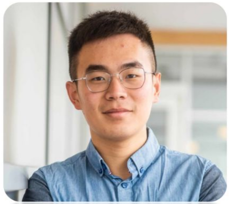
Approximately Equivariant Networks for Imperfectly Symmetric Dynamics



Rui Wang*
UC San Diego

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Northeastern University

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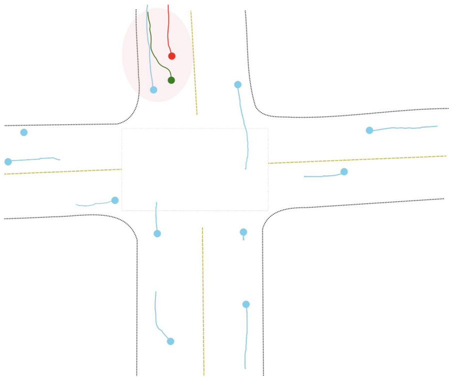
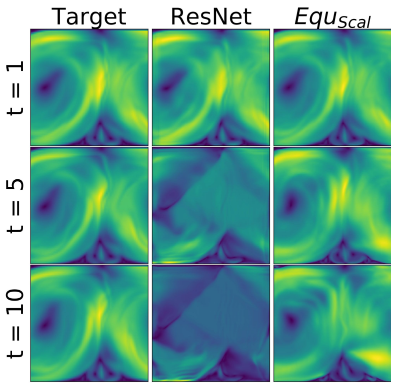
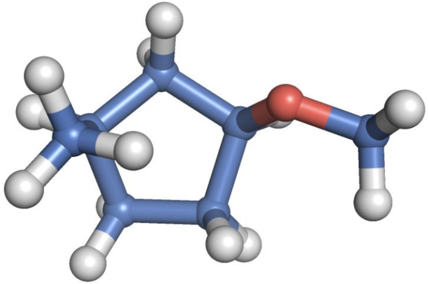
International Conference on Machine Learning (ICML) 2022

Symmetry and Equivariant Networks

➔ **Success of Equivariant Networks:**

Cohen & Welling. (2016); Ravanbakhsh et al. (2017); Konder & Trivedi (2018); Walters et al.(2021); Wang et al.(2021); Shi et al.(2021)



Why Do We Need Symmetry?

Incorporate symmetry as inductive bias into models

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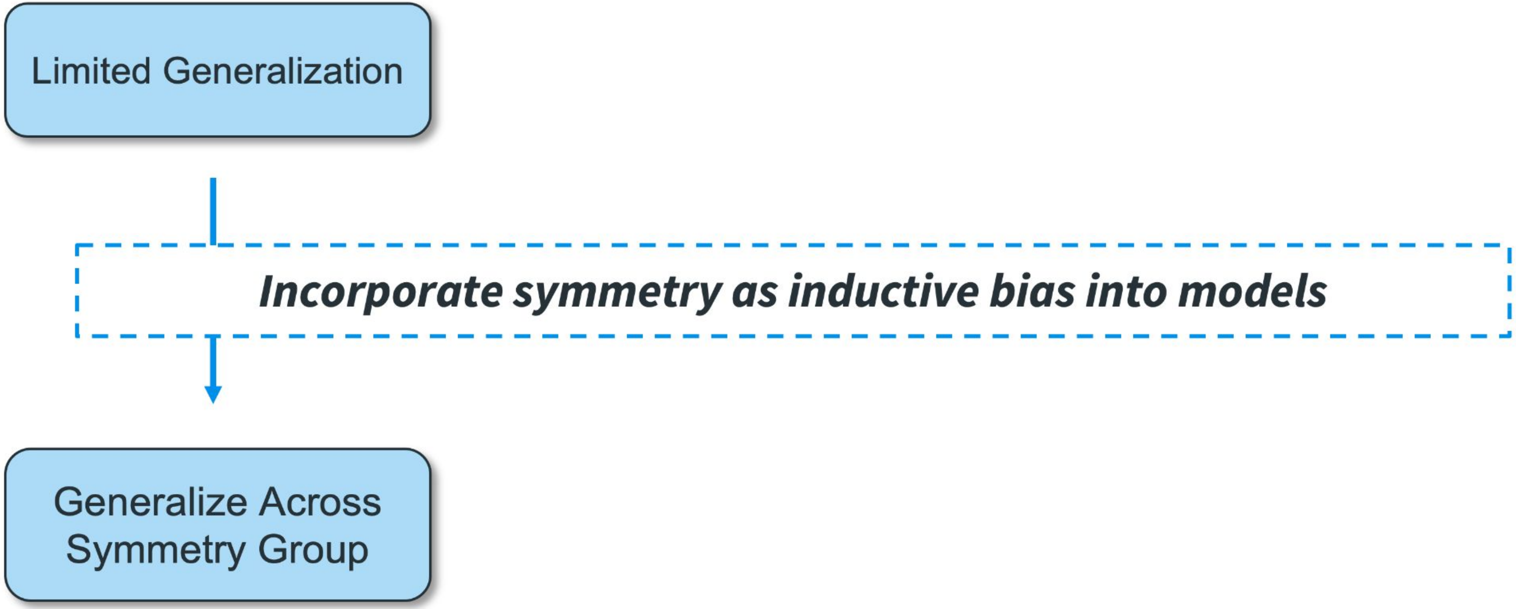

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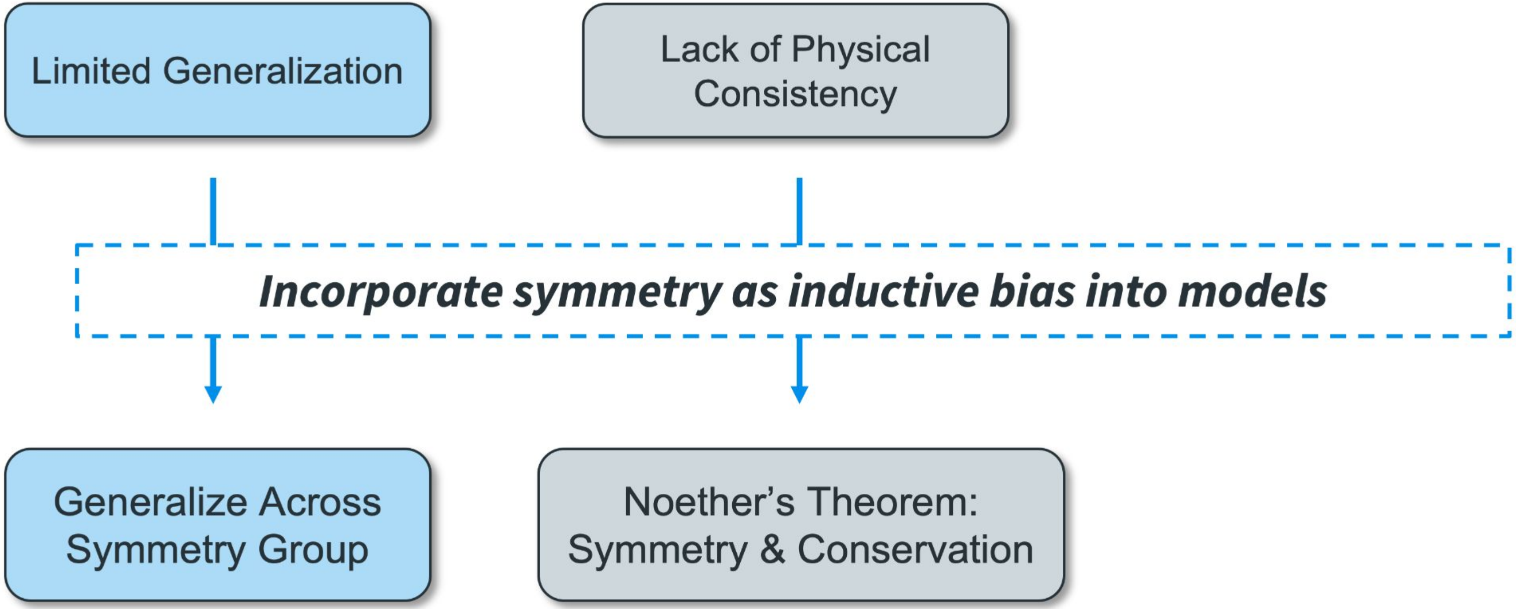

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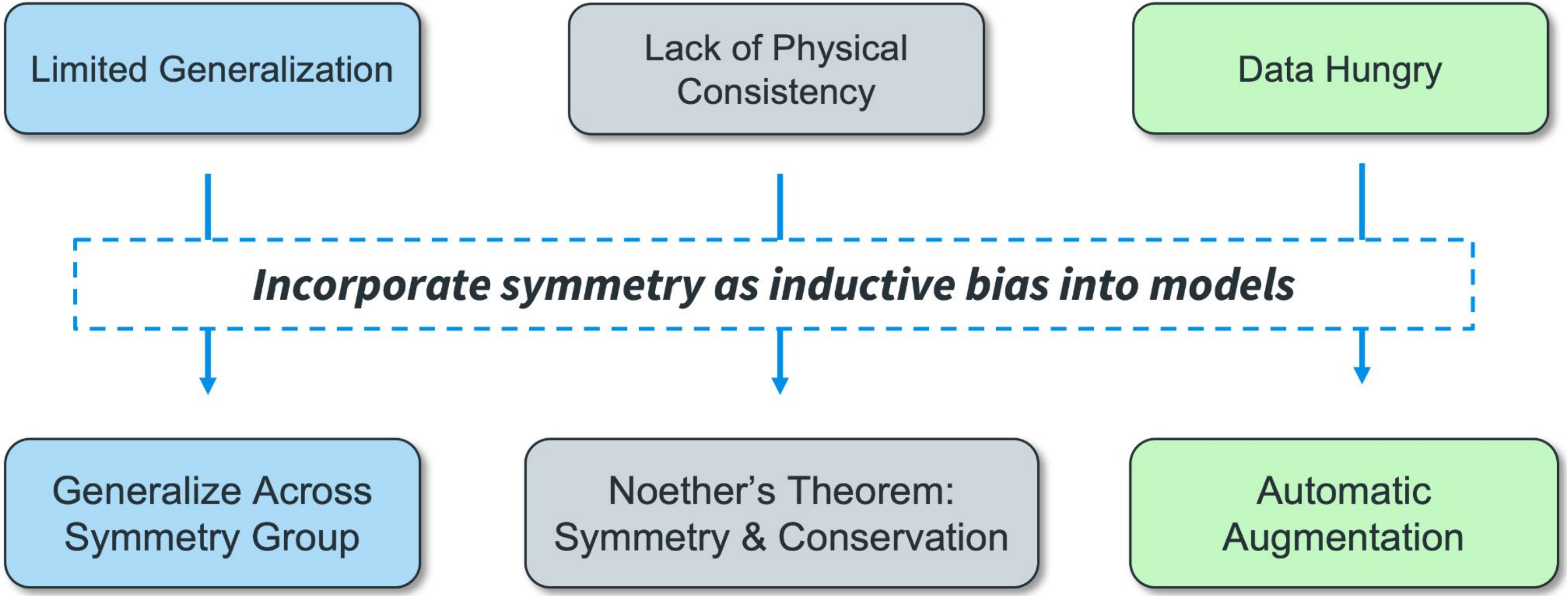

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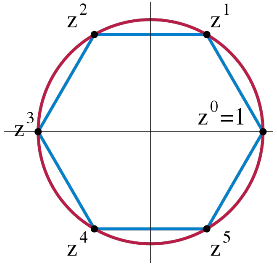

✓ **Group**: A set G with an associative binary operation

$$\circ : G \times G \to G; \qquad 1 \in G; \qquad \forall g \in G, \exists g^{-1} \in G.$$

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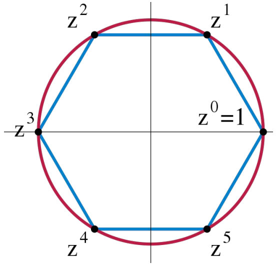
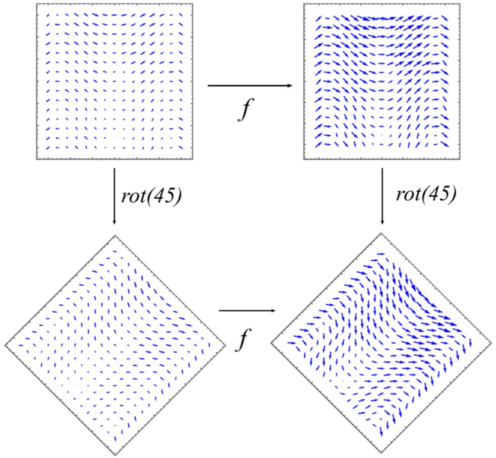


✓ **Equivariance:** a function $f : X \to Y$ and a group G, ρ_{in} acts on X and ρ_{out} acts on Y

G-**equivariant**: $f(\rho_{in}(g)x) = \rho_{out}(g)f(x)$



But Real-World Data Rarely Conforms to Strict Symmetry

G**-approx-equiv**: $|f(\rho_{in}(g)x) - \rho_{out}(g)f(x)| < \varepsilon$

➔ Even if the governing equations are symmetric, varying external forces, boundary conditions, or noisy data may break symmetry.

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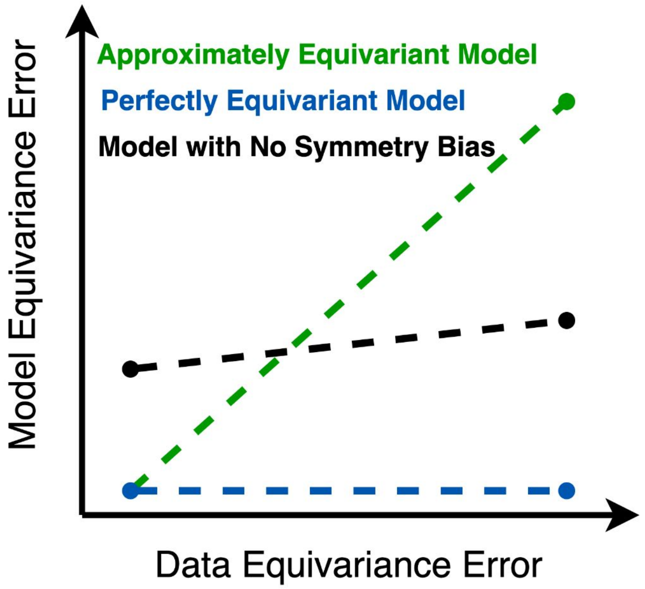

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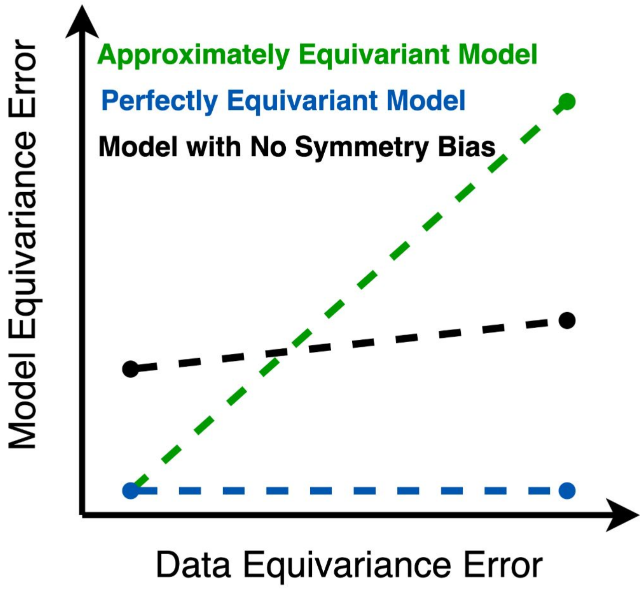

- Ideal models should **automatically** learn the **correct amount of symmetry**.

Strict Equivariance → Approximate Equivariance

Relaxing weight-sharing constraints in Equivariant Networks by

introducing group element dependent parameters

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❖ **Group Convolution**

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Relaxing weight-sharing constraints in Equivariant Networks by

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❖ **Relaxed Group Convolution**

$$[f \star_G \Psi](g) = \sum_{h \in G} f(h)\Psi(g^{-1}h) \longrightarrow [f \tilde{\star}_G \Psi](g) = \sum_{h \in G} \sum_{l=1}^{L} f(h) \boxed{w_l(h)} \Psi_l(g^{-1}h)$$

Strict Equivariance → Approximate Equivariance

- **Steerable Convolution** $\Phi(hx) = \rho_{\text{out}}(h)\Phi(x)\rho_{\text{in}}(h^{-1}), \ \forall h \in H$

$$\sum_{\mathbf{y}\in\mathbb{Z}^2} \sum_{l=1}^{L} (w_l \odot \Phi_l(\mathbf{y})) f_{\text{in}}(\mathbf{x}+\mathbf{y})$$

$$w \in \mathbb{R}^{c_{\text{out}} \times c_{\text{in}} \times L}$$

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$$w \in \mathbb{R}^{c_{\text{out}} \times c_{\text{in}} \times L} \qquad w : K^2 \to \mathbb{R}^{c_{\text{out}} \times c_{\text{in}} \times L}$$

Strict Equivariance → Approximate Equivariance

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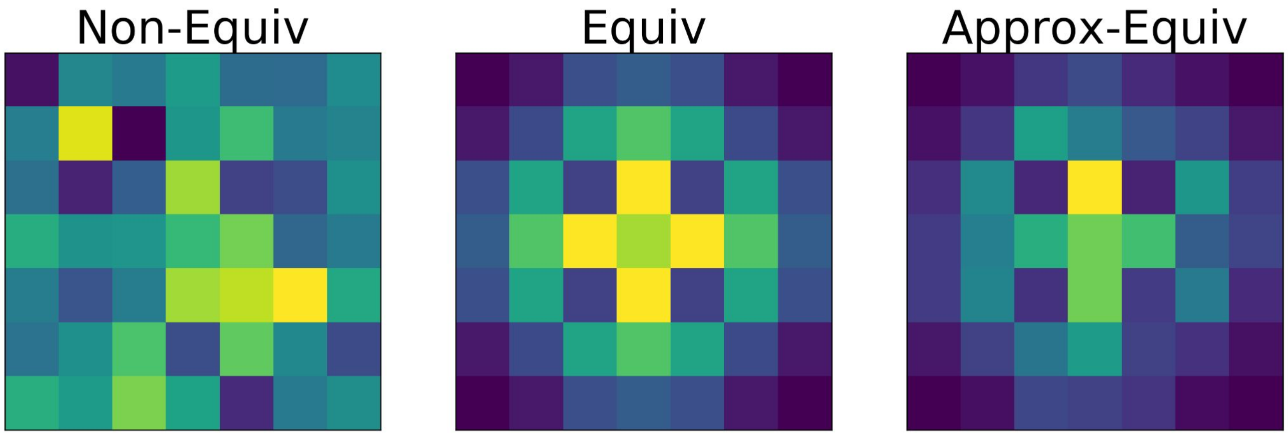

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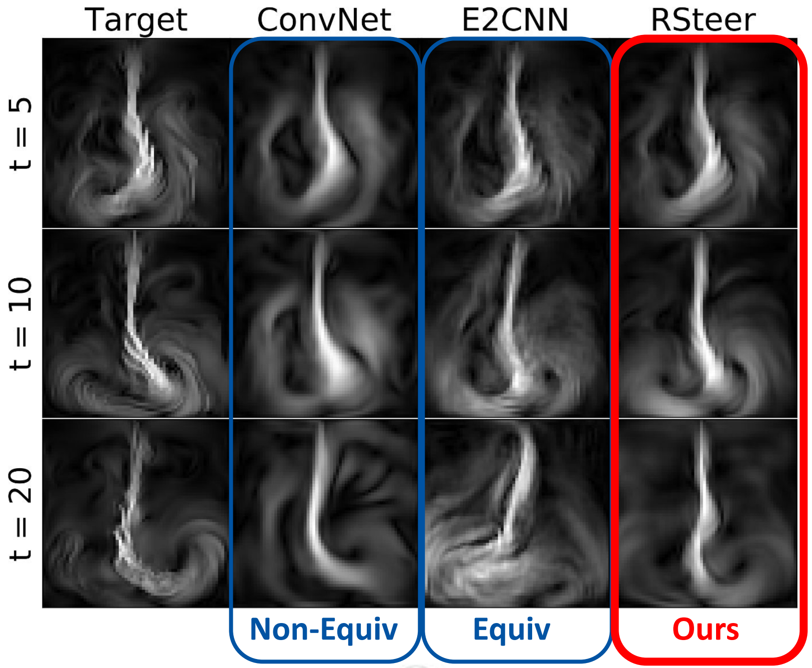
Improved Prediction on Fluid Dynamics

The buoyant force varies with the inflow positions to break the **rotation** symmetry



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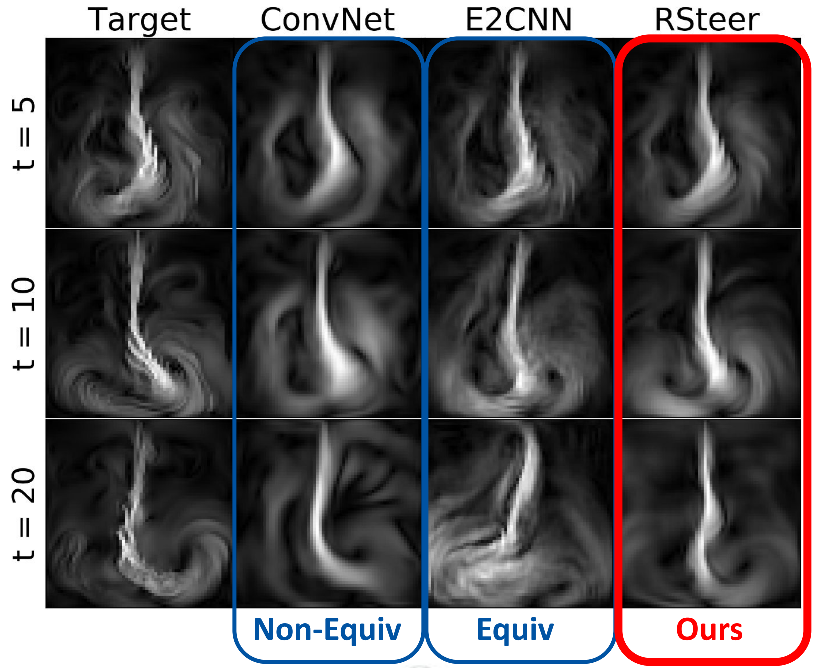
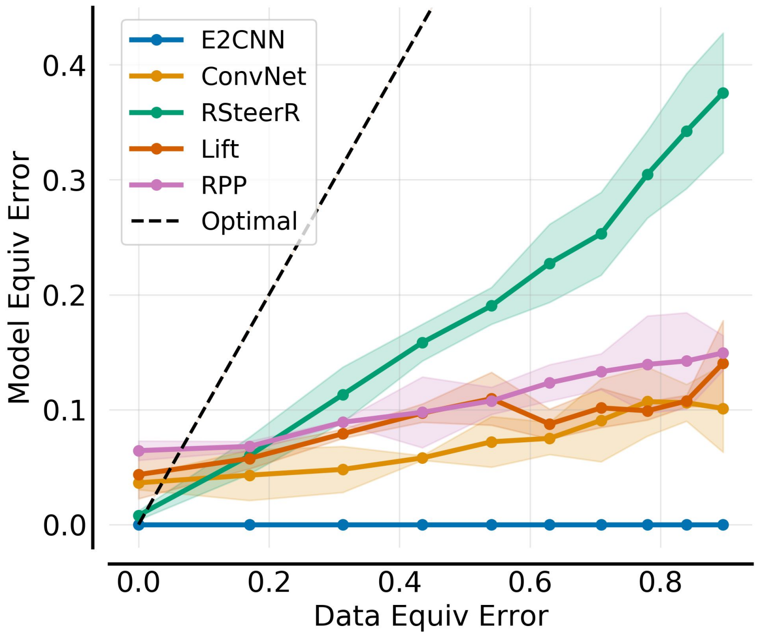


Learning Different Levels of Equivariance



Conclusion

- We propose new classes of **approximately equivariant** networks by **relaxing the weight-sharing schemes**.
- Our proposed networks **outperform** models with no symmetry bias or with overly strict symmetry constraints on **both simulations and real-world data**.
- Future work includes applying our work to graph neural networks, theoretical analysis and designing approx-equiv tensor field networks.

Thanks for Listening !

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https://github.com/Rose-STL-Lab/Approximately-Equivariant-Nets