Bilevel Learning for Inverse Problems

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Joint work with:
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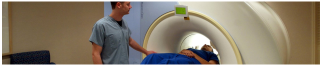
The Leverhulme Trust

Engineering and Physical Sciences Research Council

THE FARADAY INSTITUTION

Outline

1) Motivation



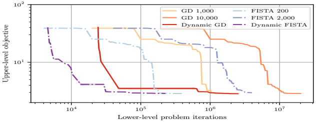
$$\min_x \frac{1}{2}\|Ax - y\|_2^2 + \lambda \mathcal{R}(x)$$

2) Bilevel Learning

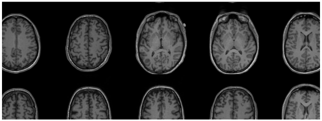
$$\min_{x,y} f(x, y)$$

$$x \in \arg\min_z g(z, y)$$

3) Efficient solution?
Yes, e.g. inexact DFO algorithms
Ehrhardt and Roberts JMIV 2021



4) High-dimensional learning?
Yes, e.g. learn MRI sampling
Sherry et al. IEEE TMI 2020



Inverse problems

$$Ax = y$$

x : desired solution

y : observed data

A : mathematical model

Goal: recover x given y

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Hadamard (1902): We call an inverse problem $Ax = y$ **well-posed** if

(1) a solution x^* **exists**

(2) the solution x^* is **unique**

(3) x^* depends **continuously** on data y.

Otherwise, it is called **ill-posed**.

Jacques Hadamard

Most interesting problems are **ill-posed**.

How to solve inverse problems?

Variational regularization ($\sim$1990)
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, ensures stability and uniqueness

λ **regularization parameter**: $\lambda \geq 0$. If $\lambda = 0$, then an original solution is recovered. As $\lambda \to \infty$, more and more weight is given to the regularizer $\mathcal{R}$.

textbooks: Scherzer et al. 2008, Ito and Jin 2015, Benning and Burger 2018

Example: Regularizers

- Tikhonov regularization: $\mathcal{R}(x) = \frac{1}{2}\|x\|_2^2$
- H^1 squared semi-norm: $\mathcal{R}(x) = \frac{1}{2}\|\nabla x\|_2^2$

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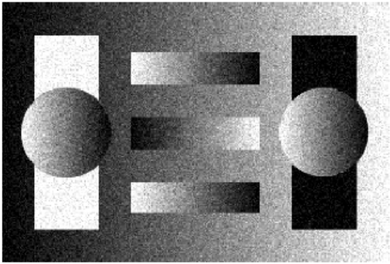
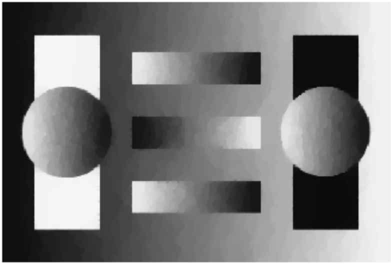
- Total Variation $\mathcal{R}(x) = \|\nabla x\|_1$ Rudin, Osher, Fatemi 1992



Noisy image



TV denoised image

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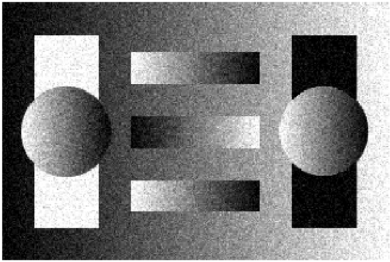
  $\mathcal{R}(x) = \|\nabla^2 x\|_1$ Hinterberger and Scherzer 2004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TV² denoised image

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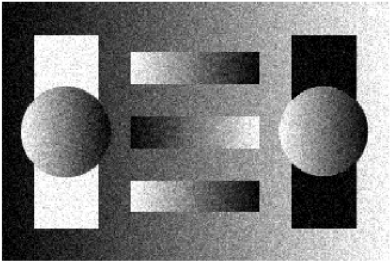
- Total Generalized Variation
  $\mathcal{R}(x) = \inf_v \|\nabla x - v\|_1 + \beta\|\nabla v\|_1$ Bredies, Kunisch, Pock 2010



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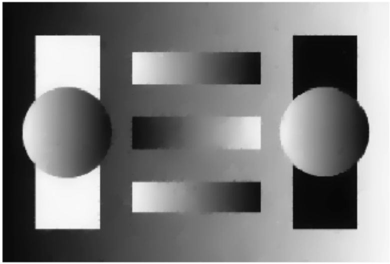

TGV^2 denoised image

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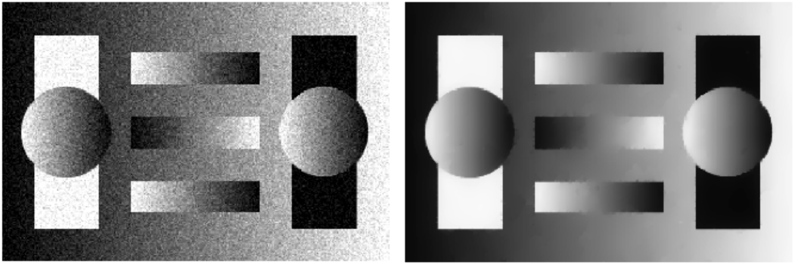


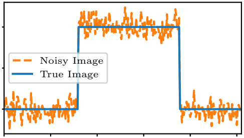
Noisy image

TGV^2 denoised image

How to choose the regularization?

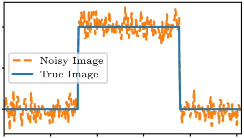
More "complicated" regularizers

$$\min_x \frac{1}{2}\|Ax - y\|_2^2 + \alpha\left(\underbrace{\sum_j \|(\nabla x)_j\|_2}_{=\mathrm{TV}(x)} \qquad\qquad\right)$$



More "complicated" regularizers

$$\min_x \frac{1}{2}\|Ax-y\|_2^2+\alpha\left(\underbrace{\sum_j \sqrt{\|(\nabla x)_j\|_2^2+\nu^2}}_{\approx \mathrm{TV}(x)}\right)$$



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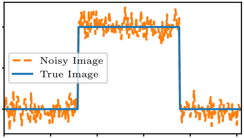

- Smooth and strongly convex
- Solution depends on choices of α, ν and ξ

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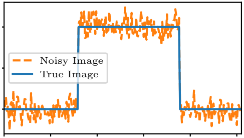
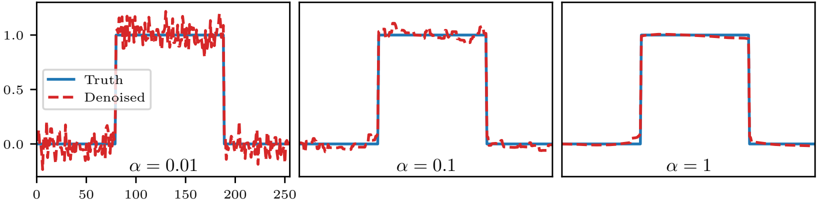


- Smooth and strongly convex
- Solution depends on choices of α, ν and ξ

Vary α ($\nu = 10^{-3}$, $\xi = 10^{-3}$)



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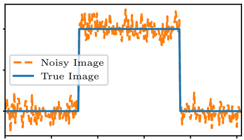

- Smooth and strongly convex
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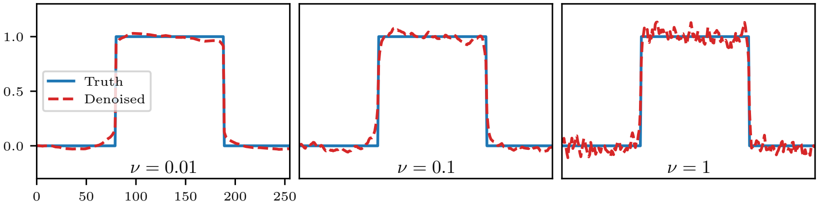
Vary ν ($\alpha = 1$, $\xi = 10^{-3}$)



More "complicated" regularizers

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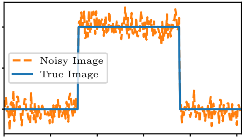
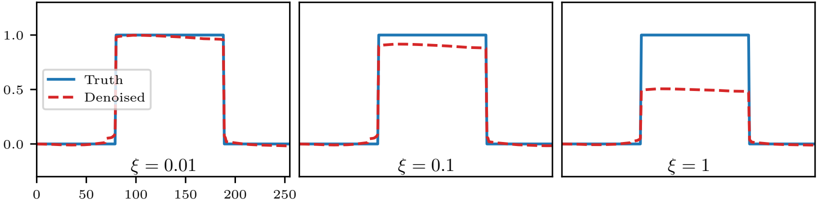


- Smooth and strongly convex
- Solution depends on choices of α, ν and ξ

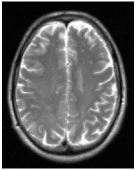
Vary ξ $(\alpha = 1,\ \nu = 10^{-3})$



How to choose all these parameters?

Example: Magnetic Resonance Imaging (MRI)

MRI scanner

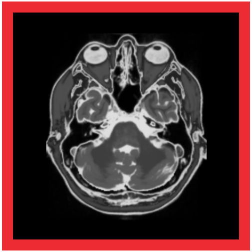


T_2^*

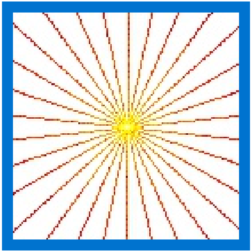
Continuous model: Fourier transform

$$Ax(s) = \int_{\mathbb{R}^2} x(s) \exp(-ist) dt$$

Dicrete model: $A = SF \in \mathbb{C}^{n \times N}$



$\longrightarrow$



Solution **not unique**.

Example: MRI reconstruction

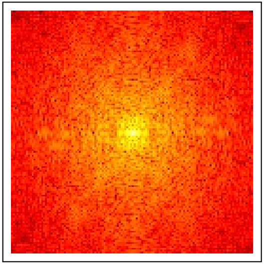
Compressed Sensing MRI:

$A = S \circ F$ Lustig, Donoho, Pauly 2007

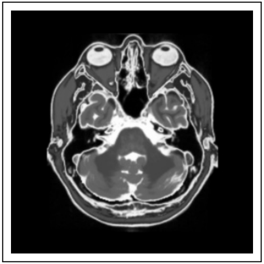
Fourier transform F, sampling $Sw = (w_i)_{i \in \Omega}$

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

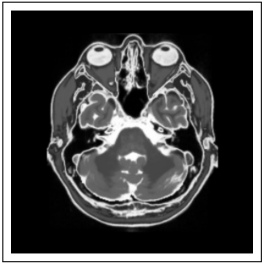
Miki Lustig



sampling $S^* y$



$\lambda = 0$



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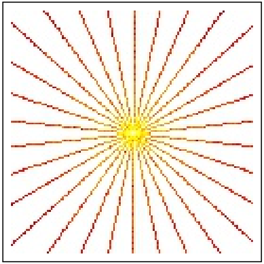

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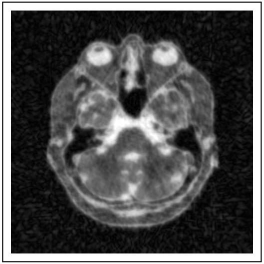

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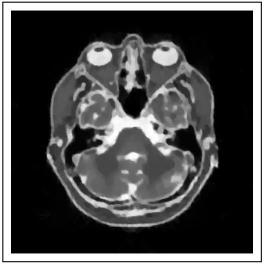

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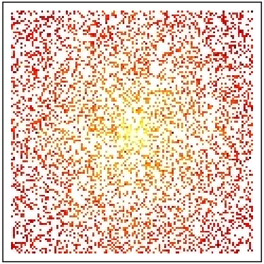

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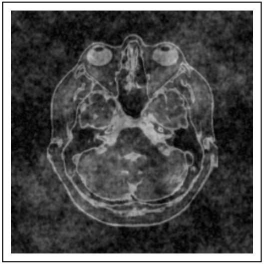

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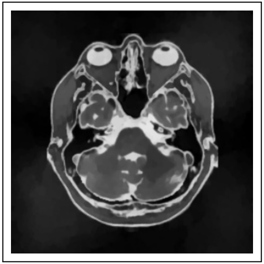

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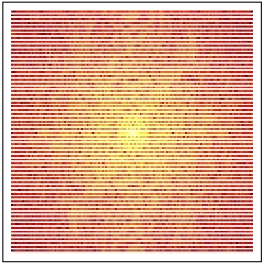

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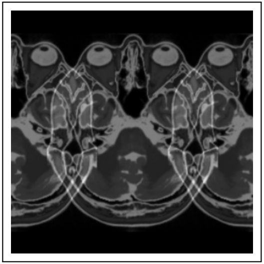

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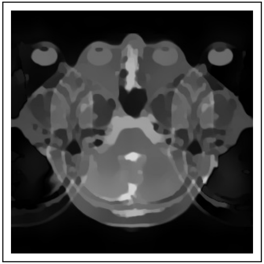

$\lambda = 10^{-3}$

How to choose the sampling Ω? Is there an optimal sampling?

Does a good sampling depend on $\mathcal{R}$ and λ?

Motivation

- **Inverse problems** can be solved via **variational regularization**

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- These models have **a number of parameters**: regularizer, regularization parameter, sampling, smoothness, strong convexity ...

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- **Inverse problems** can be solved via **variational regularization**
- These models have **a number of parameters**: regularizer, regularization parameter, sampling, smoothness, strong convexity ...
- Some of these parameters have underlying theory and heuristics but are generally still **difficult to choose** in practice

Bilevel Learning

Bilevel learning for inverse problems

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

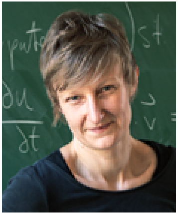
Bilevel learning for inverse problems

Upper level (learning):
Given $(x^\dagger, y), y = Ax^\dagger + \varepsilon$, solve

$$\min_{\lambda \geq 0, \hat{x}} \|\hat{x} - x^\dagger\|_2^2$$

Lower level (solve inverse problem):

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



Carola Schönlieb

von Stackelberg 1934, Kunisch and Pock 2013, De los Reyes and Schönlieb 2013

Bilevel learning for inverse problems

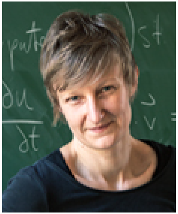
Upper level (learning):

Given $(x_i^\dagger, y_i)_{i=1}^n, y_i = Ax_i^\dagger + \varepsilon_i$, solve

$$\min_{\lambda \geq 0, \hat{x}_i} \frac{1}{n} \sum_{i=1}^{n} \|\hat{x}_i - x_i^\dagger\|_2^2$$

Lower level (solve inverse problem):

$$\hat{x}_i \in \arg\min_x \{\mathcal{D}(Ax, y_i) + \lambda \mathcal{R}(x)\}$$



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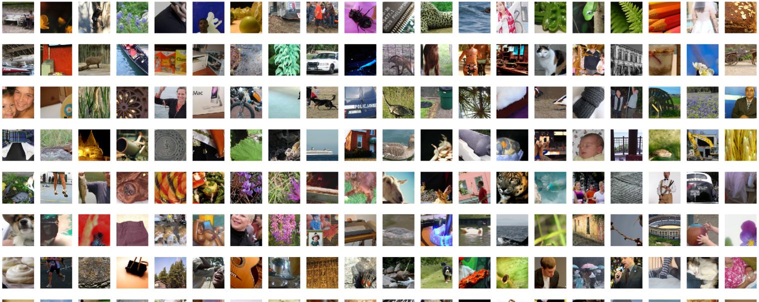

Inexact Algorithms for Bilevel Learning

Bilevel learning: Reduced formulation

Upper level:

$$\min_{\lambda \geq 0, \hat{x}} \|\hat{x} - x^\dagger\|_2^2$$

Lower level:

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

Bilevel learning: Reduced formulation

Upper level:

$$\min_{\lambda \geq 0, \hat{x}} U(\hat{x})$$

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Bilevel learning: Reduced formulation

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Lower level:

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Bilevel learning: Reduced formulation

Upper level: $$\min_{\lambda \geq 0, \hat{x}} U(\hat{x})$$

Lower level:

$$x(\lambda) := \hat{x} = \arg\min_{x} L(x, \lambda)$$

Reduced formulation: $\min_{\lambda \geq 0} U(x(\lambda)) =: \tilde{U}(\lambda)$

Bilevel learning: Reduced formulation

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$$\min_{\lambda \geq 0, \hat{x}} U(\hat{x})$$

Lower level:
$$x(\lambda) := \hat{x} = \arg\min_{x} L(x, \lambda) \quad \Leftrightarrow \quad \partial_x L(x(\lambda), \lambda) = 0$$

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Reduced formulation: $$\min_{\lambda \geq 0} U(x(\lambda)) =: \tilde{U}(\lambda)$$

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

Bilevel learning: Reduced formulation

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$$\nabla \tilde{U}(\lambda) = (x'(\lambda))^* \nabla U(x(\lambda))$$

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$$\begin{aligned} \nabla \tilde{U}(\lambda) &= (x'(\lambda))^* \nabla U(x(\lambda)) \\ &= -A^* B^{-1} \nabla U(x(\lambda)) = -A^* w \end{aligned}$$

where w solves $Bw = \nabla U(x(\lambda))$.

Algorithm for Bilevel learning

Upper level: $\min_{\lambda \geq 0, \hat{x}} U(\hat{x})$

Lower level: $x(\lambda) := \arg\min_x L(x, \lambda)$

Reduced formulation: $\min_{\lambda \geq 0} U(x(\lambda)) =: \tilde{U}(\lambda)$

- Solve reduced formulation via L-BFGS-B Nocedal and Wright 2000
- Compute gradients: Given λ
  1. Compute $x(\lambda)$, e.g. via PDHG Chambolle and Pock 2011
  2. Solve $Bw = \nabla U(x(\lambda))$, $B := \partial_x^2 L(x(\lambda), \lambda)$ e.g. via CG
  3. Compute $\nabla \tilde{U}(\lambda) = -A^* w$, $A := \partial_\lambda \partial_x L(x(\lambda), \lambda)$

Algorithm for Bilevel learning

Upper level: $\min_{\lambda \geq 0, \hat{x}} U(\hat{x})$

Lower level: $x(\lambda) := \arg\min_x L(x, \lambda)$

Reduced formulation: $\min_{\lambda \geq 0} U(x(\lambda)) =: \tilde{U}(\lambda)$

- Solve reduced formulation via L-BFGS-B Nocedal and Wright 2000
- Compute gradients: Given λ
  (1) Compute $x(\lambda)$, e.g. via PDHG Chambolle and Pock 2011
  (2) Solve $Bw = \nabla U(x(\lambda))$, $B := \partial_x^2 L(x(\lambda), \lambda)$ e.g. via CG
  (3) Compute $\nabla \tilde{U}(\lambda) = -A^* w$, $A := \partial_\lambda \partial_x L(x(\lambda), \lambda)$

This approach has a number of problems:

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

How to solve Bilevel Learning Problems?

- Most people: Ignore "problems", just compute it. e.g. Sherry et al. 2020
- Semi-smooth Newton: similar fundamental problems Kunisch and Pock 2013
- Replace lower level problem by finite number of iterations of algorithms: not bilevel anymore Ochs et al. 2015

How to solve Bilevel Learning Problems?

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Use algorithm that acknowledges difficulties:
e.g. inexact DFO Ehrhardt and Roberts 2021

Dynamic Accuracy Derivative Free Optimization

$$\min_{\theta} f(\theta)$$

Key idea: Use f_ϵ:

$$|f(\theta) - f_\epsilon(\theta)| < \epsilon$$

Accuracy as low as possible, but as high as necessary.

E.g. if

$$f_{\epsilon^{k+1}}(\theta^{k+1}) < f_{\epsilon^k}(\theta^k) - \epsilon^k - \epsilon^{k+1},$$

then

$$f(\theta^{k+1}) < f(\theta^k)$$

Dynamic Accuracy Derivative Free Optimization

$$\min_{\theta} f(\theta)$$

For $k = 0, 1, 2, \ldots$

1) Sample f_{ϵ^k} in a neighbourhood of θ_k
2) Build model $m_k(\theta) \approx f_{\epsilon^k}$
3) Minimise m_k around θ_k to get θ_{k+1}
4) If model decrease is sufficient compared to function error: accept step

Algorithm 1 Dynamic accuracy DFO algorithm for (22).

Inputs: Starting point $\theta^0 \in \mathbb{R}^n$, initial trust-region radius $0 < \Delta^0 \leq \Delta_{\max}$.

Parameters: strictly positive values $\Delta_{\max}, \gamma_{\text{dec}}, \gamma_{\text{inc}}, \eta_1, \eta_2, \eta_1', \epsilon$ satisfying $\gamma_{\text{dec}} < 1 < \gamma_{\text{inc}}$, $\eta_1 \leq \eta_2 < 1$, and $\eta_1' < \min(\eta_1, 1 - \eta_2)/2$.

Select an arbitrary interpolation set and construct m^0 (26).
for $k = 0, 1, 2, \ldots$ **do**
  repeat
    Evaluate $\widetilde{f}(\theta^k)$ to sufficient accuracy that (32) holds with η_1' (using s^k from the previous iteration of this inner repeat/until loop). Do nothing in the first iteration of this repeat/until loop.
    if $\|g^k\| \leq \epsilon$ **then**
      By replacing Δ^k with $\gamma_{\text{dec}}^i \Delta^k$ for $i = 0, 1, 2, \ldots$, find m^k and Δ^k such that m^k is fully linear in $B(\theta^k, \Delta^k)$ and $\Delta^k \leq \|g^k\|$. *[criticality phase]*
    end if
    Calculate s^k by (approximately) solving (27).
  until the accuracy in the evaluation of $\widetilde{f}(\theta^k)$ satisfies (32) with η_1' *[accuracy phase]*
  Evaluate $\widetilde{r}(\theta^k + s^k)$ so that (32) is satisfied with η_1' for $\widetilde{f}(\theta^k + s^k)$, and calculate $\widetilde{\rho}^k$ (29).
  Set θ^{k+1} and Δ^{k+1} as:

$$\theta^{k+1} = \begin{cases} \theta^k + s^k, & \widetilde{\rho}^k \geq \eta_2, \text{ or } \widetilde{\rho}^k \geq \eta_1 \text{ and } m^k \\ & \text{fully linear in } B(\theta^k, \Delta^k), \\ \theta^k, & \text{otherwise,} \end{cases} \tag{33}$$

and

$$\Delta^{k+1} = \begin{cases} \min(\gamma_{\text{inc}} \Delta^k, \Delta_{\max}), & \widetilde{\rho}^k \geq \eta_2, \\ \Delta^k, & \widetilde{\rho}^k < \eta_2 \text{ and } m^k \text{ not} \\ & \text{fully linear in} B(\theta^k, \Delta^k), \\ \gamma_{\text{dec}} \Delta^k, & \text{otherwise.} \end{cases} \tag{34}$$

  If $\theta^{k+1} = \theta^k + s^k$, then build m^{k+1} by adding θ^{k+1} to the interpolation set (removing an existing point). Otherwise, set $m^{k+1} = m^k$ if m^k is fully linear in $B(\theta^k, \Delta^k)$, or form m^{k+1} by making m^k fully linear in $B(\theta^{k+1}, \Delta^{k+1})$.
end for

Theorem Ehrhardt and Roberts 2021

If f is sufficiently smooth and bounded below, then the algorithm is globally convergent in the sense that

$$\lim_{k \to \infty} \|\nabla f(\theta_k)\| = 0\,.$$

1D Denoising Problem (learn α, ν and ξ) Ehrhardt and Roberts 2021

$$\min_{\theta} \left\{ \frac{1}{2} \sum_i \|x_i(\theta) - x_i\|_2^2 + \beta \left(\frac{L(\theta)}{\kappa(\theta)} \right)^2 \right\}$$

$$x_i(\theta) = \arg\min_x \frac{1}{2}\|x - y_i\|_2^2 + \alpha \left(\sum_j \sqrt{\|(\nabla x)_j\|_2^2 + \nu^2} + \frac{\xi}{2}\|x\|_2^2 \right)$$

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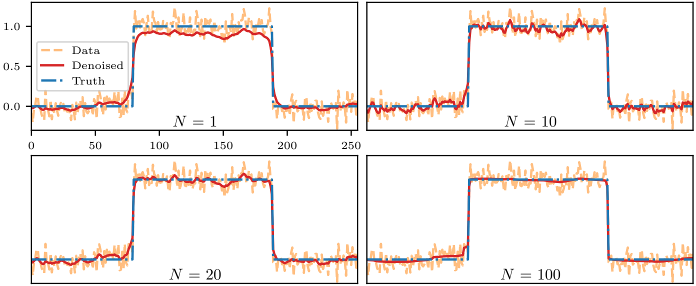
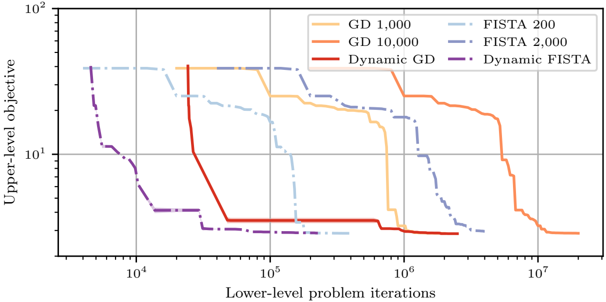
With more evaluations of $f(\theta)$, the parameter choices give better reconstructions:



Reconstruction of x_1 after N evaluations of $f(\theta)$

1D Denoising Problem (learn α, ν and ξ) Ehrhardt and Roberts 2021

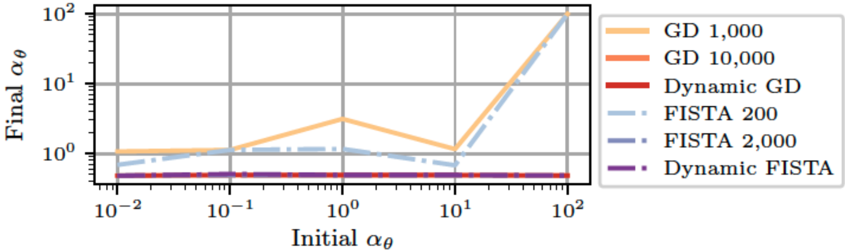
Dynamic accuracy is faster than "fixed accuracy" (at least 10x speedup):



Objective value $f(\theta)$ vs. computational effort

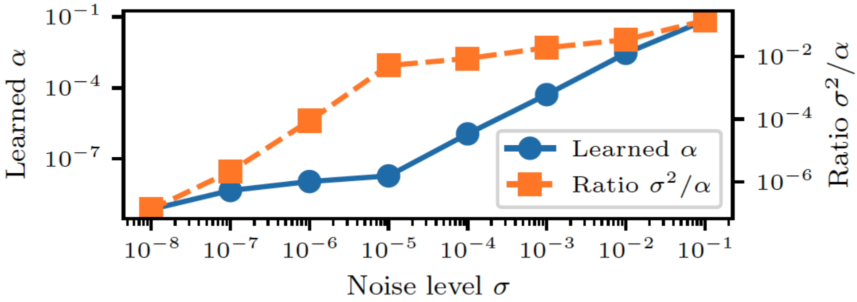
1D Denoising Problem Ehrhardt and Roberts 2021

Always learns the same parameter for sufficient accuracy.



Robustness to initialization

Denoising Problem (learn α, ν and ξ) Ehrhardt and Roberts 2021



Bilevel learning is a convergent regularization?

Learn sampling pattern in MRI

Some important works on sampling for MRI

Uninformed

- Cartesian, radial, variable density ... e.g. Lustig et al. 2007
  - ✓ simple to implement
  - ✗ not tailored to application or reconstruction method
- compressed sensing: random sampling e.g. Candes and Romberg 2007
  - ✓ mathematical guarantees
  - ✗ limited to sparse signals and sparsity promoting regularizers

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Learned

- **Largest Fourier coefficients** of training set Knoll et al. 2011
  - ✓ simple to implement, computationally light
  - ✗ not tailored to reconstruction method
- **greedy**: iteratively select "best" sample e.g. Gözcü et al. 2018
  - ✓ adaptive to dataset, reconstruction method
  - ✗ only discrete values; computationally heavy
- **Deep learning**: e.g. specify sampling as continuous parameters in network Wang et al. 2021
  - ✓ realistic and easy to implement sampling patterns
  - ✓ end-to-end
  - ✗ limited to neural network reconstruction

Learn sampling pattern in MRI

Lower level (MRI reconstruction):

$$x_i(\lambda, s) = \arg\min_x \left\{ \sum_{j=1}^{N} s_j^2 |(Fx - y_i)_j|^2 + \lambda \mathcal{R}(x) \right\} \quad s_i \in \{0, 1\}$$

Sherry et al. 2020

Learn sampling pattern in MRI

Upper level (learning):

Given **training data** $(x_i^\dagger, y_i)_{i=1}^n$, solve

$$\min_{\lambda \geq 0, s \in \{0,1\}^m} \frac{1}{n} \sum_{i=1}^{n} \|x_i(\lambda, s) - x_i^\dagger\|_2^2$$

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Sherry et al. 2020

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Sherry et al. 2020

Warm up

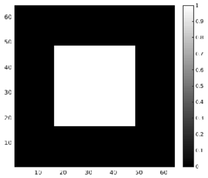
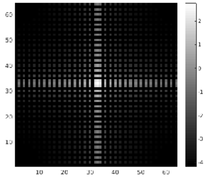
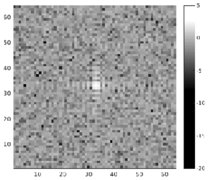


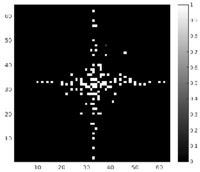
Figure: Discrete 2d bump



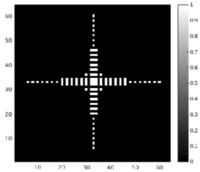
(a) Original data: $\log |y|$



(b) Noisy data: $\log |\tilde{y}|$

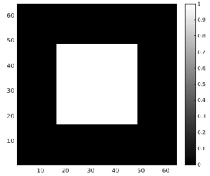


(c) Learned sampling pattern



(d) Largest 2.76% Fourier Coefficients

Warm up



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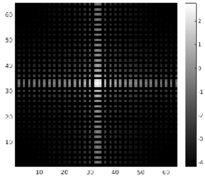

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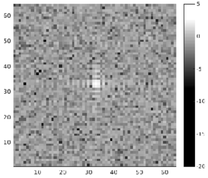

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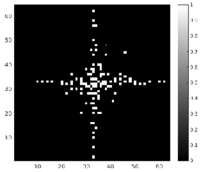

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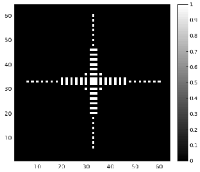

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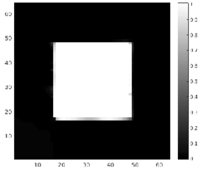
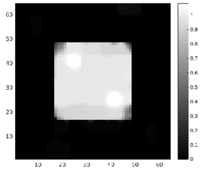


(e) Learned sampling pattern



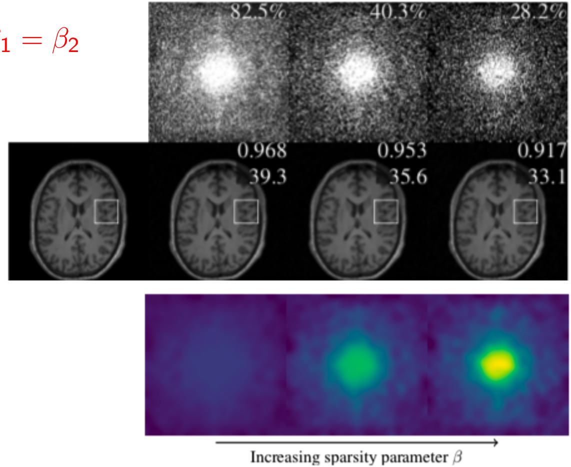
(f) Largest 2.76% Fourier Coefficients

Increasing sparsity Sherry et al. 2020

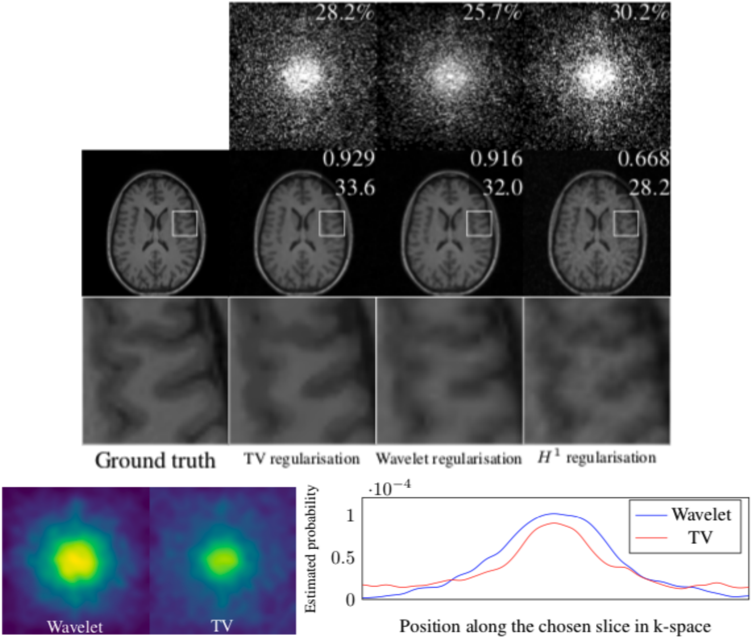
Reminder: **Upper level** (learning)

$$\min_{\lambda \geq 0, s \in [0,1]^m} \frac{1}{n} \sum_{i=1}^{n} \|x_i(\lambda, s) - x_i^\dagger\|_2^2 + \beta_1 \sum_{j=1}^{m} s_j + \beta_2 \sum_{j=1}^{m} s_j(1 - s_j)$$

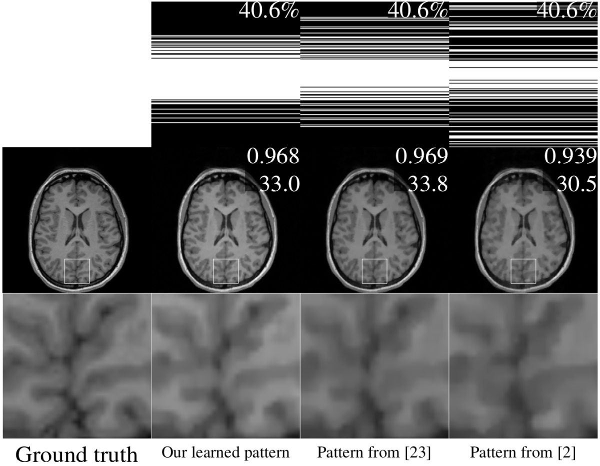
$\beta = \beta_1 = \beta_2$



Compare regularizers Sherry et al. 2020



Compare Cartesian samplings Sherry et al. 2020



	Line sampling (40.6%)	Free pattern (34.7%)
Our method	4192	6494
The method from [23]	12087	$3.90 \cdot 10^8$

number of lower-level solves

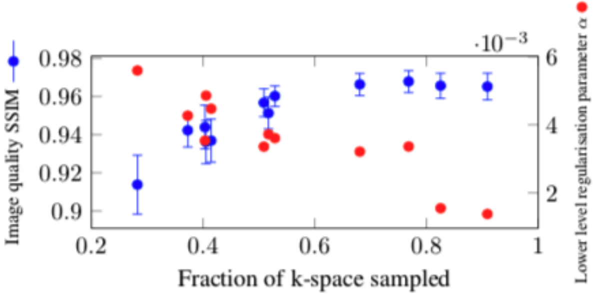
"ours" = Sherry et al. 2020

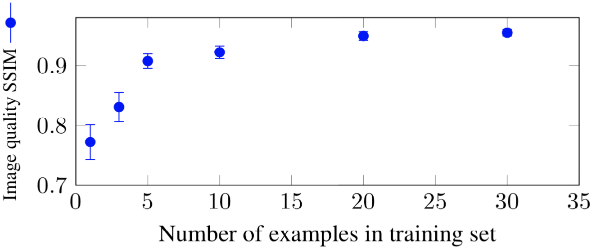
[23] = Gözcü et al. 2018

[2] = Lustig et al. 2007

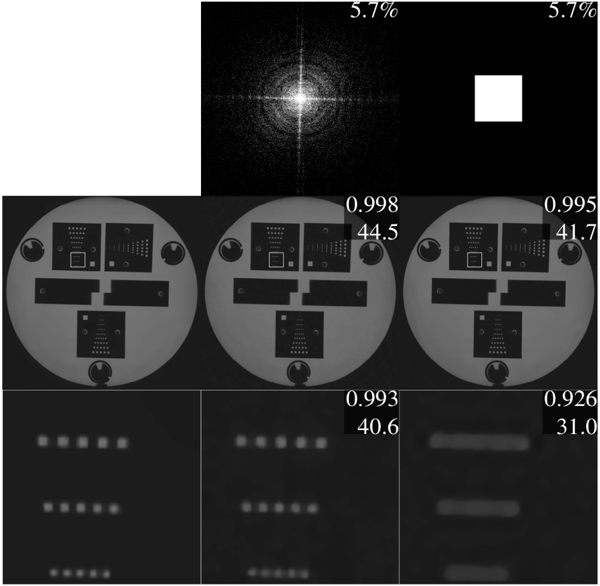
regularizer = TV

More insights: sampling and number of data Sherry et al. 2020





High resolution imaging: 1024^2 Sherry et al. 2020



Conclusions and Outlook

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- **Bilevel learning**: supervised learning framework to learn parameters in variational regularization
- **Optimization** plays a key role in bilevel learning
  - **Dynamic accuracy**: no need to specify number of iterations
  - Improved algorithms **speed up** learning significantly
  - Make learning **surprisingly robust**
- **Learned sampling** better than generic sampling
  - "Optimal" sampling **depends on regularizer**
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Future work

- **Stochastic** algorithms (like stochastic gradient descent etc)
- **Nonsmooth** or **nonconvex** lower-level problems
- **Inexact gradient** methods
- **Neural network** regularization