Laboratorio di computazione quantistica
AA 2024/2025

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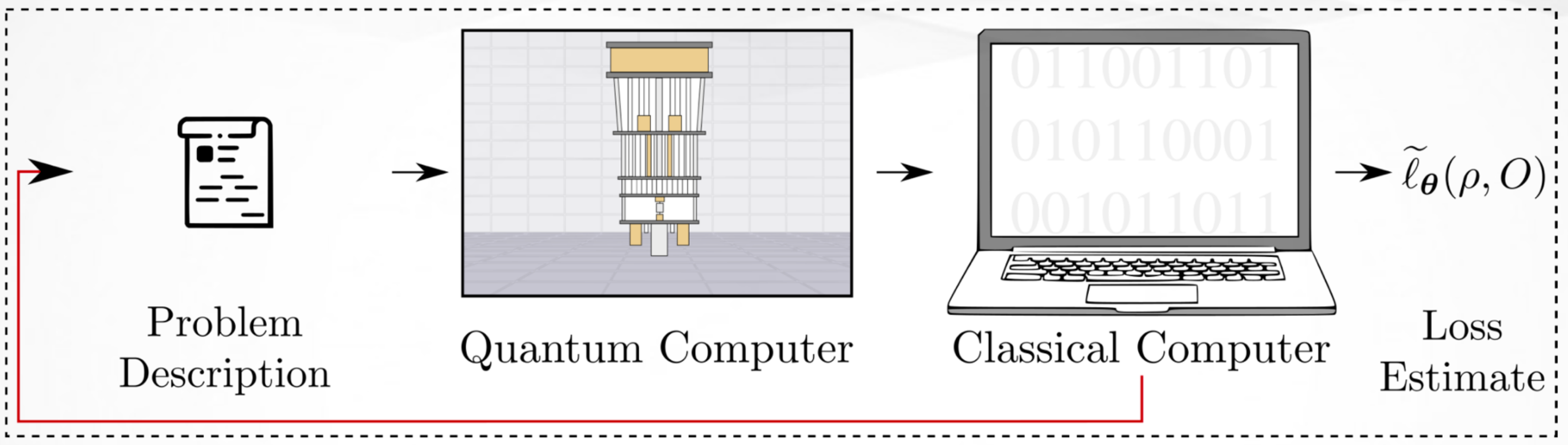
Quantum Research - CERN

CERN IT INNOVATION

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**.**



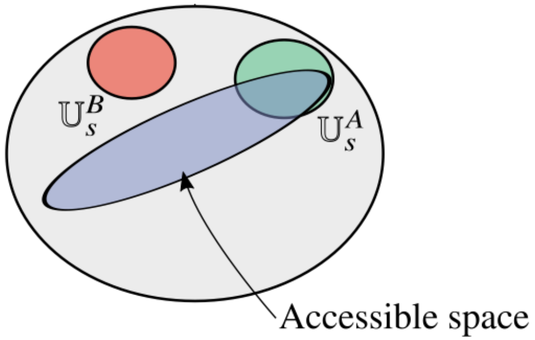
$$\ell_{\boldsymbol{\theta}}(\rho, O) = \mathrm{Tr}\left[\rho U^{\dagger}(\boldsymbol{\theta}) O U(\boldsymbol{\theta})\right]$$

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

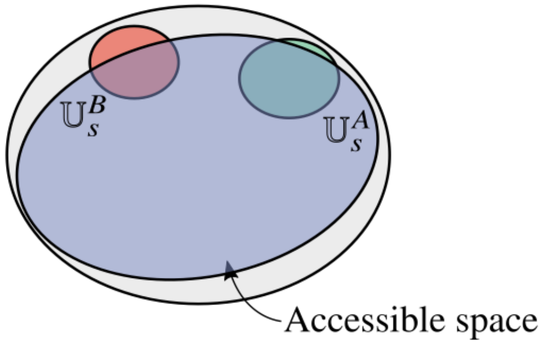
Challenges when using Parametrized Quantum Circuits

- Efficient **data handling** and data **embedding**
- Find balance: **Generalization** and **representational power** vs. **Convergence**
  - Problem of barren plateaus and vanishing gradients in optimization landscape
  - How well can we survey the Hilbert space (expressibility)?
- Current hardware limitations
  - Limited number of qubits and connectivity
  - **Quantum Noise Effects** (decoherence, measurement errors or gate-level errors)
  - Efficient interplay between classical and quantum computer
- ….

Inexpressive

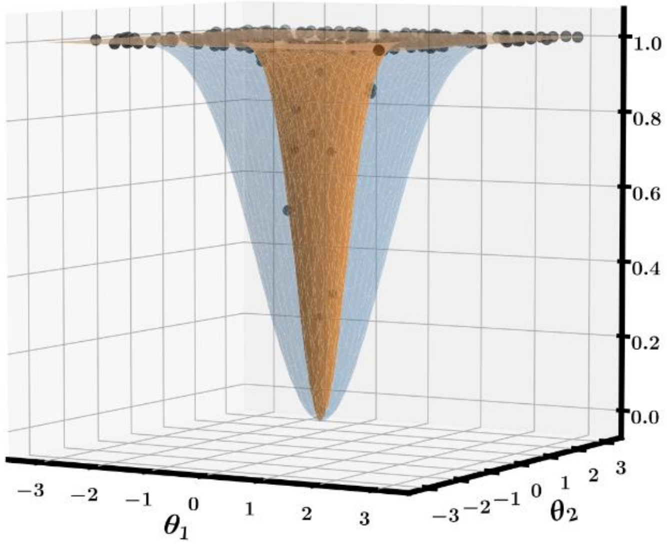


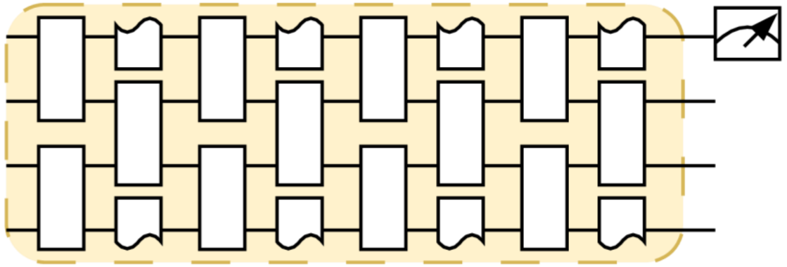
Expressive



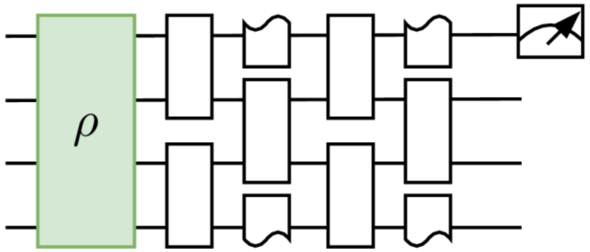
Trainability – Theoretical Limitations

Exponential Decay in the loss function $\mathrm{Var}[\ell_{\boldsymbol{\theta}}(\rho, O)] \in \mathcal{O}\left(\frac{1}{b^n}\right)$



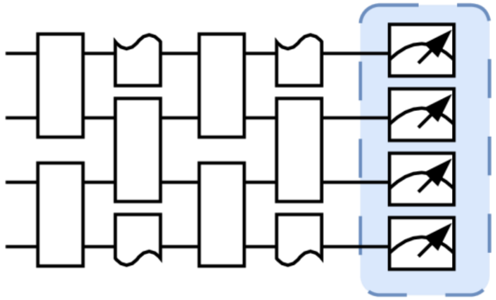


Circuit Expressivity

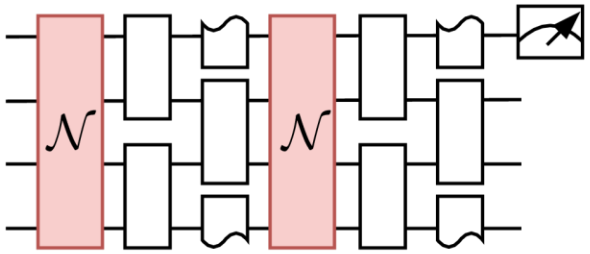


Entangled Initial State

Probabilistic
Barren plateau



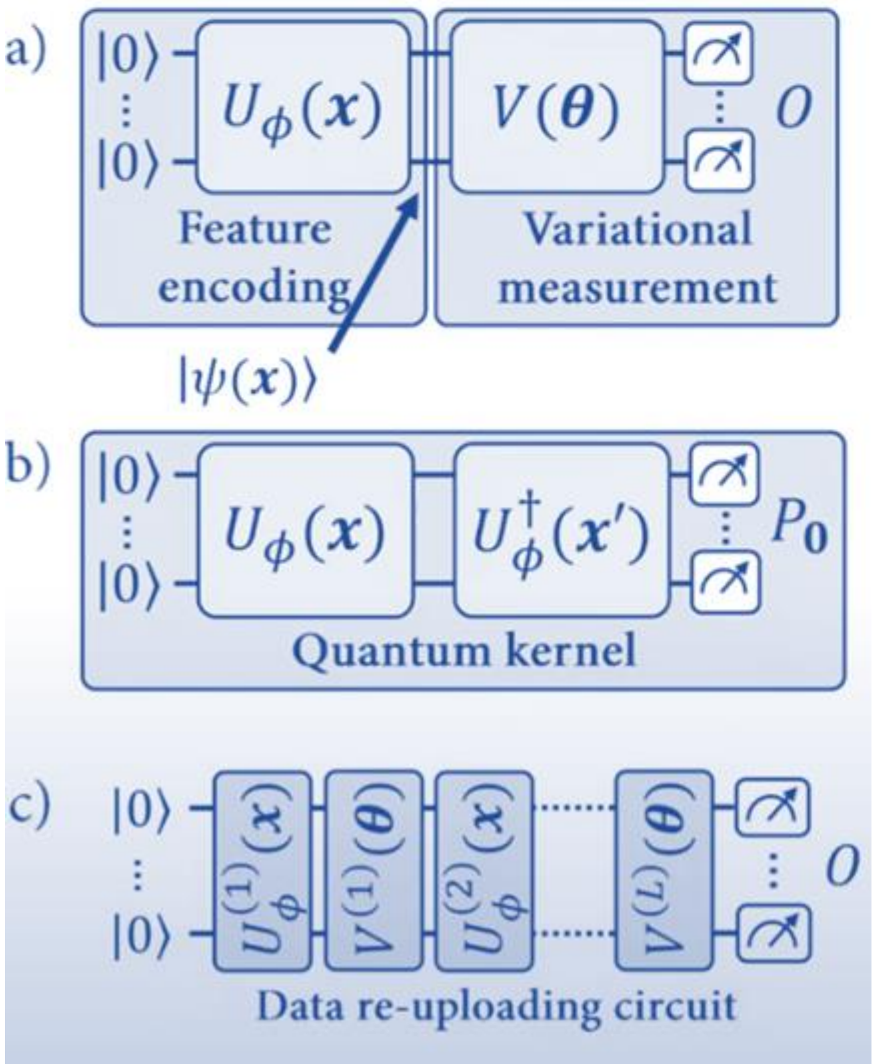
Measurement Locality



Quantum Hardware Noise

Deterministic
Barren plateau

QML models



a) Explicit quantum model:

$$f_{\boldsymbol{\theta}}(\boldsymbol{x}) = \mathrm{Tr}[\rho(\boldsymbol{x})O_{\boldsymbol{\theta}}] \qquad \rho(\boldsymbol{x}) = |\psi(\boldsymbol{x})\rangle\langle\psi(\boldsymbol{x})| \qquad O_{\boldsymbol{\theta}} = V^\dagger(\boldsymbol{\theta})OV(\boldsymbol{\theta})$$

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

b) Implicit quantum model:

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

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)

Example Applications

Quantum **Support Vector Machines** for **classification**

Quantum **Tree Tensor Networks** for pattern recognition

Quantum **Generative Adversarial Networks simulation**

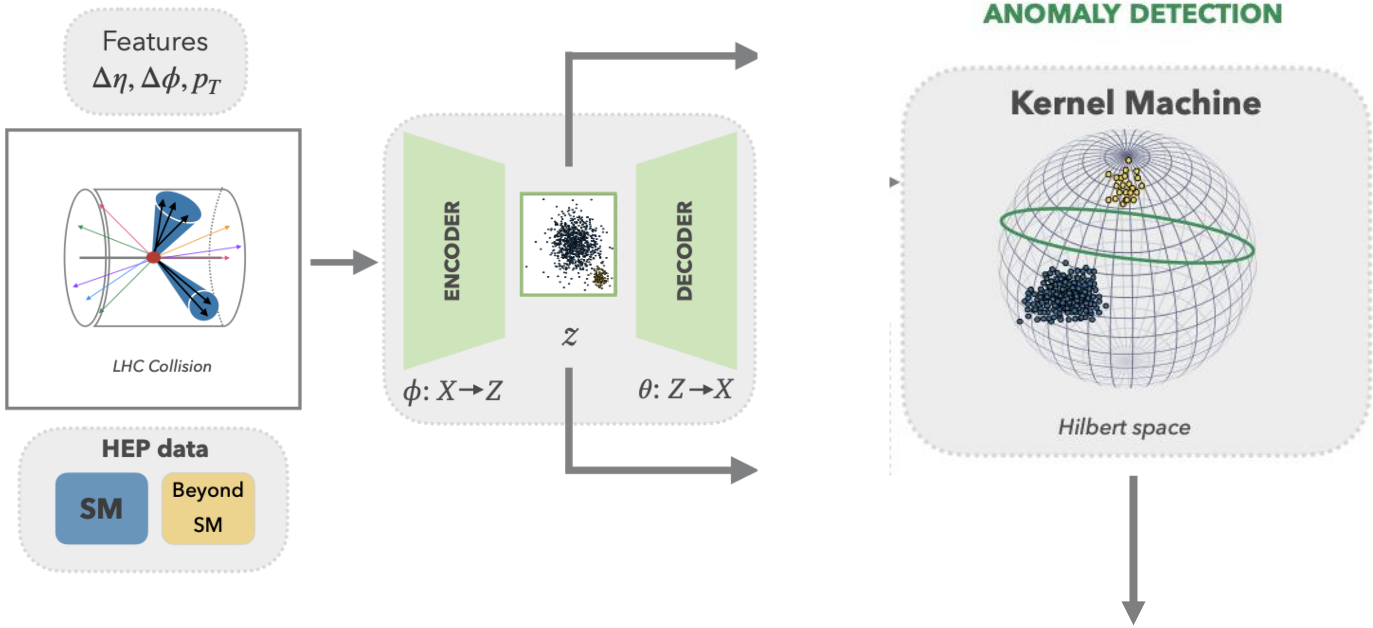
Quantum **Boltzman Machines** and reinforcement learning

Hybrid **quantum-classical data embedding**

Quantum Anomaly Detection

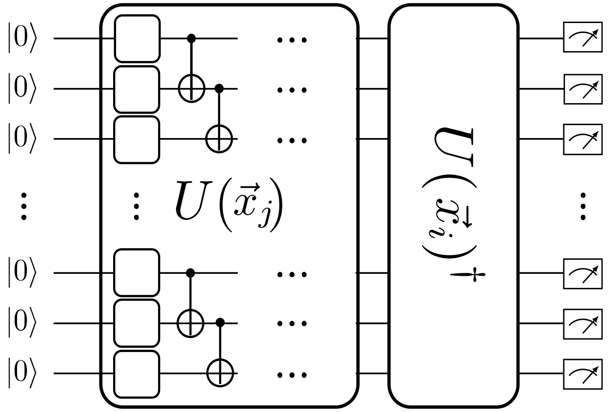
Belis V., GM, et al – *COMMSPHYS-23-1149C*

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



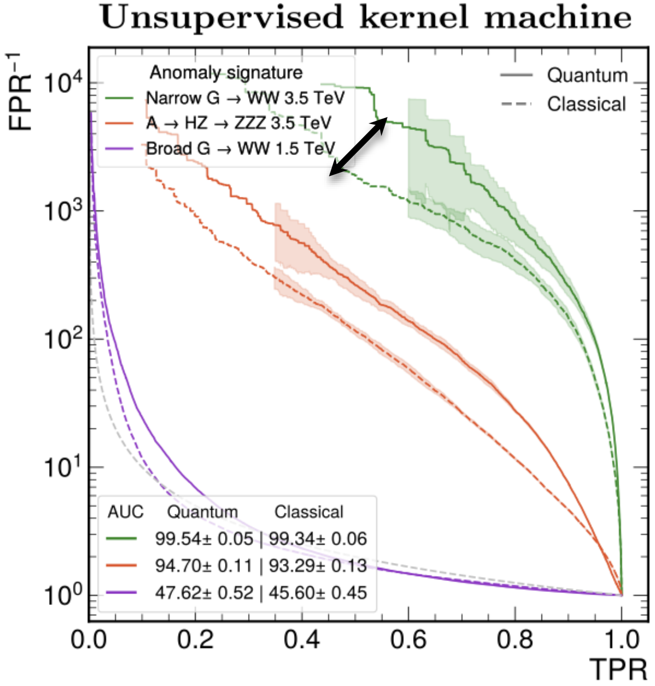
- Simulate QCD multi-jets at the LHC
- Build jet from 100 highest pt particles

Quantum Anomaly Detection

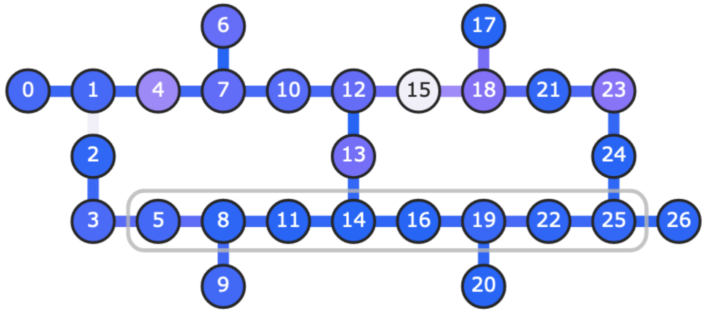
[Belis V., GM, et al – *COMMSPHYS-23-1149C*]

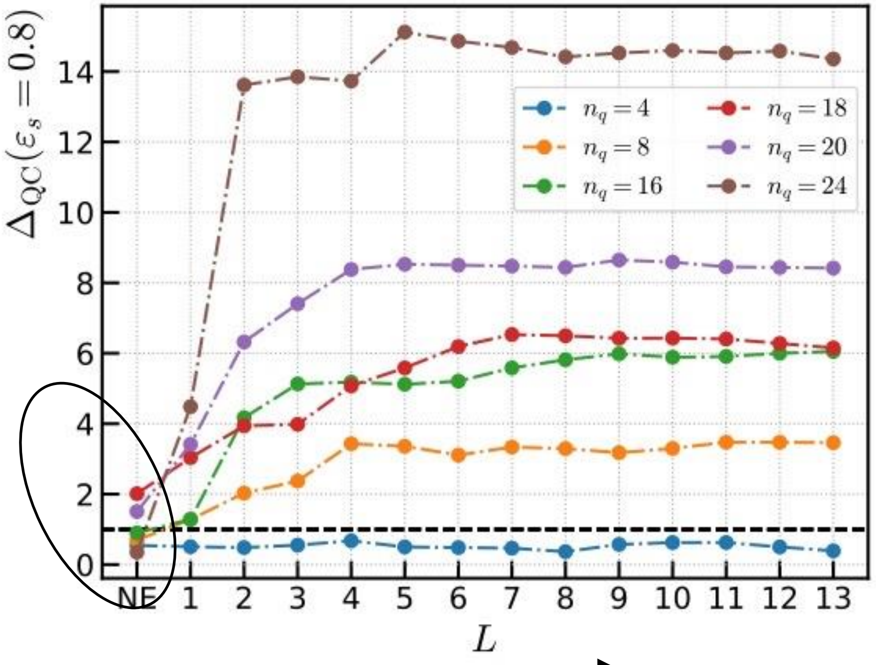
Data Analysis

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



No entanglement



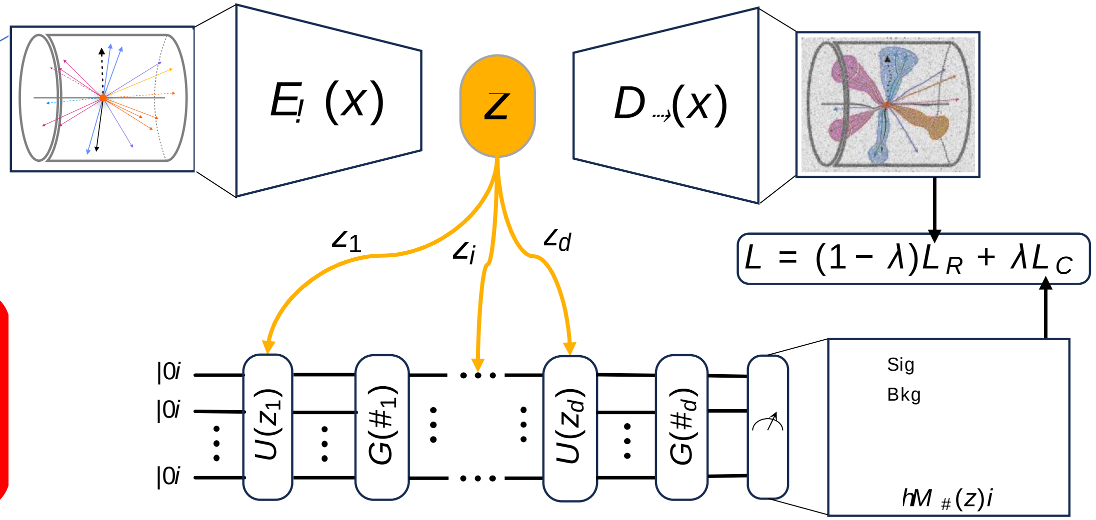


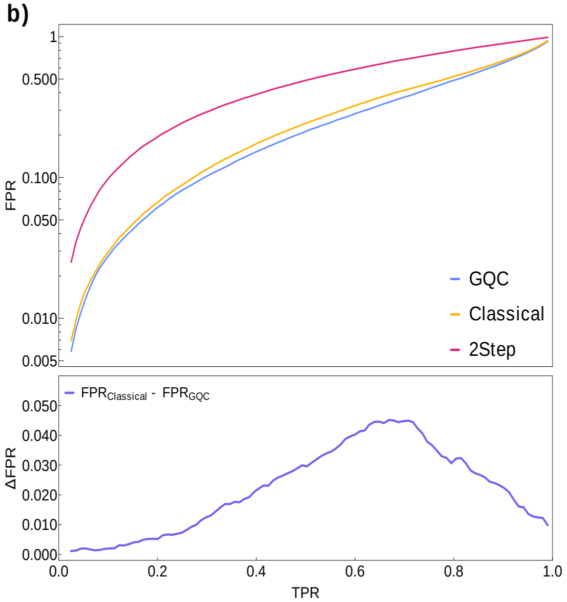
More expressive

Efficient data handling and data embedding

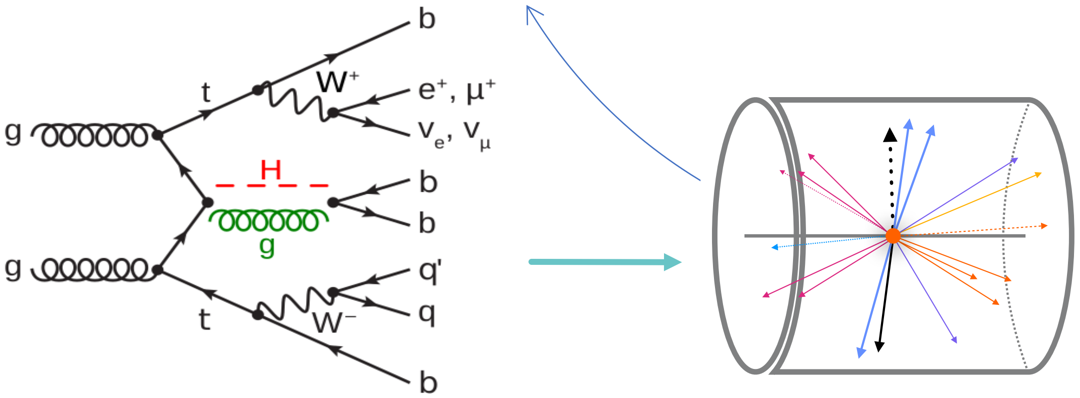
Belis V., GM, et al – *2024 Mach. Learn.: Sci. Technol. 5 035010*

Backpropagation + adjoint differentiation



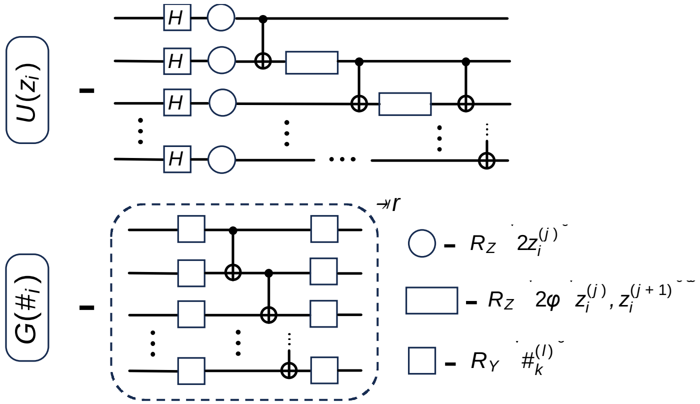


Data Analysis



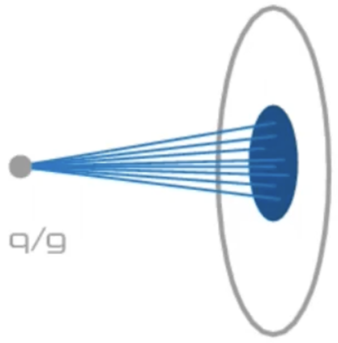
600 features

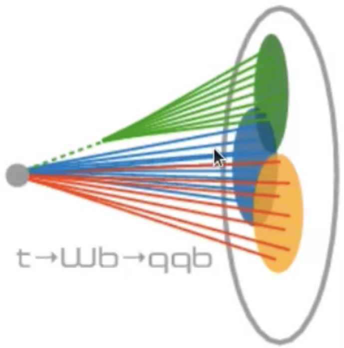
<30 features



1 - Top quark tagging – binary classification for JET

HEP QML





TO DO:

- Read and play with the classic tutorial
- Define a data compression strategy (2 steps &/or guided)
- Develop a quantum classifier (kernel/PQC)
- Discuss the performance as a function of features and data dimensionality
- Discuss exponential concentration

- Reference: https://github.com/grossiM/cometa-ML-tutorial

2 - ANNNI model noisy dynamics

Time Evolution

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

$$\kappa \equiv J_1/J_2$$

$$h \equiv \mu/J_1$$

TO DO:

- Encode the full hamiltonian of the Axial Next Nearest Neighbor Ising model for N>2
- Compute the time evolution for total magnetization or another observable
- Compare noiseless and noisy result
- Apply error mitigation

- Reference:
- https://arxiv.org/pdf/2208.08748.pdf
- https://github.com/orielkiss/qiskit-research/blob/DSV_tutorial/qiskit_research/DSV/tutorial_DSV.ipynb

3 - Quantum simulation of the Agassi model

QI + Time Evolution

The Agassi model simulates the behaviour of a two-shell nuclear system in which both the paring and quadrupole interactions are present. The model can easily be mapped to a spin system using the Jordan-Wigner transformation, and as such can be simulated on a quantum computer. This project aims to simulate the Agassi model using a quantum computing framework.
The simulation will focus on measuring the system's magnetization and concurrence, key indicators of magnetic properties and entanglement, respectively. By exploring these observables across various interaction regimes, the project seeks to analyze the interplay between quantum correlations and magnetization dynamics, leveraging quantum simulation tools to gain insights into strongly correlated systems.

TO DO:

- Represent the Agassi model Hamiltonian using qubits. Map fermionic operators to spin operators using a suitable transformation, like the Jordan-Wigner or Bravyi-Kitaev mapping.
- Apply Trotterization or Qubitization: Use techniques like Trotter-Suzuki decomposition or Variational Quantum Simulation (VQS) to simulate the Hamiltonian evolution.
- Measure magnetization and concurrence (e.g. Extract concurrence using Qiskit's state tomography tools to reconstruct the density matrix.)
- Simulate magnetization and concurrence for varying interaction parameters of the Agassi model.
- Perform classic and quantum classification of phases (you can explore supervised or unsupervised approach)

- Reference: https://doi.org/10.1016/j.physletb.2022.137133

4 - Equivariant Variational Quantum Eigensolver

~ VQE

This paper introduces equivariant quantum circuit that preserves the total spin and the translational symmetry to accurately describe singlet and triplet excited states in the J1-J2 Heisenberg model on a chain.
Ground state phase transition is detected by the energy level crossings of low-lying excited states.

$$\hat{H}_{J_1\text{-}J_2} = J_1 \sum_{r=1}^{N} \hat{\boldsymbol{S}}_r \cdot \hat{\boldsymbol{S}}_{r+1} + J_2 \sum_{r=1}^{N} \hat{\boldsymbol{S}}_r \cdot \hat{\boldsymbol{S}}_{r+2}$$

- Reference: https://arxiv.org/abs/2403.07100

TO DO:

- Reproduce results from Fig4 (1 is enough)

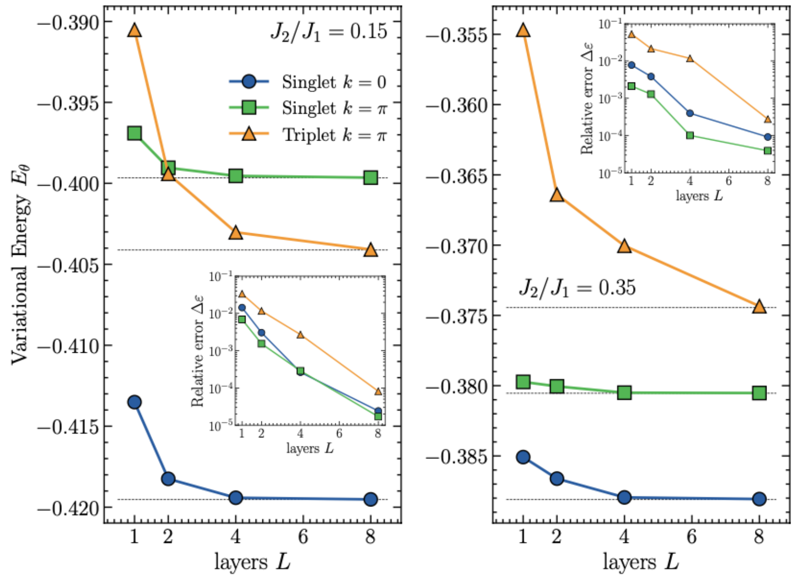
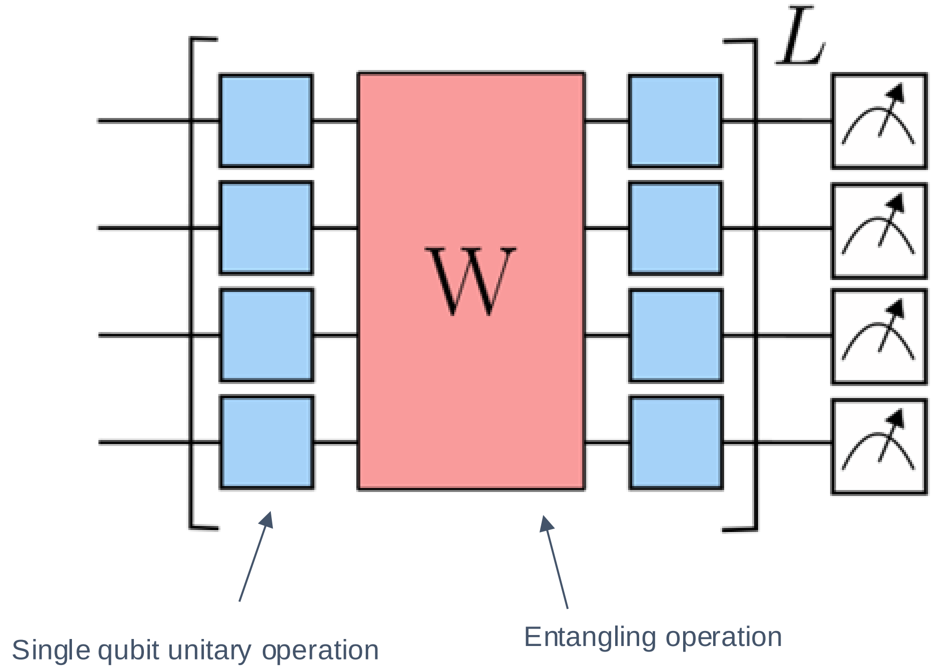
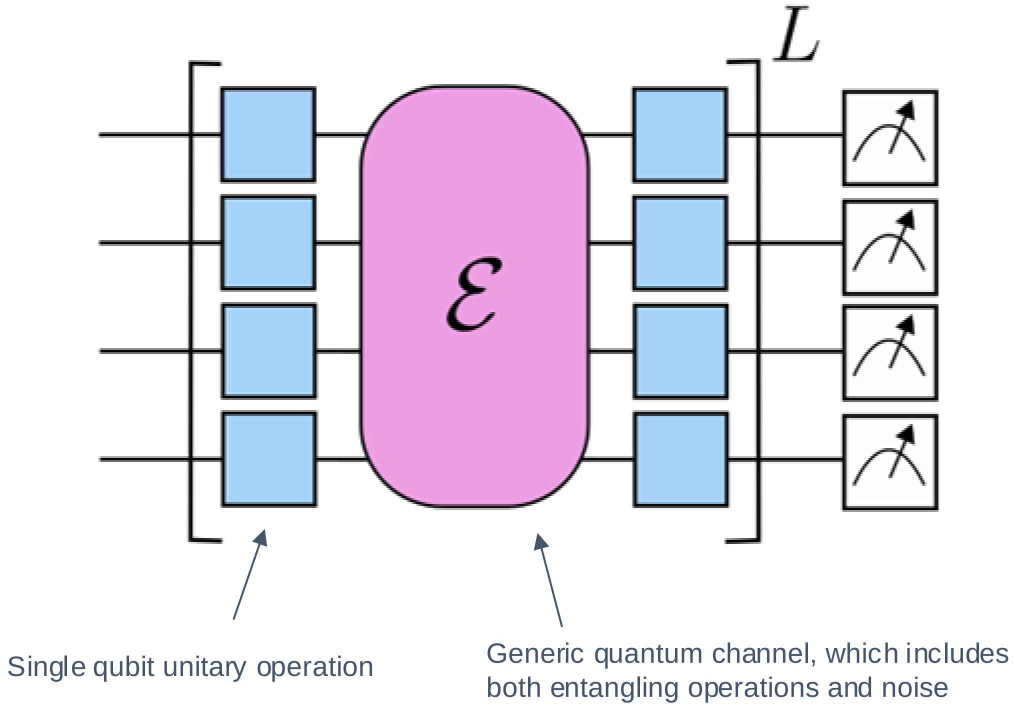


Figure 4: The variational energy for a cluster of $N = 16$ sites as a function of the number of layer $L = 1, \ldots, N/2$ for $J_2/J_1 = 0.15$ (left panel) and $J_2/J_1 = 0.35$ (right panel). The exact energies are also reported as dotted lines in both panels. The corresponding relative error $\Delta\varepsilon = |E_\theta - E_{\text{ex}}|/E_{\text{ex}}$ with respect to the exact energies is reported as insets as a function of L.

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]

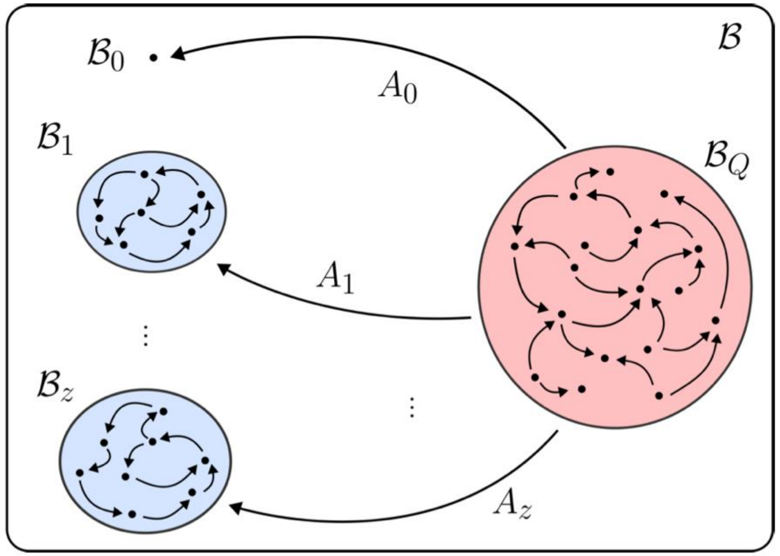
5 - Concentration in noisy PQC

QML + noise

Test the effect of non-unital noise for BP.
Change the absorption on from B_0 to B_1 with a customize ansatz (we will provide guidance and initial support). Measure the contribution to the variance with numerics or analytical solution

TO DO:

- Reproduce the numerics (see App E2, F)
- Expand the results using a different absorption



$$\mathbb{V}^{\infty}_{\rho,H} = \sum_z \frac{(\ell_\rho)_z(\ell_H)_z}{d_z} + \frac{(\ell_\rho)_z(A\ell_H)_z}{d_z}$$

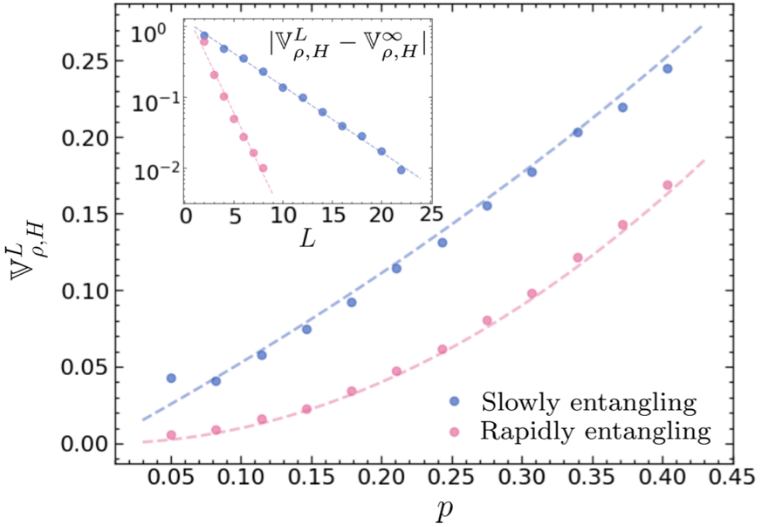


FIG. 3. Scaling of $\mathbb{V}^L_{\rho,H}$ as a function of the noise strength and the entangling power of the intermediate channel. The main figure illustrates the scaling of $\mathbb{V}^{\infty}_{\rho,H}$ with noise strength p for both rapidly entangling (pink) and slowly entangling (light blue) channels, using $L = 8$ and $L = 20$, respectively. The dotted lines represent the theoretical predictions of Eq. (25) and Eq. (24) The inset verifies the exponential convergence of $\mathbb{V}^L_{\rho,H}$ to $\mathbb{V}^{\infty}_{\rho,H}$ at $p = 0.1$, justifying the chosen number of layers. The dotted lines represent an exponential fit to the numerical data. All plots are obtained using a $n = 10$ qubit system.

- Reference:
  https://arxiv.org/pdf/2410.01893
  https://pennylane.ai/blog/2021/05/how-to-simulate-noise-with-pennylane

Thanks!

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