An adaptively inexact first-order method for bilevel optimization with application to hyperparameter learning

Joint work with Mohammad Sadegh Salehi (Bath), Matthias Ehrhardt (Bath), Subhadip Mukherjee (IIT Kharagpur)

Lindon Roberts, University of Sydney (`lindon.roberts@sydney.edu.au`)

Sydney Workshop on Mathematics of Data Science, University of Sydney
5 December 2024

Outline

1. **Bilevel learning**
2. Dynamic linesearch
3. Numerical results

Variational Regularization

Many inverse problems can be posed in the form

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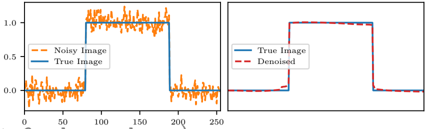
Solution depends on choices of α, ν and ξ:

Example
$(\alpha = 1,\ \nu = \xi = 10^{-3})$



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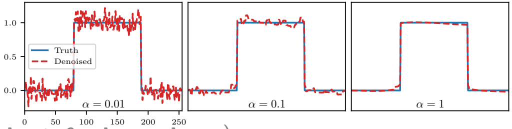

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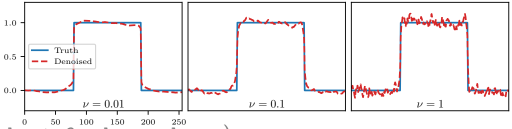

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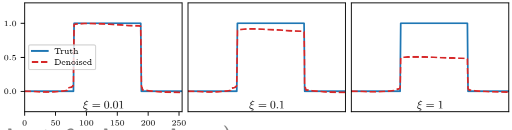

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Recovered solution depends strongly on problem parameters (e.g. α, ν and ξ)

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How to choose good problem parameters?

- Trial & error
- L-curve criterion
- **Bilevel learning** — data-driven approach

Bilevel Learning

Suppose we have training data $(x_1, y_1), \dots, (x_n, y_n)$ — ground truth and noisy observations.

Attempt to recover x_i from y_i by solving inverse problem with parameters $\theta \in \mathbb{R}^m$:

$$\hat{x}_i(\theta) := \arg\min_{x} \Phi_i(x, \theta), \qquad \text{e.g. } \Phi_i(x,\theta) = \mathcal{D}(Ax, y_i) + \theta \mathcal{R}(x).$$

Try to find θ by making $\hat{x}_i(\theta)$ close to x_i

$$\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} \|\hat{x}_i(\theta) - x_i\|^2 + \mathcal{J}(\theta),$$

with optional (smooth) term $\mathcal{J}(\theta)$ to encourage particular choices of θ.

Bilevel Optimization

The bilevel learning problem is:

$$\begin{aligned} \min_{\theta} \quad & f(\theta) := \frac{1}{n}\sum_{i=1}^{n} \|\hat{x}_i(\theta) - x_i\|^2 + \mathcal{J}(\theta), \\ \text{s.t.} \quad & \hat{x}_i(\theta) := \arg\min_{x} \Phi_i(x, \theta), \quad \forall i = 1, \ldots, n. \end{aligned}$$

- If Φ_i are strongly convex in x and sufficiently smooth in x and θ, then $\hat{x}_i(\theta)$ is well-defined and continuously differentiable.
- Upper-level problem ($\min_\theta f(\theta)$) is a smooth nonconvex optimization problem

Many use cases in data science: learning image regularizers, hyperparameter tuning, data hypercleaning, ...

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- Can't evaluate lower-level minimizers $\hat{x}_i(\theta)$ exactly, so can never get exact $f(\theta)$ or $\nabla f(\theta)$ [Kunisch & Pock, 2013; Sherry et al., 2020]
- But can evaluate f and ∇f to arbitrary accuracy (with significant computational cost) [Berahas et al., 2021; Cao et al., 2022]
- Potentially large scale: both lower-level problems and upper-level problem.
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Key question: how to find good evaluation accuracy to get (i) guaranteed convergence, (ii) without requiring hyperparameter tuning, (iii) at a reasonable computational cost?

Inexact Information

First, how do we evaluate $f(\theta)$ and $\nabla f(\theta)$? [Ehrhardt & LR, 2023]

- $\hat{x}(\theta)$ is minimiser of smooth, strongly convex problem — given ϵ, use standard first-order methods (e.g. GD) to get $x_\epsilon = x_\epsilon(\theta)$ with $\|x_\epsilon - \hat{x}(\theta)\| \leq \epsilon$

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- For an objective $g(\hat{x}(\theta))$, Implicit Function Theorem gives

$$\nabla_\theta g = -[\partial_x \partial_\theta \Phi(\hat{x}(\theta), \theta)]^T [\partial_{xx} \Phi(\hat{x}(\theta), \theta)]^{-1} \nabla_x g(\hat{x}(\theta))$$

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- Given δ, use CG to find $q_{\epsilon,\delta}$ such that $\|[\partial_{xx}\Phi(x_\epsilon, \theta)] q_{\epsilon,\delta} - \nabla_x g(x_\epsilon)\| \leq \delta$
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- Use approximate gradient $z = -[\partial_x \partial_\theta \Phi(x_\epsilon, \theta)]^T q_{\epsilon,\delta}$
- Total gradient error is $\mathcal{O}(\epsilon + \delta + \epsilon^2 + \epsilon\delta)$ with computable constants

Note: this is equivalent to an accelerated version of backpropagation applied to the lower-level solver iteration. [Mehmood & Ochs, 2020]

Inexact Linesearch

To handle inexactness, there are two key issues to resolve:

- Given $z_k \approx \nabla f(\theta_k)$ can we guarantee z_k is a descent direction?
- If no sufficient decrease (with inexact $f(\theta)$ evaluations), should we shrink stepsize or improve accuracy in f (or ∇f)?

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To be practical, we don't want to make accuracy in f or ∇f unnecessarily high (but don't want to lose convergence guarantees either).

Inexact Gradient Calculation

- Given ϵ and δ, calculate inexact lower-level minimiser x_ϵ and inexact gradient $z_k \approx \nabla f(\theta_k)$ (using CG with residual tolerance δ)
- Calculate computable upper bound ω for $\|z_k - \nabla f(\theta_k)\|$
- If $\omega \leq (1-\eta)\|z_k\|$, then use z_k (guaranteed descent direction)
- Otherwise, decrease ϵ and δ by a constant factor and start again

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Theorem

If $\|\nabla f(\theta_k)\| \neq 0$, then z_k is a descent direction for all sufficiently small ϵ and δ.

i.e. Gradient calculation terminates in finite time.

Sufficient Decrease Condition

Inexact sufficient decrease condition

- Given $\hat{\theta} = \theta_k - \alpha_k z_k$, compute $x_\epsilon(\theta_k)$ and $x_\epsilon(\hat{\theta})$ to accuracy ϵ
- Compute approximate objective values $\tilde{f}(\theta_k)$ and $\tilde{f}(\hat{\theta})$
- Inexact sufficient decrease condition is (for L-smooth and convex f):

$$\tilde{f}(\hat{\theta}) \leq \tilde{f}(\theta_k) - \lambda\alpha_k\|z_k\|^2 - \|\nabla_x f(x_\epsilon(\hat{\theta}))\|\epsilon - \|\nabla_x f(x_\epsilon(\theta_k))\|\epsilon - \frac{1}{2}L\epsilon^2$$

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- *If inexact sufficient decrease condition holds, then* $f(\hat{\theta}) \leq f(\theta_k) - \lambda \alpha_k \|z_k\|^2$.

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- *As* $\epsilon \to 0$, *we have* $[\alpha_{\text{min}}(\epsilon), \alpha_{\text{max}}(\epsilon)] \to [0, \alpha_{\text{max}}]$ *for some* $\alpha_{\text{max}} > 0$

Inexact Backtracking

Method of Adaptive Inexact Descent (MAID) (single iteration k)

1: **for** $J_{\max} = J_0, J_0+1, J_0+2, \ldots$ **do**
2: Compute inexact gradient z_k (possibly reducing ϵ and δ)
3: **for** $j = 0, \ldots, J_{\max}-1$ **do**
4: If sufficient decrease with stepsize $\alpha_k = \alpha\rho^j$, go to line 8
5: **end for**
6: Reduce ϵ and δ by constant factor *(backtracking failed, need higher accuracy)*
7: **end for**
8: Set $\theta_{k+1} = \theta_k - \alpha_k z_k$ *(successful linesearch)*
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Theorem

At each iteration k, successful linesearch occurs in finite time. Hence $\|\nabla f(\theta_k)\| \to 0$.

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Quadratic Problem

Simple linear least-squares problem (closed form for true solution):

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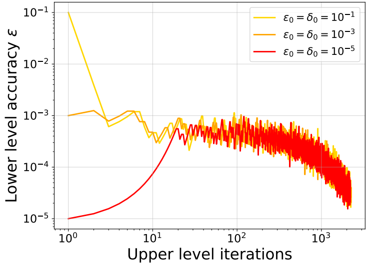
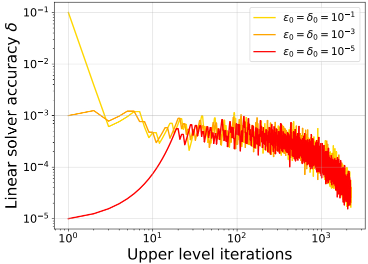
Do hyperparameters (initial accuracies ϵ and δ) matter?

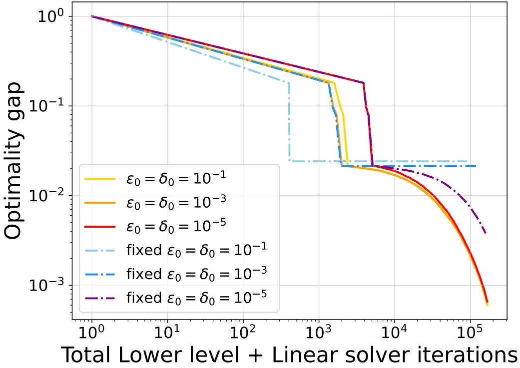


Final ϵ at each iteration



Final δ at each iteration

Dynamic accuracy is better than fixed accuracy



Optimality gap vs. computational work (lower-level + CG iterations)

Field of Experts Denoising

Field of Experts Image Denoising

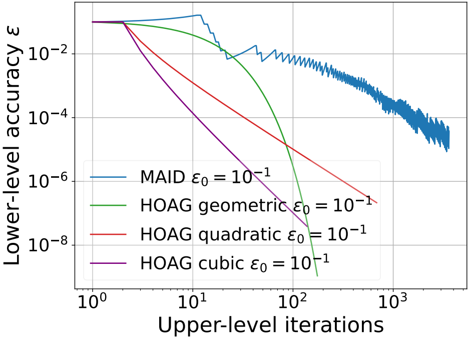
$$\min_{\theta} \; f(\theta) := \frac{1}{N}\sum_{i=1}^{N} \|\hat{x}_i(\theta) - x_i^*\|^2,$$

$$\text{s.t. } \hat{x}_i(\theta) = \arg\min_{x} \Phi_i(x,\theta) := \frac{1}{2}\|x - y_i\|^2 + \sum_{k=1}^{K} \beta_k(\theta)\|c_k(\theta) * x\|_{k,\theta} + \frac{\mu}{2}\|x\|^2.$$

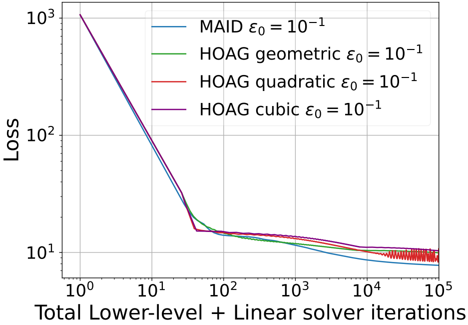
Learn $K = 30$ filters $c_k(\theta)$, smoothed ℓ_1-norms $\|\cdot\|_{k,\theta}$ and weights $\beta_k(\theta)$ to reconstruct noisy 2D images (≈ 1500 hyperparameters θ).

Using $N = 25$ training images (x_i^*, y_i) of size 96×96 pixels.

Compare MAID against HOAG (fixed accuracy schedule) [Pedregosa, 2016]



Accuracy ϵ at each iteration



Loss vs. computational work

Field of Experts Denoising

Apply learned filters on new test image

True image

Noisy (PSNR 20.3dB)

MAID (PSNR 29.7dB)

HOAG best (PSNR 28.8dB)

(Palladian Bridge, Bath, UK)

Conclusions & Future Work

Conclusions

- Bilevel learning provides a structured hyperparameter tuning method
- New linesearch method balances accuracy and computational efficiency
- Strong practical performance and robust to algorithm parameter choices
  - Outperforms other existing approaches (e.g. prescribed accuracy schedule, inexact derivative-free methods) [Pedregosa, 2016; Ehrhardt & LR, 2021]

Future Work

- Handle large training sets with SGD-type methods
- Extensions to non-strongly convex lower-level problems

Preprint: `https://arxiv.org/abs/2308.10098`

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