Exploiting Symmetries in Variational QML

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FOR QUANTUM FORMALISM
@JJ_XYZ

Based on arXiv:2205.06217

Exploiting symmetry in variational quantum machine learning

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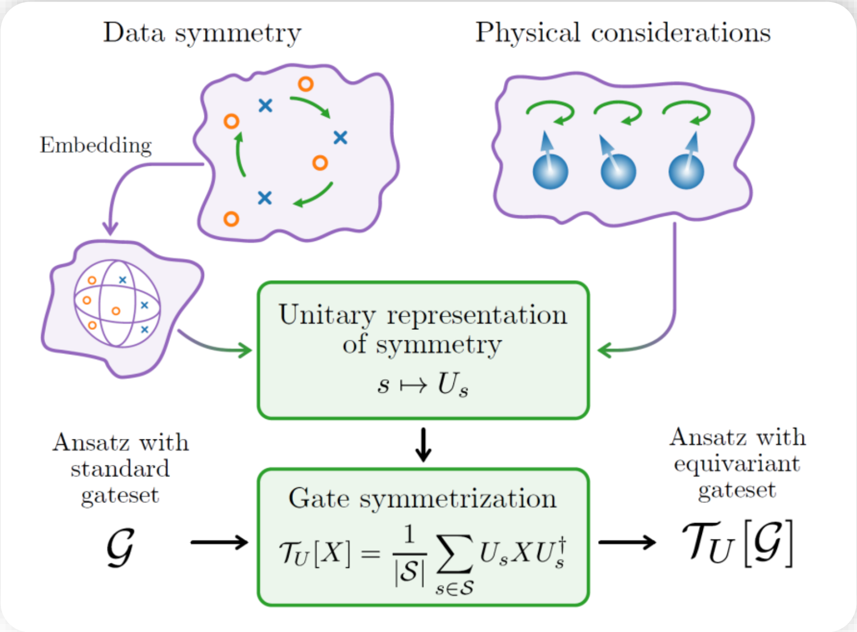
(Dated: May 12, 2022)



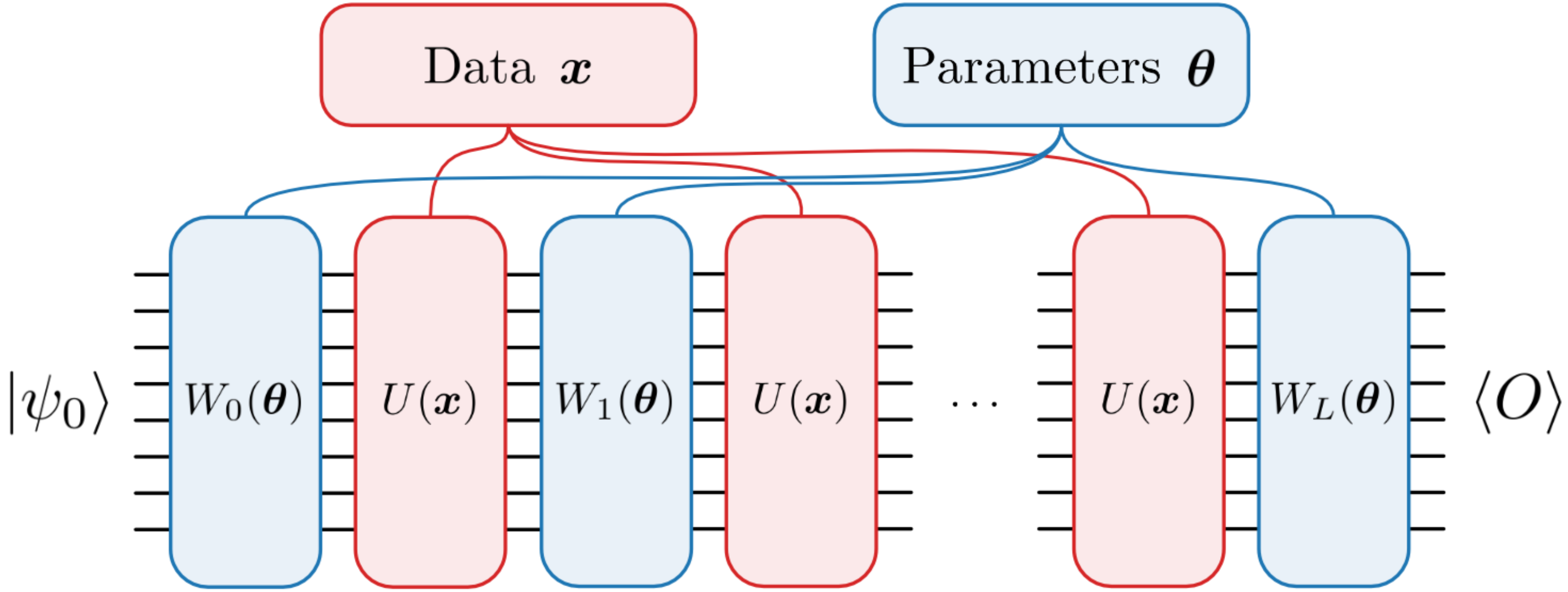





QML for Classical Data

- Classical ML has been extremely useful – can we still improve using quantum models?
- If we want to perform quantum learning on classical data, the data needs to be embedded in a quantum computer
- How to do this in a sensible way is of central importance for QML on classical data
- An embedding needs to be
  - Practical
  - Scalable
  - Useful

Variational Re-Uploading Models



How should we
› design the data embeddings?
› parametrize the trainable layers?

$\longrightarrow$

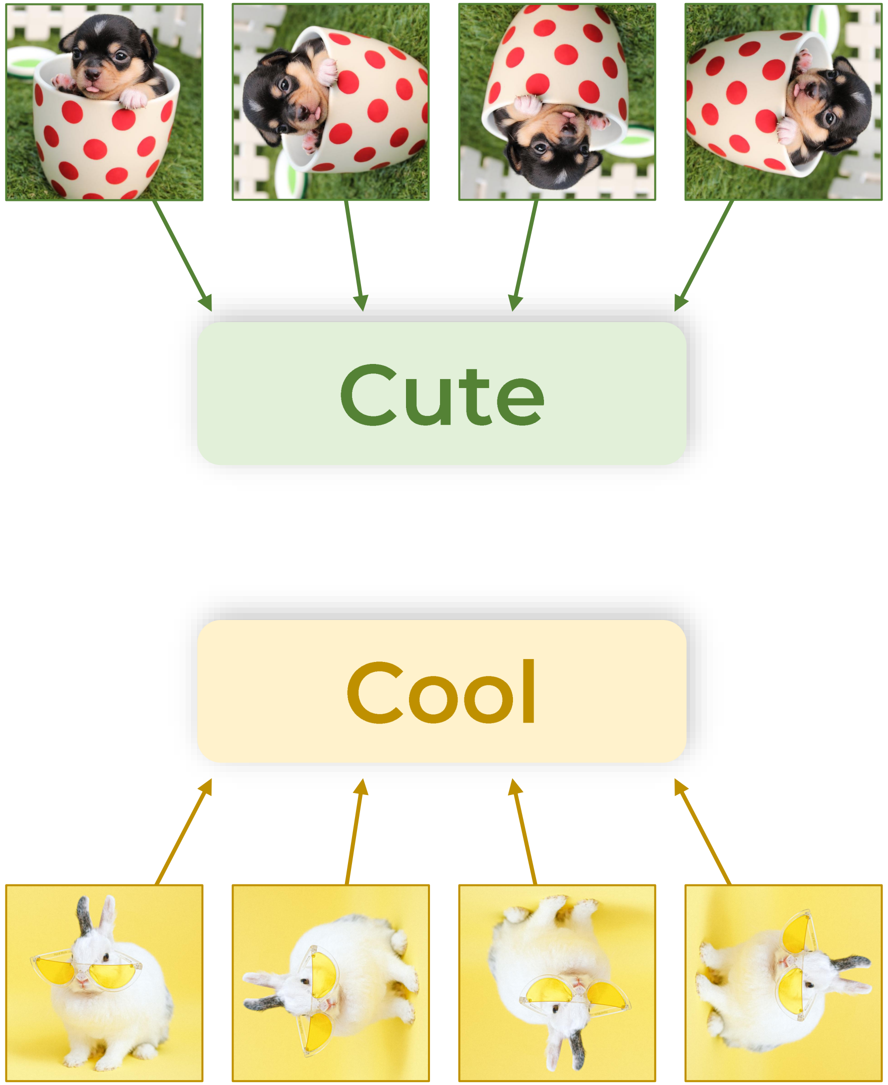
Strong need for **informed** constructions!

The Case for Symmetry

Cute

Cool

The Case for Symmetry



Label invariance under a symmetry group

$$y(V_s[\boldsymbol{x}]) = y(\boldsymbol{x}) \ \forall s \in \mathcal{S}$$

Original **representation**

$$s \mapsto V_s \in \mathbb{R}^{d \times d}$$

Extensively studied in classical machine learning in the field of **Geometric Deep Learning**

Symmetries and Embeddings

Data Embedding

$$U : \mathbb{R}^d \to \mathrm{SU}(2^n)(\simeq \mathbb{C}^{2^n \times 2^n})$$
$$\boldsymbol{x} \mapsto U(\boldsymbol{x})$$

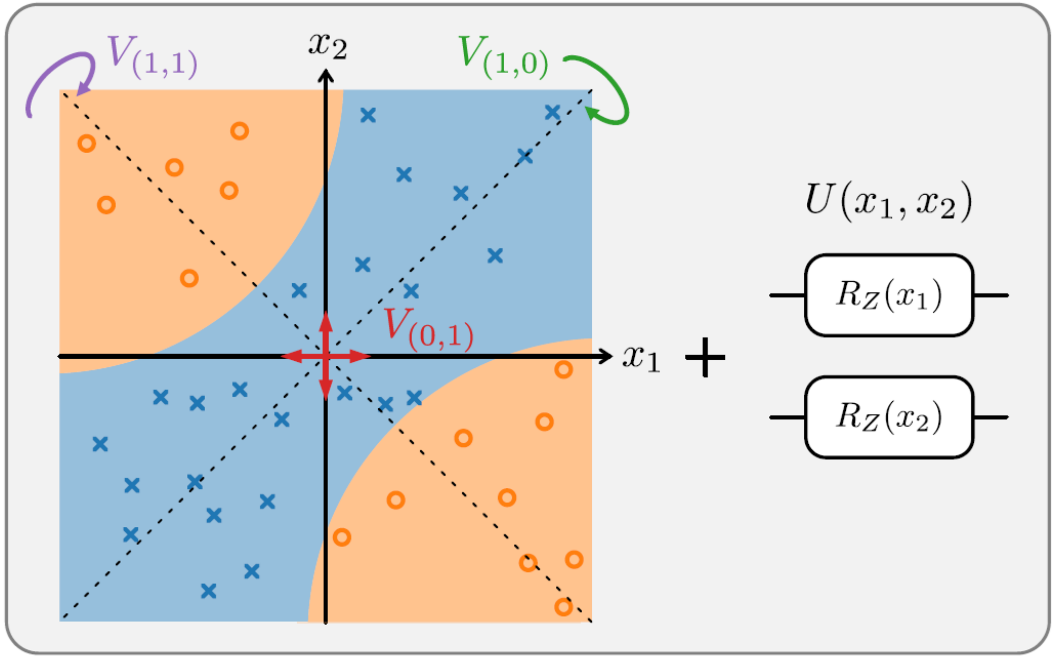
Symmetry

$$V_s : \mathbb{R}^d \to \mathbb{R}^d$$
$$\boldsymbol{x} \mapsto V_s[\boldsymbol{x}]$$

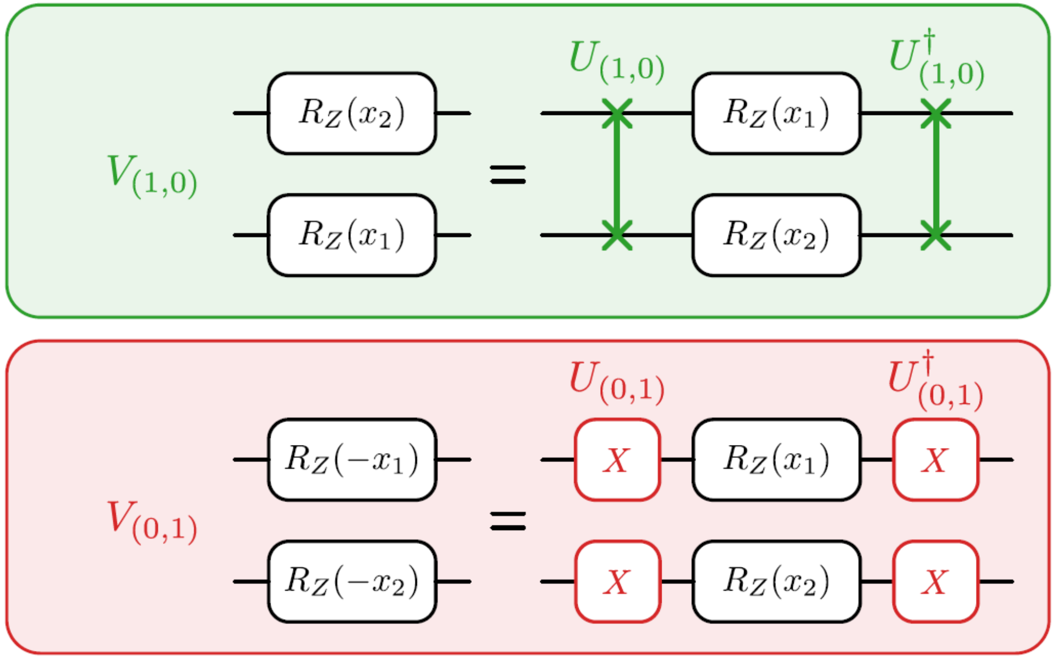
$$\begin{tikzcd} \mathbb{R}^d \arrow[r, "U"] \arrow[d, "V_s"'] & \mathrm{SU}(2^n) \arrow[d, "?"] \\ \mathbb{R}^d \arrow[r, "U"] & \mathrm{SU}(2^n) \end{tikzcd}$$

How do symmetries manifest when data is embedded in a quantum circuit?

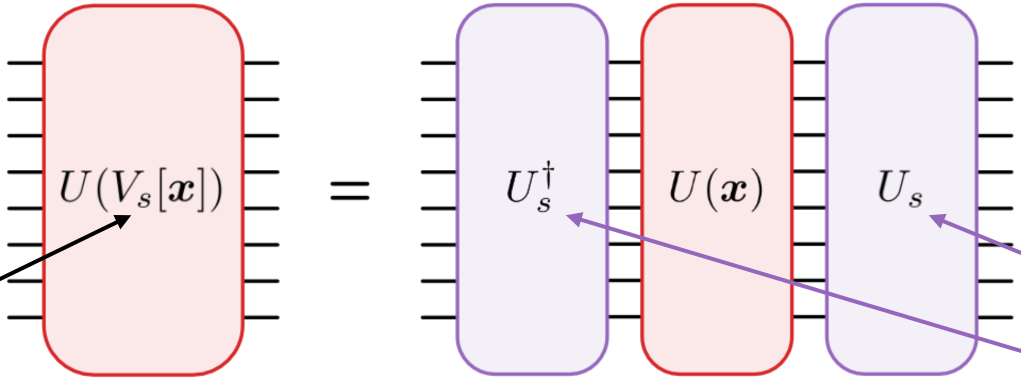
A Toy Example



$\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetric problem + Embedding



Equivariant Embeddings



Original representation

Induced representation

$$\begin{tikzcd}
\mathbb{R}^d \arrow[r, "U"] \arrow[d, "V_s"'] & \mathrm{SU}(2^n) \arrow[d, "\boxed{U_s \cdot U_s^\dagger}"] \\
\mathbb{R}^d \arrow[r, "U"] & \mathrm{SU}(2^n)
\end{tikzcd}$$

Induced Representations

› **Equivariant embeddings induce representations**

› The existence of an induced representation depends on the symmetry group, its representation on the level of the data and on the particular embedding

› For all symmetry groups a trivial embedding exists

$$U(\boldsymbol{x}) = \mathbb{I} \;\Rightarrow\; U_s = \mathbb{I} \text{ for all } s \in \mathcal{S}$$

› Faithful embeddings can only exist for groups that have faithful finite-dimensional unitary representations

Discrete Example

Three coordinates with permutation symmetry

$$\boldsymbol{x} = (x_1, x_2, x_3)$$

Embedding through mutually commuting Paulis

$$U(\boldsymbol{x}) = e^{-ix_1 XX} e^{-ix_2 YY} e^{-ix_3 ZZ}$$

Exchange through generalized Hadamard gates

$$1 \leftrightarrow 2\colon\ H_{XY} = e^{-i\frac{\pi}{2\sqrt{2}}(X+Y)}$$

Continuous Equivariant Embeddings

Data embedding

$$U(\boldsymbol{x}) = e^{-i\boxed{\mathcal{E}(\boldsymbol{x})}}$$

Data embedding into Lie algebra

$$V_s = e^{G_s}$$

Original representation

$$\begin{tikzcd} \mathbb{R}^d \arrow[r, "\mathcal{E}"] \arrow[d, "G_s"'] & \mathfrak{su}(2^n) \arrow[d, "\mathrm{ad}_{H_s}"] \\ \mathbb{R}^d \arrow[r, "\mathcal{E}"] & \mathfrak{su}(2^n) \end{tikzcd}$$

$$\begin{aligned} W_s &= U_s \cdot U_s^\dagger \\ &= \mathrm{Ad}_{U_s} \\ &= e^{\mathrm{ad}_{H_s}} \end{aligned}$$

Induced representation

$$\mathcal{E} G_s = \mathrm{ad}_{H_s} \mathcal{E}$$

Feasibility condition

Continuous Example

3D Vector with O(3) Symmetry

$$\boldsymbol{x} = (x_1, x_2, x_3)$$

$$\mathrm{O}(3) \simeq \boxed{\mathrm{SO}(3)} \rtimes \boxed{\mathbb{Z}_2}$$

Embedding on two qubits

$$U(\boldsymbol{x}) = e^{-i\boxed{(x_1 X + x_2 Y + x_3 Z)} \otimes \boxed{X}}$$

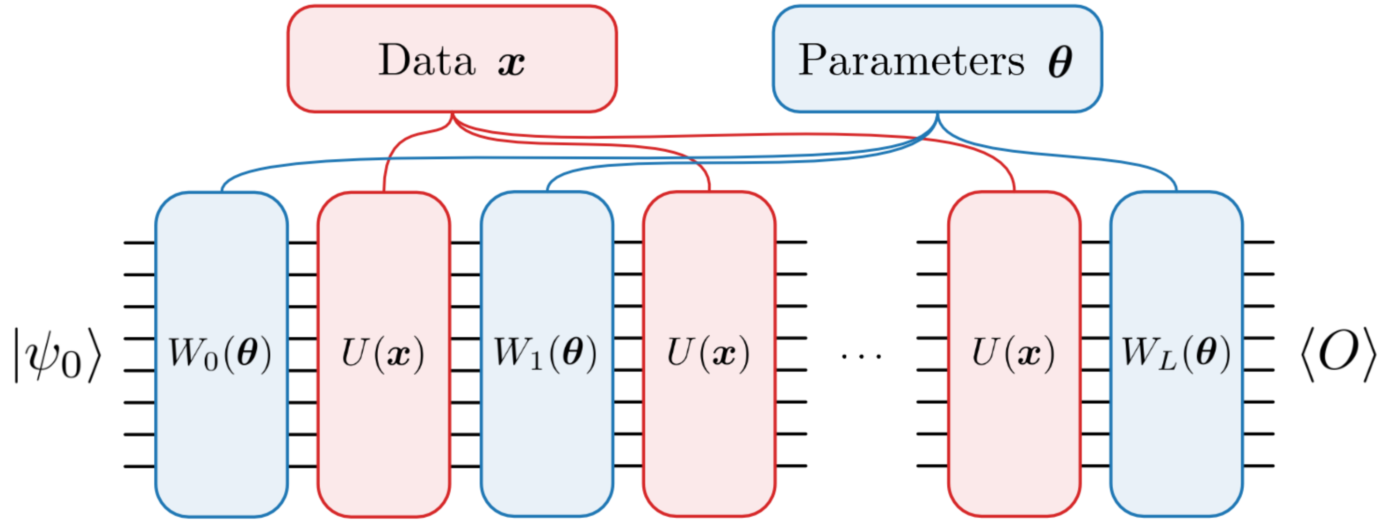
$$\boxed{\mathrm{SO}(3)} \simeq \boxed{\mathrm{SU}(2)}$$

Induced representation

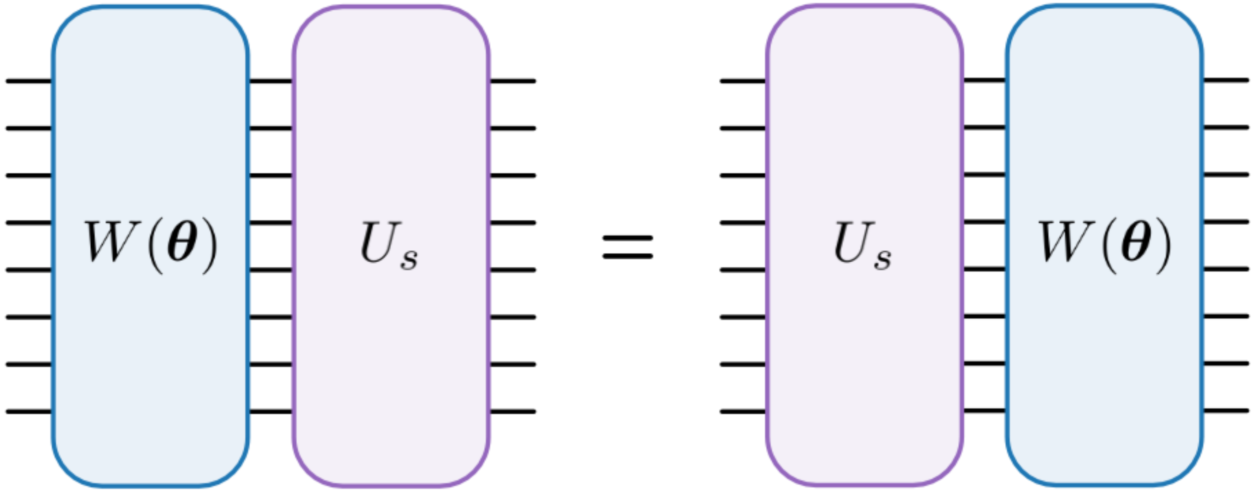
$$I^b \boxed{R_{\boldsymbol{n}}(\alpha)} \leftrightarrow \boxed{R_{\langle \boldsymbol{n}, \boldsymbol{\sigma} \rangle}}(-\alpha) \otimes Z^b$$

Invariant Models

How do we achieve **label invariance** for the whole model?

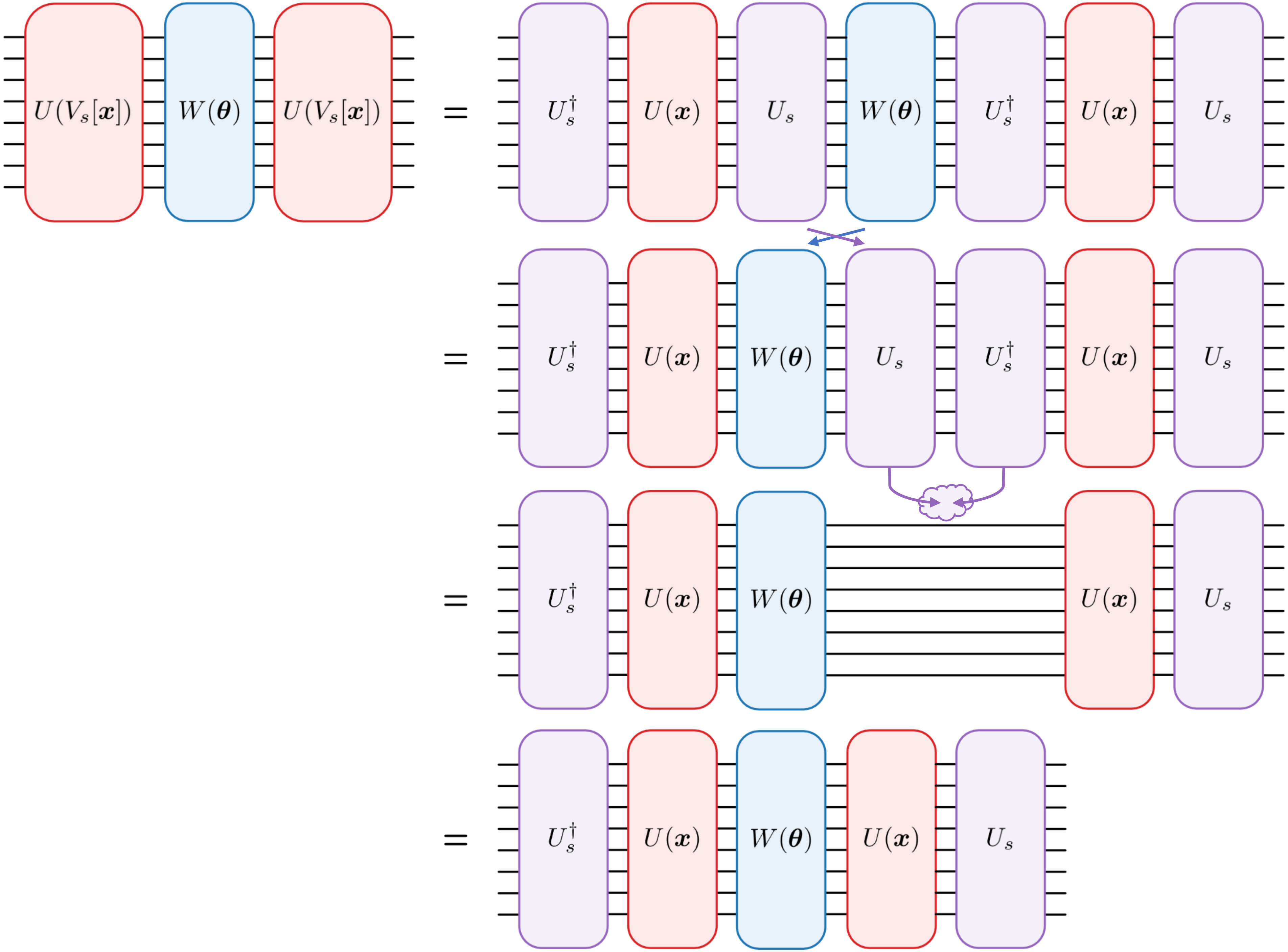


Equivariant Layers



↓

Layers need to **commute** with the induced representation


$U(V_s[\boldsymbol{x}])$
$W(\boldsymbol{\theta})$
$U(V_s[\boldsymbol{x}])$
$=$
$U_s^\dagger$
$U(\boldsymbol{x})$
U_s
$W(\boldsymbol{\theta})$
$U_s^\dagger$
$U(\boldsymbol{x})$
U_s
$=$
$U_s^\dagger$
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$U(\boldsymbol{x})$
U_s
$=$
$U_s^\dagger$
$U(\boldsymbol{x})$
$W(\boldsymbol{\theta})$
$U(\boldsymbol{x})$
U_s

Invariant Model Recipe

$$y(V_s[\boldsymbol{x}]) = y(\boldsymbol{x}) \; \forall s \in \mathcal{S}$$

Invariant input state

$$U_s|\psi_0\rangle = |\psi_0\rangle$$

Equivariant embeddings

$$U(V_s[\boldsymbol{x}]) = U_s^\dagger U(\boldsymbol{x}) U_s$$

Equivariant layers

$$U_s W(\boldsymbol{\theta}) = W(\boldsymbol{\theta}) U_s$$

Invariant observable

$$U_s O U_s^\dagger = O$$

Equivariant Gatesets

How to construct equivariant layers?

↓

Exploit the fact that concatenations of equivariant gates are again equivariant

↓

Motivates **equivariant gatesets**

Regular gateset

$$\mathcal{G} = \{G_1, G_2, \ldots\}$$

↓

Group twirl

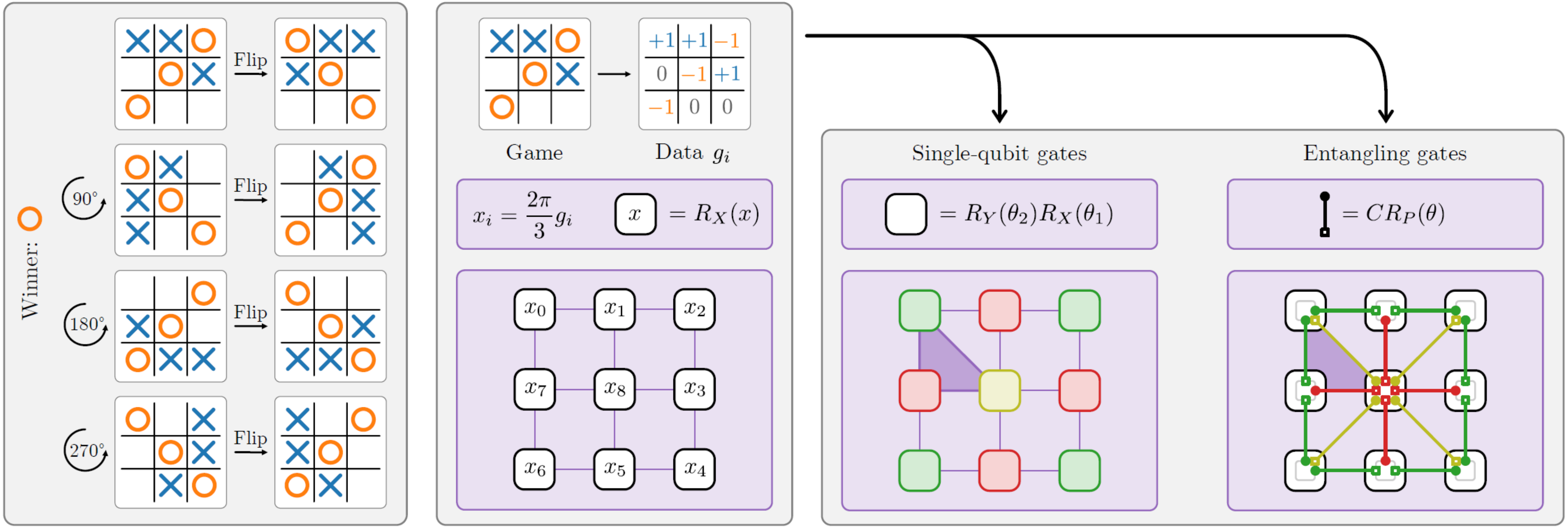
$$\mathcal{T}[G] = \frac{1}{|\mathcal{S}|} \sum_{s \in \mathcal{S}} U_s G U_s^\dagger$$

↓

Equivariant gateset

$$\mathcal{T}[\mathcal{G}] = \{\mathcal{T}[G_1], \mathcal{T}[G_2], \ldots\}$$

Tic Tac Toe



Symmetry

Encoding

Equivariant gateset

Tic Tac Toe

Compare a regular re-uploading model with a symmetrized one

Run sweeps over different depths and randomized architectures

Invariant models have similar performance in training but much better generalization performance

↓

Invariant models generically have **better generalization**

Further Results

- Analysis of different kinds of symmetries, both continuous and discrete
- Discussion of problems that can surface during the construction
- Further numerical experiments showcasing improved generalization
- We show that our techniques can also be applied to VQE and mitigate Barren Plateaus

Summary

› We need **informed choices** for parametrizations of variational quantum learning models

› **Label invariance** under a symmetry group provides such information

› We show **if and how** such information can be used to produce invariant quantum learning models

› The resulting models have less parameters and numerical experiments confirm their **better generalization**

Some Open Questions

- Are variational re-uploading models a reasonable choice for data embedding and prediction?
- What other kinds of data embeddings would be reasonable?
- Is QML for classical data a good idea in the first place? Why would embedding into the unitary group be good for classical ML tasks?

Thank you for your attention!

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