On Uncertainty Calibration for Invariant Functions

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Goal: Elucidate the generalization limits of invariant functions by proving approximation error bounds for model calibration

Preliminaries:

- Denote a map with $f : \mathcal{X} \to \mathcal{Y}$
- G a group with representations $\rho^{\mathcal{X}}, \rho^{\mathcal{Y}}$ that transform vectors in $\mathcal{X}, \mathcal{Y}$

f is *invariant* if:

$$f(x) = f(gx) \text{ for all } g \in G, x \in \mathcal{X}$$

Invariant Model class $\mathcal{H} = \{h : \mathcal{X} \to \mathcal{Y} \times [0,1]\}$ such that $h(x) = (h_Y, h_P)$ where h_P represents a confidence estimation associated with h_Y

Let Expected Calibration Error over h be defined as:

$$\mathrm{ECE}(h) = \lim_{\varepsilon \to 0} \mathbb{E}_{p \sim r(p)} \left[\left| \underbrace{\mathbb{P}(f = h_Y | p - \varepsilon < h_P < p + \varepsilon)}_{accuracy} - \underbrace{p}_{confidence} \right| \right]$$

For an indicator function $\mathbb{1}(x)$ and a probability density $q(z)$ let minority label total decent be defined:

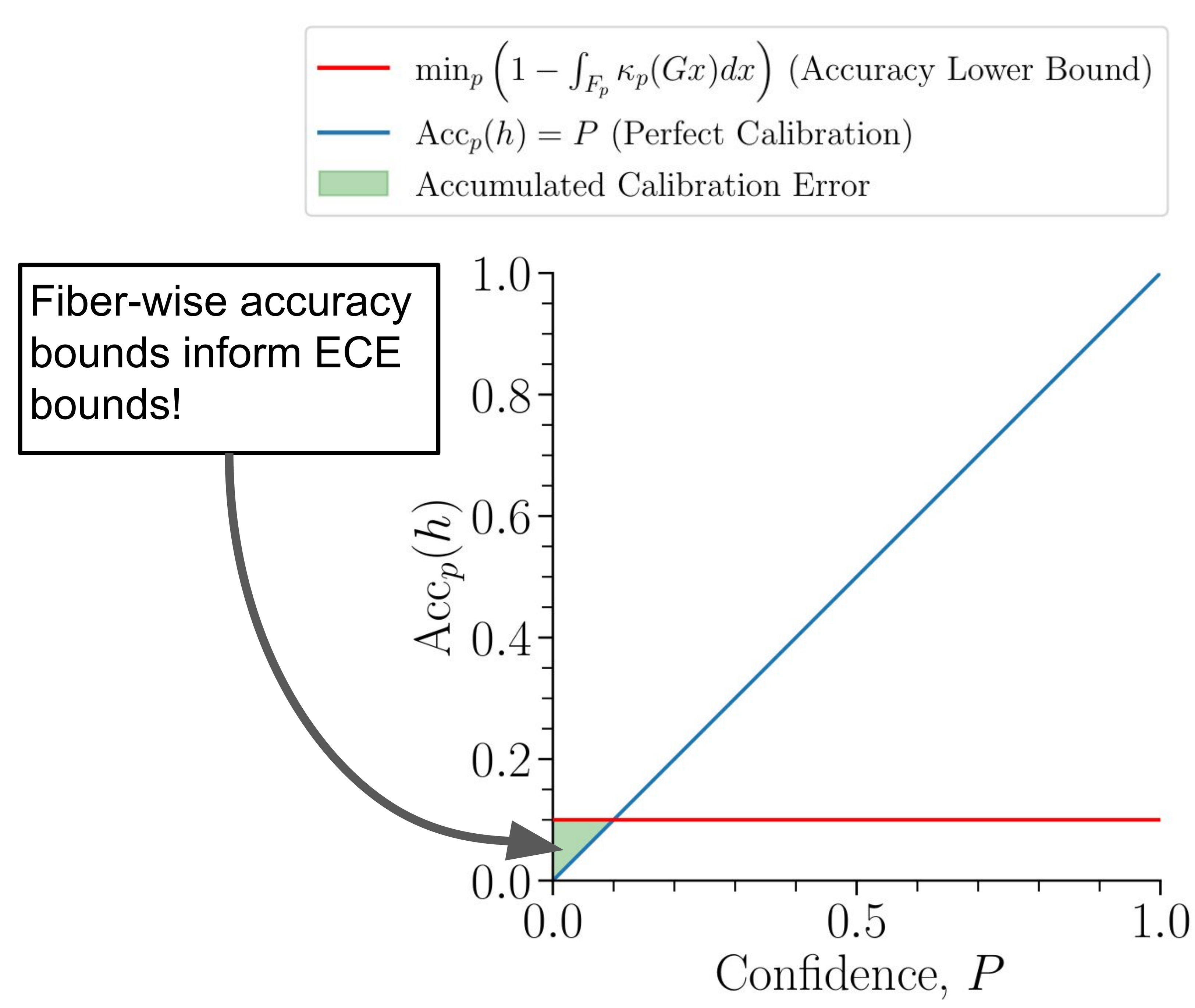
$$1 - \int_F \kappa(Gx)dx.$$

Classification Error bound is below by:

$$\kappa(Gx) = \max_{y \in Y} \int_{Gx} q(z)\mathbb{1}(f(z) \neq y))dz.$$

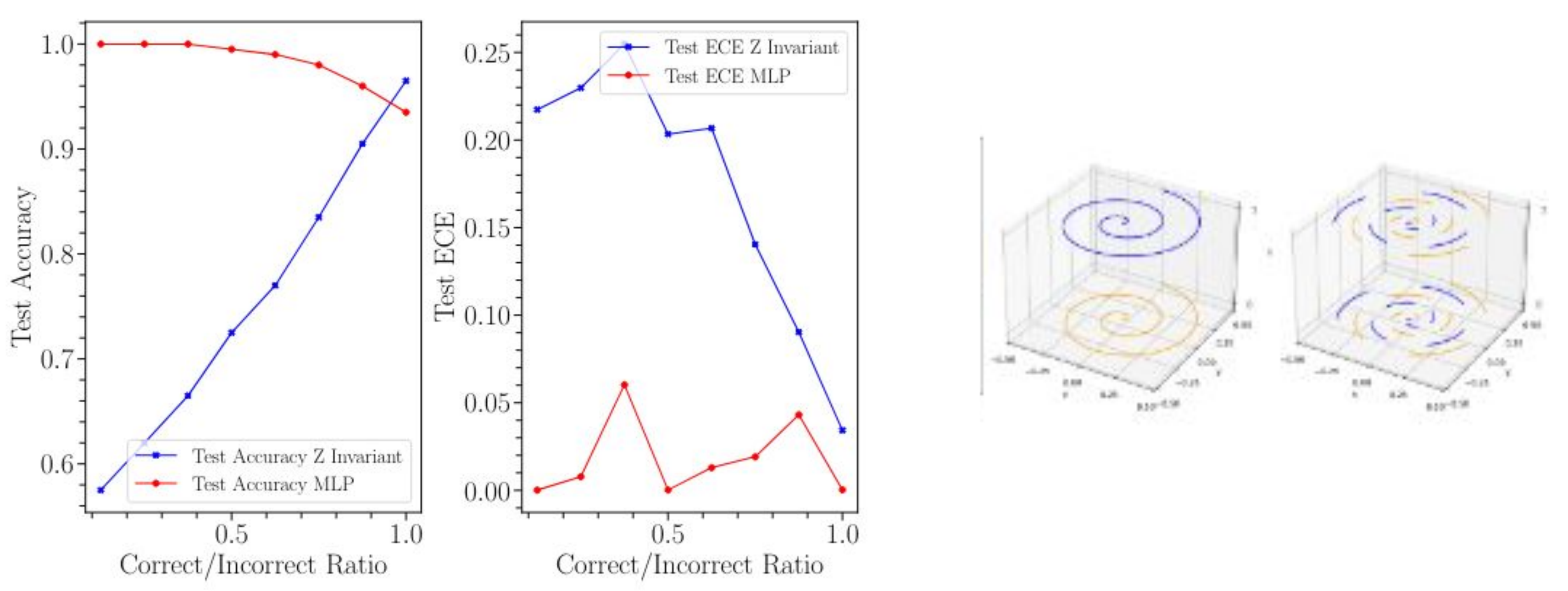
Invariant ECE Lower Bound Intuition:

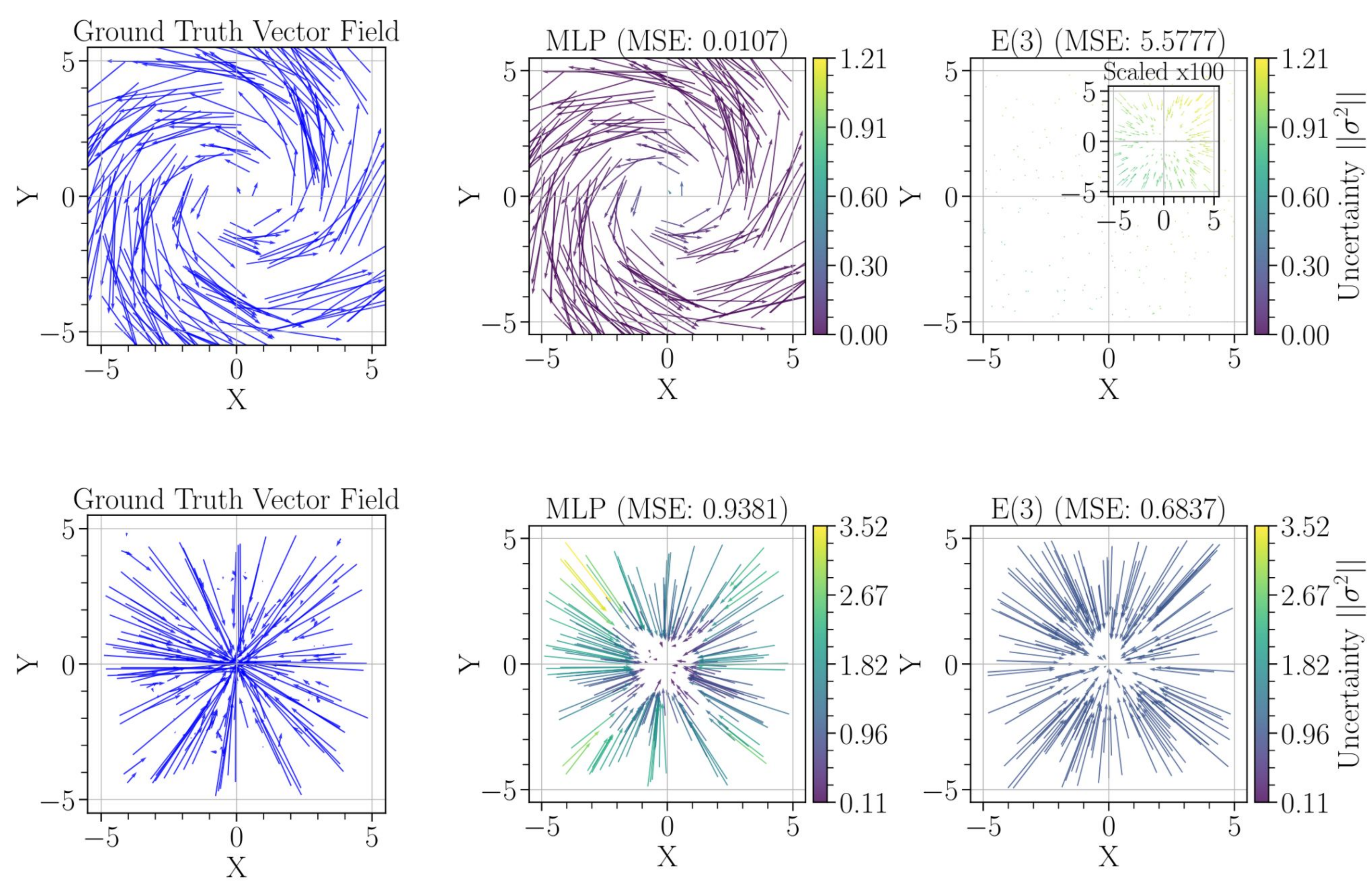
Invariant accuracy lower bound forces calibration error to accumulate!



Examples and Experiments:

Symmetry mismatch causes miscalibration!





Summary of Contributions:

- Bound calibration error for classification and regression
- Assess the disintegration of uncertainty into aleatoric and epistemic mass under symmetry constraints
- Provide illustrative examples and experiments

Main Result: Invariant ECE Bounds

Theorem 5. Denote the fundamental domain of G in a fiber $\mathcal{F}_p$ as F_p. The total minority dissent on an orbit in a fiber $\mathcal{F}_p$ is denoted $\kappa_p(Gx)$ and is defined in terms of the renormalized density $q_p(x) = q(x)/\int_{\mathcal{F}_p} q(x)dx$. Define the minimum fiber-wise classification accuracy as $m = \min_{p \in [0,1]} \left(1 - \int_{F_p} \kappa_p(Gx)dx\right)$. Then ECE is bounded below by $\int_0^m r(p)(m-p)dp$.

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References:

[1] ECE https://arxiv.org/abs/1706.04599

[2] Equi Bounds https://arxiv.org/abs/2303.04745