Representation theory for Geometric Quantum Machine Learning

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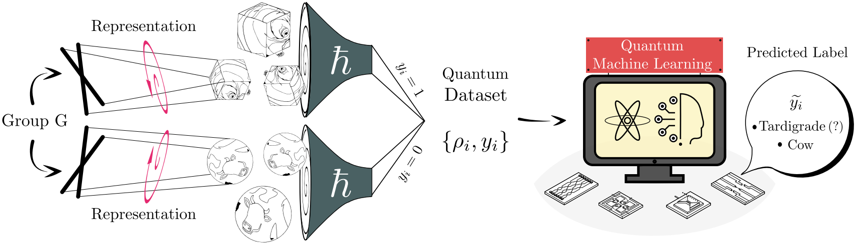
Why symmetry?

- *import: Marco Cerezo's QML Talk*
- Key QML problem: barren plateaus!
- Symmetry yields powerful inductive biases, tightly constraining search space size and structure: "a rotated tardigrade is still a tardigrade, and a rotated cow is still a cow".



Why symmetry?

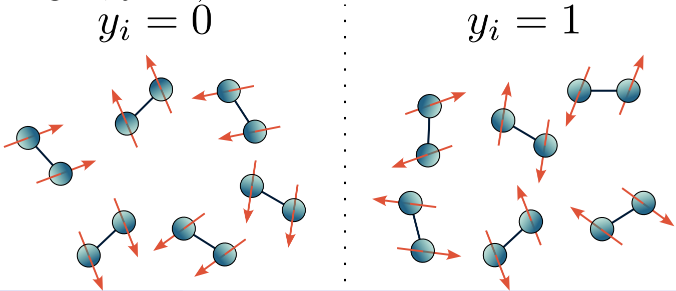
- Morally, symmetry describes "transformations which leave some property invariant".
- For QML, this means *label invariance* under some transformations of the data.
- Mathematically, symmetry is implemented by group representations.
  - Groups capture symmetry at an abstract level.
  - Representations describe how a group "acts" on a vector space, often via unitaries on a Hilbert space. This can be thought of as a more physical symmetry.
- We will define these after setting up our main example: quantum phase classification.

Ex: quantum phase classification

Heisenberg XXX chain. Local Hilbert spaces are qubits $\mathbb{C}^2$, and $J \in \mathbb{R}$ a parameter:

$$H = J \sum_{j=1}^{n-1} X_j X_{j+1} + Y_j Y_{j+1} + Z_j Z_{j+1},$$

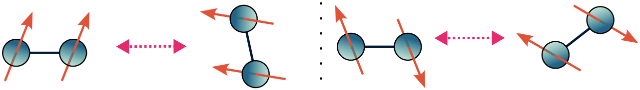
where X, Y, Z are Pauli matrices. Varying J, we get ground states which are either highly aligned (ferromagnet, $y_i = 0$) or anti-aligned (antiferromagnet, $y_i = 1$).



Ex: quantum phase classification

We can use a QML framework, like a quantum neural network, to label ground states as ferromagnets or antiferromagnets. Let $f : \mathcal{R} \to \{0, 1\}$ be a function labeling quantum states.

- *Data:* pure states $|\psi_i\rangle \in \mathcal{R}$
- *Labels:* Ferromagnetic $y_i = 0$ and antiferromagnetic $y_i = 1$
- Let's think about the structure of this problem.
  - Swapping two particles preserves alignment.
  - Identically rotating each particle preserves alignment.
- These operations may change the data, but the labels are invariant! This is a *symmetry*.



Ex: discrete symmetry

"Swapping two particles doesn't change ferromagnetism."

- Group: $G = \mathbb{Z}_2 = \{1, -1\}$ with multiplication.
- Representation space: $V = \mathbb{C}^2 \otimes \mathbb{C}^2$ (2 qubits)
- Representation R: each group element $g \in G$ gets a corresponding linear map $R_g : V \to V$,

$$R_1 \cdot |\psi_i\rangle = |\psi_i\rangle \,,$$
$$R_{-1} \cdot |\psi_i\rangle = \texttt{SWAP}\, |\psi_i\rangle \,.$$

Symmetry = Label invariance under group representation: for any quantum state $\rho_i \in \mathcal{R} \subseteq V$,

$$f(|\psi_i\rangle) = f(R_g \cdot |\psi_i\rangle), \quad \text{for all } g \in G.$$

So, $f(|\psi_i\rangle) = f(|\psi_i\rangle)$ and $f(|\psi_i\rangle) = f(\texttt{SWAP}\, |\psi_i\rangle)$.

Ex: continuous symmetry

"Rotated ferromagnets are still ferromagnets."

- Group: $G = SU(2)$
- Representation space: $V = \mathbb{C}^2 \otimes \mathbb{C}^2$ (2 qubits)
- Representation: $R_g = g^{\otimes 2}$
  - e.g. if $g = e^{itX} \in SU(2)$, then its representative $R_g : V \to V$ is

$$R_g \cdot |\psi_i\rangle = (e^{itX} \otimes e^{itX}) |\psi_i\rangle .$$

Symmetry = Label invariance under rep R of $G = SU(2)$:

$$\begin{aligned} f(|\psi_i\rangle) &= f(R_g \cdot |\psi_i\rangle) \\ &= f(g^{\otimes 2} |\psi_i\rangle). \end{aligned}$$

This is a huge inductive bias! We will eventually see that an 3D manifold of states is now identified as a single unit.

The formalities: groups

- Keep the example of rotations $G = SU(2)$ in mind, where composition (matrix multiplication) is the group operation.
- A *group* G is a set with a binary operation obeying some axioms.
  - *Binary operation:* If $g, h \in G$, then $gh \in G$. (Rotation by $h = e^{iY}$ and then rotation by $g = e^{iX}$ is the same as a rotation by $gh = e^{iX}e^{iY}$.)
  - *Identity:* There's a $\mathbb{1} \in G$, such that $g = g\mathbb{1} = \mathbb{1}g$ for any $g \in G$. (The identity matrix $e^0 = \mathbb{1} \in SU(2)$ is a rotation by 0 degrees)
  - *Inverse:* For every $g \in G$, there exists a g^{-1} with $\mathbb{1} = gg^{-1} = g^{-1}g$. (Every rotation $g = e^{i\theta X}$ has a reverse rotation $g^{-1} = e^{-i\theta X}$)
  - *Associativity:* if $g, h, k \in G$, then

    $$g(hk) = (gh)k.$$

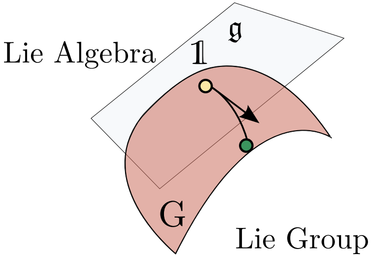
    (You can be lazy with order of operations)

Discrete and continuous groups

$G = SU(2)$ is a *Lie group* or *continuous group*, meaning it's also a manifold (we can parameterize it with coordinates).[1]

- $\implies$ We can draw continuous paths in G and take derivatives along these paths.
- Ex: time evolution with infinitesimal generator $iX \in \mathfrak{su}(2)$:

$$\{U_t := e^{itX} \mid t \in \mathbb{R}\} \text{ is a path in } SU(2)$$



[1] Matrix groups, like $SO(n)$ or $GL(n)$, are often Lie groups, and many commonly appearing Lie groups are matrix groups.

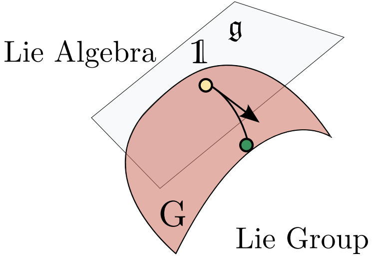
Discrete and continuous groups

Taking directional derivatives along paths in G gives a vector space with matrix commutator $[\cdot,\cdot]$: this is a *Lie algebra* $\mathfrak{g}$.

- Ex: Take the path of rotations $\{U_t = e^{itX}\}$. The infinitesimal generator is then

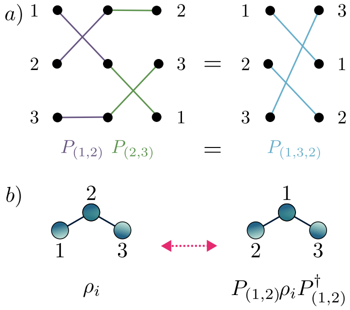
$$\frac{d}{dt}U_t\Big|_{t=0} = iXe^0 = iX \in \mathfrak{su}(2).$$

  In fact, Paulis X, Y, Z form a basis for $\mathfrak{su}(2)$, and the commutation relations tell us about its Lie algebra structure!



Discrete and continuous groups

- If the underlying set is discrete, we have a *discrete group*.
- Key example: the symmetric group S_n of permutations on n letters.
  - Two-particle swap is a special case: $S_2 \cong \mathbb{Z}_2 = \{1, -1\}$.
  - The symmetric group commonly arises in quantum as *tensor index permutations*, like qubit swaps.



Representation theory

- A *representation* R of a group G on a vector space V is a homomorphism $R : G \to \mathrm{GL}(V)$, the general linear group (invertible matrices on V)
  - *Homomorphism* just means that this map respects the group structure: if $g, h \in G$ and $V = \mathbb{C}^n$, then R_g, R_h are $n \times n$ complex matrices obeying
$$R_g R_h = R_{gh}.$$
- The first and most boring example: the trivial representation, where $V = \mathbb{C}$ and
$$R_g = \mathbb{1}, \quad \text{for all } g \in G.$$
Sanity check: if $G = \mathbb{Z}_2$, and $g = 1, h = -1$, then
$$\mathbb{1} = R_{-1} = R_1 R_{-1} = \mathbb{1}\mathbb{1} = \mathbb{1}.$$

Representation theory: $G = \mathbb{Z}_2$

- Let $V = \mathbb{C}$ and define the representation

$$R_1 = \mathbb{1}, R_{-1} = -\mathbb{1}.$$

Sanity check:

$$\mathbb{1} = R_1 = R_{-1}R_{-1} = (-\mathbb{1})(-\mathbb{1}) = \mathbb{1}.$$

Seems to work! Let's revisit the earlier two-qubit swap example.

Representation theory: $G = \mathbb{Z}_2$

- Let $V = \mathbb{C}^2 \otimes \mathbb{C}^2$ and recall:

$$R_1 = \mathbb{1}$$
$$R_{-1} = \texttt{SWAP}.$$

Sanity check: if $|\psi_i\rangle \in V$, then

$$\begin{aligned} |\psi_i\rangle = R_1 \cdot |\psi_i\rangle &= (R_{-1} \cdot R_{-1}) \cdot |\psi_i\rangle \\ &= R_{-1} \cdot (\texttt{SWAP}\,|\psi_i\rangle) \\ &= \texttt{SWAP}(\texttt{SWAP}\,|\psi_i\rangle) \\ &= |\psi_i\rangle \end{aligned}$$

- Onto the continuous examples! Same group laws, but more structure because we can take derivatives to pass to the Lie algebra $\mathfrak{g}$.

Representation theory: $G = SU(2)$

- *Defining representation:*[2] This is the rep where the representative matrices are the same as in the group itself.
  - If $G = SU(2)$, then let $V = \mathbb{C}^2$ and define the rep $U : V \to V$ to be $U_g := g$. We often write U for unitary reps.
- We can build new representations by *tensoring* $\otimes$ and *direct summing* $\oplus$. Let's revisit the ferromagnet example and do some rep theory to see what it can do for us!
- Two identically rotating qubits: $V = \mathbb{C}^2 \otimes \mathbb{C}^2$, and the rep is $g \mapsto U_g \otimes U_g$.
- Now, one of the most useful lemmas in the business.

[2] Physicists often call this the fundamental representation. Mathematicians have a slightly wider definition for "fundamental reps" which includes the defining rep.

A powerful lemma

Simultaneous Block-Diagonalization:
Let $U : G \to GL(V)$ a rep of G and $H = H^*$ such that

$$[U_g, H] = 0 \quad \text{for all } g \in G.$$

Then, for any eigenvector $|\psi\rangle$ with eigenvalue λ, $U_g |\psi\rangle$ is also an eigenvector of H with eigenvalue λ.
Proof:

$$H(U_g |\psi\rangle) = U_g H |\psi\rangle = U_g \lambda |\psi\rangle = \lambda(U_g |\psi\rangle).$$

Tensor rep of $G = SU(2)$

- It's pretty easy to see that for all $g \in SU(2)$,

$$[U_g \otimes U_g, \texttt{SWAP}] = 0.$$

$\implies$ Use the lemma! Then, diagonalizing $\texttt{SWAP}$, which acts as $\mathbb{1}$ on the symmetric subspace $\texttt{Sym}$ spanned by $\{|11\rangle, |10\rangle + |01\rangle, |00\rangle\}$ and $-\mathbb{1}$ on the antisymmetric subspace $\texttt{Alt}$ spanned by $\{|10\rangle - |01\rangle\}$, gives a block-diagonal structure for the representative matrices $U_g \otimes U_g$:

$$U_g \otimes U_g = \begin{pmatrix} \multicolumn{3}{c}{\boxed{}} & \begin{matrix} 0 \\ 0 \\ 0 \end{matrix} \\ 0 & 0 & 0 & \Box \end{pmatrix}, \quad g \in SU(2).$$

- These are *invariant subspaces* of the rep space $V = \texttt{Sym} \oplus \texttt{Alt}$. Are they the smallest invariant subspaces, aka *irreducible*?

Reducibility and the Lie algebra

- `Alt` is 1 dimensional, so irreducible.
- Theme: Lie groups are tricky, but their Lie algebras (directional derivatives) are vector spaces and easier to work with.
- *Theorem:* a rep space V is irreducible under a Lie group G if and only if it is irreducible under its Lie algebra $\mathfrak{g}$.
- So, we can work with the directional derivatives, i.e. the Paulis $\mathfrak{su}(2)$. For instance, $e^{itZ} \in SU(2)$, so passing to a representation of $\mathfrak{su}(2)$ on V by taking derivatives,

$$-i\frac{d}{dt}(e^{itZ} \otimes e^{itZ})\Big|_{t=0} = Z \otimes \mathbb{1} + \mathbb{1} \otimes Z.$$

  With these, it will be much easier to see that there's no invariant subspace under the Lie algebra representation.

Angular momentum operators = Lie algebra representation of $\mathfrak{su}(2)$

Work on the basis $\{|11\rangle, |10\rangle + |01\rangle, |00\rangle\}$ of `Sym`:

$$(Z \otimes \mathbb{1} + \mathbb{1} \otimes Z)|11\rangle = -2|11\rangle$$
$$(Z \otimes \mathbb{1} + \mathbb{1} \otimes Z)(|10\rangle + |01\rangle) = 0(|10\rangle + |01\rangle)$$
$$(Z \otimes \mathbb{1} + \mathbb{1} \otimes Z)|00\rangle = 2|00\rangle$$

Define "creation" and "annihilation" operators $\widetilde{\sigma}^{\pm} = \sigma^{\pm} \otimes \mathbb{1} + \mathbb{1} \otimes \sigma^{\pm}$ in the image of this $\mathfrak{su}(2)$ representation where $\sigma^{\pm} = \frac{1}{2}(X \mp iY)$, i.e.

$$|0\rangle \xmapsto{\sigma^{+}\cdot} |1\rangle \xmapsto{\sigma^{+}\cdot} 0, \qquad |1\rangle \xmapsto{\sigma^{-}\cdot} |0\rangle \xmapsto{\sigma^{-}\cdot} 0.$$

No invariant subspace, so `Sym` an irreducible representation!

$$|11\rangle \xmapsto{\tilde{\sigma}^{-}\cdot} \big(|10\rangle + |01\rangle\big) \xmapsto{\tilde{\sigma}^{-}\cdot} 2|00\rangle$$
$$|00\rangle \xmapsto{\tilde{\sigma}^{+}\cdot} \big(|10\rangle + |01\rangle\big) \xmapsto{\tilde{\sigma}^{+}\cdot} 2|11\rangle .$$

The irreducibility payoff

- Back to the ferromagnet: can calculate (using Lie algebra) that the Hamiltonian H has

$$[U_g \otimes U_g, H] = 0.$$

$\implies$ Simultaneous Block-Diagonalization! $V = \texttt{Sym} \oplus \texttt{Alt}$.

- You cleverly calculate for some J that $|00\rangle$ is a ground state of energy λ. But $|00\rangle \in \texttt{Sym}$, and $\texttt{Sym}$ is irreducible, so you immediately know *all* of $\texttt{Sym}$ are ground states!
- "Rotated ferromagnet is still a ferromagnet" $\implies$ Our state labels are irreducible representations of $SU(2)$!

$$\texttt{Sym} \iff \text{ferromagnet}, \qquad \texttt{Alt} \iff \text{antiferromagnet}.$$

What just happened?

- We saw a symmetry in the problem: "rotated ferromagnets are still ferromagnets".
  - In other words, the Heisenberg Hamiltonian H is invariant under this symmetry and by the lemma, the symmetry respects the energy labels.
- The symmetry is realized by the tensor representation $g \mapsto U_g \otimes U_g$ of $G = SU(2)$ on two qubits $V = \mathbb{C}^2 \otimes \mathbb{C}^2$.
- The representation $U_g \otimes U_g$ can be broken into a block-diagonal structure $V = \texttt{Sym} \oplus \texttt{Alt}$, and there is no smaller block-diagonal structure (irreducible).
  - Key was passing from Lie Group G to Lie algebra $\mathfrak{g}$, since linear things are easier.
- Irreducibility cut down number of possible states to explore from 4 dimensions to 2, and "ferro/antiferro" labels happened to coincide with irreducibles.

Just the beginning

- The symmetry program has been one of the most successful programs in science, across quantum field theory, condensed matter, classical machine learning...A key reason is that *symmetry gives block diagonal structures which reduce problems.*
- In QML, the natural extension is to look at symmetry transformations on data spaces which leave labels invariant. This gives inductive biases, which *reduces problems.*
- Exciting evidence: in arXiv:2210.09974[3], it was analytically shown that permutation-equivariant QNNs "do not suffer from barren plateaus, quickly reach overparametrization, and generalize well from small amounts of data".

[3] Schatzki, Larocca, Nguyen, Sauvage, Cerezo 2022 preprint

Just the beginning

- There are many QML tasks (and other quantum algorithms) which possess natural symmetry that is not being exploited: these may make difficult analysis and numerics problems tractable!
- When data has a symmetry (and the algorithm commutes with this symmetry[4]), we have an inductive bias, which may be able to reduce circuit and sample complexities, as well as kill barren plateaus and other trainability hurdles.
- My favorite example: unsupervised learning of ground state quantum phase diagrams for models with more interesting symmetries, like other Lie types $SO(n), Sp(n) \ldots$.

[4] When a function commutes with a symmetry, this is called *equivariance*.