Inexact Algorithms for Bilevel Learning

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14 January, 2025

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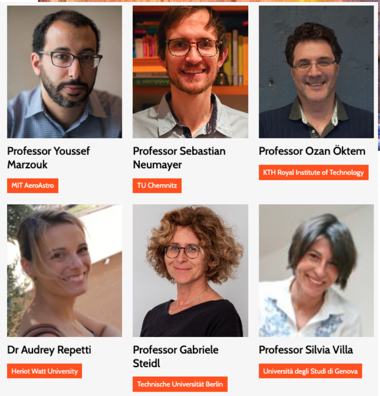
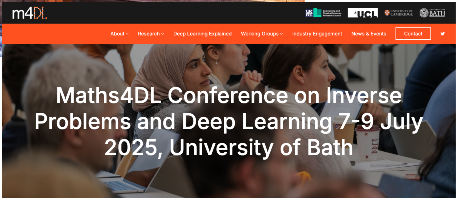
Engineering and Physical Sciences Research Council

Inverse Problems and Deep Learning: 7-9 July 2025

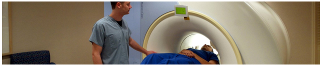




Deadline: 28 Feb 2025

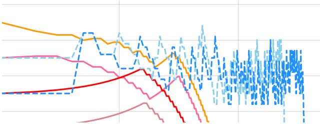
Outline

1) Bilevel learning of a regularizer



$$\min_x \frac{1}{2}\|Ax - y\|_2^2 + \lambda\mathcal{R}(x)$$

2) Inexact learning strategy



3) Numerical results

4) Inexact Piggyback

Inverse problems and Variational Regularization

$$Ax = y$$

x : desired solution

y : observed data

A : mathematical model

Goal: recover x given y

Variational regularization

Approximate a solution x^* of $Ax = y$ via

$$\hat{x} \in \arg\min_x \left\{ \mathcal{D}(Ax, y) + \lambda \mathcal{R}(x) \right\}$$

$\mathcal{D}$ **data fidelity**: related to noise statistics

$\mathcal{R}$ **regularizer**: penalizes unwanted features, stability

$\lambda \geq 0$ **regularization parameter**: weights data and regularizer

Scherzer et al. '08, Ito and Jin '15, Benning and Burger '18

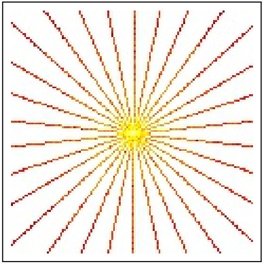
Example: Magnetic Resonance Imaging (MRI)

MRI Reconstruction Lustig et al. '07

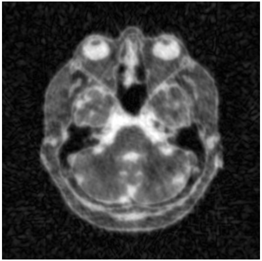
Fourier transform F, sampling $Sw = (w_i)_{i \in \Omega}$

$$\min_{x} \left\{ \sum_{i \in \Omega} |(Fx)_i - y_i|^2 + \lambda \|\nabla x\|_1 \right\}$$

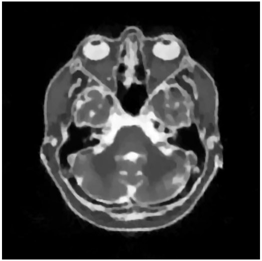
MRI scanner



data



poor choice



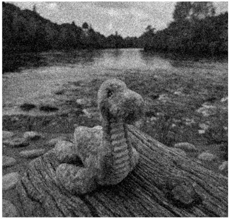
good choice

More Complicated Regularizers

Fields-of-Experts (FoE) Roth and Black ’05

$$\mathcal{R}(x) = \sum_{k=1}^{K} \lambda_k \|\kappa_k * x\|_{\gamma_k}$$

E.g. 48 kernels $7 \times 7 = 2448$ parameters



noisy

poor choice

well-trained

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Input Convex Neural Networks (ICNN) Amos et al. '17, Mukherjee et al. '24'

$$\mathcal{R}(x) = z_K,$$
$$z_{k+1} = \sigma(W_k z_k + V_k x + b_k), k = 0, \dots, K-1, z_0 = x$$

constraints on σ and W_k, e.g. 2 layers, 2000 parameters

- Convex Ridge Regularizers (CRR) Goujon et al. '22, ≈ 4000 parameters
- ...

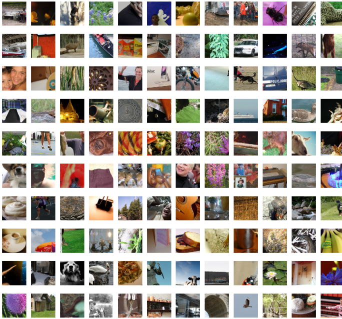
Bilevel learning for inverse problems

Upper level (learning):
Given $(x_i, y_i)_{i=1}^n, y_i \approx Ax_i$, solve

$$\min_{\theta} \frac{1}{n} \sum_{i=1}^{n} \|\hat{x}_i(\theta) - x_i\|_2^2$$

Lower level (solve inverse problem):

$$\hat{x}_i(\theta) = \arg\min_x \{\mathcal{D}(Ax, y_i) + \mathcal{R}_\theta(x)\}$$



von Stackelberg 1934, 2003, Haber and Tenorio '03, Kunisch and Pock '13,

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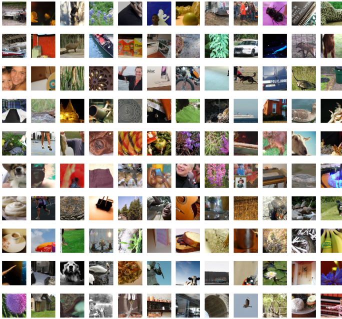

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- contrastive learning Hinton '02
- fitting prior distribution Roth and Black '05
- adversarial training Arjovsky et al. '17
- adverserial regularization Lunz et al. '18
- ...

Inexact Learning Strategy

Exact Approaches for Bilevel learning

Upper level: $$\min_{\theta} f(\theta) := g(\hat{x}(\theta))$$

Lower level: $$\hat{x}(\theta) := \arg\min_{x} h(x, \theta)$$

Access to **function values** $f(\theta)$

1) Compute $\hat{x}(\theta)$
2) Evaluate $f(\theta) := g(\hat{x}(\theta))$

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Lower level: $$\hat{x}(\theta) := \arg\min_{x} h(x, \theta)$$

Access to **gradients** $\nabla f(\theta)$

$$0 = \partial_x^2 h(\hat{x}(\theta), \theta)\hat{x}'(\theta) + \partial_\theta \partial_x h(\hat{x}(\theta), \theta) \quad \Leftrightarrow \quad \hat{x}'(\theta) = -B^{-1}A$$

$$\nabla f(\theta) = (\hat{x}'(\theta))^* \nabla g(\hat{x}(\theta)) = -A^* w, \quad \text{with } Bw = b$$

$$A = \partial_\theta \partial_x h(\hat{x}(\theta), \theta), \quad B = \partial_x^2 h(\hat{x}(\theta), \theta), \quad b = \nabla g(\hat{x}(\theta))$$

1) Compute $\hat{x}(\theta)$
2) Solve $Bw = b$
3) Compute $\nabla f(\theta) = -A^* w$

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This strategy has a number of problems:

- $\hat{x}(\theta)$ has to be computed
- Derivative assumes $\hat{x}(\theta)$ is exact minimizer
- Large system of linear equations has to be solved

Inexact Approaches for Bilevel learning

Upper level: $\min_{\theta} f(\theta) := g(\hat{x}(\theta))$

Lower level: $\hat{x}(\theta) := \arg\min_{x} h(x, \theta)$

Approximate function values $f_\varepsilon(\theta) \approx f(\theta)$:

1) Compute $\hat{x}_\varepsilon(\theta)$ to ε accuracy: $|\hat{x}_\varepsilon(\theta) - \hat{x}(\theta)| < \varepsilon$
2) Evaluate $f_\varepsilon(\theta) := g(\hat{x}_\varepsilon(\theta))$

Approximate gradients $z(\theta) \approx \nabla f(\theta)$:

$$A_\varepsilon = \partial_\theta \partial_x h(\hat{x}_\varepsilon(\theta), \theta), \quad B_\varepsilon = \partial_x^2 h(\hat{x}_\varepsilon(\theta), \theta), \quad b_\varepsilon = \nabla g(\hat{x}_\varepsilon(\theta))$$

1) Compute $\hat{x}_\varepsilon(\theta)$ to ε accuracy: $|\hat{x}_\varepsilon(\theta) - \hat{x}(\theta)| < \varepsilon$
2) Solve $B_\varepsilon w = b_\varepsilon$ to δ accuracy: $\|B_\varepsilon w - b_\varepsilon\| < \delta$
3) Compute $z(\theta) = -A_\varepsilon^* w$

Construction of Inexact Algorithms

Wish list:

- use gradients
- adaptive step-sizes (e.g. via backtracking): as large as possible as small as necessary, **maximize progress**
- adaptive accuracy: as low as possible as high as necessary, **minimize compute**

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Existing algorithms:

1) Zero-order: DFO-LS Ehrhardt and Roberts '21
   - adaptive accuracy using recent research in derivative-free optimization
   - does not scale well due to lack of gradients
2) First-order: HOAG Pedregosa '16
   - A-prior chosen accuracy ε_k
   - Convergence with stepsize $\alpha = 1/L$

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Ingredients:

- inexact gradient as descent direction
- inexact backtracking

Inexact Gradient as a Descent Direction

Assumptions:

- h is strongly convex and L_h-smooth
- g is L_g-smooth
- $\nabla_x^2 h(x, \theta)$ and $\nabla_{x\theta}^2 h(x, \theta)$ are Lipschitz

Lemma: Let $\|e_k\| \leq (1-\eta)\|z_k\|$, $\eta \in (0,1), e_k := z_k - \nabla f(\theta_k)$. Then $-z_k$ is a descent direction for f at θ_k.

Prop: Let $\hat{x}_k := \hat{x}_{\varepsilon_k}(\theta_k)$. There exists computable c_i:

$$\|e_k\| \leq c_1(\hat{x}_k)\varepsilon_k + c_2(\hat{x}_k)\delta_k + c_3\varepsilon_k^2 =: \omega_k$$

Inexact Gradient as a Descent Direction

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1) Given ε_k, δ_k, compute $\hat{x}_k, z_k$ and ω_k
2) If $\omega_k > (1-\eta)\|z_k\|$, go to step 1) with smaller ε_k, δ_k

Theorem: If $\|\nabla f(\theta_k)\| > 0$, then z_k is a descent direction for all sufficiently small ε_k, δ_k.

Sufficient Decrease with Inexact Gradients

$$\theta_{k+1} = \theta_k - \alpha_k z_k$$

- $U_{k+1} := g(\hat{x}_{k+1}) + \|\nabla g(\hat{x}_{k+1})\| \varepsilon_{k+1} + \frac{L_{\nabla g}}{2} \varepsilon_{k+1}^2 \geq f(\theta_{k+1})$
- $L_k := g(\hat{x}_k) - \|\nabla g(\hat{x}_k)\| \varepsilon_k - \frac{L_{\nabla g}}{2} \varepsilon_k^2 \leq f(\theta_k)$

Theorem: If $U_{k+1} + \eta \alpha_k \|z_k\|^2 \leq L_k$, then

$$f(\theta_{k+1}) + \eta \alpha_k \|z_k\|^2 \leq f(\theta_k).$$

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Theorem: If $U_{k+1} + \eta \alpha_k \|z_k\|^2 \leq L_k$, then

$$f(\theta_{k+1}) + \eta \alpha_k \|z_k\|^2 \leq f(\theta_k).$$

Theorem: Let f be L_f-smooth and $\nabla f(\theta_k) \neq 0$.
If $\varepsilon_k, \varepsilon_{k+1} > 0$ are small enough, then there exists $\alpha_k > 0$, such that $U_{k+1} + \eta \alpha_k \|z_k\|^2 \leq L_k$.

Method of Adaptive Inexact Descent (MAID)

One iteration:

1) Compute inexact gradient z_k (possibly reducing ε_k, δ_k)
2) Attempt backtracking to compute α_k; if failed, go to step 1) with smaller ε_k, δ_k
3) Update estimate: $\theta_{k+1} = \theta_k - \alpha_k z_k$
4) Increase accuracies $\varepsilon_{k+1}, \delta_{k+1}$ and inital step size α_{k+1}

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Theorem: Let f be bounded below. Then MAID's iterates θ_k satisfy $\|\nabla f(\theta_k)\| \to 0$.

Numerical Results

TV denoising: MAID vs DFO-LS (2 parameters)

$$h(x,\theta) = \frac{1}{2}\|x - y_t\|^2 + \underbrace{e^{\theta[1]} \sum_i \sqrt{|\nabla_1 x_i|^2 + |\nabla_2 x_i|^2 + (e^{\theta[2]})^2}}_{\text{smoothed TV}}$$

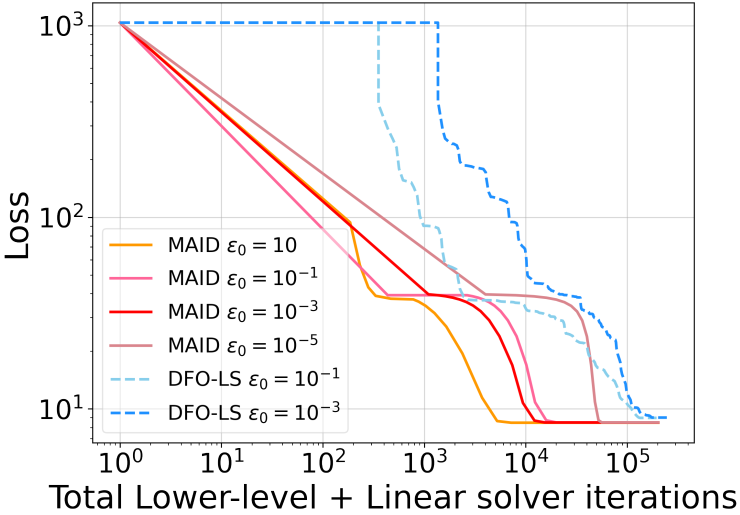
Noisy, PSNR=20.0

DFO-LS, 26.7

MAID, 26.9

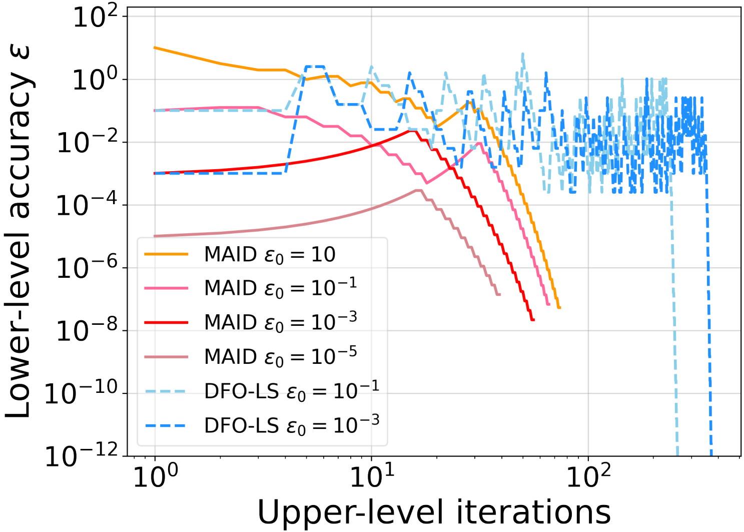
- similar image quality

TV denoising: MAID vs DFO-LS (2 parameters)



- Robustness to initial accuracy ε_0
- MAID particularly initially faster

TV denoising: MAID vs DFO-LS (2 parameters)



- MAID adapts accuracy, converge to same values in similar trend

FoE denoising: MAID vs HOAG ($\approx$ 2.5k parameters)

$$h(x,\theta) = \frac{1}{2}\|x-y\|^2 + e^{\theta[0]} \sum_{k=1}^{K} e^{\theta[k]} \|c_k * x\|_{\theta[K+k]}$$

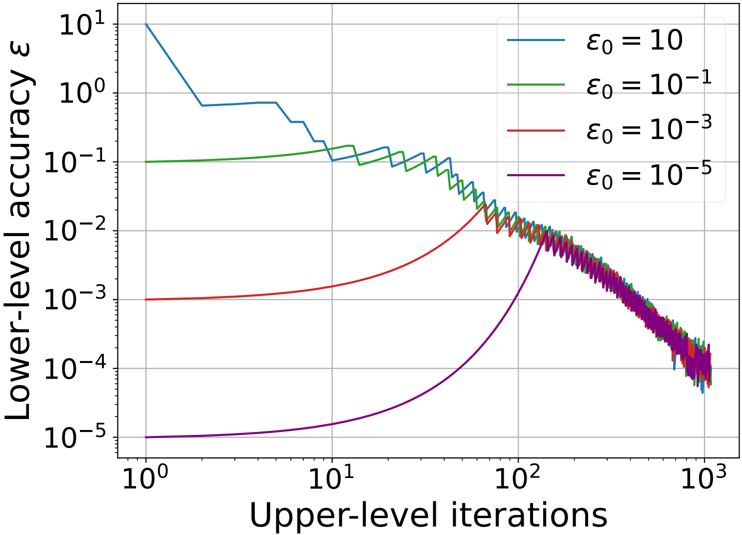
Noisy, PSNR=20.3

HOAG^2, 28.8

MAID, 29.7

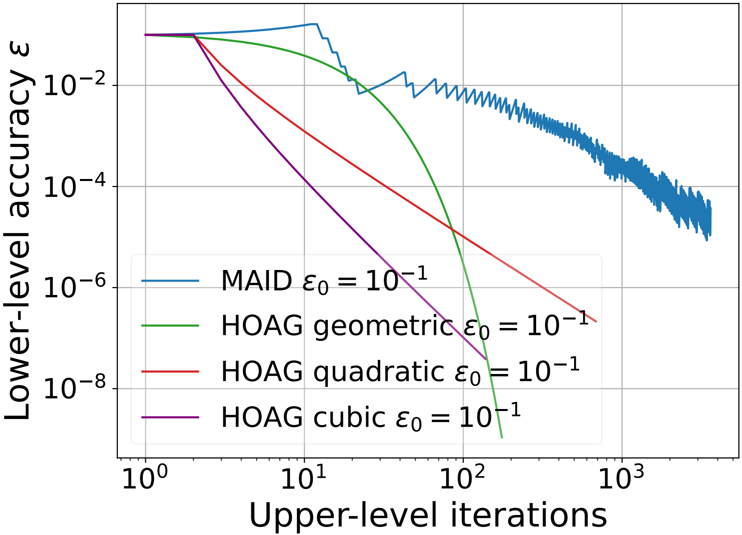
- MAID learns better regularizer than all HOAG variants; here best quadratic $\varepsilon_k = C/k^2$

FoE denoising: MAID vs HOAG ($\approx$ 2.5k parameters)



- MAID automatically tunes best accuracy schedule

FoE denoising: MAID vs HOAG ($\approx$ 2.5k parameters)



- accuracy schedule important; here slower decay better

Inexact Piggyback for Bilevel learning

Upper level: $\min_{\theta} \mathcal{L}(\theta) := \ell_1(\hat{x}(\theta)) + \ell_2(\hat{y}(\theta))$

Lower level: $\hat{x}(\theta), \hat{y}(\theta) := \arg\min_x \max_y \langle \theta x, y \rangle + g(x) - f^*(y)$

If g and f^* are regular enough, gradients can be computed via

$$\nabla \mathcal{L}(\theta) = \hat{y}(\theta) \otimes \hat{X}(\theta) + \hat{Y}(\theta) \otimes \hat{x}(\theta)$$

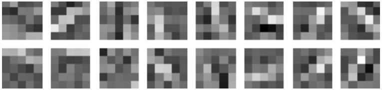
where $\hat{X}(\theta), \hat{Y}(\theta)$ solve another saddle-point problem of a similar form involving $\nabla^2 g(\hat{x}(\theta))$, $\nabla^2 f^*(\hat{y}(\theta))$, $\nabla \ell_1(\hat{x}(\theta))$ and $\nabla \ell_2(\hat{x}(\theta))$

Idea: this is of the same form as for MAID.

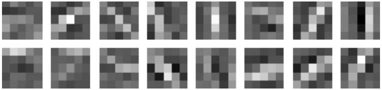
Problems of this form:

- learning discretisations of TV Chambolle and Pock '21
- training ICNNs after primal-dual reformulation Wong et al. '24

Learning TV discretisations



non-adaptive



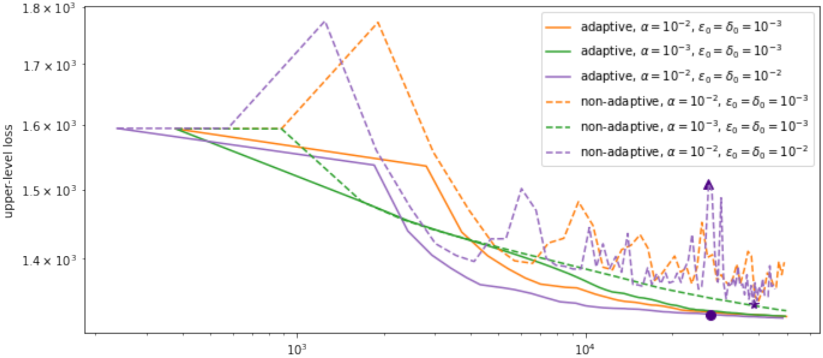
adaptive

standard TV
PSNR = 25.82 dB

non-adaptive
PSNR = 26.63 dB

adaptive
PSNR = 26.90 dB

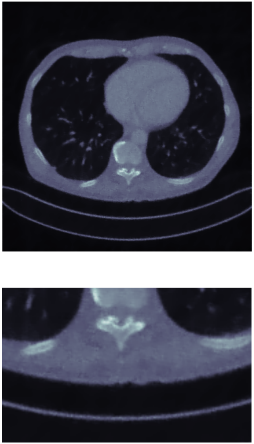
Learning TV discretisations II



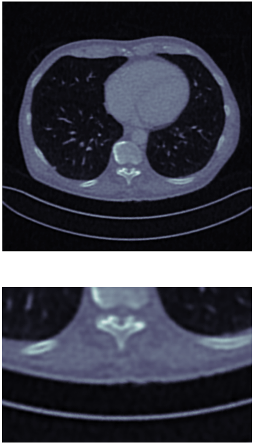
compute

- results still depend on parameters
- sensitivity much reduced

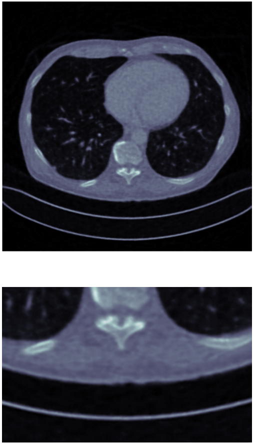
CT Reconstruction



ICNN-AR, PSNR=29.3



ICNN-Bilevel, 31.4



LPD, 34.2

Conclusions & Future Work

Conclusions

- **Bilevel learning**: supervised learning for variational regularization; computationally very hard
- **Accuracy** in the optimization algorithm is important; stability and efficiency
- **MAID** is a first-order algorithm with adaptive accuracies for descent and backtracking
- **High-dimensional** parametrizations can be learned; e.g. FoE, ICNN (a few thousand parameters)

Future work

- **Smart accuracy** schedule; can we disentangle accuracies ε, δ and step size α
- **Stochastic** variants for training from large data