Exploring hybrid quantum-classical neural networks for particle tracking

CERN openlab summer student lightning talks

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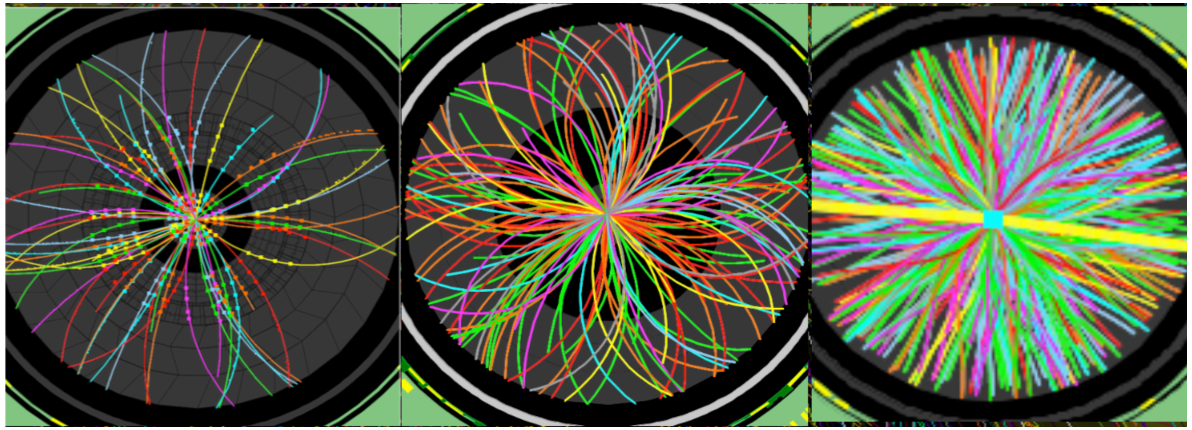
The track reconstruction task



Increasing number of pile-up events at the LHC (2010-2012) [1].

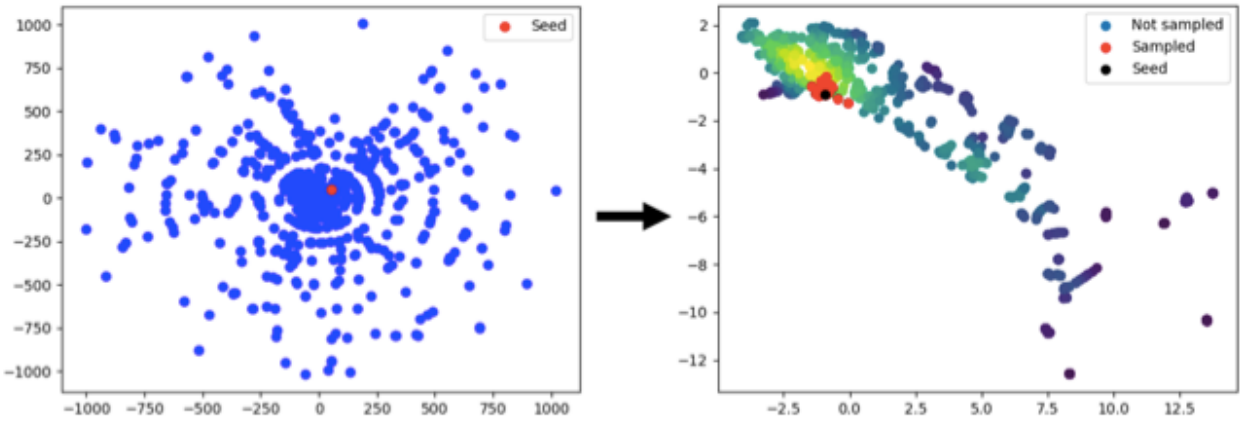
- Update to HL-LHC: significant increase of complexity and size of data
- ML techniques are being explored, to tackle the complex task of reconstructing the particle paths

- This work builds up on the Exa.TrkX project [2]: using graph neural networks for particle track reconstruction
- Previously explored quantum graph neural networks show promising results [3]
- Working with the publicly available TrackML dataset [4]

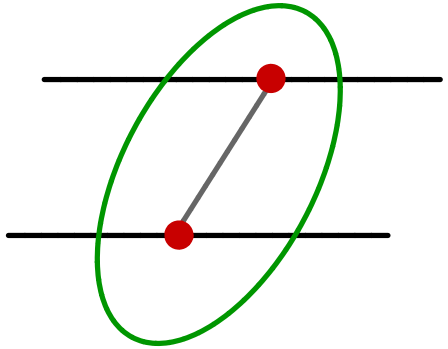
[1] https://indico.fnal.gov/event/14207/contributions/24393/attachments/15565/19803/AllScientistRetreat_PreMeeting_LHC_final.pdf, Slide 7
[2] N. Choma et al. Track seeding and labelling with embedded-space neural networks arXiv:2007.00149
[3] C. Tüysüz et al., "A quantum graph neural network approach to particle track reconstruction," 2020.
[4] https://www.kaggle.com/c/trackml-particle-identification/data

Learning the embedding

Data pipeline



Visualization of the Exa.TrkX embedding [4].



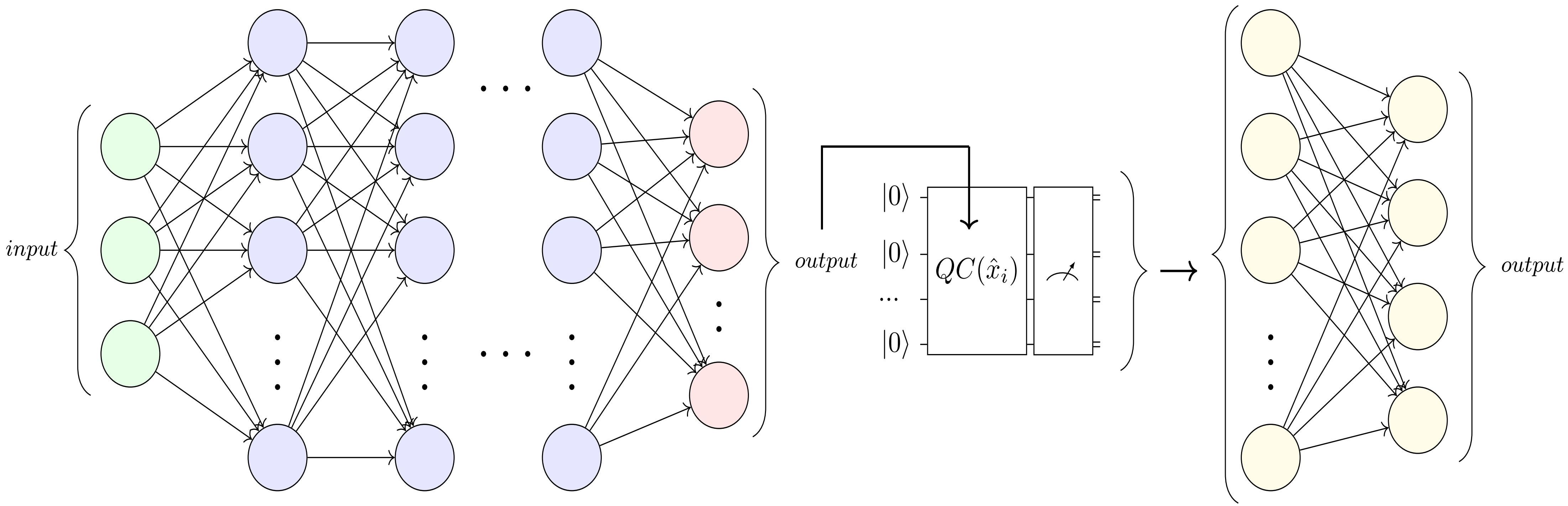
A single doublet.

First preprocessing steps of the data → **Embeddings of pairs of hits (label: true, false)** → **Graph construction and classification with GNN**

[4] N. Choma et al. Track seeding and labelling with embedded-space neural networks arXiv:2007.00149

The quantum-classical network

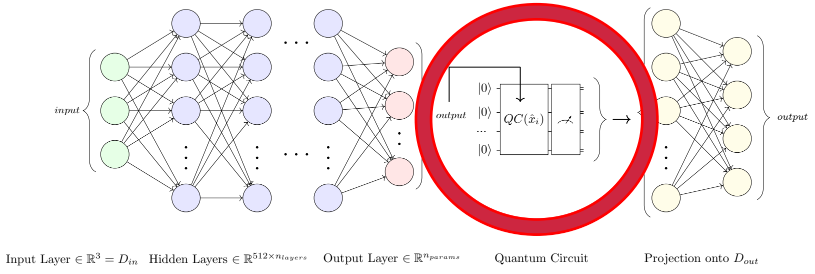
Architecture of the hybrid network

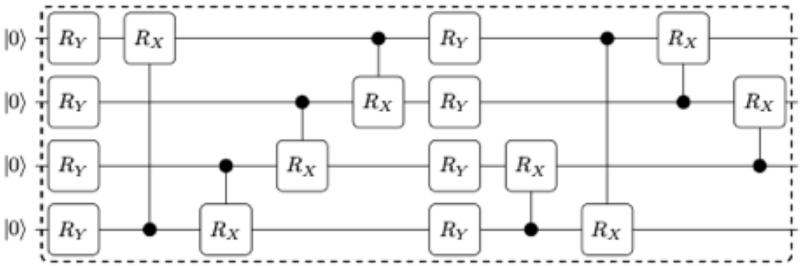


Input Layer $\in \mathbb{R}^3 = D_{in}$ Hidden Layers $\in \mathbb{R}^{512 \times n_{layers}}$ Output Layer $\in \mathbb{R}^{n_{params}}$ Quantum Circuit Projection onto D_{out}

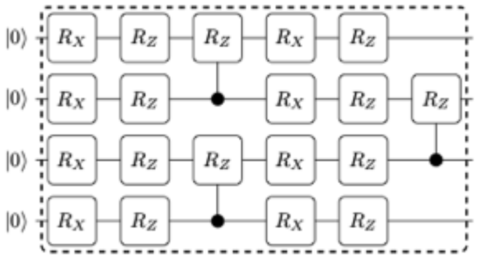
Examples of used quantum circuits

Circuit number	Number of parameters $n_{parameters}$	Entanglement (the higher the better) [1]	Expressibility (the lower the better) [1]	Average training time per batch (= 100 samples)
5	28	0.29	0.05	37 s ± 8 s
7	19	0.21	0.10	20 s ± 4 s
11	12	0.54	0.13	14 s ± 4 s
14	16	0.49	0.02	16 s ± 4 s

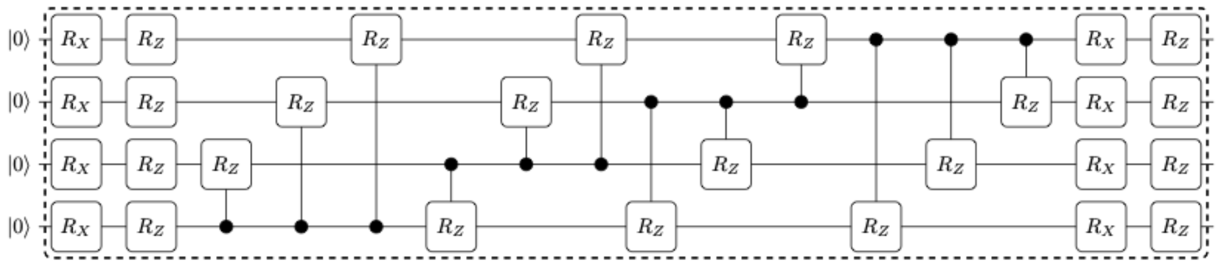




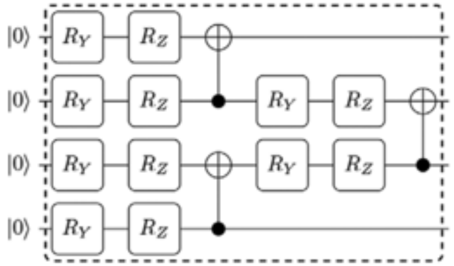
Circuit 14



Circuit 7



Circuit 5



Circuit 11

[1] and circuit architectures from: http://dx.doi.org/10.1002/qute.201900070, values reproduced by C. Tüysüz and A. Açar

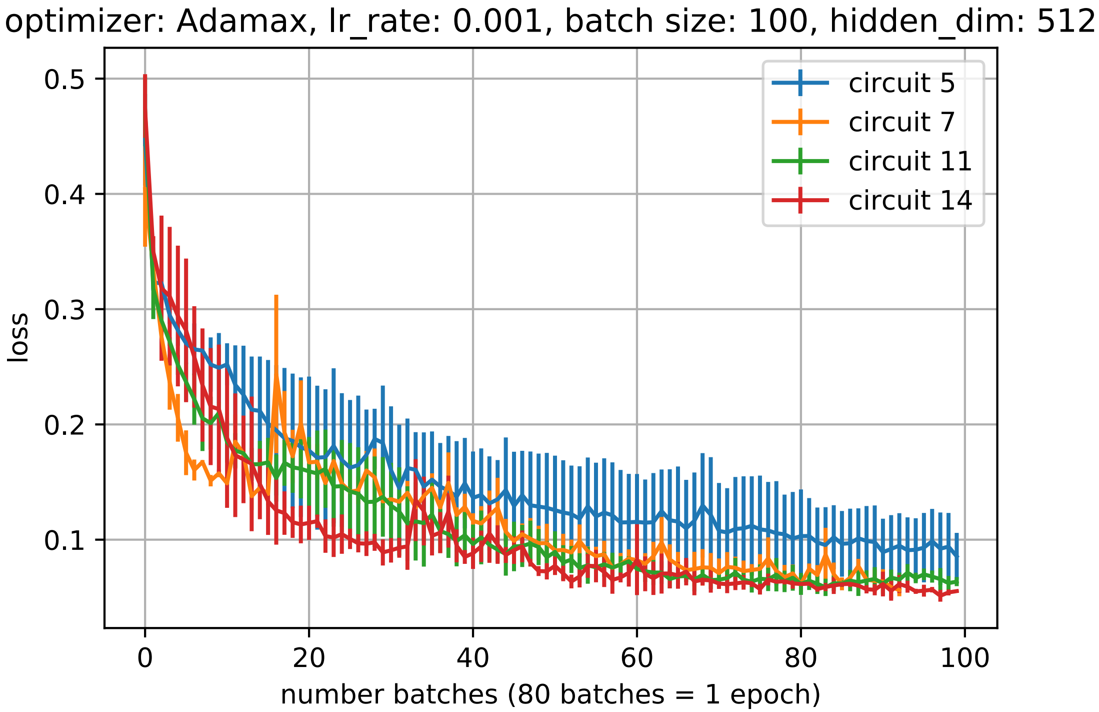
Preliminary results

Problems:

- Long training times for simulation: *O(days)*
- Behavior of loss function strongly dependents on initialization (e.g. circuit 5)

Future work :

- Different quantum circuit architectures
- Replace classical MLP layers with quantum circuits
- More qubits (8 vs. 4 qubits)
- Speed-up through GPU usage
- More training data



Validation loss of the hybrid network with the respective quantum circuit.

Thank you!
Are there any questions?

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And thanks to my mentors: Sofia Vallecorsa, Daniel Dobos, Kristiane Novotny, Cenk Tüysüz

BACKUP

Quantum Gates

Initial state on the Bloch sphere: $|0\rangle = \binom{1}{0}$

Used 1-qubit gates:

- Rotational gate with one parameter (eg. RX) acting on initial $|\mathbf{0}\rangle$ state:

$$R_x(\theta)|0\rangle = \begin{pmatrix} \cos(\theta/2) & -i\sin(\theta/2) \\ -i\sin(\theta/2) & \cos(\theta/2) \end{pmatrix} \cdot \begin{pmatrix} 1 \\ 0 \end{pmatrix} = \begin{pmatrix} \cos(\theta/2) \\ -i\sin(\theta/2) \end{pmatrix}$$

Used 2-qubit gates:

- CNOT gate: $$CNOT = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & 1 & 0 & 0 \\ 0 & 0 & 0 & 1 \\ 0 & 0 & 1 & 0 \end{pmatrix}$$

- Conditional rotational gates (e.g. CRX): $$CRX(\theta) = \begin{pmatrix} 1 & 0 & 0 & 0 \\ 0 & \cos(\theta/2) & 0 & -i\sin(\theta/2) \\ 0 & 0 & 1 & 0 \\ 0 & -i\sin(\theta/2) & 0 & \cos(\theta/2) \end{pmatrix}$$