Towards Robust Learning to Optimize with Theoretical Guarantee

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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

Learning to Optimize

ML/DL Model + Training

- Benefits
  - Better optimality (potential).
  - Better convergence/efficiency [1].

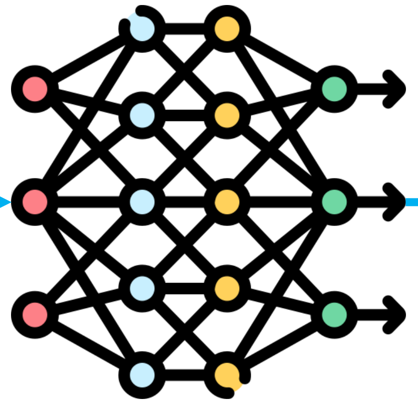
[1]. Jialin Liu, Xiaohan Chen, Zhangyang Wang, Wotao Yin, and HanQin Cai. Towards Constituting Mathematical Structures for Learning to Optimize. In ICML, 2023.

How does L2O work?

- Workflow of L2O (Inference)

Given initial point x_i^0

$$x_i^0 \in \boxed{N(0,1)}, \boxed{f\left(x_i^0\right)}$$



x_i^*

A distribution

A class of objective

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

① x OOD

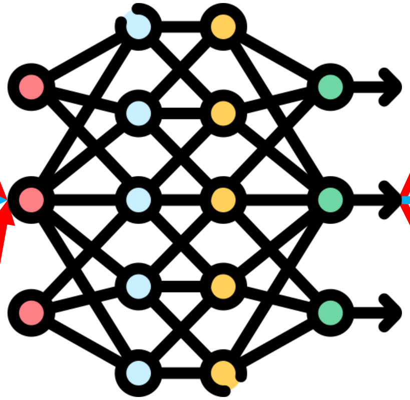
$x^0 \in N(10,1),\ f(x)$

In-Distribution (InD)

$x^0 \in N(0,1),\ f(x)$

② f OOD

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



$x^* \in D'$

$x^* \neq x^*$

$x^* \in D$

$x^* \neq x^* + 10$

$x^* \in D''$

Theoretical Convergence Analysis

- Convergence of Single-Iteration (Smooth Case)

$$
\begin{aligned}
&F'(x_k + s_k) - F'(x_{k-1} + s_{k-1}) \\
&\le \boxed{-\frac{\|\nabla f'(x_{k-1} + s_{k-1})\|^2}{2L}} \qquad \text{Convergence of Gradient-Descent} \\
&\left.\begin{aligned}
&+ L\| \operatorname{diag}(\mathbf{J}_{1,k-1} s') \nabla f'(x_{k-1} + s_{k-1})\|^2 \\
&+ L\|\frac{\nabla f'(x_{k-1} + s_{k-1}) - \nabla f(x_{k-1})}{2L} - \mathbf{J}_{2,k-1} s'\|^2.
\end{aligned}\right\} \text{Deterioration w.r.t. OOD}
\end{aligned}
$$

Theoretical Convergence Rate Analysis

- Convergence Rate (Smooth Case)

$$\min_{k=1,\ldots,K} F'(x_k + s_k) - F'(x^* + s^*)$$

$$\le \boxed{\frac{L}{2}\|x_0 - x^* + s_0 - s^*\|^2 - \frac{L}{2}\|x_K - x^* + s_K - s^*\|^2}$$

Convergence Rate of [Gradient-Descent]

$$+ \frac{L}{K}\sum_{k=1}^{K}(x_k + s_k - x^* - s^*)^\top$$

$$\Big(x_k + s_k - \big(x_{k-1} + s_{k-1} - \frac{\nabla f'(x_{k-1} + s_{k-1})}{L}\big)\Big).$$

Deterioration w.r.t. OOD

Convergence Improvement

- Upper Bound Relaxation

$$\begin{aligned}
&F'(x_k + s_k) - F'(x_{k-1} + s_{k-1}) \\
&\le -\frac{\|\nabla f'(x_{k-1} + s_{k-1})\|^2}{2L} \\
&+ \frac{\|\nabla f'(x_{k-1} + s_{k-1}) - \nabla f(x)\|^2}{2L} \\
&+ \left(LC_1^2 n \|\nabla f'(x_{k-1} + s_{k-1})\|^2 + 2LC_2^2 n\right) \boxed{\|s'\|^2}.
\end{aligned}$$

OOD vector,
NN's input feature

- Improve upper bound: Magnitude reduction.
  - Our approach: Input Feature Simplification.

A New L2O Model with Gradient-Only Input

- New Model Formulation Based on [1]

$$
\begin{aligned}
x_k =& x_{k-1} - \mathbf{R}_k \nabla f(x_{k-1}) - \mathbf{R}_k g_k - \mathbf{Q}_k v_{k-1} - b_{1,k}, \\
v_k =& (\mathbf{I} - \mathbf{B}_k) G_k + \mathbf{B}_k G_{k-1} - b_{2,k}, \\
G_k :=& \mathbf{R}_k^{-1} (x_{k-1} - x_k - \mathbf{Q}_k v_{k-1} - b_{1,k}),
\end{aligned}
$$

- Learn $\mathbf{R}, \mathbf{Q}, \mathbf{B}$. Details at

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

Empirical Outperformance

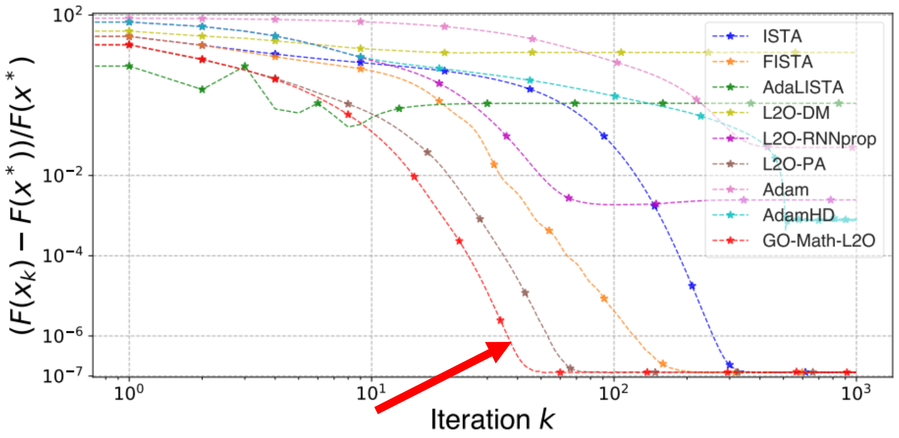


Figure 1. LASSO Regression: InD.

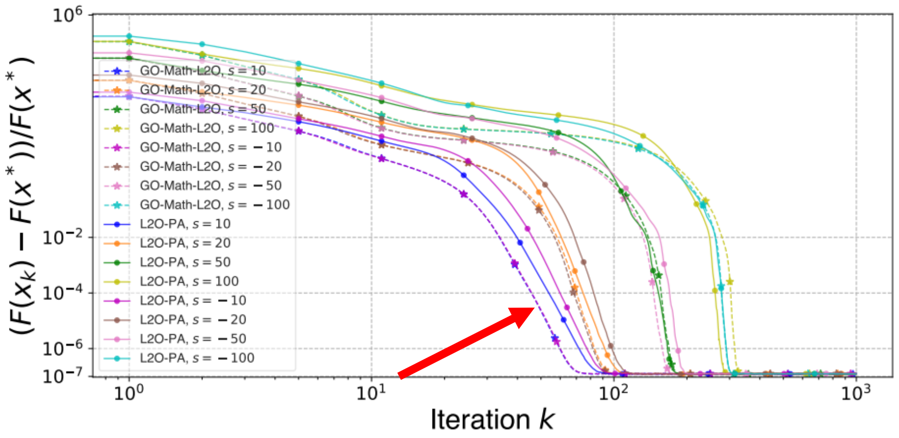


Figure 3. LASSO Regression: OOD by Trigger 1.

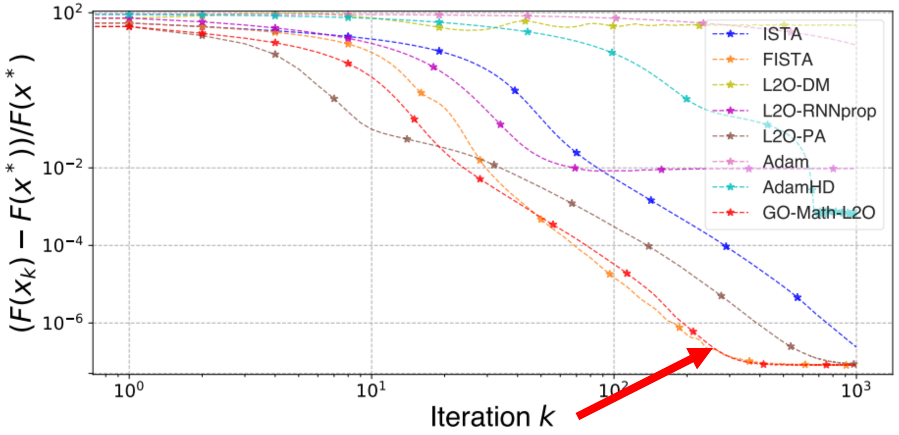


Figure 2. LASSO Regression: Real-World OOD.

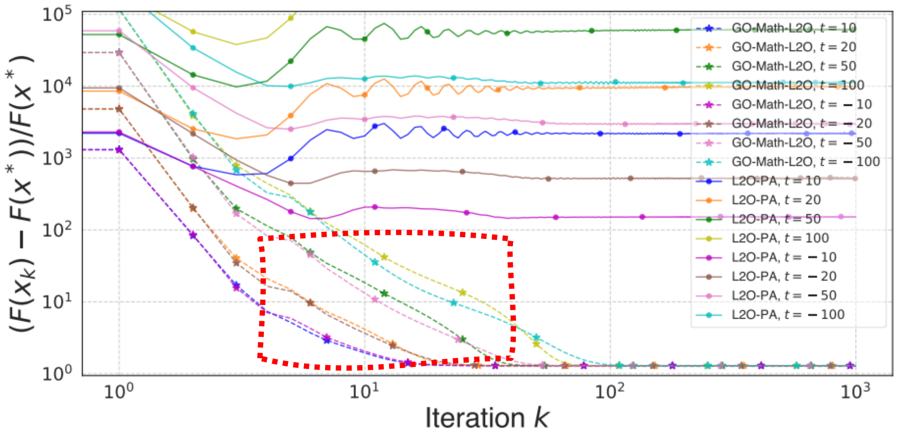


Figure 4. LASSO Regression: OOD by Trigger 2.

Empirical Outperformance

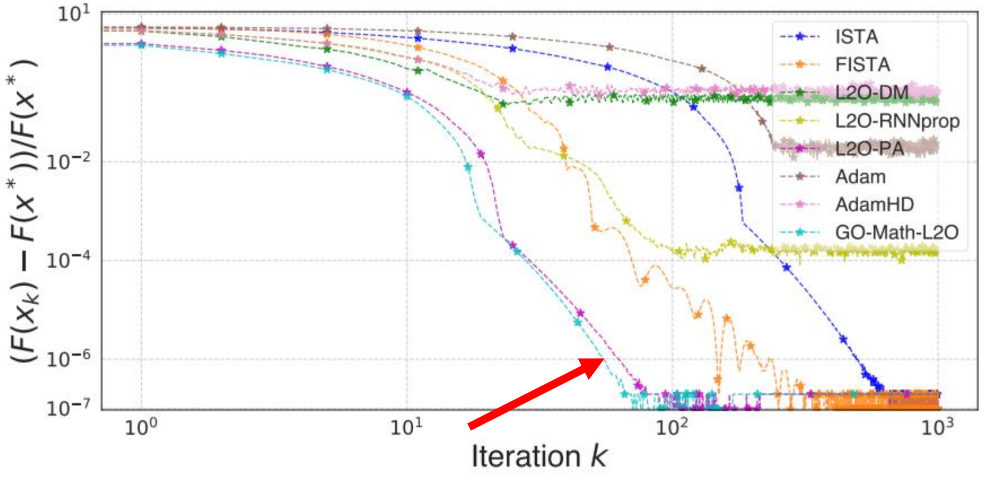


Figure 14. Logistic Regression: Real-World Ionoshpere Dataset.

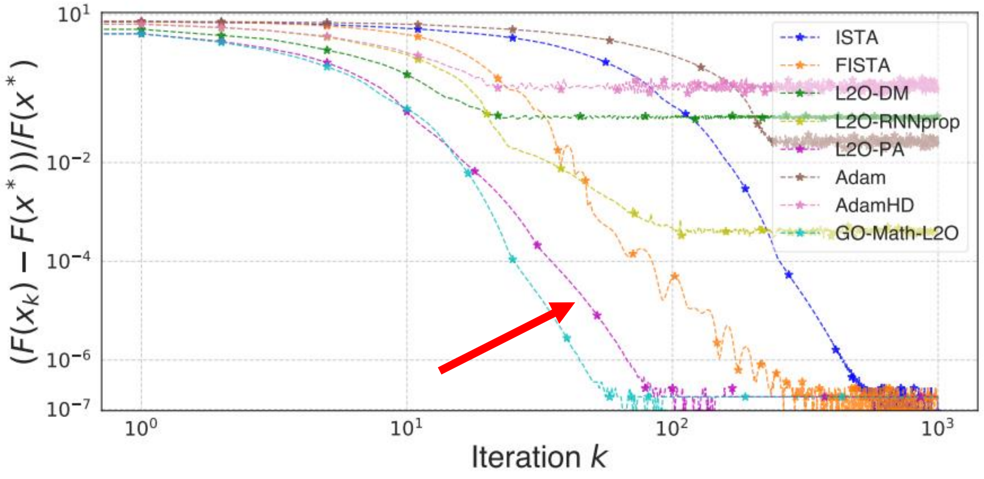


Figure 15. Logistic Regression: Real-World Spambase Dataset.

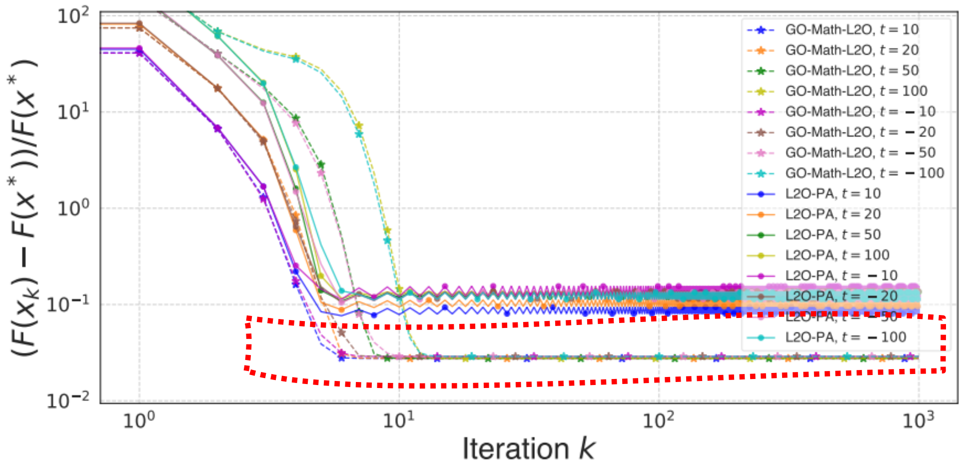


Figure 17. Logistic Regression: OOD by Trigger 2.

Thank You!

Project at NetX-lab/GoMathL2O-Official (github.com)

Paper

Code

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