LancBiO: Dynamic Lanczos-aided Bilevel Optimization via Krylov Subspace

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March 30, 2025

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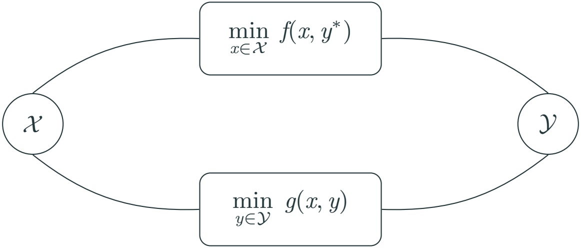
Bilevel Optimization (BiO) Problems

Standard formulation

Bilevel Optimization (BiO)

$$
\begin{aligned}
\min_{x \in \mathcal{X}} \quad & f(x, y^\star) \\
\text{s.t.} \quad & y^\star \in \arg\min_{y \in \mathcal{Y}} \; g(x, y)
\end{aligned}
$$

The nested structure couples the **upper level** and **lower level**



Applications

Model selection [Kunapuli et al., 2008; Giovannelli et al., 2021]

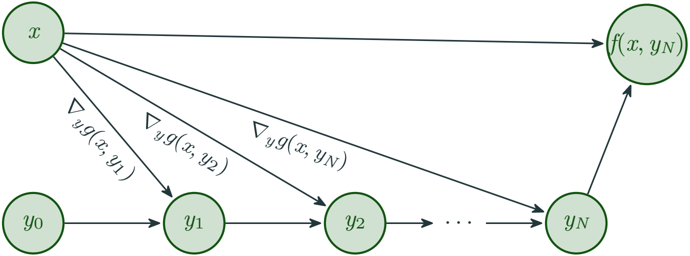
Hyper-parameters optimization [Franceschi et al., 2018; Bao et al., 2021]

Data poisoning [Liu et al., 2024]

Reinforcement learning [Hong et al., 2023; Chakraborty et al., 2024; Thoma et al., 2024; Yang et al., 2025]

...

Main idea



Existing works

- Algorithm Designs: [Domke, 2012; Franceschi et al., 2018; Shaban et al., 2019; Grazzi et al., 2020]
- Theoretical Analysis: [Ji, 2021; Gu and Huang, 2022; Zhang et al., 2024]

- Value function based reformulation:

$$\min_{x \in \mathcal{X}, y \in \mathcal{Y}} f(x, y), \qquad \text{s.t. } g(x, y) \leq g^*(x)$$

- Optimality condition based reformulation:

$$\min_{x \in \mathcal{X}, y \in \mathbb{R}^{d_y}} f(x, y), \qquad \text{s.t. } \nabla_y g(x, y) = 0$$

Algorithm	Objective functions		Reference
	Upper-Level	Lower-Level	
Smoothing PG	Smooth	Convex constraint	[Lin-Xu-Ye, 2014]
BOME	Smooth	PL	[Liu-Ye-Wright-Stone-Liu, 2022]
PBGD	Smooth	PL	[Shen-Chen, 2023]
F2SA	Smooth	Strongly Convex	[Kwon-Kwon-Wright-Nowak, 2023]
———	Slater's Constraint Qualification		[Dempe-Dutta, 2012]
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II. Reformulation based methods

- Value function based reformulation

$$\min_{x \in \mathcal{X}, y \in \mathcal{Y}} f(x, y), \qquad \text{s.t. } g(x, y) \le g^*(x)$$

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Scenario of interest: $g(x, \cdot)$ is strongly convex

$$y^*(x) = \arg\min_{y \in \mathbb{R}^{d_y}} g(x, y)$$

By optimality condition & implicit function theorem

$$0 \equiv \nabla_y g(x, y^*(x)) \Rightarrow \nabla^2_{xy} g(x, y^*(x)) + \nabla_x y^*(x)^\top \nabla^2_{yy} g(x, y^*(x)) = 0$$

Hyper-gradient computation

$$\begin{aligned} \nabla \phi(x) &:= \nabla f(x, y^\star(x)) \\ &= \nabla_x f(x, y^\star(x)) + \nabla_x y^\star(x)^\top \nabla_y f(x, y^\star(x)) \\ &= \nabla_x f(x, y^\star) - \nabla^2_{xy} g(x, y^\star) \left[\nabla^2_{yy} g(x, y^\star)\right]^{-1} \nabla_y f(x, y^\star) \end{aligned}$$

Hyper-gradient

$$\nabla\phi(x) = \nabla_x f(x, y^\star) - \nabla^2_{xy} g(x, y^\star) \left[\nabla^2_{yy} g(x, y^\star)\right]^{-1} \nabla_y f(x, y^\star)$$

Main difficulties

- Solving the lower-level problem to obtain $y^*(x)$
- ★ Approximating the **Hessian inverse vector product**

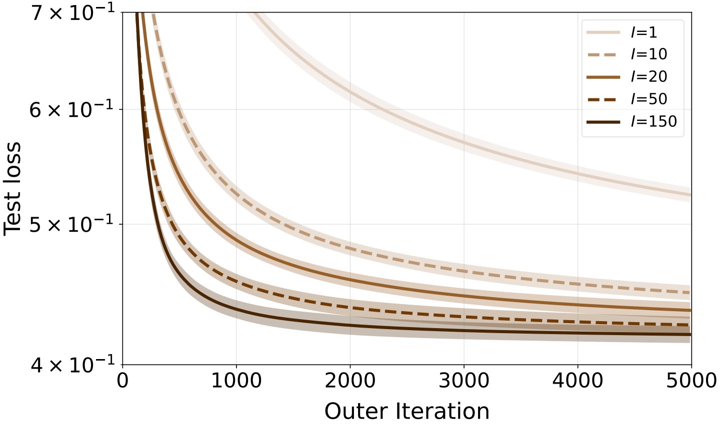
$$v^*(x) := \left[\nabla^2_{yy} g(x, y^*(x))\right]^{-1} \nabla_y f(x, y^*(x))$$

Vanilla update rule

$$\mathbf{1}\times : x^+ = x - \beta \left(\nabla_x f(x, y) - \nabla^2_{xy} g(x, y) \left[\nabla^2_{yy} g(x, y)\right]^{-1} \nabla_y f(x, y)\right)$$

$$\mathbf{N}\times : y^+ = y - \alpha \nabla_y g(x, y)$$

An observation



The more accurate v^*, the more enhanced descent!

How to tackle v^*: approximation principle

- Neumann Series approximation when $\rho(A) < 1$

$$A^{-1} = \sum_{i=0}^{\infty} (I - A)^i$$

[Ghadimi and Wang, 2018; Chen et al., 2021; Ji, 2021]

- At each iteration, solve a linear system approximatively:

$$\begin{aligned}
\mathbf{1}\times &: \nabla^2_{yy} g(x, y)\, v \approx \nabla_y f(x, y) \\
\mathbf{1}\times &: x^+ = x - \beta \left(\nabla_x f(x, y) - \nabla^2_{xy} g(x, y)\, v \right) \\
\mathbf{N}\times &: y^+ = y - \alpha \nabla_y g(x, y)
\end{aligned}$$

where v can be obtained by

- GD [Arbel and Mairal, 2022]
- CG [Yang et al., 2023]
- LS [Xiao et al., 2023]

How to tackle v^*: amortization principle

- Two time-scale **single** loop algorithm [Hong et al., 2020]

$$\mathbf{1}\times : x^+ = x - \beta_k \left(\nabla_x f(x, y) - \nabla^2_{xy} g(x, y) \left[\nabla^2_{yy} g(x, y) \right]^{-1} \nabla_y f(x, y) \right)$$

$$\mathbf{1}\times : y^+ = y - \alpha_k \nabla_y g(x, y)$$

- Dynamically approximate (**auxiliary**) variables [Dagréou et al., 2022]

$$\mathbf{1}\times : v^+ = v - \gamma \left(\nabla^2_{yy} g(x, y)\, v - \nabla_y f(x, y) \right)$$

$$\mathbf{1}\times : x^+ = x - \beta \left(\nabla_x f(x, y) - \nabla^2_{xy} g(x, y)\, v^+ \right)$$

$$\mathbf{1}\times : y^+ = y - \alpha \nabla_y g(x, y)$$

How to tackle the Hessian inverse vector product v^* in BiO

- Approximation principle
- Amortization principle

How to adhere to these two principles

- Subspace methods for efficient Approximation: [Yuan, 2014; Carmon and Duchi, 2018]
- Subspace iteration for reasonable Amortization: [Yuan, 1995; Saad, 2011]

A Subspace Technique

Revisit hyper-gradient

Recall the hyper-gradient

$$\nabla \phi(x_k) = \nabla_x f(x_k, y_k^\star) - \nabla^2_{xy} g(x_k, y_k^\star) \left[\nabla^2_{yy} g(x_k, y_k^\star) \right]^{-1} \nabla_y f(x_k, y_k^\star)$$

and its estimator

$$\widetilde{\nabla} \varphi(x_k, y_k, v_k) := \nabla_x f(x_k, y_k) - \nabla^2_{xy} g(x_k, y_k)\, v_k$$

Geometric interpretation

$$\min_{v \in \mathcal{S}_k} \; m_k(v) := \frac{1}{2} v^\top \nabla^2_{yy} g(x_k, y_k)\, v - \nabla_y f(x_k, y_k)^\top v$$

$$\mathcal{S}_k = \mathbb{R}^{d_y} \implies v_k = \nabla^2_{yy} g(x_k, y_k)^{-1} \nabla_y f(x_k, y_k) := A_k^{-1} b_k$$

Low-dimensional subspace?

Krylov subspace [Krylov, 1931]:

$$\mathcal{K}_N(A, b) := \operatorname{span}\left\{b, Ab, A^2 b, \dots A^{N-1} b\right\}$$

- $\mathcal{K}_N(A, b)$ provides a good estimate for $A^{-1}b$ [Carmon and Duchi, 2018]
- An observation

$$\mathcal{K}_N(A, b) = \mathcal{K}_N(I - \eta A, b)$$

Neumann series approximation

- When $\rho(\eta A) < 1$, for some $N \in \mathbb{N}$

$$A^{-1}b = \eta \sum_{i=0}^{\infty} (I - \eta A)^i b \in \mathcal{K}_N(A, b)$$

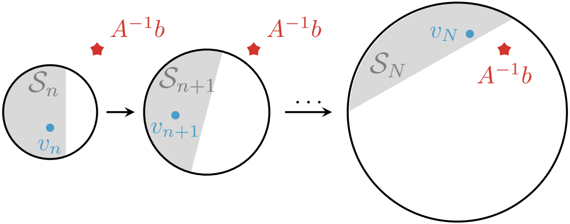
Constructing 2-D subspace in Krylov

Given $v_n \in \mathcal{K}_{\mathbf{n}}(A, b)$, an initial approximation of $A^{-1}b$

$$v_n = \sum_{i=0}^{n-1} c_i (I - \eta A)^i b \approx A^{-1} b$$

Recursively, we can choose

$$v_{n+1} \in \mathcal{S}_{n+1} := \operatorname{span}\{b, (I - \eta A) v_n\} \subseteq \mathcal{K}_{n+1}(A, b)$$



$$\mathcal{K}_n(A, b) \subseteq \mathcal{K}_{n+1}(A, b) \subseteq \cdots \subseteq \mathcal{K}_N(A, b)$$

Extend the thoughts in BiO context

- $A_k \approx A_{k-1}, b_k \approx b_{k-1}$ for consecutive iterations
- $\mathcal{S}_k = \operatorname{span}\{b_k, (I - \eta A_k) v_{k-1}\}$

SubBiO

$$\mathbf{1}\times : \mathcal{S}_k := \operatorname{span}\{b_k, (I - \eta A_k) v_{k-1}\}$$

$$\mathbf{1}\times : v_k := \underset{v \in \mathcal{S}_k}{\arg\min} \; m_k(v) := \frac{1}{2} v^T A_k v - b_k v$$

$$\mathbf{1}\times : x_{k+1} = x_k - \beta \left(\nabla_x f(x_k, y_k) - \nabla^2_{xy} g(x_k, y_y) \, v_k \right)$$

$$\mathbf{1}\times : y_{k+1} = y - \alpha \nabla_y g(x_k, y_k)$$

Two-dimensional subproblem

- Subproblem in SubBiO

$$\min_{z \in \mathbb{R}^2} \frac{1}{2} z^\top (S_k^\top A_k S_k) z - b_k^\top S_k z$$

☹ Projecting Hessian $S_k^T A_k S_k$ costs $O(\mathbf{2}n^2)$

- $A_k v_{k-1}$: $O(n^2)$
- $\nabla^2_{xy} g(x_k, y_k) v_k$: $O(n^2)$

SubBiO costs $O(\mathbf{4}n^2)$ per iteration!

A Dynamic Lanczos-aided Framework

- How to reduce $O(4n^2)$ while preserving the advantages of Krylov subspace?

Motivation

- How to reduce $O(4n^2)$ while preserving the advantages of Krylov subspace?
- Main computation comes from the projection of Hessian A_k

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- How to reduce $O(4n^2)$ while preserving the advantages of Krylov subspace?
- Main computation comes from the projection of Hessian A_k
- It's reasonable to consider the Lanczos Process

Lanczos iteration algorithm

Lanczos process [Lanczos, 1950] computes the eigenvalues and corresponding eigenvectors of symmetric matrix.

- Construct Krylov subspace

$$\mathcal{K}_k(A, b) = \operatorname{span}\left\{b, Ab, \ldots, A^{k-1}b\right\}$$

  and an orthogonal basis Q_k
- Project A to the Krylov subspace, $T_k = Q_k^T A Q_k$
- Compute eigenvalues and eigenvectors of T_k

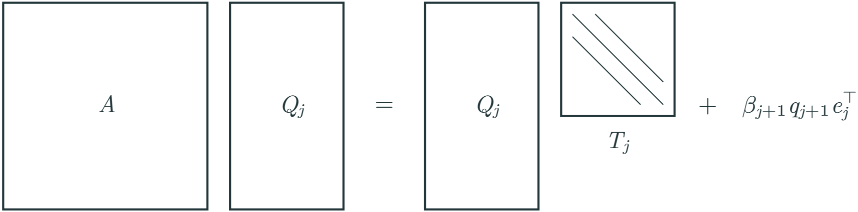
Goal

- Maintain an **orthogonal basis** $Q_j = [q_1, \ldots, q_j]$ of $\mathcal{K}_j(A, b)$
- Keep the (approximate) projection matrix T_j **tridiagonal**

Iterates

$$u_j = Aq_j - \beta_j q_{j-1} \qquad \alpha_j = q_j^\top u_j \qquad \omega_j = u_j - \alpha_j q_j$$
$$\beta_{j+1} = \|\omega_j\| \qquad q_{j+1} = \omega_j / \beta_{j+1}$$

Tridiagonalization



Dynamic Lanczos process in BiO

Core principles

- Incrementally construct subspaces $\mathcal{S}_k$
- Dynamically solve quadratic subproblems:

$$v_k := \arg\min_{v \in \mathcal{S}_k} \; m_k(v) := \frac{1}{2} v^T A_k v - b_k^T v$$

Adapt standard Lanczos process in BiO

$$\begin{aligned} u_j &= A_j q_j - \beta_j q_{j-1} \\ \alpha_j &= q_j^\top u_j \\ \omega_j &= u_j - \alpha_j q_j \\ \beta_{j+1} &= \|\omega_j\| \\ q_{j+1} &= \omega_j / \beta_{j+1} \end{aligned}$$

$$T_j = \left(\begin{array}{cc:c} \multicolumn{2}{c:}{T_{j-1}} & \mathbf{0} \\ \cdashline{3-3} & & \beta_j \\ \hdashline \mathbf{0} & \beta_j & \alpha_j \end{array} \right).$$

Lanczos process is inherently unstable!

[Paige, 1980; Meurant and Strakoš, 2006]

Two ”Res” strategies

Restart mechanism

- Restart subspaces each m steps
- Mitigate the accumulation of difference among $\{A_1, \ldots, A_k\}$

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Residual minimization

- Minimal residual subproblems

$$\min_{\Delta v \in \mathcal{S}_k} \|(b_k - A_k \bar{v}) - A_k \Delta v\|^2$$

- Correct current $\bar{v}$, $v_k = \bar{v} + \Delta v_k$
- Collect historical information

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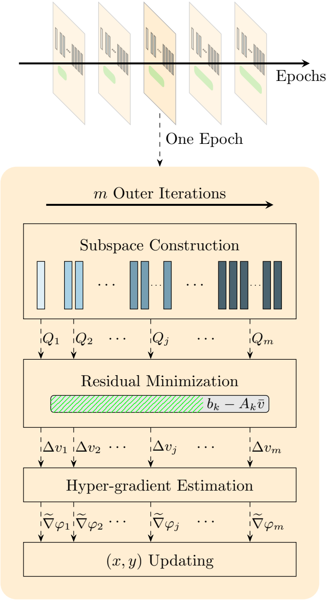


Computational complexity

- ☺Low-dimensional subproblems
- ☺No cost of Hessian projection
- LancBiO needs $O(\mathbf{2}n^2)$ instead of $O(4n^2)$ of SubBiO

Relation with existing work

Existing work [Ghadimi and Wang, 2018; Hong et al., 2020; Ji, 2021; Dagréou et al., 2022]

$$\text{stocBiO, TTSA, BSA}: v_k = \eta \sum_{i=0}^{N} (I - \eta A_k)^i b_k$$

$$\text{SOBA}: v_k = v_{k-1} - \eta (A_k v_{k-1} - b_k)$$

Ours

$$\text{SubBiO}: v_k = \arg\min_{v \in \mathcal{S}_k^{\mathrm{Sub}}} m_k(v) := \frac{1}{2} v^T A_k v - b_k v$$

$$\text{LancBiO}: v_k \approx \arg\min_{v \in \mathcal{S}_k^{\mathrm{Lanc}}} m_k(v) := \frac{1}{2} v^T A_k v - b_k v$$

Theoretical Analysis

Divide iterates into epochs of m-step dynamic Lanczos process

$$\varepsilon_{st}^{h} := \left(1 + \frac{L_{gx}}{\mu_g}\right) \|x_{mh+s} - x_{mh+t}\| + \|y_{mh+s} - y_{mh+s}^{*}\|$$

$$\varepsilon_{j}^{h} := \max_{1 \leq s,t \leq j} \varepsilon_{st}^{h}$$

Proposition

The dynamic Lanczos process in LancBiO with normalized q_1 and α_j, β_j, q_j satisfies

$$A_j^{*} Q_j = Q_j T_j + \beta_{j+1} q_{j+1} e_j^{\top} + \delta Q_j, \quad \text{for } j = 1, 2, \ldots, m,$$

with $\|\delta q_j\| \leq L_{gyy} \varepsilon_j$

Theorem

Within each epoch, set the step size $\theta \sim \mathcal{O}(1/m)$ for y and the step size for x as zero in the first m_0 steps, and the others as $\lambda \sim \mathcal{O}(1/m^4)$, then the iterates $\{x_k\}$ satisfy

$$\frac{m}{K(m-m_0)} \sum_{\substack{k=0,\\ (k \bmod m) > m_0}}^{K} \left\|\nabla \varphi\left(x_k\right)\right\|^2 = \mathcal{O}\left(\frac{m\lambda^{-1}}{K(m-m_0)}\right)$$

where m is the subspace dimension and $m_0 \sim \Omega(\log m)$

Numerical Experiments

Default settings

Compared methods

- **TTSA**: first single-loop algorithm [Hong et al., 2020]
- **stocBiO**: double-loop, truncated Neumann Series [Ji, 2021]
- **AmIGO**: double-loop, GD or CG [Arbel et al., 2022]
- **SOBA**: single-loop, auxiliary variable v [Dagréou et al., 2022]
- **F2SA**: penalty-based method [Kwon et al., 2023]
- **HJFBiO**: Hessian/Jacobian-free method [Huang, 2024]

Running platform

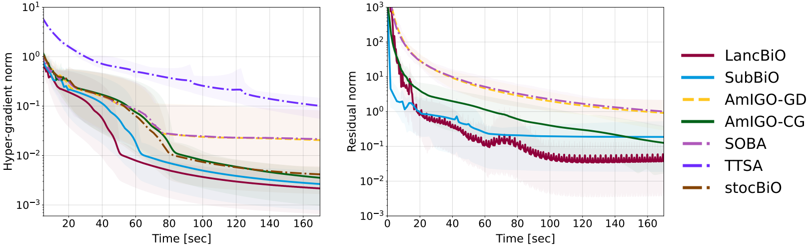
- Intel® Xeon® Gold 6330 CPUs & NVIDIA A800 GPU
- Python 3.8.0 + Pytorch 1.13.1

Synthetic problem

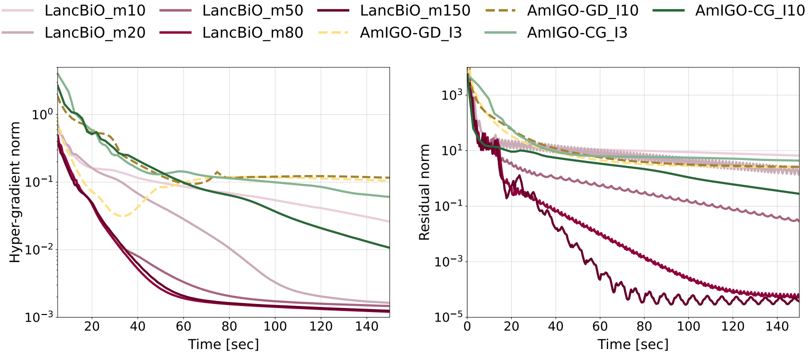
$$\min_{x \in \mathbb{R}^d} \quad f(x, y) := c_1 \cos\left(x^\top D_1 y\right) + \tfrac{1}{2} \left\| D_2 x - y \right\|^2,$$

$$\text{s. t.} \quad y^* = \arg\min_{y \in \mathbb{R}^d} g(x, y)$$

$$:= c_2 \sum_{i=1}^{d} \sin(x_i + y_i) + \log\left(\sum_{i=1}^{d} e^{x_i y_i}\right) + \frac{1}{2} y^\top \left(D_3 + G\right) y,$$



Influence of the subspace dimension m

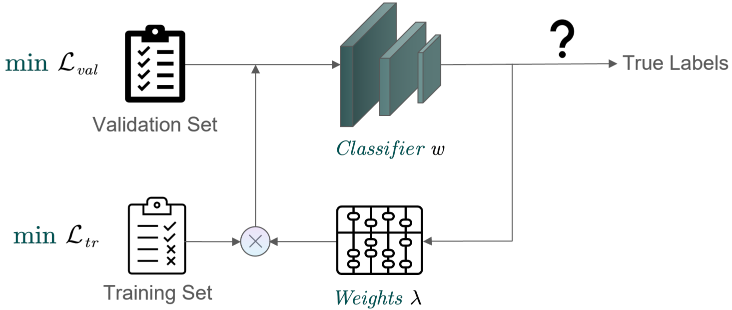


- ☺ Increases in m enhance the convergence of the residual norm
- ☺ When $m = 50$, the estimate of v^* is sufficiently accurate

Data hyper-cleaning

Goal: train a classifier in a corrupted setting where some labels of training data are replaced by random class numbers

- **Upper level**: data weights λ
- **Lower level**: classifier defined by deep nets w

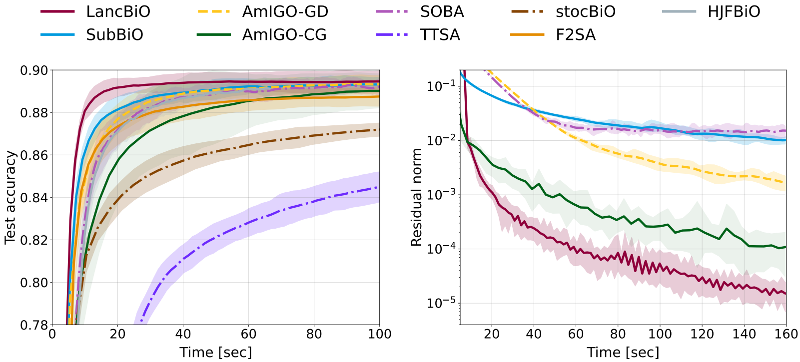


Goal: train a classifier in a corrupted setting where some labels of training data are replaced by random class numbers

BiO formulation:

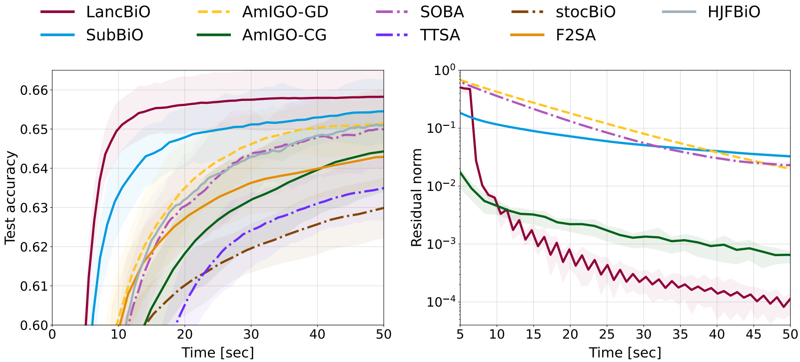
$$\begin{aligned}
\min_{\lambda} \quad & \mathcal{L}_{val}(\lambda, w^*) = \frac{1}{|\mathcal{D}_{\text{val}}|} \sum_{(x_i, y_i) \in \mathcal{D}_{\text{val}}} L(w^* x_i, y_i) \\
\text{s.t.} \quad & w^* = \arg\min_{w} \ \mathcal{L}_{tr}(w, \lambda) \\
& \quad := \frac{1}{|\mathcal{D}_{\text{tr}}|} \sum_{(x_i, y_i) \in \mathcal{D}_{\text{tr}}} \sigma(\lambda_i) L(w x_i, y_i) + C_r \|w\|^2
\end{aligned}$$

Test on MNIST (pollution rate=0.8)

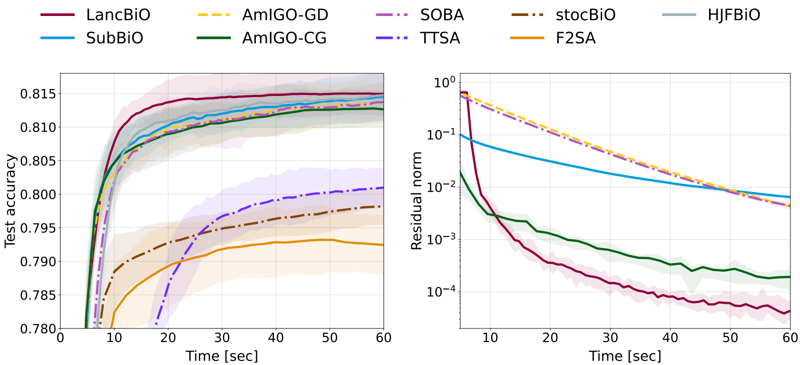


- ☺ LancBiO reaches the plateau fastest
- ☺ LancBiO achieves the lowest residual norm and best accuracy
- ☺ Hessian-vector products averages at $(1 + \frac{1}{m})$ per outer iteration

Test on Kuzushiji-MNIST (pollution rate=0.6)



Test on Fashion-MNIST (pollution rate=0.5)



Subspace-based methods exhibit robust performance

Conclusion and perspectives

Take-home notes

- First subspace technique in BiO
- Improved numerical performance
- Analysis to tackle instability of constructing Krylov subspaces in BiO
- Extension to stochastic settings

References

- **Yan Yang**, Bin Gao, Ya-xiang Yuan. *LancBiO: dynamic Lanczos-aided bilevel optimization via Krylov subspace.* ICLR (2025)
- Code is publicly available from https://github.com/UCAS-YanYang/LancBiO