# Approximate Equivariance and Generalization

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Boston Symmetry Day

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Northeastern University

$$f(g(x)) = g(f(x))$$

# G-Equivariance

$$\begin{tikzcd} L(X_1) \arrow[r, "\mathbb{T}_g"] \arrow[d, "\phi"] & L(X_1) \arrow[d, "\phi"] \\ L(X_2) \arrow[r, "\mathbb{T}'_g"] & L(X_2) \end{tikzcd}$$

A note on the title
(let's see if we can get to displacement structures!).

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- Real world symmetries are rarely exact
- Not to be confused with partial symmetries.

# Approximate Equivariance

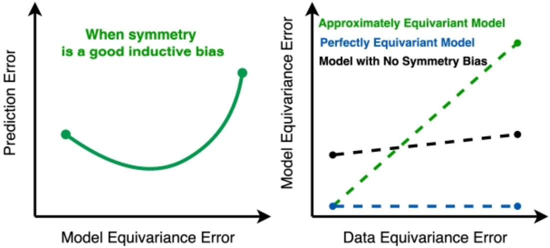


*Figure from: Wang, Walters, and Yu ICML 2022*

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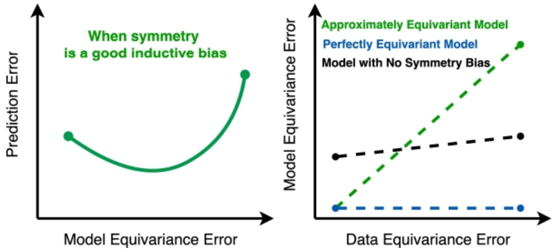


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- There is a common intuition that there is a *sweet spot* for balancing between model and data equivariance that can lead to good generalization
- How do we show this is the case?

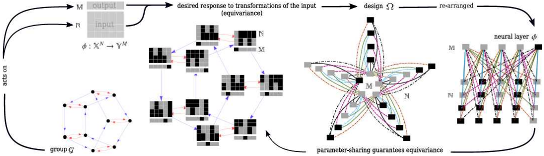
## Some Theoretical Developments

An Approximate Survey

# Some Axes of Theoretical Development

## 1 Architectural Characterizations

- Discrete groups: Equivariance and Parameter Sharing. Ravanbaksh, Schneider, Poczos, ICML 2017



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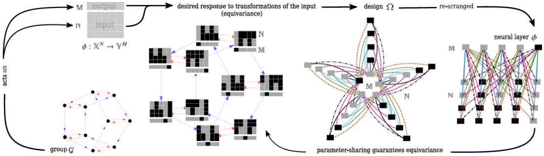


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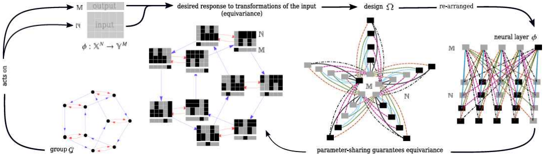


- Convolution $\iff$ Equivariance (Kondor & Trivedi); scalar fields, general compact groups, ICML 2018.
- Convolution $\iff$ Equivariance (Cohen, Geiger, & Weiler); steerable case, general compact groups, NeurIPS 2020

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- Characterization of Linear Layers:
  - $\mathbb{S}_n$, Maron, Ben-Hamu, Shamir, Lipman, ICLR 2019
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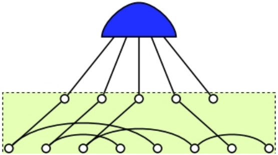

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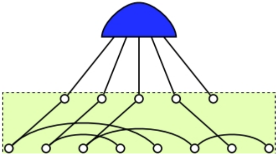

- Similar for Quantum group equivariant neural networks.

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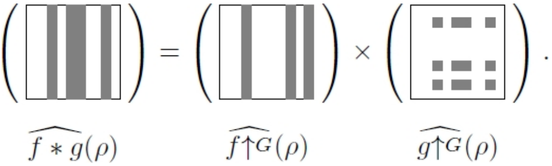
2 Fourier picture

- For scalar fields, Kondor & Trivedi, 2018



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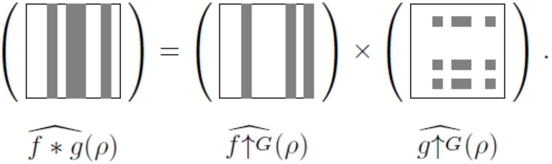


- For the steerable case, Xu, Lei, Dobriban, & Daniilidis, ICML 2022.

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4 More Universality Results

- Barron's analogue for equivariant networks, Lawrence 2022.

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- Behboodi, Cesa, & Cohen, NeurIPS 2022.

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- e.g. Wang, Zhu, Park, Platt, & Walters

Mircea Petrache
Pontificia Universidad Católica de Chile

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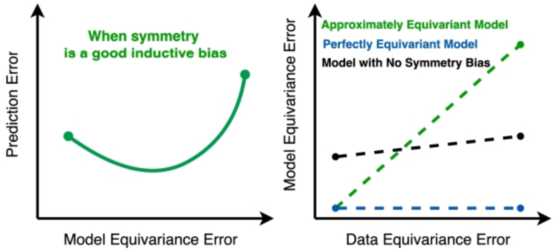
- Overall Goal: Theoretically understand the dependence of optimal model equivariance for data with pre-specified symmetries.

# Approximate Equivariance

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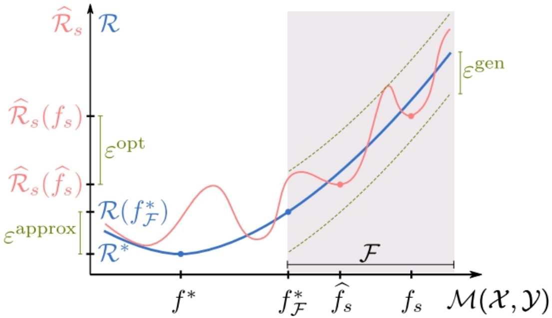
# How does the picture look like?




*Courtesy: J. Berner*

- Blue is the exemplary risk, red is the empirical risk [with respect to the projected space of measurable functions $\mathcal{M}(\mathcal{X}, \mathcal{Y})$)]
  - $\mathcal{R}^*$ is the so-called Bayes Risk.
  - Usual picture: Error: $\varepsilon^{\text{approx}} + \varepsilon^{\text{opt}} + \varepsilon^{\text{gen}}$

## Generalization Error

## Improved Generalization with Equivariance

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- Reminder: Usually care about $\sup_{f \in \mathcal{F}} Pf - P_n f$

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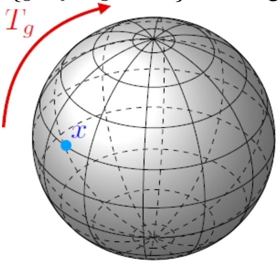

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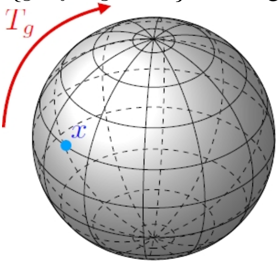


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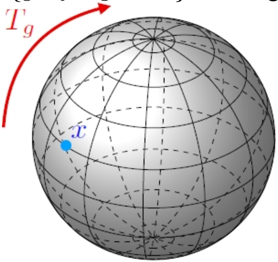


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- $g$ is a random variable, uniformly distributed over compact $G$
- More: Ulf Grenander, *Probabilities on Algebraic Structures* 1967

# Preliminary: Family of Invariant Functions

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**Lemma**

*Assume $\tilde{\mathcal{F}}$ consists of $G$-equivariant functions, and $\mathcal{F}$ consists of $G$-invariant functions. Let $D^G := \frac{1}{|G|}\int_G g \cdot D dg$, then generalization errors for $\tilde{\mathcal{F}}$ for $D$ and $D^G$ are the same.*

# Invariant Functions

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- Equivalent to concentration bounds.
- Let's focus on bounds roughly of the type:

$$\mathbb{P}\left[\sup_{\mathcal{F}}(P - P_n)f \geq \mathcal{R}(\mathcal{F}_Z) + \epsilon\right] \leq 2\exp\left(-\frac{\epsilon^2 n}{2\|\mathcal{F}\|_\infty}\right),$$

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- $Z_i = (X_i, Y_i)$, and $\sigma = (\sigma_1, \sigma_2, \ldots, \sigma_n)$ are the so-called Rademacher random variables, distributed uniformly over $\{-1, 1\}^n$

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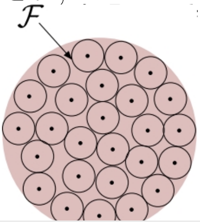
- Use this covering number: $\mathcal{N}(\mathcal{F}, t, \|\cdot\|_\infty) :=$
$\min \left\{ k : \exists \{f_1, \ldots, f_k\} \subset \mathcal{F}, \max \; \min \; \|f_j - f\|_\infty \leq t \right\}$



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- There are two equivalent ideas that can help improve generic bounds of the type discussed

# What happens with $G$-Equivariance? – Idea 1

1. Replace $\mathcal{F}$ by a set of $G$-orbit representatives $\mathcal{F}^0$
   - Probabilities and expectations don't change

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- Instead of $f_1, \dots, f_k$, take their orbits $G \cdot f_1, \dots, G \cdot f_k$
- Need to analyze the covering number $\mathcal{N}^G(\mathcal{F}, t, \|\cdot\|_\infty) :=$ $\min\left\{k : \exists\{f_1, \dots, f_k\} \subset \mathcal{F}, \max_{f\in\mathcal{F}} \min_{1\leq j\leq k}\left(\min_{g\in G}\|g\cdot f_j - f\|_\infty\right)\right\}$

# Improvement with $G$-Equivariance

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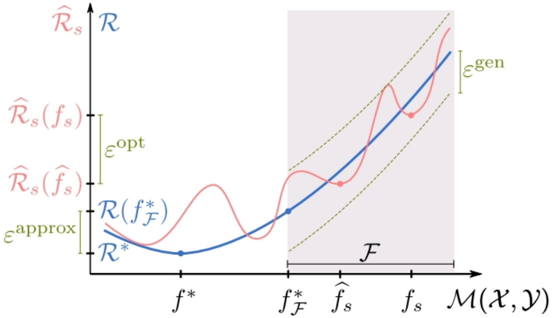
  - Reduce covering number problem for $\mathcal{X} \times \mathcal{Y}$ to independent problems
  - Each problem deals with orbit representatives $\mathcal{X}_0$ and covering $G$
- Has appeared in some works in different contexts (Chen *et al.*, 2023).

# Improvement with $G$-Equivariance

- Can get bounds for $G$-equivariance... but then what?

# Only Part of the Story




*Courtesy: J. Berner*

- Blue is the exemplary risk, red is the empirical risk
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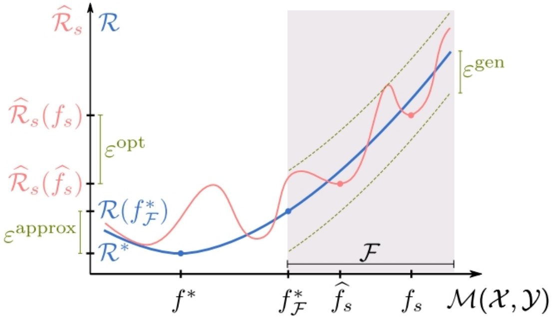


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  - Have only considered the generalization error!

## Approximation Error

### Model Equivariance versus Data Equivariance

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# Sketch of Idea: First Steps

- Fix random variables $(X, Y) \backsim D$, denote $\mathcal{X}_0$ as G-orbit representatives in $\mathcal{X}$

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- $g$ and $\bar{X}$ are now random variables $\implies$ distributions of $g \cdot \bar{X}, Y \simeq (X, Y)$
- Distributions of the three objects can be obtained by suitable projections:
  - Of $\bar{X}$, denoted $D_{\bar{X}} = \pi_{X_0} \pi_X D$
  - Of $g$, denoted $D_g = D_{g|\bar{X}} D_{\bar{X}}$
  - Of $Y$, denoted $D_Y = D_{Y|g,\bar{X}} D_{g|\bar{X} D_{\bar{X}}}$

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- Replace $x$ by $X$, and obtain:

$$AppErr_{equi}(D, \ell) = \mathbb{E}_{\bar{X}} \min_y \mathbb{E}_{g|\bar{X}} \mathbb{E}_{Y|g,\bar{X}} \ell(y, Y)$$

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- Can obtain explicit formulae in many cases, also reasonably easy to compute

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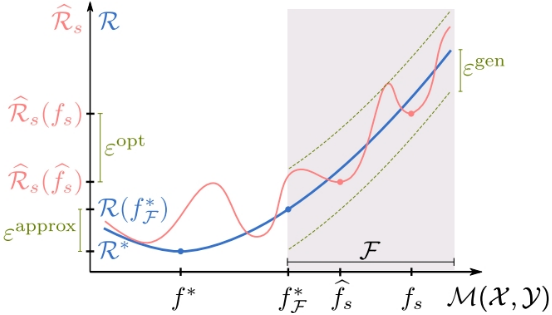


*Courtesy: Wang, Walters, and Yu*

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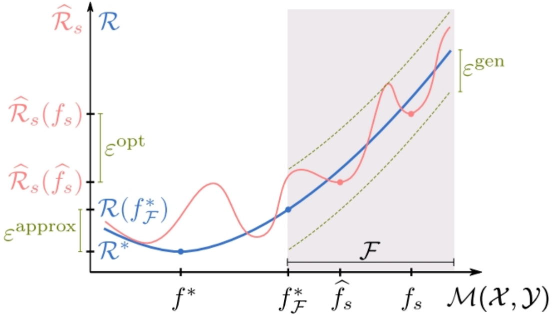


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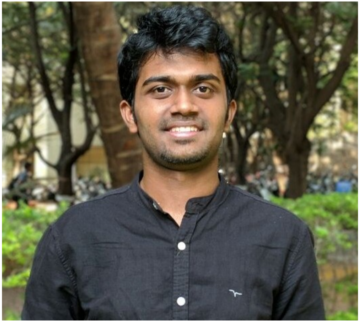
- Note: Skipped handling optimization error. But the picture remains similar with added caveats.

Learning Partial Symmetries

Exploiting Displacement Structure



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