Improving Equivariant Networks with Probabilistic Symmetry Breaking

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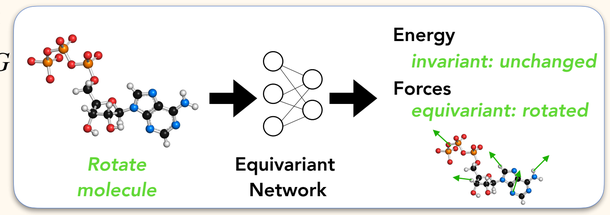
Background: Symmetries in ML

Equivariance:

$f : X \to Y, g \in G$

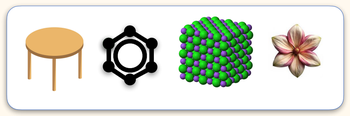
$f(gx) = gf(x)$

Benefits in generalization, sample complexity



Equivariant functions can't break symmetries…

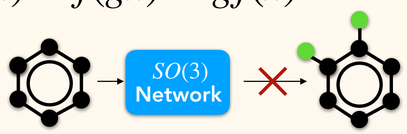
Many objects are themselves inherently symmetric:



Equivariance preserves data symmetries: for all group elements g,

$$x = gx \to f(x) = f(gx) = gf(x)$$

This is restrictive: an equivariant network can't turn a symmetric input into an asymmetric output



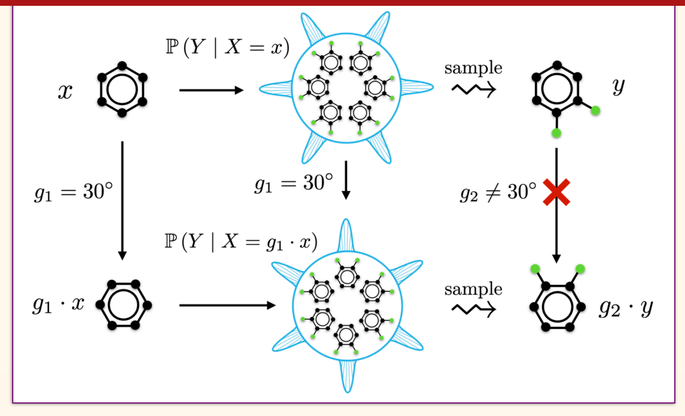
But: retaining the inductive bias of equivariance on asymmetric inputs is still desirable.

	Generalization benefits	Can break symmetries
Non-equivariant model	✗	✓
Equivariant model	✓	✗
Symmetry-breaking (goal)	✓	✓

How do we achieve this? First, observe that any of these outputs is equally good:

Suggests: learn a map to equivariant *distributions* $f : X \to \mathcal{P}(Y)$, such that individual samples from $f(x)$ can break the symmetry of x

Equivariant distributions can break symmetries



Equivariant networks **can't break symmetries**, which is **problematic for generative models**. We use symmetry-breaking positional encodings to ***minimally*** **break symmetry**.

Probabilistic Representation Theorem

***How can we learn* equivariant distributions?**

→ **requires a source of randomness ("noise outsourcing", e.g. [2])**

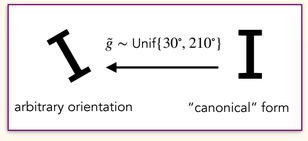
Theorem: $Y \,|\, X$ is equivariant iff, for some $f : X \times G \times (0,1) \to Y$ jointly equivariant in X and g (i.e. $f(hx, hg, \epsilon) = hf(x, g, \epsilon)$), $\epsilon \sim \text{Unif}(0,1)$, and $\tilde{g} \,|\, X$ as defined below,

$$Y \overset{a.s.}{=} f(X, \tilde{g}, \epsilon)$$

Asymmetric output · *Symmetric input* · *"Equivariant randomness" to break symmetries* · *"Arbitrary randomness"*

$\tilde{g}$ should have as little randomness as possible to distinguish among the symmetrically equivalent outputs, e.g.

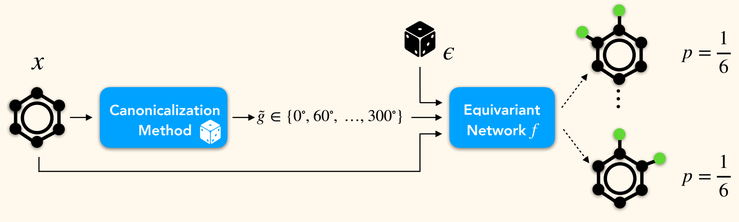
Canonicalization conveniently provides this randomness



Generalization to "noise injection": can let $\tilde{g}$ more generally be a random variable with no self-symmetries and $\tilde{g} \,|\, X \sim h\tilde{g} \,|\, hX$

→ Sometimes easier to compute, e.g. to avoid solving graph automorphism! Also, applies to [3]

Symmetry-Breaking Positional Encodings



To make an equivariant network f break symmetries, we use canonicalization to sample a random $\tilde{g}$ and add it as input

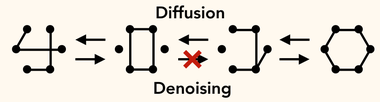
Algorithm 1 SymPE: Symmetry-Breaking Positional Encodings

Inputs: input $x \in \mathcal{X}$
Learnable parameters: learned vector $v \in \mathcal{V}$, equivariant neural network parameters θ, canonicalization parameters ϕ
Sample $\tilde{g} \sim h_\phi(x)$ ▷ Sample group element for canonicalization
$\tilde{v} \leftarrow \tilde{g}v$ ▷ Apply group element to learned vector
Return $f_\theta(x \oplus \tilde{v})$ ▷ Forward pass with positional encoding

Experiments

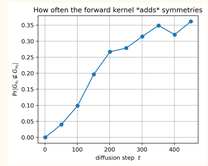
Graph Generation with Diffusion Models

Problem: Noising process is likely to introduce symmetries that cannot be denoised



Experiment: DiGress discrete diffusion with graph transformer, using SymPE with sorting canonicalization to break symmetries

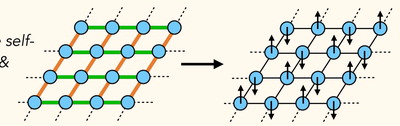
Method	NLL
DiGress	129.7
DiGress + noise	126.5
DiGress + SymPE	30.3

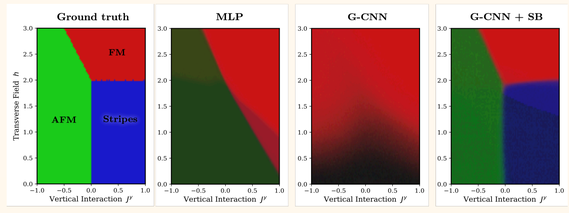


Ising Model

Task: Given vertical and horizontal interaction strengths (J_x, J_y), output a configuration (up or down spin for each node in the grid graph) of minimal energy

Interaction strengths have self-symmetry: reflections & translations · *Energy function has symmetry: rotations, translations, and reflections*

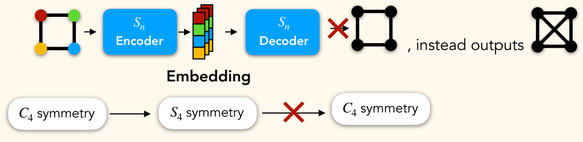




Phase of predicted ground states. Green: antiferromagnetic, Red: ferromagnetic, Blue: Stripes, Black: No order.

Graph Autoencoder

Problem: An S_n-equivariant encoder with per-node embeddings can spuriously introduce extra symmetry, which an S_n-equivariant decoder cannot break.



Solution: Break symmetries via sorting a learned scalar embedding per-node, where sorting breaks ties

Experiment: Erdös-Renyi random graphs from [4] with GNN auto encoder architecture

Method	% Correct Edges
No symmetry-breaking	3.9
Noise (randomly initialized node features)	2.3
Randomly permuting instead of sorting	1.3
Passing in Laplacian encodings directly (no sorting)	0.98
Our method: sorting learned embeddings	0.77

References

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