Towards Robust Learning to Optimize with Theoretical Guarantees

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1. Introduction and Motivation

- What is Learning to Optimize (L2O)?

Optimization Problem: $\min_x f(x)$, $x \in R^n, f: R^n \to R$ → Human-Designed Algorithm: Gradient Descent

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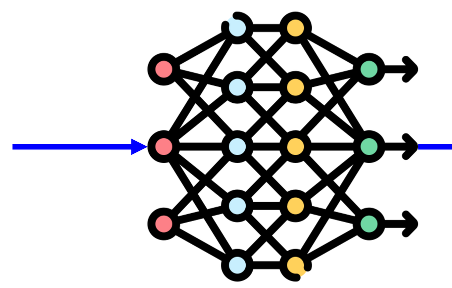
Learning to Optimize: ML/DL Model + Training

- Benefits
  - Better optimality (potential).
  - Better convergence/efficiency [1].
- Workflow of L2O (Inference, Toy example):

Given initial point x_i^0

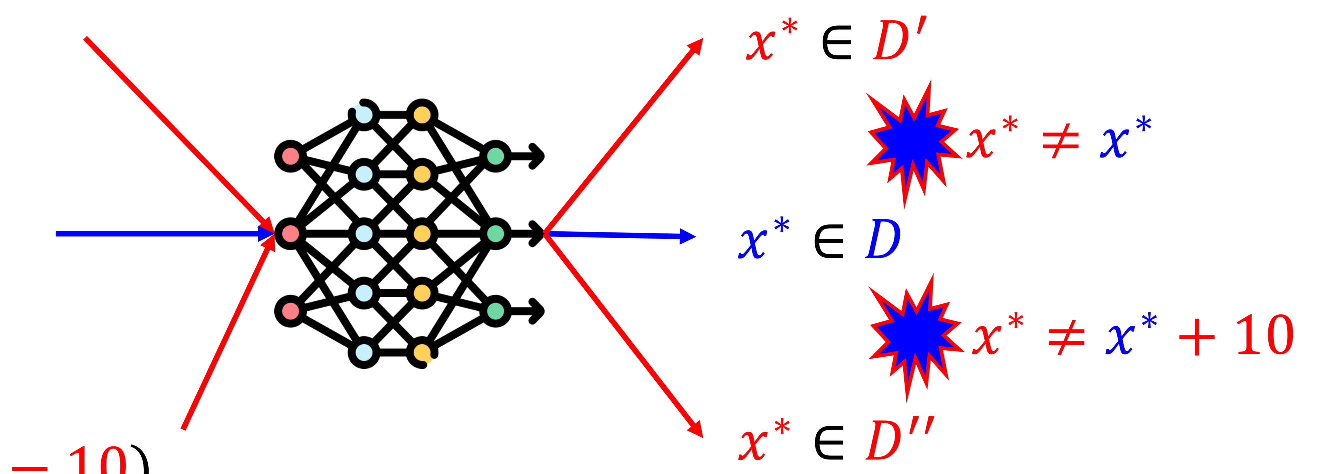
$x_i^0 \in N(0,1), f(x_i^0)$ →  → x_i^*

- L2O Model 's Failure in Out-of-Distribution (OOD) Scenarios

① x OOD
$x^0 \in N(10,1),\ f(x)$

In-Distribution (InD)
$x^0 \in N(0,1),\ f(x)$

② f OOD
$x^0 \in N(0,1),\ f = f(x-10)$



- Q1, How does OOD influence the behavior of x ?
  - Motivation 1: Convergence Analysis in OOD Scenarios.
- Q2, Can we achieve better x^* in OOD scenarios ?
  - Motivation 2: Convergence Improvement in OOD Scenarios.

2. Methods (Step-by-Step, Paper at)

- Backbone L2O Model: Math-Inspired L2O [1]
  - L2O model construction: Necessary condition of convergence.
  - SOTA empirical convergence.

1. Definition:
   - Optimization Problem

   $\min_x f(x) + r(x), x \in R^n$. $f, r: R^n \to R$, f: smooth, r: non-smooth, proper.
   - L2O OOD Definition (Fixed Dimensional Space):

   Define InD Problems ⟶ L2O OOD: Solving OOD Problems
     - Two OOD cases: Initial point x^0 and objective f.
2. OOD Formulation: Formulate OOD with OOD-InD **Difference**
   - Sequences(trajectory in the paper): Variable and Input Feature (defined in terms of objective and variable).

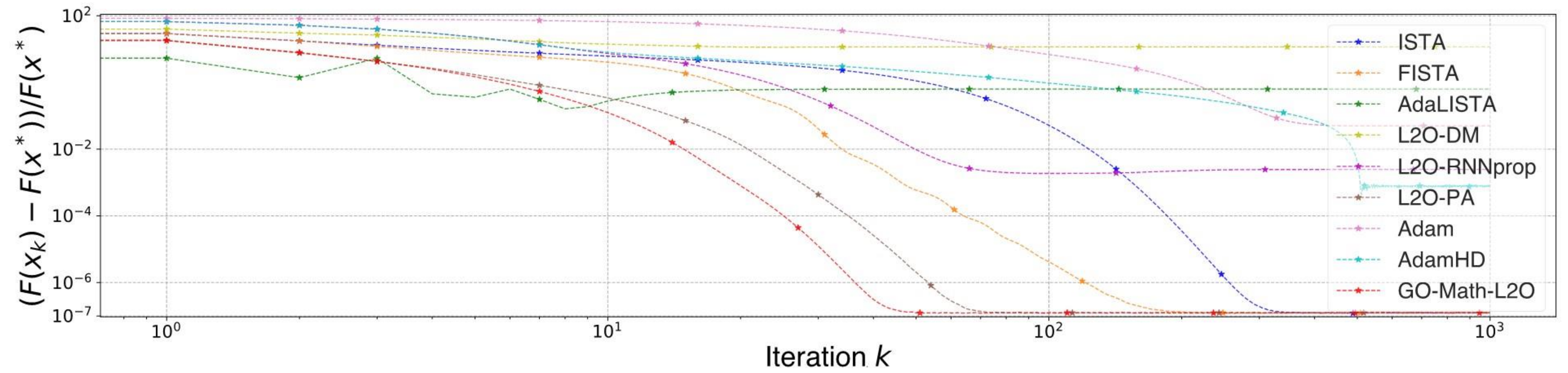
   OOD Sequences − InD Sequences = Virtual Sequences (Extent of OOD)
3. L2O Model's **OOD Behavior** (Output) Formulation:
   - Formulate OOD behavior by InD behavior.
   - Eq. (3) in the paper, extension of Mean Value Theorem for Vector-Valued Function.

   $d(\text{OOD Input Feature}) = d(\text{InD Input Feature}) + \mathbf{J}_d(\text{Difference}) = d(z) + \mathbf{J}_d s'$

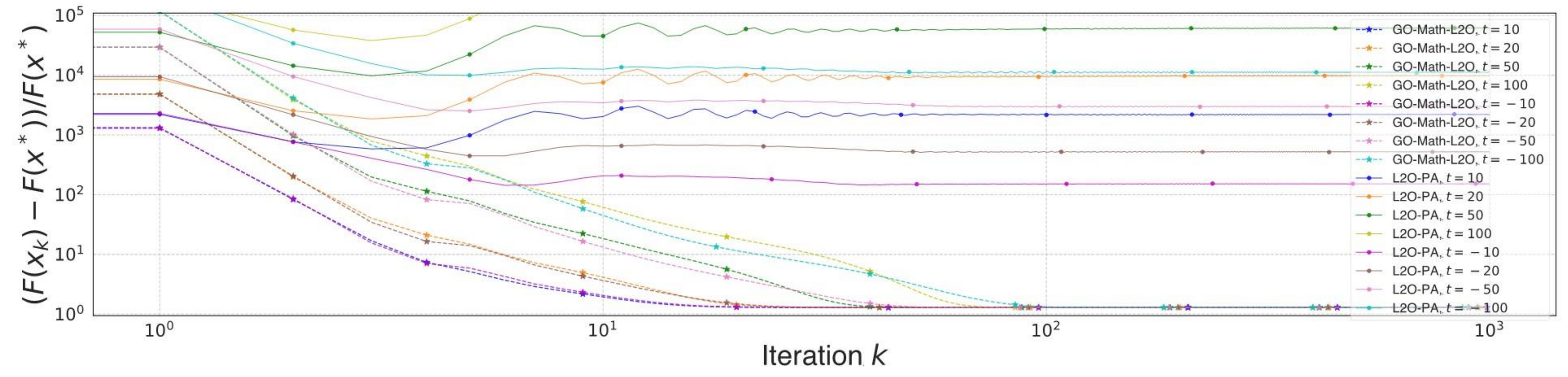
   Bounded "Jacobian" Matrix; Virtual Feature
4. Convergence Analysis: **Convergence Rate Upper Bound**
   - Training-free: Stabilize L2O model's InD behavior by optimal upper bound.
   - OOD Convergence Analysis:
     - Split OOD sequence into InD part and virtual part.
     - InD: Deterministic convergence.
     - OOD: Formulated by virtual variable.
5. Convergence Improvement:
   - Upper bound relaxation on convergence rate: Magnitude of input feature determines convergence rate.
   - Improvement Strategy: Reduce input features.
   - Proposed method: A gradient-only math-inspired L2O model.
     - Eliminate variable-related features.
     - Posterior non-smooth sub-gradient construction.

3. Results（Project at ）

1. Theoretical Results
- InD case: Lemma 1, Corollary 1 in the paper.
  - In general, convergence rate of L2O is as best as a conventional algorithm.
- OOD case: Theorems 1 and 2, Lemmas 2 and 3 in the paper.
  - Convergence rate is deteriorated by $\mathcal{O}(\text{virtual variable})$ $\mathcal{O}(\text{gradient})$.
  - Convergence rate is upper bounded by $\mathcal{O}(\|\text{virtual variable}\|)$.
2. Empirical Results (Our Model: GO-Math-L2O)
- InD Outperformance



- OOD Outperformance over SOTA Math-Inspired L2O [1]



References

[1]. Jialin Liu, Xiaohan Chen, Zhangyang Wang, Wotao Yin, and HanQin Cai. Towards Constituting Mathematical Structures for Learning to Optimize. In ICML, 2023.