Quantum Computing for High energy physics: CERN perspective

Workshop on Tensor Networks and (Quantum) Machine Learning for High-Energy Physics

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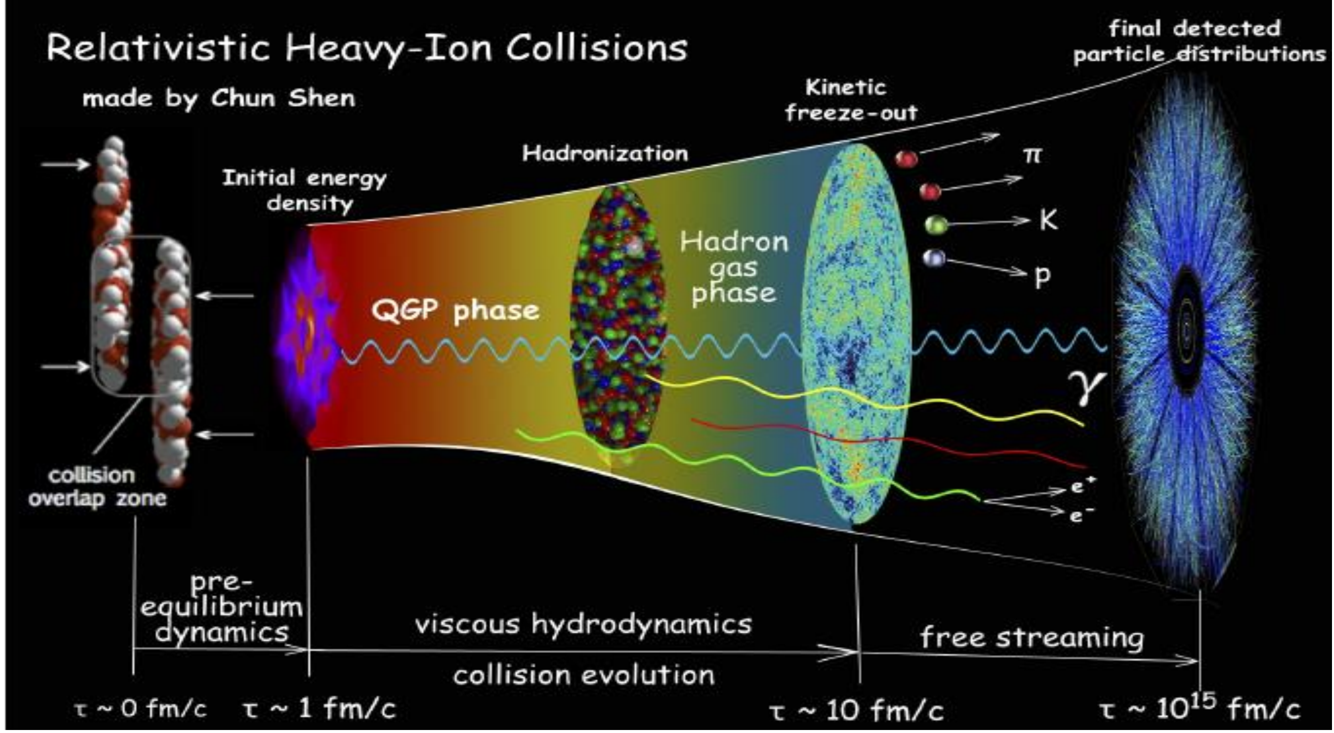
QUANTUM TECHNOLOGY INITIATIVE

Motivation

Theoretical challenge

- Non-zero chemical potential (QCD phase diagram)
- Real time dynamics

  → heavy ion collisions, scattering quenches



From: 10.1051/epjconf/20159700025
Cartoon of the time evolution of an ultra-relativistic heavy-ion collision

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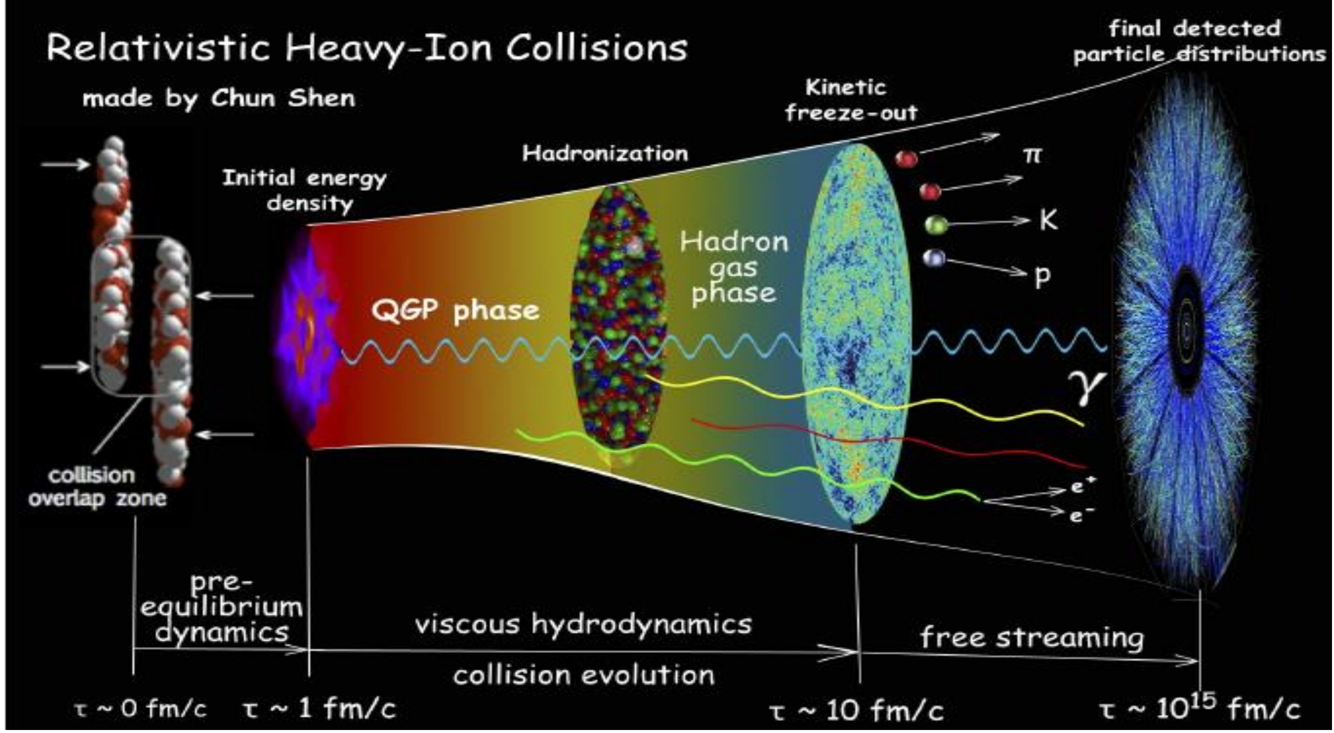

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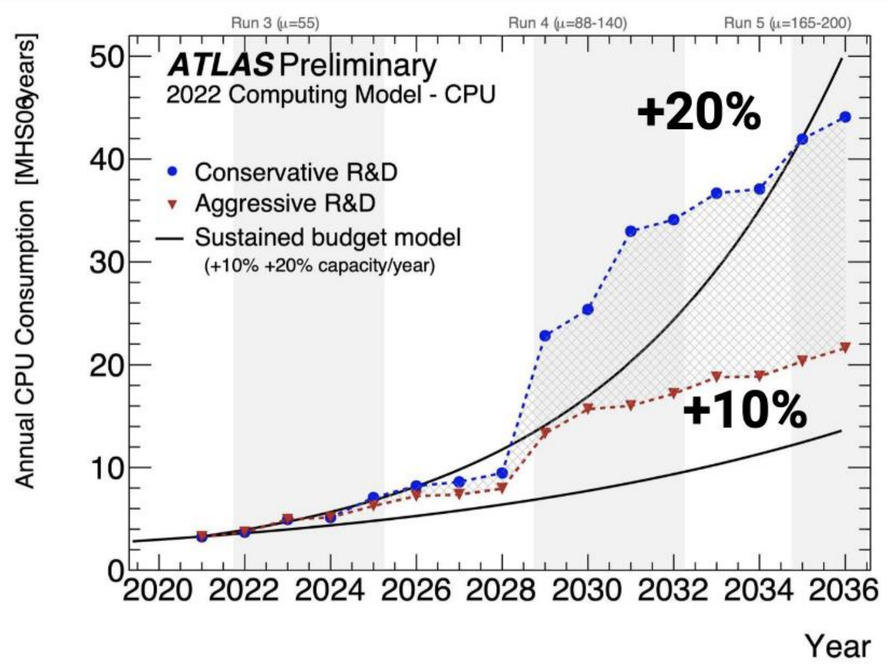
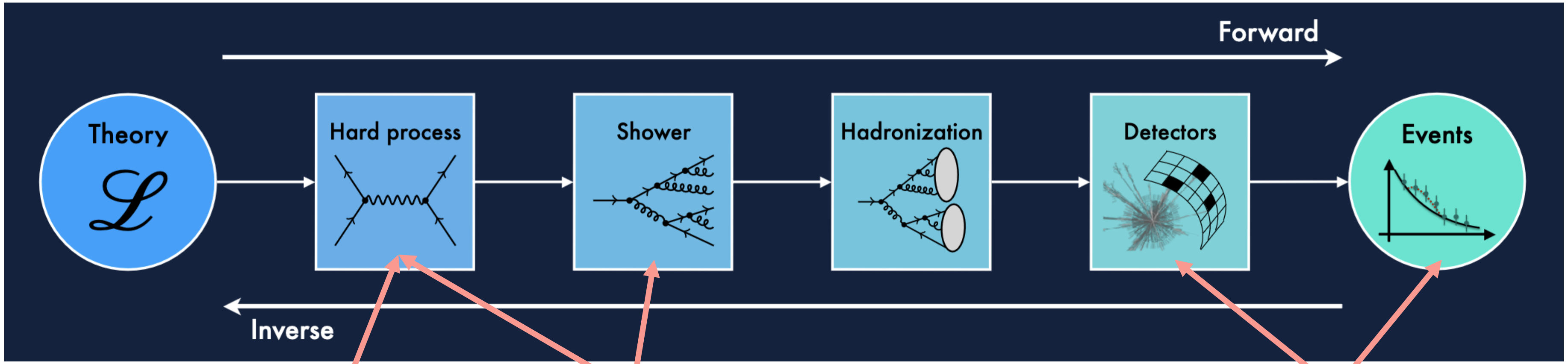


From HL-LHC Projections - ATLAS Software and Computing HL-LHC Roadmap

Computing challenge for High-Lumi LHC

- Simulation and analysis

  → need: new technology, algorithms and methods



interference [2110.10112]

Bell inequalities [2102.11883, 2203.05582]

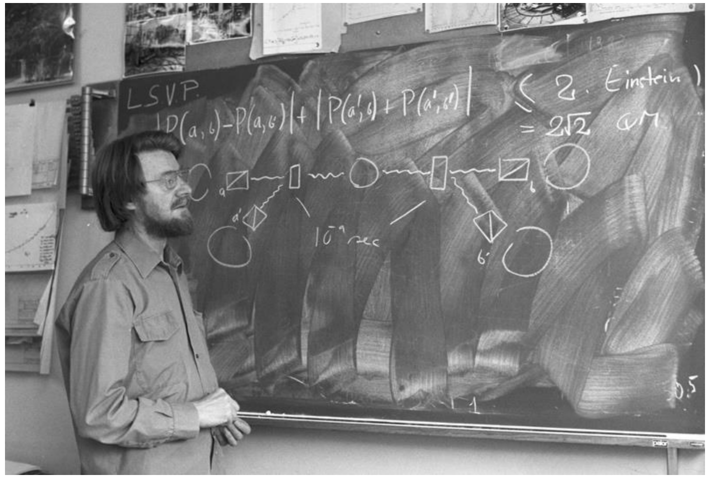
entanglement [1703.02989]

spin correlations [1907.03729]

Fundamental motivation

Utilise information and correlations inherent in HEP data.

Exploit "quantum remnants" in data.



Quantum Machine Learning Challenge

CERN examples

Discussion

Quantum Machine Learning Challenge

CERN examples

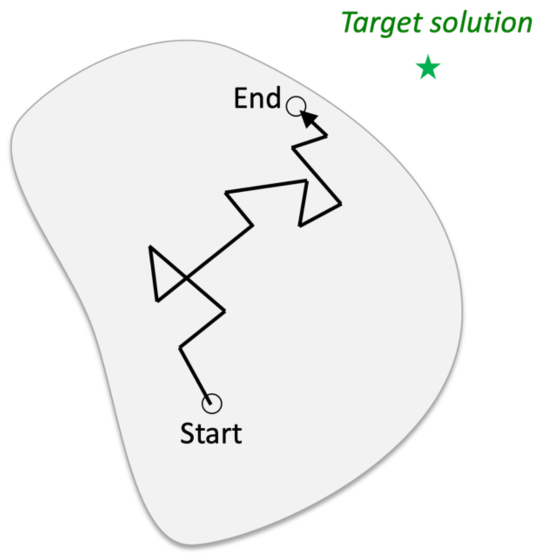
Discussion

Model Space and Learning Algorithms

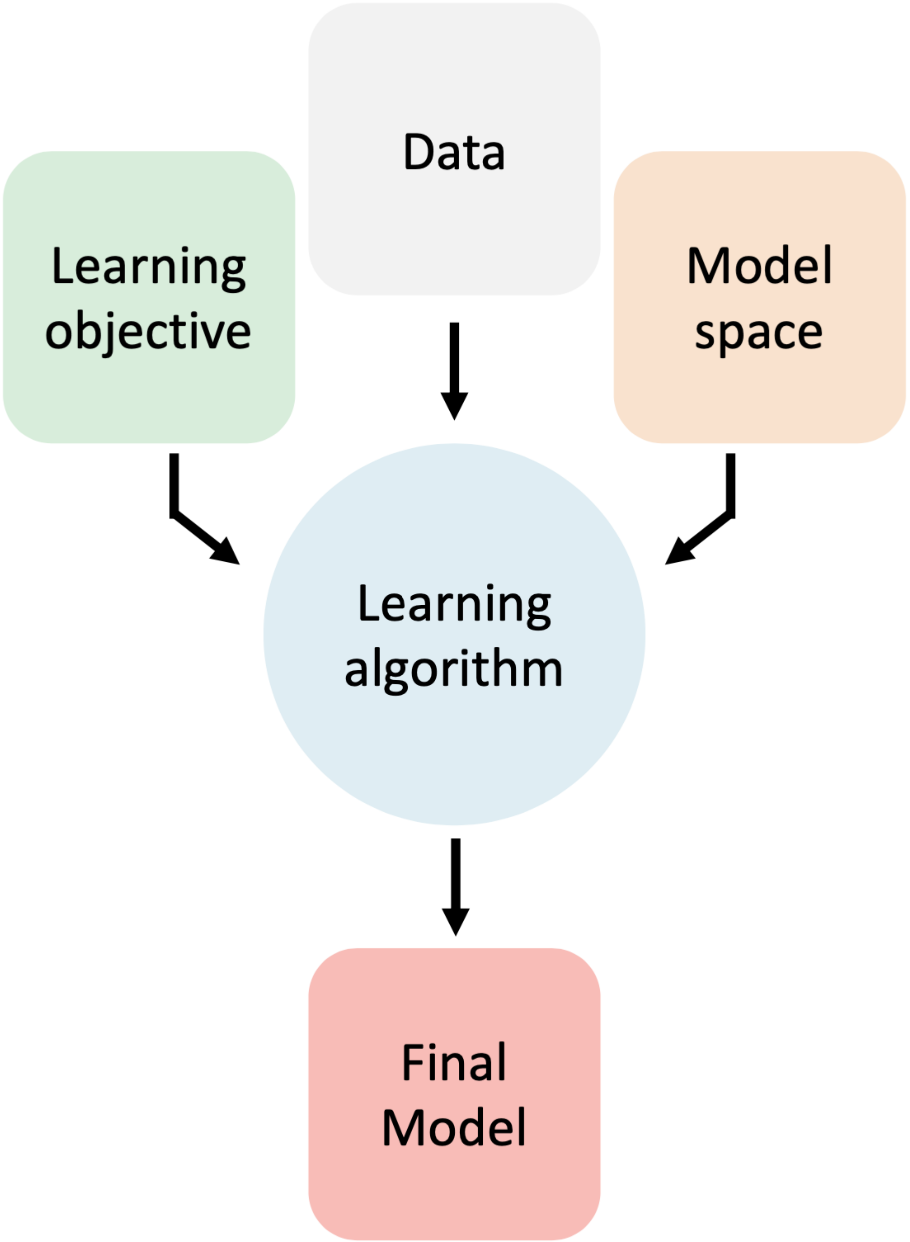
- Choose type of model
  - Each set of parameters is a point in space of models
- Need to find the best model parameters for loss
- **Learning is like a search** through space of models,

guided by the data

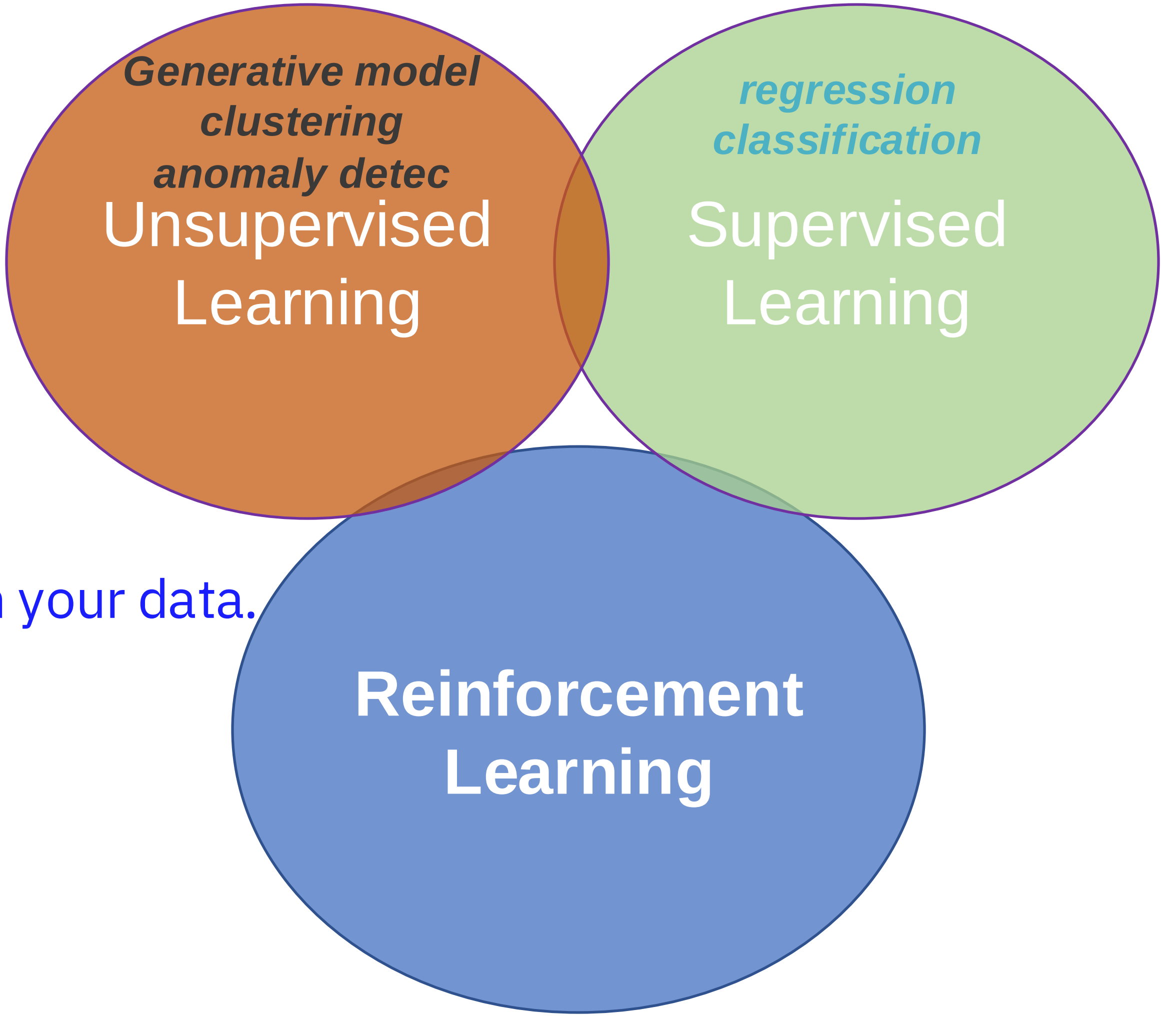
- Various possibilities
  - Exhaustive search
  - Closed for solutions (rare)
  - Iterative optimization



Space of Possible Models



Machine Learning + QC



Supervised ML

Labeled data, i.e., data with defined output.

A model is trained giving this data and you have direct evaluation.

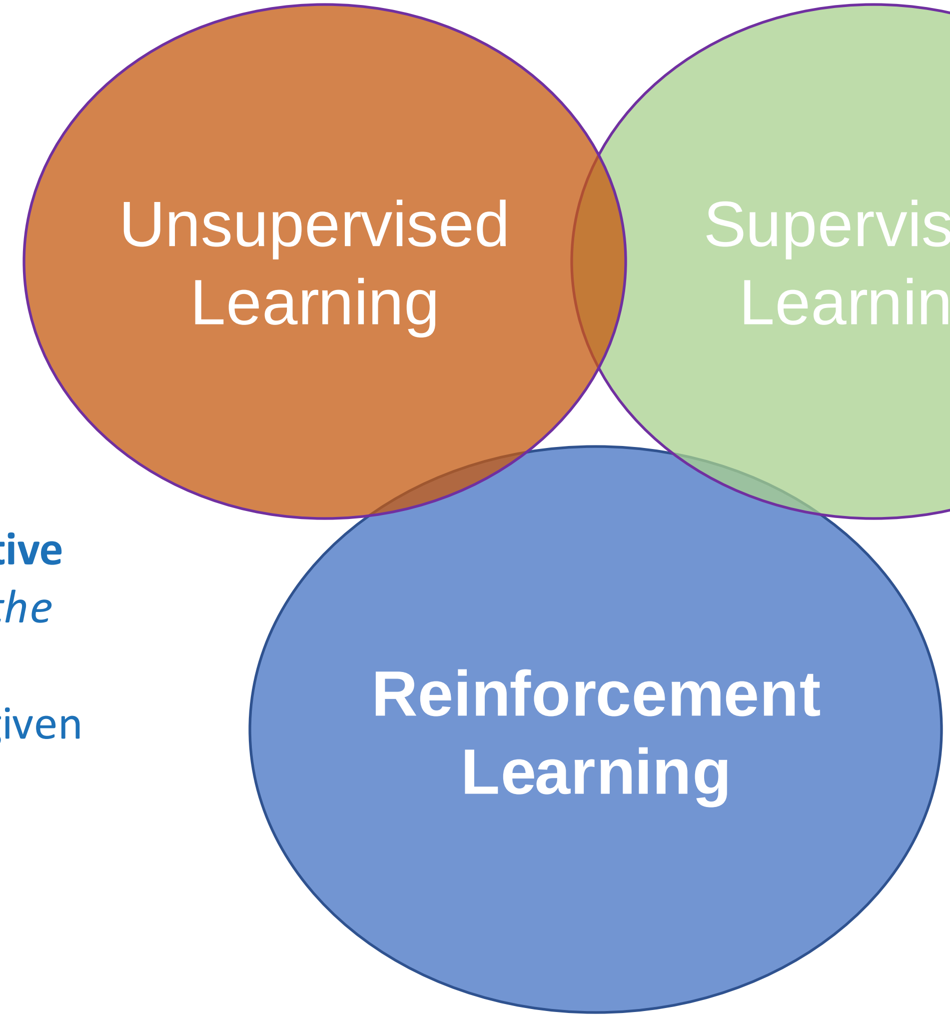
Unsupervised ML

Unlabeled data.

ML finds patterns in your data.

Indirect evaluation.

Quantum Machine Learning



Supervised ML

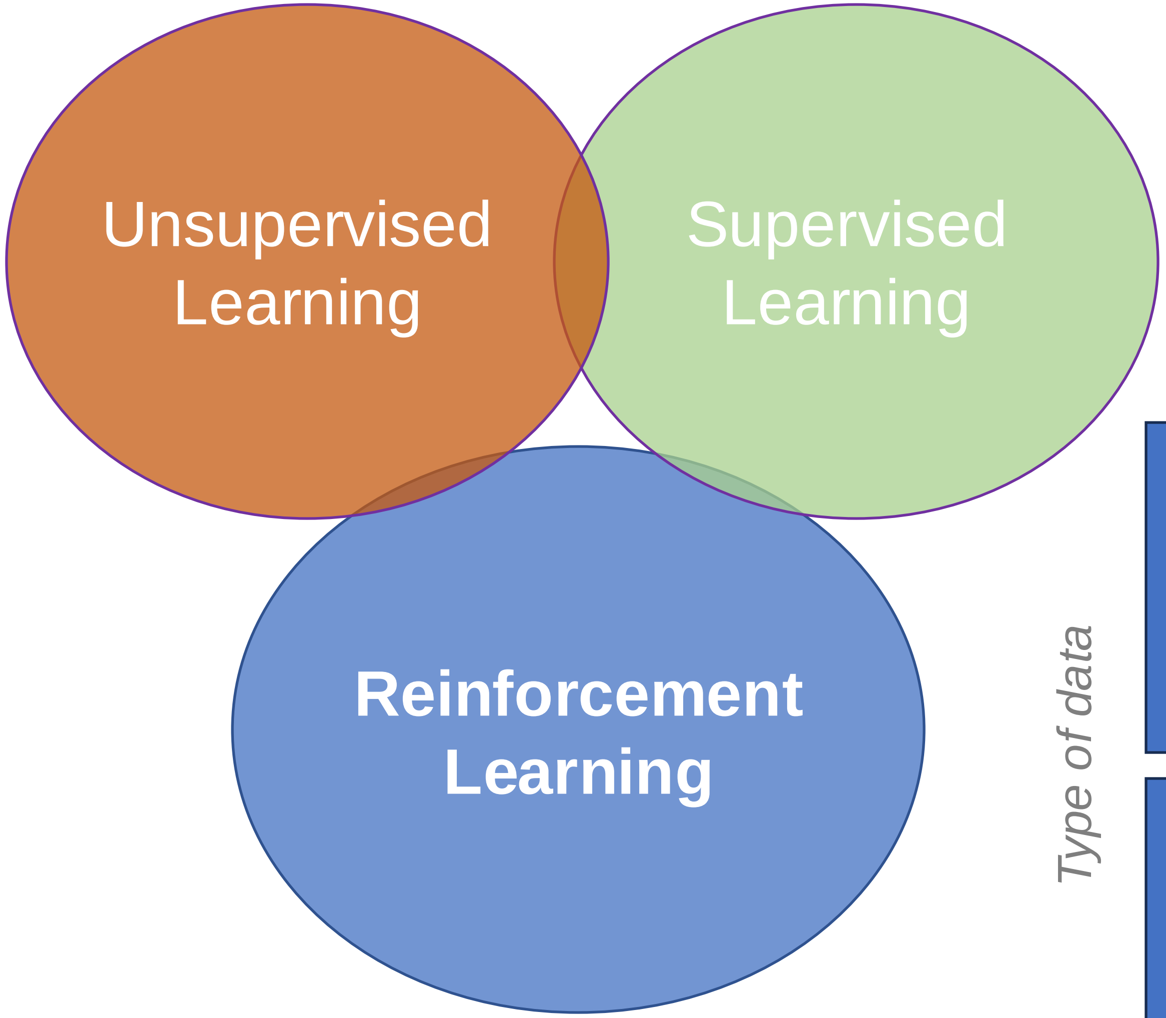
e.g., **Quantum Classifier**: aims to learn *input-output relation* of labeled dataset $f: x_{in} \mapsto x_{out}$ by optimizing quantum network

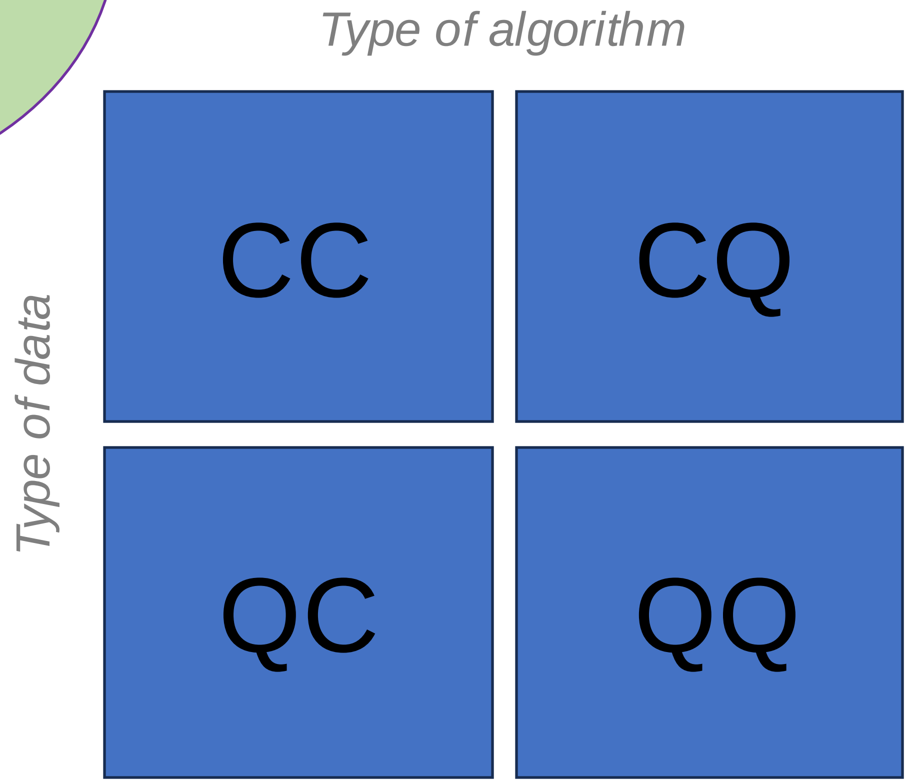
Unsupervised ML

e.g., **Quantum Generative Models**: aims to *learn the underlying probability distribution* $\pi(y)$ of a given data set and *generates samples* from it using quantum network

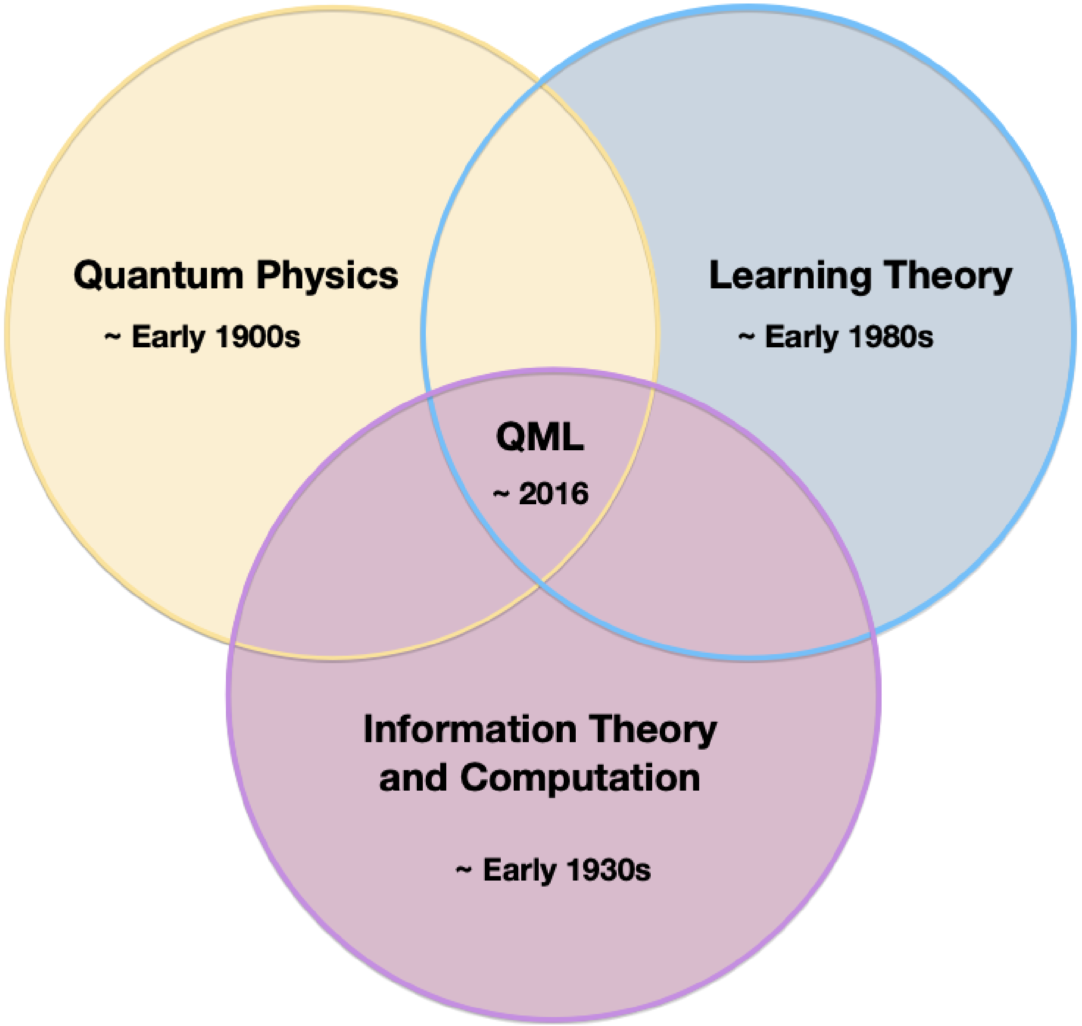
→ See Elias' talk ☺

Quantum Machine Learning

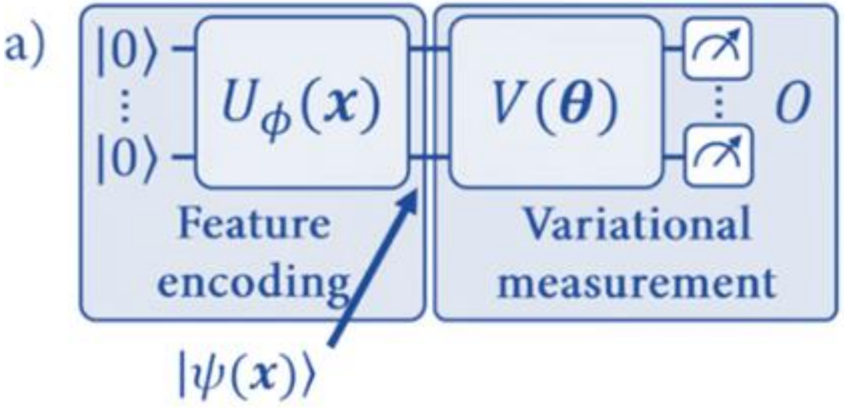




Quantum Machine Learning (QML)



QML models



a) Explicit quantum model:

$$\rho(\boldsymbol{x}) = |\psi(\boldsymbol{x})\rangle\langle\psi(\boldsymbol{x})|$$

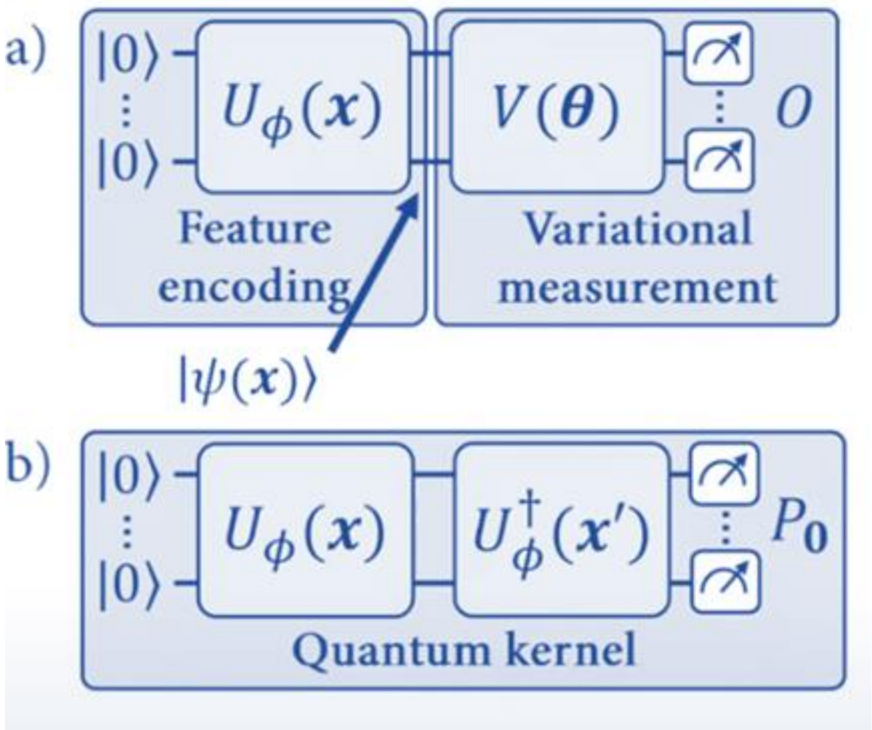
$$f_{\boldsymbol{\theta}}(\boldsymbol{x}) = \mathrm{Tr}[\rho(\boldsymbol{x})O_{\boldsymbol{\theta}}]$$

$$O_{\boldsymbol{\theta}} = V^\dagger(\boldsymbol{\theta})OV(\boldsymbol{\theta})$$

A linear model with a restricted $\boldsymbol{w}$

S.Jerbi at al., Quantum Machine Learning Beyond Kernel Methods – Nature Communications 14, 517 (2023)

QML models



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A linear model with a restricted $\boldsymbol{w}$

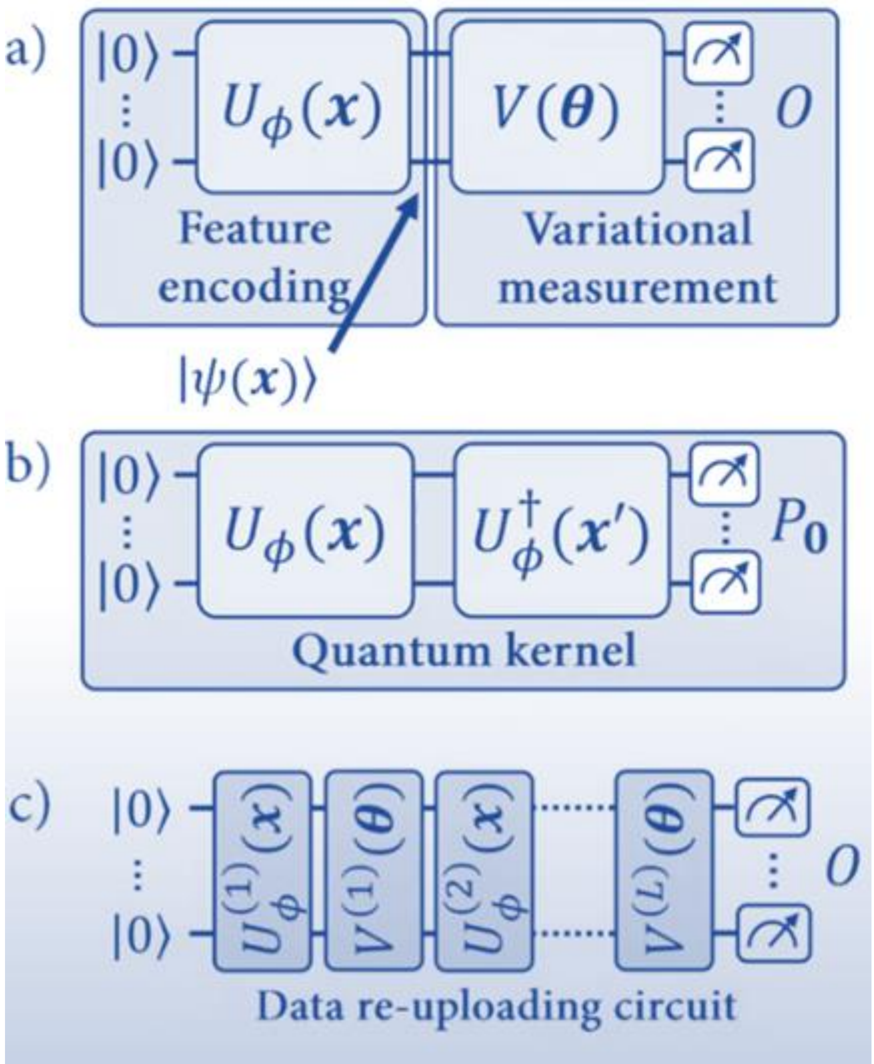
b) Implicit quantum model:

$$f_{\boldsymbol{\alpha}}(\boldsymbol{x}) = \mathrm{Tr}\left[\rho(\boldsymbol{x})O_{\boldsymbol{\alpha},\mathcal{D}}\right] \qquad O_{\boldsymbol{\alpha},\mathcal{D}} = \sum_{m=1}^{M} \alpha_m \rho(\boldsymbol{x}^{(m)})$$

A kernel linear model

S.Jerbi at al., Quantum Machine Learning Beyond Kernel Methods – Nature Communications 14, 517 (2023)

QML models



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$\boxed{\text{A linear model with a restricted } \boldsymbol{w}}$

b) Implicit quantum model:

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$\boxed{\text{A kernel linear model}}$

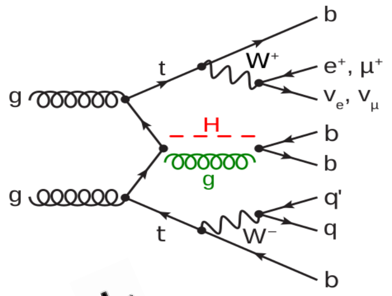
c) Data re-uploading model:

$$f_{\boldsymbol{\theta}}(\boldsymbol{x}) = \mathrm{Tr}[\rho(\boldsymbol{x},\boldsymbol{\theta})O_{\boldsymbol{\theta}}]$$

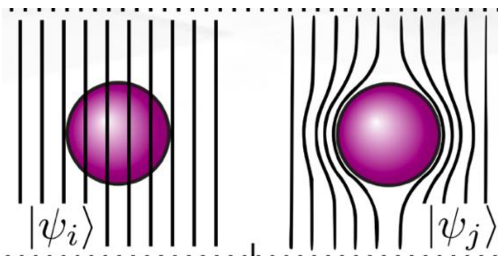
S.Jerbi at al., Quantum Machine Learning Beyond Kernel Methods – Nature Communications 14, 517 (2023)

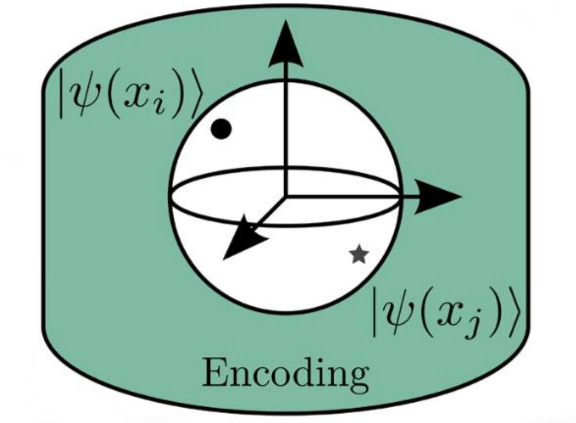
QML Pipeline

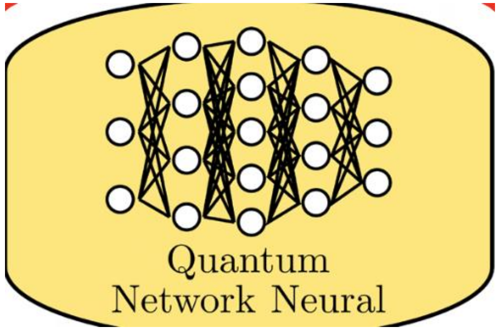
Classical Data



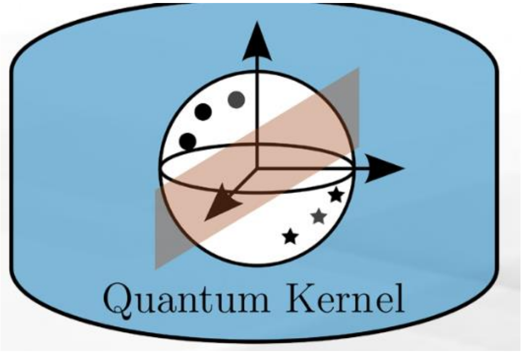
Quantum Data







training



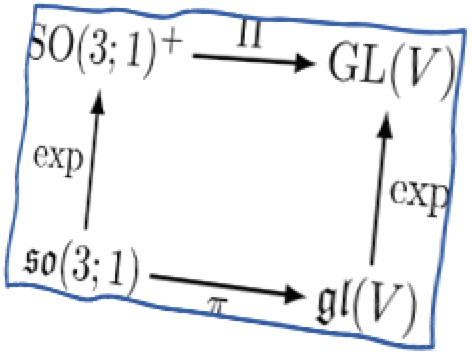
Theoretically: $P(0) = \mathrm{Tr}[|0\rangle\langle 0|\rho]$.
In practice: $P(0) = \frac{N_0}{N}$ with a statistical precision of order $\frac{1}{\sqrt{N}}$

Signal/Background
Paramagnetic/Ferromagnetic
prediction

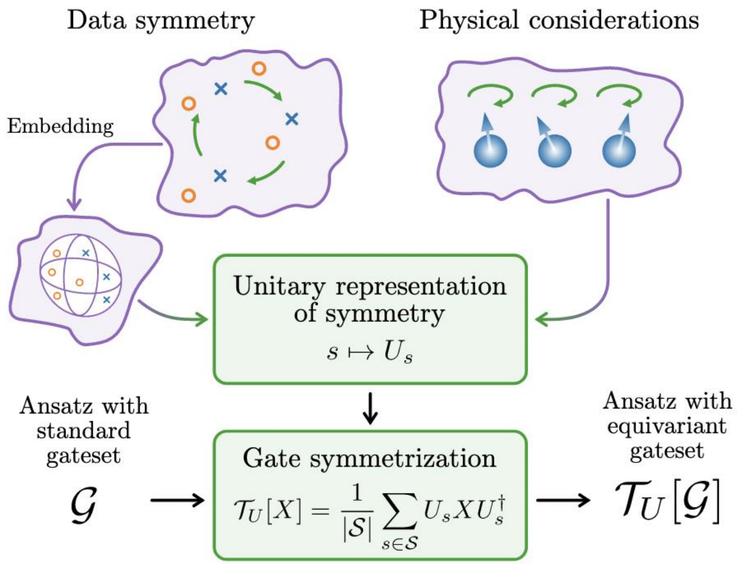
QML models implementations for NISQ

Variational algorithms - EXPLICIT

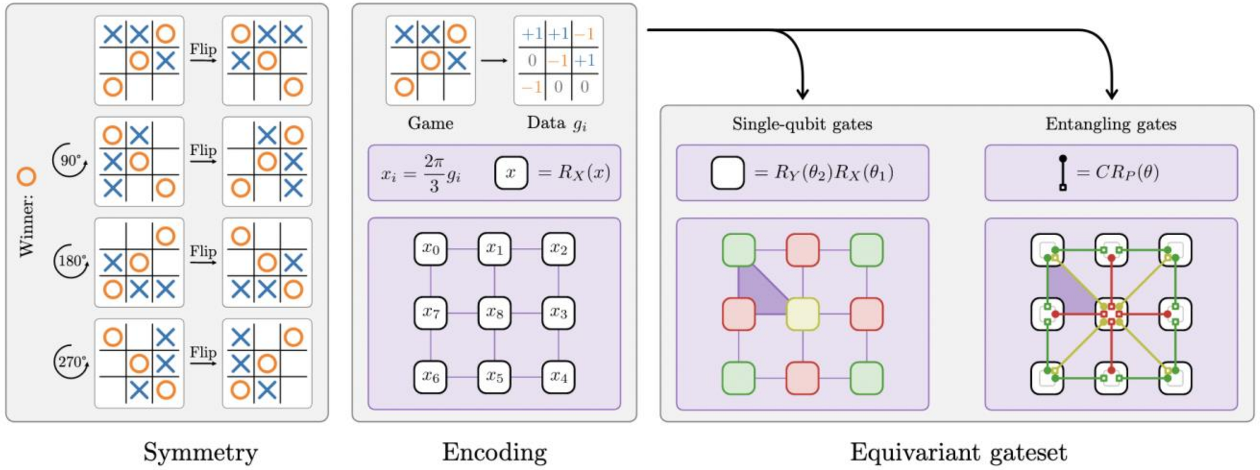
- Flexible parametric ansatz: design can leverage data symmetries[1,2]
- Can use **gradient-free** methods or **stochastic gradient-descent**
- **Data Embedding** can be **learned**
- **Better generalization[2,3]**



https://github.com/fizisist/LorentzGroupNetwork



A unitary representation of a symmetry group S can arise from data symmetries when the data points are suitably encoded or alternatively from physical considerations of a variational problem[2].

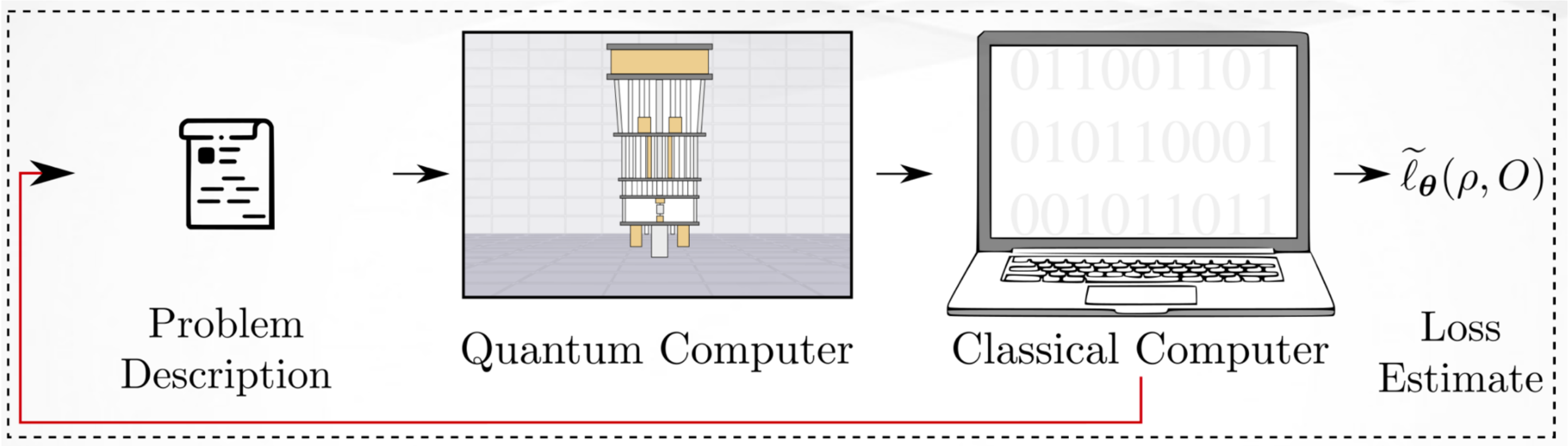


1-A. Bogatskiy et al. "Lorentz group equivariant neural network for particle physics." PMLR, 2020
2-J. Meyer et al "Exploiting symmetry in variational quantum machine learning", PRX Quantum 4, 010328 (2023)
3-S.Jerbi at all., Quantum Machine Learning Beyond Kernel Methods Nature Communications 14, 517 (2023)

Variational Quantum Algorithms

Variational Quantum Algorithms have many similarities with classical machine learning.
To devise a first quantum machine learning model, few details need to be added, namely **data encoding** and **cost data dependence.**

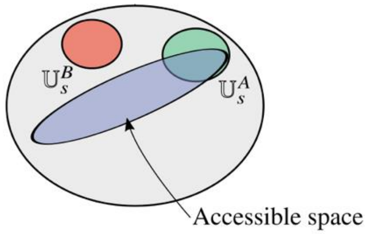
The loss/cost function is obtained by classically post-processing the measurement results, including data dependence**.**



$$\ell_{\boldsymbol{\theta}}(\rho, O) = \mathrm{Tr}\left[\rho U^{\dagger}(\boldsymbol{\theta}) O U(\boldsymbol{\theta})\right]$$

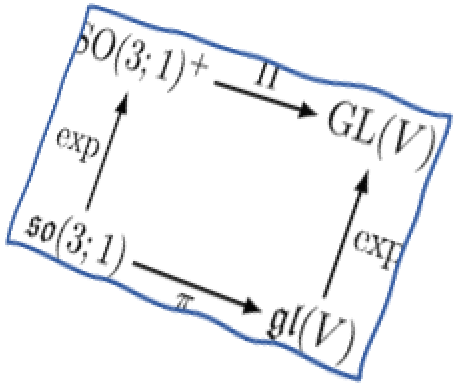
The Hilbert space can serve as an ***exponentially big feature space***

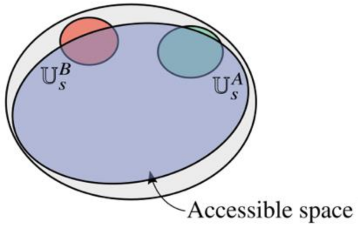
Variational Quantum Algorithms – the Challenge



1. **<u>Efficient data handling and data embedding</u>**
2. **<u>Ansatz choice</u>**

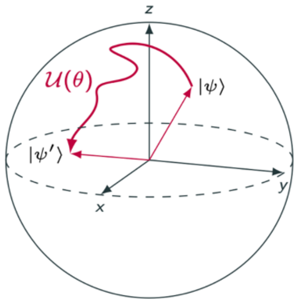
   Can we find the most suitable ansatz for the given problem?
   How well can we survey the Hilbert space (SYMMETRY?!)?





3. **<u>Trainability</u>**

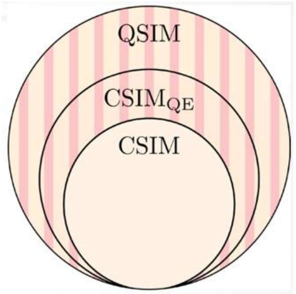
   Can the parameters be updated?



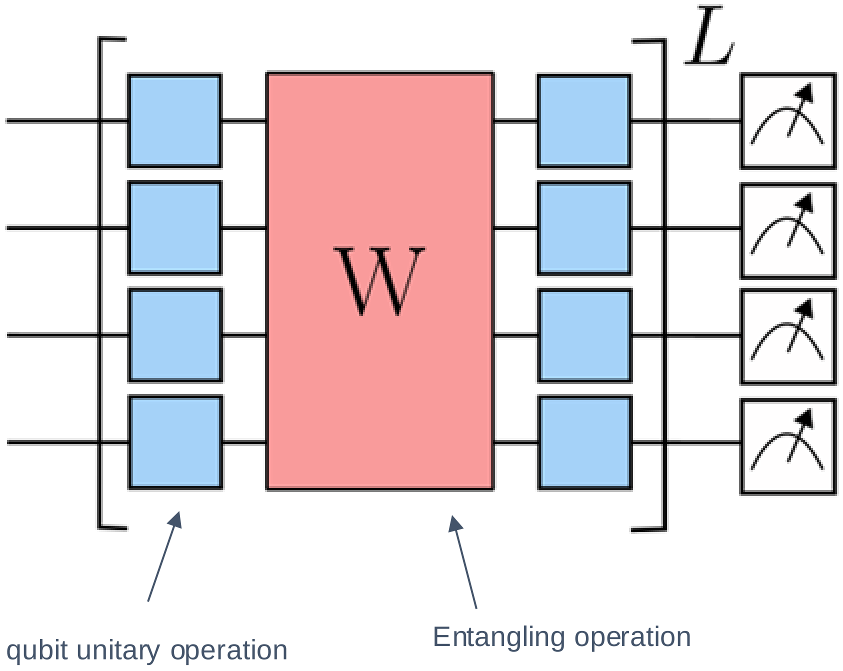
4. **<u>Classical Simulability</u>**

   Are the quantum simulations classically simulable?
   No need for a quantum computer!?

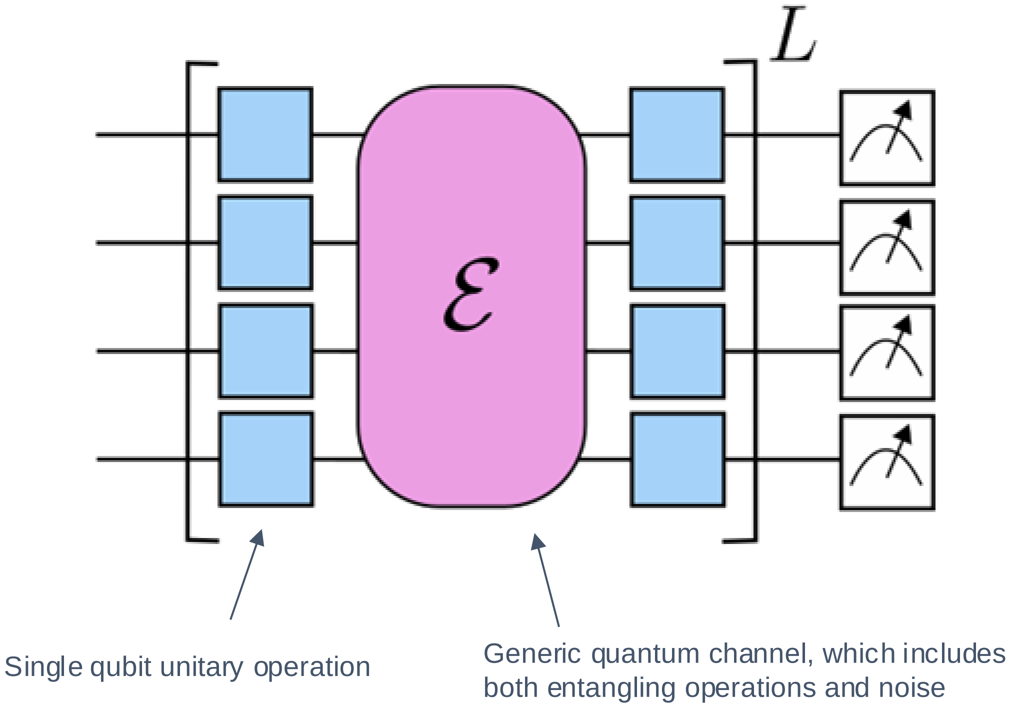
   Just because we can simulate a loss, does not mean it is practical to do so!



What about noise? Non-unitary QML



Add noise



The presence of noise is often overlooked in such analyses

→ Symmetry breaking in geometric quantum machine learning in the presence of noise

[MG et al. PRX Quantum 5, 030314]

→ Estimates of loss function concentration in noisy parametrized quantum circuits

[G. Crognaletti., GM, et al – arXiv:2410.01893]

Quantum Machine Learning Challenge

CERN examples

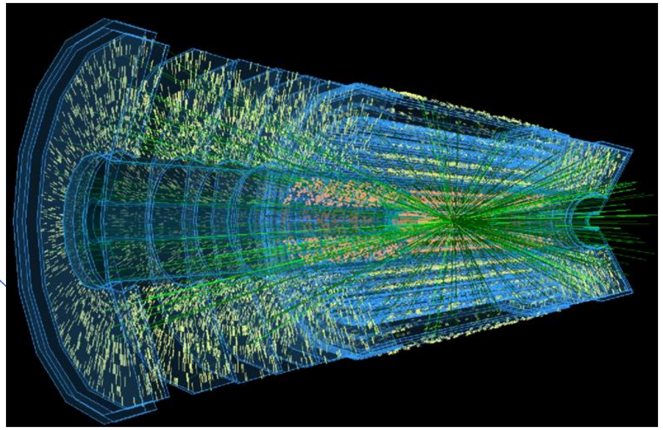
Discussion

HEP Pipeline

Theory

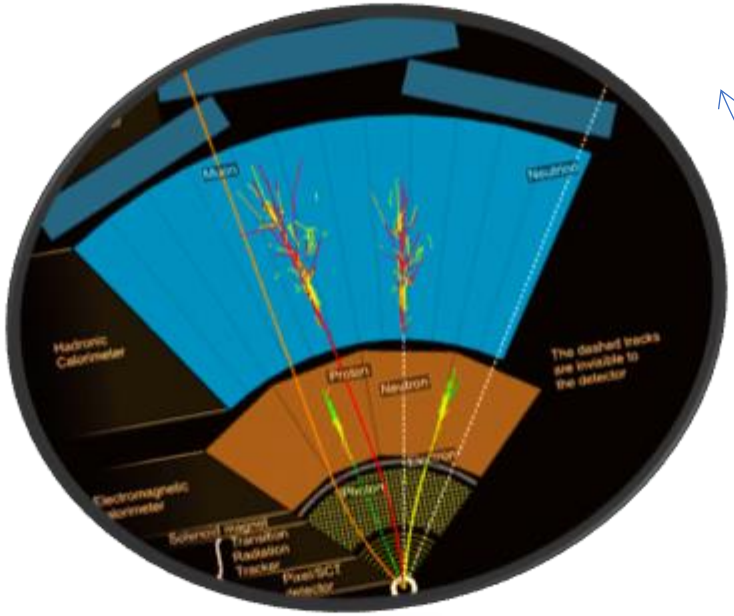
Calculate (differential) cross sections

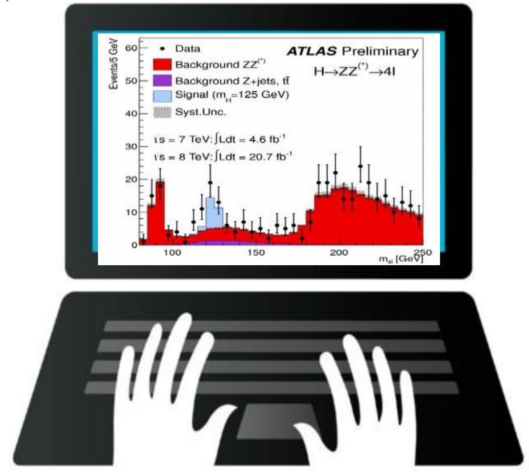
$$d\sigma = \frac{1}{\text{flux}} dx_a dx_b\, f(x_a) f(x_b)\, d\Phi_n \left\langle\, |M_{\lambda,c,\ldots}(p_a, p_b \mid p_1, \ldots, p_n)|^2 \,\right\rangle$$



Data Generation

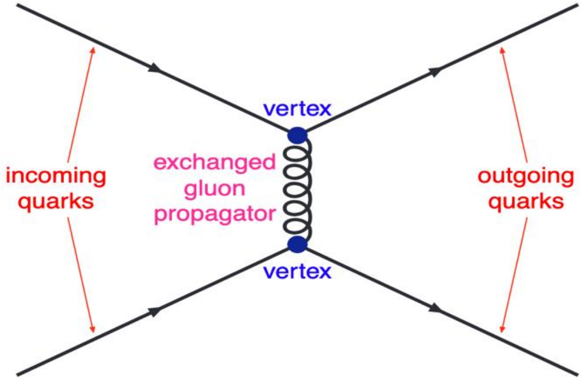
Data Analysis





Feature Extraction

Theory



3 billions CPU hours/year
15% is MC integration

phase-space factor

integrand

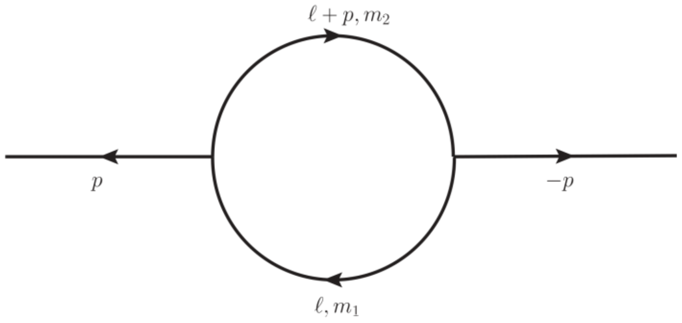
$$\sigma = \frac{1}{F}\int d\Phi |M|^2 \Theta(\Phi - \Phi_c)$$

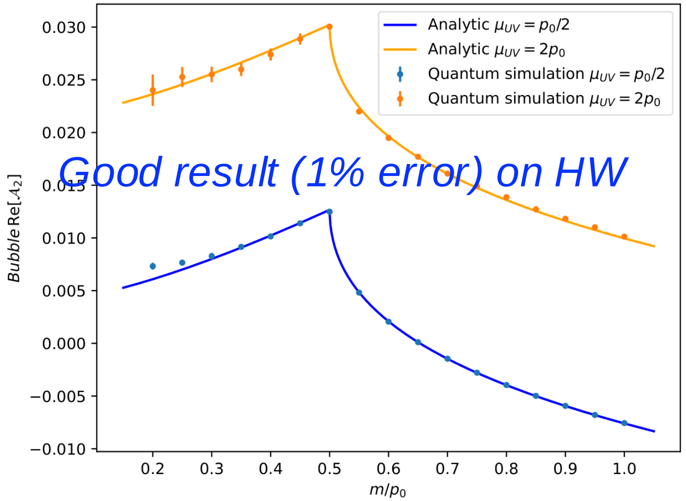
phase-space cuts

probability distributions/
matrix element

Agliardi, Grossi, Pellen, Prati "**Quantum integration of elementary particle processes**." https://doi.org/10.1016/j.physletb.2022.137228

Theory

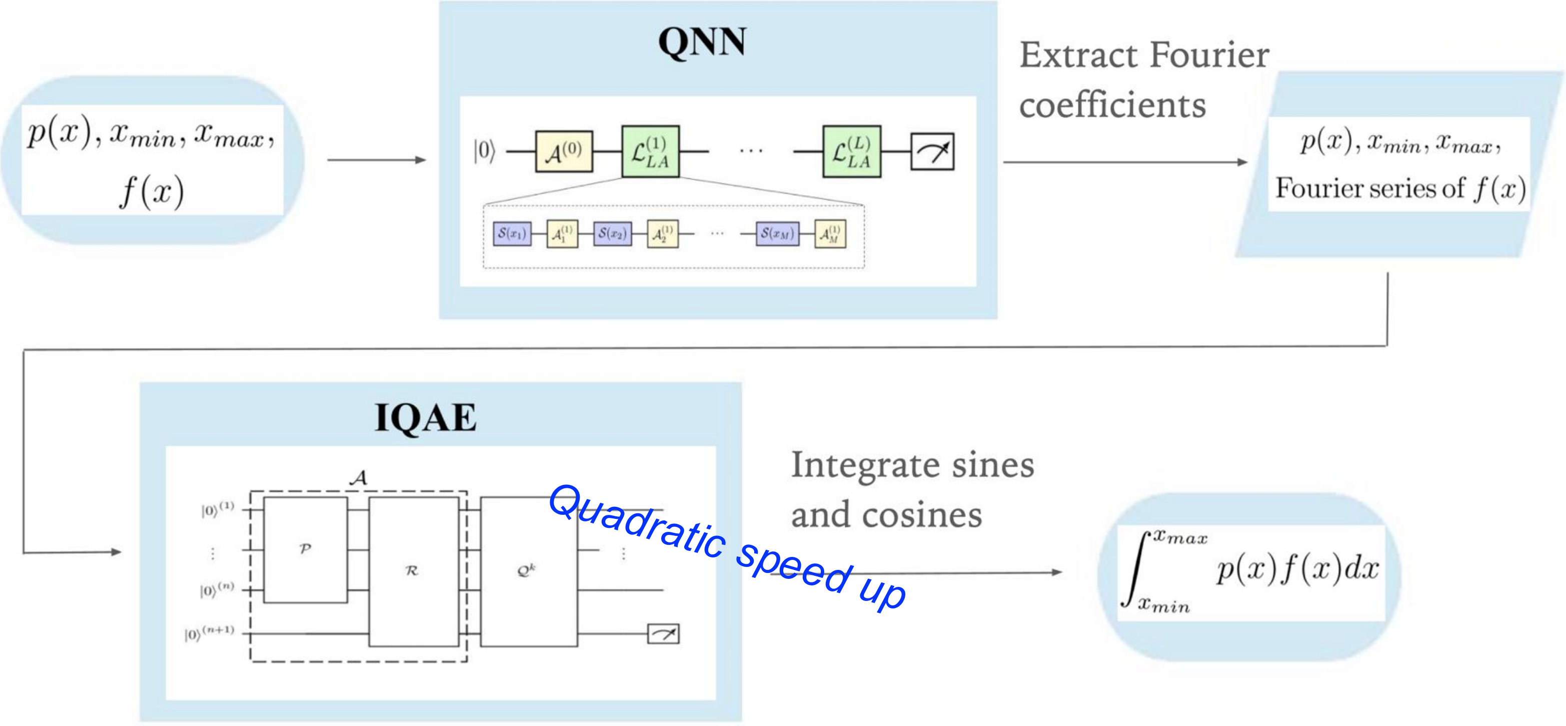




Good result (1% error) on HW

Loop Feynman integral (Bubble)

$$\mathcal{A}_2^{(1)}(p, m_1, m_2) = \int_\ell \prod_{i=1}^{2} G_F(q_i) = \int_\ell \frac{1}{(\ell^2 - m_1^2 + \imath 0)\,((\ell + p)^2 - m_2^2 + \imath 0)}$$

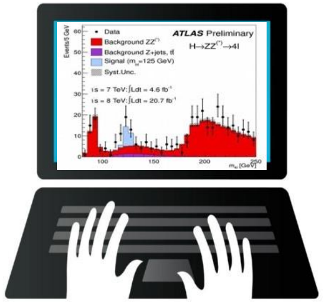


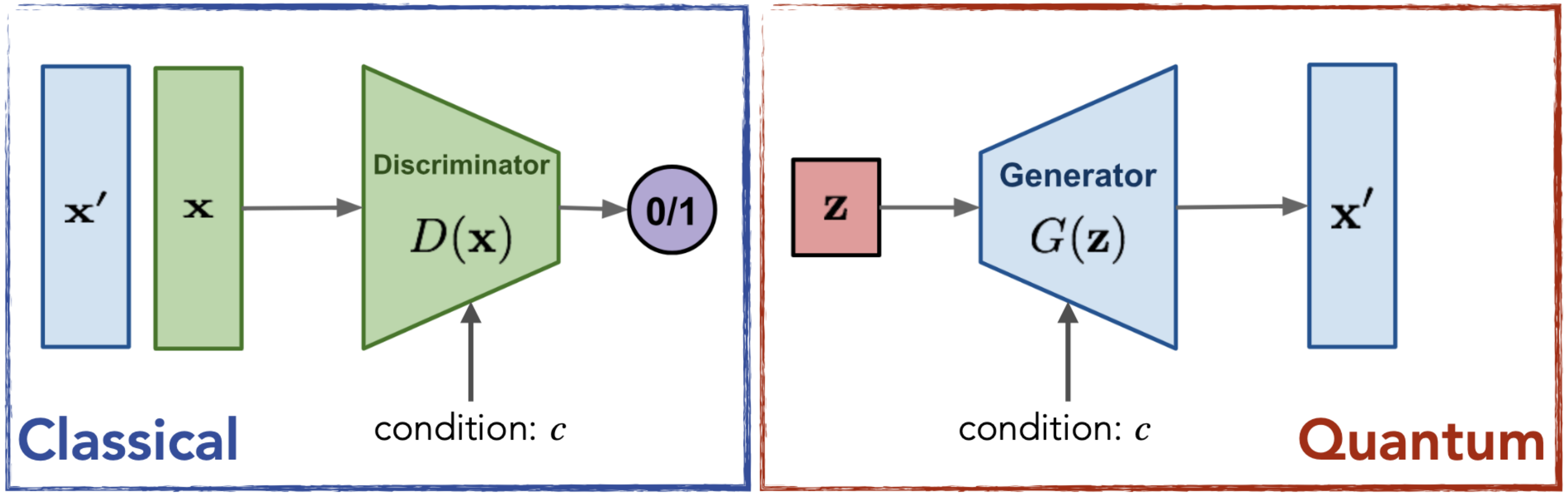
Quadratic speed up

PhysRevD.110.074031 *- Martinez de Lejarza, GM., et al.*
Loop Feynman integration on a quantum computer

CERN QUANTUM TECHNOLOGY INITIATIVE

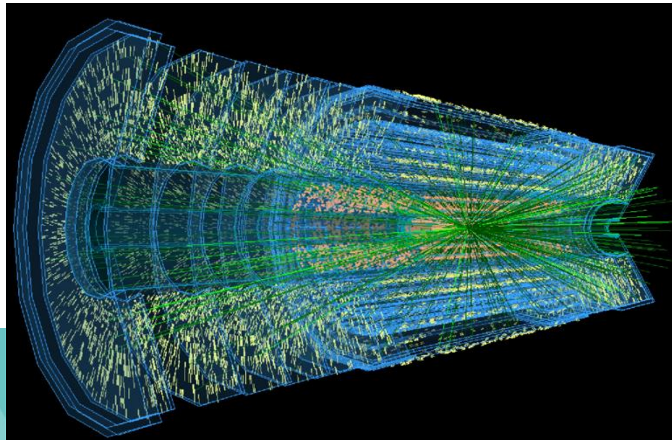
- **Generative Adversarial Networks :** two networks competing, generator produces fake data, and a discriminator distinguishes between real and fake data
- **Quantum GAN (QGAN) replaces the generator network by a parameterised quantum circuit**



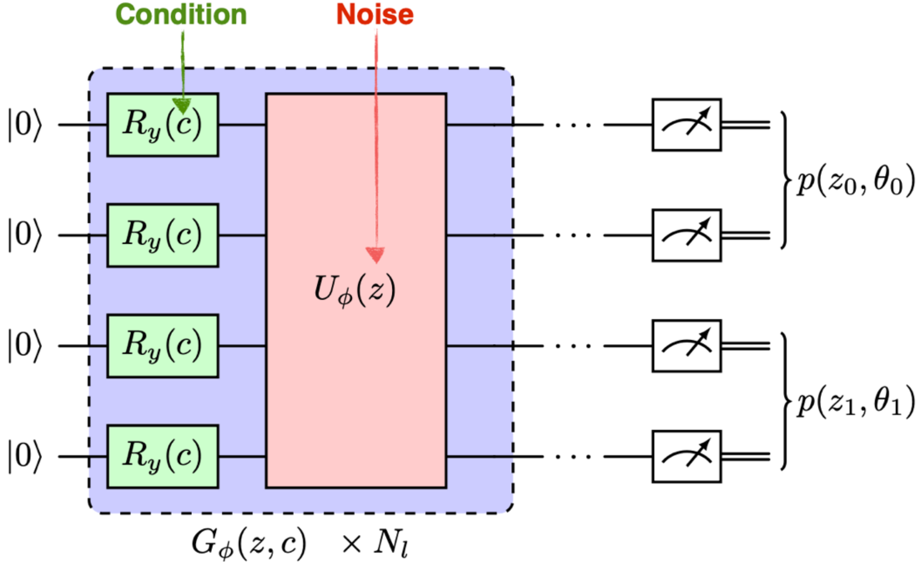


Data Generation

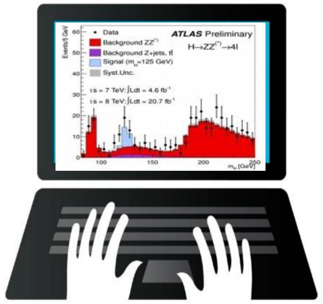
- How can quantum simulators model particle interactions described by SOTA hadronization model?
- Can quantum generative model provide better results in terms of more accurate physics description?
- Can we offer an alternative to the traditional MC or classic GM with QC?



MG, Y. Haddad, V. Croft, C. Tusyz in preparation

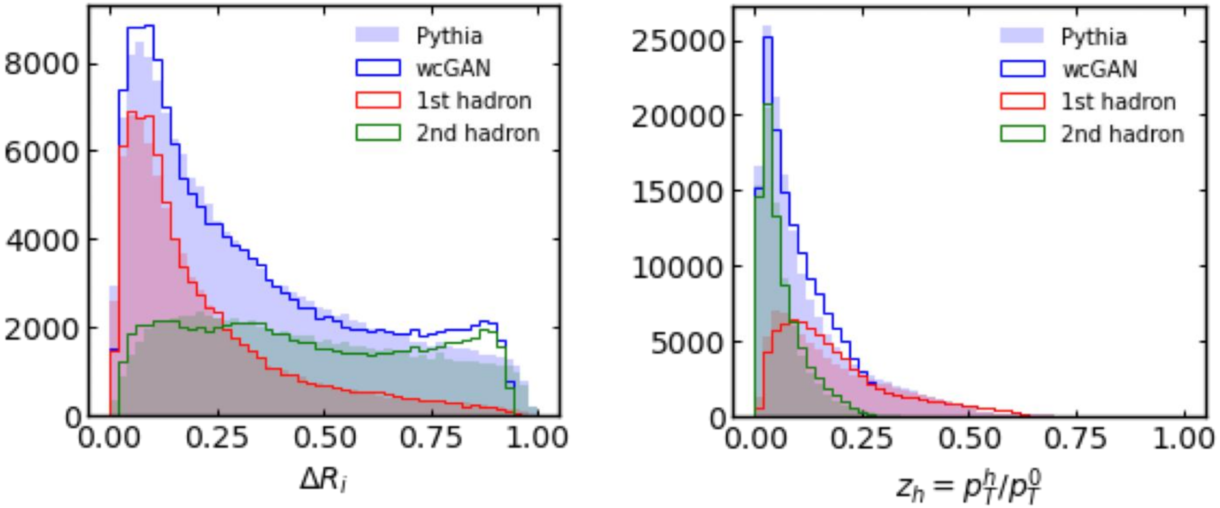


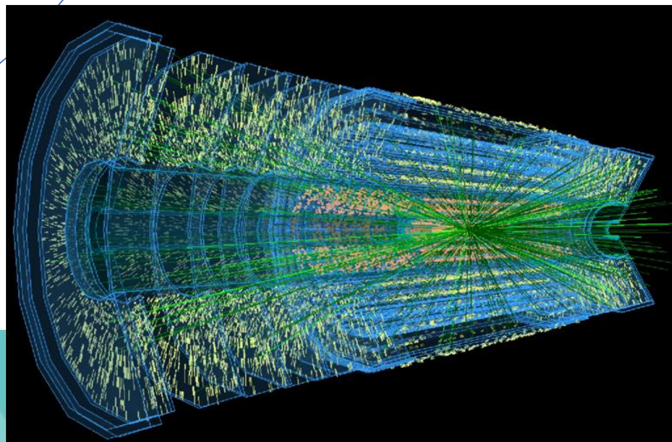
- Data: anti-k_T ($R = 0.4$) jets generated with Pythia8 ($p_T > 30$ GeV)
- Each jet constitent represented by two features:
  - Momentum fraction $z_i = p_T^i / p_T^{jet}$
  - Angle with reference to the jet axis $\theta_i = \Delta R_i / R$
- 1 qubit = 1 feature: $\hat{x} = \{\langle \sigma_Z^0 \rangle, \langle \sigma_Z^1 \rangle, \ldots, \langle \sigma_Z^n \rangle\}$
- Style-based approach (*): the noise is inserted in every gate: $\phi_i \to \phi_i = w \cdot z + b$
  - The noise z, is sampled from $\mathcal{U}(0,1)$
- Jet p_T included as condition via R_y rotations in styled-base approach: $c \to c = w \cdot c + b$



Style-based Hybrid QGAN for *hadronization*

Data Generation

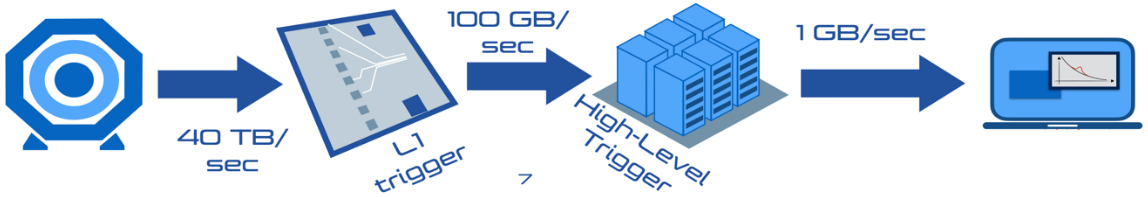




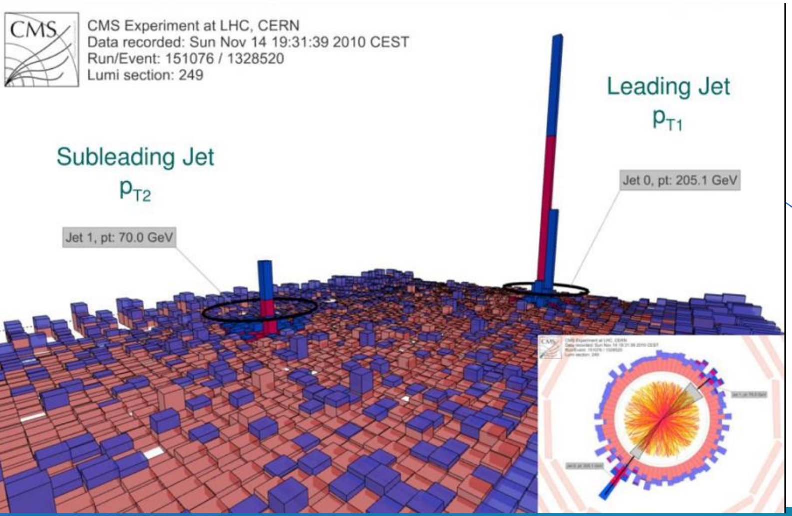
The Quantum GAN captures the distributions of the first and second emissions, reproduce their dependence with the jet scale

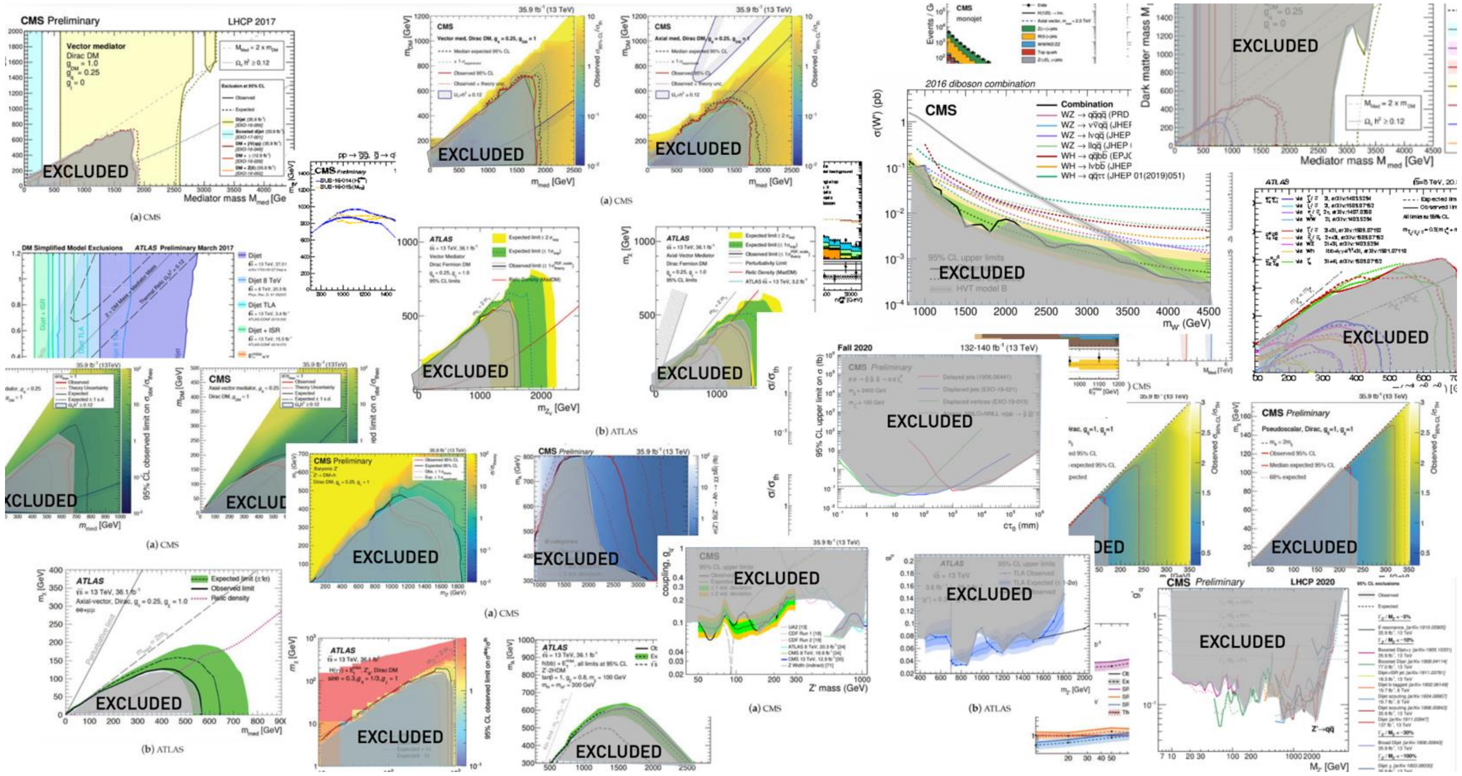
MG, Y. Haddad, V. Croft, C. Tusyz in preparation

Where is NEW PHYSICS?
Are we using the right data?



Data Analysis

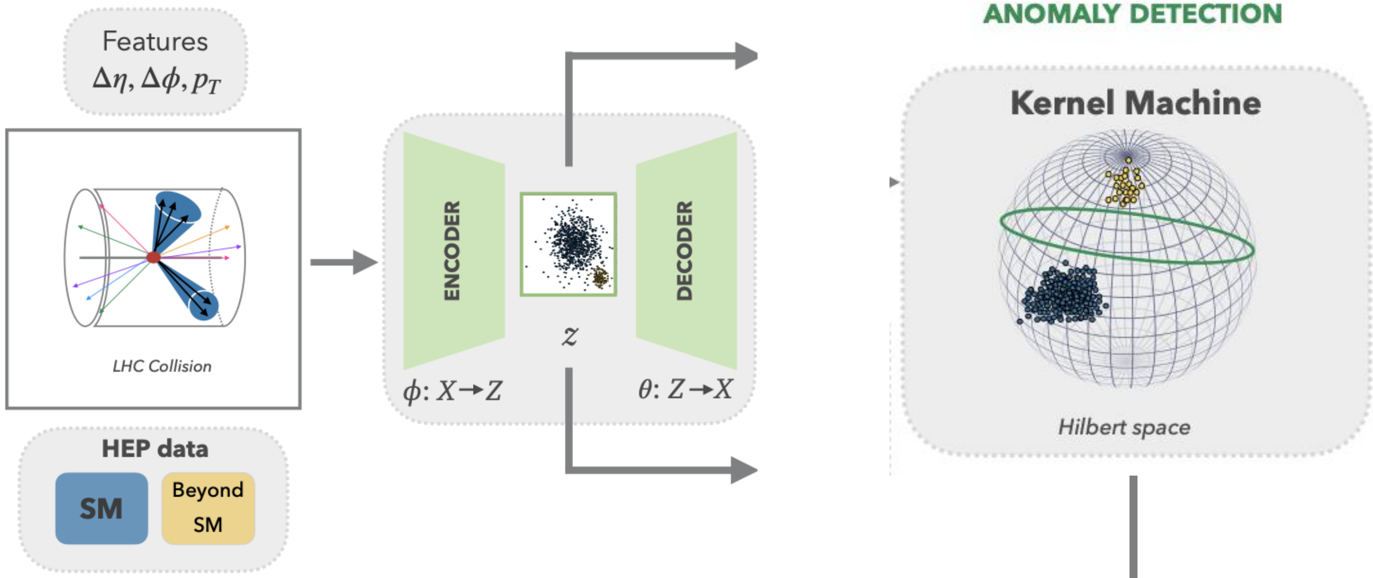




Quantum Anomaly Detection

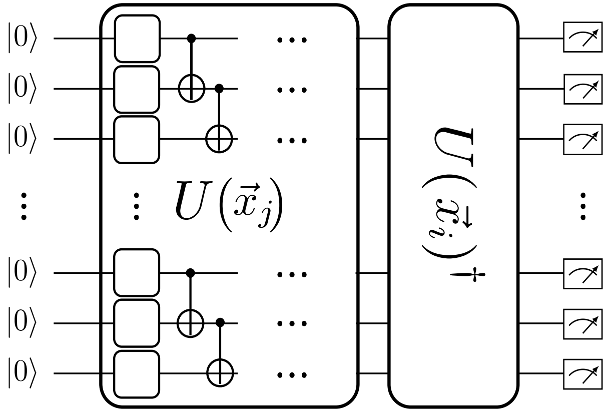
[Belis V., GM, et al – *COMMSPHYS-23-1149C*]

Data Analysis



$$\mathbb{R}^{300} \to \mathbb{R}^{\ell}\ , \ell = 4, 8{,}16$$

$\Delta\eta$	$\Delta\eta$	$\Delta\eta$	$\Delta\eta$	$\cdots$	$\Delta\eta$	$\Delta\eta$	$\Delta\eta$	$\Delta\eta$
$\Delta\phi$	$\Delta\phi$	$\Delta\phi$	$\Delta\phi$	$\cdots$	$\Delta\phi$	$\Delta\phi$	$\Delta\phi$	$\Delta\phi$
p_T	p_T	p_T	p_T	$\cdots$	p_T	p_T	p_T	p_T

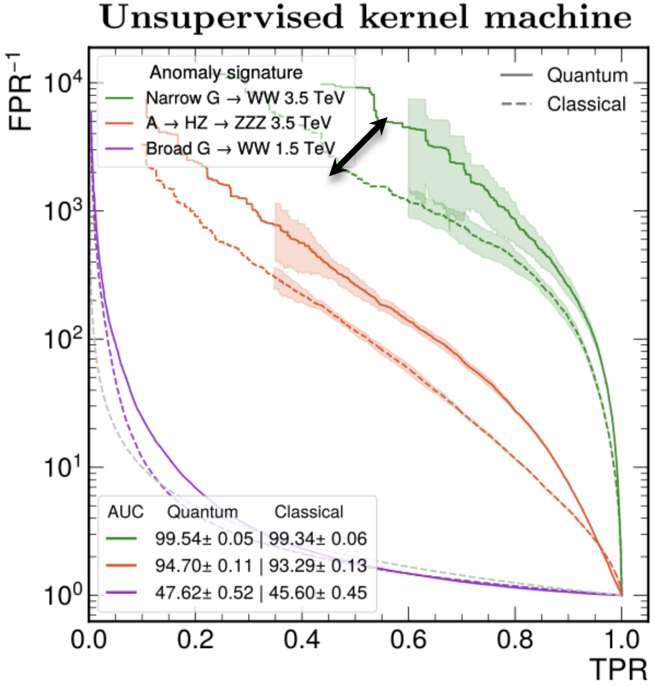


- Simulate QCD multi-jets at the LHC
- Build jet from 100 highest pt particles

Quantum Anomaly Detection

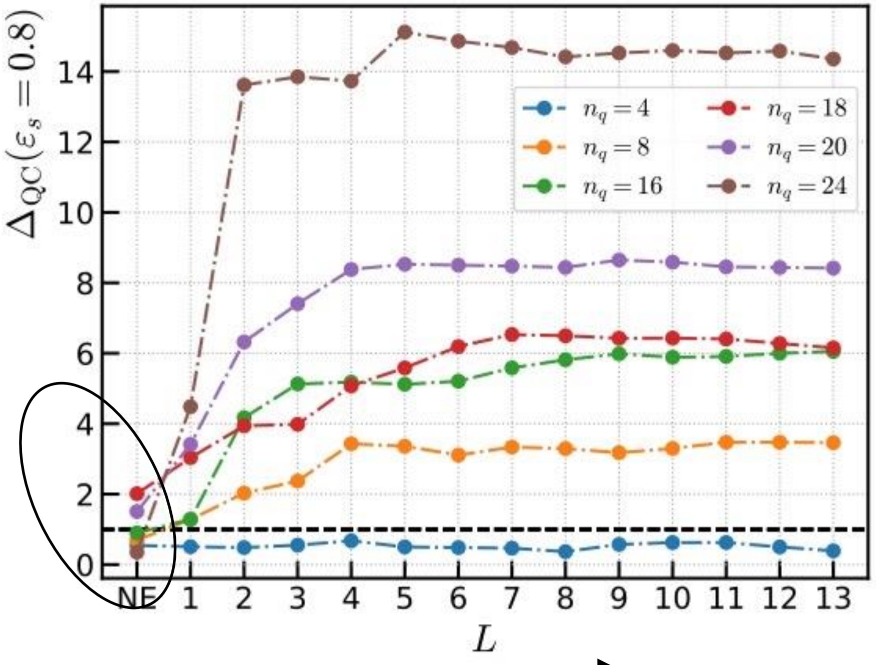
[Belis V., GM, et al – *COMMSPHYS-23-1149C*]

- Importance of intrinsically quantum properties of the feature map
- Up to **14 times** the performance of the classical model for 24 qubits!

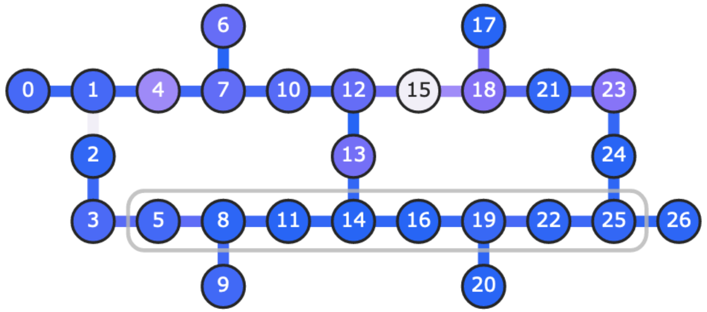


Data Analysis

No entanglement



More expressive



Quantum Machine Learning Challenge

CERN examples

Discussion

QC research directions in HEP

QC4HEP working group

Concrete challenges

- What are the most promising applications?
- How to **define performance metrics** and validate results?

Experimental data has high dimensionality

- Can we train **Quantum Machine Learning** algorithms effectively?

Experimental data is shaped by physics laws

- Can we leverage them to build better algorithms?
- Can we train the loss on a classical device, and sample on quantum (GENERATIVE MODELs)
- Quantum Error Mitigation is the way, waiting for scalable ERROR CORRECTION

PRX QUANTUM **5**, 037001 (2024)

Roadmap

Quantum Computing for High-Energy Physics: State of the Art and Challenges

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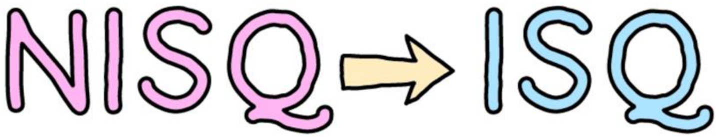
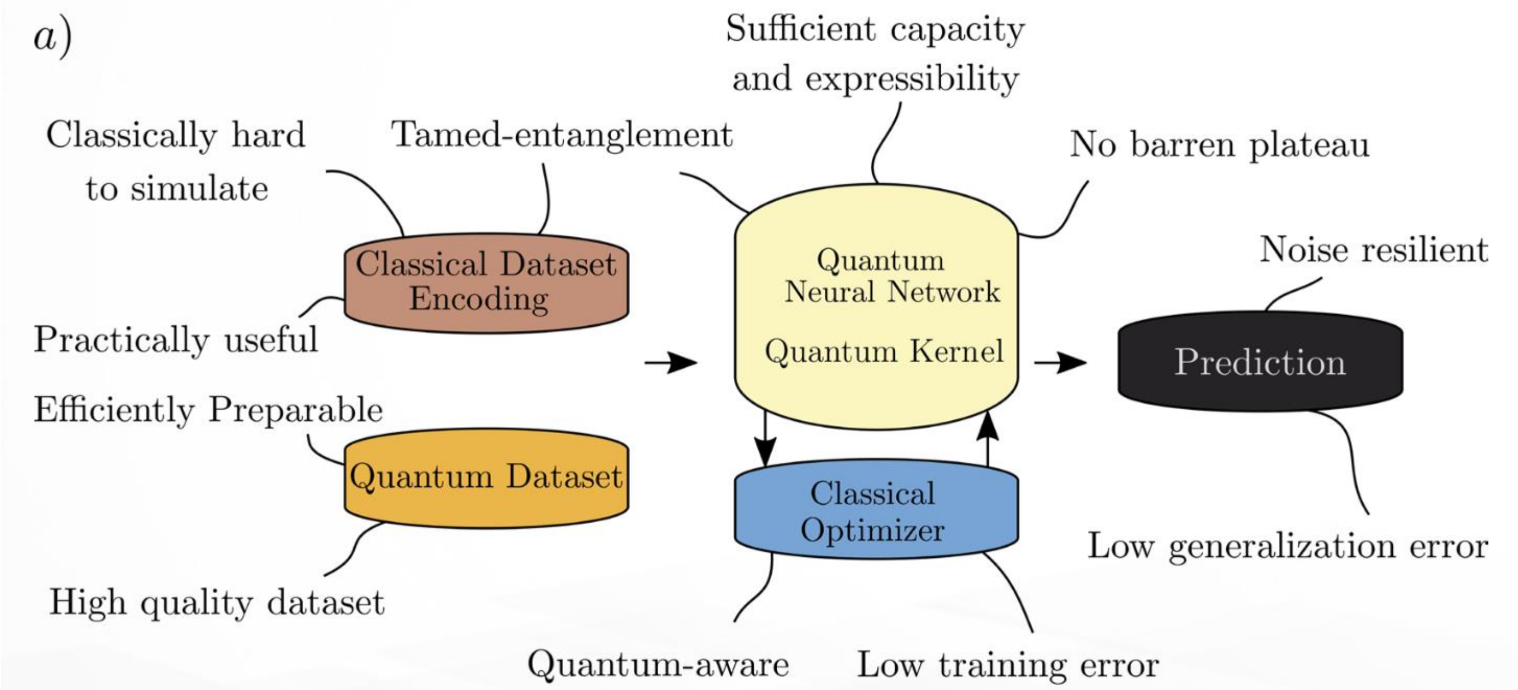


Variational Quantum Algorithms – Summary

- VQA can't be trusted any more than classical machine learning
- VQA requires linear algebra and python
- Some success has been achieved for small problem sizes (N< 30 qubits)
- We do not yet have the hardware required to test these algorithms at scale



Perspective*: Challenges and opportunities in quantum machine learning,* M. Cerezo, et al., Nature Comp. Sc., 2, 567 (2022).

Quantum Algorithms – Summary

Conventional quantum algorithms

→ come with provable guarantees

→ require significant knowledge of quantum information, group theory, physics, etc.

Query complexity: classical versus quantum

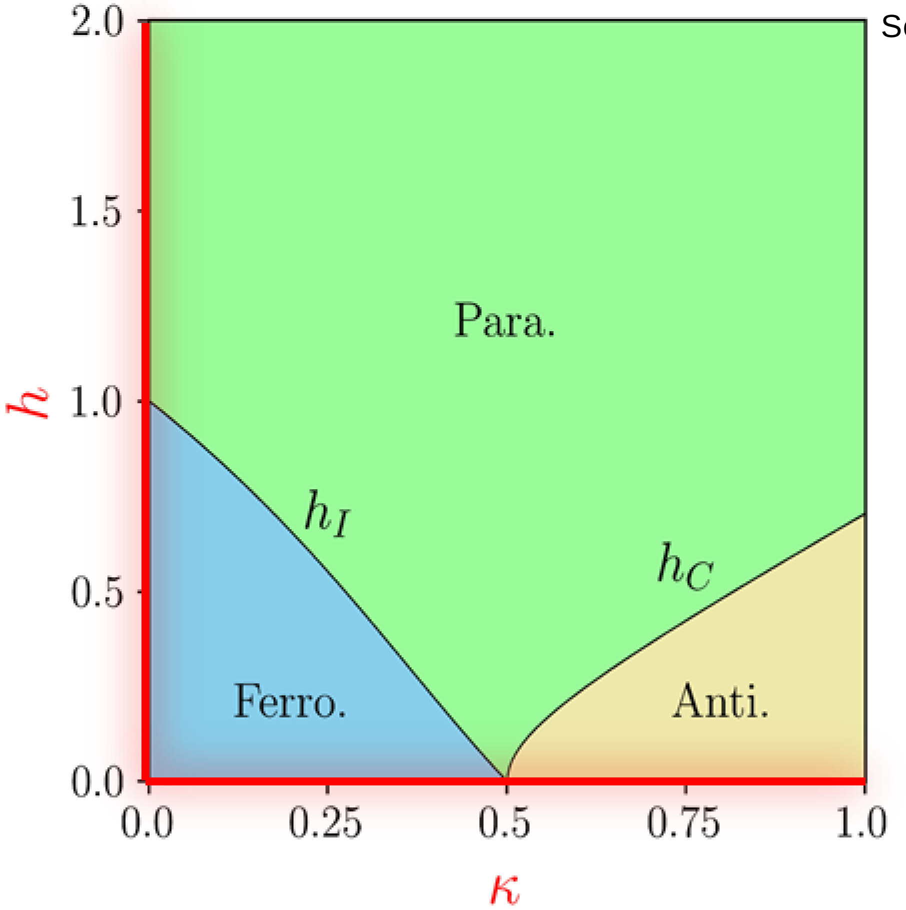
	Determ. machine (worst case)	Quantum computer
Deutsch	2	1
Deutsch–Jozsa	$2^n/2+1$	1
Bernstein–Vazirani	n	1
Grover	2^n-1	$O(\sqrt{2^n})$
Simon	$2^n/2+1$	$O(n)$
Period finding	$O(r)$	$O(1)$

The Physics model: Axial Next Nearest Neighbor Ising (ANNNI)

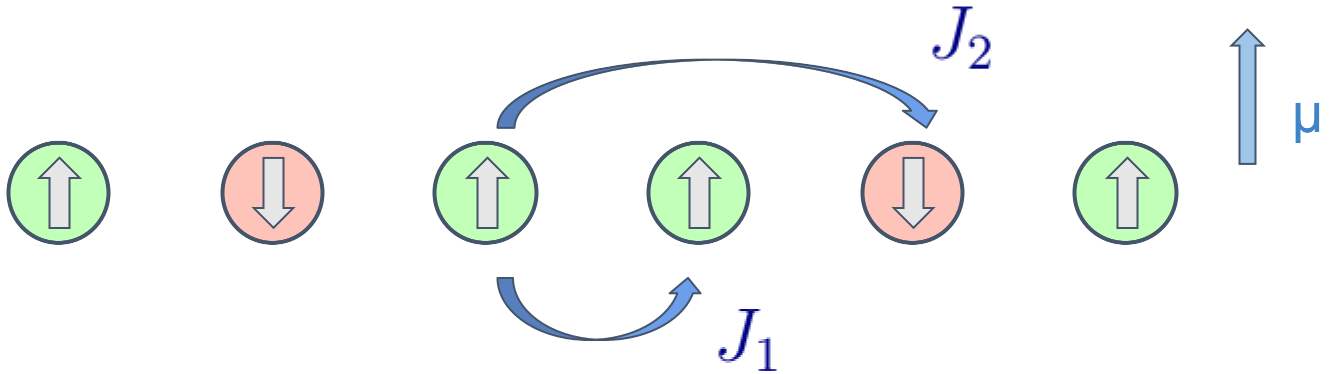
$$\mathcal{H} = -J_1 \sum_{i=1}^{N} \sigma_x^i \sigma_x^{i+1} - \kappa\, \sigma_x^i \sigma_x^{i+2} - h\, \sigma_z^i$$

$\kappa \equiv J_1/J_2$

$h \equiv \mu/J_1$



Senk, *Physics Reports*, **170**, 4 (1988)



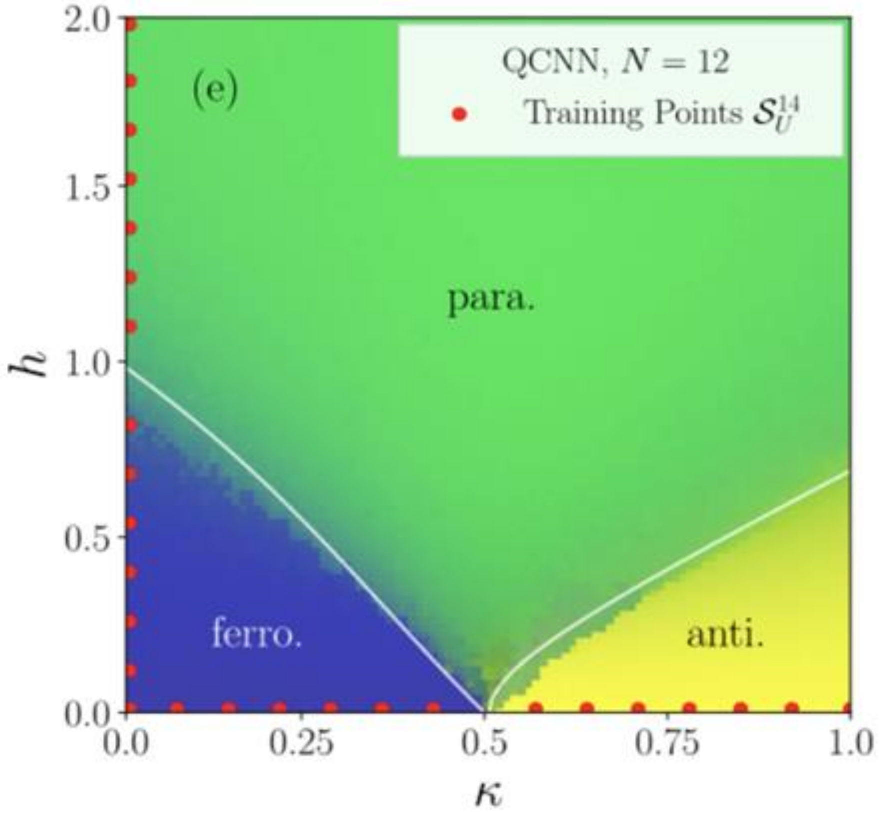
Integrable only for:

- $h = 0,\ \forall\kappa$ (x-axis)
- $\kappa = 0,\ \forall h$ (y-axis)

QML for quantum data: drawing phase diagrams

1. **Supervised classification of the ground state**
2. Quantum states are **exponentially hard to save classically**.
   - Generate quantum states with VQE
3. **Bottleneck** from access to classical training labels
   - Train in integrable subregions
   - Generalize to a full model

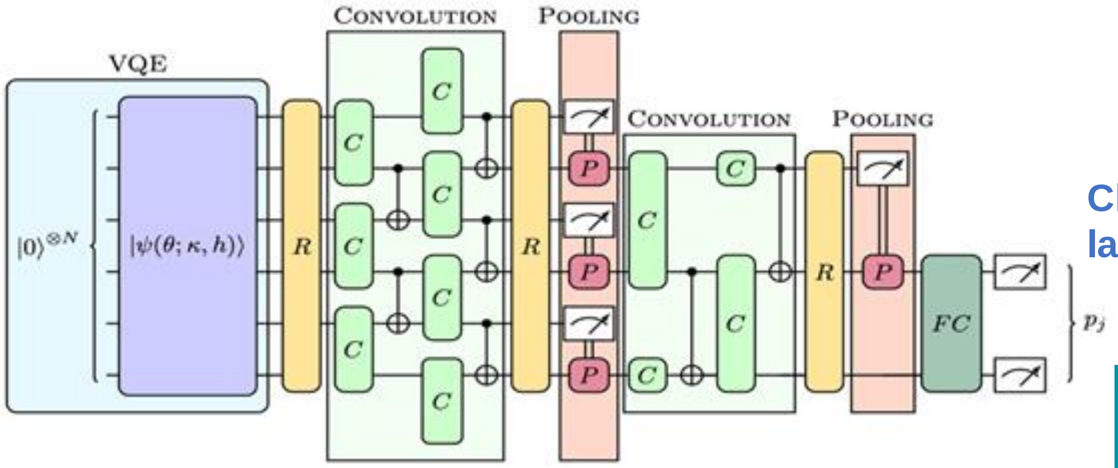
Monaco, at al. Physical Review B 107.8 (2023): L081105



QCNN output using 12 qubits:95% accuracy

Quantum data

Quantum classifier



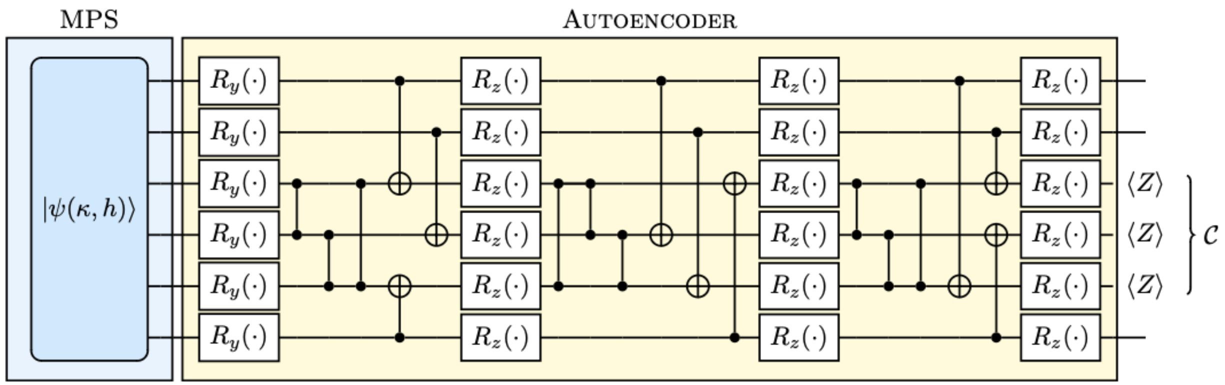
Classical label

QML using TN

Exploring the Phase Diagram of the quantum one-dimensional ANNNI model
https://arxiv.org/abs/2402.11022

- *Unsupervise: Quantum Autoencoder to learn an effective unitary operation capable of compressing all the information*
- *All anomaly detection models were trained to compress the point (κ, h) = (0, 0) of the Hamiltonian*

- *Training: single state selected to achieve compression*
- *Cost is assigned to compressed state allowing the outline of all phases*



$$\mathcal{U}(\vec{\theta})|\psi\rangle^N = |0\rangle^{\otimes K} \otimes |\phi\rangle^{N-K}$$

$$\mathcal{C} = \frac{1}{2} \sum_{j \in q_T} (1 - \langle \sigma_j^z \rangle),$$

loss function

QML using TN

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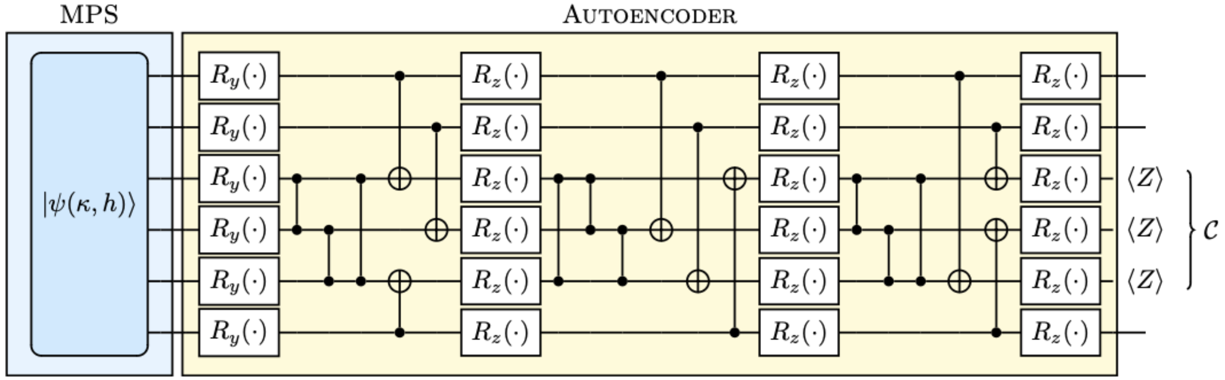

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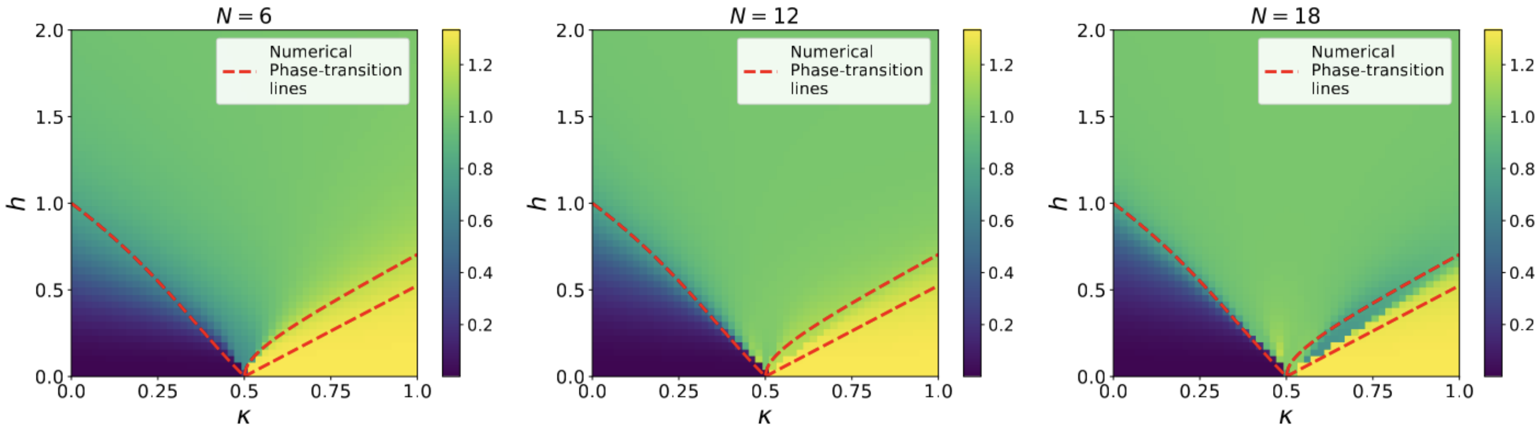

FIG. 13: Compression Scores $\mathcal{C}$ of the AD circuits trained on the $(\kappa, h) = (0, 0)$ point of the ANNNI model phase diagram at different system sizes N: 6 (left), 12 (middle), and 18 (right). The scores are showcased as a function of the interaction strength ratio ($\kappa = -J_2/J_1$) and the external magnetic field ($h = B/J_1$). Lower compression scores indicate better disentanglement of trash qubits from others, as defined by eq. 2.

Conclusion

NISQ → ISQ

- Complexity & learning theory mostly gives us insights into **worst-case behavior**

  → ML: Learning theory predicted deep neural networks to not be trainable

  Benchmarking can help us to understand the behavior on specific instances
- We need to make a comparison of **computational cost** - may lead to poly advantages!
- Change the goal: quantum advantage will be unlikely in many cases **BUT** we can identify promising paths for **hybrid computational advantages (TN + QML?)**
- We can train the loss on a classical device, and sample on quantum (GENERATIVE MODELs)

  → larger devices for high-quality data?
- What’s the role of data?
- Community goal is bridging the gap between near-term and fault-tolerant quantum machine learning

QT4HEP 2025 - save the date