An Online Learning Approach to Interpolation and Extrapolation in Domain Generalization

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Outline

1 Introduction

2 Preliminaries

3 Online Domain Generalization Game

4 Interpolation Formal Results

5 Extrapolation Formal Results

6 Conclusion and Discussion

Background

OOD

The success of machine learning algorithms assumes that the data are I.I.D., an assumption that is often broken in practice.

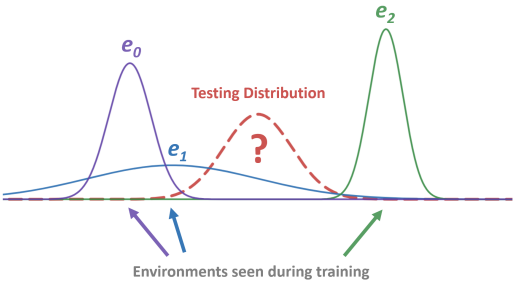
Out-of-Distribution (OOD) generalization: testing distribution is unknown and differs from the training distribution

Background

Domain Generalization

Assumption: training data comprised of distinct distributions or "environments".

Domain Generalization: given several domains, learn a model that can generalize to an unseen test data which relates to the observed domains.



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How do future test distributions relate to the groups encountered during training?

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How can we ensure good out-of-distribution performance?

- **Goal**: minimize risk over worst-case combination of groups.

Motivation

Shortcomings of Prior Works

Prior work lacks formal justification of Empirical Risk Minimization's (ERM) ability to "interpolate" the training distributions and "extrapolate" beyond them.

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Prior work lacks formal justification of Empirical Risk Minimization's (ERM) ability to "interpolate" the training distributions and "extrapolate" beyond them.

Other shortcomings of prior work:

1. Lack of theoretical guarantees on replacements to ERM
2. Strictly consider worst-case performance, which is not representative of the real-world

There is a need for a robust measure of OOD generalization that allows for a comparison of computational and statistical properties among domain generalization algorithms.

Contributions

Under the notion of inter- and extrapolation based on the re-weighting of sub-groups:

1. Extrapolation is computationally harder than interpolation.
2. The statistical complexity of inter- and extrapolation not too different.

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Convex Hull

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where $\lambda \in \nabla_E$ is a vector of convex coefficients (∇_E is the $E - a$ simplex) - in other words, within the convex hull of training distributions.

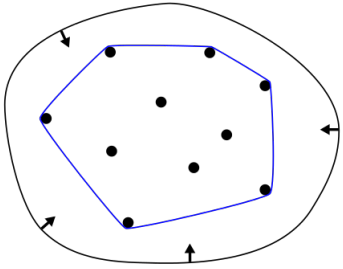

Figure: convex hull

Extrapolation

Bounded Affine Combinations

Recall that $\lambda \in \nabla_E$ is a vector of convex coefficients. The proposed test distributions can be defined as bounded affine combinations of the environments:

$$\sum_{e \in \mathcal{E}} \lambda_e = 1, \lambda_e \geq -\alpha . \forall e \in \mathcal{E}.$$

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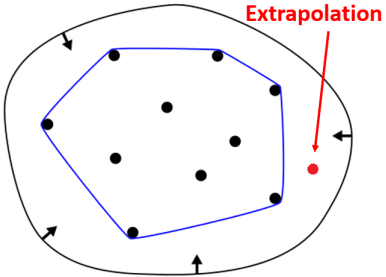
$$\sum_{e \in \mathcal{E}} \lambda_e = 1, \lambda_e \geq -\alpha . \forall e \in \mathcal{E}.$$

Note: the resulting function is not guaranteed to be a probability distribution, but can be framed as a re-weighting of the environment *risks*.



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Consider Domain Generalization as a continuous game of online learning - with a *player* and *adversary*.

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Each Round:

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Goal: Adapt better to unseen distributions as more distributions are seen, i.e. $\downarrow$ per-round regret.

Game Preliminaries

1. Let B be a convex set of potential predictors.
   Assume for all $\lambda \in \Delta_E$, β that minimizes p^λ is in B.
2. For any $\beta \in B$ and all $e \in \mathcal{E}$, the expected loss under p^e is finite

Game

- **Input:** Convex parameter space B, distributions $\{P_{XY}\}_{e\in\mathcal{E}}$, strongly convex loss $\ell : B \times (\mathcal{X} \times \mathcal{Y})$

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$$\lambda_t = \{\lambda_{t,e}\}_{e\in\mathcal{E}}, \lambda_{t,e} \geq 0, \forall e \in \mathcal{E}.$$

  3. Define $f_t(\beta) := \mathbb{E}_{(x,y)\sim p^{\lambda_t}}[\ell(\beta, (x, y))]$, where $p^{\lambda_t} = \sum_{e\in\mathcal{E}} \lambda_{t,e} p^e$.
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- **end for**
- Player suffers regret

$$R_T = \sum_{t=1}^{T} f_t(\hat{\beta}_t) - \min_{\beta\in B} \sum_{t=1}^{T} f_t(\beta).$$

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Single-round loss guarantees good performance in the worst-case, but this is not representative of future test environments in the real-world.

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Goal

When can we achieve sublinear regret rates?

Sublinear regret implies recovery of model with best average over all distributions in limit – minimax.

Recovers invariant predictor if it is indeed the best.

Theoretical Contribution

Regret Rates

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2. the statistical complexity (minimax) $\underbrace{\Theta(\log T),\ \Theta(\sqrt{T})}_{\text{unclear in what sense}}$ respectively, is not too different.

Conclude that ERM is minimax for both interpolation and extrapolation.

Lemma 1

Lemma

Recall that $\mathcal{R}^\lambda(\beta)$ is defined as the risk of β on the distribution p^e. Then for all finite λ,

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Takeaway: When an adversary chooses convex coefficients, they are equivalently choosing a loss function f_t that is a convex combination of individual environment risks $\{f_e\}_{e=1}^E$.

Theorem 1

Kreuger et al. (2020) show that the regret rate when an adversary can play arbitrary strongly convex functions of losses is $\mathcal{O}(\log t)$.

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Takeaway: We may expect that restricting the adversary to playing within the convex hull of a limited number of functions might be expected to affect the asymptotic statistical complexity.

Even with full knowledge of the adversary's limited selection, no algorithm can surpass $\mathcal{O}(\log t)$ – achieved by Follow-The-Leader (ERM).

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Consider an "oblivious" adversary (sequence of loss functions selected at start of game).

For general Lipschitz functions, against an oblivious adversary:

- no deterministic strategy can guarantee sublinear regret,
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- no deterministic strategy can guarantee sublinear regret,
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Follow–The–Perturbed–Leader (FTPL) can achieve Information-Theoretic regret lower bound of $\Omega(\sqrt{T})$ (Suggala & Netrapalli, 2020).

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Takeaway: Surprisingly, even with relaxing the general Lipschitz function to bounded affine combinations of strongly convex losses - fully know by the player - the game remains equally hard.

Proof of Theorem 2

Proof.

Part 1/2. We will show that for any deterministic algorithm, there exists a sequence of loss functions with regret bounded by $\mathcal{O}(T)$. Assume $\lambda_e > -\alpha \, \forall e$. Define

$$f_{e_1}(x) = x^2, \qquad f_{e_2} = x^4 + \frac{1}{2\alpha}x^2.$$

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ii. if $|x| \geq 1$, then $f_t = f_{e_1}$.

Observe that in case i. the loss $f_t(x) \geq 0$, and in case ii. $f_t(x) \geq 1$.

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Now consider the best actions in hindsight. If $a \leq \frac{T}{2}$, then $x^* = 0$ suffers 0 loss and the player's regret is at least $b = T - a \geq \frac{T}{2}$.

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On the other hand, if $a > \frac{T}{2}$, then for any x, the player suffers a loss of

$$-a\alpha x^4 + (a/2 + a\alpha + b)x^2 \leq a\alpha(x^2 - x^4) + (a + b)x^2 = (a\alpha(1 - x^2) + T)x^2. \quad (1)$$

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We can chose $x^* = \sqrt{1 + \frac{3}{\alpha}}$ and the player suffers regret $\geq \frac{T}{2}$. In either case, the player suffers $\mathcal{O}(T)$ regret. □

Deterministic vs. Randomized Algorithms

What about randomized algorithms?

Theorem 3

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Even with a randomized algorithm against an oblivious adversary playing bounded affine combinations, achieving sublinear regret is NP-hard.

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Even with a randomized algorithm against an oblivious adversary playing bounded affine combinations, achieving sublinear regret is NP-hard.

Takeaway: Again, we cannot seem to achieve a sublinear regret rate for extrapolation.

When we consider the definitions in this paper, we realize there is a exponentially large gap, in the sense of computational complexity, between interpolation and extrapolation.

Theorem 4

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Against an oblivious adversary playing bounded affine combinations, the achievable regret is lower bounded as $\Omega(\sqrt{T})$ – with oracle access to approximate minimzation of a non-convex function.

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Against an oblivious adversary playing bounded affine combinations, the achievable regret is lower bounded as $\Omega(\sqrt{T})$ – with oracle access to approximate minimzation of a non-convex function.

Takeaway: Recall that FTPL has a minimax lower bound of $\Omega(\sqrt{T})$ for an oblivious adversary playing arbitrary Lipschitz functions - FTPL *is just a noise variant of ERM*.

It turns out that that $\Omega(\sqrt{T})$ remains minimax for bounded affine combinations, that is, we cannot outperform ERM.

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Takeaway

Divide domain generalization into two tasks i) interpolation and ii) extrapolation:

1. the computation complexity difference between the two is exponential, but
2. the statistical complexity (minimax) $\underbrace{\Theta(\log T), \Theta(\sqrt{T})}_{\text{unclear in what sense}}$ respectively, is not too different.

Discussion

1. Clarification of similarity of bounds.
2. In practice, the performance of ERM does not seem to match these results
3. Violated assumptions in practice
   - Linearity
4. Degree of extrapolation ($-\alpha$)
5. Definition of interpolation/extrapolation can (perhaps should) be reconsidered
6. Worst-case average loss is not the same as worst-case loss – the latter is still important

Questions?

Thanks for you attention!

Appendix I

Algorithm 1 Convex OFTPL

Input: Perturbation Distribution P_{PRTB}, number of samples m, number of iterations T
Denote $\nabla_0 = 0$
for $t = 1 \dots T$ **do**
    Let g_t be the guess for ∇_t
    for $j = 1 \dots m$ **do**
        Sample $\sigma_{t,j} \sim P_{\text{PRTB}}$
        $\mathbf{x}_{t,j} \in \operatorname{argmin}_{\mathbf{x} \in \mathcal{X}} \langle \nabla_{0:t-1} + g_t - \sigma_{t,j}, \mathbf{x} \rangle$
    end for
    Let $\mathbf{x}_t = \frac{1}{m} \sum_{j=1}^{m} \mathbf{x}_{t,j}$
    Play $\mathbf{x}_t$ and observe loss function f_t
end for

Appendix II

Algorithm 2 Nonconvex OFTPL

Input: Perturbation Distribution P_{PRTB}, number of samples m, number of iterations T
Denote $f_0 = 0$
for $t = 1 \dots T$ **do**
    Let g_t be the guess for f_t
    for $j = 1 \dots m$ **do**
        Sample $\sigma_{t,j} \sim P_{\text{PRTB}}$
        $\mathbf{x}_{t,j} \in \operatorname{argmin}_{\mathbf{x} \in \mathcal{X}} f_{0:t-1}(\mathbf{x}) + g_t(\mathbf{x}) - \sigma_{t,j}(\mathbf{x})$
    end for
    Let P_t be the empirical distribution over $\{\mathbf{x}_{t,1}, \mathbf{x}_{t,2} \dots \mathbf{x}_{t,m}\}$
    Play $\mathbf{x}_t$, a random sample generated from P_t
    Observe loss function f_t
end for