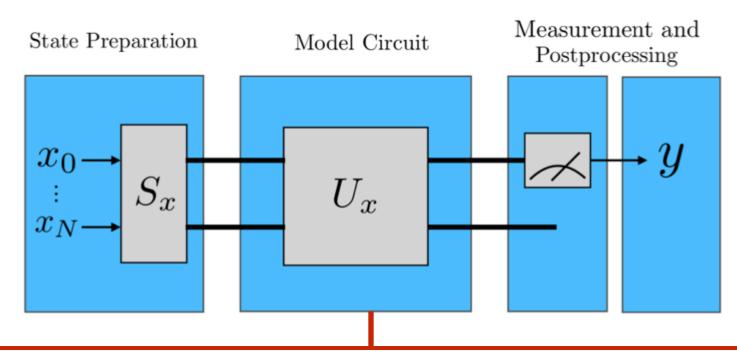
$$x \mapsto S_x |\phi\rangle = S_x |0\rangle^{\otimes n} = |x\rangle$$

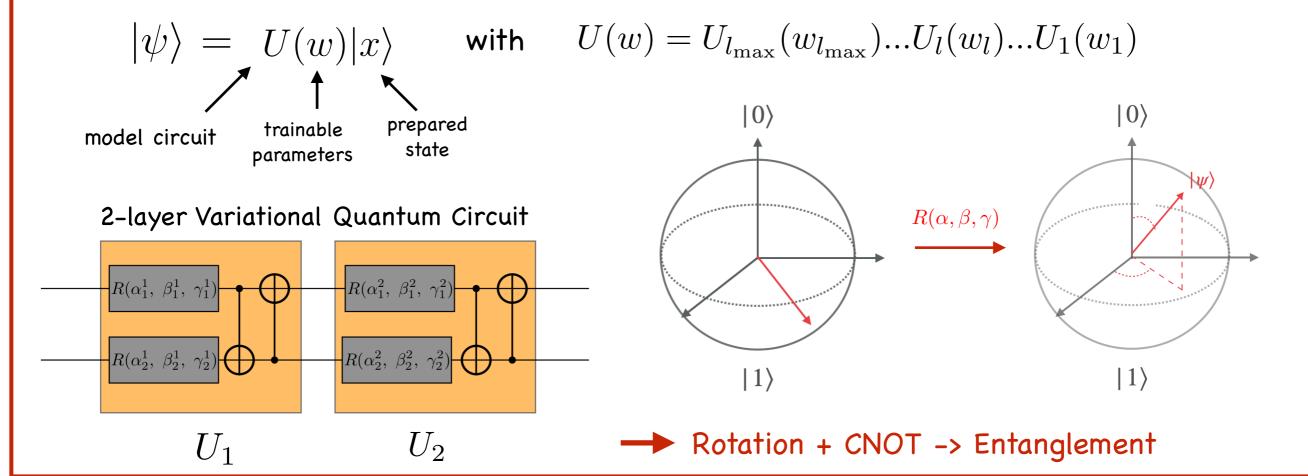
e.g. angle encoding

$$|x\rangle = \bigotimes_{i=1}^{n} \cos(x_i)|0\rangle + \sin(x_i)|1\rangle$$

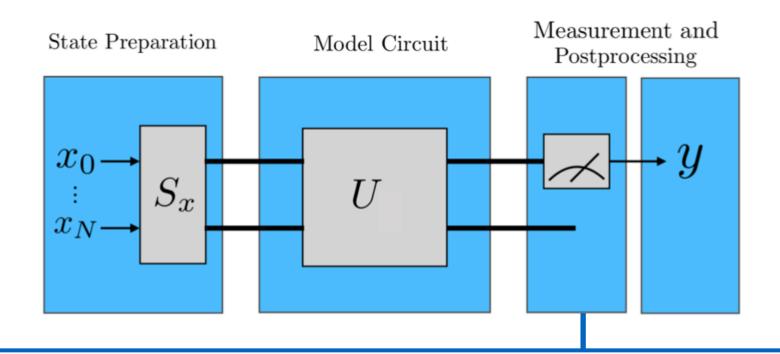


Quantum Machine Learning with a Variational Quantum Circuit





Quantum Machine Learning with a Variational Quantum Circuit

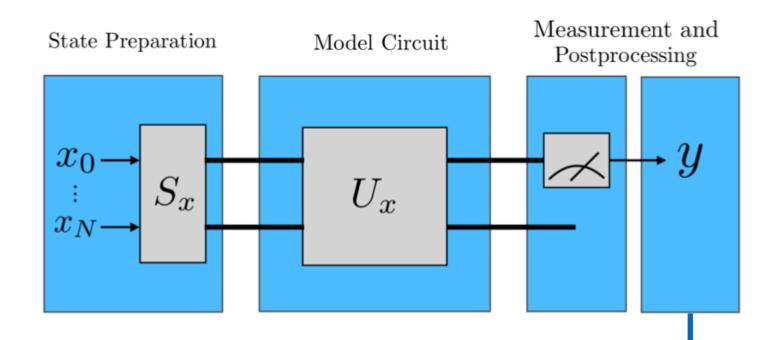


- Entangled state shares information across qubits
- Evaluate expectation value of qubits to construct loss for supervised S vs B classification one qubit sufficient

$$\mathbb{E}(\sigma_z) = \langle 0|S_x(x)^{\dagger}U(w)^{\dagger}\hat{O}U(w)S_x(x)|0\rangle = \pi(w,x) \quad \text{ for } \quad \hat{O} = \sigma_z \otimes \mathbb{I}^{\otimes (n-1)}$$

- Quantum network output: $f(w, b, x) = \pi(w, x) + b$
- Changing operator and loss => VQE, VQT, ... (simulate QFT)

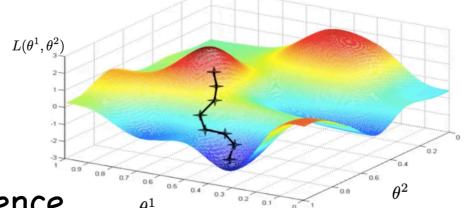
Quantum Machine Learning with a Variational Quantum Circuit



Hybrid approach (QC to calculate exp. value, CC to optimise U operator)

21

 $\text{Loss function} \quad L = \frac{1}{n} \sum_{i=1}^n \left[y_i^{\text{truth}} - f(w,b,x_i) \right]^2 \quad \text{L}(\theta^1,\theta^2)$ label (signal, bkg), supervised learning



 Quantum gradient descent - for fast convergence Fubiny-Study metric underlies geometric

structure of VQC parameter space: $\theta_{t+1} = \theta_t - \eta g^+ \nabla L(\theta)$

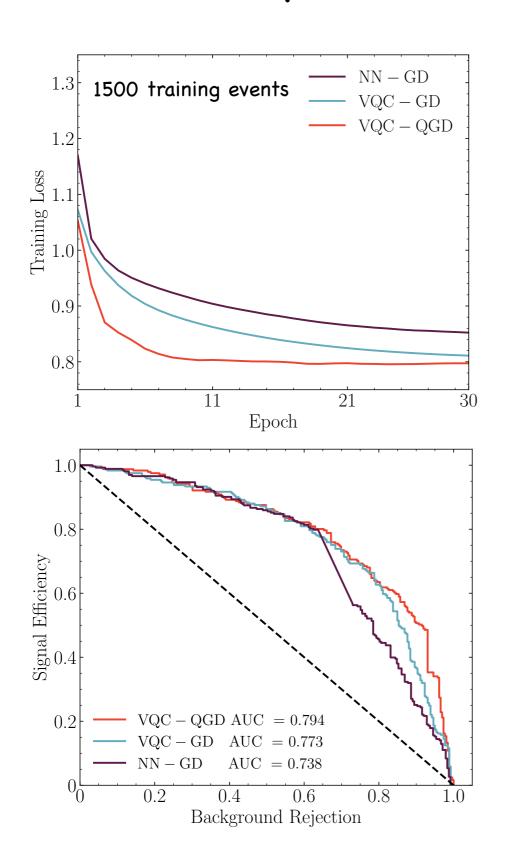
$$\theta_{t+1} = \theta_t - \eta g^+ \nabla L(\theta)$$

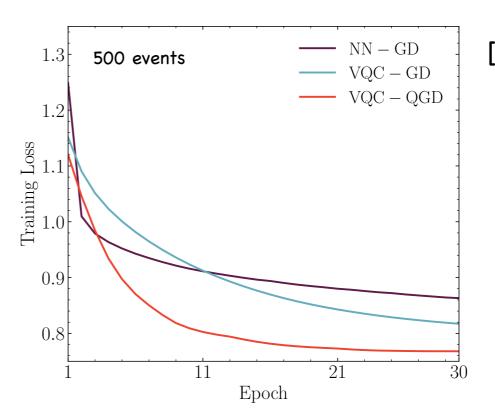
[Chenq '10]

[Blance, MS '20]

[Abbas et al '20]

Gate quantum machine learning in action





[Blance, MS '20]

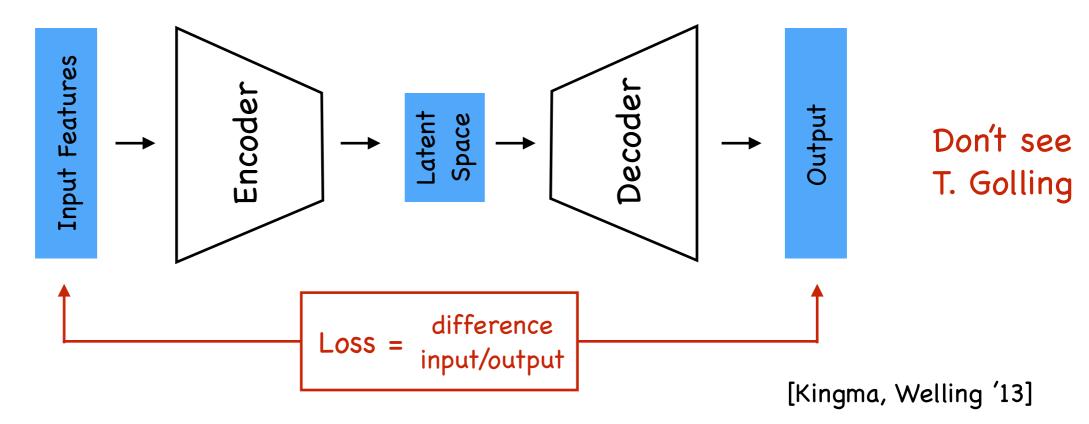
QC device vs simulator

Device	Accuracy (%)
PennyLane default.qubit	72.6
ibmq_qasm_simulator	72.6
ibmqx2	71.4

• Applied to pp o t ar t vs pp o Z' o t ar t lept. top dec for 2d feature space only p_{T,b_1} and E_T

Autoencoder for unsupervised learning

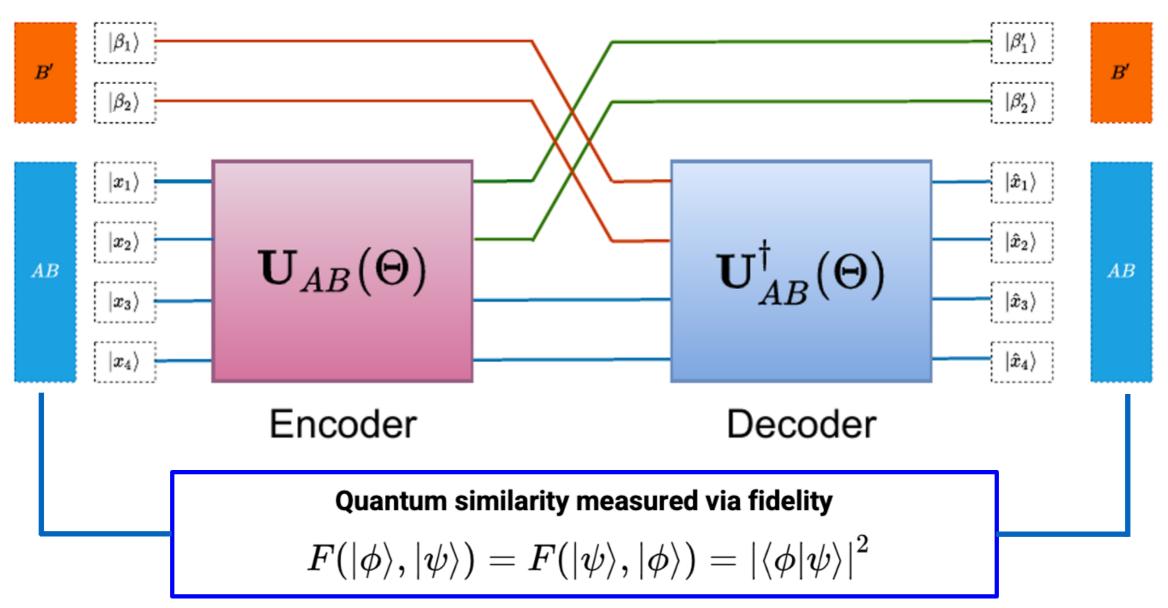
Most popular NN-based anomaly detection method



- in first step input is encoded into information bottleneck
- between input/output layer and bottleneck can be several hidden layers (conv./deep NNs) -> highly non-linear
- after bottleneck decoding step
- Reconstructed output is then compared with input via loss-function (often MSE)
- NN is trained such that input and output high degree of similarity

Unsupervised learning with quantum-gate Autoencoder

[Ngairangbam, MS, Takeuchi '21]



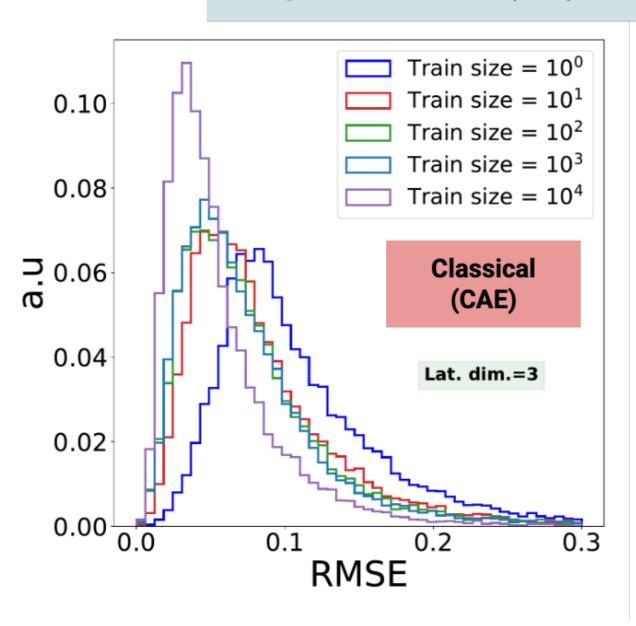
Induce information bottleneck by discarding states of B system after encoding, and replacing with reference states B' with no connection with the encoder.

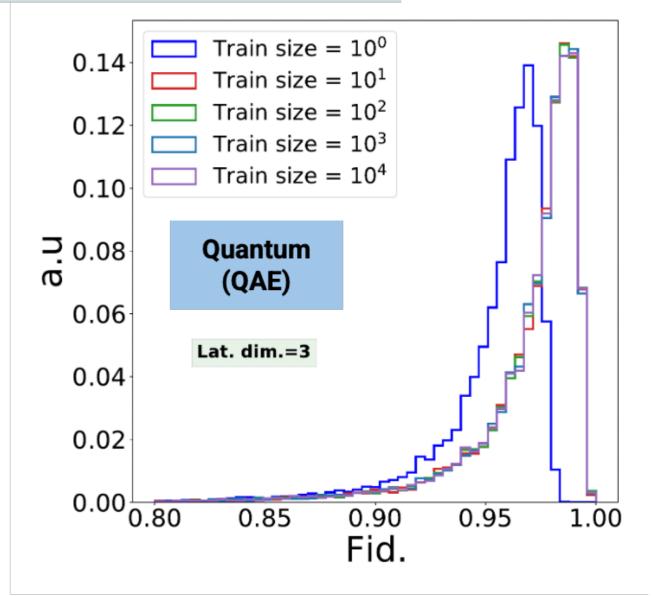
Future Accelerators

Michael Spannowsky

Results: Training size dependence

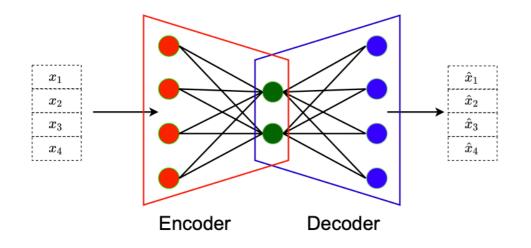
Dependence of (BG) test loss on training size

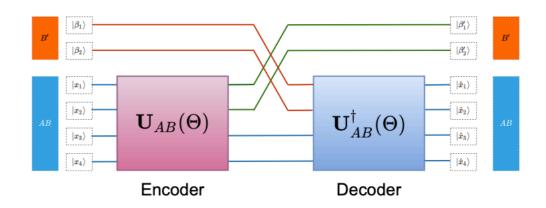


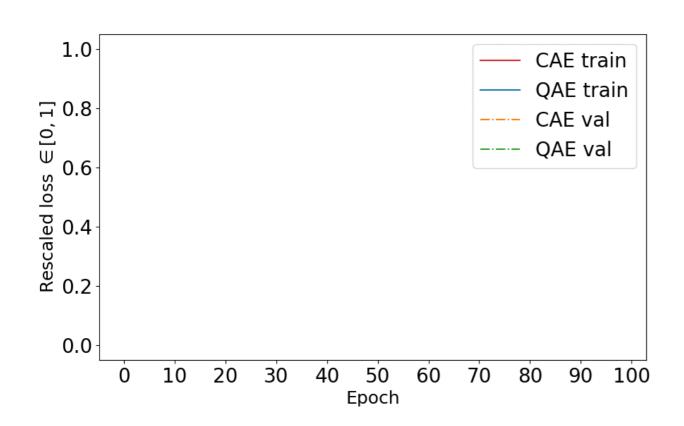


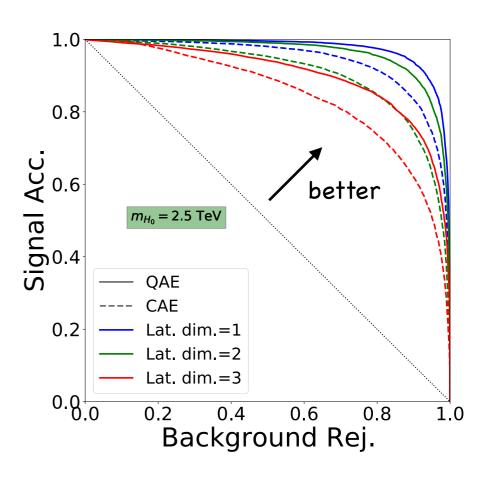
Classical autoencoder

Quantum autoencoder









Much faster training and better performance for Quantum autoencoder

In our test case, outcome prevails for much larger classical networks

Adiabatic quantum computing

 Adiabatic quantum computing (AQC) proposed as application of quantum adiabatic theorem to solve optimisation problems [Farhi, Goldstone, Gutmann '00]

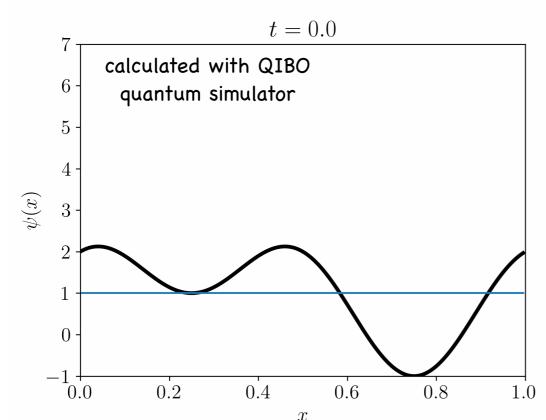
• Turns out to equivalent to quantum circuit model, i.e. it is universal

[Aharonov, et al '07]

ullet States that if system prepared in ground state $|\psi_0
angle$ of Hamiltonian ${\cal H}$

If Hamiltonian changed smoothly and slowly enough system remains in ground state

A time variation of the Hamiltonian from \mathcal{H}_I to \mathcal{H}_P is implemented according to: $\mathcal{H}(t) = (1 - s(t))\mathcal{H}_I + s(t)\mathcal{H}_P \quad t \in [0, T] \quad s: [0, \tau] \to [0, 1]$



$$H = (1 - t) \frac{p^2}{2m^2} + t V(x)$$

encode problem/optimisation task here

Quantum annealing: Non-universal but powerful?

• Specific Hamiltonian. What does the "anneal" mean?

$$\mathcal{H}_{QA}(t) = \sum_{i} \sum_{j} J_{ij} \sigma_i^Z \sigma_j^Z + \sum_{i} h_i \sigma_i^Z + \Delta(t) \sum_{i} \sigma_i^X$$

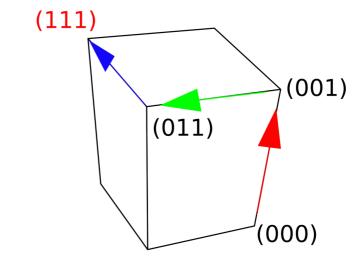
final Hamiltonian (encodes actual problem)

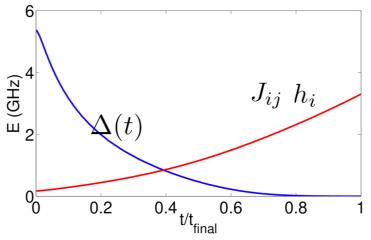
initial Hamiltonian
(ground state = superposition of qubits with 0 and 1)

 $\Delta(t)$ induces bit-hopping in the Hamming/Hilbert space

Anneal idea: transition from ground state of initial
 Hamiltonian into ground state of problem Hamiltonian

 The idea is to dial this parameter to land in the global minimum (i.e. the solution) of some "problem space" described by J, h:

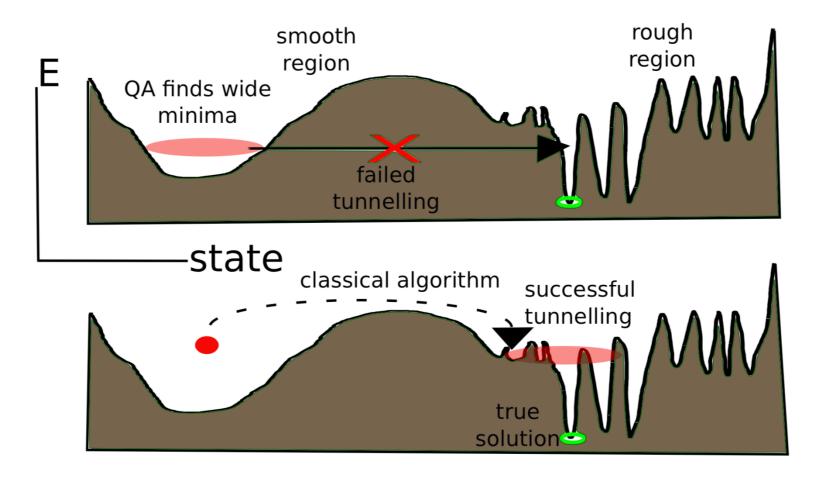




28

Thermal (classical) and Quantum Annealing are complementary:

- \bullet Thermal tunnelling is fast over broad shallow potentials $\sim e^{-{\rm height}/T}$ (Quantum "tunnelling" is exponentially slow)
- Quantum tunnelling is fast through tall thin potentials $\sim e^{-\sqrt{\mathrm{height}} \times \mathrm{width}/\hbar}$ (Thermal "tunnelling" is exponentially slow Boltzmann suppression)
- Hybrid approach can be useful depending on solution landscape



A quantum laboratory for QFT and QML

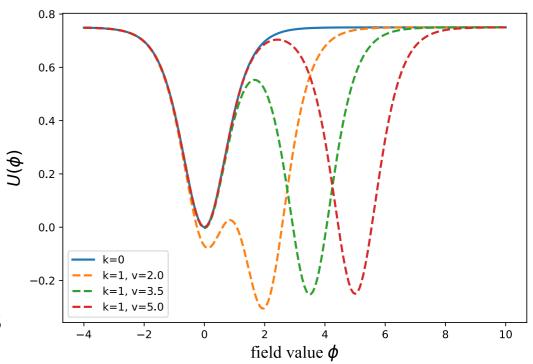
- going beyond the reach of classical computers -
- Using the spin-chain approach for field theories discussed before, we can encode a QFT on a quantum annealer and study its dynamics directly.

[Abel, MS '20]

- To show that the system is a true and genuine quantum system we investigate if the state can tunnel from a meta-stable vacuum into a the true vacuum.
- Choose a potential of interest:

 $U(\phi) = \frac{3}{4} \tanh^2 \phi - k(t) \operatorname{sech}^2 (c(\phi - v))$ where $\phi = \eta/\eta_0$ time dependent

 $\phi(t)$ is the field and c, v are dimless constants



• For real-time evolution of field theory on QA see [Fromm, Philipsen, Winterowd '22]

The tunnelling probability in a QFT is calculated by evaluating the path-integral in Euclidean space around the action's critical points using the steepest gradient-descent method

$$\langle \eta_i | \eta_f \rangle_E = \int \mathcal{D} \delta \eta \, e^{-\hbar^{-1} \int dt \left(\frac{m(\dot{\eta}_{cl} + \delta \dot{\eta})^2}{2} + U(\eta_{cl} + \delta \eta) - E_0 \right)} \quad = A e^{-\hbar^{-1} S_{E,cl}} \quad \text{quantum annealer}$$

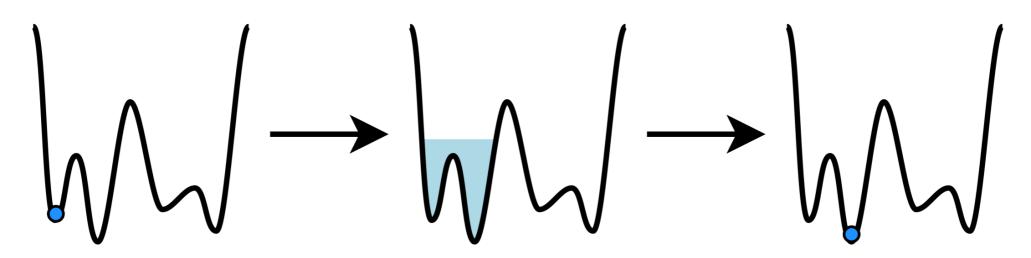
For the tunnelling rate $\Gamma=|\langle \eta_i|\eta_f\rangle_E|^2 \approx e^{-2\hbar^{-1}S_{E,cl}}$ with $S_{E,cl}=\int_{\eta_+}^{\eta_e}d\eta\sqrt{2m(U-E_0)}$

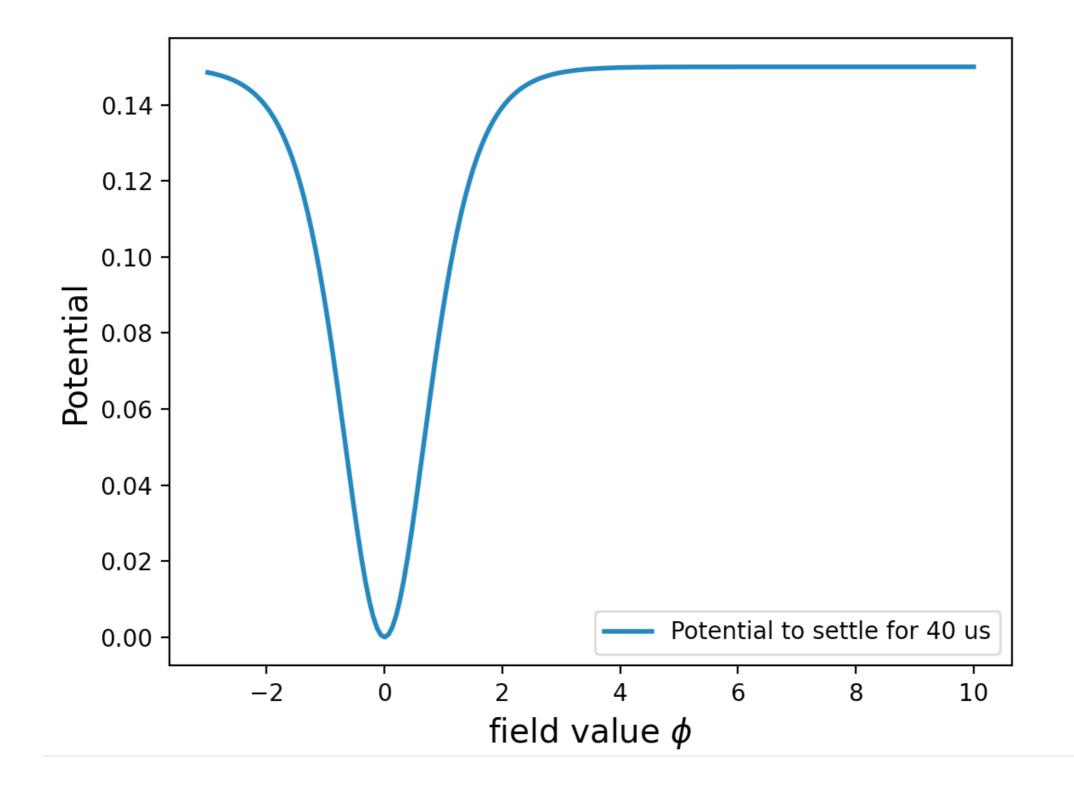
Exponent is object of interest: $\hbar^{-1}S_E \approx \gamma^{-\frac{1}{2}} \int_{\phi_+}^{\phi_e} \sqrt{\frac{3}{4} \tanh^2 \phi - \mathrm{sech}^2(\phi - v)} \, d\phi$ with $\gamma \stackrel{\mathrm{def}}{=} \hbar^2/2m\eta_0^2$

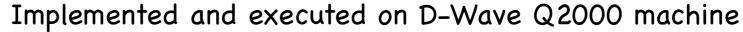
$$\log \Gamma \approx -2\hbar^{-1} S_E \approx \sqrt{\frac{3}{\gamma}} \left(\frac{5}{3} - v\right)$$

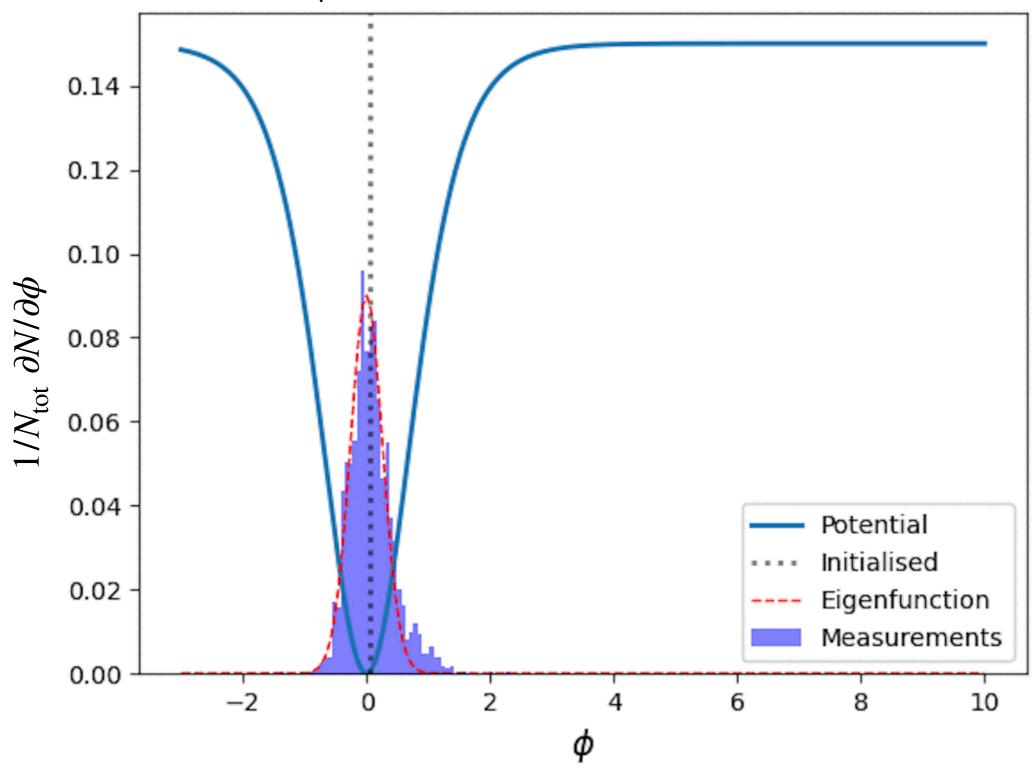
D-Wave reverse annealing

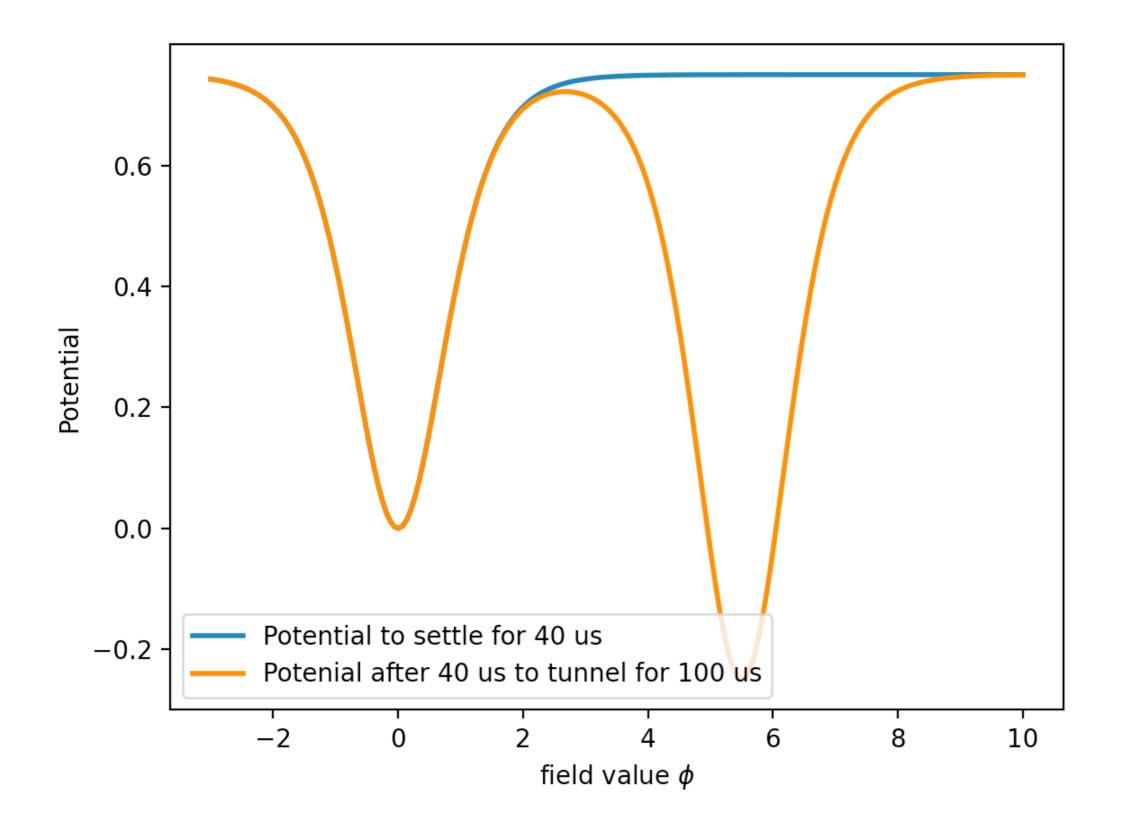
starts at sq=1 (classical) -> sq < 1 (quantum) -> measurement in sq=1 (classical)

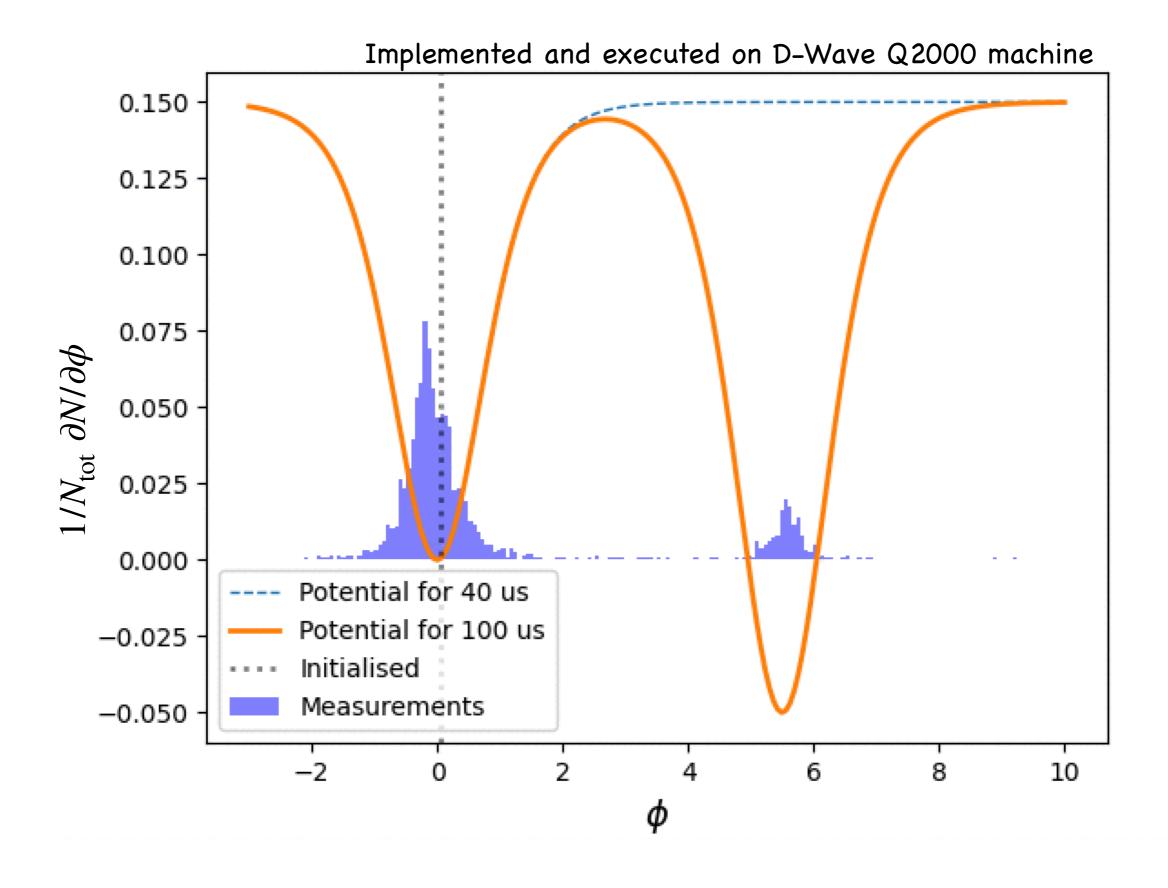




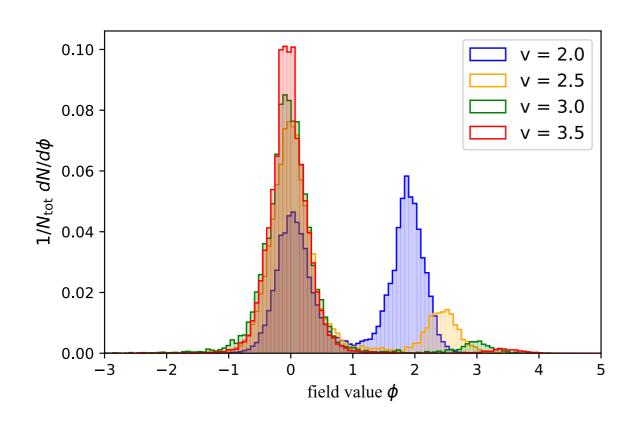








Results: it decays with v as expected

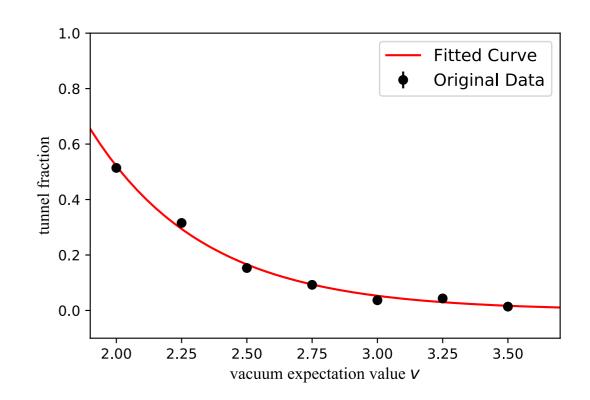


Perform tunnelling for

$$t_{\mathrm{tunnel}} = 100 \mu s$$
 at $s_q = 0.7$

Theory:
$$\log \Gamma = 3.0 \times (1.66 - v)$$

Exp:
$$\log \Gamma = 2.29 \times (1.71 - v)$$



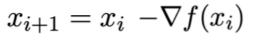
Optimisation comparison quantum vs classical

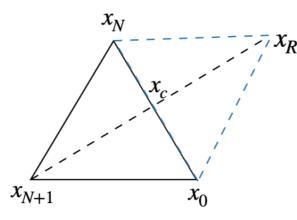
gradient descent

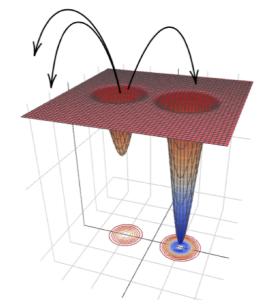
Nelder-Mead

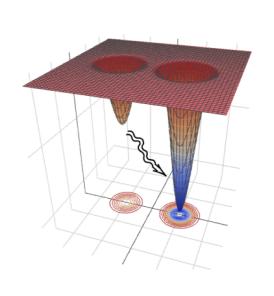
Thermal Annealing

Quantum Annealing



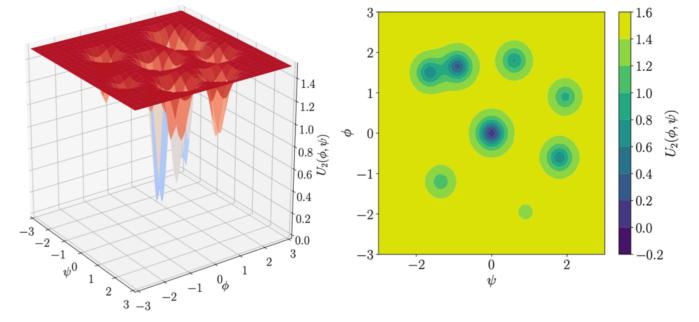






Applied to several examples in [Abel, Blance, MS '21], let's show one here:

Multi-well potential

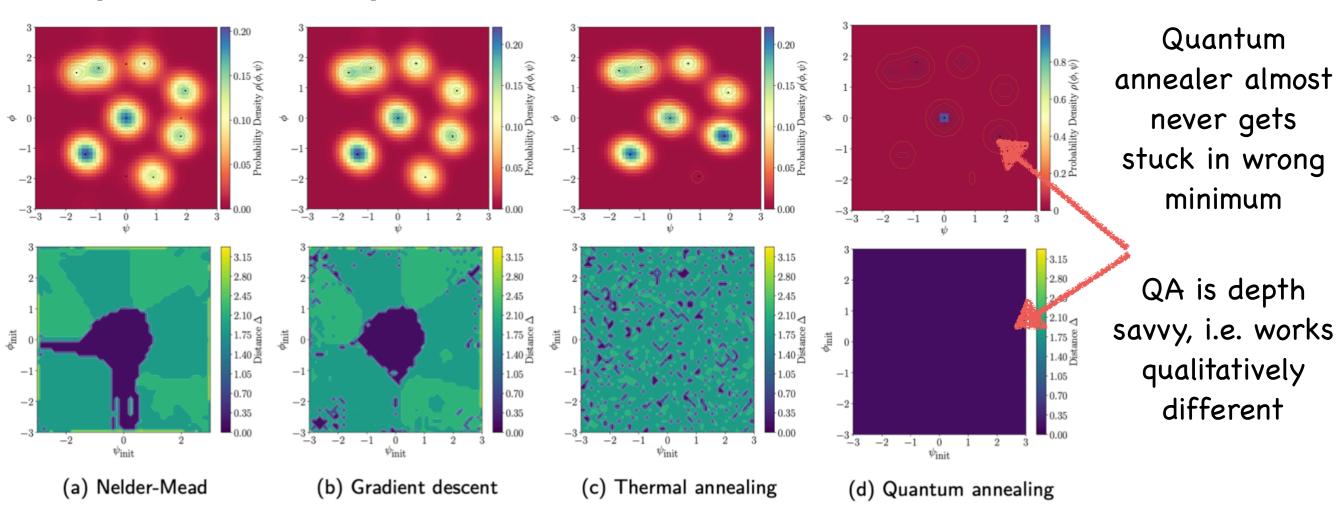


Results for Multi-well potential

 Quantum algorithms finds global minimum of potential reliably and fast!

Method	$\mathbf{Time/run} (\mu \mathbf{s})$			
Nelder-Mead	4900			
Gradient Descent	2900			
Thermal Annealing	$5 imes 10^5$			
Quantum Annealing	115			

[Abel, Blance, MS '21]





Clear advantage

Completely Quantum Neural Networks

Structure of node i, in layer L
$$L_i(x) = g\left(\sum_i w_{ij}x_i + b_i
ight)$$

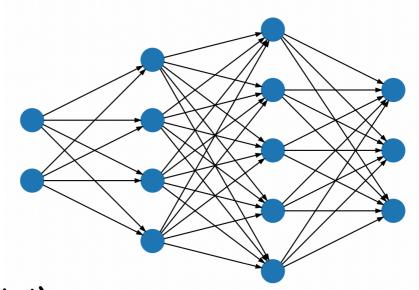
Network output in final layer $Y = L^{(n)} \circ \ldots \circ L^{(0)}$

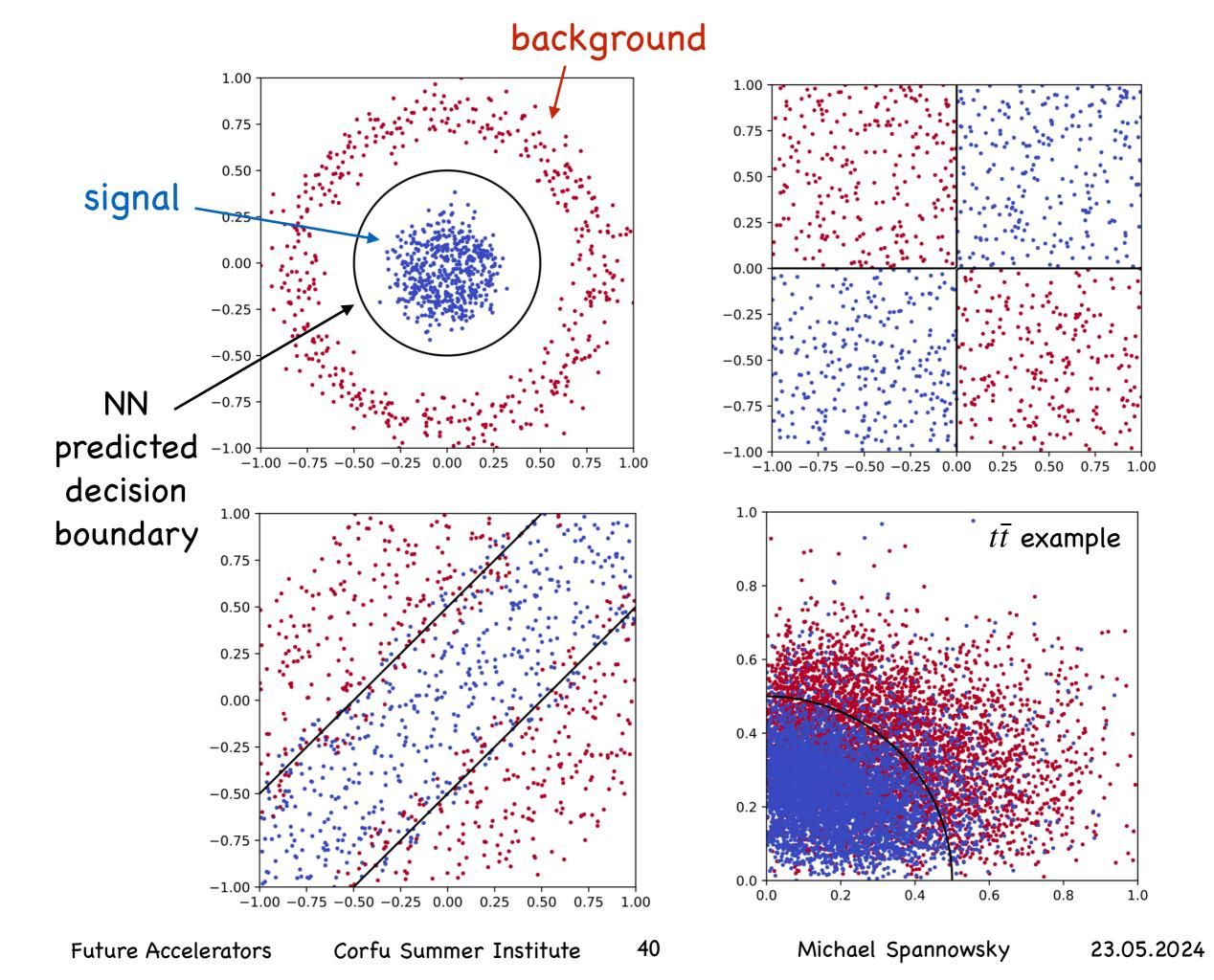
$$Y = L^{(n)} \circ \ldots \circ L^{(0)}$$

Loss function
$$\mathcal{L}(Y) = \frac{1}{N_d} \sum_a |y_a - Y(x_a)|^2$$

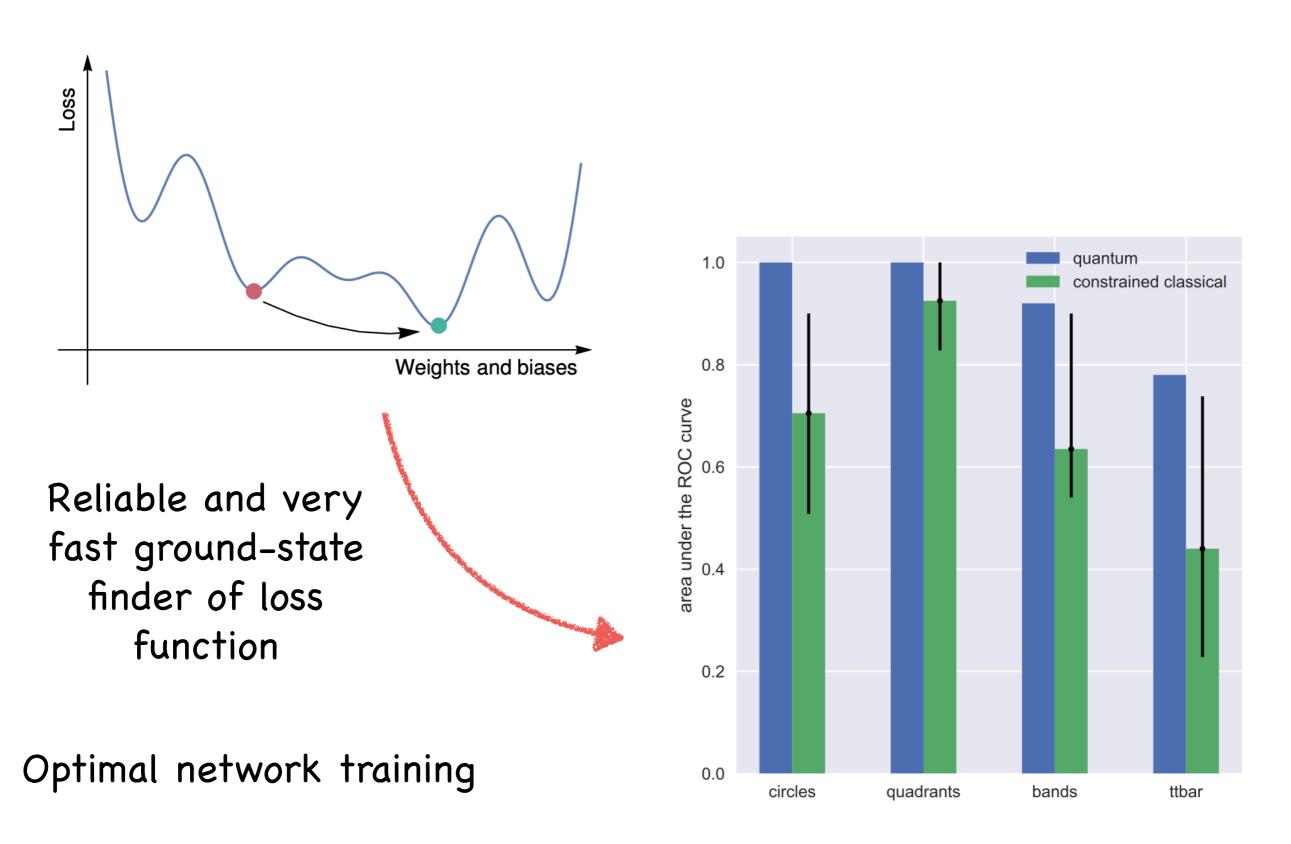
[Abel, Criado, MS '22]

- Developed binary encoding of weights (discretised)
- Polynomial approximation of activation function
- Reduction of binary higher-order polynomials into quadratic ones (Ising model)





Completely Quantum Neural Networks



Application to differential equations and variational methods

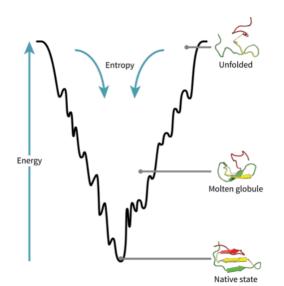
Define your mathematical task as an optimisation problem

$$\mathcal{F}_m(\vec{x}, \phi_m(\vec{x}), \nabla \phi_m(\vec{x}), \cdots, \nabla^j \phi_m(\vec{x})) = 0$$

Build the full function, here a DE into the loss function, incl boundary conditions

$$\begin{split} \mathcal{L}(\{w,\vec{b}\}) &= \frac{1}{i_{\text{max}}} \sum_{i,m} \hat{\mathcal{F}}_m(\vec{x}^i, \hat{\phi}_m(\vec{x}^i), \cdots, \nabla^j \hat{\phi}_m(\vec{x}^i))^2 \\ &+ \sum_{\text{B.C.}} (\nabla^p \hat{\phi}_m(\vec{x}_b) - K(\vec{x}_b))^2 \;, \\ &\text{[Piscopo, MS, Waite '19]} \end{split}$$

identify trial solution with network output $\hat{\phi}_m(\vec{x}) \equiv N_m(\vec{x}, \{w, \vec{b}\})$

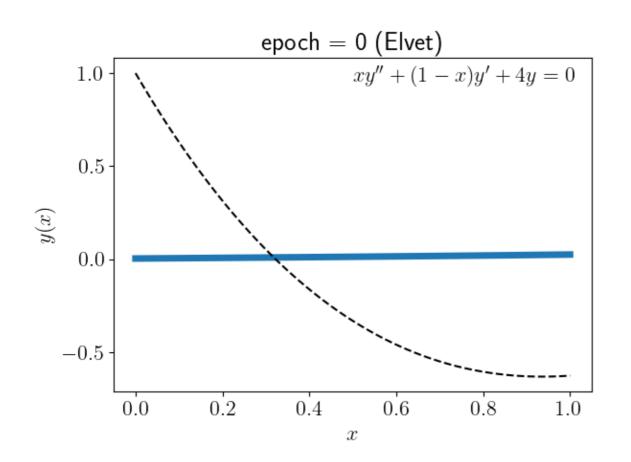


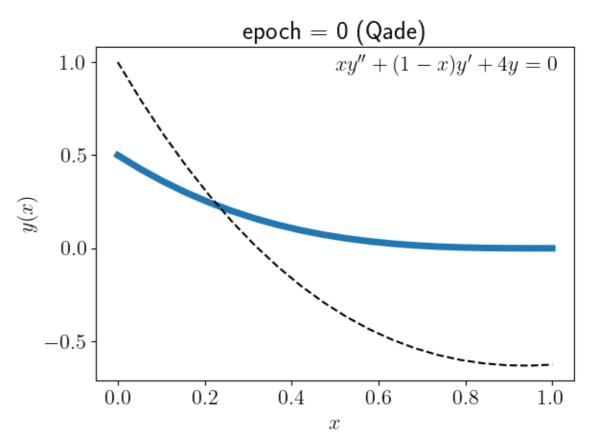
QADE: Solving differential equations with a quantum annealer

[Criado, MS '22]

Example Laguerre differential equation:

$$xy'' + (1-x)y' + 4y = 0$$
 with $y(0) = 1$ and $y(1) = L_4(1)$





Classical Neural Network https://gitlab.com/elvet/elvet

Quantum algorithm http://gitlab.com/jccriado/qade

[Piscopo, MS, Waite '19] [Araz, Criado, MS '21]

QFitter

Example Higgs EFT fit:

[Criado, Kogler, MS '22]

$$\mathcal{L} = \frac{c_{u3}y_{t}}{v^{2}}(\phi^{\dagger}\phi)(\bar{q}_{L}\tilde{\phi}u_{R}) + \frac{c_{d3}y_{b}}{v^{2}}(\phi^{\dagger}\phi)(\bar{q}_{L}\phi d_{R})$$

$$+ \frac{ic_{W}g}{2m_{W}^{2}}(\phi^{\dagger}\sigma^{a}D^{\mu}\phi)D^{\nu}W_{\mu\nu}^{a} + \frac{c_{H}}{4v^{2}}(\partial_{\mu}(\phi^{\dagger}\phi))^{2}$$

$$+ \frac{c_{\gamma}(g')^{2}}{2m_{W}^{2}}(\phi^{\dagger}\phi)B_{\mu\nu}B^{\mu\nu} + \frac{c_{g}g_{S}^{2}}{2m_{W}^{2}}(\phi^{\dagger}\phi)G_{\mu\nu}^{a}G^{a\mu\nu}$$

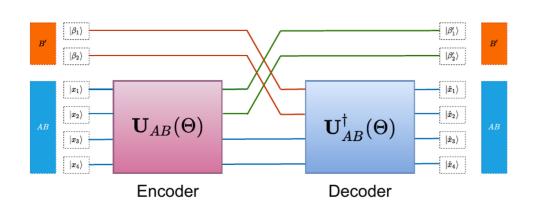
$$+ \frac{ic_{HW}g}{4m_{W}^{2}}(\phi^{\dagger}\sigma^{a}D^{\mu}\phi)D^{\nu}W_{\mu\nu}^{a}$$

$$+ \frac{ic_{HB}g'}{4m_{W}^{2}}(\phi^{\dagger}D^{\mu}\phi)D^{\nu}B_{\mu\nu} + \text{h.c.}$$

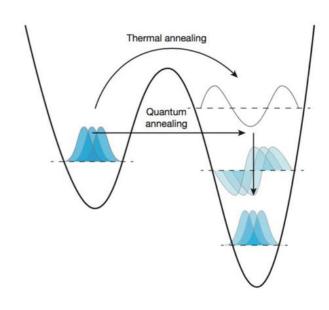
$$\chi^2 = \sum_{ij} V_a C_{ab}^{-1} V_b \qquad V_a = O_a^{(\text{exp})} - O_a^{(\text{th})}(c)$$

- Fast and reliable state-of-the-art Higgs, ELW, ... fits
- Convergence no problem for non-convex $\Delta\chi^2=\chi^2-\chi^2_{\rm min}$ functions

Formulation	Method	Fit time	c_{HW}	c_H	c_g	c_{γ}	χ^2
Standard	Minuit (initial $c_{HW} = 0$) Minuit (initial $c_{HW} = -0.05$) Simulated annealing (initial $c_{HW} = 0$) Simulated annealing (initial $c_{HW} = -0.05$)	$642\mathrm{s}$	-0.050 -0.009	$0.039 \\ 0.100$	1.4×10^{-5} -9.7×10^{-6} 1.4×10^{-5} 1.4×10^{-5}	$-1.0 \times 10^{-4} \\ 3.7 \times 10^{-6}$	$\begin{array}{c} 135 \\ 4110 \end{array}$
QUBO	Simulated annealing (Class A) Simulated annealing (Class B) Quantum annealing	$6.4 \mathrm{s}$ $6.4 \mathrm{s}$ $0.2 \mathrm{s}$	-0.045	-0.175	-3.0×10^{-5} -3.7×10^{-5} 1.9×10^{-5}	1.8×10^{-4}	3910 228 68



Summary



- Quantum Computing is exciting research area that rapidly expands,
 supported through private and public sector. Many methods to be invented.
 - → Can exploit QM prop: entanglement, superposition principle and tunnelling
- HEP is inherently quantum mechanical, thus description in terms of quantum computing should be advantageous
 - → Suitable theory description needed for QC devices
 - → Path to an application yielding quantum advantage



• For quantum advantage in real-world applications need development of technical realisation of quantum computers (size, fault tolerance, type of operations,...)