Embedding of particle tracking data using hybrid quantum classical neural networks

25th International Conference on Computing in High-Energy and Nuclear Physics

20.05.2021

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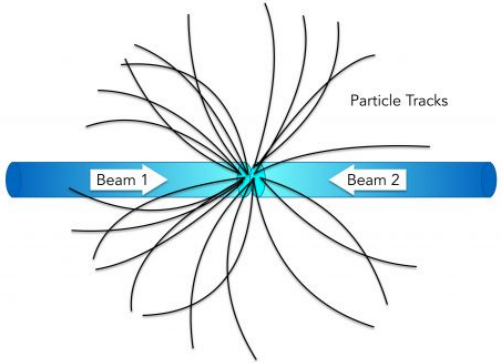
Outline

- The particle track reconstruction problem and data set
- The embedding within the data processing pipeline
- Quantum circuit model architectures and training results
- Comments on future improvements

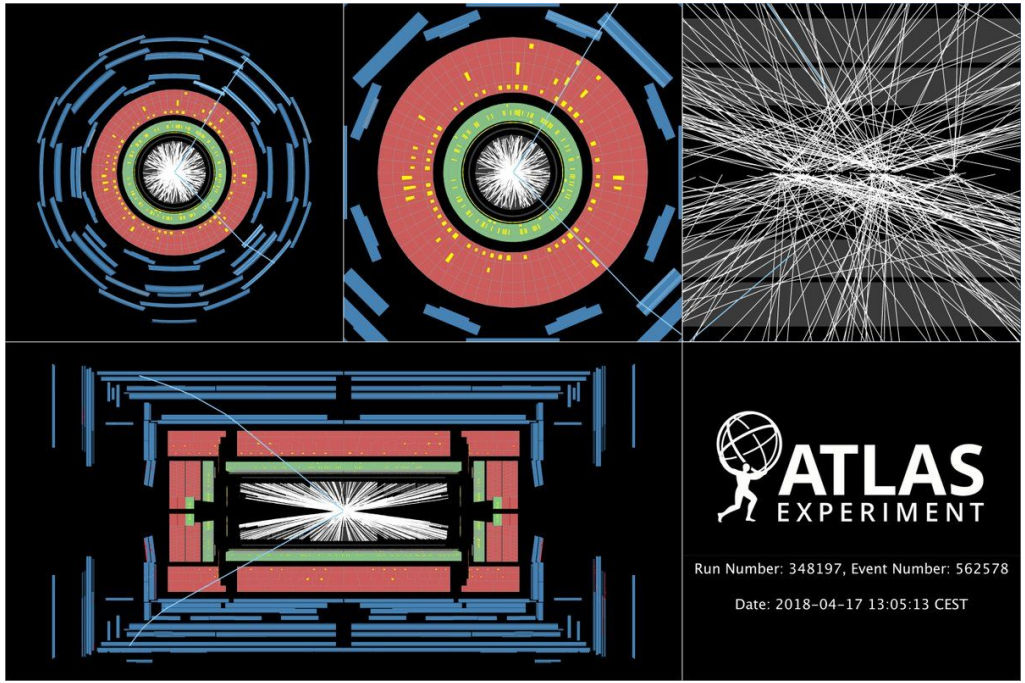
Large Hadron Collider (LHC)

and particle track reconstruction



https://atlas.cern/updates/atlas-news/counting-collisions

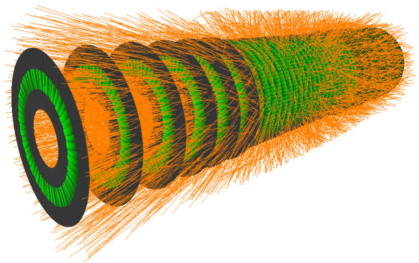
An event view from ATLAS Experiment

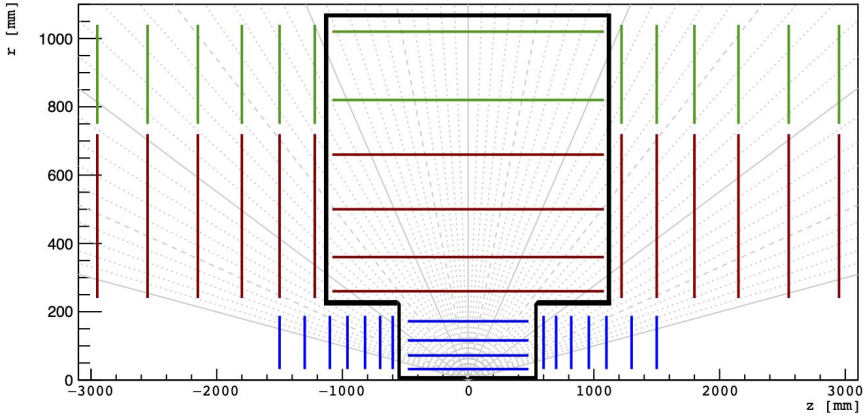


https://cds.cern.ch/record/2315786

TrackML Dataset

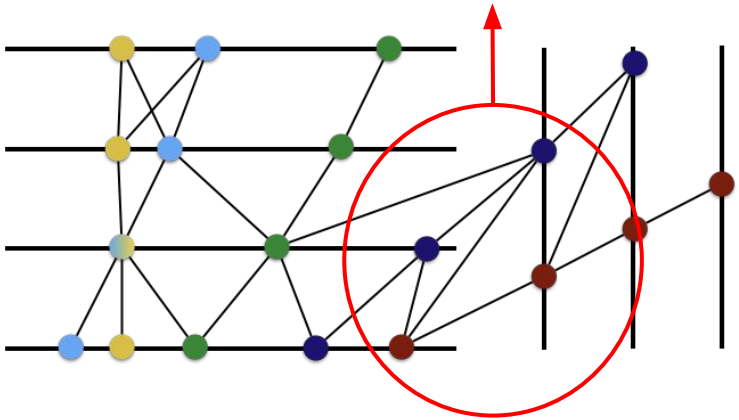
https://www.kaggle.com/c/trackml-particle-identification/overview





Contains: 10k collision events (200 soft QCD interactions)
(arXiv: 1904.06778)

endcaps produce a lot of ambiguity and therefore many track candidates, we omit endcaps as we want to limit our model to simpler cases.

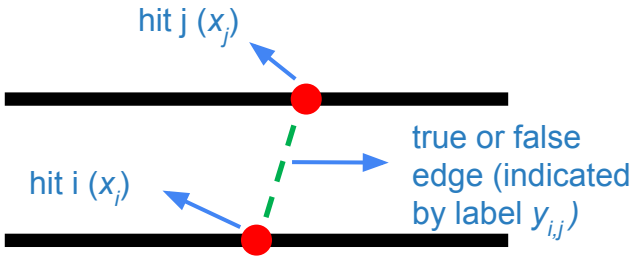


Retrieved from: Farrell et al. 2018 (arXiv: 1810.06111)

Learning the embedding of the hit data set

The data processing pipeline

First preprocessing steps of the data set → Embedding of pairs of hits (doublets): $\Phi(x_i, \theta)$ in 4D embedding space → Graph construction and classification with (quantum) GNN



A doublet in original space.

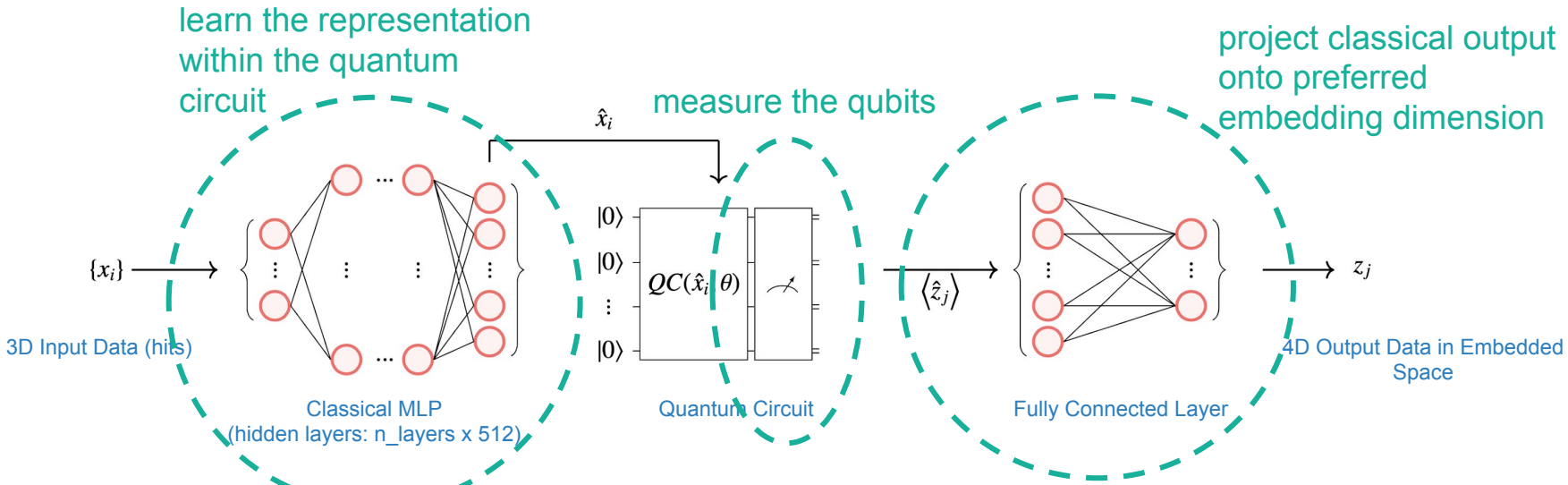
Hinge Embeddig Loss:

$$s_n = (x_i, x_j, y_{i,j})$$

$$loss(s_n) = \begin{cases} \max\{0, \|\Phi(x_i,\theta) - \Phi(x_j,\theta)\|_2\}, & \text{if } (x_i, x_j) \text{ belong to the same trajectory} \\ 0, & \text{if } (x_i, x_j) \text{ belong to different trajectories.} \end{cases}$$

Similar to Choma et al. 2020 (arXiv: 2007.00149)

Hybrid Neural Network architecture



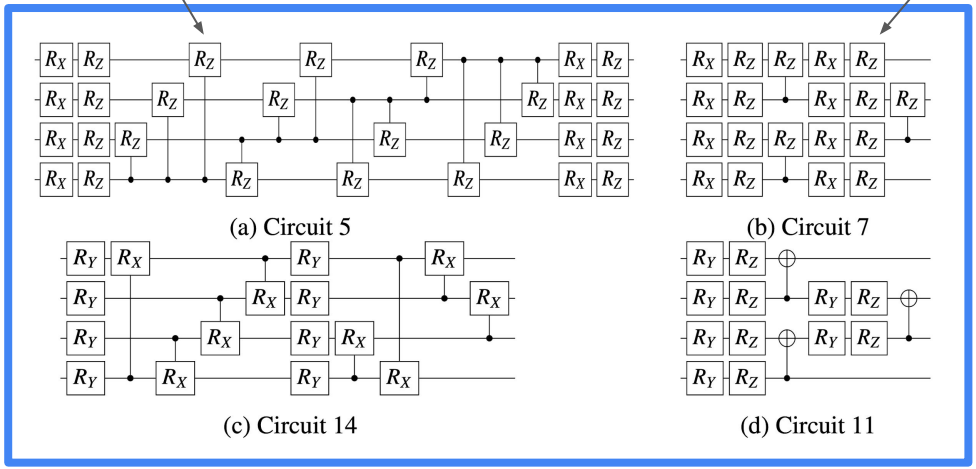
General model of the hybrid architecture

MLP adapted from: Choma et al. 2020 (arXiv: 2007.00149)

Quantum Circuit Approach

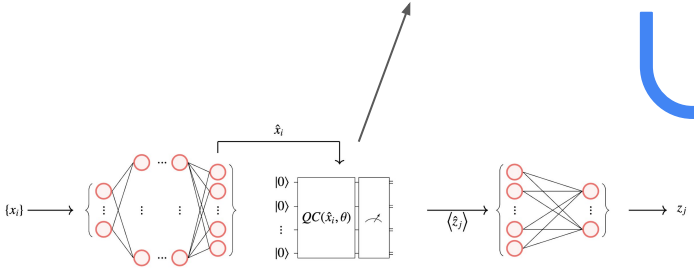
$$CR_Z(\hat{x}_i) = \mathbb{1} \otimes |0\rangle\langle 0| + \exp\left(-i\frac{\hat{x}_i}{2}\sigma_Z\right) \otimes |1\rangle\langle 1|$$

$$R_Z(\hat{x}_i) = \exp\left(-i\frac{\hat{x}_i}{2}\sigma_Z\right)$$



- these quantum circuits were chosen due to their different values regarding entanglement and expressibility
- the 4-qubit quantum circuits encode the output of the classical MLP as angles within the rotational gates displayed

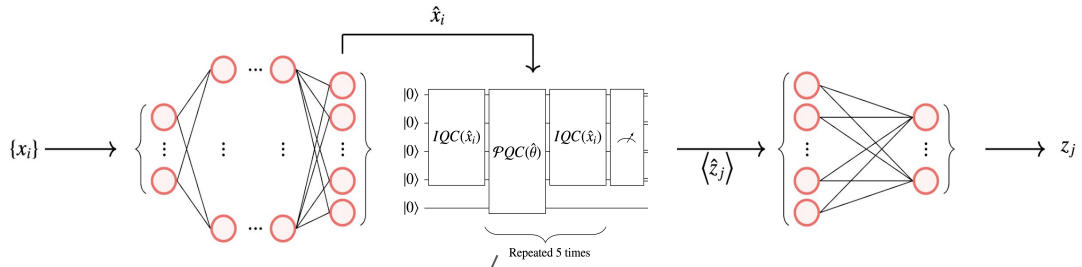
$$QC_{id} : \mathbb{R}^{n_{parameters}} \longrightarrow \mathbb{R}^{n_{measurements}}$$



Circuit	Parameters $n_{parameters}$	Entanglement (the higher the better)	Expressibility (the lower the better)
5	28	0.290	0.051
7	19	0.212	0.104
11	12	0.538	0.139
14	16	0.545	0.011

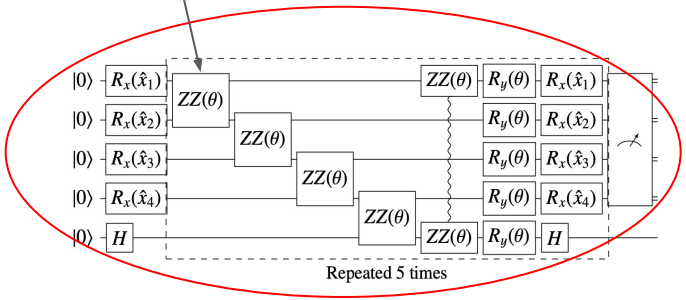
Circuits adapted from and values calculated as in: Sim et al. 2019 (arXiv:1905.10876)

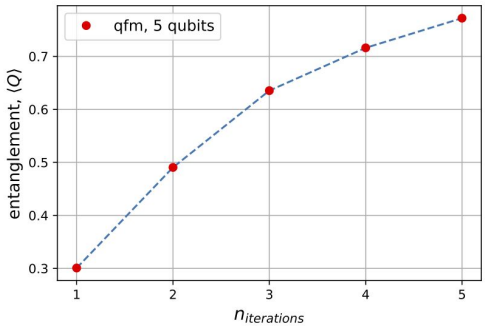
Quantum Feature Map Approach (QFM)

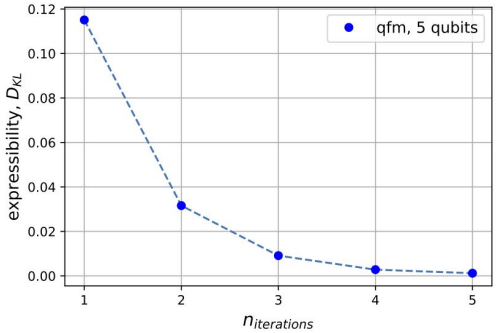


- QFM iteratively encodes the input x_i
- additionally, there are optimizable parameters θ included within the quantum circuit
- repeating blocks of the circuit as indicated on the left increases the entanglement and decreases the expressibility value, which is preferable

$$ZZ(\theta) = \exp\left(-i\frac{\theta}{2}(\sigma_Z)^{\otimes 2}\right)$$





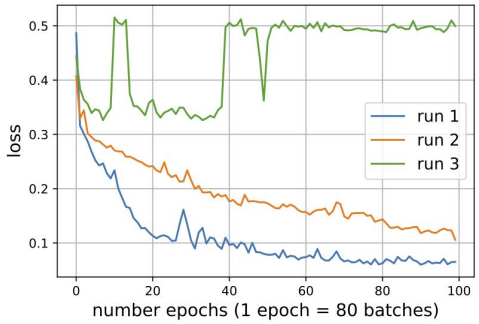


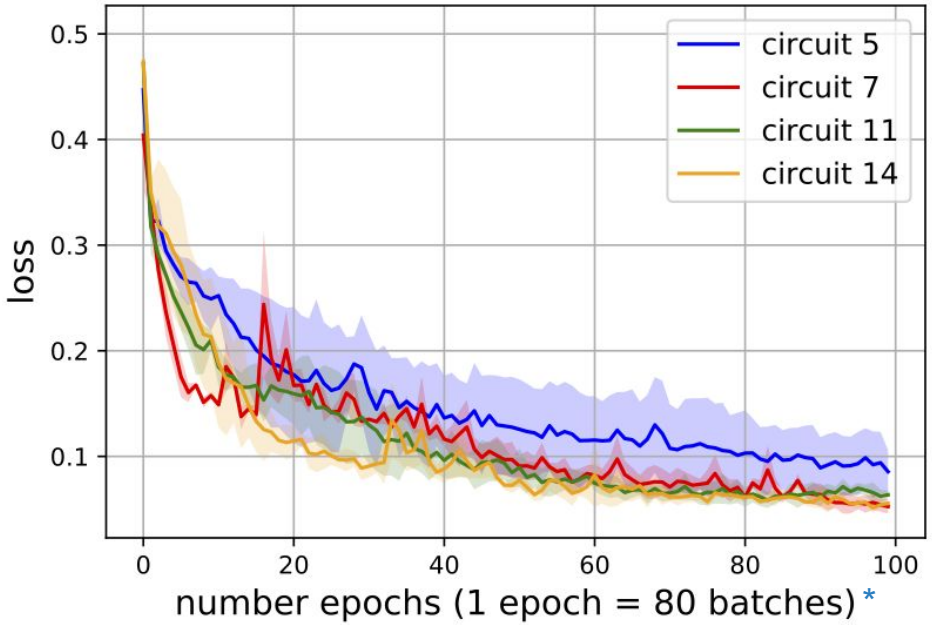
Adapted from: Lloyd et al. 2020 (arXiv:2001.03622)

Ent./Expr. values calculated as in: Sim et al. 2019 (arXiv:1905.10876)

Training results

Quantum Circuit Approach





- training time proportional to number of gates in the quantum circuit
- observation of plateaus in training/validation loss for circuit 5, which includes the highest number of QC parameters in this test

Circuit	Parameters $n_{parameters}$	Entanglement (the higher the better)	Expressibility (the lower the better)	Training time (average per batch)
5	28	0.290	0.051	$37 \pm 8s$
7	19	0.212	0.104	$20 \pm 4s$
11	12	0.538	0.139	$14 \pm 4s$
14	16	0.545	0.011	$16 \pm 4s$

Training data set: 8k hits, validation data set: 2k hits, using ADAMAX optimizer, n_layers = 10, hinge embedding loss, lr = 1e-2.

* mean and indicated std of 3 independent runs, plot without circuit 5 run 3 for better visualization

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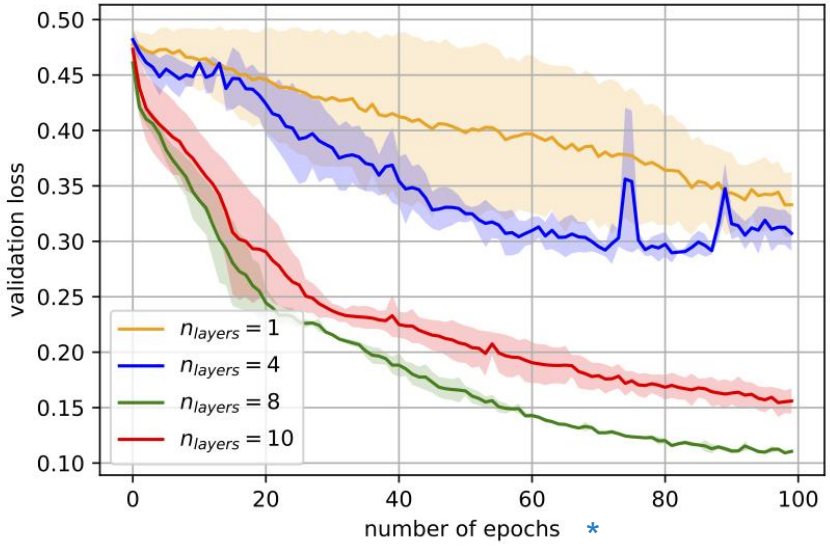
Ent./Expr. values calculated as in: Sim et al. 2019 (arXiv:1905.10876)

Training results

QFM Approach

Circuit	Parameters $n_{parameters}$	Entanglement (higher value preferred)	Expressibility (lower value preferred)	Training time (average per batch)
QFM (5 qubits) ($n_{iteration} = 5$)	74	0.772	0.001	$5min38 \pm 8s$
14 (4 qubits) ($n_{iteration} = 1$)	16	0.545	0.011	$16 \pm 4s$



- learning rate has to be lowered using this architecture by factor 0.1
- similar performance of 1 and 4 layer version, as well as for 8 and 10 classical layers
- validation loss converges to high validation loss for low number of layers
- std much higher when training with less classical layers
- possibility for better convergence when training for more than 100 epochs (especially for 8 and 10 layers)

Training data set: 8k hits, validation data set: 2k hits, using ADAMAX optimizer, hinge embedding loss, lr = 1e-3.

* mean and indicated std of 2 independent runs

Ent./Expr. values calculated as in: Sim et al. 2019 (arXiv:1905.10876)

Conclusion

How to improve?

- test different quantum encoding schemas
- explore more quantum circuits
- explore different architectures
- train on more doublet data

Challenges

- quantum models are hard to simulate and the simulation times are long, especially for larger models that include more trainable parameters

Things to explore

- explore effects when training with real hardware and noise models
- test non-hybrid quantum architectures

Contributors

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Thank you.

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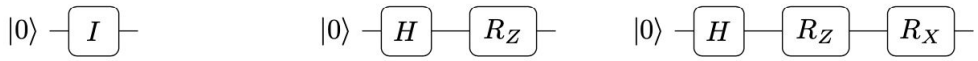
Results shown here will be published soon, with a complete overview.
The most recent version of the code will be published under https://qtrkx.github.io.

Backup Slides

Q.C. for Machine Learning

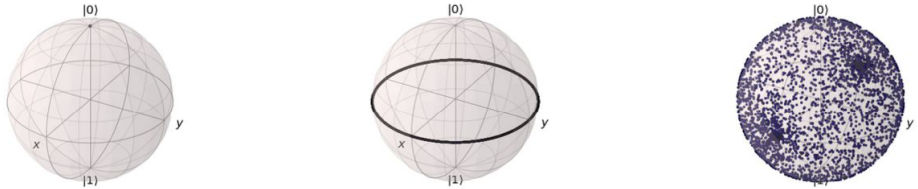
Parameterized Gates



$$RZ(\lambda) = exp(-i\frac{\lambda}{2}Z) = \begin{pmatrix} e^{-i\frac{\lambda}{2}} & 0 \\ 0 & e^{i\frac{\lambda}{2}} \end{pmatrix}$$

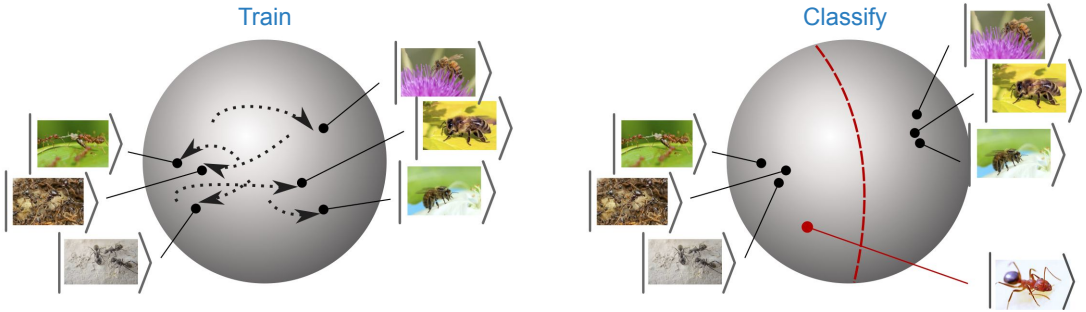
$$RX(\theta) = exp(-i\frac{\theta}{2}X) = \begin{pmatrix} \cos\frac{\theta}{2} & -i\sin\frac{\theta}{2} \\ -i\sin\frac{\theta}{2} & \cos\frac{\theta}{2} \end{pmatrix}$$

We can use parameterized gates to embed data in the Hilbert Space.



Adapted from: Sim et al. 2019 (arXiv:1905.10876)

Then, we can use other parametrized gates that we can optimize to do tasks such as classification.



Adapted from: Lloyd et al. 2020 (arXiv:2001.03622)