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Exploiting Symmetry in Variational QML

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Exploiting symmetry in variational quantum machine learning

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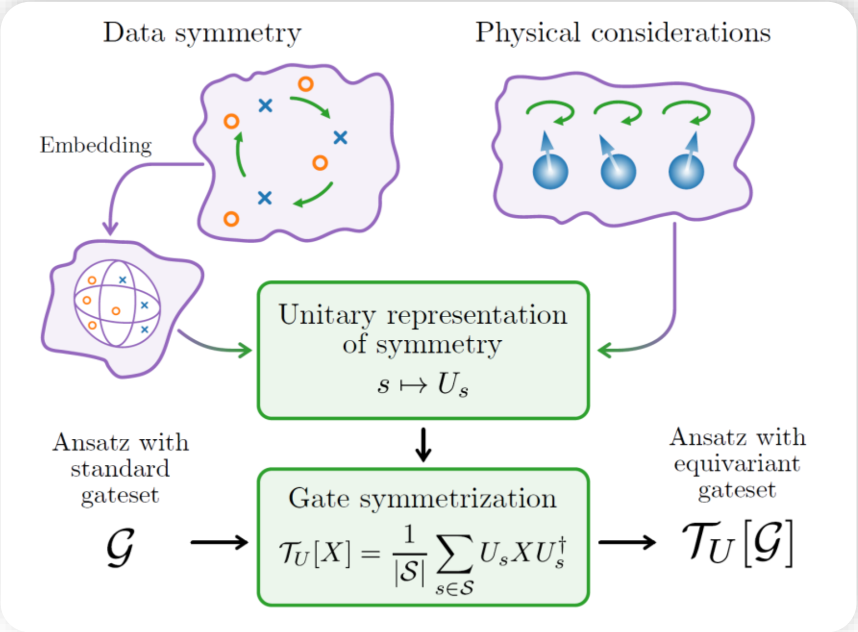
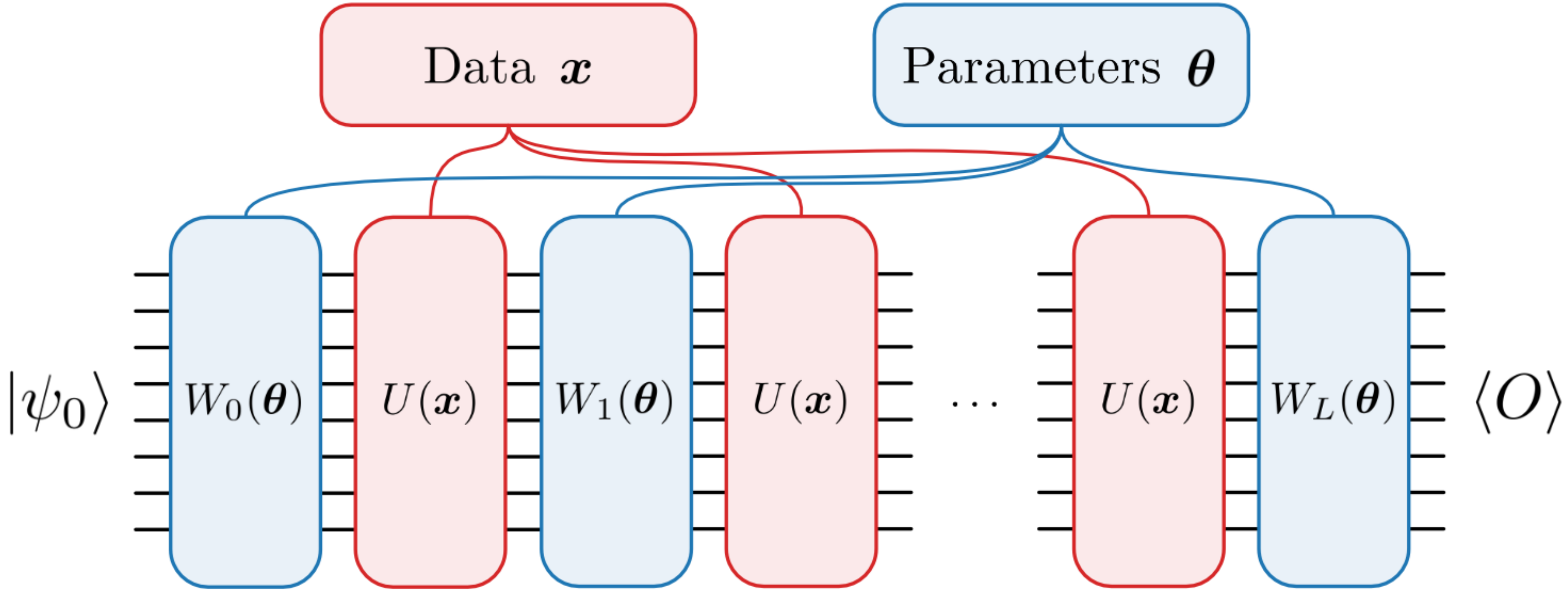







Variational Learning Models



How should we
- × design the data embeddings?
- × parametrize the trainable layers?

$\longrightarrow$

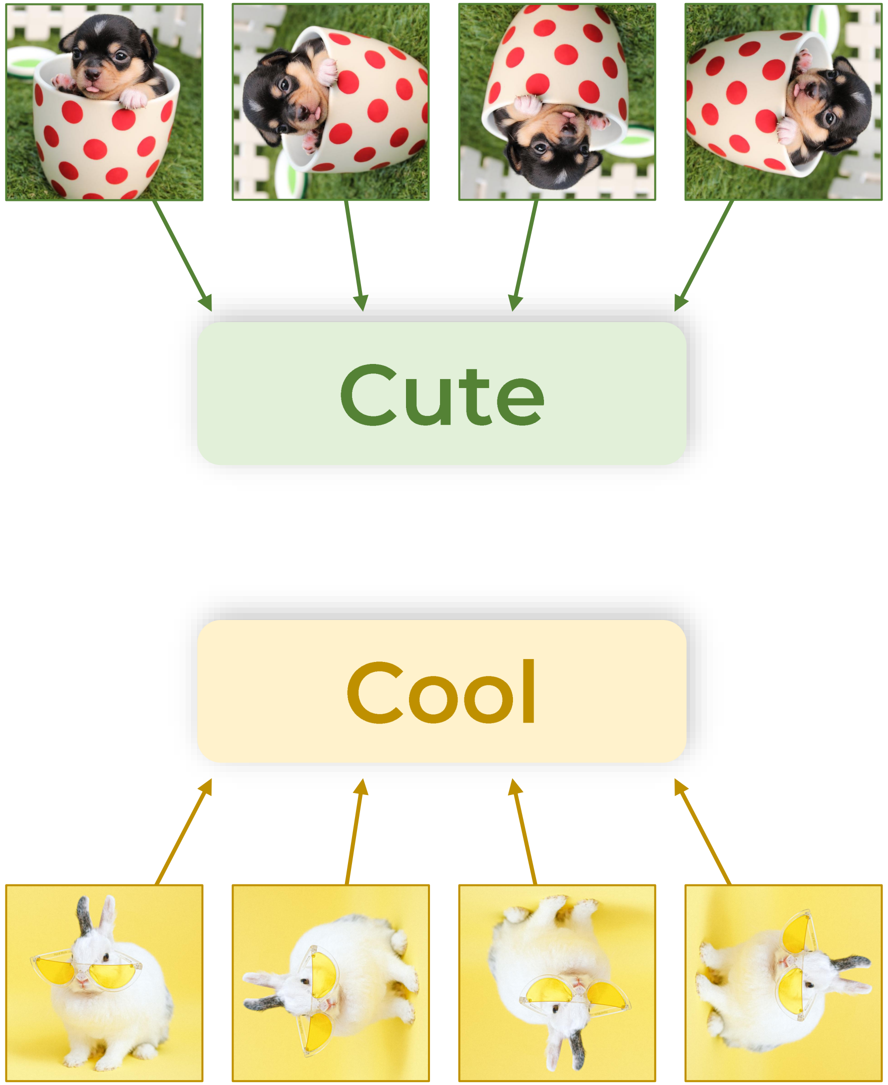
Strong need for **informed** constructions!

The Case for Symmetry

Cute

Cool

The Case for Symmetry



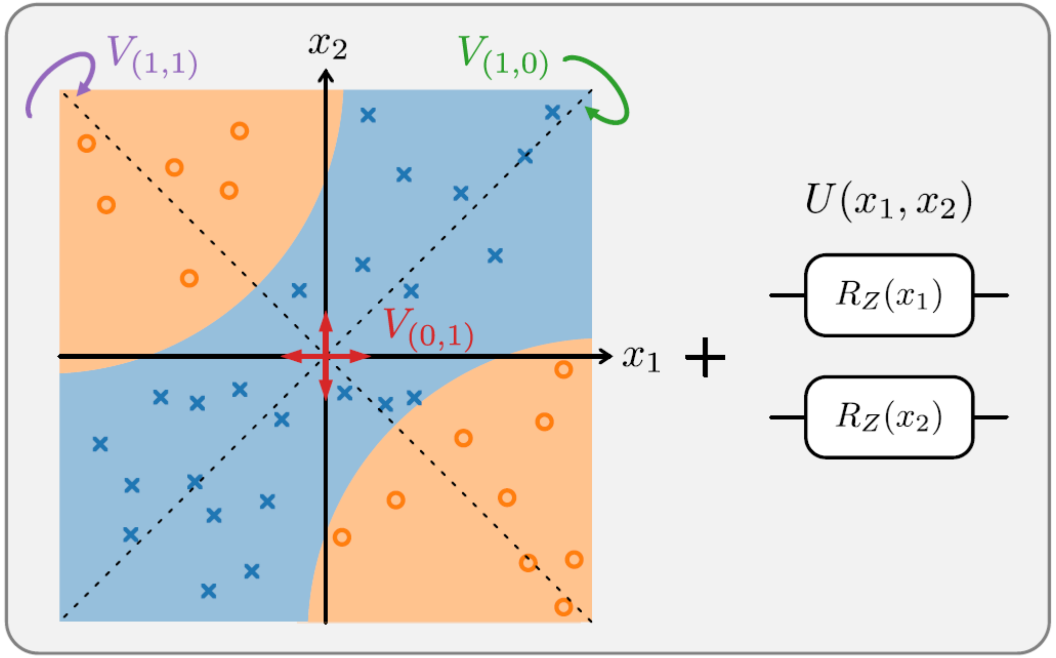
Label invariance under
a symmetry group

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

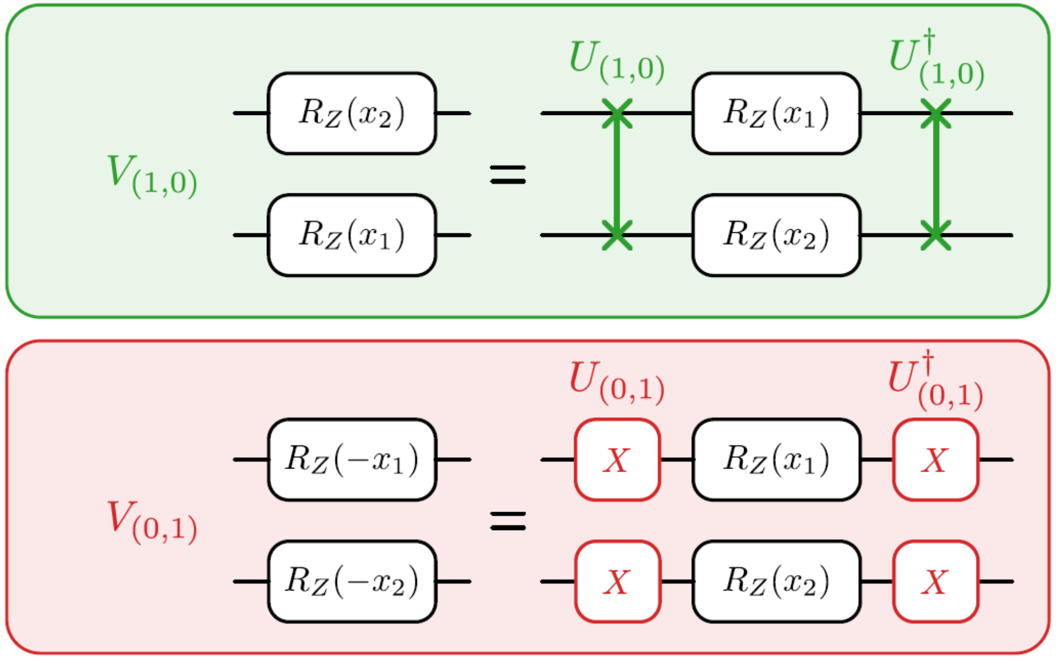
Extensively studied in classical machine learning in the field of **Geometric Deep Learning**

Symmetries and Embeddings

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

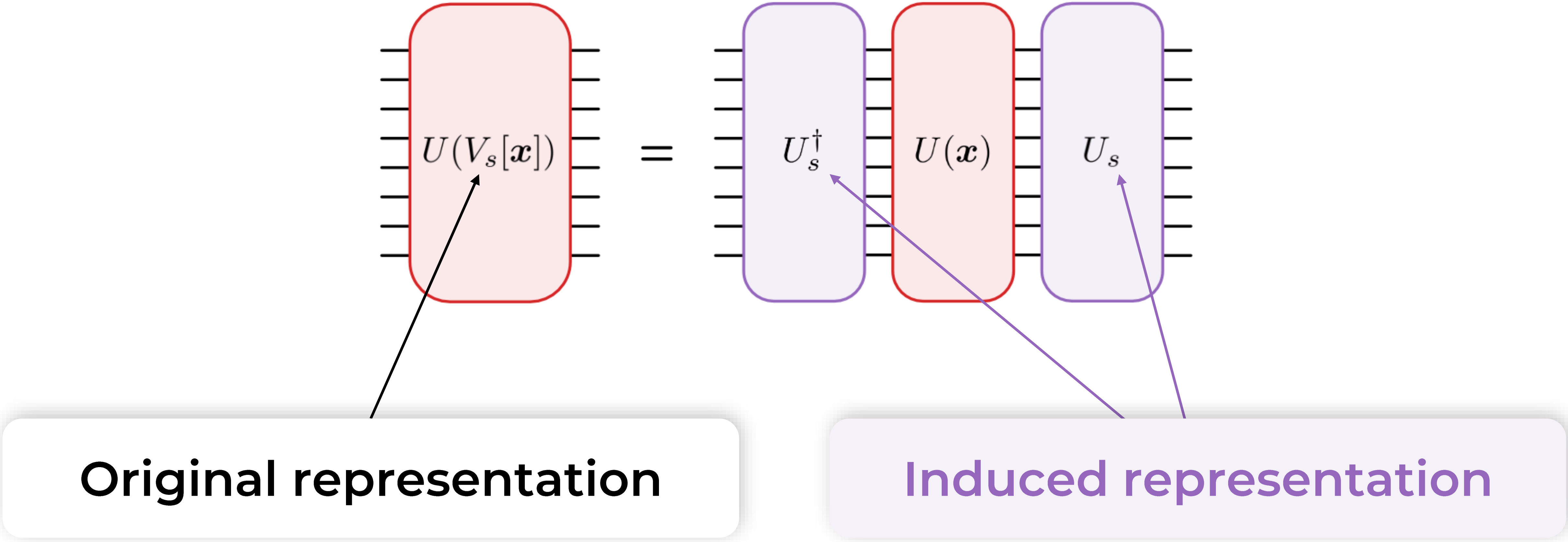


$\mathbb{Z}_2 \times \mathbb{Z}_2$ symmetric problem + Embedding

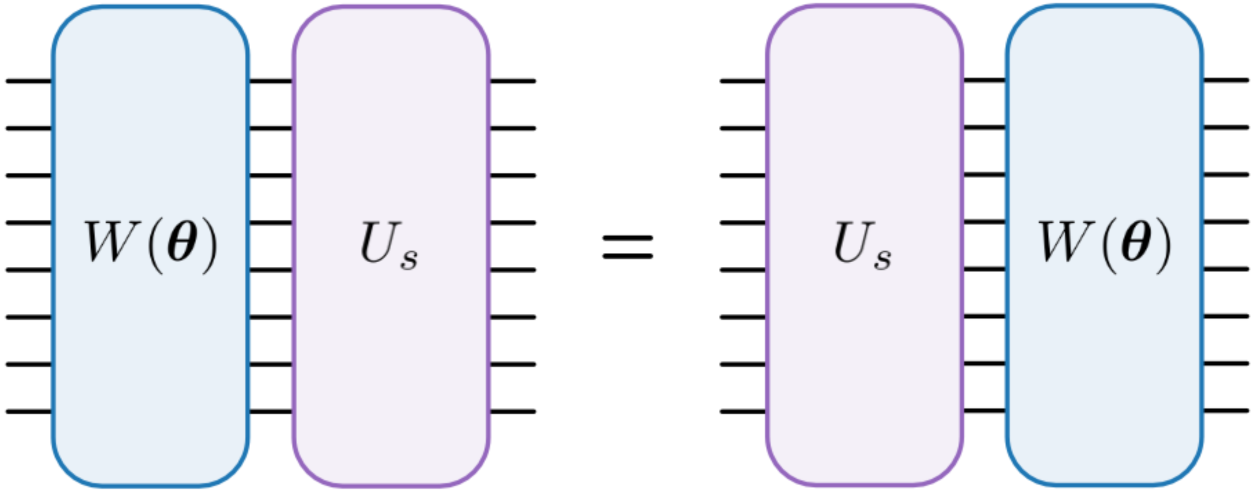


Induced representation

Equivariant Embeddings

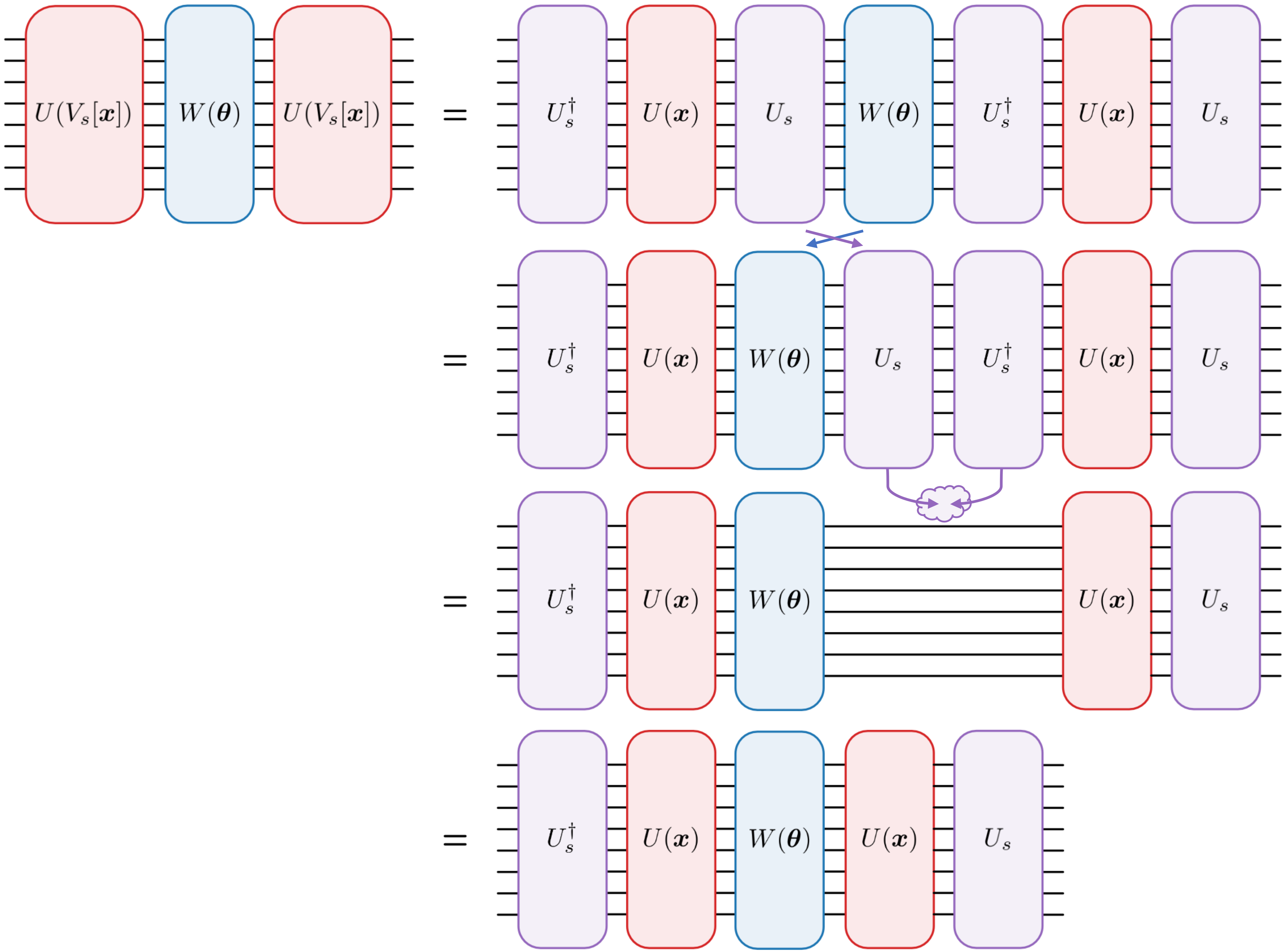


Equivariant Layers



↓

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

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

$\longrightarrow$

Equivariant embeddings

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

Equivariant layers

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

$\longrightarrow$

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

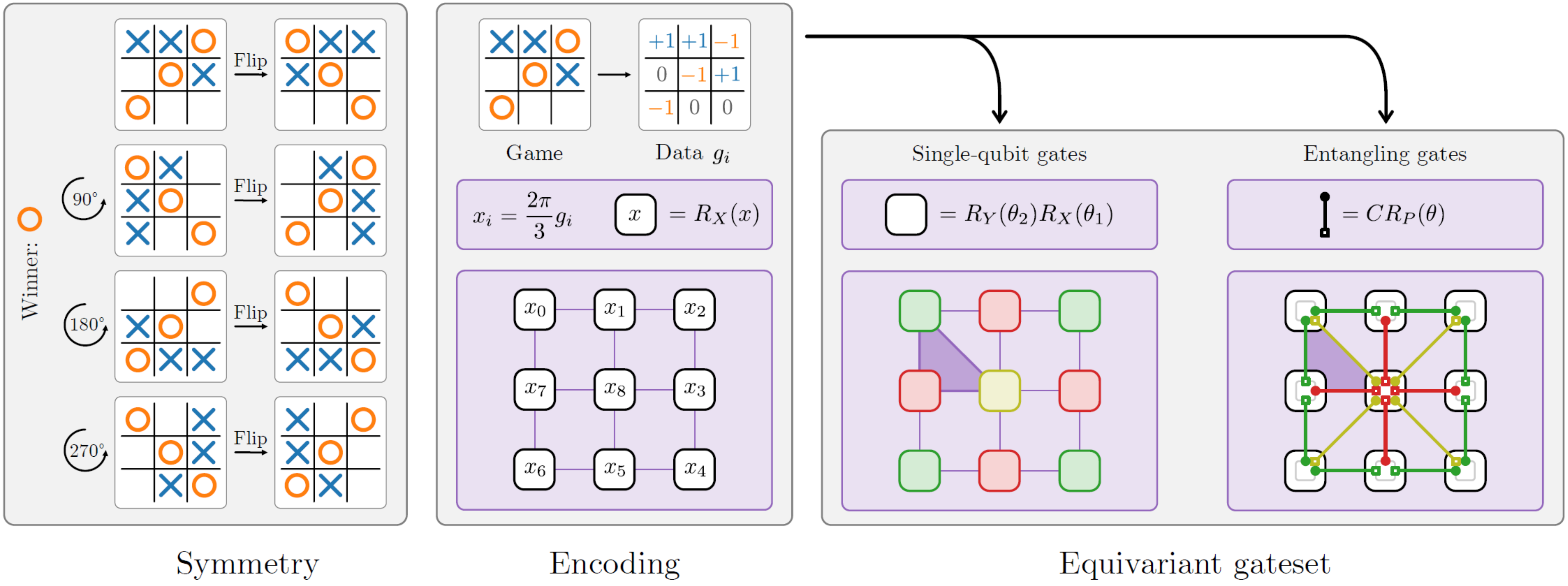
$$\mathcal{T}[G] = \frac{1}{|\mathcal{S}|}\sum_{s\in\mathcal{S}} U_s G U_s^\dagger$$

↓

Equivariant gateset

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

Tic Tac Toe



Winner:
Flip
90°
180°
270°
Game
Data g_i
+1 +1 −1
0 −1 +1
−1 0 0
$x_i = \frac{2\pi}{3} g_i$
$= R_X(x)$
x_0 x_1 x_2
x_7 x_8 x_3
x_6 x_5 x_4
Single-qubit gates
$= R_Y(\theta_2)R_X(\theta_1)$
Entangling gates
$= CR_P(\theta)$
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**

Thank you for your attention!

Slides

Paper

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