Generative Models in High Energy Physics:

from classical use cases to quantum implementations

QUANTUM
TECHNOLOGY
INITIATIVE

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AI & Quantum Research - CERN IT

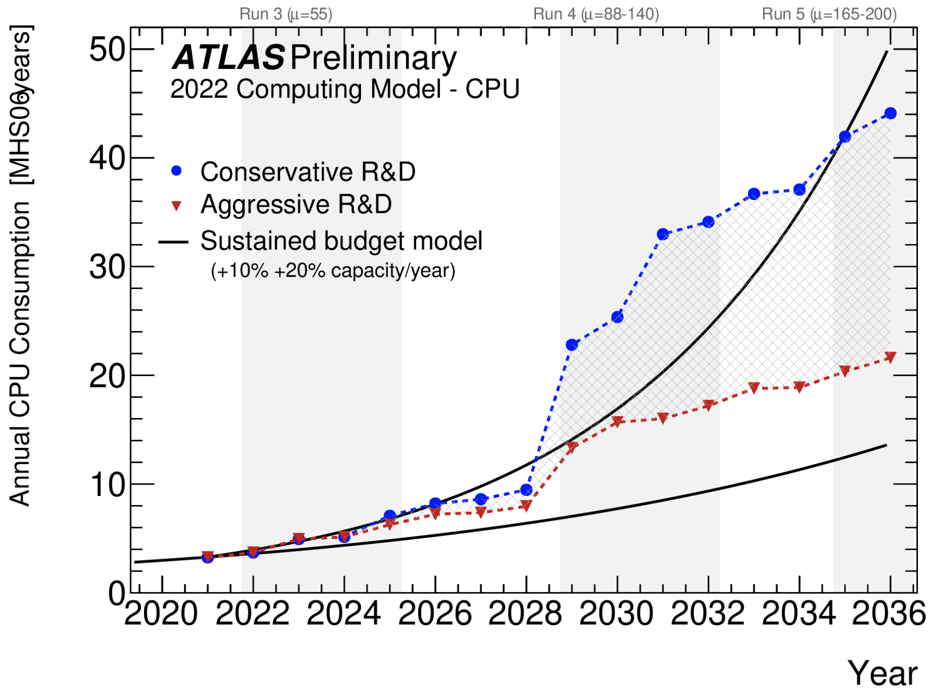
December 14th 2022

Outline

1. Computing challenges at CERN and the High Luminosity LHC
2. Deep Generative Models and representation learning
3. CERN Quantum Technology Initiative
4. Quantum Machine Learning and Applications at CERN
5. Initial results
6. Research directions
7. Summary

HL-LHC computing challenges

HL-LHC: Computing Challenges



High Luminosity LHC can do physics @ unprecedented level of precision

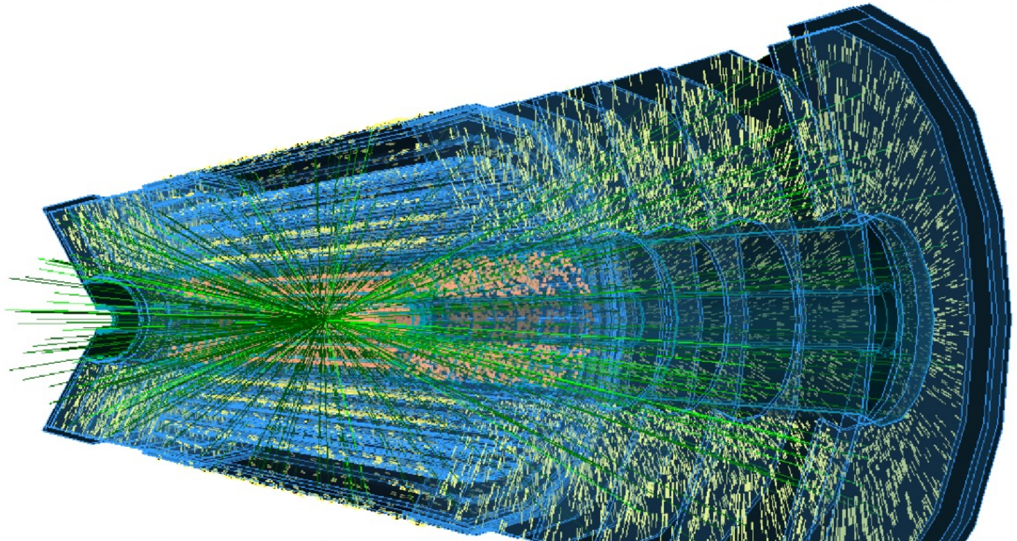
Higgs : measure fermions and bosons couplings at % level

Electro-weak sector, **top** quark, **multi-bosons** states

New physics searches, **dark matter**, etc..

Large amount of data, O(100) simultaneous collisions, high granularity detectors will require:

- **Equally accurate theoretical predictions**: improved theory calculations, faster Monte Carlo simulation
- **Fast and accurate analysis methods** (AI-based?)



ITk: new ATLAS inner detector for HL-LHC

S. Campana et al. arXiv:2203.07237

Theory and Simulation

Quantum Field Theory[1]

- Lattice QCD, Sign problems

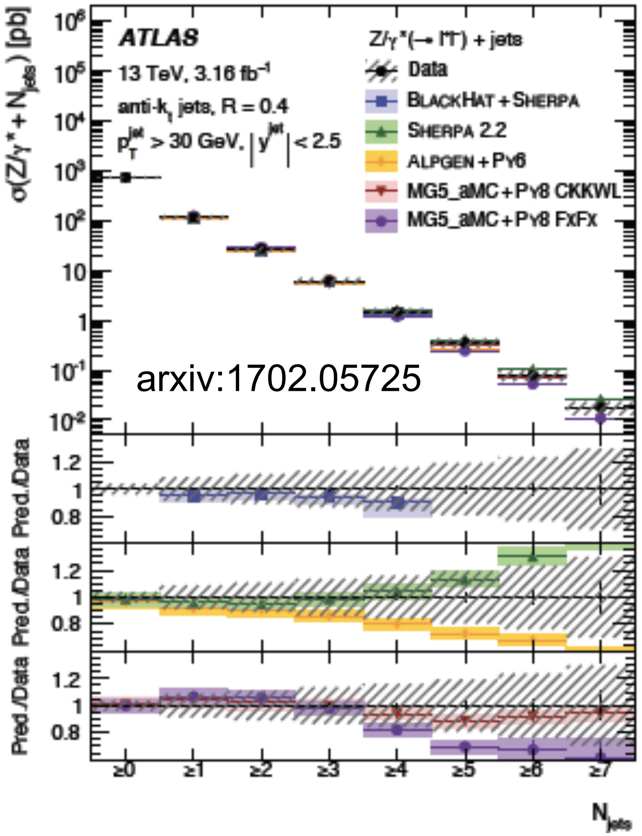
Parton showering

Event Generation & Cross section integration

Phase space sampling scales exponentially with number of final state particles[2]

- HL-LHC @ 3 10^{-3} fb^{-1} will have percent-level precision @N_{jet} = 9
- Need comparable (higher-order) MC
- N_{jet} increases with center-of-mass energy

Precision studies at FCC



Time and memory usage (Sherpa 3.x.y + HDF5) (H. Schulz 2018)

Process $W^+ +$	5j	6j*	7j*	8j†
RAM Usage	189 MB	484 MB	1.32 GB	1.32 GB
Init/startup time	3m5s / 1s	24m52s / 5s	3h6m / 18s	5h55m / 20s
Integration time	128×4h38m	256×13h53m	512×19h0m	1024×23h8m
MC uncertainty	1.0%	0.99%	2.38%	4.68%
Unweighting eff	$9.56 \cdot 10^{-5}$	$7.66 \cdot 10^{-5}$	$7.20 \cdot 10^{-5}$	$7.51 \cdot 10^{-5}$
10k evts	24h 40m	2d 11h	10d 15h	78d 1h

Numbers generated on dual 8-core Intel® Xeon® E5-2660 @ 2.20GHz
*,† Number of quarks limited to ≤6/4

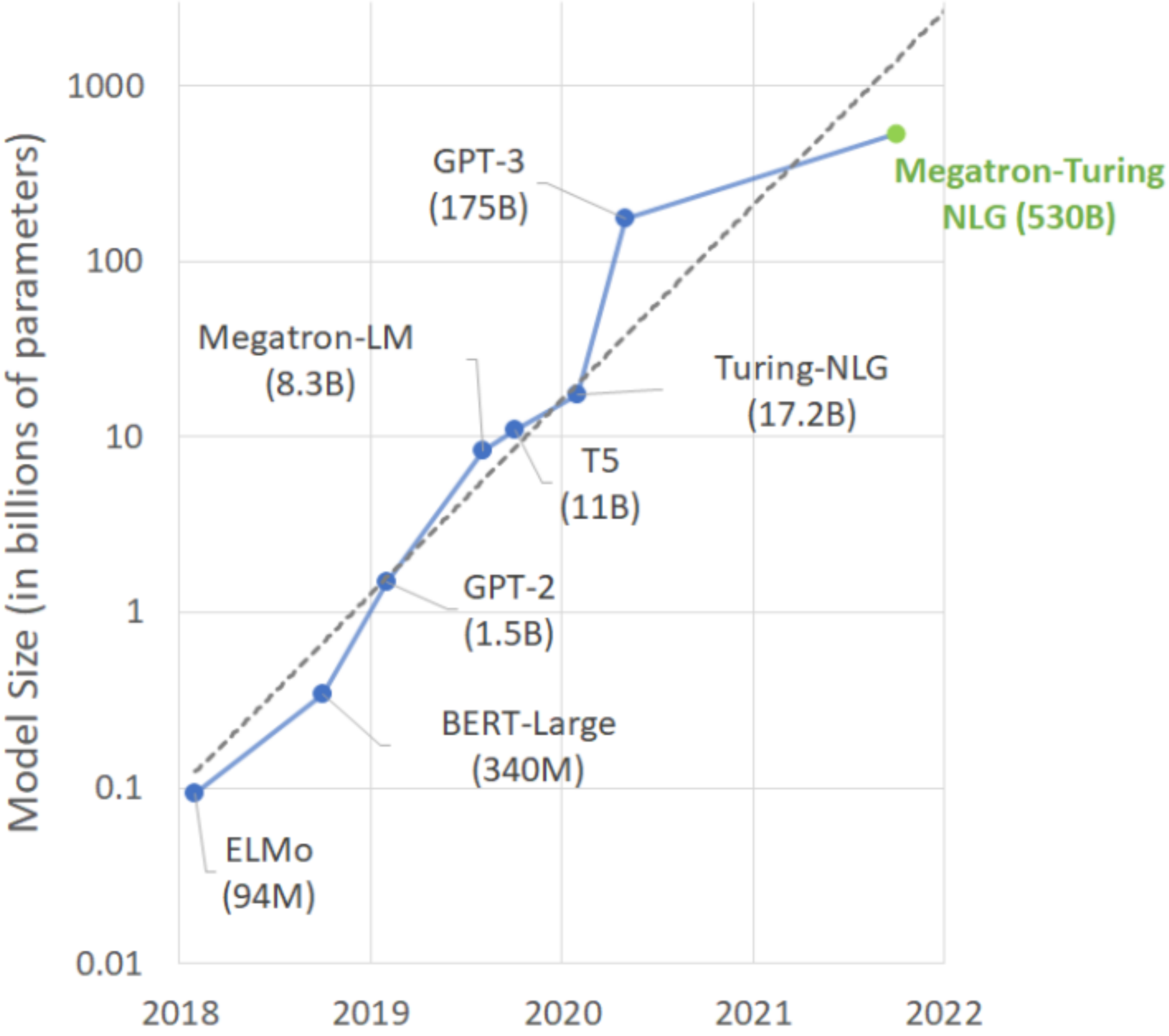
1 D. Grabowska's presentation at the CERN QTI workshop (https://indico.cern.ch/event/1098355)
2 arxiv:1905.05120

Deep Generative Models

Bommasani, Rishi, et al. "**On the opportunities and risks of foundation models.**" arXiv:2108.07258 (2021)

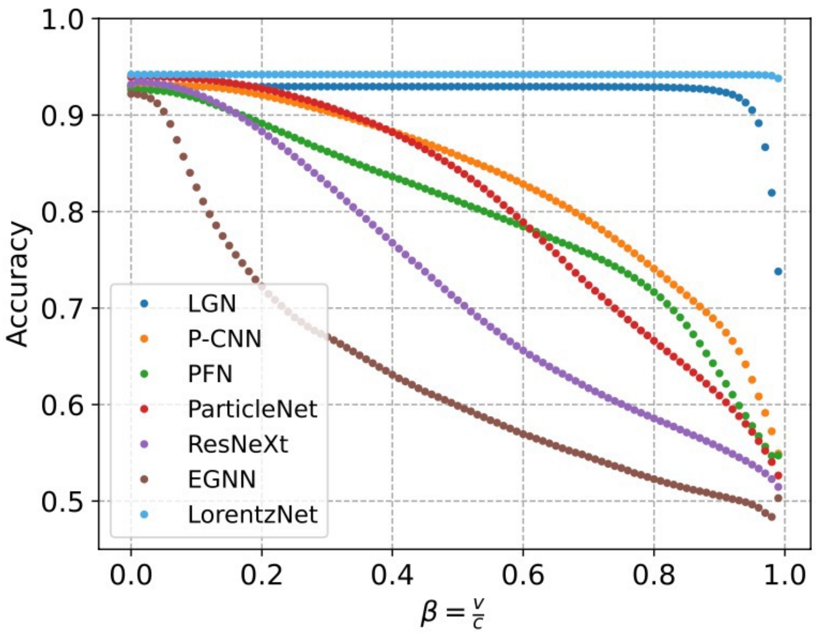
Representation Learning

- **Generative Models** learn the **representation** of an intractable probability distribution, p_{data} defined on $\mathbb{R}^n$
- Don't define explicit mathematical expression of $p_{model} \approx p_{data}$
- Trained as **generators** $\mathcal{g}: \mathbb{R}^m \rightarrow \mathbb{R}^n$ that map samples from a tractable distribution $\mathcal{Z}$ supported in $\mathbb{R}^m$ to points in $\mathbb{R}^n$



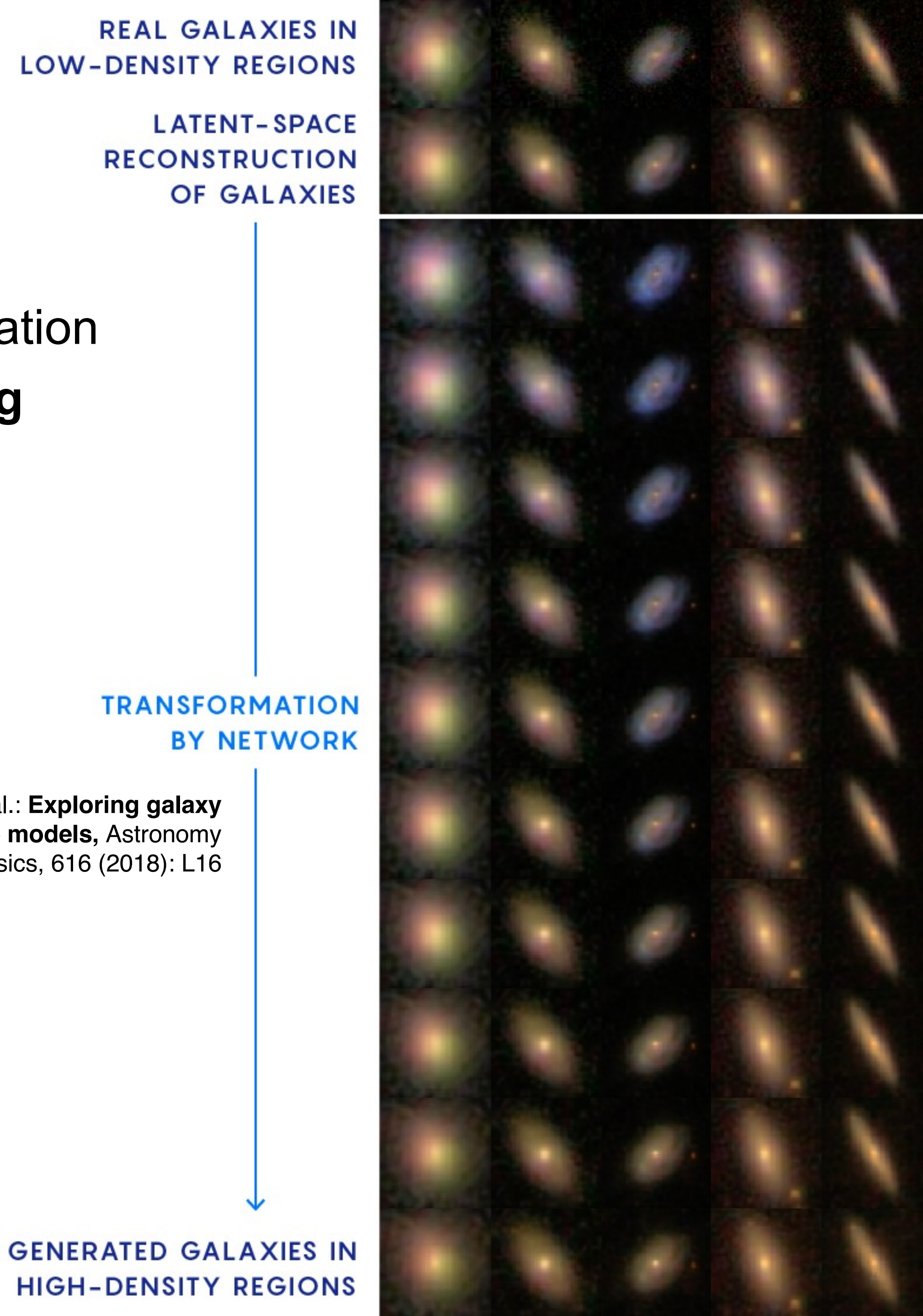
Internal representations

- **Lower-dimension manifold** representing the original information
- Beneficial to **connect representation to specific underlying symmetry group.**
- Manipulate latent space:
    - **Style** specification or **Hypothesis testing** directly in data

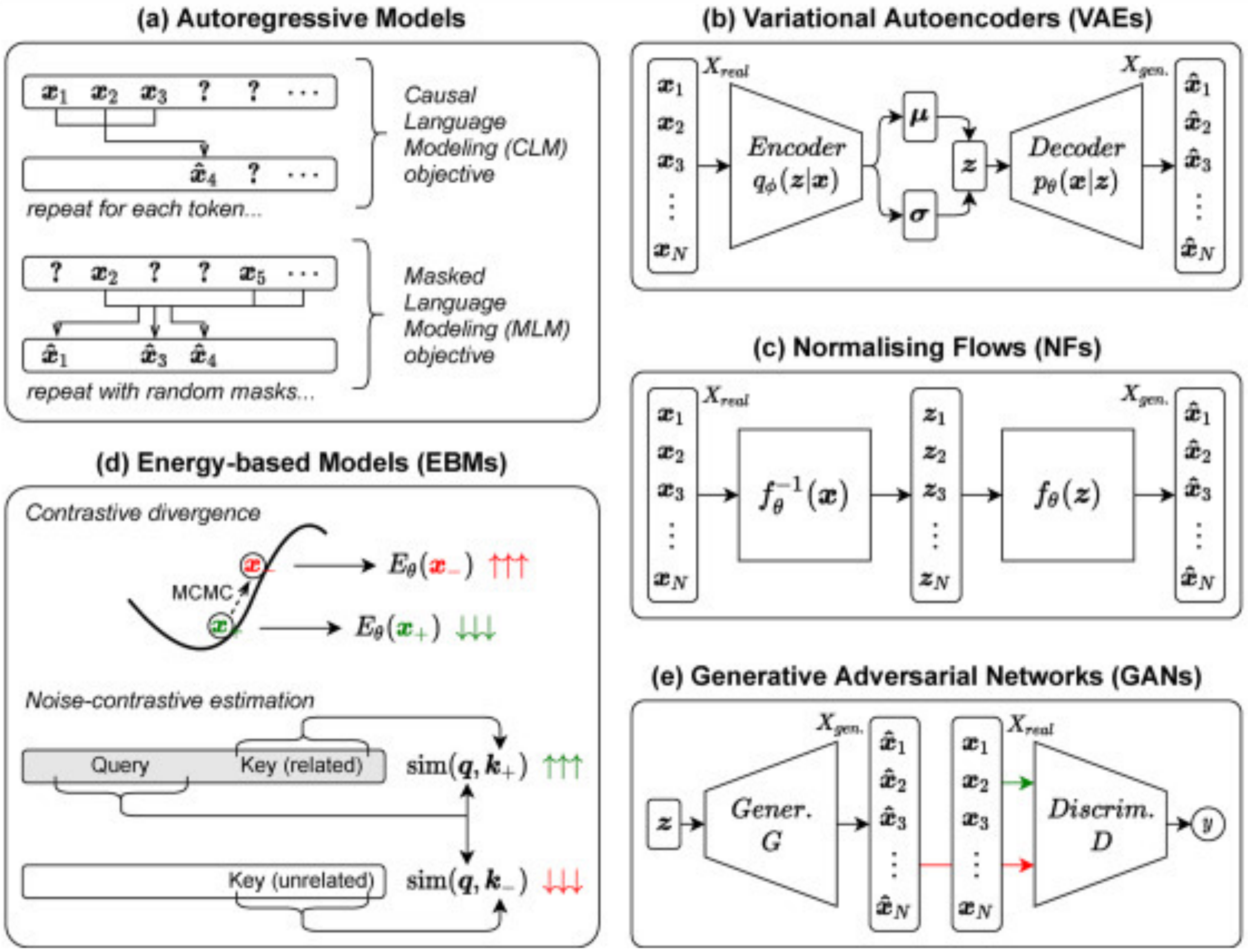


Gong, Shiqi, et al. "**An Efficient Lorentz Equivariant Graph Neural Network for Jet Tagging.**" *arXiv:2201.08187* (2022)

Kevin Schawinski et al.: **Exploring galaxy evolution with generative models,** Astronomy and Astrophysics, 616 (2018): L16



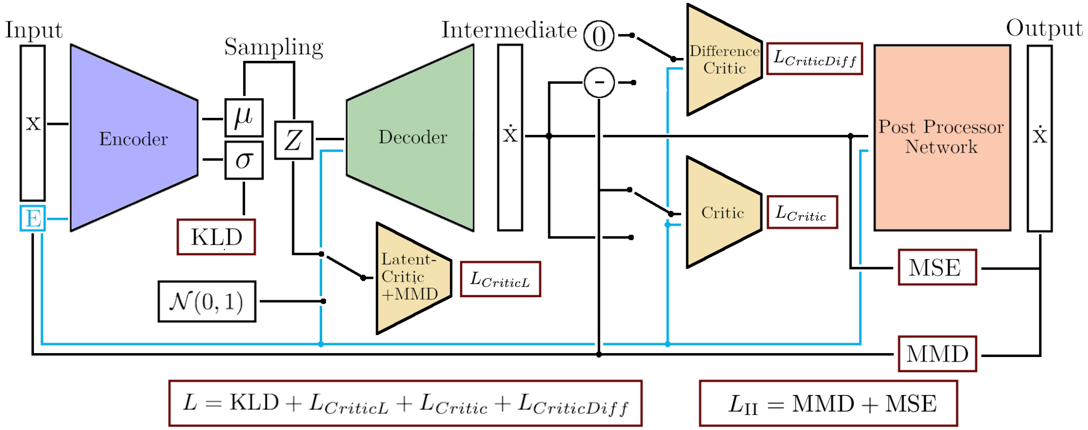
Examples

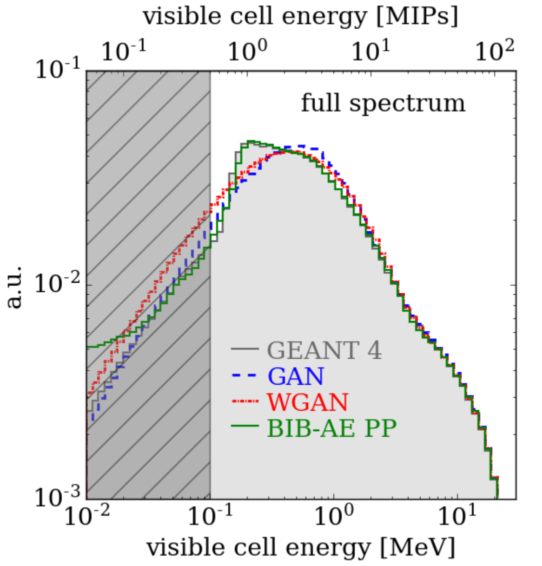

(a) Autoregressive Models
repeat for each token...
Causal Language Modeling (CLM) objective
repeat with random masks...
Masked Language Modeling (MLM) objective
(b) Variational Autoencoders (VAEs)
X_{real}
$X_{gen.}$
Encoder $q_\phi(z|x)$
Decoder $p_\theta(x|z)$
(c) Normalising Flows (NFs)
$f_\theta^{-1}(x)$
$f_\theta(z)$
(d) Energy-based Models (EBMs)
Contrastive divergence
MCMC
$E_\theta(x_-)$ ↑↑↑
$E_\theta(x_+)$ ↓↓↓
Noise-contrastive estimation
Query
Key (related)
Key (unrelated)
$\mathrm{sim}(q, k_+)$ ↑↑↑
$\mathrm{sim}(q, k_-)$ ↓↓↓
(e) Generative Adversarial Networks (GANs)
Gener. G
Discrim. D

Jason M. Allen, "**Théâtre D'opéra Spatial**", August 2022

High Energy Physics examples

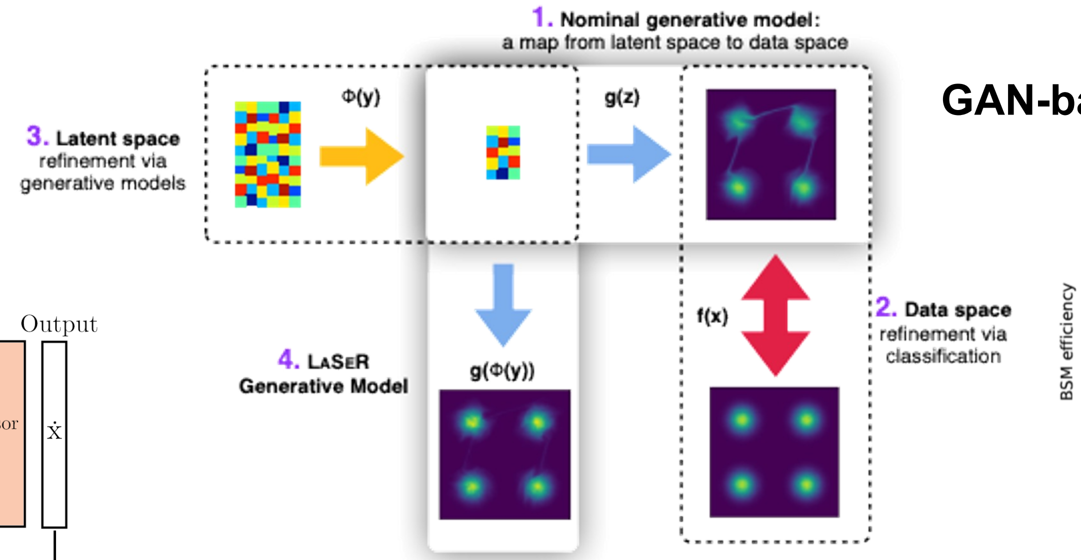
GAN – AutoEncoder hybrid





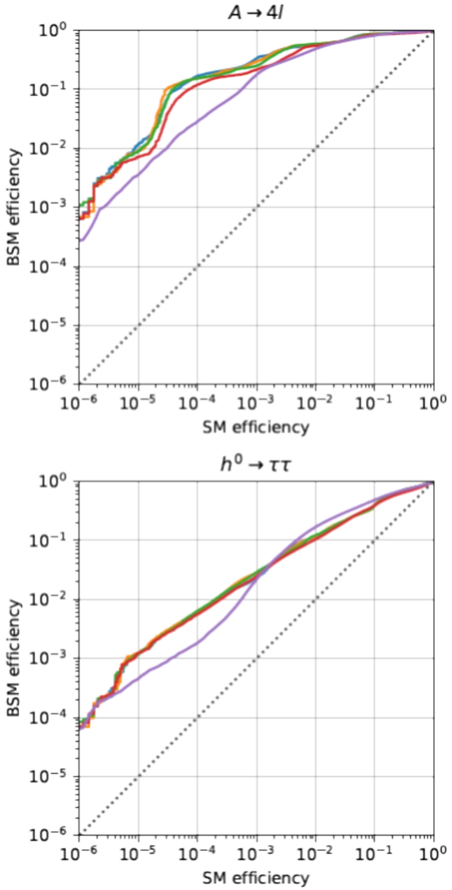
Buhmann, Erik, et al. "**Getting high: high fidelity simulation of high granularity calorimeters with high speed.**" *Computing and Software for Big Science* 5.1 (2021): 1-17.

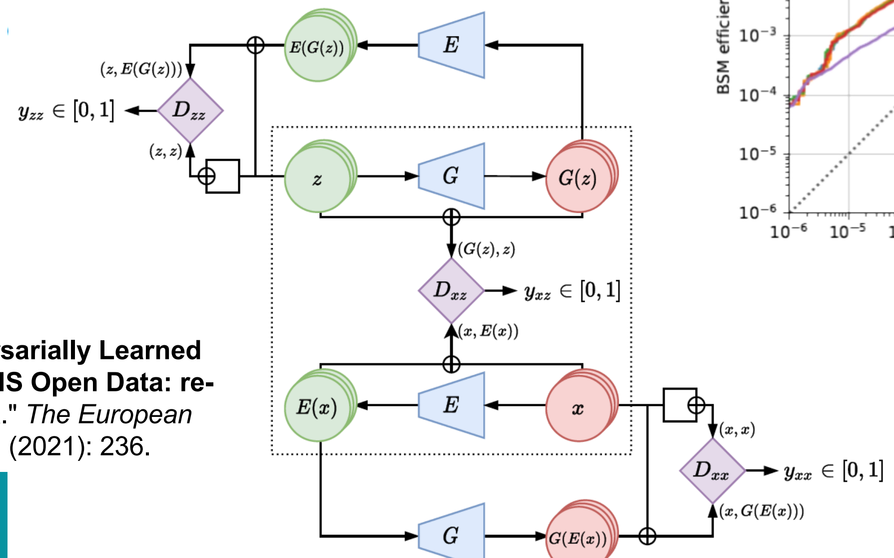
Latent space refinement



Winterhalder, Ramon, Marco Bellagente, and Benjamin Nachman. "**Latent Space Refinement for Deep Generative Models.**" *arXiv preprint arXiv:2106.00792* (2021).

GAN-based anomaly detection

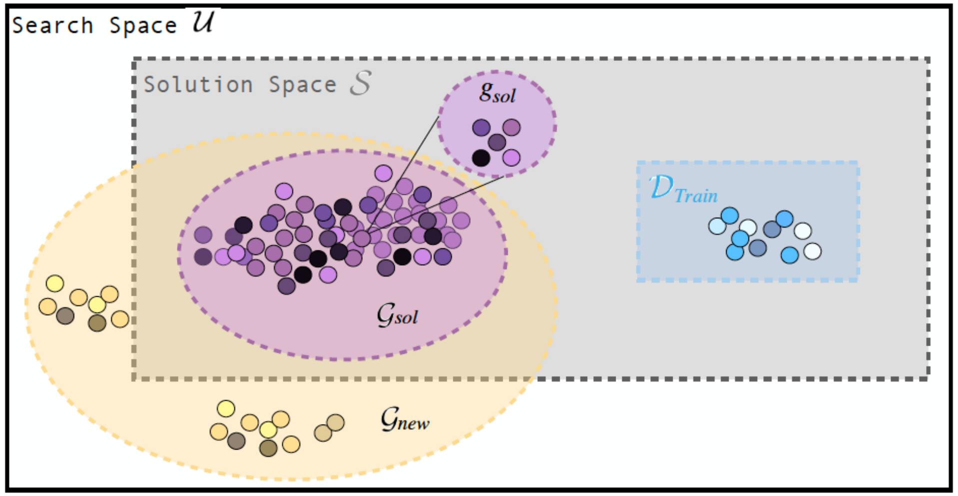




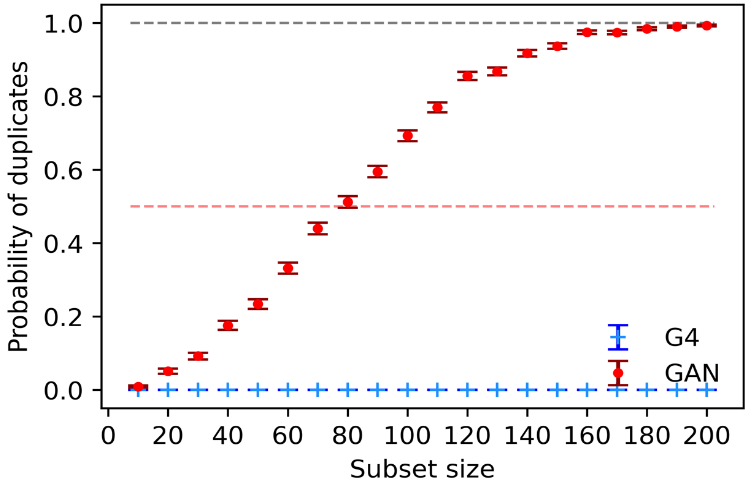
Knapp, Oliver, et al. "**Adversarially Learned Anomaly Detection on CMS Open Data: re-discovering the top quark.**" *The European Physical Journal Plus* 136.2 (2021): 236.

Generalization & limitations

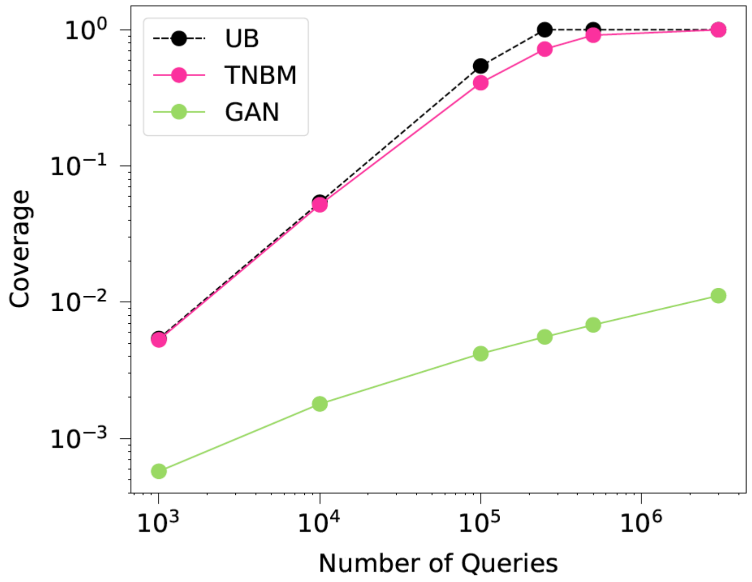
- Assessing generalisation is **particularly complex** in case of unsupervised learning and generative modeling
  - **Definitions** and **metrics**
  - **Comparison** among models
  - **Continuous** vs **discrete**
- Typical optimisation metrics might favor «copying»



Evaluating Generalization in Classical and Quantum Generative Models, K. Gili, M. Mauri and A. Perdomo-Ortiz, arxiv: 2201.0877 (2022)



Jaruskova, K. and Vallecorsa S. "**Estimating the Support Size of GANs for High Energy Physics Detector Simulation**."ML4PS NEURIPS2021



Quantum Computing at CERN

The CERN Quantum Technology Initiative

CERN established the QTI in 2020

- Roadmap in 2021
- Publicly available on Zenodo

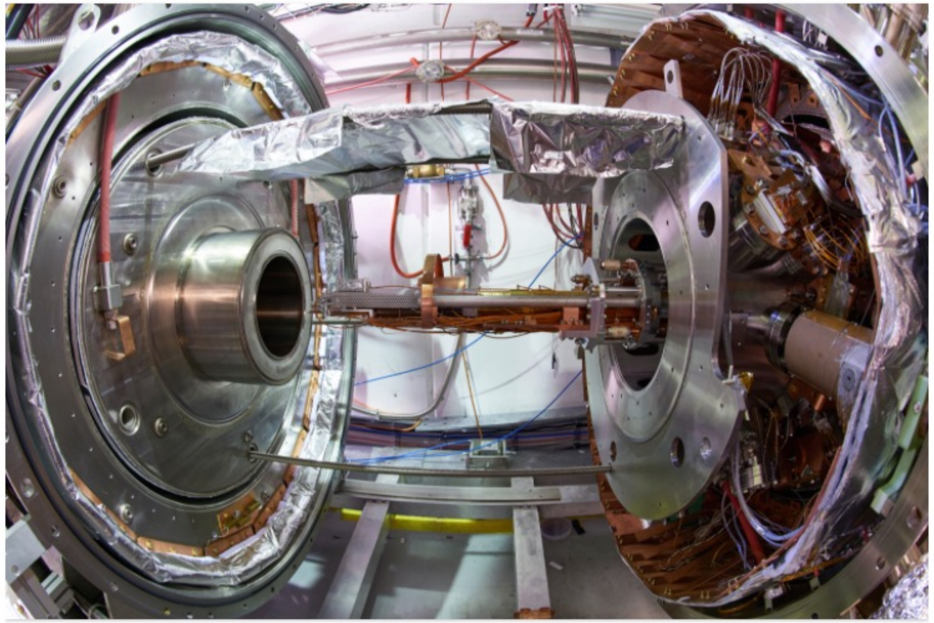
https://doi.org/10.5281/zenodo.5553774

Voir en français

CERN meets quantum technology

The CERN Quantum Technology Initiative will explore the potential of devices harnessing perplexing quantum phenomena such as entanglement to enrich and expand its challenging research programme

30 SEPTEMBER, 2020 | By Matthew Chalmers



The AEgIS 1T antimatter trap stack. CERN's AEgIS experiment is able to explore the multi-particle entangled nature of photons from positronium annihilation, and is one of several examples of existing CERN research with relevance to quantum technologies. (Image: CERN)

T1 - Scientific and Technical Development and Capacity Building

T2 - Co-development

APPLICATIONS | NEWS

CERN unveils roadmap for quantum technology

4 November 2021

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Credit: CERN

T3 - Community Building

T4 - Integration with national and international initiatives and programmes

International Conference on Quantum Technologies for High-Energy Physics (QT4HEP22)

CERN | QUANTUM TECHNOLOGY INITIATIVE

1–4 Nov 2022
CERN
Europe/Zurich timezone
There is a live webcast for this event.

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- Lodging
- Financial Sponsorships
- Swiss power plugs

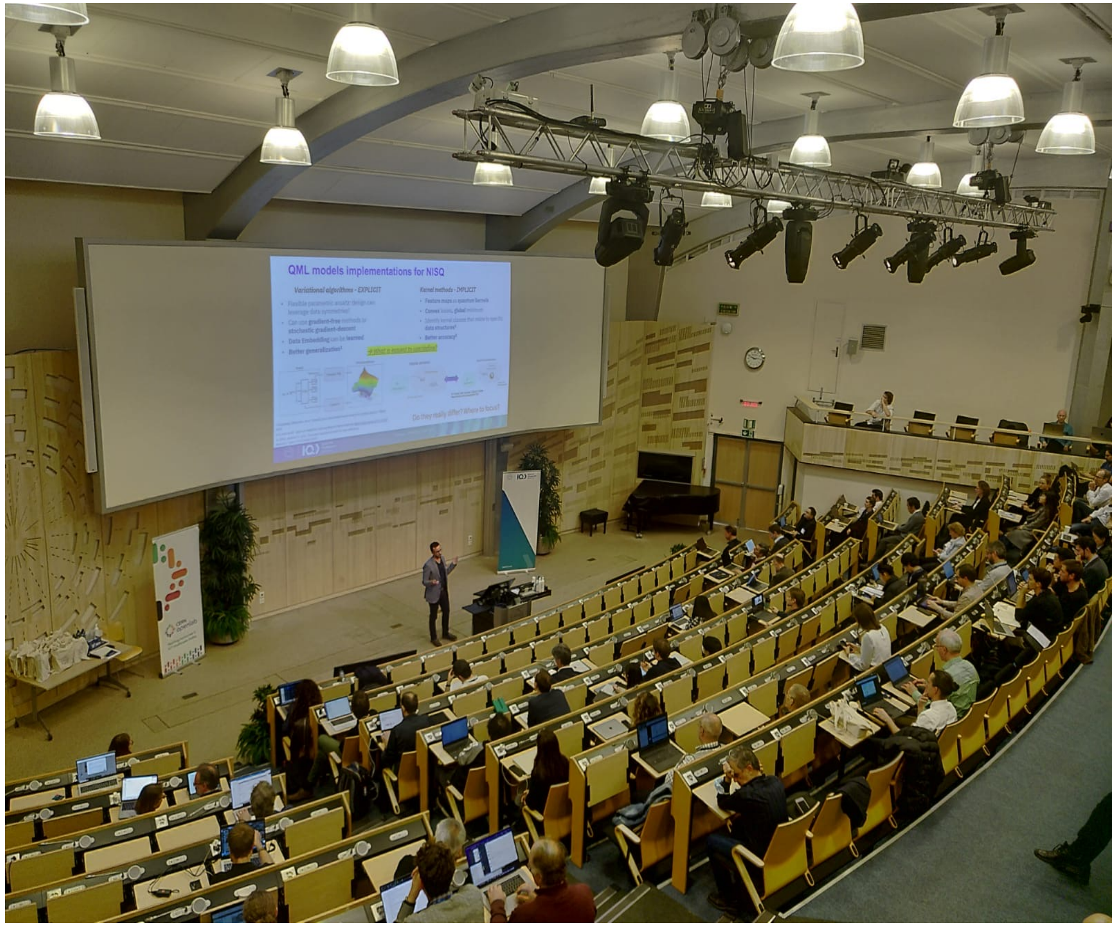
Contact

QT4HEP-conference@c...

Registration deadline extended until Friday, 28 October for the International Conference on Quantum Technology for High-Energy Physics, which will be hosted at CERN on 1–4 November 2022.

Following CERN's successful workshop on quantum computing in 2018, this is the first edition of the #QT4HEP conference taking place to further investigate the nascent quantum technology and its great promise to support scientific research.

Bringing the whole community together, we aim to foster common activities and knowledge sharing, discuss the recent developments in the quantum science field and keep looking for activities within HEP — and beyond — that can most benefit from the application of quantum technologies.



Collaboration ecosystem

Organizations and Projects

QUANTUM FLAGSHIP

QuantHEP

esa

Industry

Atos

IBM

Cambridge Quantum Computing

IDQ

Microsoft

Xanadu

intel

aws Amazon Braket

PASQAL

Google

DESY.

EPFL

ETH zürich

UK NATIONAL QUANTUM TECHNOLOGIES PROGRAMME

lrz

TUM

INFN Istituto Nazionale di Fisica Nucleare

Universitas Studiorum Insubriae

Orta Doğu Teknik Üniversitesi – Middle East Technical University, Northern Cyprus Campus

Universidad de Oviedo

Universitas Studii Paduani

University of Waterloo – Concordia cum veritate

cnrs IN2P3

iit ISTITUTO ITALIANO DI TECNOLOGIA

QuTech

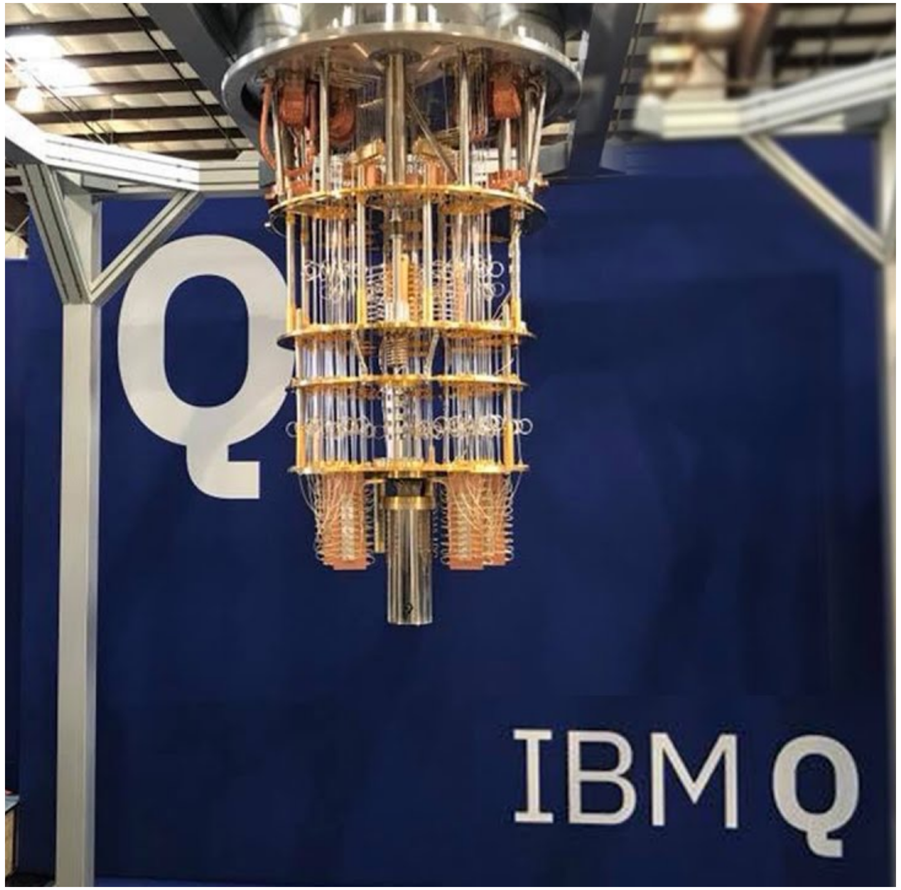
ICEPP The University of Tokyo

Fermilab

Oak Ridge National Laboratory

Academia, Research Labs and Agencies

CERN Quantum Hub



CERN is a **Hub Member** of the **IBM Quantum Network** since 2021

Access to IBM hardware based on quotas for Hub members and projects

Agreement for an initial 3-years phase

Hub members

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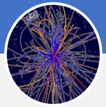
INFN

Going Beyond Classically Computable Problems

Building Experience on the Possibilities and Limits of Quantum Computing
for **Chemistry** and **Physics Challenges**

Scientific Objectives



- Assess the **areas of potential quantum advantage** in HEP (QML, classification, anomaly detection, tracking)
- Develop **common libraries of algorithms, methods, tools**; benchmark as technology evolves
- Collaborate to the development of shared, **hybrid classic-quantum infrastructures**

Computing & Algorithms

- Identify and develop techniques for **quantum simulation** in collider physics, QCD, cosmology within and beyond the SM
- Co-develop quantum computing and sensing approaches by providing **theoretical foundations** to the identifications of the areas of interest

Simulation & Theory

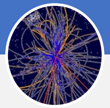
- Develop and promote **expertise in quantum sensing** in low- and high-energy physics applications
- Develop quantum sensing approaches with emphasis on **low-energy particle physics measurements**
- Assess **novel technologies and materials** for HEP applications

Sensing, Metrology & Materials

- **Co-develop CERN technologies relevant to quantum infrastructures** (time synch, frequency distribution, lasers)
- Contribute to the **deployment and validation of quantum infrastructures**
- Assess requirements and **impact of quantum communication on computing applications** (security, privacy)

Communications & Networks

Quantum Computing Objectives at CERN



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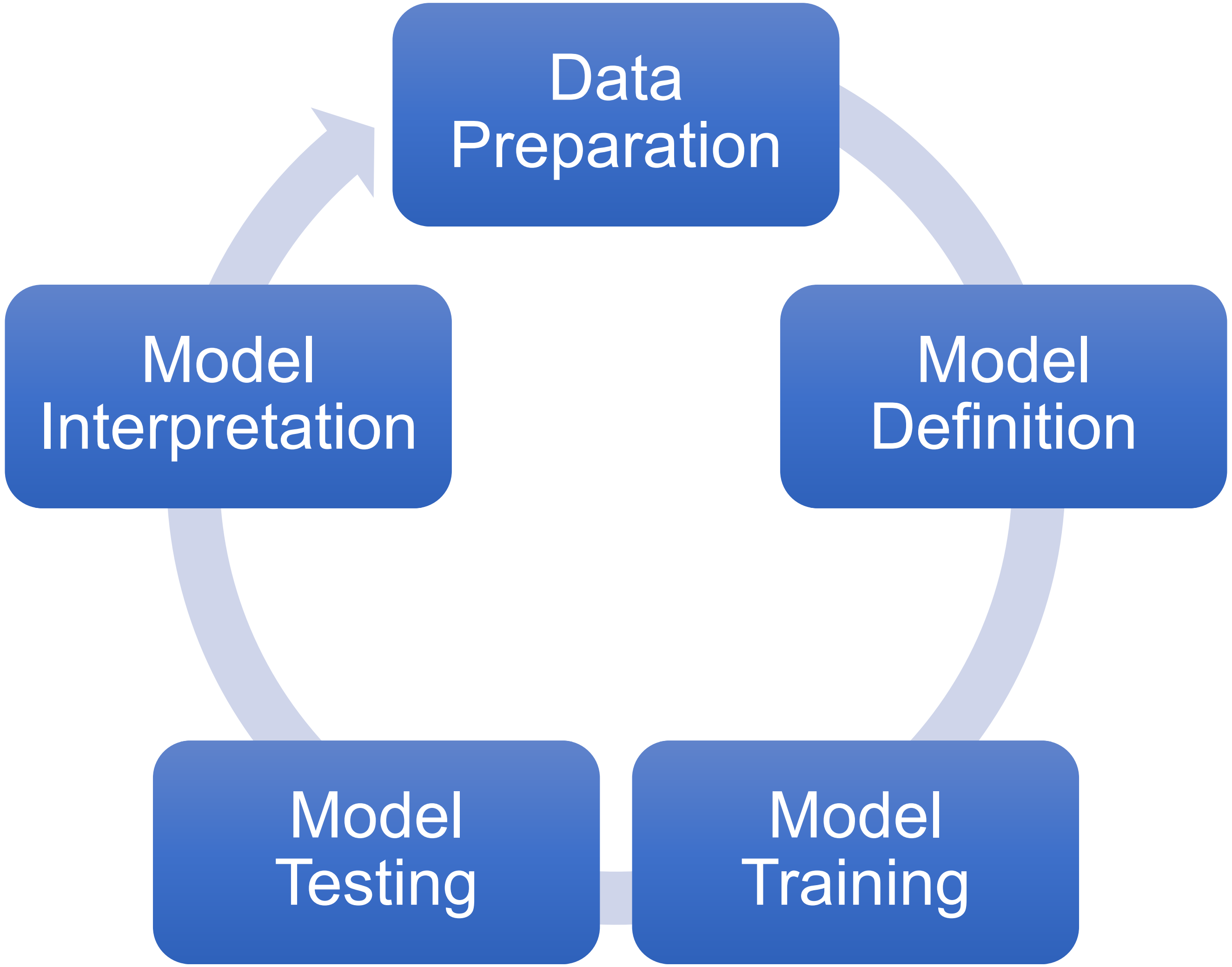
Computing & Algorithms

- Baseline for **application prioritisation** and **systematisation**
- **Formal approach** to algorithms, methods, error characterisation and correction
  - **Quantum Machine Learning**
    - Increasing use of ML in many computing and data analysis flows
    - Can be built as **hybrid models** where quantum computers act as accelerators
    - Efficient data handling is a challenge
  - **Algorithms beyond QML**
- **Test different hardware**
- Contribute to the development of a **quantum infrastructure**

Machine Learning Model Lifecycle



Investigating the full QML Lifecycle

Quantum advantage of many known QML algorithms is impeded by **I/O bottleneck**

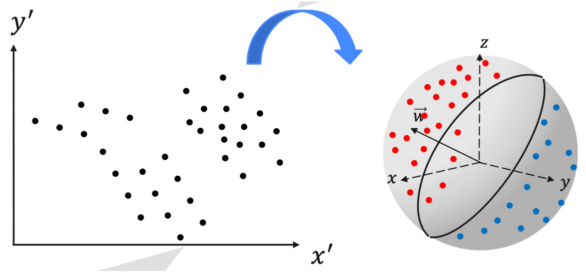
Data Preparation

Model Definition

Model Training

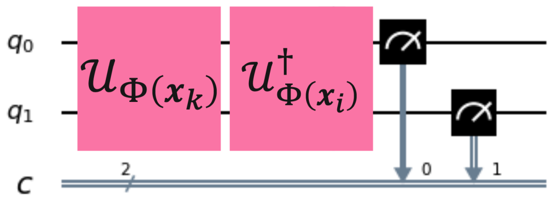
Model Testing

Model Interpretation

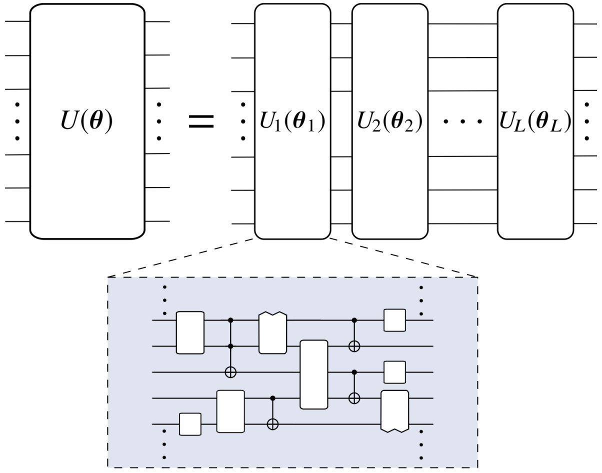


Data Reduction
Data Encoding [1,2,3]

Read Out



Trainability (BP…)



[1] Robust data encodings for quantum classifiers, Ryan LaRose and Brian Coyle, Phys. Rev. A 102, 032420

[2] Quantum convolutional neural network for classical data classification, https://arxiv.org/pdf/2108.00661.pdf

[3] Quantum Support Vector Machines for Continuum Suppression in B Meson Decays, https://arxiv.org/abs/2103.12257

Model definition

Variational algorithms - EXPLICIT

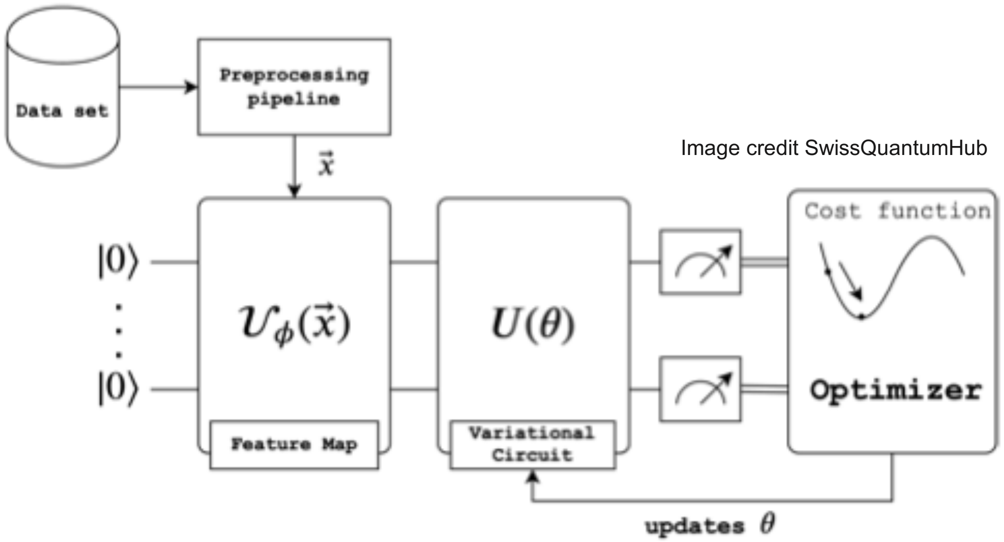


Image credit SwissQuantumHub

Define a **parametric quantum circuit** with trainable parameters ϑ

$$U(x, \vartheta)$$

Given an observable *O*, build a model

$$y(x, \vartheta) = \langle 0 | U^\dagger(x, \vartheta) O U(x, \vartheta) | 0 \rangle$$

- **Trained using gradient-free** or **gradient-based** optimization in a classical loop
- **Data Embedding** $\mathcal{V}_\phi(x)$ can be **learned**
- Improve performance by designing architectures to **leverage data symmetries**[1]
- Aim at quantum circuits that are **hard to simulate classically**

[1] Bogatskiy, Alexander, et al. "**Lorentz group equivariant neural network for particle physics.**" *International Conference on Machine Learning*. PMLR, 2020.

Model definition

Kernel methods - IMPLICIT

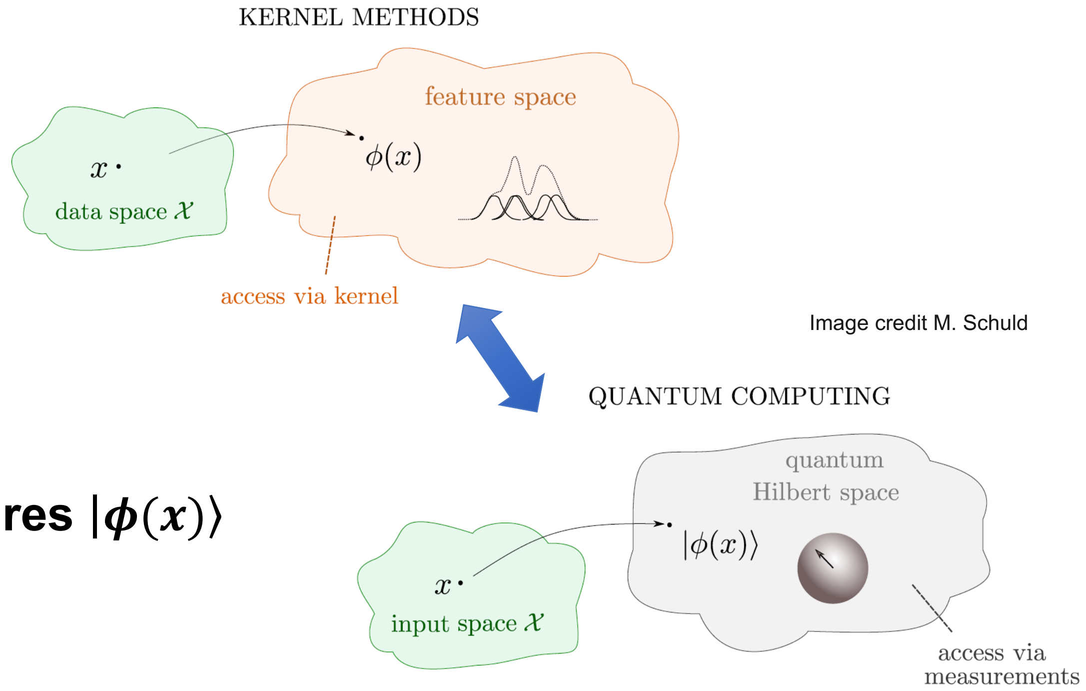


Image credit M. Schuld

Feature maps as **quantum kernels**

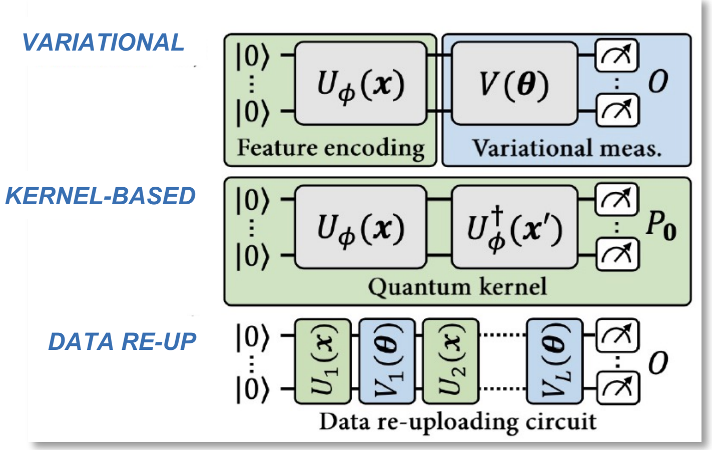
Use quantum computers to create **classically intractable features** $|\boldsymbol{\phi}(\boldsymbol{x})\rangle$

- Build inner product of feature vectors → $O(N_{data}^2)$
- Use classical **kernel-based training**
  - **Convex** losses**, global** minimum
- Identify classes of kernels that relate to specific data **structures**[1]
- Given a variational circuit of the form $U(x, \vartheta) = \mathcal{V}_\vartheta U_\phi(x)$, can define a quantum kernel method with better accuracy: $|\boldsymbol{\phi}(\boldsymbol{x})\rangle = U_\phi(x)|0\rangle$
- **Classically: not all machine learning models can be described by kernel methods.**

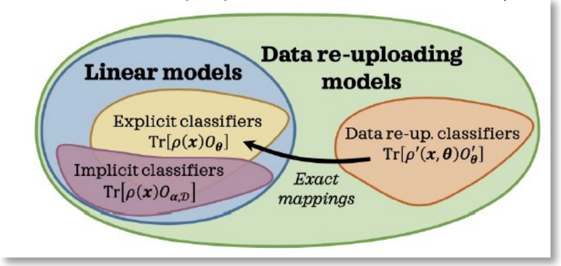
Schuld, Maria. "Supervised quantum machine learning models are kernel methods." *arXiv preprint arXiv:2101.11020* (2021).

[1] Glick, Jennifer R., et al. "**Covariant quantum kernels for data with group structure**." *arXiv preprint arXiv:2105.03406* (2021).

Equivalent interpretations?



Jerbi, Sofiene, et al. "**Quantum machine learning beyond kernel methods**." *arXiv preprint arXiv:2110.13162* (2021).

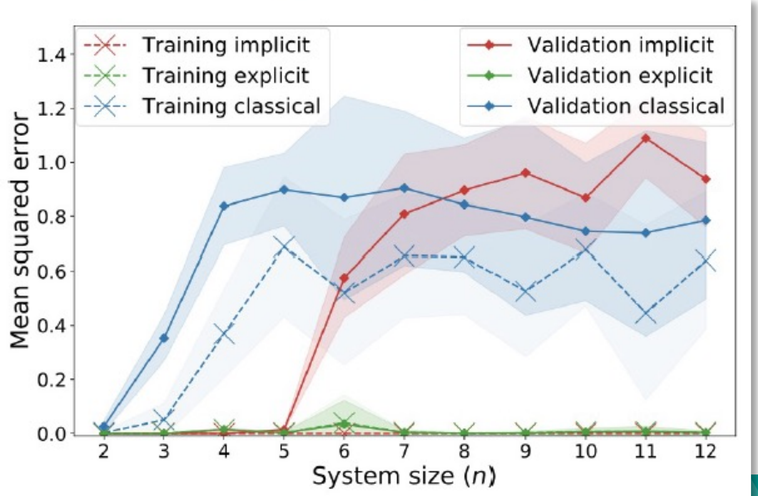


Characterize models behaviour, similarities among them and **link to data properties.**

Ex:

- Data Re-Uploading circuits: alternating data encoding and variational layers.
  - Represented as **explicit linear models** (variational) in larger feature space

  → can be reformulated as **implicit models** (kernel)
- Representer theorem: implicit models achieve **better accuracy**
  - Explicit models exhibit **better generalization** performance



PCA on 28x28 fashion-MNIST dataset, ZZ feature encoding + hardware-efficient variational unitary

Model Convergence and Barren Plateau

The size of the Hilbert space requires compromises between **expressivity**, **convergence** and **generalization**

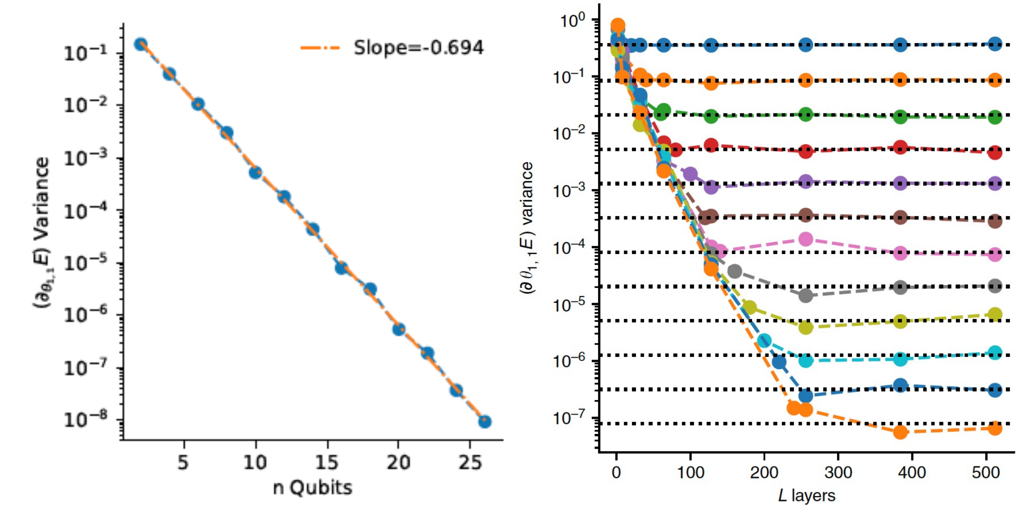
Classical gradients **vanish exponentially** with the number of layers (J. McClean *et al.*, arXiv:1803.11173)

- Convergence still possible if gradients consistent between batches.

Quantum gradient decay exponentially in the number of qubits

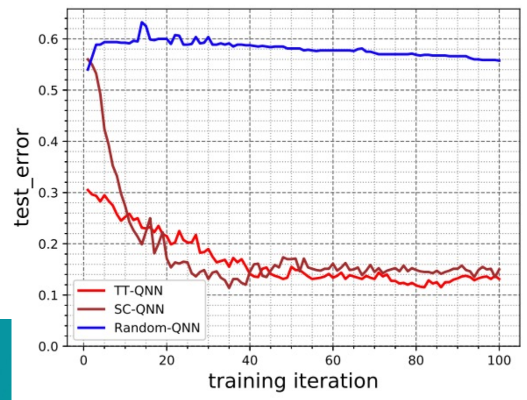
- Random circuit initialization
- Loss function locality in shallow circuits (M. Cerezo *et al.*, arXiv:2001.00550)
- Ansatz choice: TTN, CNN (Zhang *et al.*, arXiv:2011.06258, A Pesah, *et al.*, *Physical Review X* 11.4 (2021): 041011.)
- Noise induced barren plateau (Wang, S *et al.*, Nat Commun 12, 6961 (2021))

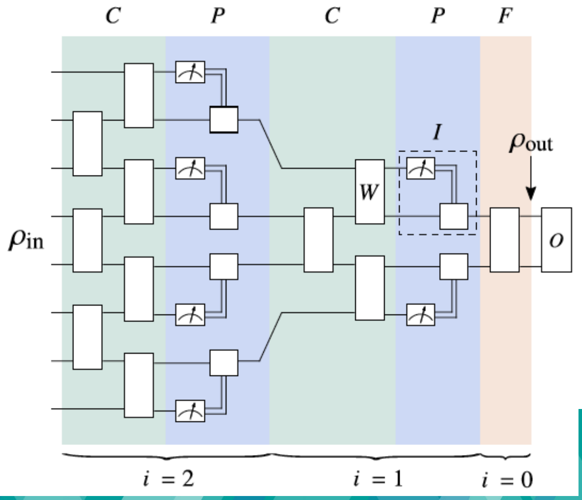
J. McClean *et al.*, arXiv:1803.11173



QCNN: A Pesah, *et al.*, *Physical Review X* 11.4 (2021): 041011

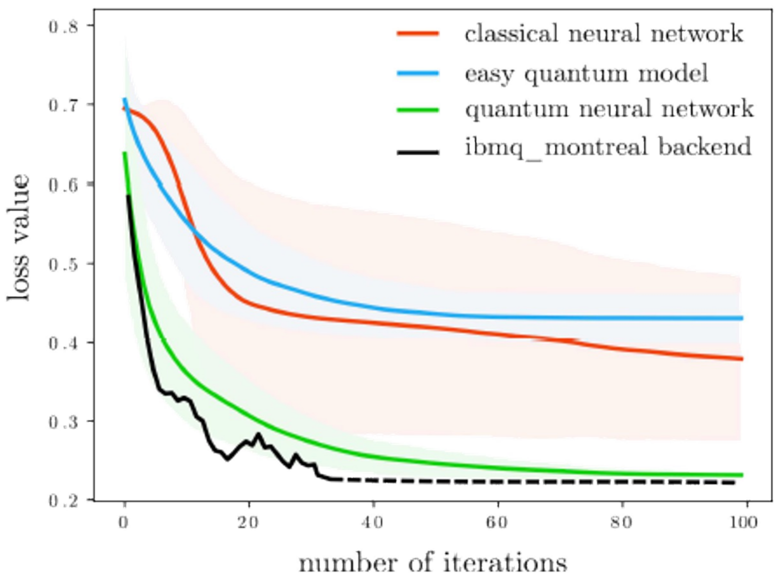
TTN for MNIST classification (8 qubits), Zhang *et al.*, arXiv:2011.06258





Defining quantum Advantage for QML

Abbas, Amira, et al. "**The power of quantum neural networks.**" *Nature Computational Science* 1.6 (2021): 403-409.



Different possible definitions

Runtime speedup

Sample complexity

Representational power

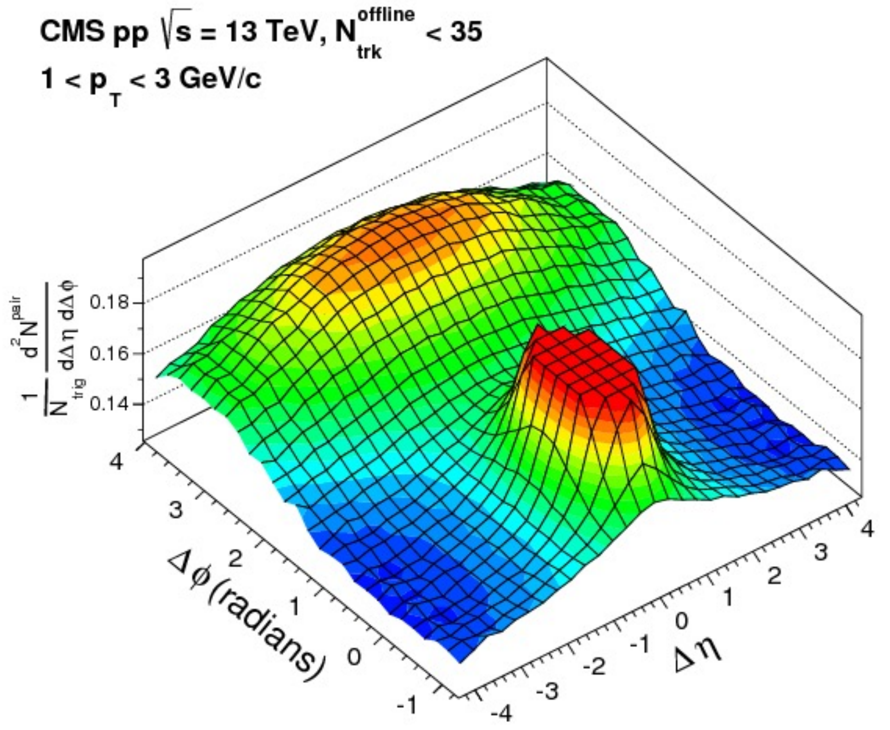
Classical Intractability: a quantum algorithm that cannot be efficiently simulated classically

- No established recipe for classical data
- Need to use the whole exponential advantage in Hilbert space, but will it converge ?

(Algorithm expressivity vs convergence and generalization)

Kübler, Jonas, Simon Buchholz, and Bernhard Schölkopf. "**The inductive bias of quantum kernels.**" Advances in Neural Information Processing Systems 34 (2021).
Huang, HY., Broughton, M., Mohseni, M. et al. **Power of data in quantum machine learning**. Nat Commun 12, 2631 (2021). https://doi.org/10.1038/s41467-021-22539-9

Practical advantage



Khachatryan, Vardan, et al. "**Measurement of Long-Range Near-Side Two-Particle Angular Correlations in p p Collisions at s= 13 TeV**." *Physical review letters* 116.17 (2016): 172302.

Practical implementation vs asymptotic complexity

Data embedding
NISQ vs ideal quantum devices
Realistic applications

Performance metrics and fair comparison to classical models

HEP data is classical, but originally produced by quantum processes. It is these **intrinsically quantum correlations** we are trying to identify

A change of paradigm could reflect in interesting insights

- What are natural building blocks for QML algorithms?
- How can we construct useful bridges between QC and learning theory?
- How can we make quantum software ready for ML applications?

Quantum information with top quarks in QCD
Yoav Afik, Juan Ramón Muñoz de Nova
https://arxiv.org › abs › 2101.10307

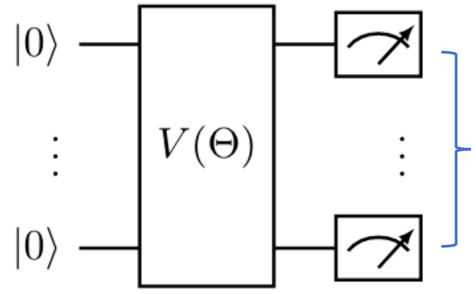
Schuld, Maria, and Nathan Killoran. "**Is quantum advantage the right goal for quantum machine learning?**." *arXiv preprint arXiv:2203.01340* (2022).

Quantum Generative Models

Delgado and Hamilton, arXiv:2203.03578 (2022)
Zoufal, et al., *npj Quantum Inf* **5**, 103 (2019)
Leadbeater et al., *Entropy* **2021**, *23*, 1281.
Amin, et al. *Physical Review X* 8.2 (2018): 021050.

QCBM

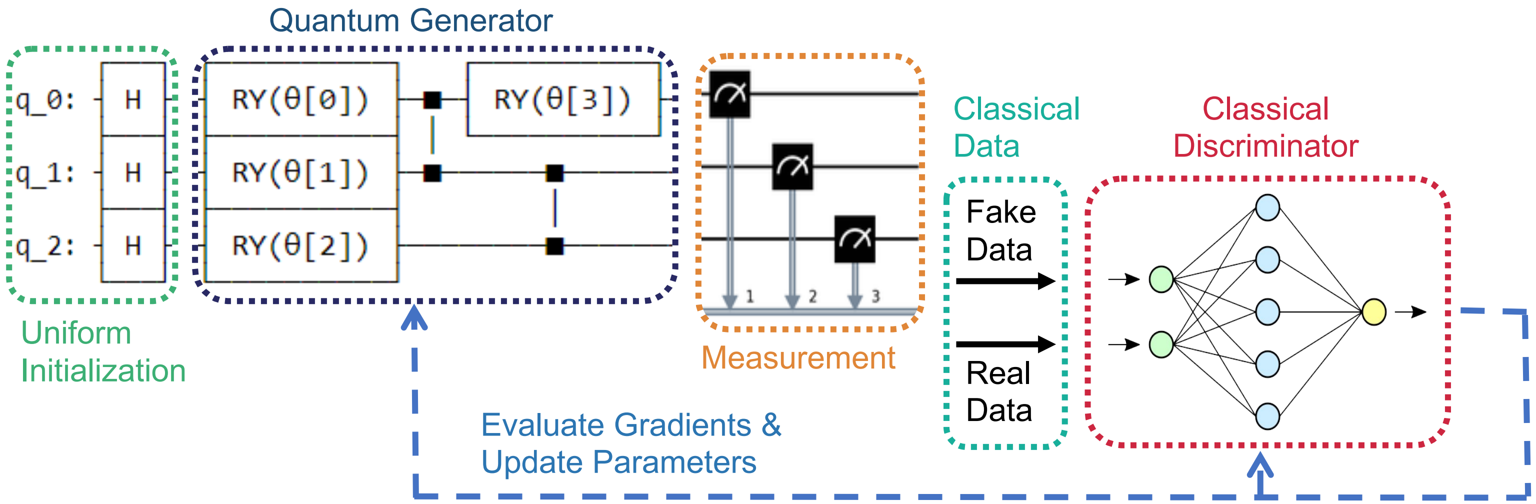
Sample variational pure state $|\psi(\theta)\rangle$ by projective measurement through **Born rule**: $\mathbf{p}_{\boldsymbol{\theta}}(\mathbf{x}) = |\langle \mathbf{x}|\boldsymbol{\psi}(\boldsymbol{\theta})\rangle|^2$.



n dimensional binary strings map to 2^n bins of the discretized dataset.

QGAN

Multiple implementations, mostly classical-quantum hybrid



QBM

Network of stochastic binary units with a quadratic energy function that follows the Boltzman distribution (Ising Hamiltonian)

$$H = -\sum_a b_a \sigma_a^z - \sum_{a,b} w_{ab} \sigma_a^z \sigma_b^z$$

Typical metrics:

$$D_{\mathrm{KL}}(P \| Q) = \sum_i P(i) \log\left(\frac{P(i)}{Q(i)}\right)$$

$$\mathrm{MMD}(\mathbb{P}_r, \mathbb{P}_g) = \left(\mathbb{E}_{\substack{\mathbf{x}_r, \mathbf{x}_r' \sim \mathbb{P}_r, \\ \mathbf{x}_g, \mathbf{x}_g' \sim \mathbb{P}_g}} \left[k(\mathbf{x}_r, \mathbf{x}_r') - 2k(\mathbf{x}_r, \mathbf{x}_g) + k(\mathbf{x}_g, \mathbf{x}_g')\right]\right)^{\frac{1}{2}}$$

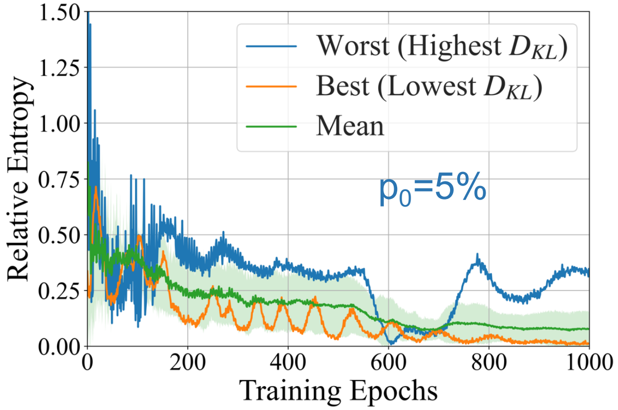
Our results so far..

- **Multiple QML prototypes for different applications**
  - We can build expressive models and we can train them ☺
- **Increasing level of precision**
- **Robustness against noise ?**

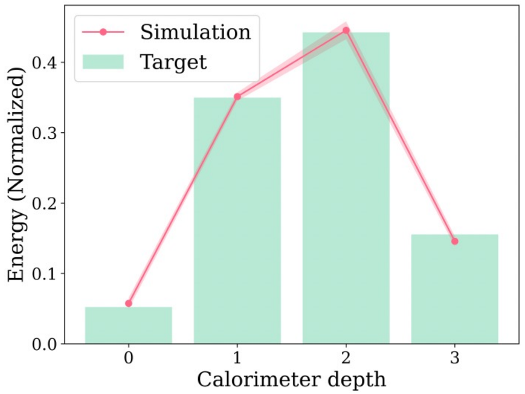
- **Scale is still a problem on current quantum hardware**
  - Complex data pre-processing
- **Generalization**
- **Empirical results → Need theoretical grounding**

QML at CERN

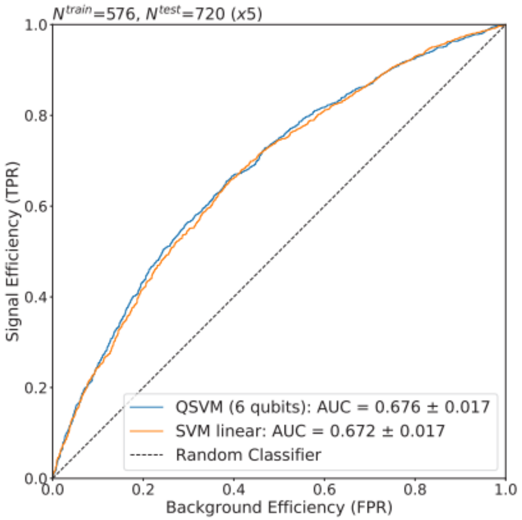
Borras, Kerstin, et al. "**Impact of quantum noise on the training of quantum Generative Adversarial Networks**." *arXiv preprint arXiv:2203.01007* (2022).



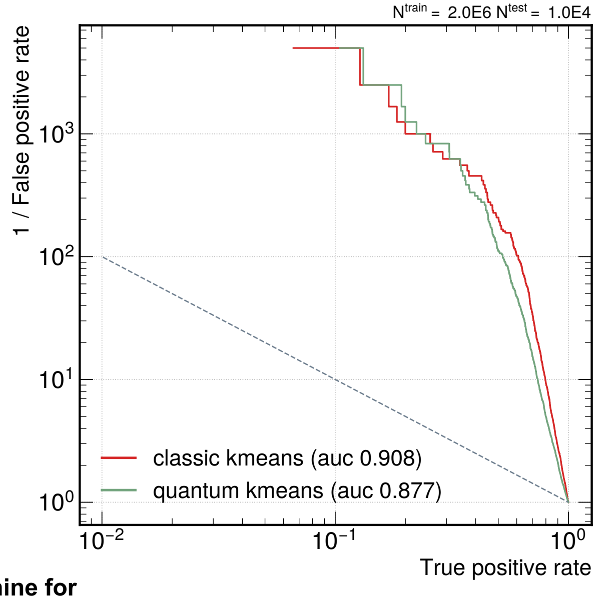
Chang S.Y. *et al.,* **Running the Dual-PQC GAN on Noisy Simulators and Real Quantum Hardware**, QTML2021, ACAT21



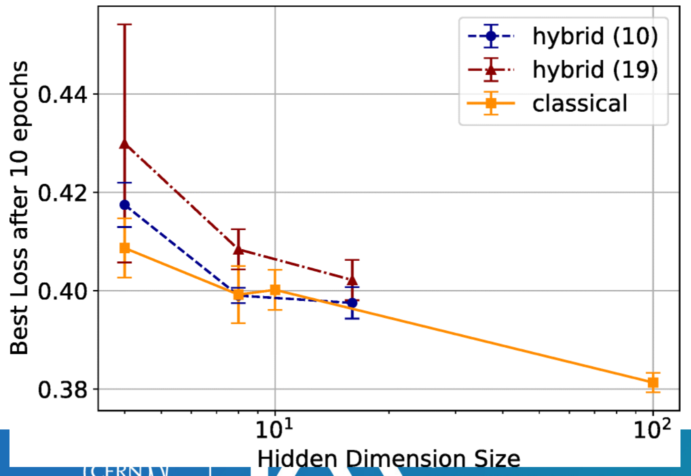
Vasilis Belis, Samuel González-Castillo, Christina Reissel, Sofia Vallecorsa, Elías F. Combarro, Günther Dissertori, and Florentin Reiter. **Higgs analysis with quantum classifi**ers. EPJ Web of Conferences, 251:03070, 2021



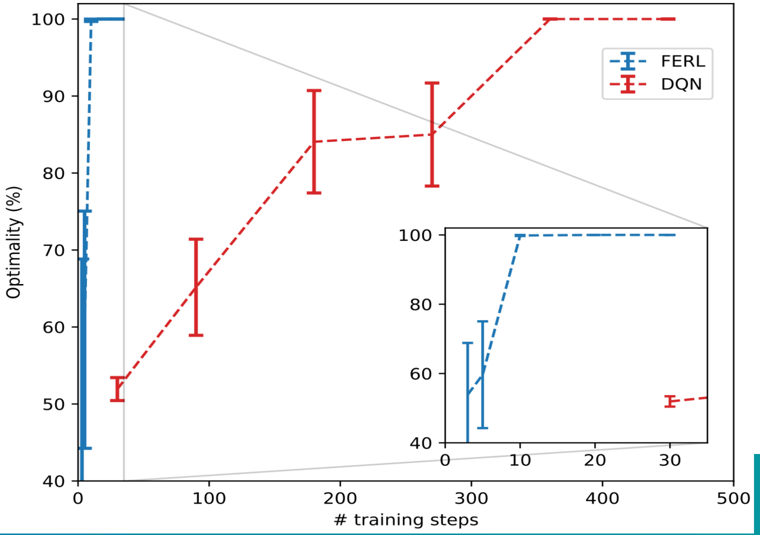
Kinga Wozniak, **Unsupervised clsutering for a Randall–Sundrum Graviton at 3.5TeV narrow resonance, 5th IML workshop, May 2022**



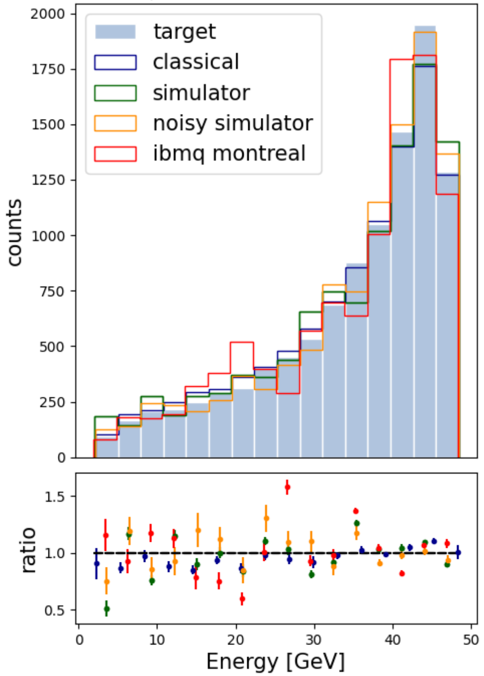
Tüysüz, Cenk, et al. "**Hybrid quantum classical graph neural networks for particle track reconstruction**." *Quantum Machine Intelligence* 3.2 (2021): 1-20.



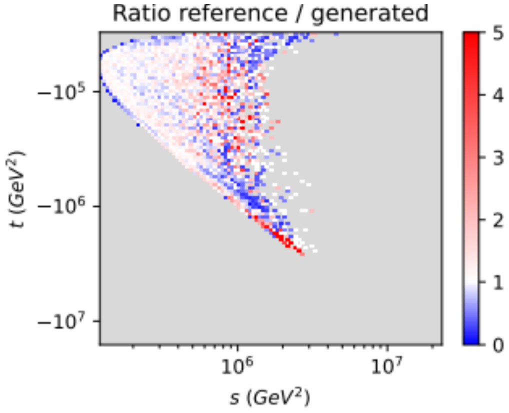
M. Shenk, V. Kain, **Quantum Reinformcement Learning**, BQiT 2021, 2022 CERN openlab Tech Workshop



O. Kiss, **Quantum Born Machine for event generation**, ACAT2021



Bravo-Prieto, Carlos, et al. "**Style-based quantum generative adversarial networks for Monte Carlo events**." *arXiv preprint arXiv:2110.06933* (2021).

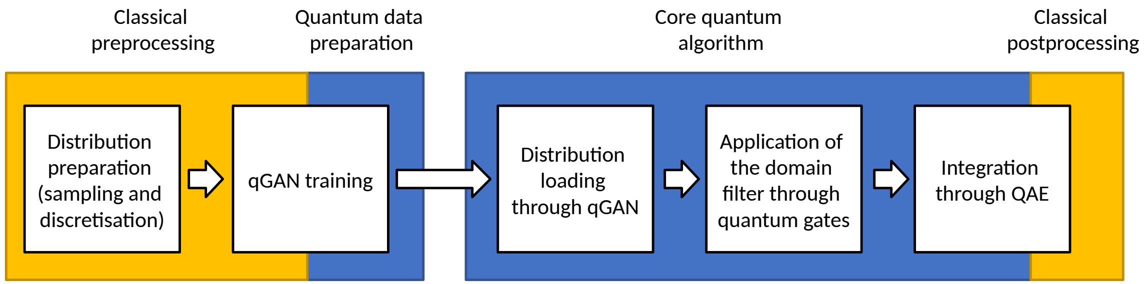


Agliardi, Gabriele, et al. "**Quantum integration of elementary particle processes**." *arXiv preprint arXiv:2201.01547* (2022)

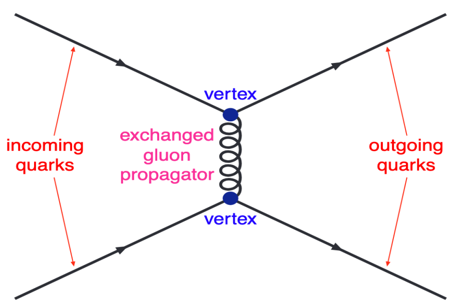
qGAN for quantum data preparation

Cross section integration using **Quantum Amplitude Estimation**

Data encoding affects quality of integration



Electroweak example:



phase-space factor

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

matrix element

phase-space cuts

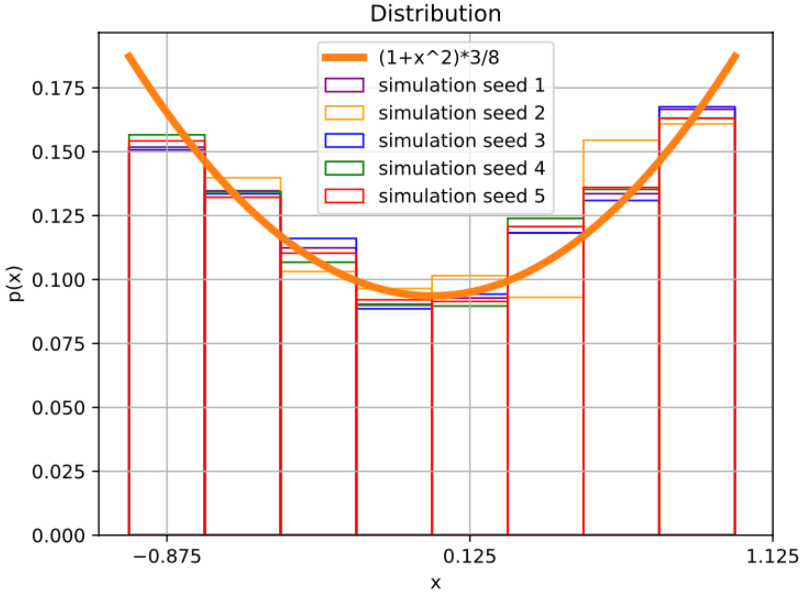
qGAN for data embedding

Test on $1 + x^2$ distribution:

- 10k events, 3 qubits, circular entanglement

$$G(\phi)\,|\psi_{in}\rangle = |g(\phi)\rangle = \sum_{i=0}^{N-1} \sqrt{p_g^i(\phi)}\,|i\rangle$$

Loading	Difference per bin [%] Min.	Max.	Average	σ_x
Direct	+0.207	−1.88	1.35	1.80×10^{-3}
qGAN default	+2.36	−21.1	8.51	0.0118
qGAN optimised	−0.995	−12.4	4.65	7.00×10^{-3}



qGAN for event generation

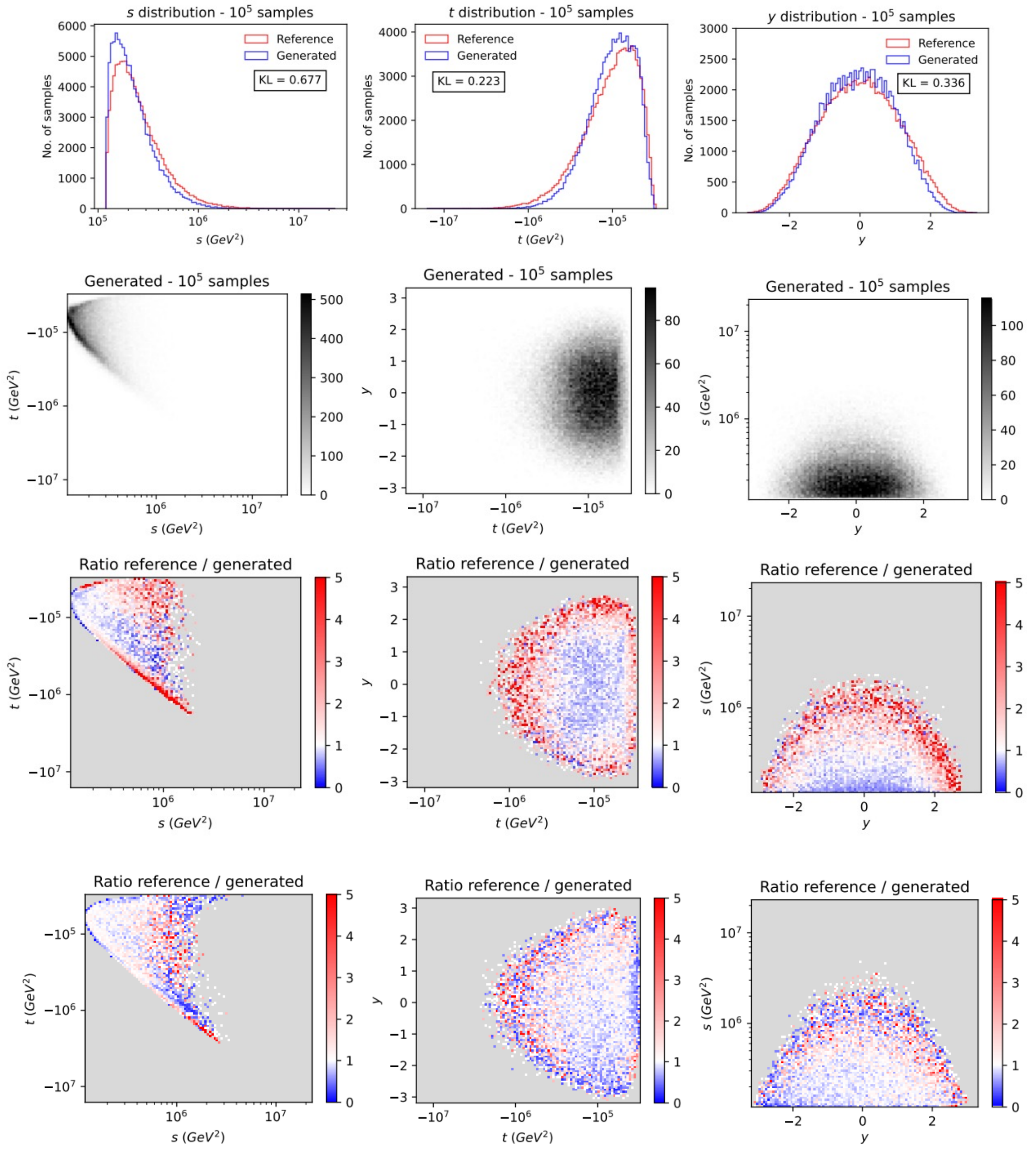
Generate Mandelstam (*s,t*) + *y* variables for **t-tbar production**

Introduce a **style-based** approach

	$pp \to t\bar{t}$ **LHC events**
Qubits	3
D_{latent}	5
Layers	2
Epochs	3×10^4
Training set	10^4
Batch size	128
Parameters	62
U_{ent}	2 sequential CR_y gates

IBM Q Santiago

Quantum simulator

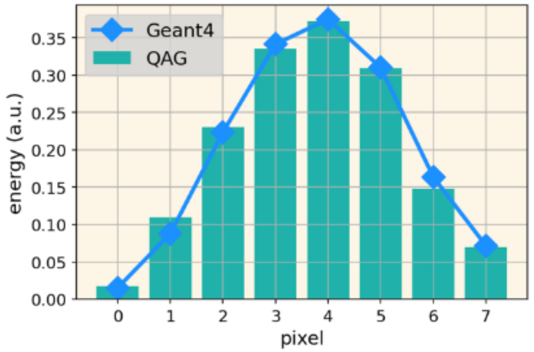


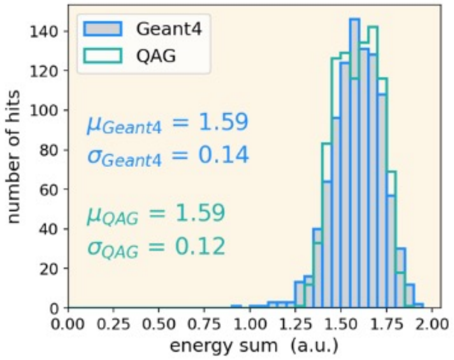
Bravo-Prieto et al. "**Style-based quantum generative adversarial networks for Monte Carlo events**." Quantum 6, 777 (2022) , *arXiv preprint arXiv:2110.06933* (2021).

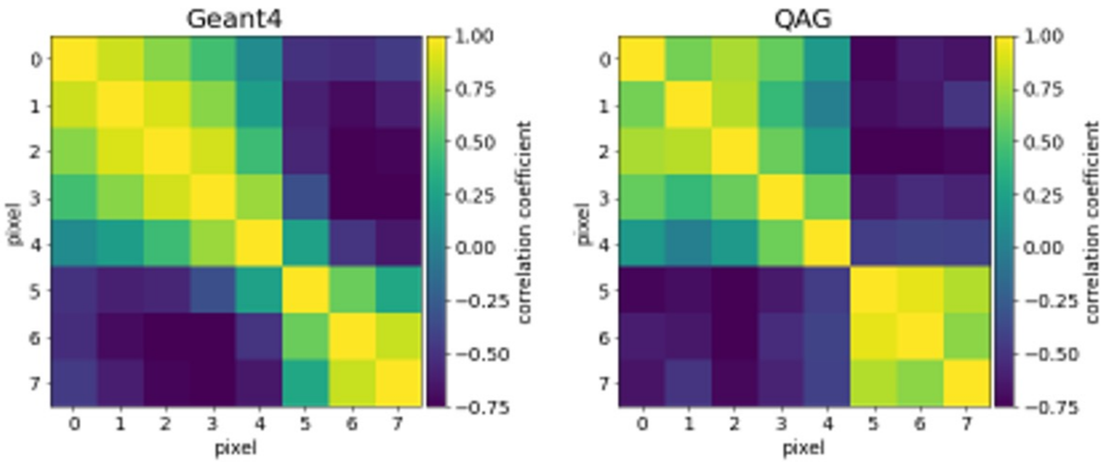
The case of detector simulation

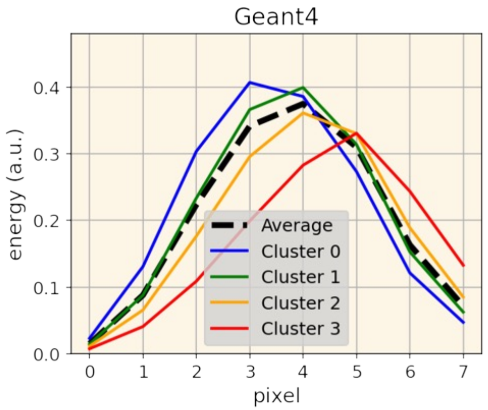
QML can realistically simulate the energy deposited by particles in a detector

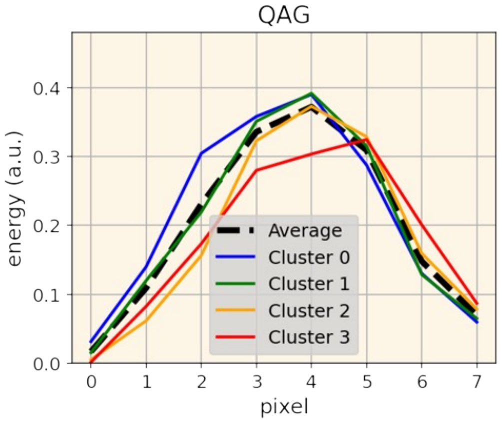
QNN (MMD loss)





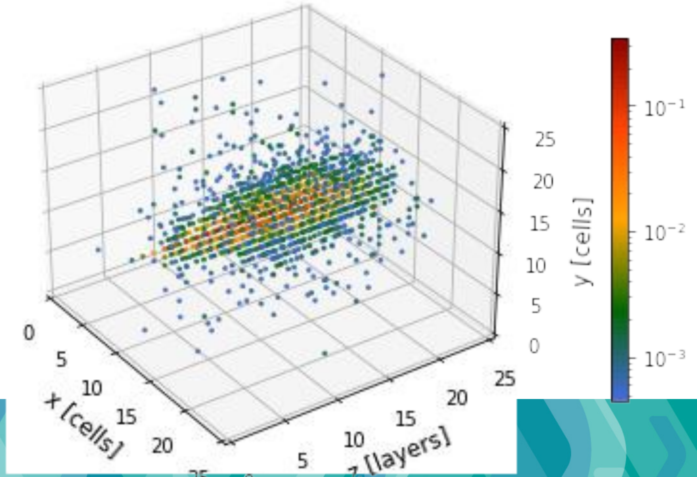






Scale is the main problem

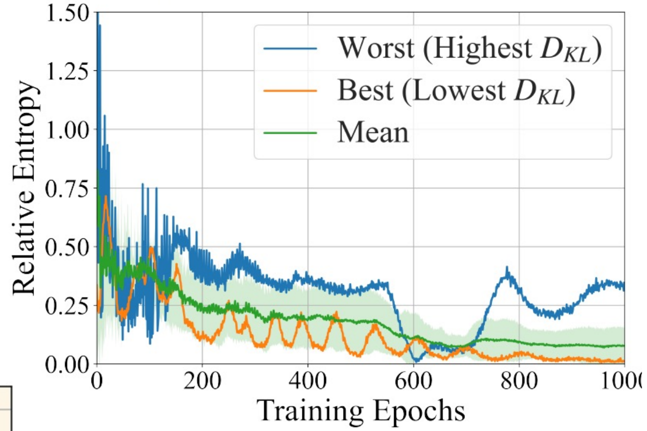
Entirely change the formulation?

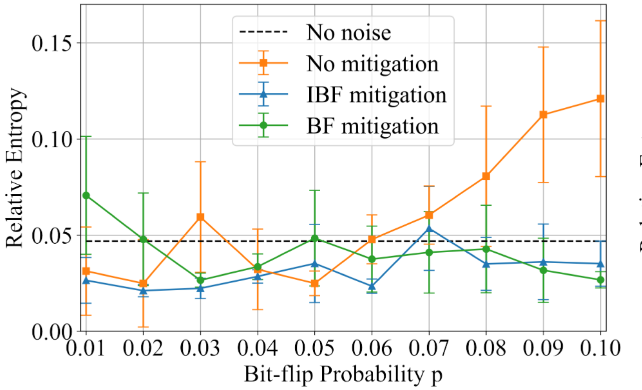


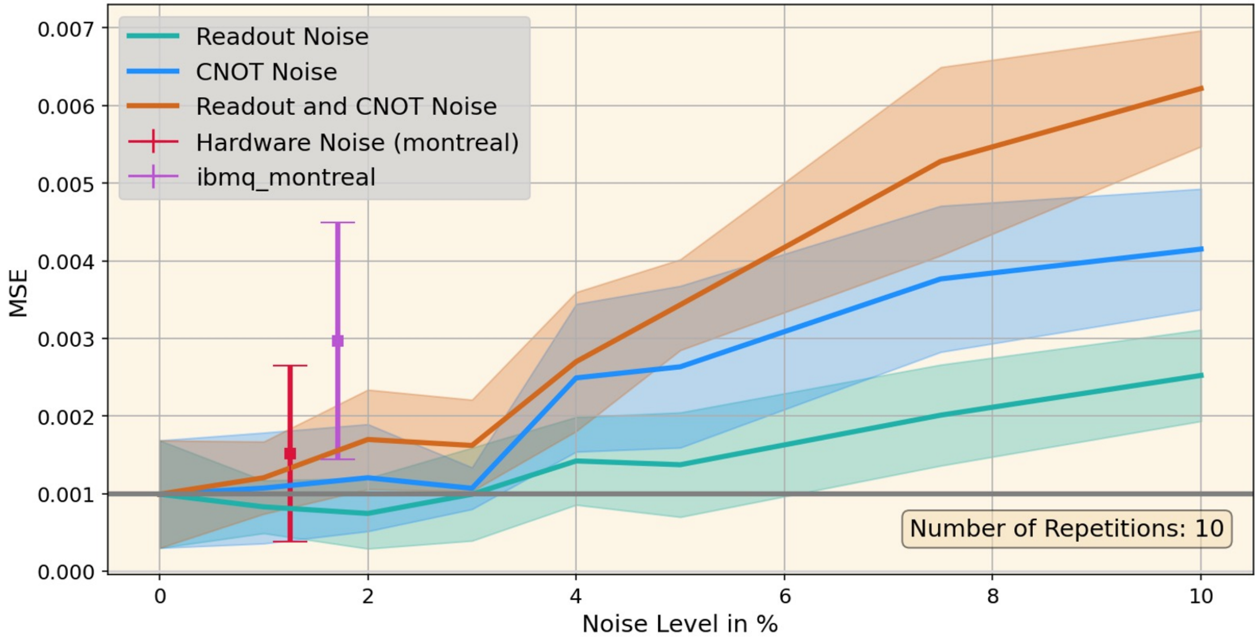
Borras, Kerstin, et al. "**Impact of quantum noise on the training of quantum Generative Adversarial Networks**." ACAT2021, *arXiv preprint arXiv:2203.01007* (2022).

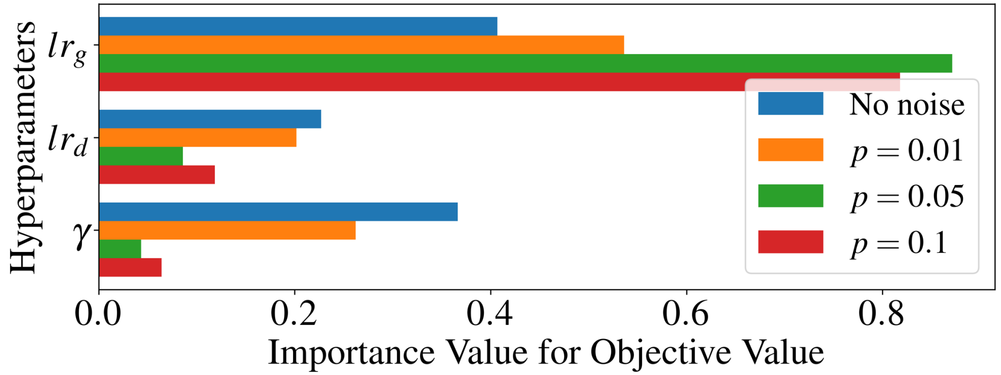
Robustness against noise

QML training process seems **robust against noise** (error mitigation is needed in extreme cases)







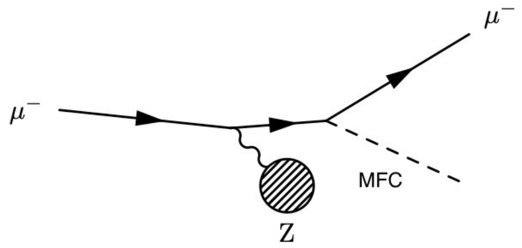


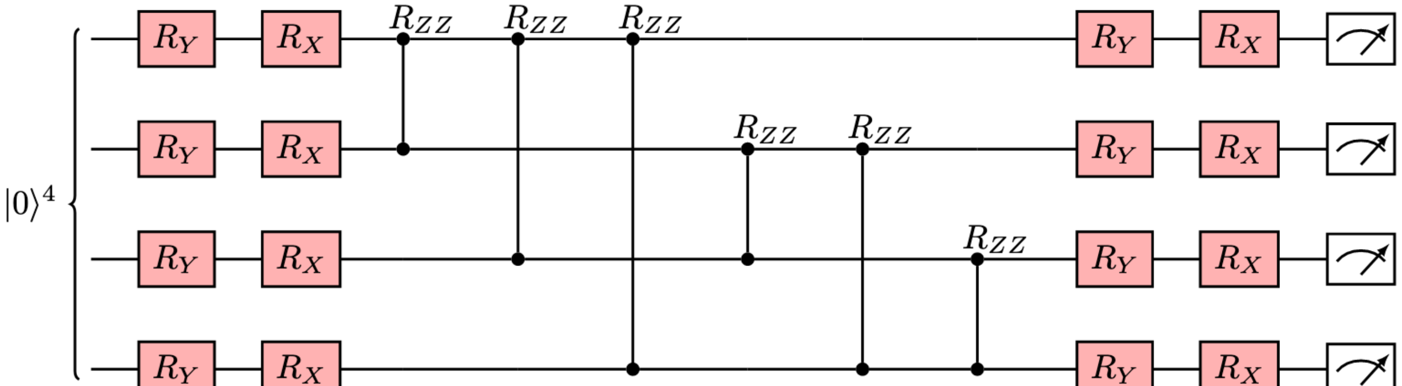
QCBM for event generation

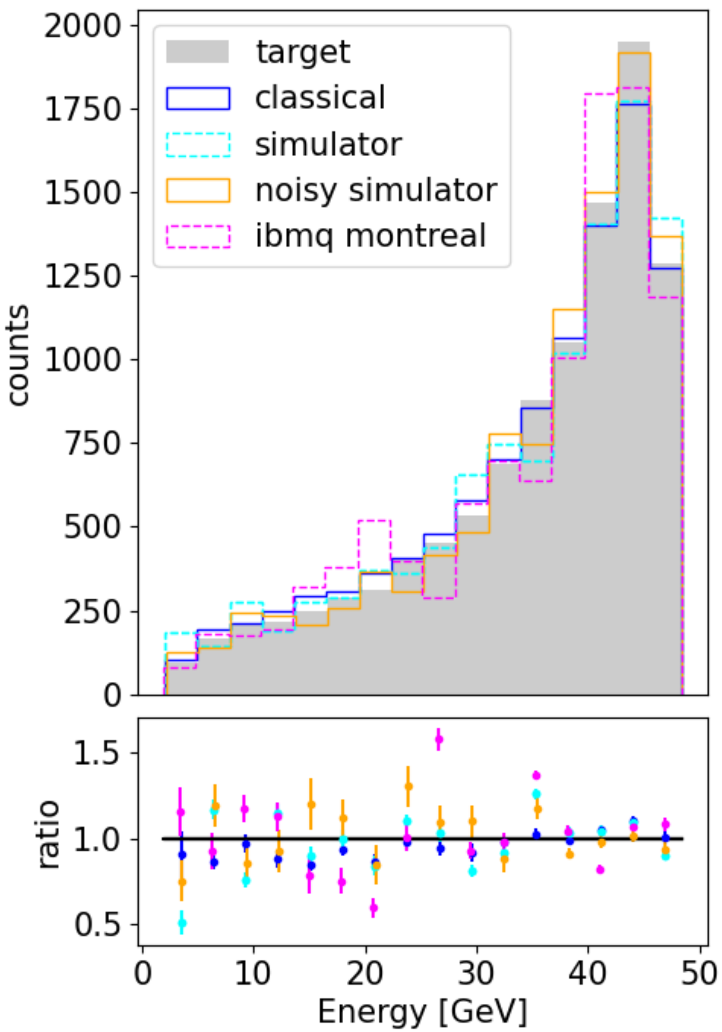
Muon Force Carriers, in muon fixed-target experiments (FASER) or muon interactions in calorimeters (ATLAS)[1].

Generate multivariate distribution (E, p_t, η)

Maximum Mean Discrepancy for training





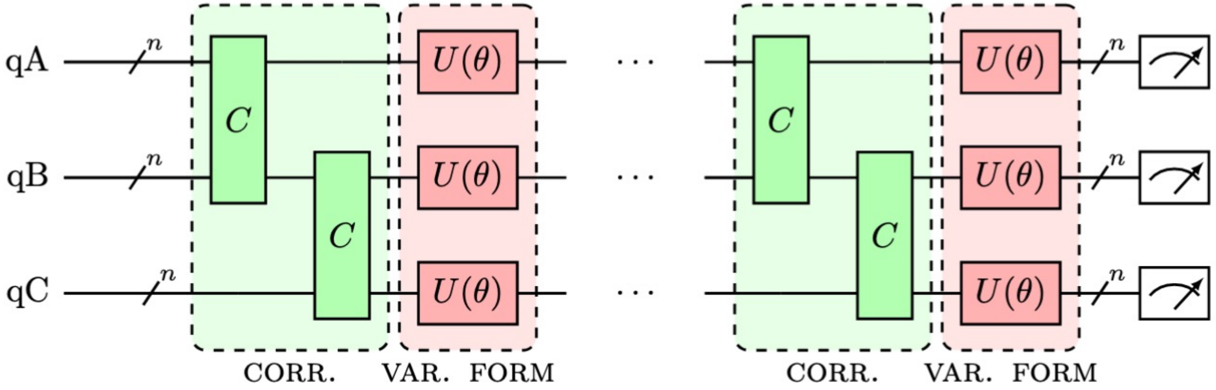


1 Galon, I, Kajamovitz, E et al. "**Searching for muonic forces with the ATLAS detector**". In: Phys. Rev. D 101, 011701 (2020)

Kiss, Grossi, *et al.*, *Phys. Rev. A* **106**, 022612 (2022)

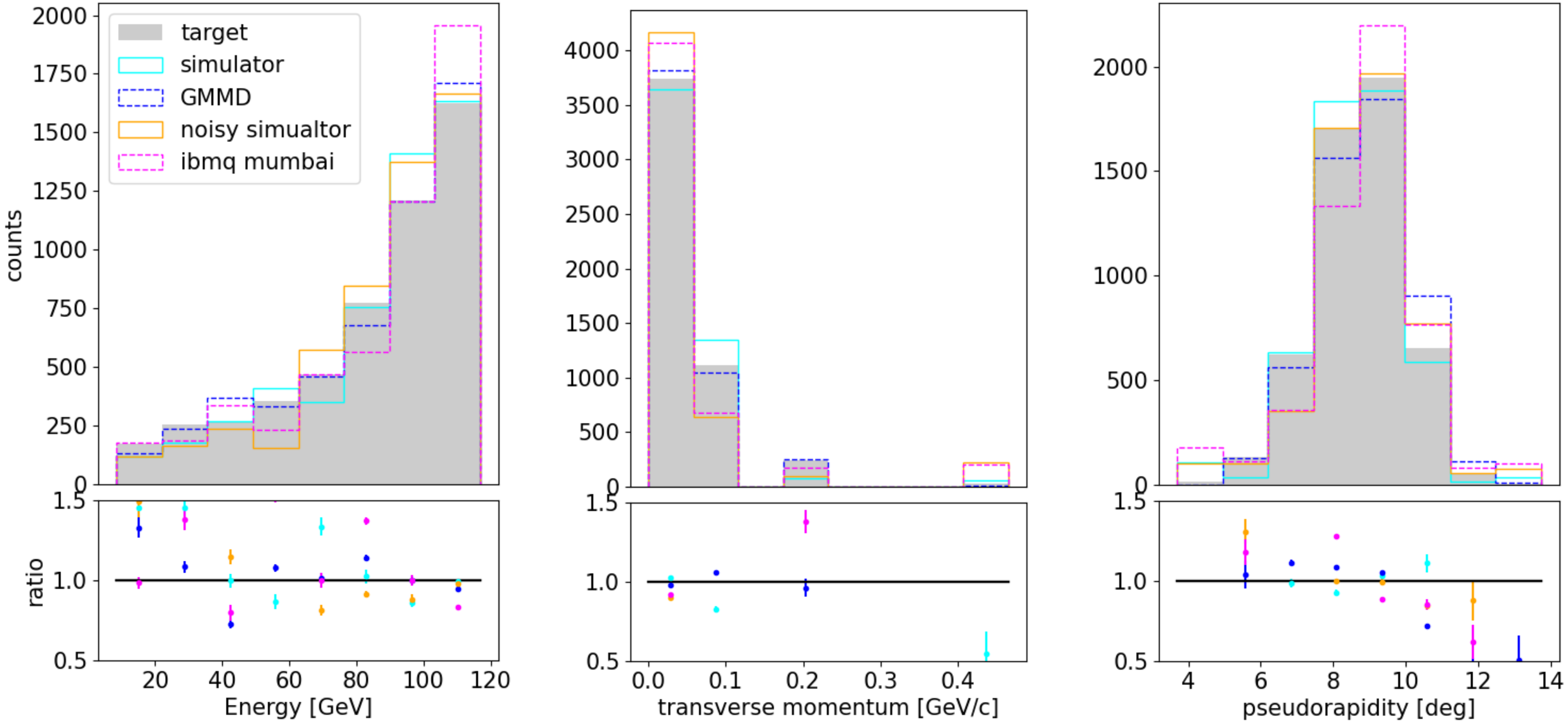
Multivariate PDFs

UNIVERSITÉ DE GENÈVE
FACULTÉ DES SCIENCES

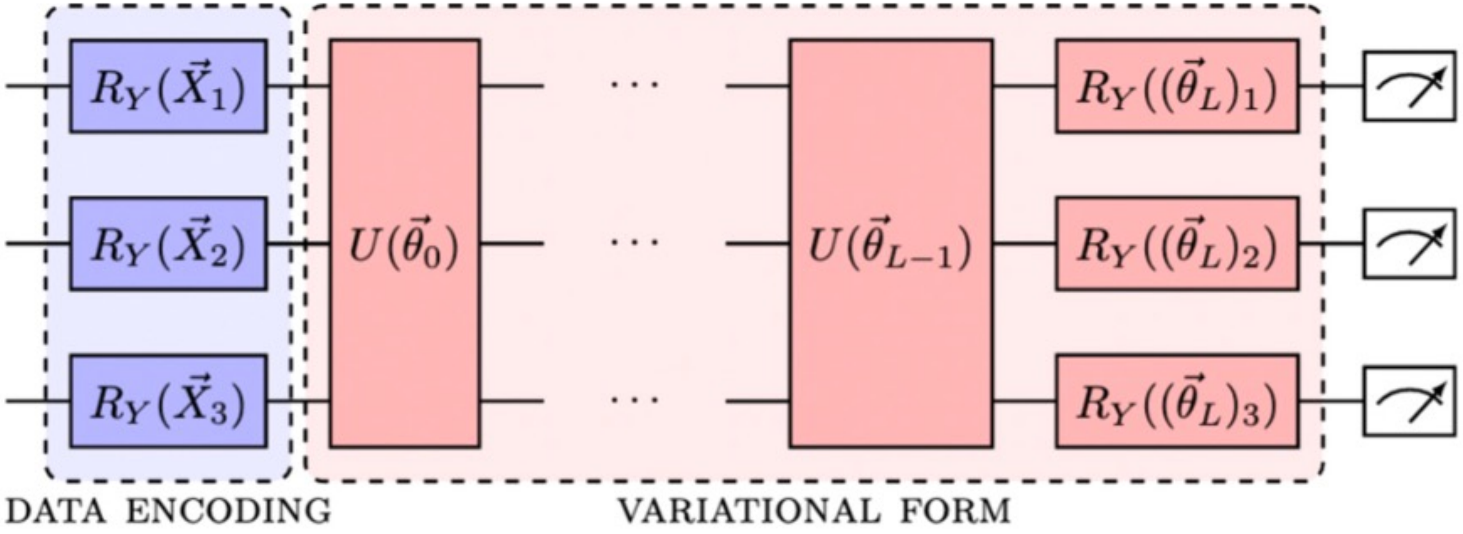


Simulation	Noisy simulation	IBMQ Mumbai	Classical
0.12	0.06	0.06	0.01

Mean difference between the correlations in the MC and generated samples



Conditional probability distribution

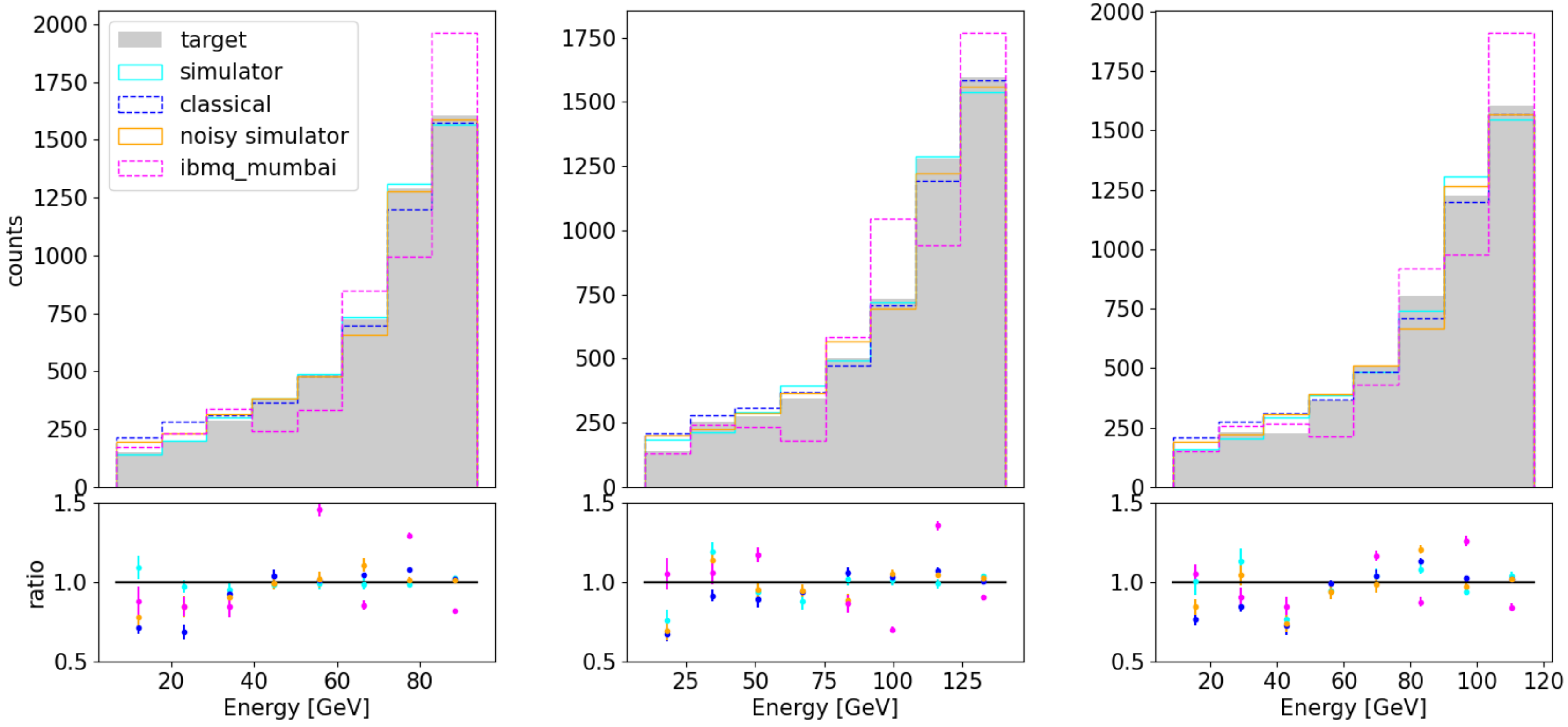


We want to **modelize** $p(y|x)$ where x is the incoming energy E_{in}.

1. Data re-uploading does not improve the sampling.

2. Training on hardware is important to assimilate the noise.

a) train: 100 GeV   b) train 150 GeV   c) test 125 GeV



Research directions

Correlate expected model performance to data set properties

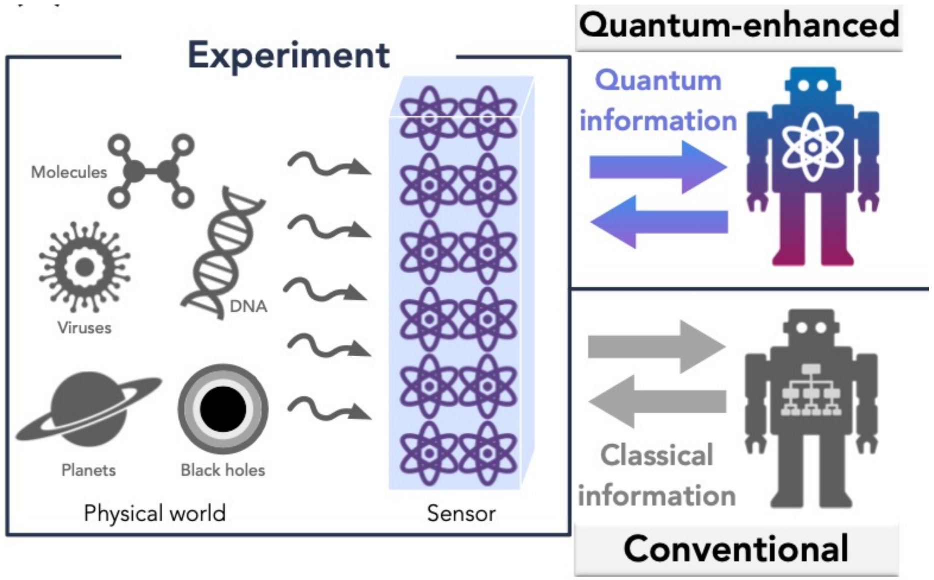
Trainability vs expressivity robustness studies

Evaluating generalisation

Quantum vs classical data

Algorithms beyond QML

Quantum machine learning for quantum data



Huang, *et al.*, *Science* **376**, 6598 (2022)

Work directly with quantum states.

Task: Drawing phase diagrams

1. **Supervised classification** using a convolutional QNN using the groundstates as input data.

2. Advantageous since quantum states are **exponentially hard to save classically**.

3. **Bottleneck**: we need access to classical training labels! Interpolation does not work

Cong, *et al.*, *Nat. Phys.* **15**, 1273–1278 (2019)

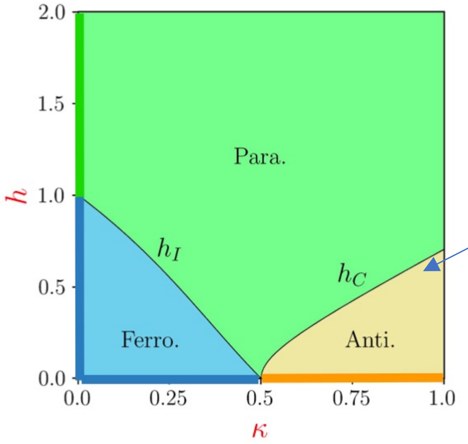
Setting the stage

- **Train in easy (integrable) subregions**
- **Generalize to a full model[1]**
- Model: Axial Next Nearest Neighbor Ising (ANNNI) Hamiltonian:

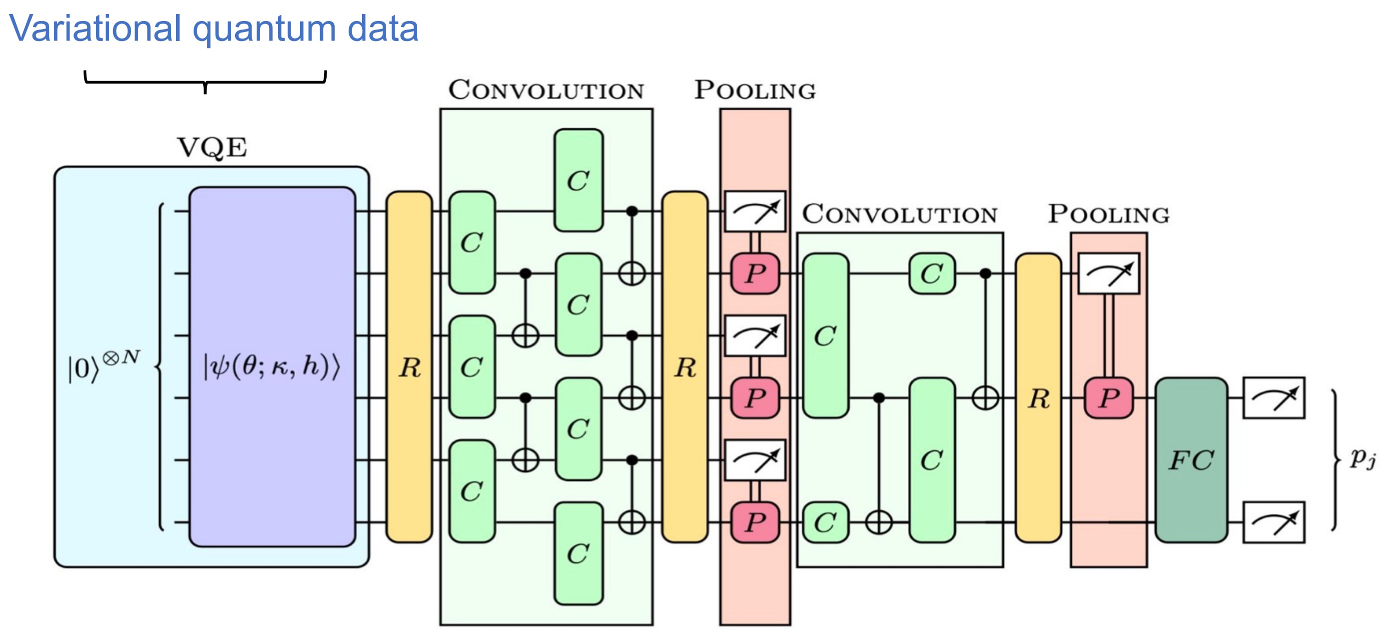
$$H = J \sum_{i=1}^{N} \sigma_x^i \sigma_x^{i+1} - \kappa \sigma_x^i \sigma_x^{i+2} + h \sigma_z^i,$$

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

Which is integrable for $\kappa = 0$ or $h = 0$.



Monte Carlo, DMRG



Binary Cross-entropy

Loss: $$\mathcal{L} = -\frac{1}{|\mathcal{S}_X^n|} \sum_{(\kappa,h)\in\mathcal{S}_X^n} \sum_{j=1}^{K} y_j(\kappa,h) \log\left(p_j(\kappa,h)\right)$$

Labels:

- [0,1] ferromagnetic
- [1,0] antiphase
- [1,1] paramagnetic
- [0,0] trash label

Monaco, at al. arXiv: 2208.08748 (2022)

Results

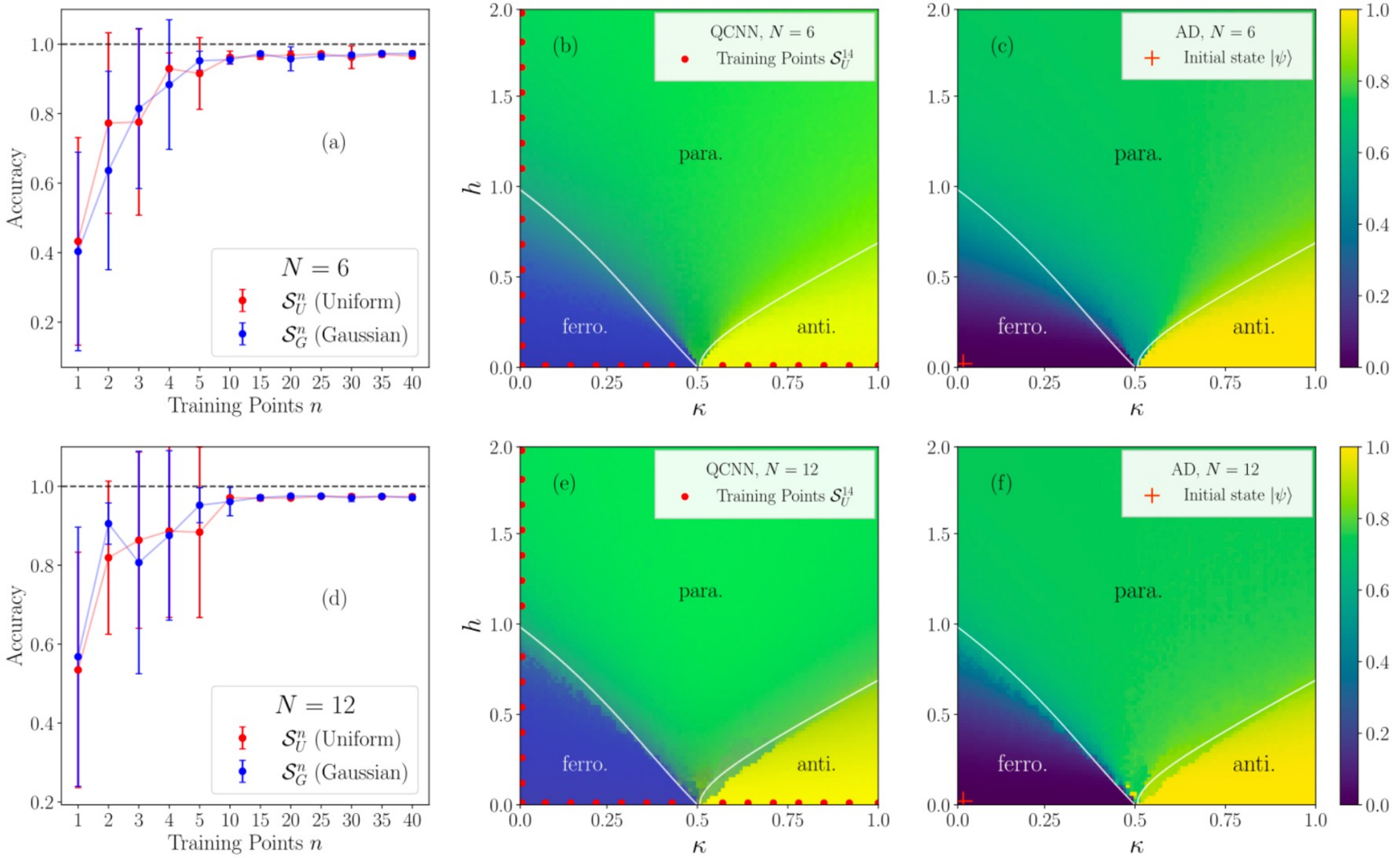
Learn a similarity function between the data.

Kottman, *et al.*, *Phys. Rev. Research* **3**, 043184 (2021))

Size of training set | QCNN (95%) | Autoencoder

N = 6

N = 12



1. Out of Distribution Generalization? [M..Caro et al., Out-of-distribution generalization for learning quantum dynamics, https://arxiv.org/abs/2204.10268]
2. Performance increases with the system's size.
3. Adresses the bottlneck of needing expensive training labels.
4. QCNN gives quantitative predictions [Banchi et all., Generalization in Quantum Machine Learning: A Quantum Information Standpoint, PRX QUANTUM 2, 040321 (2021)]

Other possible applications

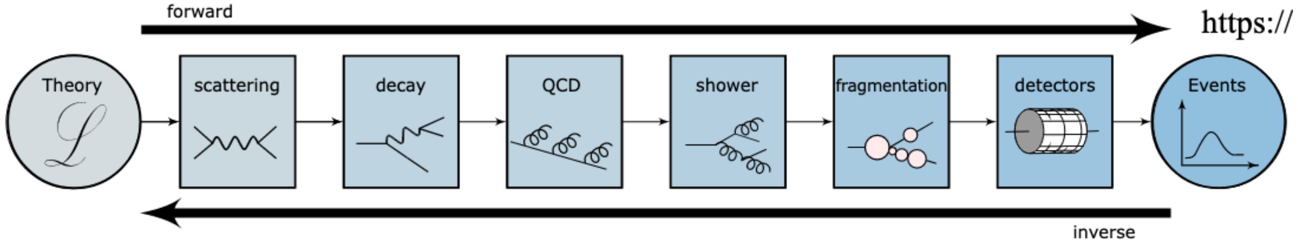
Inversion problem

Detectors measure the results of particle interactions with matter

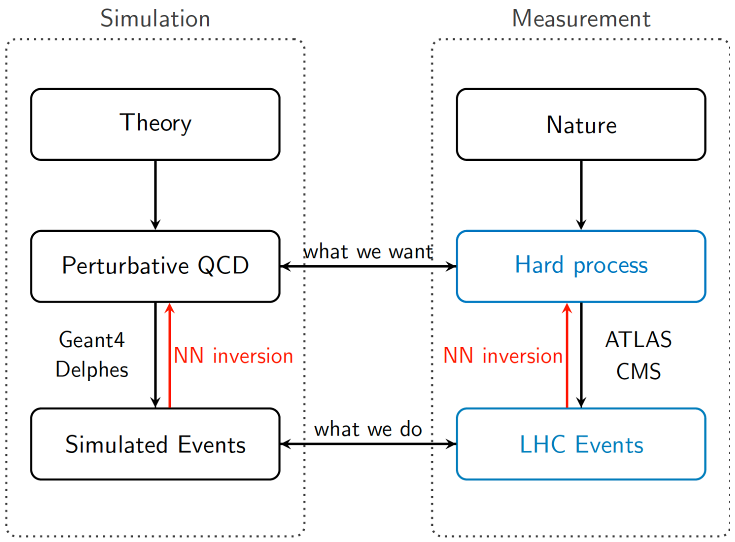
- Need **particle production processes**

Go back from experiments to theory:

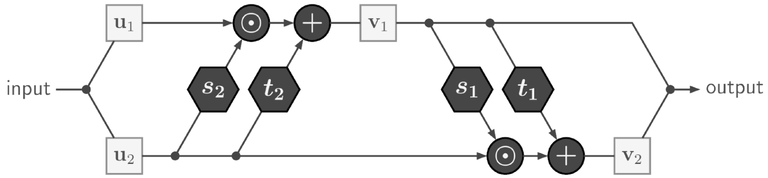
- **Disentangle** production process from the experimental setup
- Bayesian problem

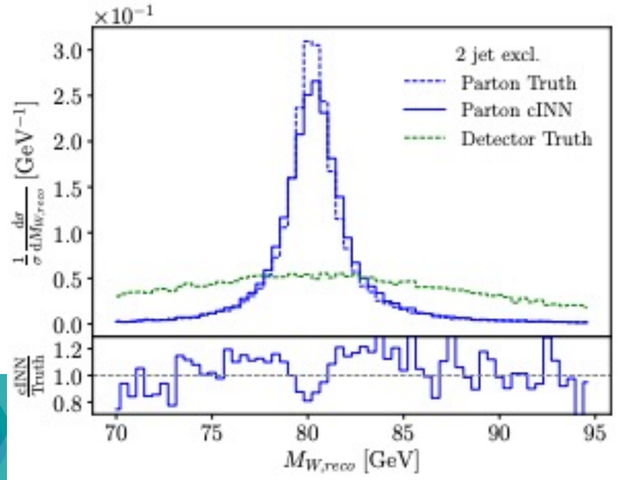


Shown
https://



Invertible networks and normalising flows

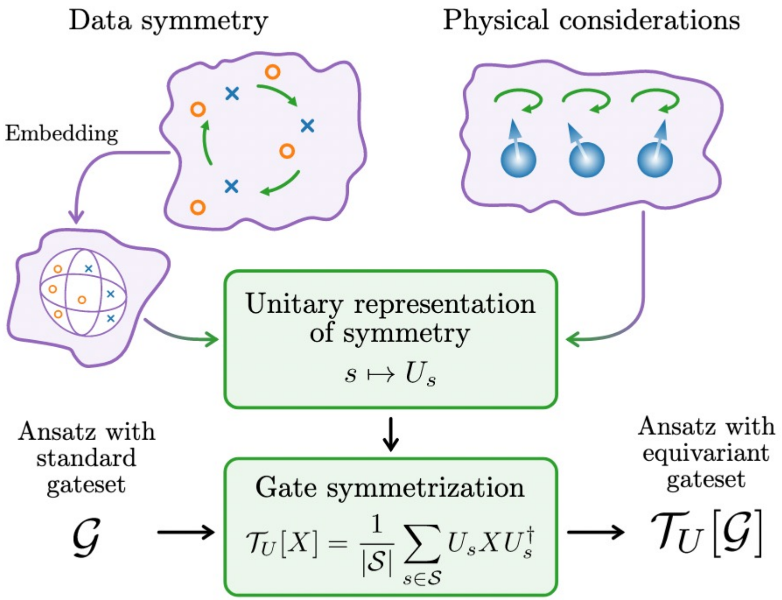




arxiv:1808.04730
arxiv:2006.06685

Introducing symmetry groups

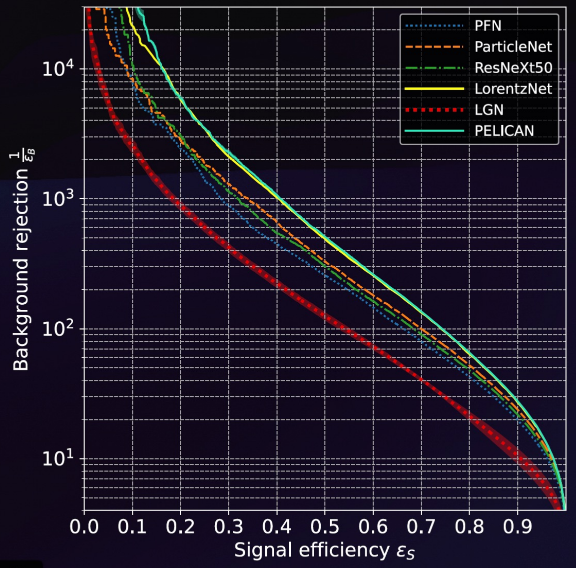
A **unitary representation** of a **symmetry group** S can arise from data symmetries when the data points are suitably **encoded** or alternatively from **physical considerations of a variational problem**[2].



Top-tagging performance

Alexander Bogatskiy, ML4Jets , Nov 2022

- State of the art top-tagger with 8x fewer params of the previous best tagger
- Exact invariance massively improves sample efficiency



Architecture	Accuracy	AUC	$1/\epsilon_B$	# Params
LGN	0.929(1)	0.964(14)	424 ± 82	4.5k
PFN	0.932	0.982	891 ± 18	82k
ResNeXt	0.936	0.984	1122 ± 47	1.46M
ParticleNet	0.938	0.985	1298 ± 46	498k
LorentzNet	0.942	0.9868	2195 ± 173	220k
Our work	0.9425(1)	0.9869(1)	2289±204	46k

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", https://arxiv.org/abs/2205.06217
3-S.Jerbi at all., Quantum Machine Learning Beyond Kernel Methods https://arxiv.org/abs/2110.13162
4- Glick, Jennifer R., et al. "Covariant quantum kernels for data with group structure." arXiv:2105.03406 (20

Perspective

The CERN QTI is studying impact of Quantum Technologies in High Energy Physics:

- Some **preliminary hints** of advantage
- So far.. we can do «**as good as classical methods**». In many cases, limitations are hardware-related
- Need more **robust studies** to estimate **performance** and drive **model development**

We are now formulating a **longer term research plan**

- Identify cases where quantum approach could be **more effective** than classical algorithms**...**
- …

CERN Quantum Technology Initiative

Accelerating Quantum Technology Research and Applications

Thank you!

Next November @CERN:

QML
QUANTUM MACHINE LEARNING
2023

A priori methodology to assess Quantum Advantage

Complexity theory can set a rigorous upper bound on prediction error [1]

$$\mathbb{E}_{\mathbf{x}}|h(\mathbf{x}) - y(\mathbf{x})| \leq \mathcal{O}\left(\sqrt{\frac{s_{K,\lambda}(N)}{N}}\right)$$

Metrics implemented in QuASK[2]

- Geometric Difference – $g_{CQ}(\lambda)$
- Approximate Dimension – d
- Model Complexity – $s_{K,\lambda}(N)$

geometry test

- $g_{CQ} << \sqrt{N}$
  - ***dimensionality test***
    - $d << N$ → ***Classical*** ✓
    - ***else*** → ***Classical Quantum*** ✓/✗
- $g_{CQ} \propto \sqrt{N}$
  - ***complexity test***
    - $s_C << N$ → ***Classical*** ✓
    - $s_Q << N$, $s_C \approx N$ → ***Potential QA***
    - ***else*** → ***Classical Quantum*** ✓/✗

Constraints:

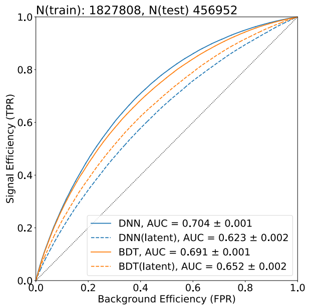
- Encoding (feature) map of classical and quantum kernels
- Data structure - complex distribution function, dimensionality of the input space…
- Optimization of relevant parameters λ, γ

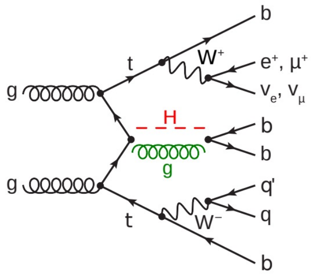
1 HY. Huang et al, Nature Communication **12**, 2631 (2021)
2 F.Di Marcantonio et all., QuASK -- arXiv:2206.15284
https://quask.readthedocs.io/en/latest/#

F. Di Marcantonio et al., The Role of Data in Projected Quantum Kernels: the Higgs Boson Discrimination.

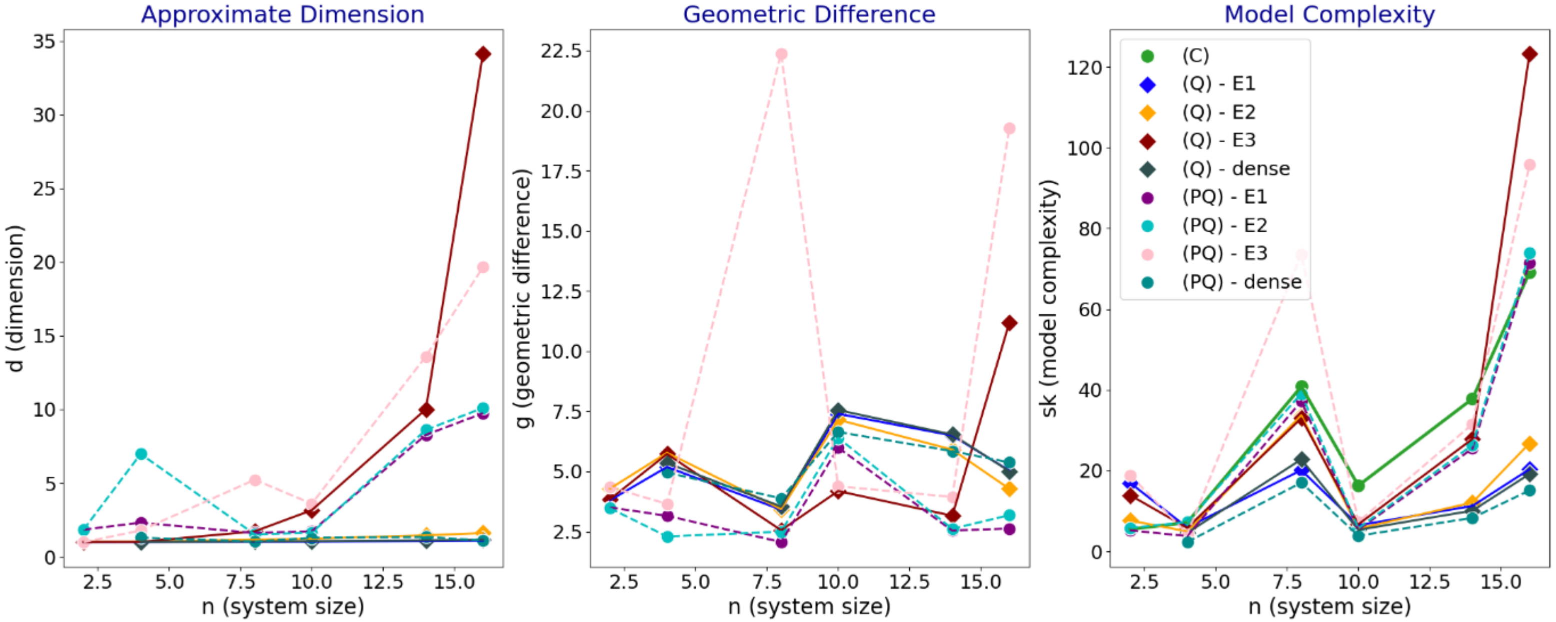
Analize the performance of quantum kernels

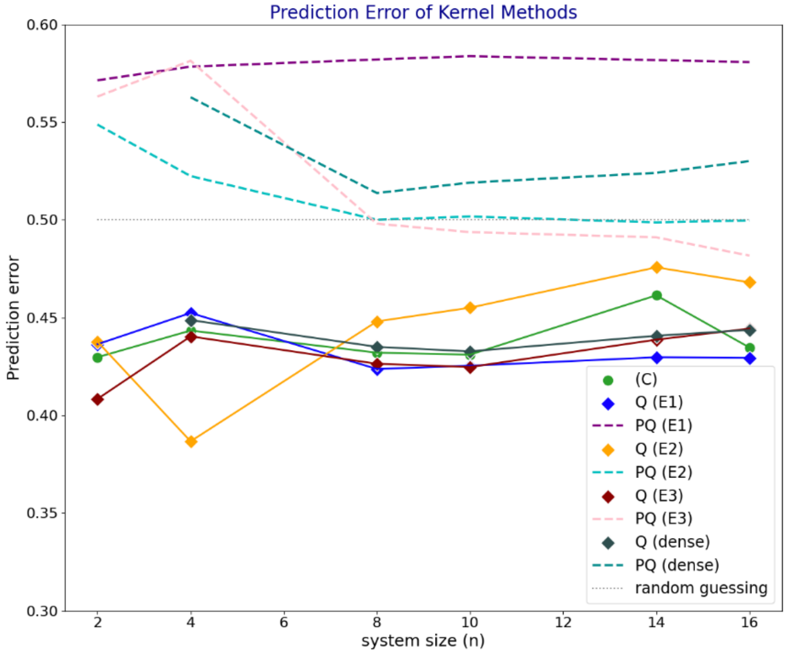
- Focus on **H(tbb) classification**
- quantum kernels keep data in low-dimensional Hilbert spaces
- model complexity increases with the number of qubits for all ML models.
- Model complexity are similar (sometimes below classical models)
- Projected kernels don’t help





V. Belis, EPJ Web of Conferences 251, 03070 (2021)





QUANTUM TECHNOLOGY INITIATIVE

Definition and loading of probability distributions – exact loading

Class that implements the (complex amplitude) initialization of some flexible collection of qubit registers.

Implements a recursive initialization algorithm, including optimizations [1].

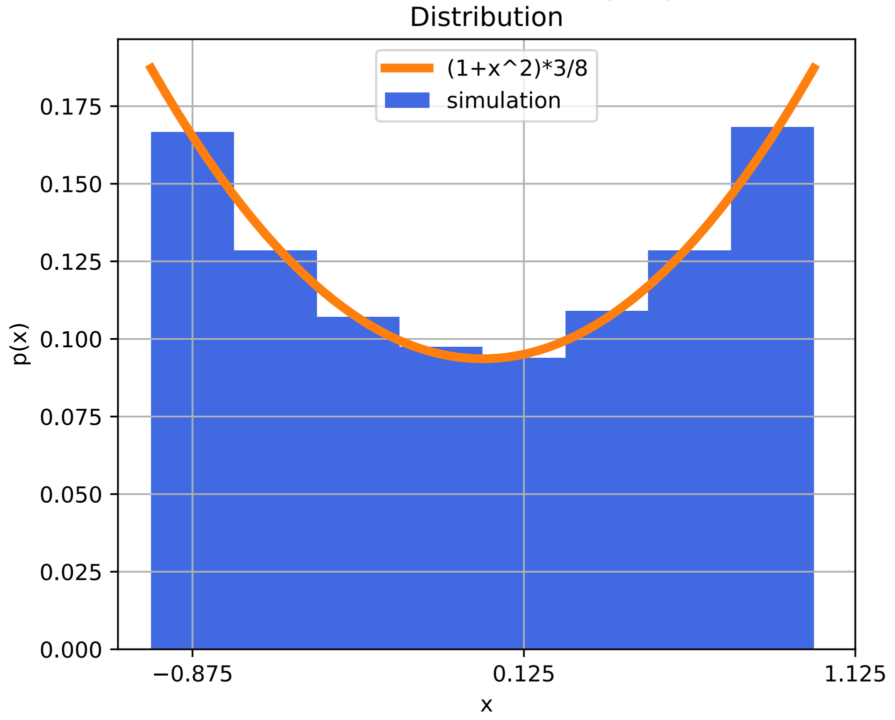
Note that Initialize is an Instruction and not a Gate since it contains a reset instruction, which is not unitary.

Discrepancies from the truth by no more than 2% and is on average around 1%.

Quality of the exact loading is directly dependent on the statistics of the sample given as input.

NB we assume <u>truth distribution is unknown analytically</u>

 # gates scales as O(2n)

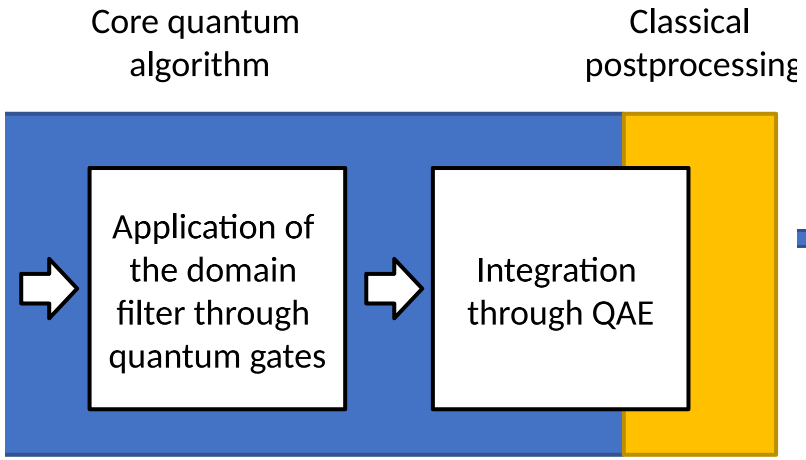


Loading	Difference per bin [%] Min.	Max.	Average	σ_x
Direct	$+0.207$	-1.88	1.35	1.80×10^{-3}

[1] "Synthesis of Quantum Logic Circuits" https://arxiv.org/abs/quant-ph/0406176v5

Integration of probability distributions - QAE

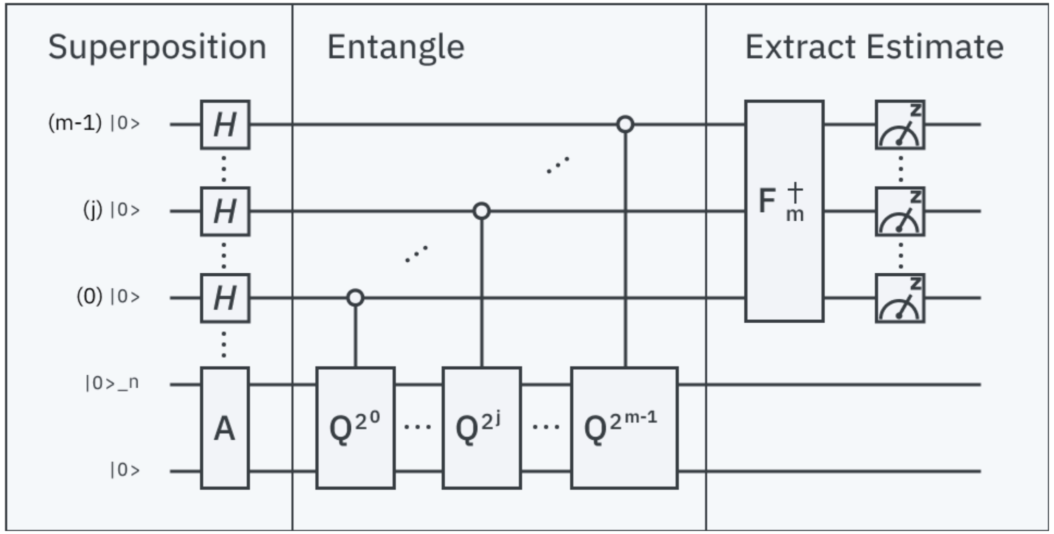
$$\sigma = \frac{1}{F}\int d\Phi\, \underset{\text{probability distributions}}{|M|^2}\, \overset{\text{integrand}}{\Theta(\Phi - \Phi_c)}$$



$$I = \int dx\, \underset{\text{probability distributions}}{f(x)}\, \overset{\text{integrand}}{g(x)}$$

- The **Quantum Amplitude Estimation**, grounded on QPE, is a tool to perform Monte Carlo-like simulations on quantum computers, with an almost quadratic speedup

- Different implementations of QAE:
  - original QAE implementation by Brassard et al;
  - **Iterative Amplitude Estimation** which does not rely on Quantum Phase Estimation (QPE) but is only based on Grover's Algorithm, which reduces the required number of qubits and gates;
  - Maximum Likelihood Amplitude Estimation which limit resorting to expensive controlled operations;



Chang S.Y. *et al.*, Running the Dual-PQC GAN on Noisy Simulators and Real Quantum Hardware, QTML2021, ACAT21

qGAN Benchmarks on hardware

Train models using **noisy simulator** and test the inferen
trapped-ion (IONQ) quantum hardware

- For IBMQ machines, choose the qubits with the lowest

Device	Readout error CX error	$D_{KL}/D_{KL,ind}$ $(\times 10^{-2})$
ibmq_jakarta	0.028 $1.367 \cdot 10^{-2}$	0.14 ± 0.14 6.49 ± 0.54
ibm_lagos	0.01 $5.582 \cdot 10^{-3}$	0.26 ± 0.11 6.92 ± 0.71
ibmq_casablanca	0.026 $4.58 \cdot 10^{-2}$	4.03 ± 1.08 6.58 ± 0.81
IONQ	NULL $1.59 \cdot 10^{-2}$	1.24 ± 0.74 10.1 ± 5.6

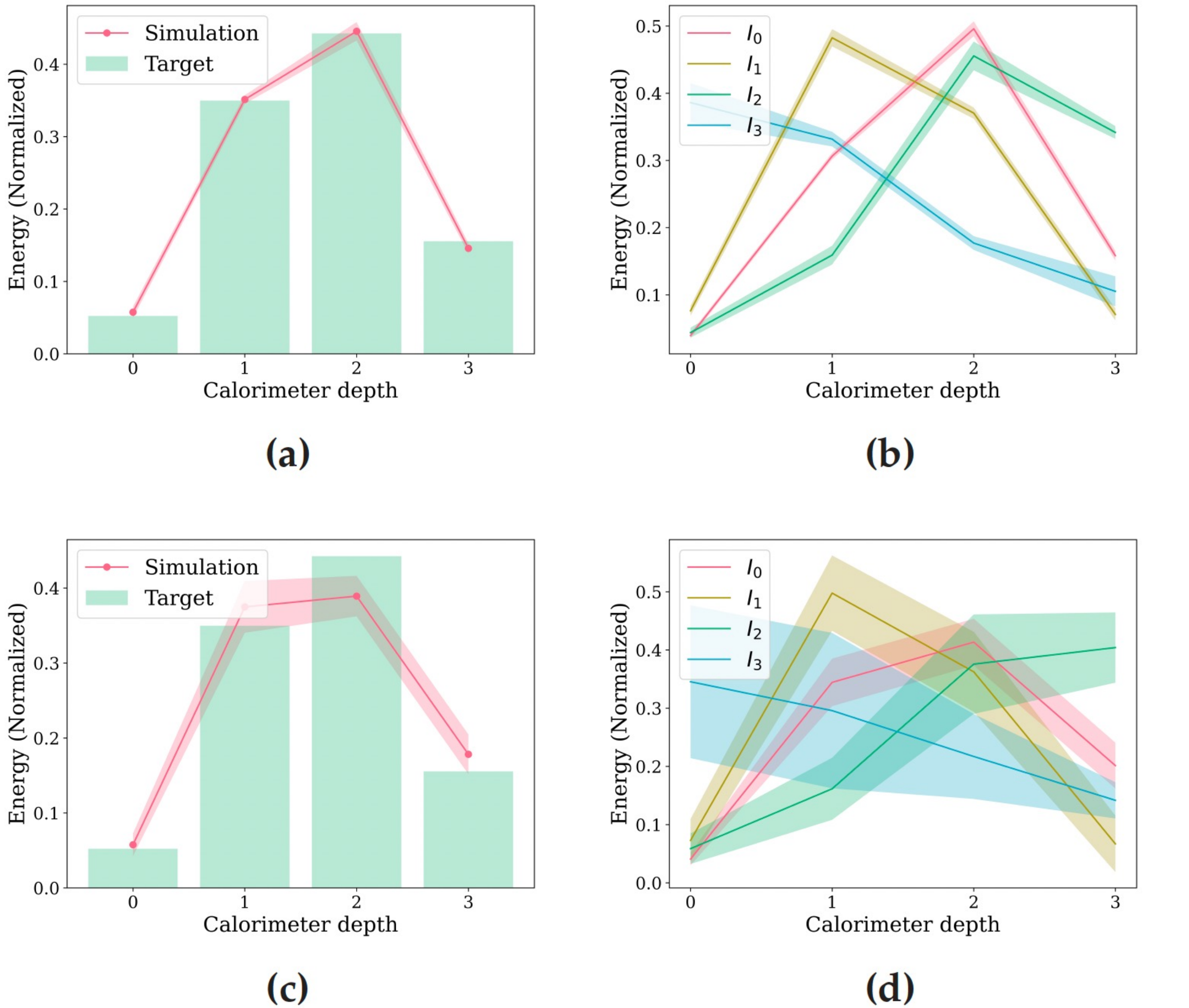


Figure 4: Mean (a,c) and individual images (b,d) obtained by inference test on ibmq_jakarta (a,b) and IONQ (c,d).

Quantum sensing

Change of quantum state caused by the interaction with an external system:

- **transition between superconducting and normal-conducting**
- **transition of an atom from one state to another**
- **change of resonant frequency of a system (quantized)**

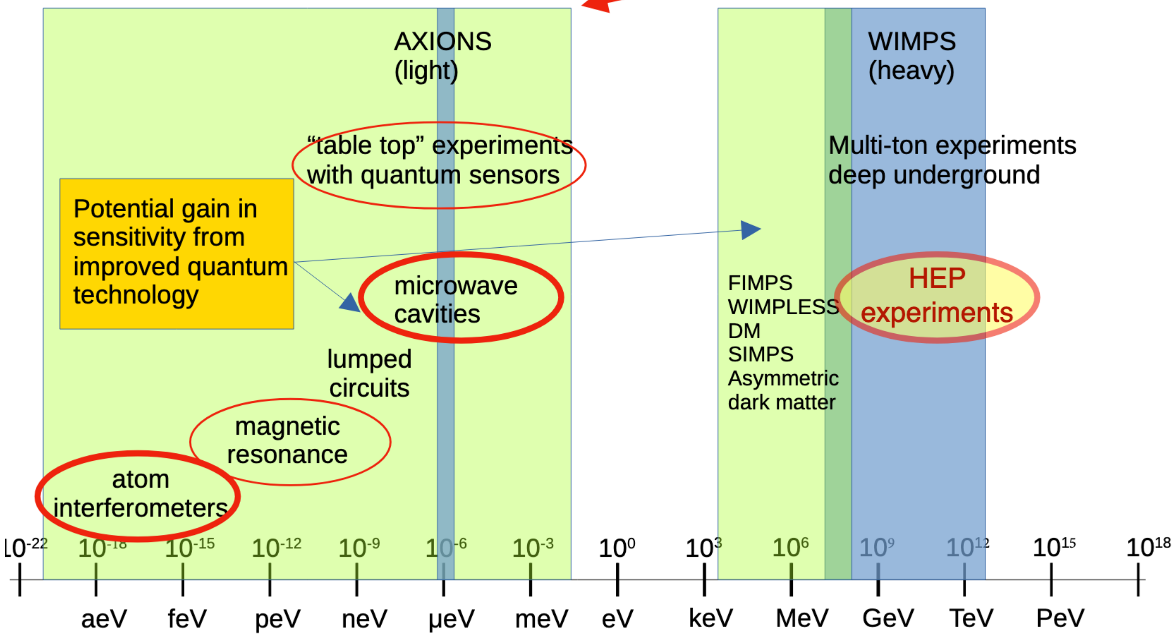
quantum sensors & particle physics: what are we talking about?

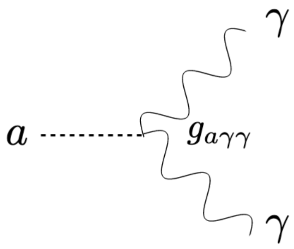
Axions, ALP's, DM & non-DM UL-particle searches

cavity size = axion size
axion mass = unknown

$$F \sim g_{a\gamma}^2 m_A^2 B^4 V^2 T_{sys}^{-2} G^4 Q,$$

system noise temperature
cryo-amplifiers JJPA





(but not only…)