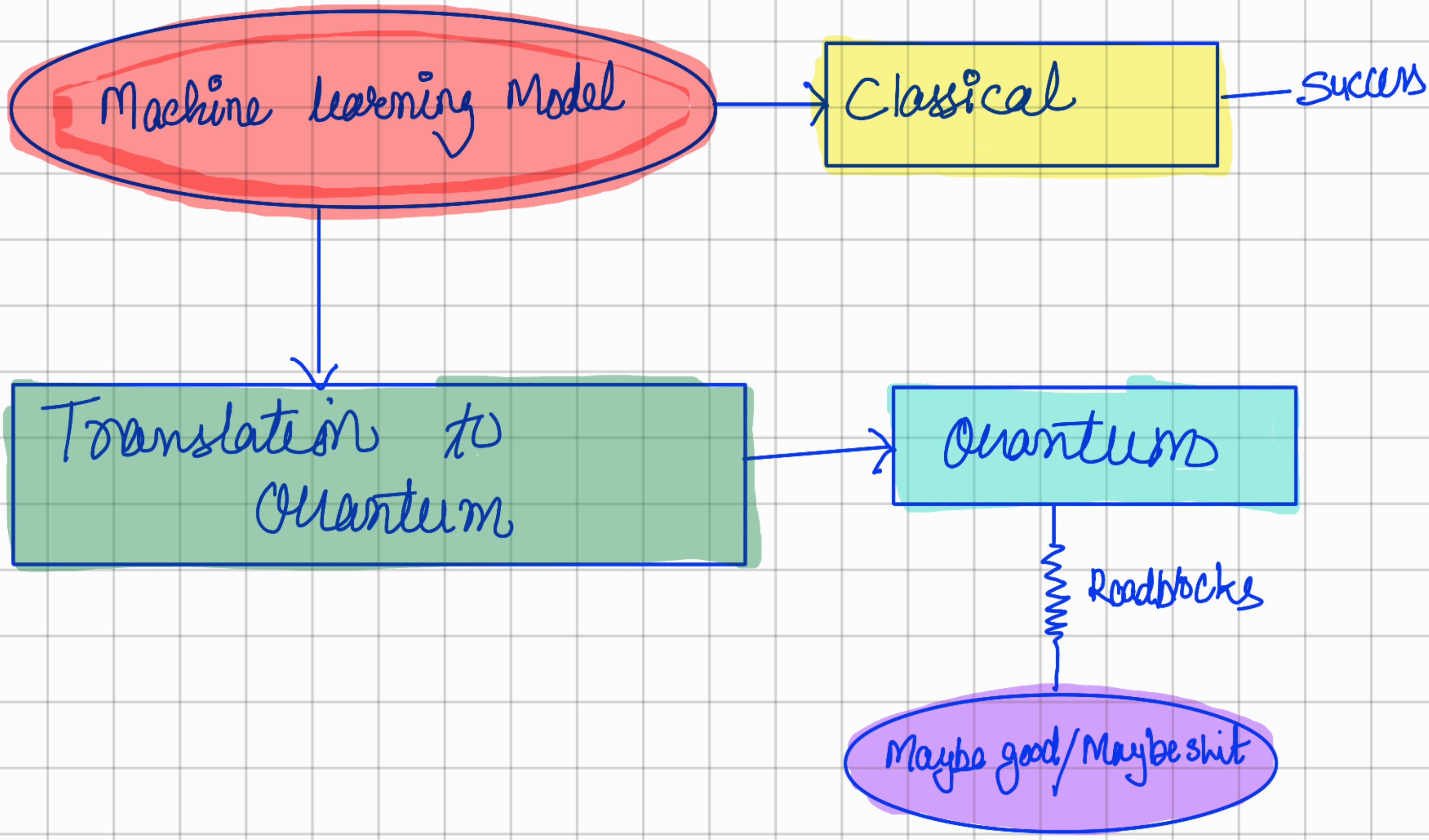
Group Representation Theory → make the model more quantum aware.



Due to the success of classical geometric deep learning, there have been several efforts to create QML models with strong inductive bias that respect the underlying structure and symmetries of the data over which they act.

Strong inductive bias: restrict the space of the functions explored by the QML model by imposing task-specific knowledge or assumptions

A model tailored to a given task will have better performance

analysing the symmetries of datasets

GROUP THEORY

REPRESENTATION THEORY

studies abstract algebraic objects called groups
which are sets equipped by binary operation for combining elements

studies abstract algebraic objects called groups
which are collections of linear transformations acting on a vector space.

Groups encode abstract symmetries, and representations describe the concrete actions of these symmetries.

They are crucial to manipulate the symmetries underlying the data. These can be used to create equivariant quantum neural networks and measurement operators as well as to understand how different representations of the same symmetry group can access different types of information in a quantum state.

Quantum Machine Learning

Let's start with a simple classification of labeled data task.

One has a repeated access to the dataset of the form

$$S = \{\rho_i, y_i\}_{i=1}^{N}$$

ρ_i are the n-qubit states $\in R$ in domain R in a Hilbert space with dimension $(d = 2^n)$

y_i are the real-valued labels in some label domain Y

$$f: R \to Y \Rightarrow f(\rho_i) = y_i$$

Train a model $h_\theta : R \to Y$

trainable

How the model is defined?

parameters

What are the inductive biases encoded in the mode?

The goal is to somehow encode the information about the symmetries of the data in S into the model?

Quantum Machine Learning Model

$$h_\theta(\rho_i) = \mathrm{Tr}\left[\mathcal{W}_\theta(\rho_i^{\otimes k}) M_i\right]$$ (the model)

$$\mathcal{W}_\theta : \mathcal{B}(\mathcal{H}^{\otimes k}) \longrightarrow \mathcal{B}(\mathcal{H}^{\otimes k'})$$

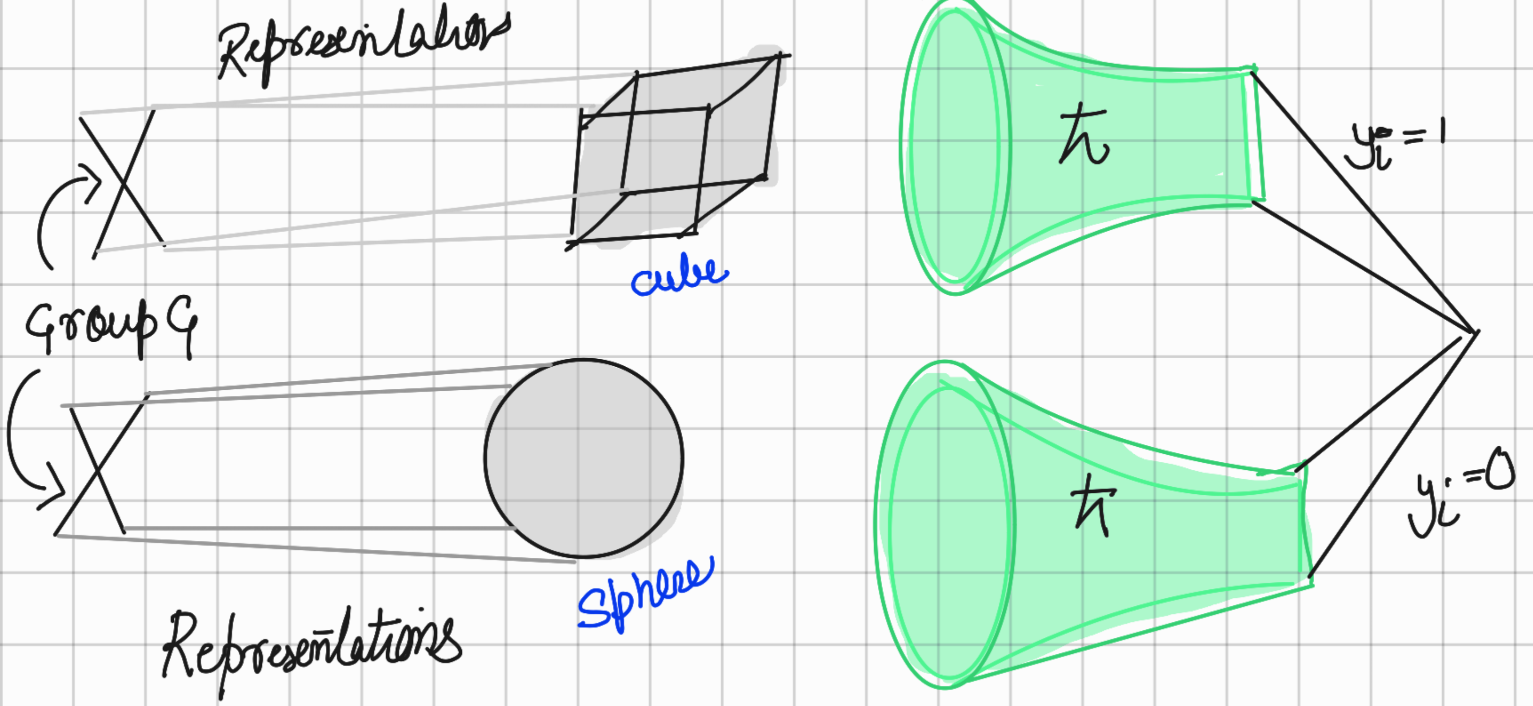
this is trainable parameterized quantum channel

and

M_i is a potentially data-dependent Hermitian measurement operator.

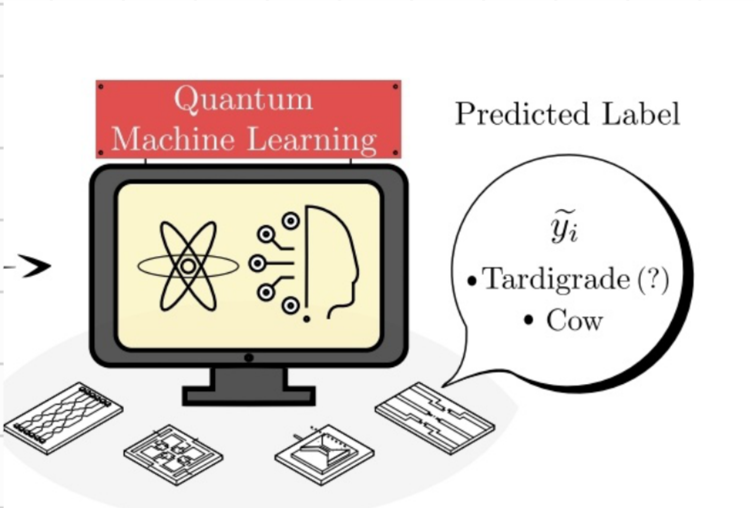
$\mathcal{B}(\mathcal{H}^{\otimes k})$ denotes the space of bounded linear operator on $\mathcal{H}^{\otimes k}$

Symmetries and groups in QML



Quantum Dataset

$\{\rho_i, y_i\}$



consider a task of classifying between spherical cows and cubic tardigrades whose information are encoded into the quantum states. The spherical cow is still spherical, and as such the QML model should be able to accurately classify it regardless of how the cow was rotated.

Symmetries and groups in QML

What is symmetry? Something that is left unchanged after the transformation. We'll refer to the transformation as some unitary applied on a quantum state.

$$\rho \longrightarrow U \rho U^{\dagger}$$

(wigner theorem guarantees that all symmetry transformations of quantum states preserving inner products are unitary or anti unitary)

Proposition 1: Let G be the set of all unitary symmetry transformations, such that for any $U \in G$, the map

$\rho \to U\rho U^{\dagger}$ leaves some properties of ρ unchanged.

Then $\mathcal{G}$ forms a group.

it follows all properties of group

$U, V \in \mathcal{G}$

$U \cdot V \in \mathcal{G}$ $\Rightarrow$ $\rho \to U\rho U^{\dagger} \to V \cdot U \rho U^{\dagger} \cdot V^{\dagger}$

Associativity, existence of identity, existence of invrs.

Associativity : $U, V, W \in \mathcal{G}$, then

$$(W \cdot V) \cdot U = W \cdot (V \cdot U)$$

Identity : $\mathbb{1} \cdot U = U \cdot \mathbb{1} = U$ and $\mathbb{1} \in \mathcal{G}$

Inverse : $U \in \mathcal{G}$, $\exists$ $U^{\dagger} \in \mathcal{G}$ s.t $U \cdot U^{\dagger} = U^{\dagger} \cdot U = \mathbb{1}$

inverse conjugate.

Definition I (Label Invariance) : The action of the group $\mathcal{G}$ is said to leave the data labels y_i invariant, if

$$\boxed{f(U\rho_i U^{\dagger}) = f(\rho_i) = y_i} \quad \forall \rho_i \text{ with label } y_i, \ \forall U \in \mathcal{G}$$

if the states are themselves invariant, label invariance is immediately satisfied.

$$U\rho U^{\dagger} = U$$

but there may be a case where the states are not invariant, but we still have label invariance.

$\Rightarrow$ $U\rho U^{\dagger} \neq \rho$ but

$\Rightarrow \quad U\rho U^\dagger \neq \rho$, but

$$f(U\rho U^\dagger) = f(\rho)$$

Dataset $S = \{\rho_i, y_i\}_{i=1}^{N}$ drawn from $R \times Y$ $\quad \rho_i \in R$, $y_i \in Y$

such that the label y_i associated to the state ρ_i is assigned according to some function $f: R \to Y$

$$f(\rho_i) = y_i$$

We want our QML model h_θ to be invariant under G and we focus on two condition

> equivariance under G of the parameterized quantum channel

> equivariance of the measurement operator.

How to ensure that a QML model h_θ is invariant under G?

i) Equivariance under G of the parametrized quantum channel

$$\mathcal{W}_\theta\left(U^{\otimes k} \rho_i^{\otimes k} (U^\dagger)^{\otimes k}\right) = U^{\otimes k'} \mathcal{W}_\theta\left((\rho_i)^{\otimes k}\right) (U^\dagger)^{\otimes k'}$$

$$\forall U \in G$$

where the QML model is:

$$h_\theta(\rho_i) = \mathrm{Tr}\left[\mathcal{W}_\theta\left(\rho_i^{\otimes k}\right) M_i\right] \quad \text{(the model)}$$

$h_\theta(\rho_i) = \mathrm{Tr}[\mathcal{W}_\theta(\rho_i^{\otimes k}) M_i]$ (Internal)

$$\mathcal{W}_\theta : B(\mathcal{H}^{\otimes k}) \longrightarrow B(\mathcal{H}^{\otimes k'})$$

ii) Equivariance of the Measurement operator:

$$[M, U^{\otimes k'}] = 0 \quad , \forall U \in \mathcal{G}$$

commutator

Let's prove Label invariance:

Proof:

$$h_\theta(U\rho U^\dagger) = \mathrm{Tr}[\mathcal{W}_\theta((U\rho U^\dagger)^{\otimes k}) M_i]$$

making use of equivariance under $\mathcal{G}$

$$\Rightarrow \mathrm{Tr}[U^{\otimes k'} \mathcal{W}_\theta([\rho_i]^{\otimes k})(U^\dagger)^{\otimes k'} M_i]$$

$$\Rightarrow \mathrm{Tr}[\mathcal{W}_\theta([\rho_i])^{\otimes k} (U^\dagger)^{\otimes k'} M_i U^{\otimes k}]$$

$$\Rightarrow \mathrm{Tr}[\mathcal{W}_\theta([\rho_i])^{\otimes k} M_i]$$

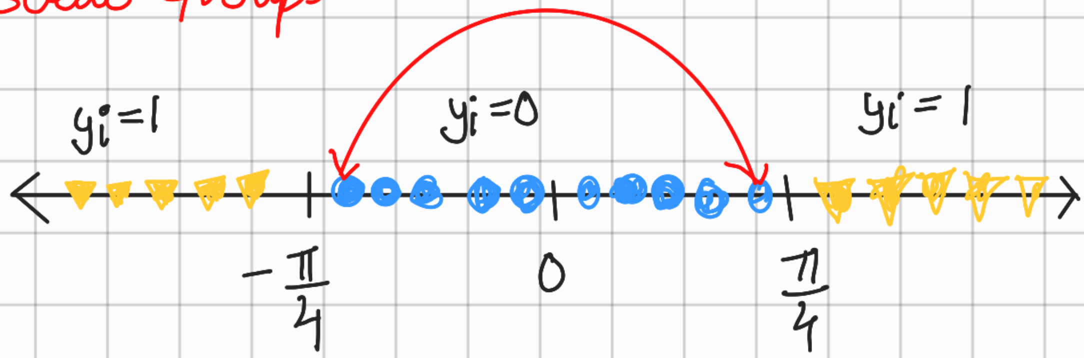
$$\Rightarrow h_\theta(\rho_i) \qquad \forall U \in \mathcal{G}$$

Equivariant Quantum Neural Network is passing the action of the symmetry from their input to their output.

Equivariant measurement leads to the models that absorb the action of symmetry the actions of symmetry.

Examples of discrete and continuous symmetries in QML
$\in \mathbb{Z}$ $\in \mathbb{R}$

Discrete Groups.

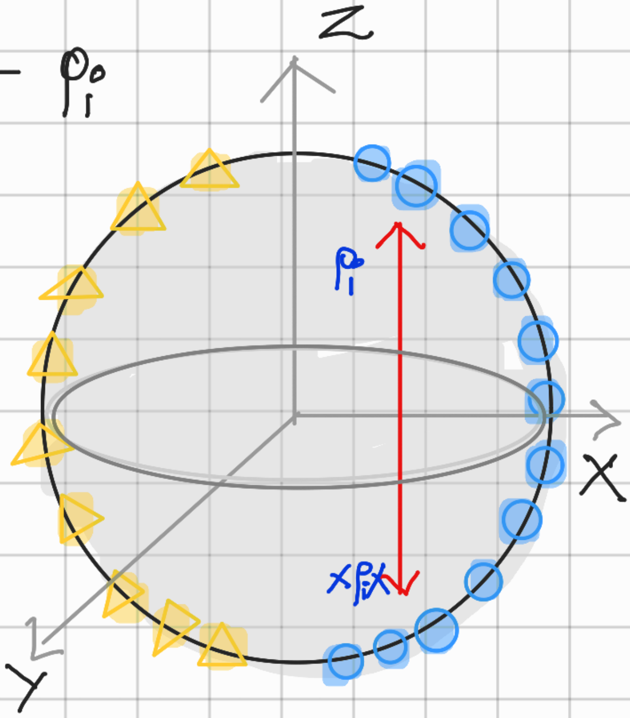


we want to distinguish blue circles ($y_i=0$) from yellow △ ($y_i=1$)

Here the labels of the data are invariant under translation $x \to -x$

$|+\rangle$ —— $\boxed{R(x_i)}$ —— ρ_i

$$R(\theta) = e^{-i\theta Y}$$



We can see that the labels are invariant under the bit flip transformation.

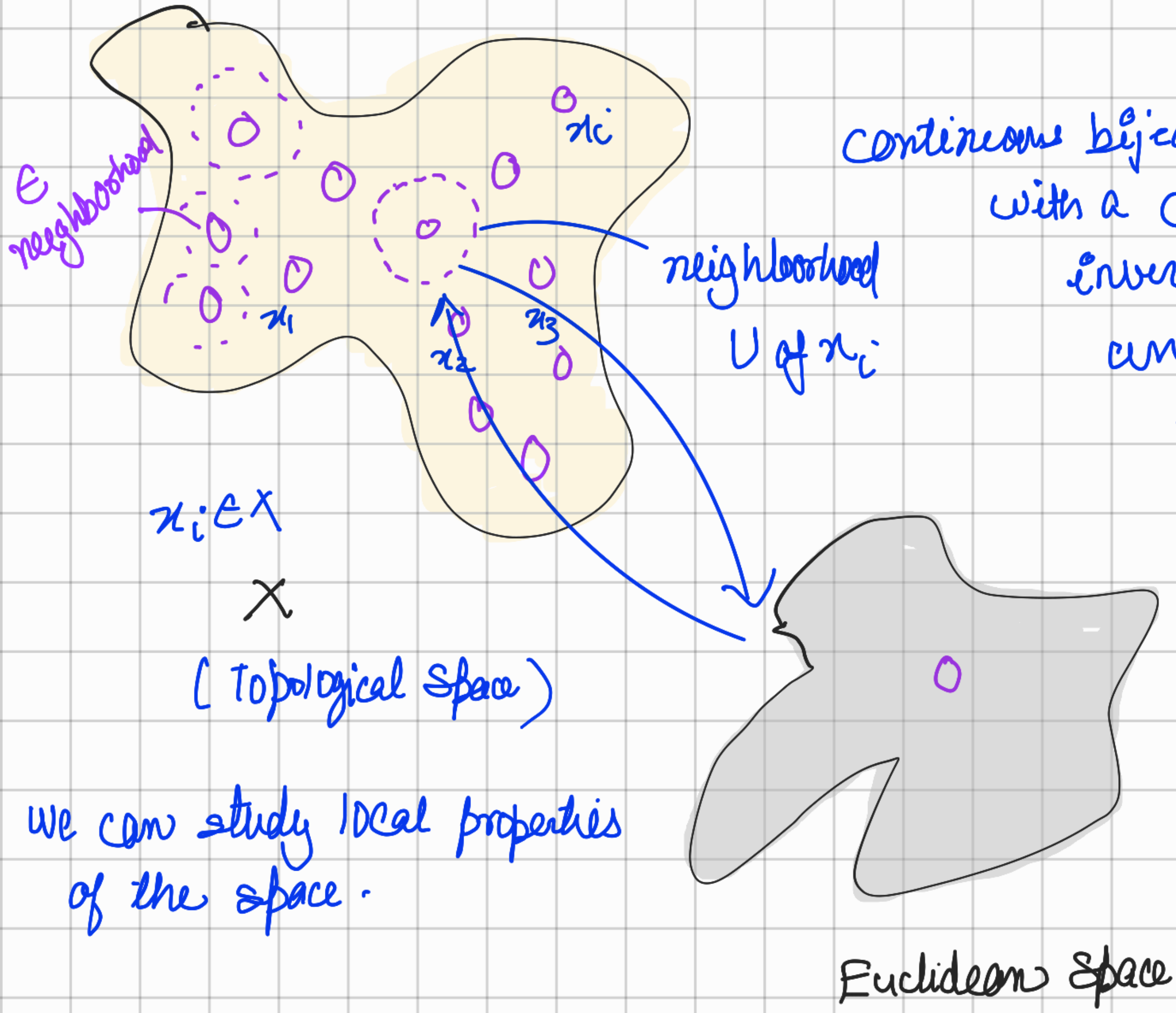
$$G_{bflip} = \{\mathbb{1}, X\}$$

group is discrete, only has two elements.

Continuous Groups.

(locally homeomorphic to an Euclidean Space)

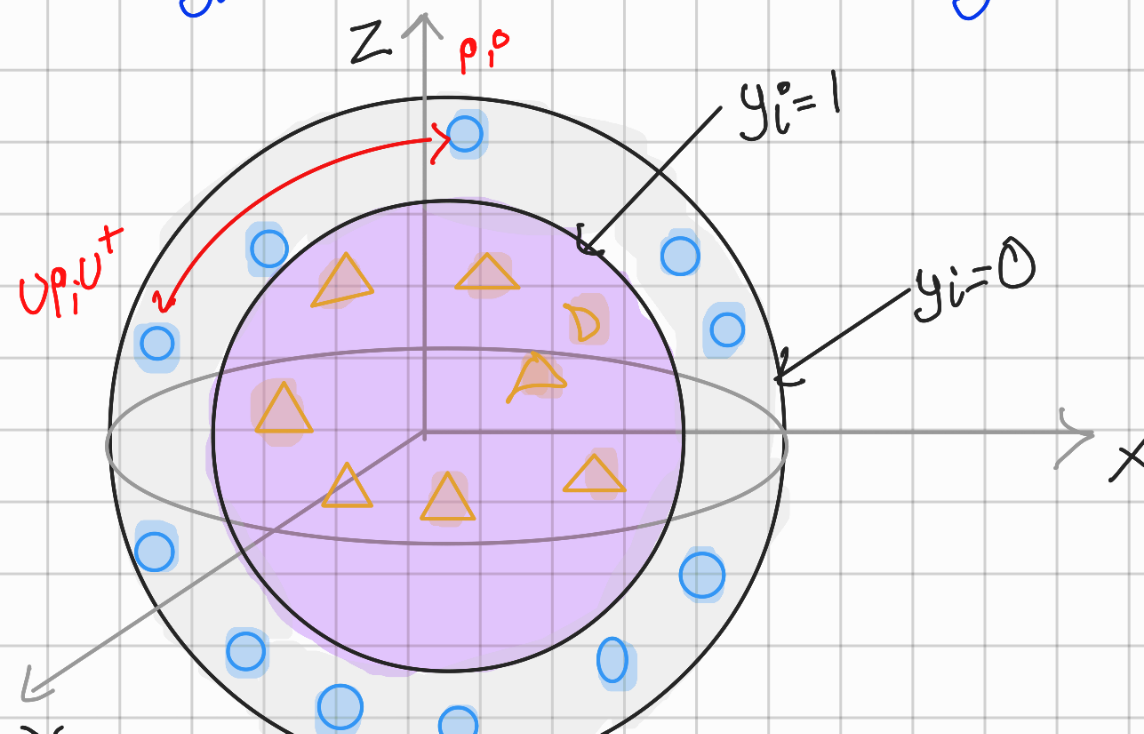
this means that at each point within that topological space you can find a neighbourhood that looks very much like a portion of Euclidean space.



continuous bijective function with a continuous inverse b/w U and some Euclidean spa.

We can study local properties of the space.

Eg: Binary QML classification, where we want to classify single-qubit pure states (states on the surface of the bloch) with $y_i = 0$ and mixed states with $y_i = 1$



Here the task was to classify single-qubit pure state with mixed states. $y_i = 0$ (pure) $y_i = 1$ (mixed). Since purity is a spectral property it gets preserved by action of any Unitary

$$G_{uni} = \{ U \in SU(2) \}$$

Continuous group with infinitely many Unitaries

where the unitaries can take the form

$$U = c_0 \mathbb{I} + (c_1 X + c_2 Y + c_3 Z)$$

$$c_0 \in \mathbb{R}$$
$$\sum_{i=0}^{3} c_i^2 = \mathbb{I}$$

continuous groups are also manifolds, they contain additional structure lacked by discrete groups.

LIE GROUPS

It is a mathematical structure that combines the properties of a smooth manifold and a group. They are used to describe symmetries and transformations in various areas.

we can construct a smooth path in a Lie group, that basically means that we can define continuous functions that map a real interval to the Lie group in a smooth and differentiable manner.

i.e

directional derivatives of continuous group paths

Eg: Exponentiation of every element X of the Lie Algebra leads to an element of the Lie group $e^X = g$

$$\mathfrak{g} = \{ X \in \mathbb{C}^{d \times d} \mid e^X \in G \}$$

(we'll see them in more detail later)

Let's explore the connection between symmetries and groups.

Abstractifying Physical Symmetries to Goal

i) identify the symmetry of data and then abstractify them

connect a physical symmetry group with some familiar abstract mathematical group.

Groups encode abstract symmetries, and representation describe concrete symmetries.

Representations provide a way to implement the symmetries described by the group in a tangible and practical manner.

This process is highly heuristic and general process do not exist

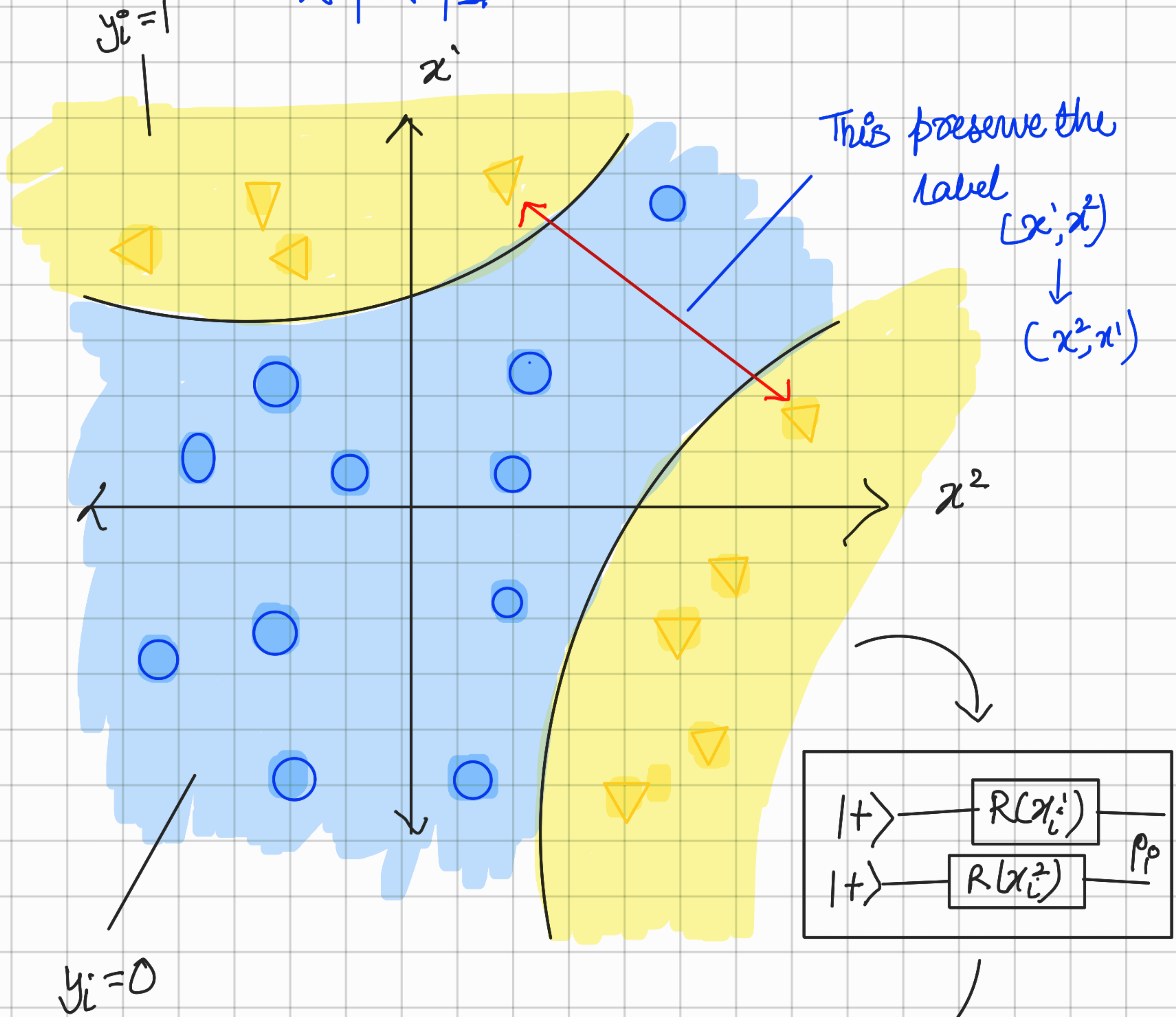
one physical symmetry group (representations) can be identified with several abstract groups.

$$G_{bflip} = \{ \mathbb{1}, X \}$$

Cayley Table

	$\mathbb{1}$	X
$\mathbb{1}$	$\mathbb{1}$	X
X	X	$\mathbb{1}$

$\mathbb{Z}_2$



$$\rho_i = SWAP \, \rho_i \, SWAP$$

$$G_{SWAP} = \{\mathbb{1}, SWAP\}$$