Towards Constituting Mathematical Structures for Learning to Optimize

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(Most slides are generously shared by **Dr. Jialin Liu, Dr. Xiaohan Chen**, and **Dr. Wotao Yin**, Alibaba DAMO)

Outline

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Learning to Optimize

Consider an optimization problem

$$\min_{\mathbf{x} \in \mathbb{R}^n} F(\mathbf{x})$$

Instead of manually designing an iterative algorithm

$$\mathbf{x}_{k+1} = \mathcal{T}_F(\mathbf{x}_k)$$

One may learn an update rule from data

$$\mathbf{x}_{k+1} = \mathcal{T}_F(\mathbf{x}_k; \theta)$$

where the parameter θ is obtained by minimizing a *loss function*

$$\min_{\theta \in \Theta} \mathbb{E}_{F \in \mathcal{F}} L(\mathbf{x}_K(\theta))$$

The set $\mathcal{F}$ consists of all instances of interest.

The process of minimizing the loss function is named *training*.

Such methodology is named *Learning to Optimize (L2O)*.

Examples

Example I: Learned ISTA (LISTA) [Gregor and LeCun, 2010]

- LASSO: $\mathcal{F} = \{(1/2)\|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2 + \lambda\|\mathbf{x}\|_1 : \mathbf{A} \in \mathbb{R}^{m\times n}, \mathbf{b} \in \mathbb{R}^m\}$
- Choose a baseline algorithm ISTA: $\mathbf{x}_{k+1} = \mathrm{prox}_{\theta_k}(\mathbf{x}_k - \alpha_k \mathbf{A}^\top(\mathbf{A}\mathbf{x}_k - \mathbf{b}))$
- Parameterization: $\mathbf{x}_{k+1} = \mathrm{prox}_{\theta_k}(\mathbf{W}_{1,k}\mathbf{x}_k + \mathbf{W}_{2,k}\mathbf{b})$

Example II: Learning a rule for step size [Xiong et al., 2022]

- Deep learning:
  $\mathcal{F} = \{f(\mathbf{x}) : f$ is the loss function of training neural networks$\}$
- Choose a baseline algorithm SGD: $\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha_k \mathbf{g}_k$, where $\mathbf{g}_k$ is the stochastic gradient.
- Parameterization: $\alpha_k = \mathrm{NN}(\mathbf{x}_k, \mathbf{g}_k; \theta)$.

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- Parameterization: $\alpha_k = \mathrm{NN}(\mathbf{x}_k, \mathbf{g}_k; \theta)$.

Sample instances from $\mathcal{F}$ and Learn an algorithm.

The learned algorithm works well on unseen instances in $\mathcal{F}$.

Discussions and Motivations

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L2O provides a uniform tool to obtain customized algorithms without domain knowledge.

Questions:

- Can we find principles from learned algorithms?
- Can we use domain knowledge to regularize the models?

ML vs OPT

Machine learning (ML) is *induction*

- (problems, answers) are given for training
- ML learns to give answers in the future

Optimization (OPT) is *prescription*

- (problems, evaluations) are given, not answers
- OPT finds answers with best evaluations

Learning to optimize (L2O) combines ML and OPT to obtain “better” solutions “faster”, by learning from records of optimization.

Classic vs Learned

Classic OPT:

- Experts hand-built algorithms based on theory and experience
  For example, Simplex Method and Nesterov Accelerated Gradient Method
- Algorithms are written as iterations in a few lines
- Practitioners pick an algorithm to use

L2O:

- Experts propose L2O templates and training procedures
- Practitioners
  - pick an L2O template
  - prepare training data
  - apply a training procedure

  $\rightarrow$ obtain a trained algorithm for future problems
- Practitioners are more involved in the design process

Papers and Coauthors

This talk is based on the following articles:

- J. Liu, X. Chen, Z. Wang, W. Yin, and H. Cai. "Towards Constituting Mathematical Structures for Learning to Optimize." ICML 2023.
- X. Chen, J. Liu, Z. Wang, and W. Yin. "Hyperparameter Tuning is All You Need for LISTA." NeurIPS 2021.
- J. Liu, X. Chen, Z. Wang, and W. Yin. "ALISTA: Analytic weights are as good as learned weights in LISTA." ICLR 2019.
- X. Chen, J. Liu, Z. Wang, and W. Yin. "Theoretical Linear Convergence of Unfolded ISTA and its Practical Weights and Thresholds." NeurIPS 2018.

Outline

LASSO and ISTA

LASSO: assume $\mathbf{b} = \mathbf{A}\mathbf{x}_* +$ noise; recover $\mathbf{x}_*$ by solving

$$\min_{\mathbf{x}} \frac{1}{2}\|\mathbf{A}\mathbf{x} - \mathbf{b}\|_2^2 + \lambda\|\mathbf{x}\|_1$$

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Iterative soft-thresholding algorithm (ISTA):

$$\mathbf{x}_{k+1} = \eta_{\lambda\alpha}\left(\mathbf{x}_k - \alpha\mathbf{A}^\top(\mathbf{A}\mathbf{x}_k - \mathbf{b})\right)$$

- convergence requires a proper stepsize α or line search
- the gradient-descent step reduces $\frac{1}{2}\|\mathbf{A}\mathbf{x} - \mathbf{b}\|^2$
- the soft-thresholding step $\eta_{\lambda\alpha}(\cdot)$ reduces $\lambda\|\mathbf{x}\|_1$

Learned ISTA [Gregor and LeCun, 2010]

Introduce scalar $\theta = \lambda\alpha$ and matrices $\mathbf{W}_1 = \alpha\mathbf{A}^\top$ and $\mathbf{W}_2 = \mathbf{I} - \alpha\mathbf{A}^\top\mathbf{A}$.

Rewrite ISTA as

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Rewrite ISTA as

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Introduce $\theta_k, \mathbf{W}_{1,k}, \mathbf{W}_{2,k}$, $k = 0, 1, \ldots, K-1$, as free parameters and define

$$\mathbf{x}_{k+1} = \eta_{\theta_k}(\mathbf{W}_{1,k}\mathbf{b} + \mathbf{W}_{2,k}\mathbf{x}_k), \quad k = 0, 1, \cdots, K-1.$$

Once $\{\theta_k, \mathbf{W}_{1,k}, \mathbf{W}_{2,k}\}_{k=0}^{K-1}$ are determined, we obtain a new algorithm.

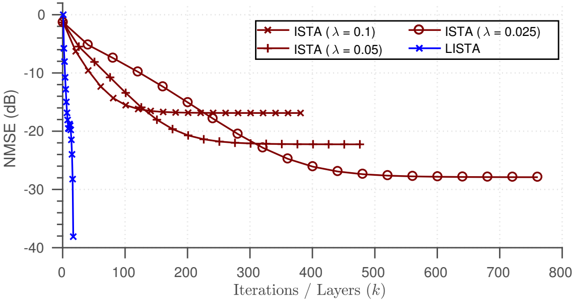
Find parameters such that the algorithm converges very fast for a set of LASSO instances with the same $\mathbf{A}$.

Fix random matrix $\mathbf{A}$, generate a set of sparse $\mathbf{x}_{*,i}$, with varying supports, and $\mathbf{b}_i = \mathbf{A}\mathbf{x}_{*,i} + \text{noise}_i$. Form the training set $\mathcal{F} = \{(\mathbf{x}_{*,i}, \mathbf{b}_i)\}$.

Fix a small $K > 0$, and train the parameters by applying SGD to

$$\min_{\{\theta_k, \mathbf{W}_{1,k}, \mathbf{W}_{2,k}\}_{k=0}^{K-1}} \mathbb{E}_{(\mathbf{x}_*, \mathbf{b}) \in \mathcal{F}} \left\| \mathbf{x}_K(\mathbf{b}) - \mathbf{x}_* \right\|_2^2 .$$

After the NN is trained with $K = 16$:



The trained NN is called Learned ISTA (LISTA).

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Theorem

Assume no noise. If LISTA has $\mathbf{x}_k \to \mathbf{x}_*$ as $k \to \infty$ uniformly for all sparse $\mathbf{x}_*$, then the parameters $\{\theta_k, \mathbf{W}_{1,k}, \mathbf{W}_{2,k}\}_{k=0}^{\infty}$ must satisfy the relation

$$\mathbf{W}_{2,k} + \mathbf{W}_{1,k}\mathbf{A} \to \mathbf{I}, \quad \text{as } k \to \infty.$$

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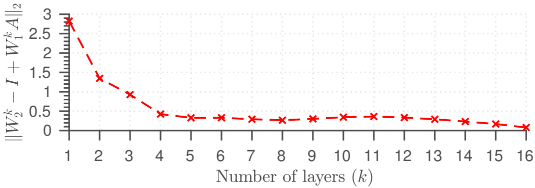
Indeed, training confirms the claims:



Therefore, we enforce

$$\mathbf{W}_{2,k} = \mathbf{I} - \mathbf{W}_{1,k}\mathbf{A},$$

for all k, yielding the iteration:

$$\mathbf{x}_{k+1} = \eta_{\theta_k}(\mathbf{x}_k + \mathbf{W}_{1,k}(\mathbf{b} - \mathbf{A}\mathbf{x}_k)).$$

We call it *weight coupling (CP).*

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Parameters

$$\mathcal{O}(n^2K + mnK) \xrightarrow{\text{reduce}} \mathcal{O}(mnK),$$

significant reduction if $m < n$ (which is often the case).

After this reduction, training also appears to be more stable.

Empirical Settings

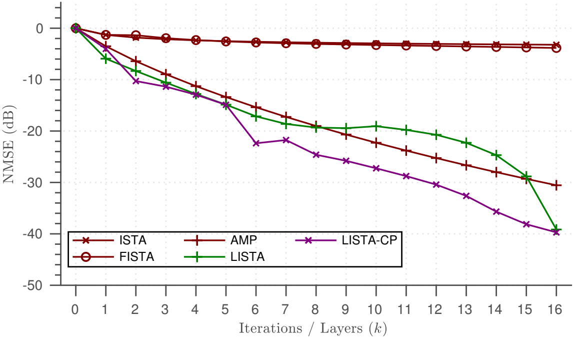
Normalized MSE (NMSE) in dB:

$$\mathrm{NMSE}(\hat{\mathbf{x}}, \mathbf{x}_*) = 20 \log_{10} \left(\|\hat{\mathbf{x}} - \mathbf{x}_*\|_2 / \|\mathbf{x}_*\|_2 \right)$$

Tests:

- $m = 250$, $n = 500$, sparsity $s \approx 50$.
- $\mathbf{A}_{ij} \sim \mathcal{N}(0, 1/\sqrt{m})$, iid. $\mathbf{A}$ is column-normalized.
- Magnitudes were sampled from standard Gaussian.

Weight coupling (CP)



CP stabilizes intermediate results.

Same final recovery quality.

Outline

A general L2O model

Consider $\min_{\mathbf{x}\in\mathbb{R}^n} F(\mathbf{x})$.

A baseline manually designed algorithm: gradient descent with momentum:

$$\begin{aligned}\mathbf{v}_{k+1} =& \beta_k \mathbf{v}_k + (1-\beta_k)\nabla F(\mathbf{x}_k),\\ \mathbf{x}_{k+1} =& \mathbf{x}_k - \alpha_k \mathbf{v}_{k+1}, \qquad k = 0,1,2,\ldots\end{aligned}$$

Andrychowicz et al. [2016] proposed to learn a parameterized algorithm:

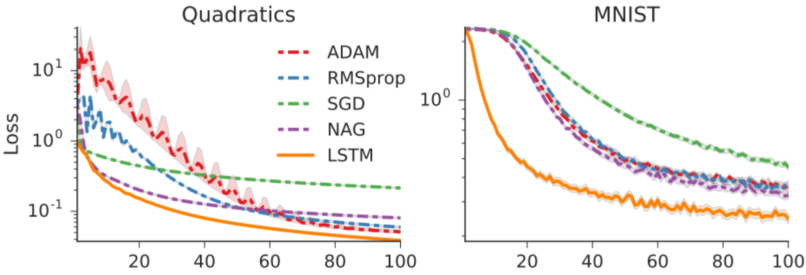
$$\begin{aligned}\mathbf{d}_k, \mathbf{h}_k =& \mathrm{LSTM}\Big(\mathbf{x}_k, \nabla F(\mathbf{x}_k), \mathbf{h}_{k-1}; \phi\Big)\\ \mathbf{x}_{k+1} =& \mathbf{x}_k - \mathbf{d}_k\end{aligned}$$

by minimizing a loss function

$$\min_{\phi} \mathbb{E}_{F\in\mathcal{F}} \sum_{k=1}^{K} F(\mathbf{x}_k)$$

Term “LSTM” means a long short-term memory cell.

Numerical results



Some discussions

Observation: The learned update rule may diverge on unseen instances.
This is still an active topic in the literature. [Wichrowska et al., 2017, Wu et al., 2018, Metz et al., 2019, Chen et al., 2020, Harrison et al., 2022, Metz et al., 2022]

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Preparations:

- Assumptions on the objective function F:

(Smooth case) $F(\mathbf{x}) = f(\mathbf{x})$, where f is convex and differentiable with Lipschitz continuous gradient
(Nonsmooth case) $F(\mathbf{x}) = r(\mathbf{x})$, where r is proper, closed and convex.
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- Assumptions on the update direction $\{\mathbf{d}_k\}$

Basic settings for smooth case

The update direction $\mathbf{d}_k$ is generated by $\mathrm{LSTM}\big(\mathbf{x}_k, \nabla f(\mathbf{x}_k), \mathbf{h}_{k-1}; \phi\big)$

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Let's consider a more general update rule

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \mathbf{d}_k(\mathbf{x}_k, \nabla f(\mathbf{x}_k))$$

where $\mathbf{d}_k$ is an operator picked from

$$\mathcal{D}_C(\mathbb{R}^{2n}) = \Big\{\mathbf{d} : \mathbb{R}^{2n} \to \mathbb{R}^n \;\Big|\; \mathbf{d} \text{ is differentiable, } \|\mathrm{J}\mathbf{d}(\mathbf{z})\|_{\mathrm{F}} \le C,\ \forall \mathbf{z} \in \mathcal{Z}\Big\}.$$

- Training needs derivatives of $\mathbf{d}_k$.
- Many existing parameterization approaches yield $\mathbf{d}_k \in \mathcal{D}_C(\mathbb{R}^{2n})$.

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- (Asympototic Fixed Point Condition) Formally, we relax it and assume

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The two assumptions are coined as *(GC)* and *(FP)*, respectively.

A Preliminary Result

Theorem

For any f and any operator sequence $\{\mathbf{d}_k\}_{k=0}^{\infty}$ that satisfies (GC) and (FP), there exist $\mathbf{P}_k \in \mathbb{R}^{n\times n}$ and $\mathbf{b}_k \in \mathbb{R}^n$ satisfying

$$\mathbf{d}_k(\mathbf{x}_k, \nabla f(\mathbf{x}_k)) = \mathbf{P}_k \nabla f(\mathbf{x}_k) + \mathbf{b}_k,$$

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- A "good" update rule is not totally free.
- It covers many optimization algorithms, such as accelerated GD, quasi-Newton methods, etc.
- Instead of learning $\mathbf{d}_k$, one may learn a *preconditioner* $\mathbf{P}_k$ and a *bias* $\mathbf{b}_k$

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \mathbf{P}_k\big(\mathbf{x}_k; \phi\big)\nabla f(\mathbf{x}_k) - \mathbf{b}_k\big(\mathbf{x}_k; \psi\big),$$

Nonsmooth case

On nonsmooth problems $\min_{\mathbf{x}} r(\mathbf{x})$, a direct extension to gradient descent is sub-gradient descent: $\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha_k \mathbf{g}_k,\ \mathbf{g}_k \in \partial r(\mathbf{x}_k)$.

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An implicit rule like proximal point algorithm (PPA) converges much better:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha_k \mathbf{g}_{k+1}, \quad \mathbf{g}_{k+1} \in \partial r(\mathbf{x}_{k+1}).$$

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On nonsmooth problems $\min_{\mathbf{x}} r(\mathbf{x})$, a direct extension to gradient descent is sub-gradient descent: $\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha_k \mathbf{g}_k,\ \mathbf{g}_k \in \partial r(\mathbf{x}_k)$.

Such explicit rule suffers from convergence issues.

An implicit rule like proximal point algorithm (PPA) converges much better:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \alpha_k \mathbf{g}_{k+1}, \quad \mathbf{g}_{k+1} \in \partial r(\mathbf{x}_{k+1}).$$

Back to L2O, we choose an implicit rule:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \mathbf{d}_k(\mathbf{x}_{k+1}, \mathbf{g}_{k+1}), \quad \mathbf{g}_{k+1} \in \partial r(\mathbf{x}_{k+1}).$$

Implicit rule:

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \mathbf{d}_k(\mathbf{x}_{k+1}, \mathbf{g}_{k+1}), \quad \mathbf{g}_{k+1} \in \partial r(\mathbf{x}_{k+1}). \tag{1}$$

Theorem

For each r and any $\{\mathbf{d}_k\}_{k=0}^{\infty}$ that satisfies (GC) and (FP), there exist $\mathbf{P}_k \in \mathbb{R}^{n\times n}$ and $\mathbf{b}_k \in \mathbb{R}^n$ such that (1) *yields*

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \mathbf{P}_k \mathbf{g}_{k+1} - \mathbf{b}_k, \quad \mathbf{g}_{k+1} \in \partial r(\mathbf{x}_{k+1}),$$

with $\mathbf{P}_k$ is bounded and $\mathbf{b}_k \to \mathbf{0}$ as $k \to \infty$. If we further assume $\mathbf{P}_k \succ \mathbf{0}$, $\mathbf{x}_{k+1}$ can be uniquely determined through $\mathbf{x}_{k+1} = \mathbf{prox}_{r,\mathbf{P}_k}(\mathbf{x}_k - \mathbf{b}_k)$.

The proximal operator $\mathbf{prox}_{r,\mathbf{P}_k}$ is defined with $\mathbf{prox}_{r,\mathbf{P}}(\bar{\mathbf{x}}) := \arg\min_{\mathbf{x}} r(\mathbf{x}) + \frac{1}{2}\|\mathbf{x}-\bar{\mathbf{x}}\|^2_{\mathbf{P}^{-1}}$.

- Global Convergence and Asymptotic Fixed Point Condition imply (1) yields a structure.
- A generalized proximal point algorithm. Fix $\mathbf{P}_k = \alpha\mathbf{I}, \mathbf{b}_k = \mathbf{0}$, it reduces to PPA.

Composite Case

Consider the composite case $\min_{\mathbf{x}} f(\mathbf{x}) + r(\mathbf{x})$. We analyze a mixed rule

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \mathbf{d}_k(\mathbf{x}_k, \nabla f(\mathbf{x}_k), \mathbf{x}_{k+1}, \mathbf{g}_{k+1}), \quad \mathbf{g}_{k+1} \in \partial r(\mathbf{x}_{k+1}). \tag{2}$$

Theorem

For any $f, r, \{\mathbf{d}_k\}_{k=0}^{\infty}$ that satisfies (GC) and (FP), there exist $\mathbf{P}_k \in \mathbb{R}^{n\times n}$ and $\mathbf{b}_k \in \mathbb{R}^n$ such that (2) *yields*

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \mathbf{P}_k(\nabla f(\mathbf{x}_k) - \mathbf{g}_{k+1}) - \mathbf{b}_k, \;\; \mathbf{g}_{k+1} \in \partial r(\mathbf{x}_{k+1}),$$

with $\mathbf{P}_k$ is bounded and $\mathbf{b}_k \to \mathbf{0}$ as $k \to \infty$. If we further assume $\mathbf{P}_k \succ \mathbf{0}$, $\mathbf{x}_{k+1}$ can be uniquely determined given $\mathbf{x}_k$ through

$$\mathbf{x}_{k+1} = \mathbf{prox}_{r,\mathbf{P}_k}(\mathbf{x}_k - \mathbf{P}_k \nabla f(\mathbf{x}_k) - \mathbf{b}_k). \tag{3}$$

With $\mathbf{P}_k = \alpha \mathbf{I}, \mathbf{b}_k = \mathbf{0}$, (3) reduces to Proximal Gradient Descent (PGD).

Longer Horizen

Introduce an extra variable $\mathbf{y}_k$ that encodes historical information

$$\mathbf{y}_k = \mathbf{m}(\mathbf{x}_k, \mathbf{x}_{k-1}, \cdots, \mathbf{x}_{k-T}).$$

Insert $\mathbf{y}_k$ to the previous update rule

$$\mathbf{x}_{k+1} = \mathbf{x}_k - \mathbf{d}_k(\mathbf{x}_k, \nabla f(\mathbf{x}_k), \mathbf{x}_{k+1}, \mathbf{g}_{k+1}, \mathbf{y}_k, \nabla f(\mathbf{y}_k)), \quad \mathbf{g}_{k+1} \in \partial r(\mathbf{x}_{k+1})$$

Theorem

Suppose $T = 1$. For any $f, r, \mathbf{m}, \{\mathbf{d}_k\}_{k=0}^{\infty}$ that satisfies (GC) and (FP), there exist $\mathbf{P}_{1,k}, \mathbf{P}_{2,k}, \mathbf{A}_k \in \mathbb{R}^{n\times n}$ and $\mathbf{b}_{1,k}, \mathbf{b}_{2,k} \in \mathbb{R}^n$ satisfying

$$\begin{aligned}
\mathbf{x}_{k+1} &= \mathbf{x}_k - (\mathbf{P}_{1,k} - \mathbf{P}_{2,k})\nabla f(\mathbf{x}_k) - \mathbf{P}_{2,k}\nabla f(\mathbf{y}_k) - \mathbf{b}_{1,k} \\
&\qquad - \mathbf{P}_{1,k}\mathbf{g}_{k+1} - \mathbf{B}_k(\mathbf{y}_k - \mathbf{x}_k), \ \mathbf{g}_{k+1} \in \partial r(\mathbf{x}_{k+1}), \\
\mathbf{y}_{k+1} &= (\mathbf{I} - \mathbf{A}_k)\mathbf{x}_{k+1} + \mathbf{A}_k\mathbf{x}_k + \mathbf{b}_{2,k}
\end{aligned}$$

for all $k = 0, 1, 2, \cdots$, with $\{\mathbf{P}_{1,k}, \mathbf{P}_{2,k}, \mathbf{A}_k\}$ bounded and $\mathbf{b}_{1,k} \to \mathbf{0}, \mathbf{b}_{2,k} \to \mathbf{0}$ as $k \to \infty$.

L2O Model and Parameterization

If we further assume $\mathbf{P}_{1,k}$ is uniformly symmetric positive definite, then we can substitute $\mathbf{P}_{2,k}\mathbf{P}_{1,k}^{-1}$ with $\mathbf{B}_k$ and obtain

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\hat{\mathbf{x}}_k &= \mathbf{x}_k - \mathbf{P}_{1,k}\nabla f(\mathbf{x}_k), \\
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\end{aligned}$$

We suggest using diagonal matrices for $\mathbf{P}_{1,k}, \mathbf{B}_k, \mathbf{A}_k$ in practice:

$$\mathbf{P}_{1,k} = \mathrm{diag}(\mathbf{p}_k), \quad \mathbf{B}_k = \mathrm{diag}(\mathbf{b}_k), \quad \mathbf{A}_k = \mathrm{diag}(\mathbf{a}_k),$$

where $\mathbf{p}_k, \mathbf{b}_k, \mathbf{a}_k \in \mathbb{R}^n$ are vectors.

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$$

where $\mathbf{p}_k, \mathbf{b}_k, \mathbf{a}_k \in \mathbb{R}^n$ are vectors.

We model $\mathbf{p}_k$, $\mathbf{a}_k$, $\mathbf{b}_k$, $\mathbf{b}_{1,k}$, $\mathbf{b}_{2,k}$ as the output of LSTM:

$$
\begin{aligned}
\mathbf{o}_k, \mathbf{h}_k &= \mathrm{LSTM}\Big(\mathbf{x}_k, \nabla f(\mathbf{x}_k), \mathbf{h}_{k-1}; \phi_{\mathsf{LSTM}}\Big),\\
\mathbf{p}_k, \mathbf{a}_k, \mathbf{b}_k, \mathbf{b}_{1,k}, \mathbf{b}_{2,k} &= \mathrm{MLP}(\mathbf{o}_k; \phi_{\mathsf{MLP}}).
\end{aligned}
$$

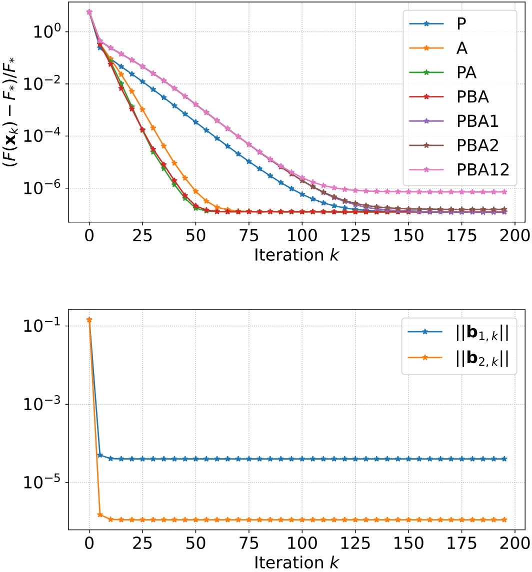
Ablation Study

We compare

- **PBA12**: $\mathbf{p}_k$,$\mathbf{a}_k$,$\mathbf{b}_k$,$\mathbf{b}_{1,k}$,$\mathbf{b}_{2,k}$ are all learnable.
- **PBA1**: $\mathbf{p}_k$,$\mathbf{a}_k$,$\mathbf{b}_k$,$\mathbf{b}_{1,k}$ are learnable; $\mathbf{b}_{2,k} = \mathbf{0}$.
- **PBA2**: $\mathbf{p}_k$,$\mathbf{a}_k$,$\mathbf{b}_k$,$\mathbf{b}_{2,k}$ are learnable; $\mathbf{b}_{1,k} = \mathbf{0}$.
- **PBA**: $\mathbf{p}_k$,$\mathbf{a}_k$,$\mathbf{b}_k$ are learnable; $\mathbf{b}_{2,k} = \mathbf{b}_{1,k} = \mathbf{0}$.
- **PA**: $\mathbf{p}_k$,$\mathbf{a}_k$ are learnable; $\mathbf{b}_{2,k} = \mathbf{b}_{1,k} = \mathbf{0}$; $\mathbf{b}_k = \mathbf{1}$.
- **P**: only $\mathbf{p}_k$ is learnable; $\mathbf{a}_k = \mathbf{b}_{2,k} = \mathbf{b}_{1,k} = \mathbf{0}$; $\mathbf{b}_k = \mathbf{1}$.
- **A**: only $\mathbf{a}_k$ is learnable; $\mathbf{b}_{2,k} = \mathbf{b}_{1,k} = \mathbf{0}$; $\mathbf{b}_k = \mathbf{1}$; $\mathbf{p}_k = (1/L)\mathbf{1}$.

on more challenging LASSO settings: $\mathbf{A}$ is not fixed; each LASSO instance takes an independently generated $\mathbf{A}$.

Ablation study: Results



Final model

We adopt (**PA**) and fix $\mathbf{b}_{1,k} = \mathbf{b}_{2,k} = \mathbf{0}$ and $\mathbf{b}_k = \mathbf{1}$.

$$
\begin{aligned}
\mathbf{o}_k, \mathbf{h}_k &= \mathrm{LSTM}\Big(\mathbf{x}_k, \nabla f(\mathbf{x}_k), \mathbf{h}_{k-1}; \phi_{\mathsf{LSTM}}\Big), \\
\mathbf{p}_k, \mathbf{a}_k &= \mathrm{MLP}(\mathbf{o}_k; \phi_{\mathsf{MLP}}), \\
\mathbf{x}_{k+1} &= \mathbf{prox}_{r,\mathbf{p}_k}\Big(\mathbf{y}_k - \mathbf{p}_k \odot \nabla f(\mathbf{y}_k)\Big), \\
\mathbf{y}_{k+1} &= \mathbf{x}_{k+1} + \mathbf{a}_k \odot (\mathbf{x}_{k+1} - \mathbf{x}_k).
\end{aligned}
$$

Instead of learning the update rule, we suggest learning a preconditioner $\mathbf{p}_k$ and an accelerator $\mathbf{a}_k$.

Comparison: In-Distribution Test

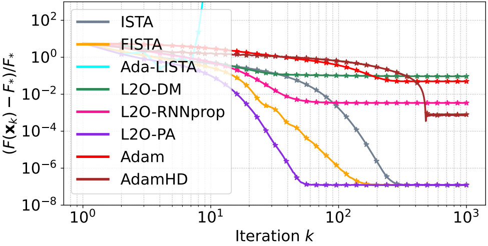


Figure: LASSO: Train and test on synthetic data.

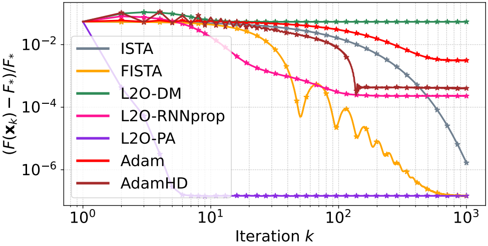


Figure: Logistic: Train and test on synthetic data.

Comparison: Out-of-Distribution Test

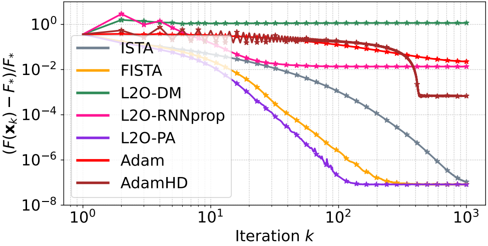


Figure: LASSO: Train on synthetic data and test on real data (BSDS500).

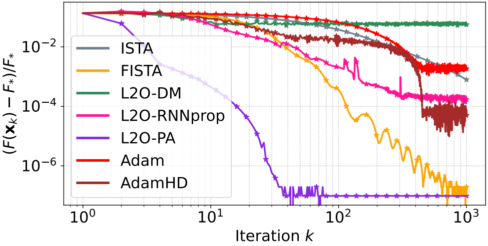


Figure: Logistic: Train on synthetic data and test on real data (Ionosphere).

Outline

Further analysis

Recall LISTA-CP model:

$$\mathbf{x}_{k+1} = \eta_{\theta_k}(\mathbf{x}_k - \mathbf{W}_{1,k}(\mathbf{A}\mathbf{x}_k - \mathbf{b})).$$

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Assume $\mathbf{b} = \mathbf{A}\mathbf{x}_* +$ noise, where $\mathrm{supp}(\mathbf{x}_*)$ is uniformly distributed.

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Assume $\mathbf{b} = \mathbf{A}\mathbf{x}_* +$ noise, where $\mathrm{supp}(\mathbf{x}_*)$ is uniformly distributed.

Liu et al. [2019] shows that the recovery error and convergence rate only depend on

$$\sup_k \max_{1 \le i \ne j \le n} |\mathbf{w}_{i,k}^\top \mathbf{a}_j|$$

- $\mathbf{w}_{i,k}$ is the i-th column of $\mathbf{W}_{1,k}$; $\mathbf{a}_j$ is the j-th column of $\mathbf{A}$.
- $\mathbf{W}_{1,k}$ are scaled such that $\mathbf{w}_{i,k}^\top \mathbf{a}_i = 1$ for all $i = 1, 2, \cdots, n$.
- One might minimize the non-diagonal terms of $\mathbf{W}_{1,k}^\top \mathbf{A}$ independently for each k.
- An extension to *mutual coherence* in compressive sensing.

Parameter reduction: tie W_1 across iterations

Inspired by the analysis, let us try $\mathbf{W}_{1,k}$ tied for all k. Write it as $\mathbf{W}$.

- Tied LISTA (TiLISTA) iteration:

$$\mathbf{x}_{k+1} = \eta_{\theta_k}(\mathbf{x}_k - \gamma_k \mathbf{W}^\top(\mathbf{A}\mathbf{x}_k - \mathbf{b})).$$

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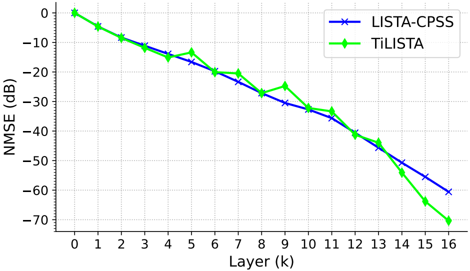
Parameters:

$$\mathcal{O}(mnK) \xrightarrow{\text{reduce}} \mathcal{O}(mn + K),$$

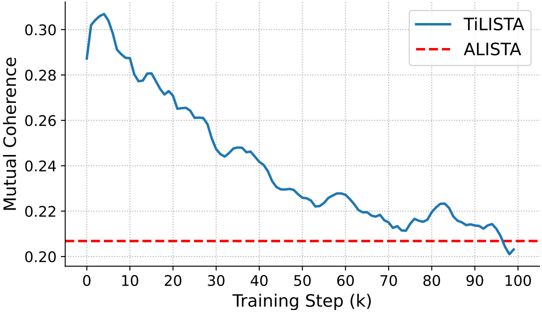
We learn only step sizes $\{\gamma_k\}_k$ and thresholds $\{\theta_k\}_k$ and a single matrix $\mathbf{W}$.



TiLISTA works even slightly better than LISTA-CPSS

Observation

We scale $\mathbf{W}$ such that $\mathbf{w}_i^\top \mathbf{a}_i = 1$ for $i = 1, \ldots, n$ and then measure $\max_{1 \leq i \neq j \leq n} |\mathbf{w}_i^\top \mathbf{a}_j|$ in TiLISTA. Compare it to ALISTA (next slide).



Good W needs to have small mutual coherence to A.

Analytic LISTA (ALISTA)

We use this principle to determine $\mathbf{W}$ *without training* [Liu et al., 2019] .

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Two steps:

1. Compute approximately optimal $\tilde{\mathbf{W}}$:

$$\tilde{\mathbf{W}} \in \underset{\mathbf{W} \in \mathbb{R}^{m \times n}}{\operatorname{argmin}} \left\| \mathbf{W}^\top \mathbf{A} \right\|_F^2, \text{ s.t. } \mathbf{w}_i^\top \mathbf{a}_i = 1, \ \forall i = 1, 2, \cdots, n,$$

   which is a convex quadratic program (QP).

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   which is a convex quadratic program (QP).

2. With $\tilde{\mathbf{W}}$ fixed, learn $\{\gamma_k, \theta_k\}_k$ from data

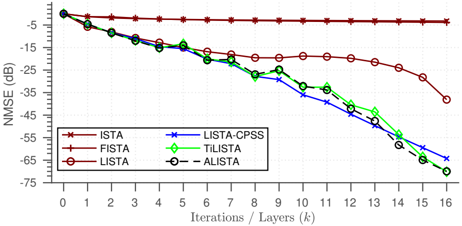
Parameters:

$$\mathcal{O}(mn + K) \stackrel{\text{reduce}}{\longrightarrow} \mathcal{O}(K).$$

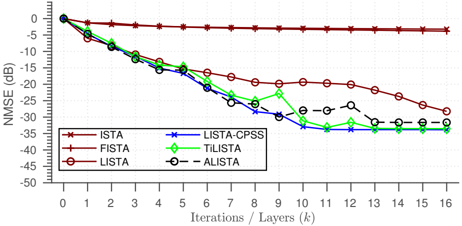
Training takes only minutes.

Numerical evaluation

Noiseless case
(SNR=∞)



Noisy case
(SNR=30dB)



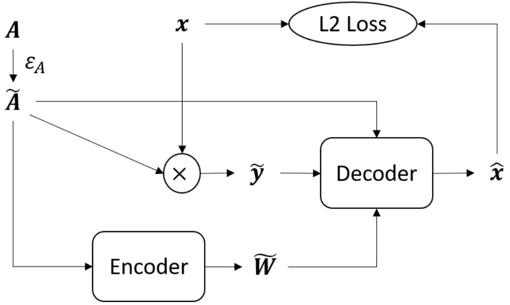
Robust ALISTA

Consider $\tilde{y} = \tilde{A}x + \varepsilon$ with $\tilde{A} = A + \varepsilon_A$. Given $\tilde{A}$ and $\tilde{y}$, recover x. Must handle varying $\tilde{A}$.

Unroll an algorithm into an NN to generate $\tilde{W}$ for $\tilde{A}$.

Method:

1. train an NN (called *encoder*) with many pairs of $(\tilde{A}, \tilde{W})$
2. train an ALISTA (called *decoder*) with many $(\tilde{A}, \tilde{y}, \tilde{W}, x)$
3. jointly train them with many $(\tilde{A}, \tilde{y}, \tilde{W}, x)$

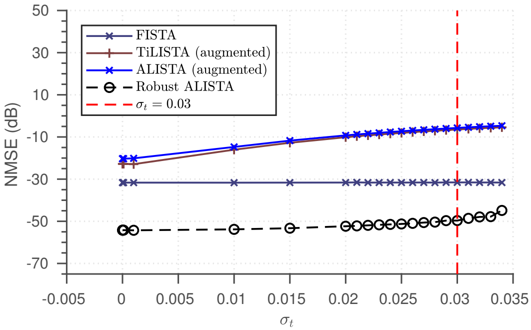


Numerical results

Fix an A. Training:

- Non-robust LISTA methods used their W matrices obtained with A.
- Robust ALISTA trained with perturbed A (Gaussian $\sigma = 0.03$).

Testing: All methods tested with perturbed A's (Gaussian $\sigma_1, \sigma_2, \cdots \leq 0.03$).



Robust ALISTA is significantly more robust.

HyperLISTA [Chen et al., 2021]

Introduce

- a hybrid-thresholding operator to bypass p^k largest entries and soft-threshold the rest
- analytic formulas for the parameters
- three hyper-parameters subject to grid search

Significance:

- allow the parameters to be "instance optimal"
- proves $\exists$ parameters to obtain *superlinear-like* error reduction

HyperLISTA learns $c_1, c_2, c_3 > 0$ and use them to set

$$\theta^k = c_1 \mu \Big\| A^{\dagger}(Ax^k - b) \Big\|_1, \qquad \text{soft threshold}$$

$$\beta^k = c_2 \mu \, \|x^k\|_0, \qquad \text{momentum stepsize}$$

$$p^k = c_3 \min\left(\log\left(\frac{\|A^{\dagger} b\|_1}{\|A^{\dagger}(Ax^k - b)\|_1} \right), n \right), \qquad \text{pass-through count}$$

The formulas are motivated by the analysis but use x^k instead of x^{true}.

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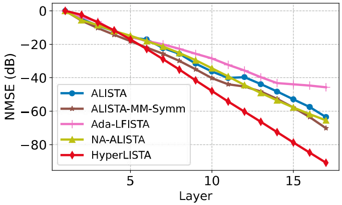
The formulas are motivated by the analysis but use x^k instead of x^{true}.

Parameters:

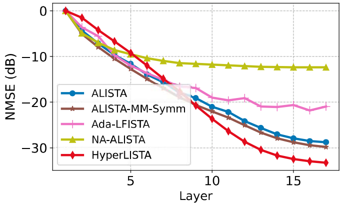
$$\mathcal{O}(K) \xrightarrow{\text{reduce}} 3.$$

Training can be done by grid search or a global optimization method.

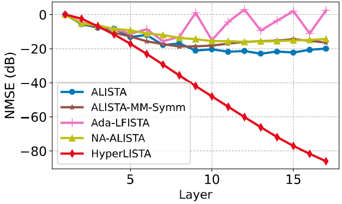
HyperLISTA is fast and robust



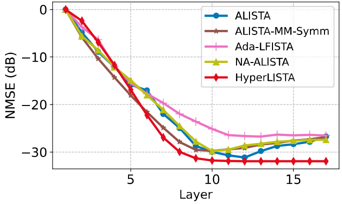
(a) Noiseless. No train/test mismatch.



(b) Sparsity ratio p changed to 0.15.



(c) Variance σ of non-zero elements changed to 2.



(d) Noise level changed to SNR=30dB.

Good analytic rules have better generalization perf.

LISTA [Gregor-LeCun, 2010] → $\left\{W_1^{(k)}, W_b^{(k)}, \alpha^{(k)}, \theta^{(k)}\right\}_{k=1}^{K}$ $\mathcal{O}(K(m+n)n)$

Eliminate W_1

LISTA-CPSS [Chen et al., 2018] → $\left\{W_b^{(k)}, \alpha^{(k)}, \theta^{(k)}\right\}_{k=1}^{K}$ $\mathcal{O}(Kmn)$

Eliminate W_b

ALISTA [Liu et al., 2019] → $\left\{\alpha^{(k)}, \theta^{(k)}\right\}_{k=1}^{K}$ $\mathcal{O}(K)$

Eliminate all parameters

HyperLISTA [Chen et al., 2021] → c_1, c_2, c_3 $\mathcal{O}(1)$

Training time: 10 hour → 6 mins

Uncovered LISTA topics

- [Moreau and Bruna, 2017] proposed to understand LISTA by the similarity between LISTA and a matrix-factorization method.
- [Xin et al., 2016] proposed learned iterative hard-thresholding-CP.
- [Wu et al., 2019] proposed gated mechanisms to improve LISTA.
- [Ito et al., 2019] proposed a minimum mean squared error (MMSE) estimator-based shrinkage function in LISTA.
- [Yang et al., 2020] proposed to use nonconvex-function-induced regularizers in LISTA.
- [Heaton et al., 2020] introduced a safeguard wrapper for LISTA methods applied to structured convex problems.
- When K is large or $K = \infty$, LISTA cannot be trained. Instead, we can use deep equilibrium[Bai et al., 2019, Winston and Kolter, 2020] and fixed-point network [Fung et al., 2022]. [Gilton et al., 2021] demonstrated better image recovery.

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