Permutation Invariant Quantum Machine Learning in Particle Physics

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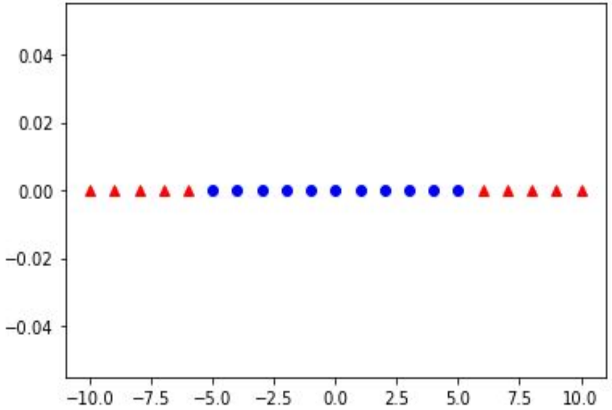
Classical Support Vector Machines

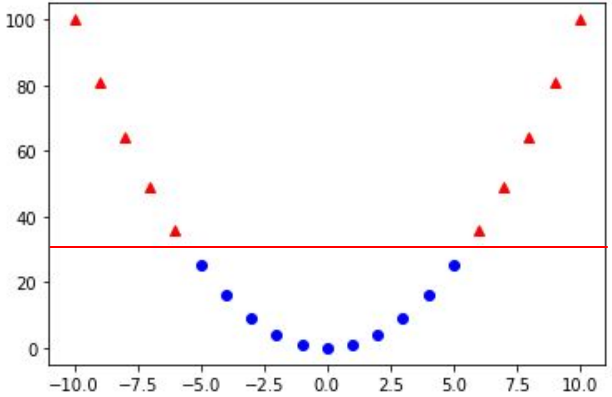
General Idea:

Encode to a higher dimensional space where the classification is easier.

Can't separate in 1D



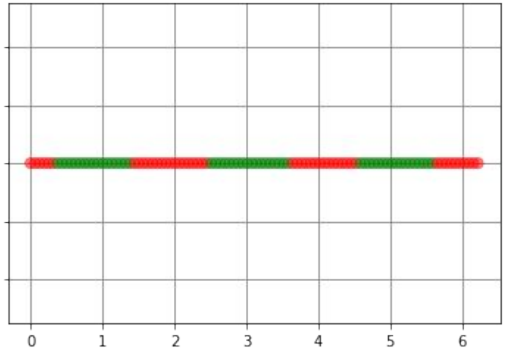
Separable in 2D



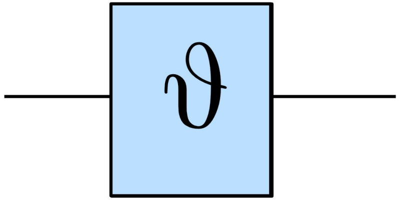
$y = x^2$

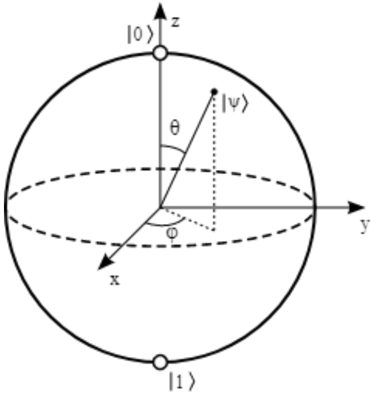
Single Qubit Encoding Example

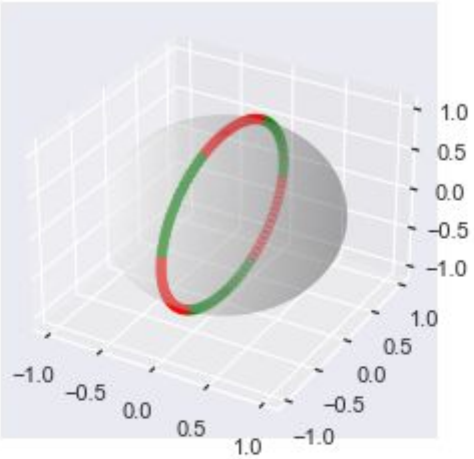
Classical 1 dimensional data. Labelled as θ



Classical data θ is input into X rotation gate angles.



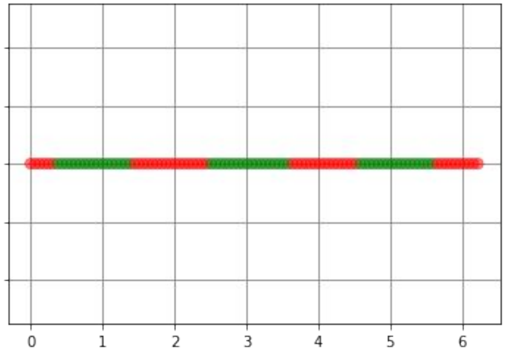




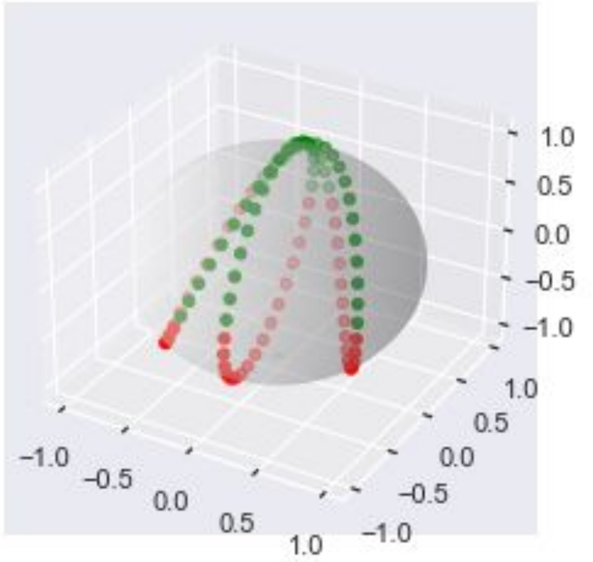
Encoding provided by a single X rotation gate on an initial 0 state

Better Encoding Circuit

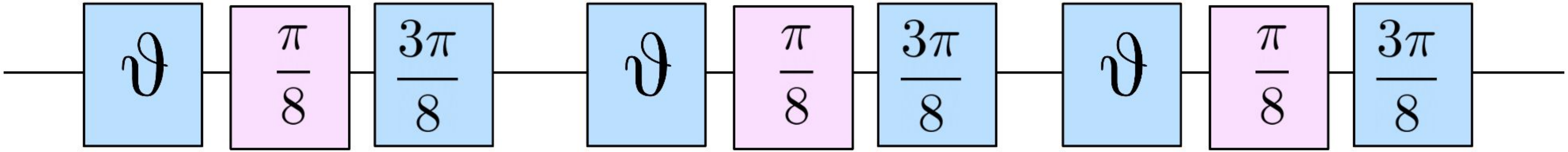
Classical 1 dimensional data



Encoding provided by circuit specific to the data

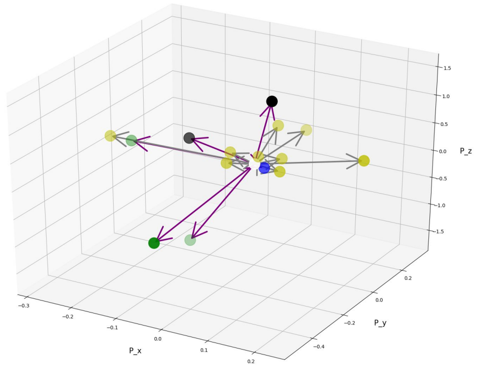


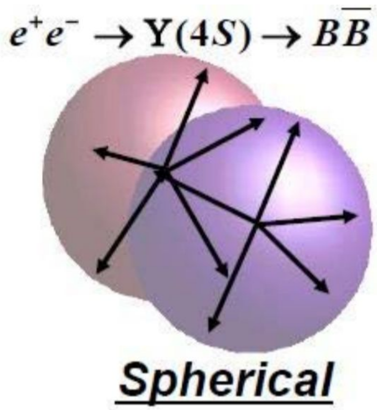
Encoding Circuit constructed for the data

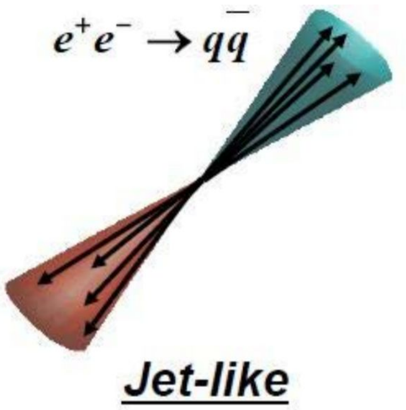


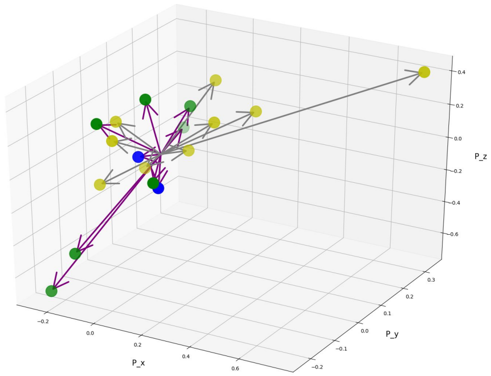
Particle Decay Classification

- Distinguish between B Meson pair and quark pair.
- Background 100 times larger (B -> K+ K- mode)
- Data consists of (p, theta, phi) for each particle in the decay.





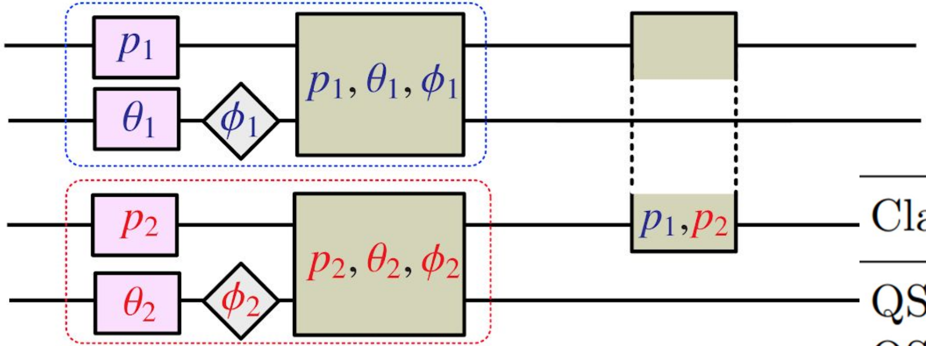




Particle Physics Quantum SVM

Particles entangled individually

Particles entangled with each other through their momenta



Classification Algorithm	AUC
QSVM - Combinatorial Encoding	0.827
QSVM - Bloch Sphere Encoding	0.861
QSVM - Separate Particle Encoding	**0.877**
Classical SVM - RBF Kernel	0.865
Classical FastBDT	0.821

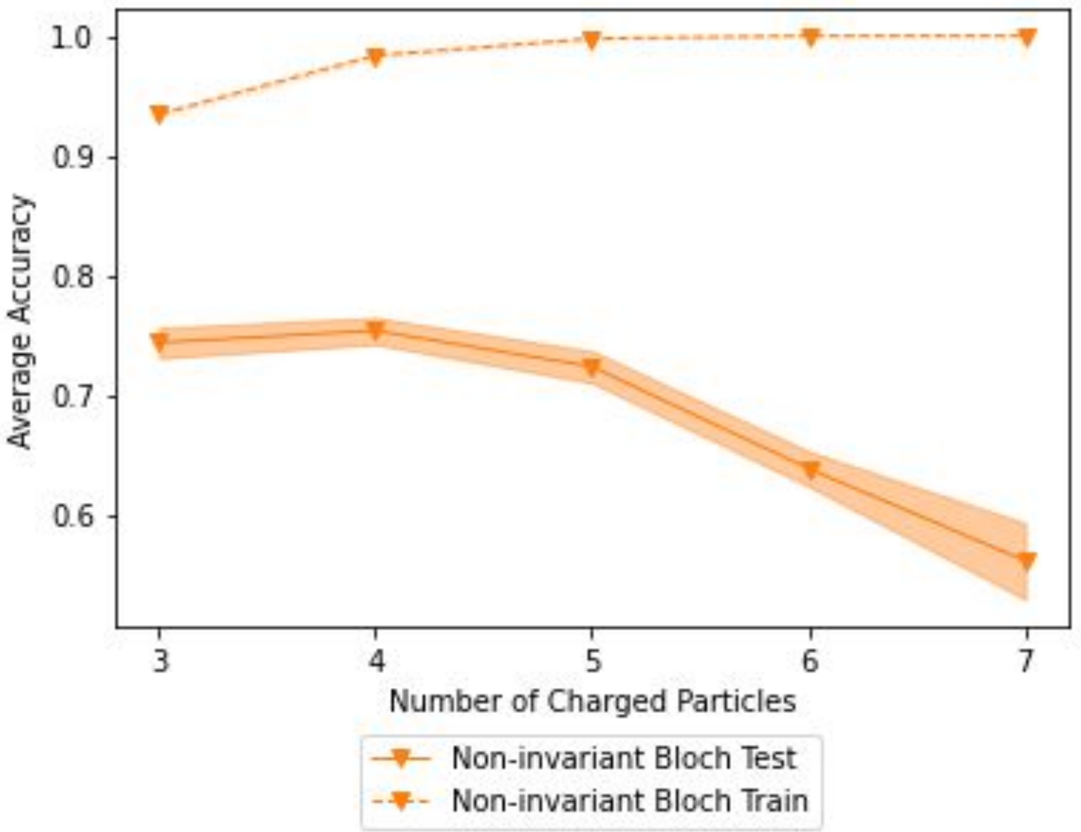
[2] Heredge, Jamie & Hill, Charles & Hollenberg, Lloyd & Sevior, Martin. (2021). Quantum Support Vector Machines for Continuum Suppression in B Meson Decays. Computing and Software for Big Science. 5. 10.1007/s41781-021-00075-x.

Poor Generalisation

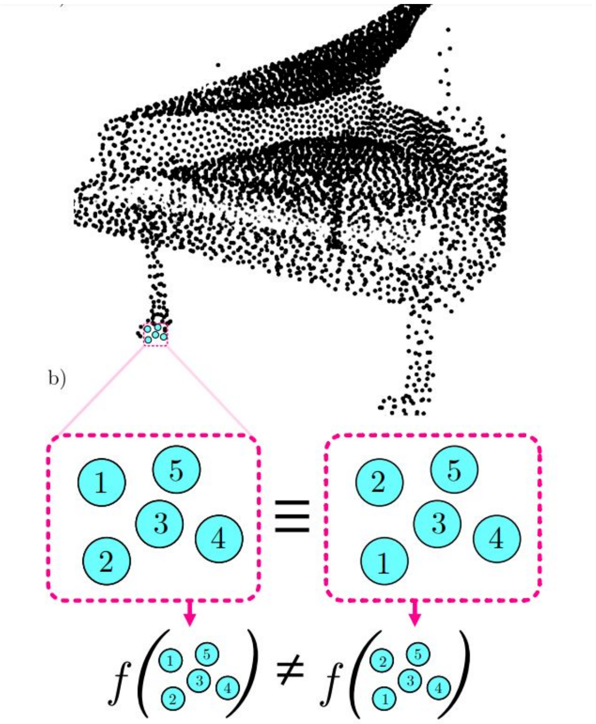
This is considering an event with 7 charged particles

As we give the algorithm more information, it starts to perform worse!

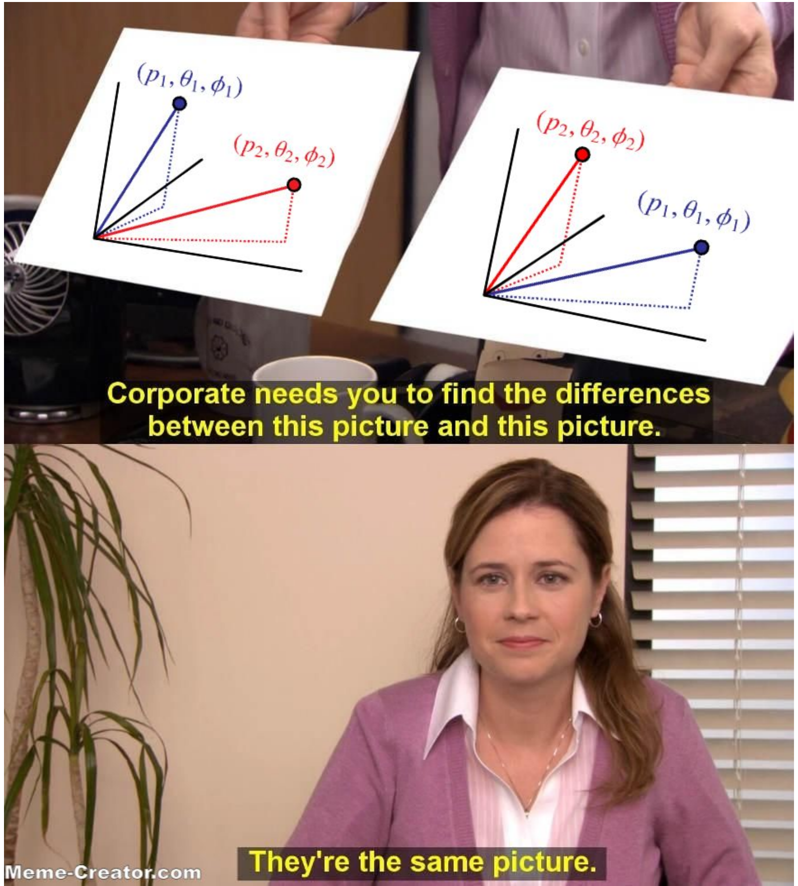
Dimensionality too large = Overfitting on training data



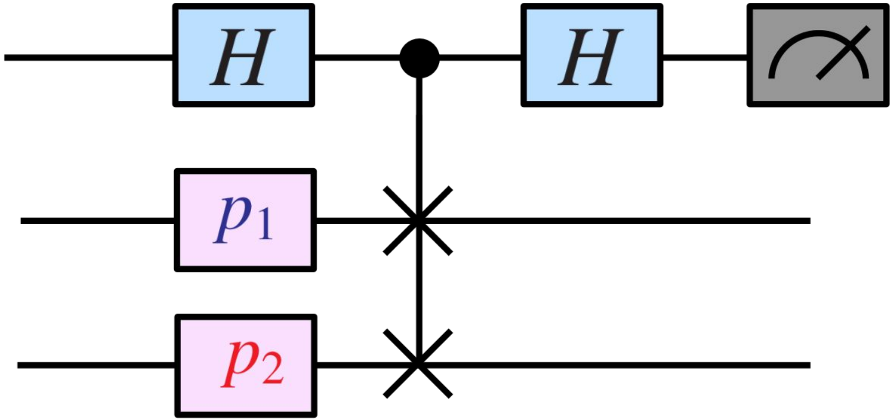
Point Order Permutation Symmetry



$$X = [x_1, y_1, z_1, x_2, y_2, z_2, ..., x_n, y_n, z_n]$$



Symmetric State Preparation



$H \rightarrow$

$$|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle + |1\rangle)|p_1\rangle|p_2\rangle$$

$CSWAP \rightarrow$

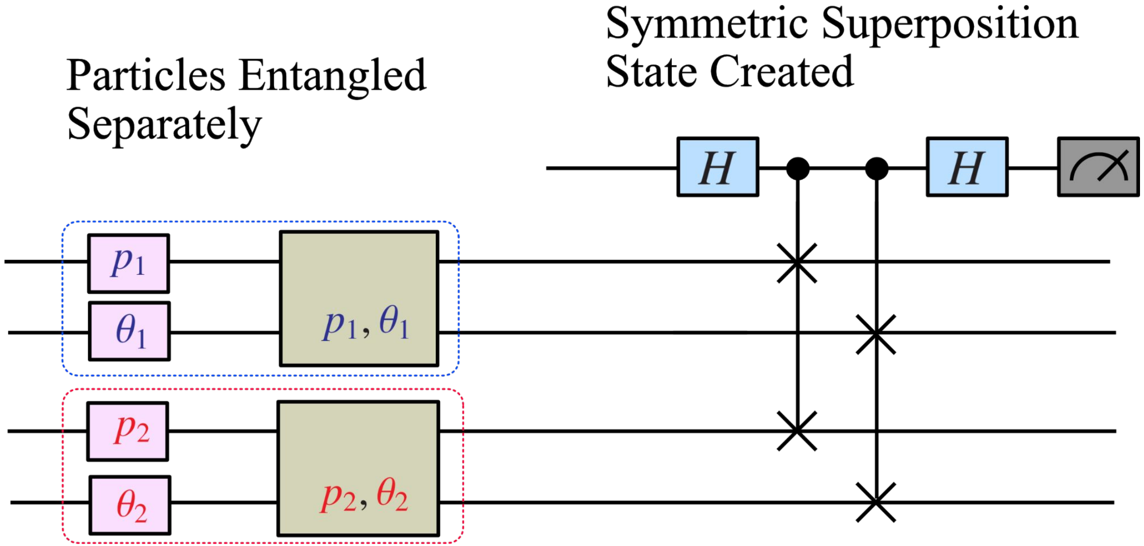
$$|\psi\rangle = \frac{1}{\sqrt{2}}(|0\rangle|p_1\rangle|p_2\rangle + |1\rangle|p_2\rangle|p_1\rangle)$$

$H \rightarrow$

$$|\psi\rangle = \frac{1}{2}\Big(|p_1\rangle|p_2\rangle + |p_2\rangle|p_1\rangle\Big)|0\rangle + \frac{1}{2}\Big(|p_1\rangle|p_2\rangle - |p_2\rangle|p_1\rangle\Big)|1\rangle$$

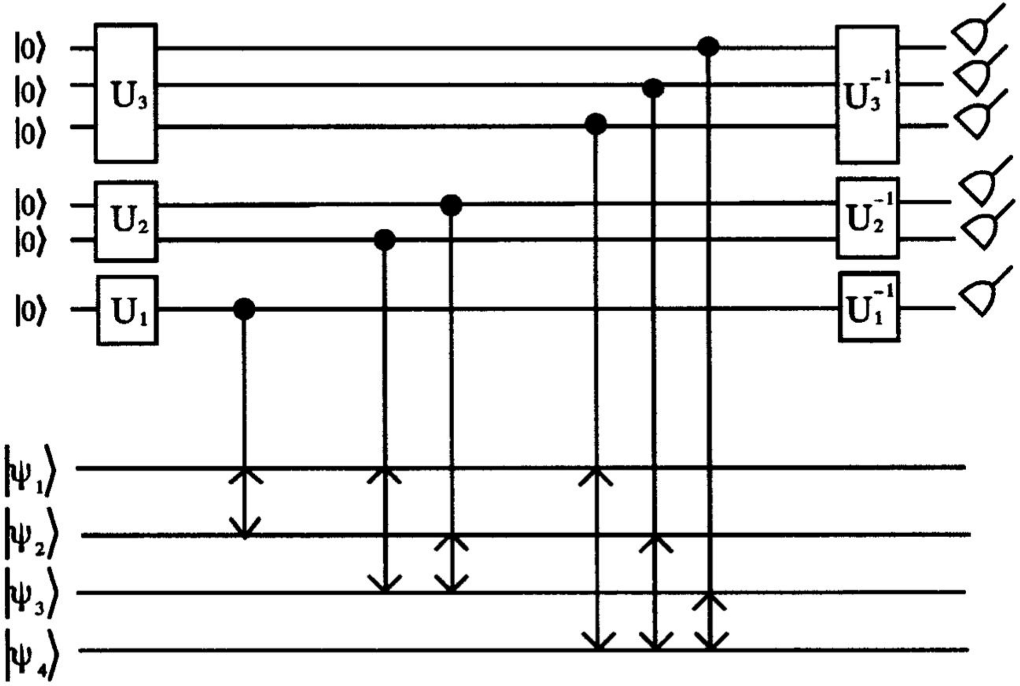
[3] Heredge, Jamie & Hill, Charles & Hollenberg, Lloyd & Sevior, Martin. (2023). Permutation Invariant Encodings for Quantum Machine Learning with Point Cloud Data https://arxiv.org/abs/2304.03601

Symmetrised Encoding



$$|\psi\rangle = \frac{1}{\sqrt{2}}\left(|p_1\rangle|p_2\rangle + |p_2\rangle|p_1\rangle\right)$$

Generalised Symmetrisation



[4] Stabilisation of Quantum Computations by Symmetrisation, Adriano Barenco, Andre` Berthiaume, David Deutsch, Artur Ekert, Richard Jozsa, Chiara Macchiavello (1996)

Reduction in Dimensionality

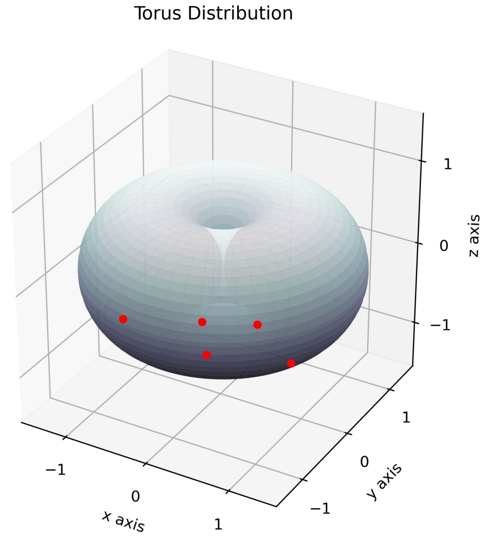
Dimension = 8

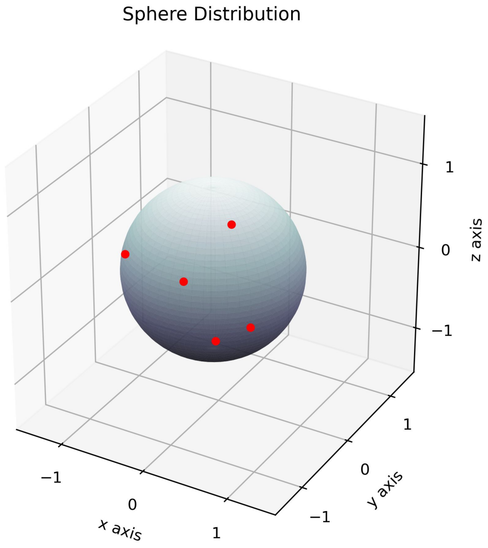
$$
\begin{aligned}
|\psi\rangle = {} & \alpha_0|0\rangle|0\rangle|0\rangle \\
& + \alpha_1|1\rangle|0\rangle|0\rangle + \alpha_2|0\rangle|1\rangle|0\rangle + \alpha_3|0\rangle|0\rangle|1\rangle \\
& + \alpha_4|1\rangle|1\rangle|0\rangle + \alpha_5|1\rangle|0\rangle|1\rangle + \alpha_6|0\rangle|1\rangle|1\rangle \\
& + \alpha_7|1\rangle|1\rangle|1\rangle.
\end{aligned}
$$

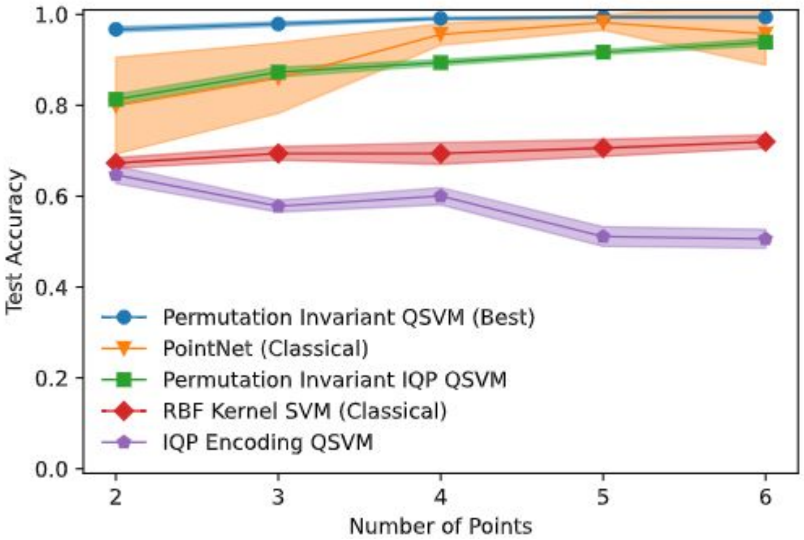
Dimension = 4

$$
\begin{aligned}
|\psi\rangle = {} & \beta_0|0\rangle|0\rangle|0\rangle \\
& + \beta_1(|1\rangle|0\rangle|0\rangle + |0\rangle|1\rangle|0\rangle + |0\rangle|0\rangle|1\rangle) \\
& + \beta_2(|1\rangle|1\rangle|0\rangle + |1\rangle|0\rangle|1\rangle + |0\rangle|1\rangle|1\rangle) \\
& + \beta_3|1\rangle|1\rangle|1\rangle.
\end{aligned}
$$

Pointcloud Shape Classification Data

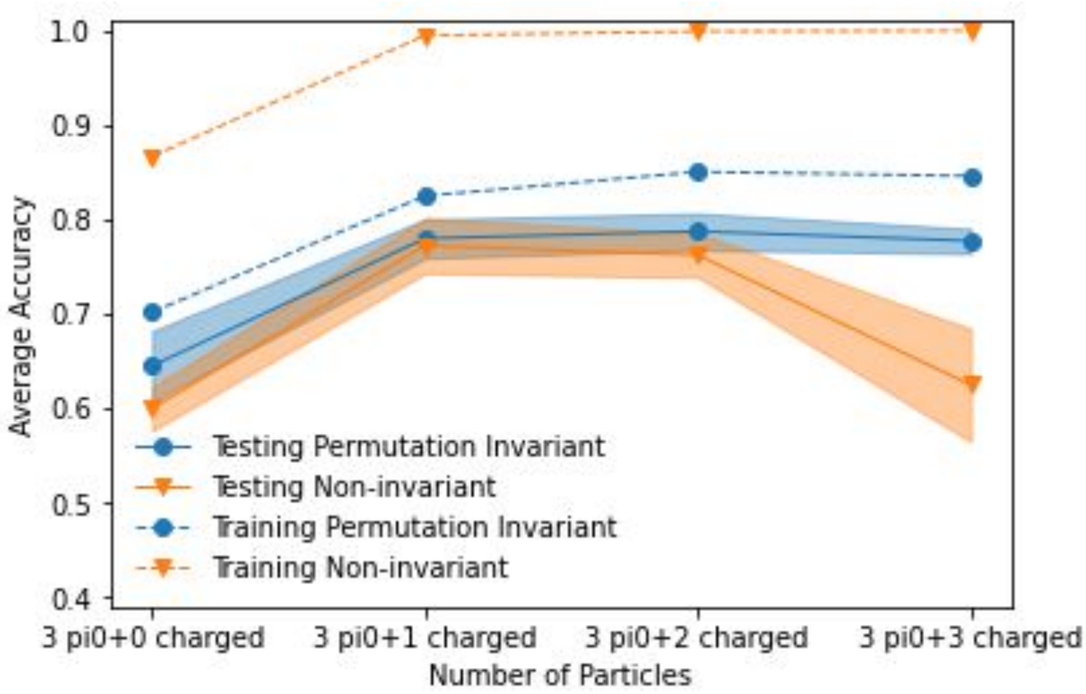




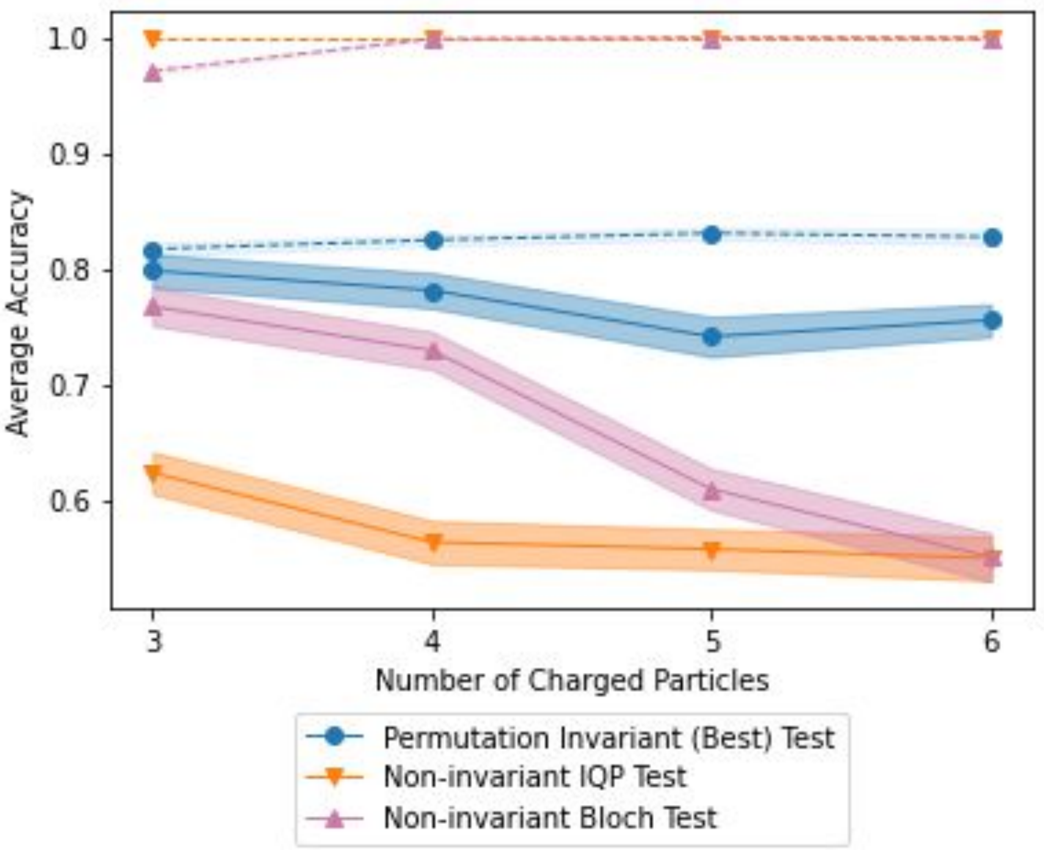


[3] Heredge, Jamie & Hill, Charles & Hollenberg, Lloyd & Sevior, Martin. (2023). Permutation Invariant Encodings for Quantum Machine Learning with Point Cloud Data https://arxiv.org/abs/2304.03601

Robust to Increasing Input Dimension



B Meson Continuum Suppression



Weightings in data:

3 particles : 20%

4 particles : 14%

5 particles : 18%

6 particles : 12%

Weighted Averages:

Permutation Invariant = 0.77
Non-invariant = 0.67

Main Points

Quantum Machine Learning suffers from a curse of dimensionality.

Particle Decay events will contain a permutation symmetry with respect to their ordering.

Capturing symmetry in the model can reduce dimensionality and improve generalisation.

References

[1] Vojtech Havlicek, Antonio D. C´orcoles, Kristan Temme, Aram W. Harrow, Abhinav Kandala, Jerry M. Chow, and Jay M. Gambetta. Supervised learning with quantum enhanced feature spaces, Nature volume 567, 209–212 (2019)

[2] Heredge, Jamie & Hill, Charles & Hollenberg, Lloyd & Sevior, Martin. (2021). Quantum Support Vector Machines for Continuum Suppression in B Meson Decays. Computing and Software for Big Science. 5. 10.1007/s41781-021-00075-x.

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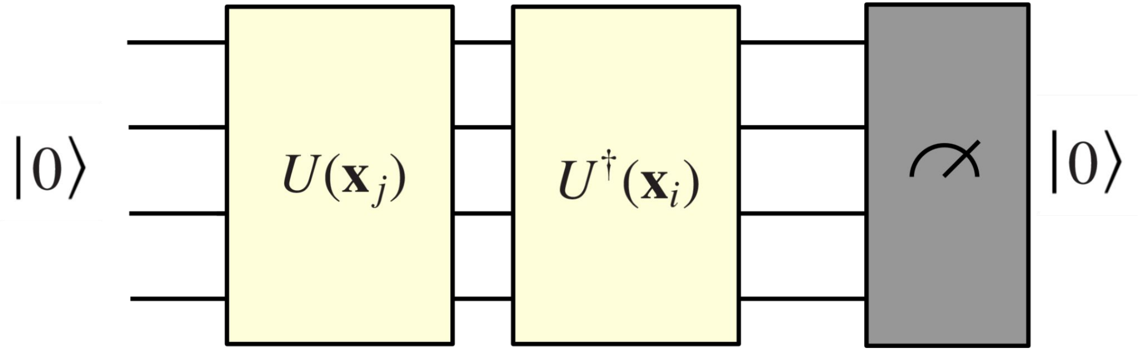
[4] Stabilisation of Quantum Computations by Symmetrisation, Adriano Barenco, Andre` Berthiaume, David Deutsch, Artur Ekert, Richard Jozsa, Chiara Macchiavello (1996)

Extra Slides

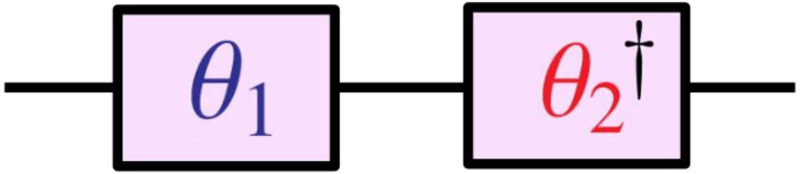
Quantum Kernel Estimator Example



Proportion of 0 State Measurements = Kernel Entry Estimate

$$|\langle \Phi(\boldsymbol{x})|\Phi(\boldsymbol{z})\rangle|^2 = |\langle 0^n|\mathcal{U}^\dagger_{\Phi(\boldsymbol{x})}\mathcal{U}_{\Phi(\boldsymbol{z})}|0^n\rangle|^2$$

Example circuit where encoding is a single rotation gate



Resulting state and consequent Kernel Entry

$$|\Phi\rangle = \cos\frac{\theta}{2}|0\rangle + \sin\frac{\theta}{2}|1\rangle$$

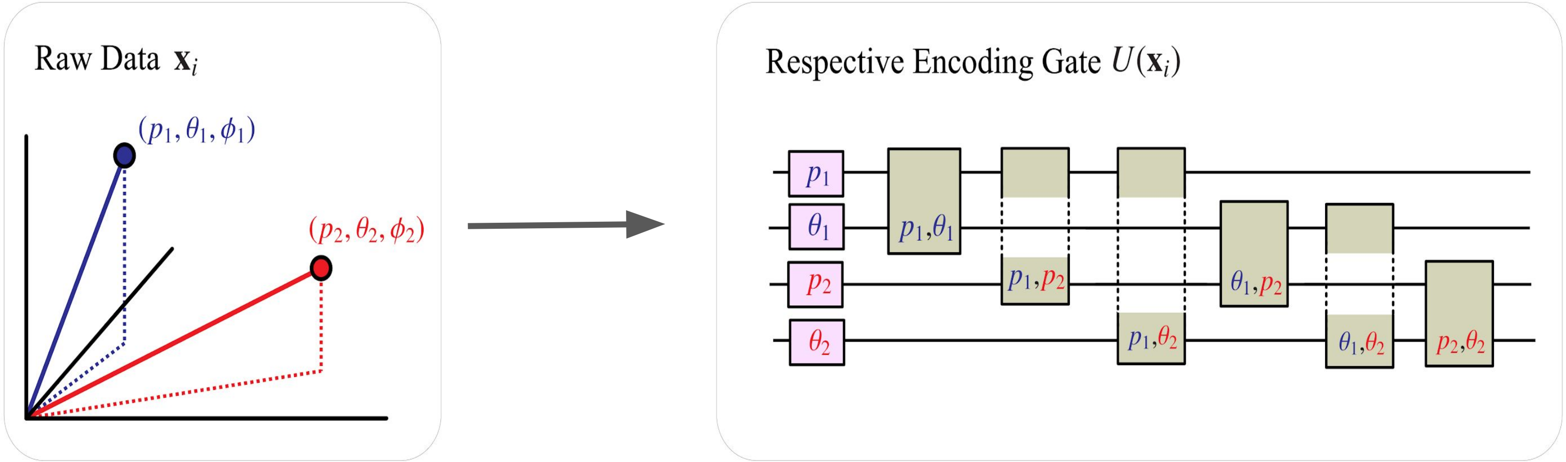
Kernel entry = $|cos(\frac{\theta_1 - \theta_2}{2})|^2$

Encoding Step

$$|\Phi(z)\rangle = \mathcal{U}_{\Phi(z)}|0^n\rangle$$

IQP Encoding

- Large number of gates
- Generic approach



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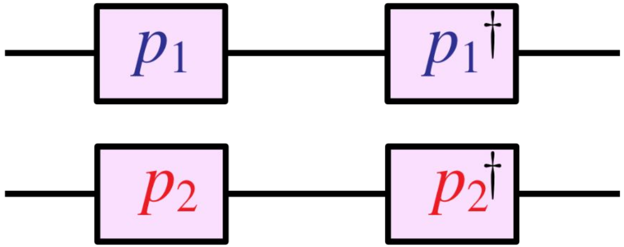
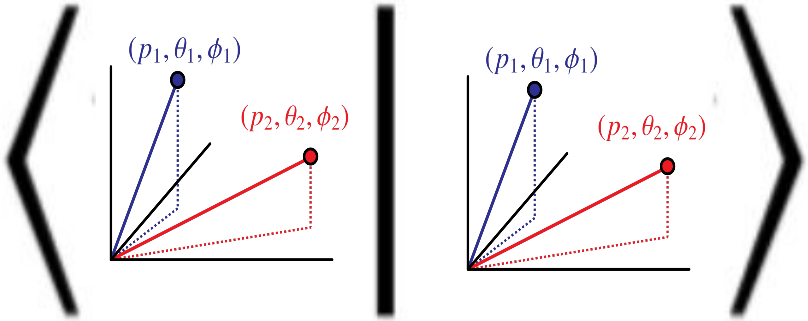
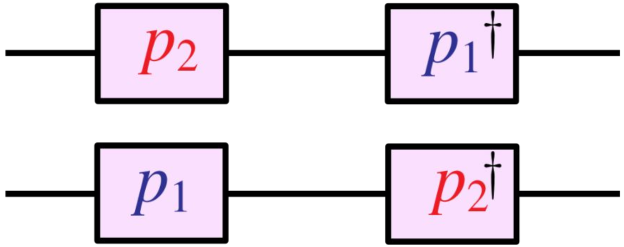
Different Results Under Point Order Permutation

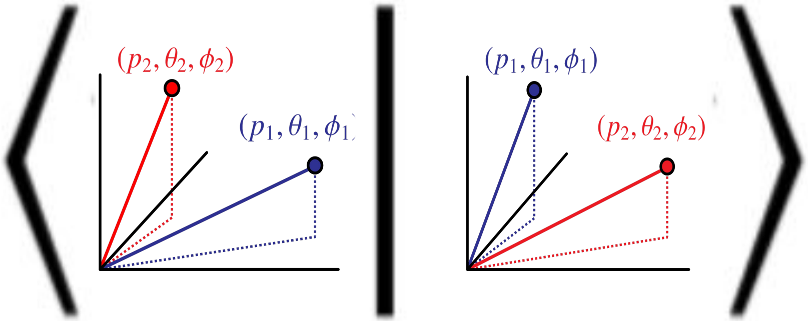
Always measure 0 state = Perfect overlap





Non-perfect overlap = Data looks different!
But they are the same picture!





Generalise Better For Large Particle Events