



Learning Provably Improves the Convergence of Gradient Descent

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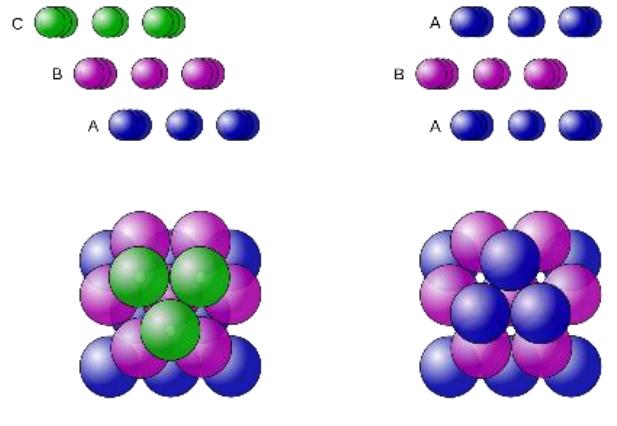


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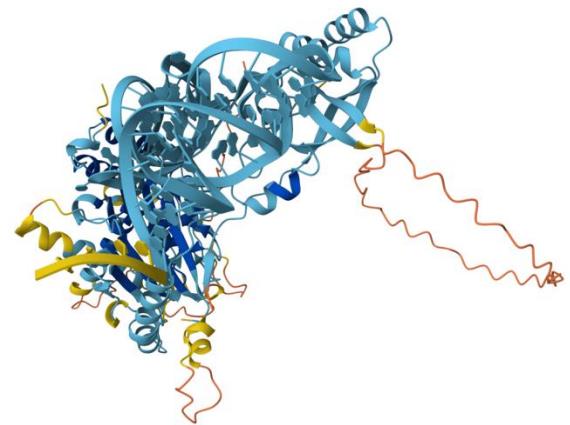


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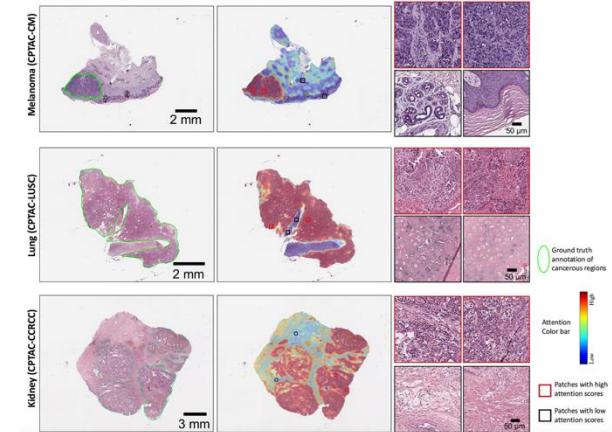
Introduction: AI for Science



基于符号逻辑的
开普勒猜想证明
[Forum of Mathematics]



AlphaFold
蛋白质预测
[Nature]



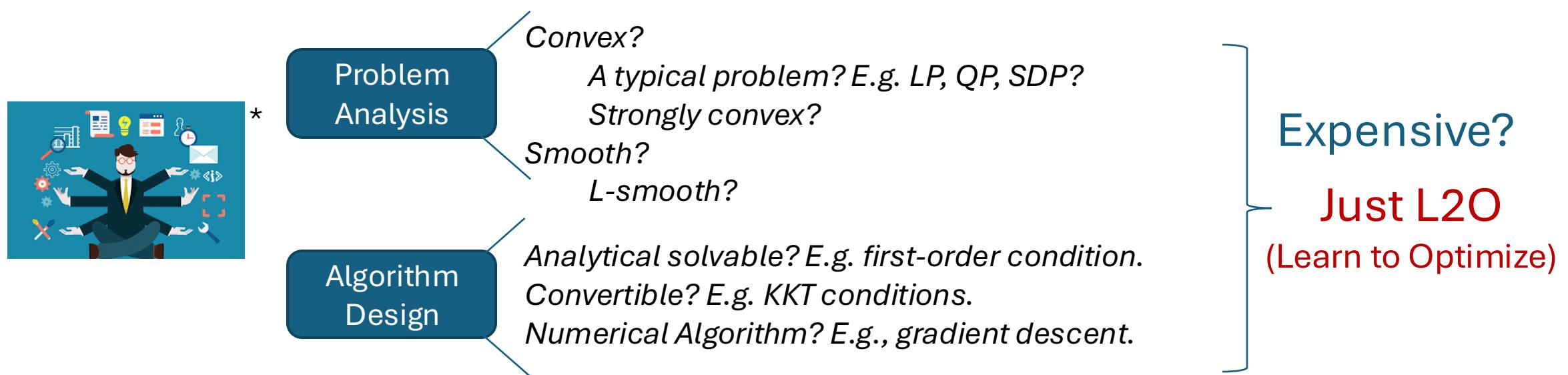
基于大模型的
病理学成像评估
[Nature]

Introduction: Mathematical Programming



$$\min_x f(x), \\ x \in \mathbb{R}^n, f: \mathbb{R}^n \rightarrow \mathbb{R}$$

- Conventional Algorithm: Human-Designed

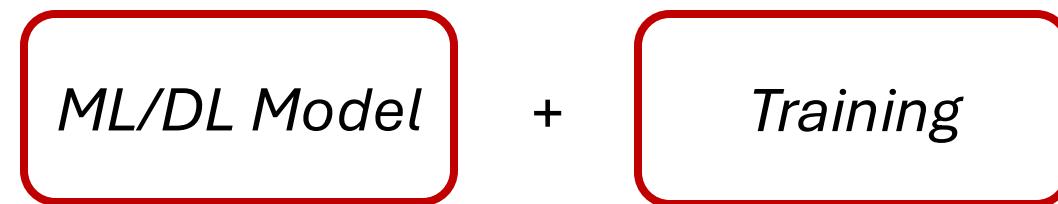


* Picture from Google

L2O: Predict Solution by Machine Learning



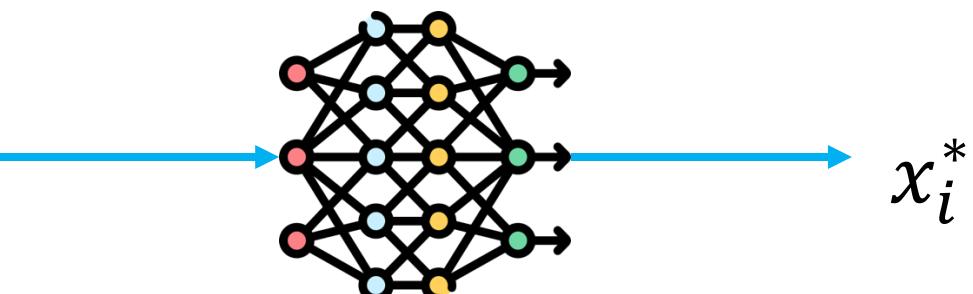
- L2O Architecture



- L2O Workflow

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

Information of Objective



Minimizer

Success of L2O in Different Scenarios



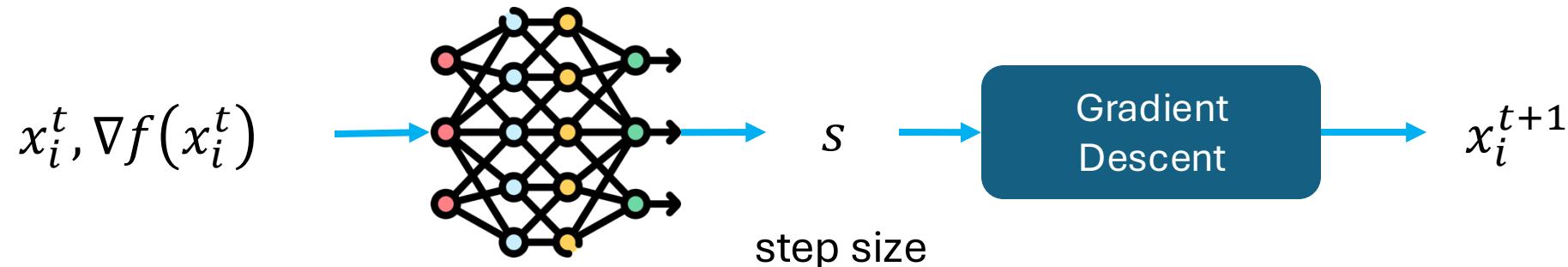
- Applications of L2O
 - Computer Networks
 - Routing: *ICLR 19, TNSE 20, CVPR 20*, etc.
 - Resource Allocation:
TSP 18, JSAC 21, TWC 23, INFOCOM 24, etc.
 - Finance
 - Decision Making: *TNNLS 16, IJCAI 21*, etc.
 - Transportation
 - Path Planning: *TITS 22, TNNLS 24*, etc.
 - Mathematical Solver:
ICLR 19, ICML 23, CVPR 24, etc.
Others: *Math Benchmark of LLM*.

Optimality.
Convergence/Efficiency [1].

Introduction: Optimization and L2O



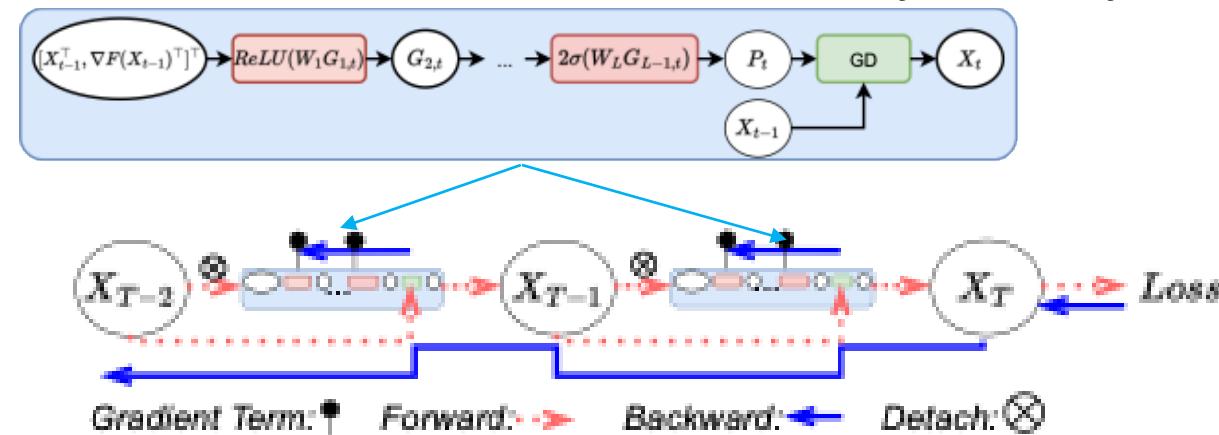
- Scenarios: General Optimization Problems
- Learning to Optimize (L2O) Architecture:
 - Unrolling (Math-L2O [Liu et al., ICML 2023])



- Problem Definition: Quadratic Programming
$$\min_x f(x), x \in R^n$$
- $f: R^n \rightarrow R$, quadratic.
- f is convex and smooth.

Analysis: Training V.S. Unrolling

- Optimization (Unrolling) Steps v.s. Training Iterations
 - Optimization Steps (Unrolling process): $x_{t-1} \rightarrow x_t$.

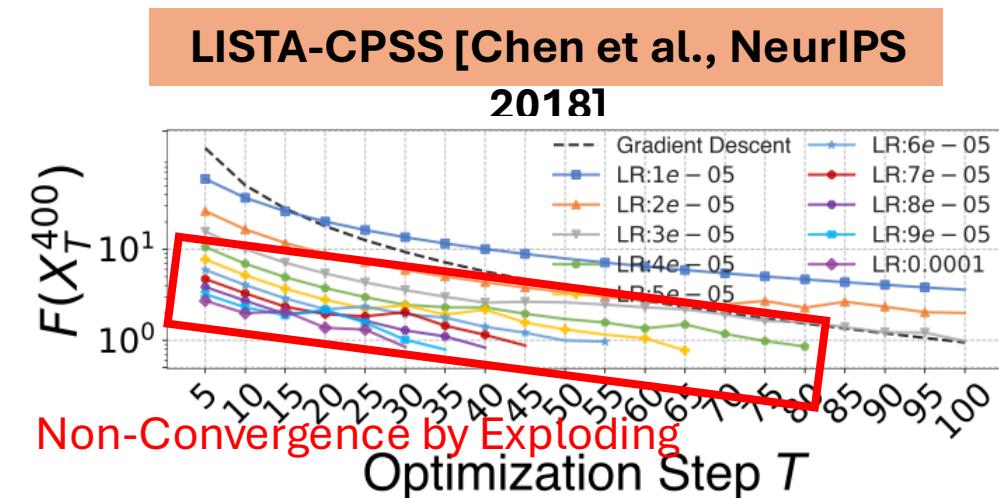
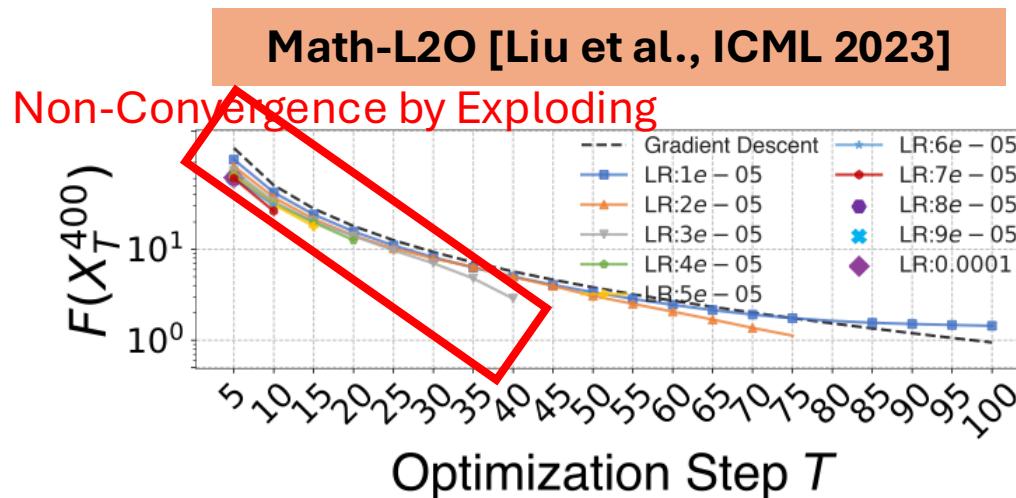


- Training Iterations: Stable T , $f(x_T^{k-1}) \rightarrow f(x_T^k)$.
- Optimization is orthogonal to training.
 - Can we have convergence of Unrolling-L2O from training?

Convergence with Different Unrolling Steps



- Objective by 100 steps, by 400 training iterations



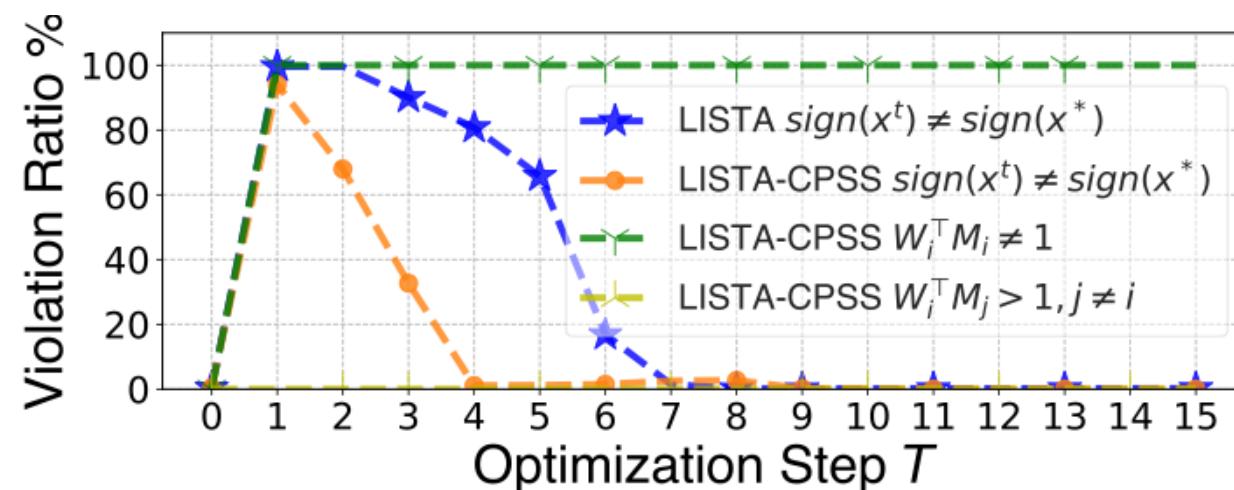
- Longer optimization (unrolling) steps require smaller learning rates.
- Larger learning rates improve convergence.

There is no guarantee that training will always converge.

Motivate our rigorous L2O convergence proof of training.

Existing Theoretical Convergence Proofs

- Rely on Strict Assumptions
 - LISTA-CPSS [Chen et al., NeurIPS 2018]
 - Sequence converges to optimum in a fixed direction: $\text{sign}(X_t) = \text{sign}(X^*)$.
 - Learnable matrix is (semi-)orthogonal to coefficient matrix in objective: $\mathbf{W}_i^\top \mathbf{M}_i = 1$ and $\mathbf{W}_i^\top \mathbf{M}_j > 1$ for all $j \neq i$.
- **Violated** by Real Training



Non-Trivial Unrolling-L2O Convergence Proof?



- A Novel Convergence Demonstration Methodology for Math-L2O (Unrolling L2O)
- Main Design:
 1. L2O Convergence Construction

Convergence alignment between training and optimization.
(NOTE: Training is orthogonal to optimization process in Unrolling L2O.)
 2. Training Convergence Demonstration.

Neural Tangent Kernel Theorem.
 3. Deterministic Initialization Method.

Initialize NN to achieve alignment.
Ensure training converge.

Design Part-I: L2O Convergence Construction



- Align **Upper Bound** of L2O Training to **Lower Bound** of Gradient Descent.

1. General Convergence Rate of L2O Training:

- k : training iteration, t : optimization step.

$$F(X_T^k) \leq r_k C(X_T^0), X_T^0 = \text{L2O}_{W_{[L]}}(X_0)$$

Some Constant Mapping

2. Convergence Rate of Gradient Descent:

$$F(X_T^0) \leq \frac{\beta}{T} \|X_0^0 - X^*\|_2^2$$

3. Alignment: Let $C(X_T^0) = F(X_T^0)$, $F(X_T^k) \leq r_k \frac{\beta}{T} \|X_0^0 - X^*\|_2^2$

4. Given constant initial point that $X_0^0 = X_0^k$, convergence rate (at step T) of L2O:

$$F(X_T^k) \leq r_k \frac{\beta}{T} \|X_0^k - X^*\|_2^2$$

Requirement: Demonstrate the convergence rate of L2O Training.



Design Part-II: Training Convergence Demonstration

- We prove it by Neural Tangent Kernel Theorem.
 - NN training: Gradient descent.
 - L-1 layer is wide: More neuron than training samples.

1. Gradient of NN Layers: By chain rule, similar to BPTT (Sec. 5.1.4, Page 86)
2. NN's outputs in L2O are upper-bounded by **inputs** (Lemma 5.3.6, Theorem 5.3.7, Page 96-97)
Help us manipulate output of NN by the given inputs.
3. Gradient is Upper-Bounded by **Objective** (Theorem 5.3.11, page 98)
Help us derive bounding target ($F(X_T^0)$) from NN's gradient of training.
4. L2O is A Semi-Smooth to Its Parameters (Theorem 5.3.13, page 99)
Help us bound dynamic of sequence with dynamic of training parameters (gradient + learning rate).
5. Linear Convergence of L2O Training (Theorem 5.3.15, page 99-100)
Conditions:
 1. *L-1 layer's singular value is **lower-bounded** by non-negative constants.*
 2. *Learning rate is **upper-bounded** by L-1 layer's singular value.*



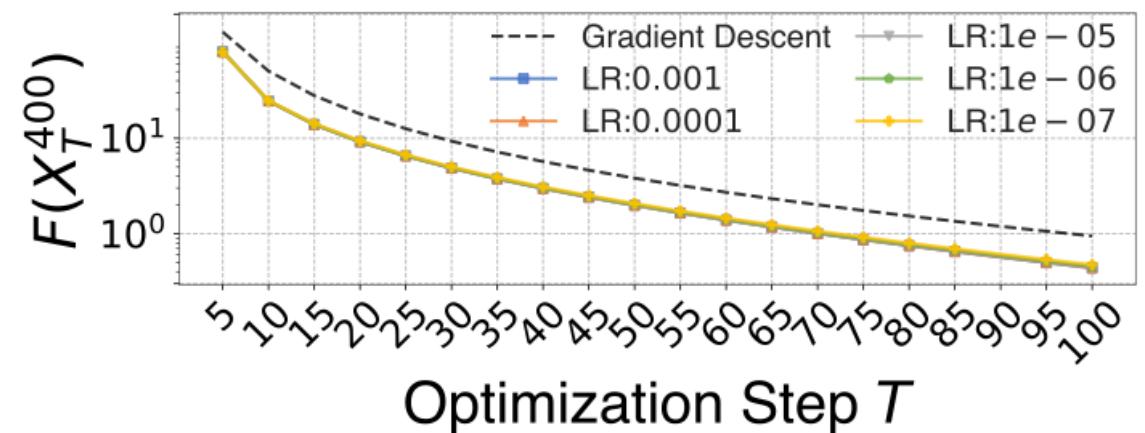
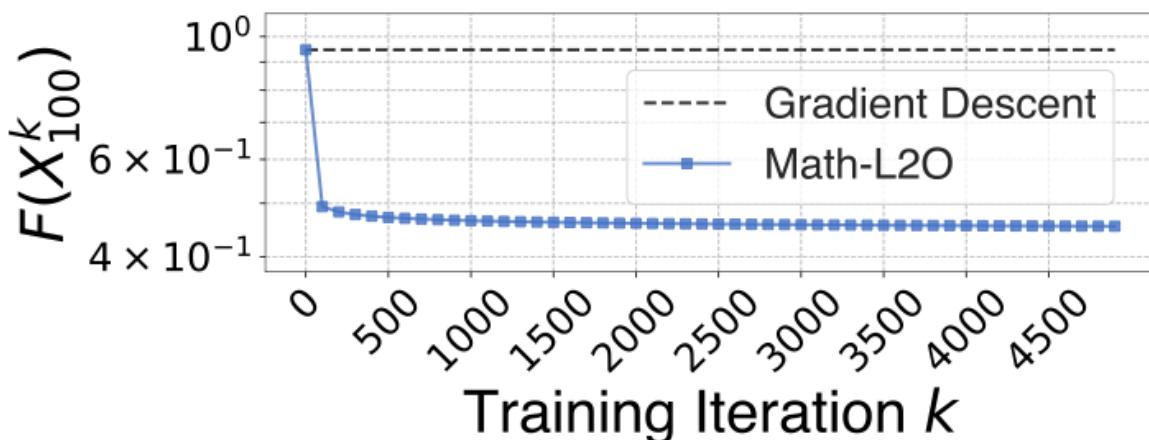
Design Part-III: Deterministic Initialization Method

1. Hold the conditions for linear training convergence rate.
2. Achieve convergence alignment.
 1. L2O generates step sizes of vanilla GD (alignment).
Let parameter matrix of last layer to be $\mathbf{0} + 2$ Sigmoid activation.
 2. Positive Singular Value
 - Non-Zero: Random generated thin matrix (transposed fat).
 - Positive: QR-decomposition + absolute operation.
 3. Enlarge Singular Value: Hold the Conditions of Linear Rate
 - Enlarge all entries of parameter matrices by a positive constant.
 - Proper positive constants : Lemmas 5.4.1-5.4.4 (pages 113-114).

Empirical Evaluation: Training Convergence

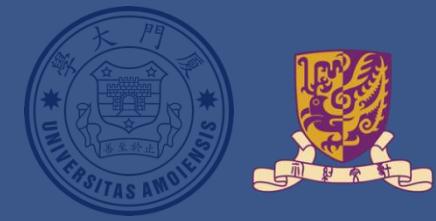


- Problem scale: Quadratic Programming, 512×400
- SOTA Unrolling:
 - Math-L2O [Liu et al., ICML 2023]
 - LISTA-CPSS [Chen et al., NeurIPS 2018]

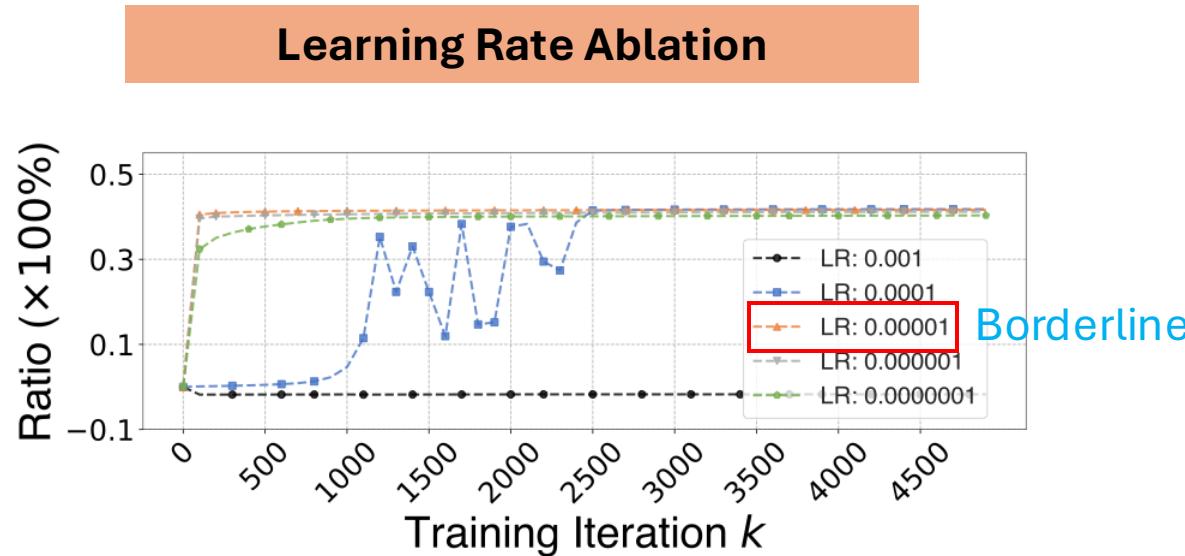


- All converge
- Robust to learning rate

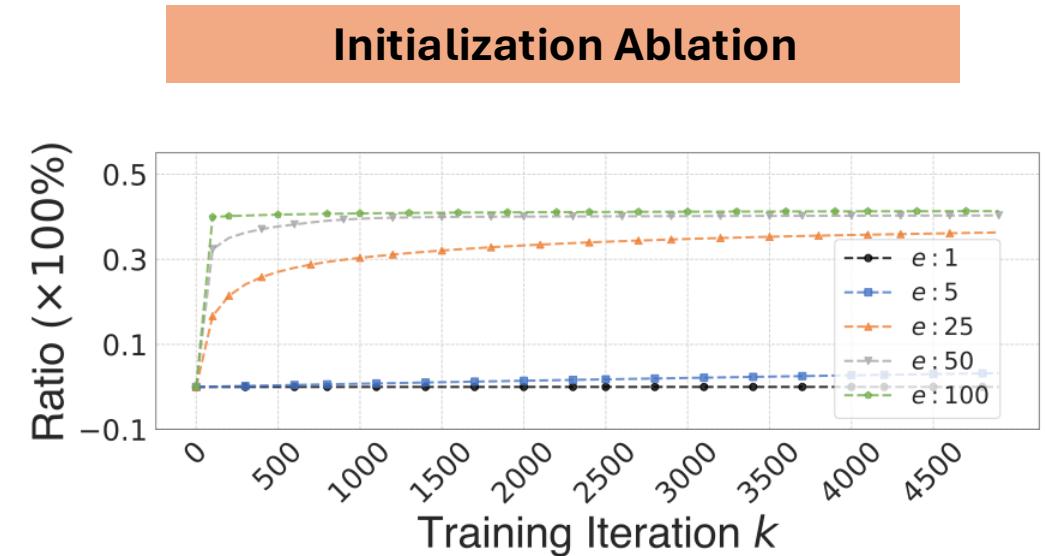
Empirical Evaluation: Ablation for Initialization and Learning Rate



- Small Scale: QP 32×25 .



- If LR is small enough, increasing LR improves convergence
- If LR is too large, convergence deteriorates.



- Increases singular value improves convergence

Thank You!

Project at <https://github.com/NetX-lab/MathL2OProof-Official>

Paper



Code



Opening!

We have:

1. Clear goal: Extend this work to a more general case.
2. Enough GPUs (for this project): 3090×4 .

We hope you are:

1. Interested in this project.
2. Good at Math (e.g., Math Competitions...)

If you are interested, drop me an email (qingyusong@xmu.edu.cn) or a WeChat message.