Bilevel Learning for Inverse Problems

Matthias J. Ehrhardt

Department of Mathematical Sciences, University of Bath, UK

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Joint work with:
F. Sherry, M. Graves, G. Maierhofer, G. Williams, C.-B. Schönlieb (all Cambridge, UK), M. Benning (Queen Mary, UK), J.C. De los Reyes (EPN, Ecuador)

L. Roberts (ANU, Australia)

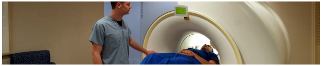
The Leverhulme Trust

Engineering and Physical Sciences Research Council

THE FARADAY INSTITUTION

Outline

1) Motivation



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

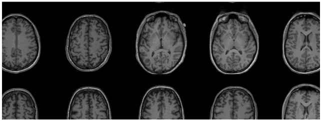
2) Bilevel Learning

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

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

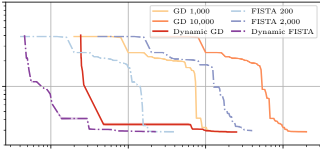
3) Learn sampling pattern in MRI

Sherry et al., "Learning the Sampling Pattern for MRI," IEEE TMI 2020.



4) Inexact algorithms

Ehrhardt and Roberts, "Inexact Derivative-Free Optimization for Bilevel Learning," JMIV 2021.



Inverse problems

$$Ax = y$$

x : desired solution

y : observed data

A : mathematical model

Goal: recover x given y

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 (∼1960): $\mathcal{R}(x) = \frac{1}{2}\|x\|_2^2$
- H^1 (∼1960-1990?) $\mathcal{R}(x) = \frac{1}{2}\|\nabla x\|_2^2$

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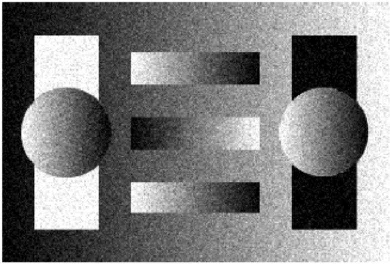
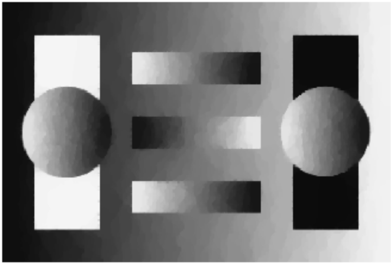
- Total Variation $\mathcal{R}(x) = \|\nabla x\|_1$ Rudin, Osher, Fatemi 1992



Noisy image



TV denoised image

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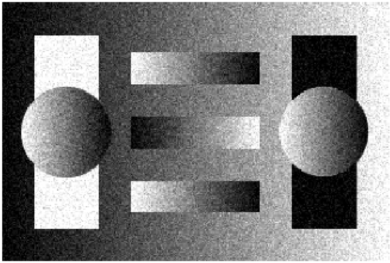

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TV² denoised image

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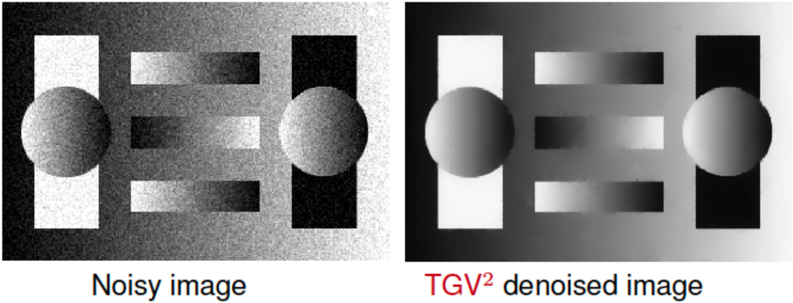
  $\mathcal{R}(x) = \inf_v \|\nabla x - v\|_1 + \beta\|\nabla v\|_1$ Bredies, Kunisch, Pock 2010



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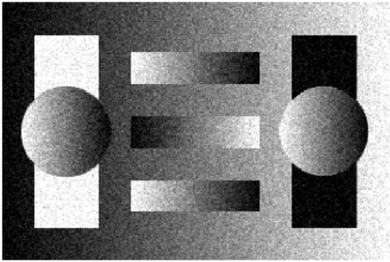
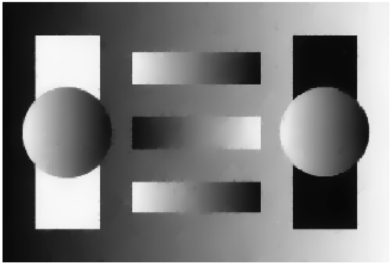


Noisy image

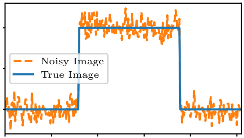


TGV^2 denoised image

How to choose the regularization?

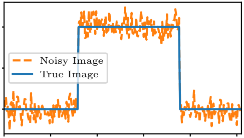
More "complicated" regularizers

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



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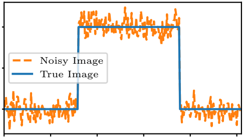
$$\min_x \frac{1}{2}\|Ax-y\|_2^2 + \alpha\left(\underbrace{\sum_j \sqrt{\|(\nabla x)_j\|_2^2 + \nu^2}}_{\approx \mathrm{TV}(x)} + \frac{\xi}{2}\|x\|_2^2\right)$$



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

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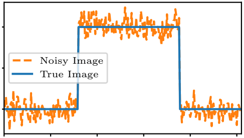
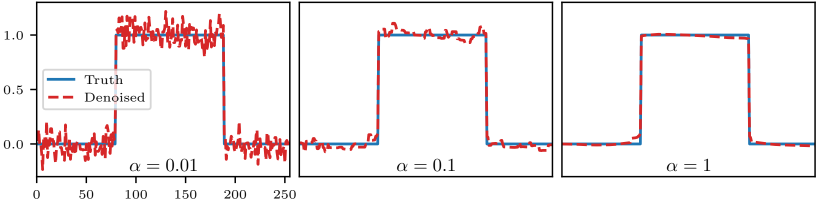


- Smooth and strongly convex
- Solution depends on choices of α, ν and ξ

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



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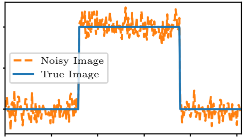

- Smooth and strongly convex
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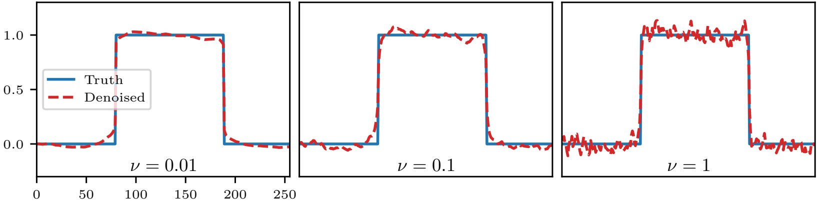
Vary ν ($\alpha = 1$, $\xi = 10^{-3}$)



More "complicated" regularizers

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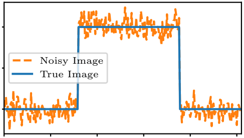
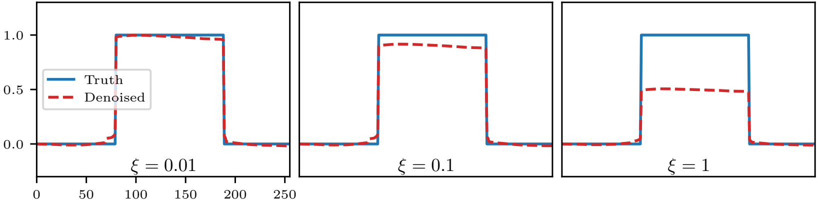


- Smooth and strongly convex
- Solution depends on choices of α, ν and ξ

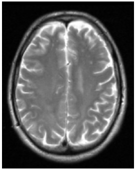
Vary ξ $(\alpha = 1,\ \nu = 10^{-3})$



How to choose all these parameters?

Example: Magnetic Resonance Imaging (MRI)

MRI scanner

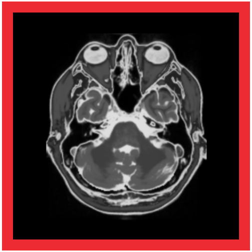


T_2^*

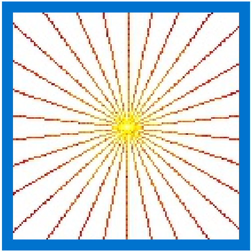
Continuous model: Fourier transform

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

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



$\longrightarrow$



Solution **not unique**.

Example: MRI reconstruction

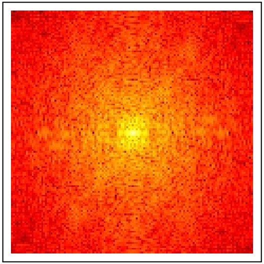
Compressed Sensing MRI:

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

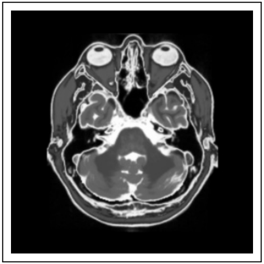
Fourier transform F, sampling $Sw = (w_i)_{i \in \Omega}$

$$\hat{x} \in \arg\min_x \left\{ \frac{1}{2} \|SFx - y\|_2^2 + \lambda \|\nabla x\|_1 \right\}$$

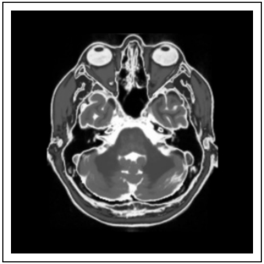
Miki Lustig



sampling $S^* y$



$\lambda = 0$



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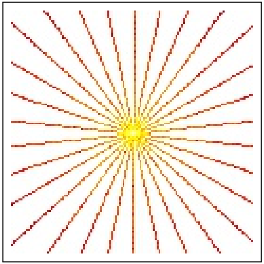

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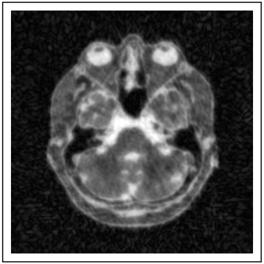

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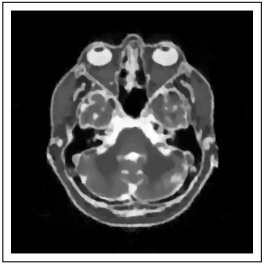

$\lambda = 10^{-4}$

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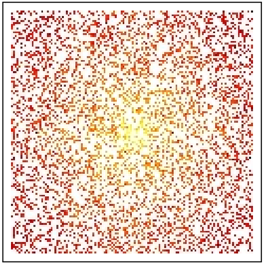
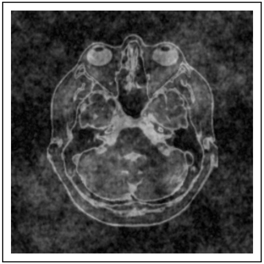
Miki Lustig



sampling $S^* y$



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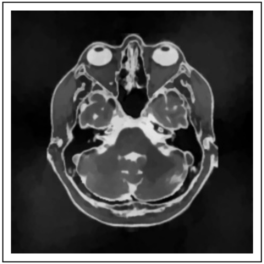

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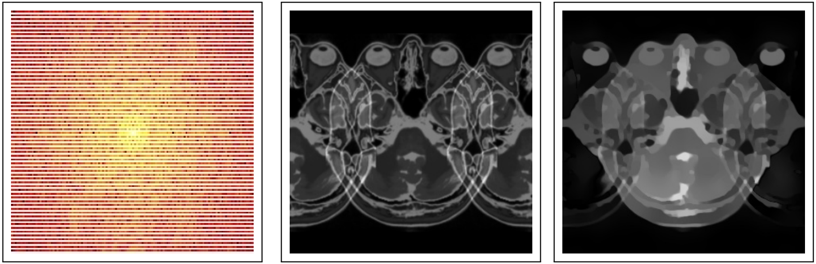

sampling $S^* y$ | $\lambda = 0$ | $\lambda = 10^{-3}$

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

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

Motivation

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

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

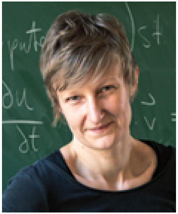
Bilevel learning for inverse problems

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

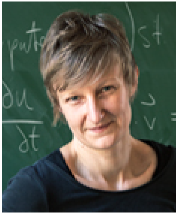
Upper level (learning):

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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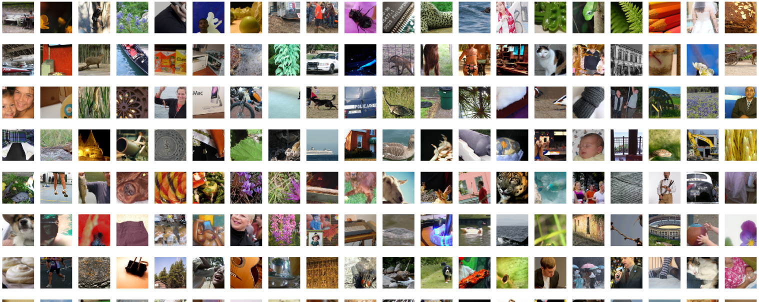
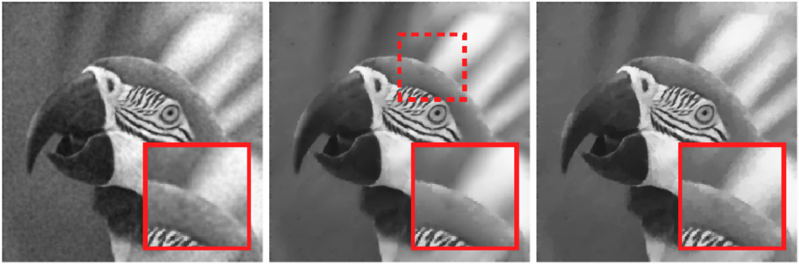


Denoising: Learning two TGV parameters.

$$\mathcal{R}(x) = \inf_v \|\nabla x - v\|_1 + \beta \|\nabla v\|_1$$



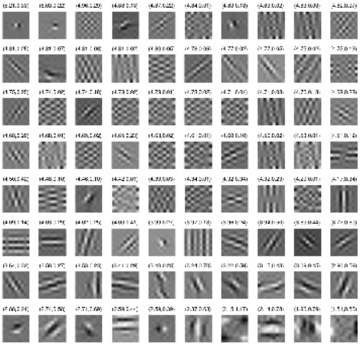
(a) Too low β / High oscillation (b) Optimal β (c) Too high β / almost TV

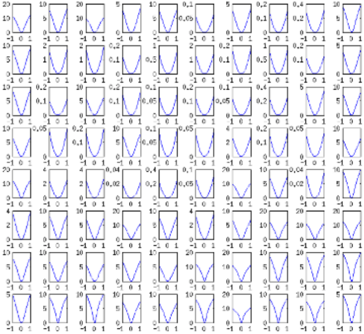
De los Reyes, Schönlieb, Valkonen 2017

Denoising: fields of experts regularisation

Learning filters K_k and potential functions ρ_k for fields of experts regularisation

$$\mathcal{R}(x) = \sum_{k=1}^{M} \sum_{i,j} \rho_k((K_k x)_{i,j})$$





Chen, Ranftl, Pock 2014

Learn sampling pattern in MRI

Learn sampling pattern in MRI

Lower level (MRI reconstruction):

$$R(\lambda, s, y) = \arg\min_x \left\{ \frac{1}{2} \| S(Fx - y) \|_2^2 + \lambda \mathcal{R}(x) \right\}$$

$$S = \mathrm{diag}(s), \quad s_i \in \{0, 1\}$$

Sherry et al. 2020

Learn sampling pattern in MRI

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

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

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Sherry et al. 2020

Warm up

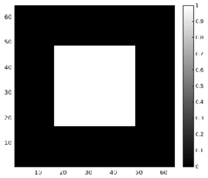
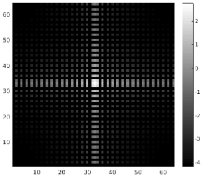
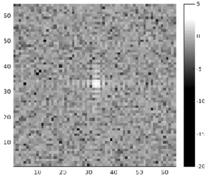


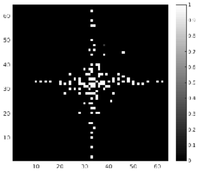
Figure: Discrete 2d bump



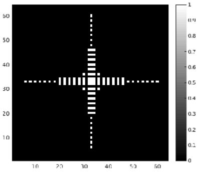
(a) Original data: $\log|y|$



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



(c) Learned sampling pattern



(d) Largest 2.76% Fourier Coefficients

Warm up

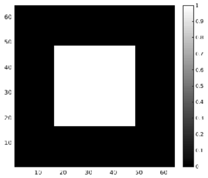
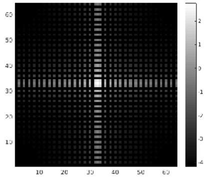


Figure: Discrete 2d bump



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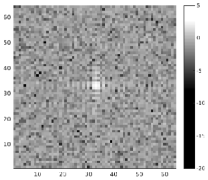
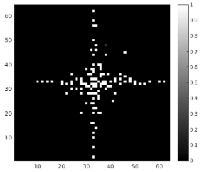
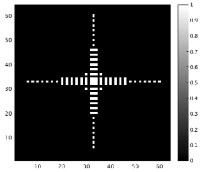


(b) Noisy data: $\log|\tilde{y}|$



(c) Learned sampling pattern



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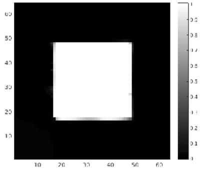
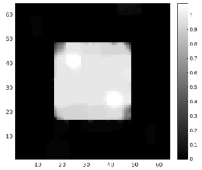
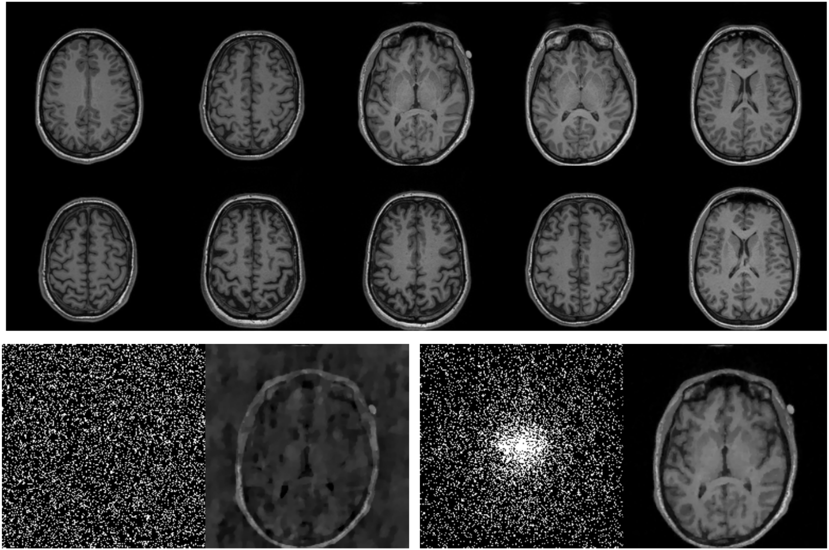


(e) Learned sampling pattern



(f) Largest 2.76% Fourier Coefficients

Classical compressed sensing versus learned Sherry et al. 2020



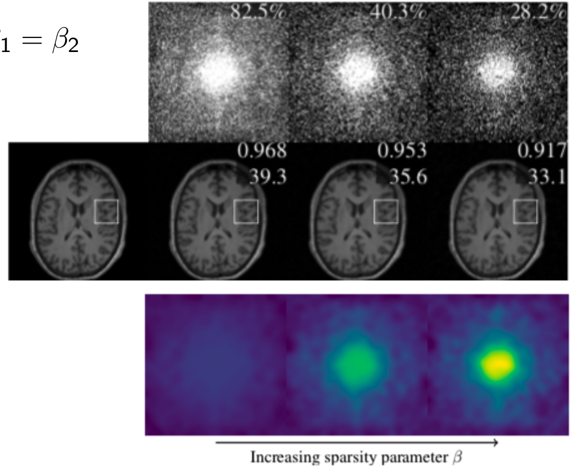
Uniform random Reconstruction Learned Reconstruction

Increasing sparsity Sherry et al. 2020

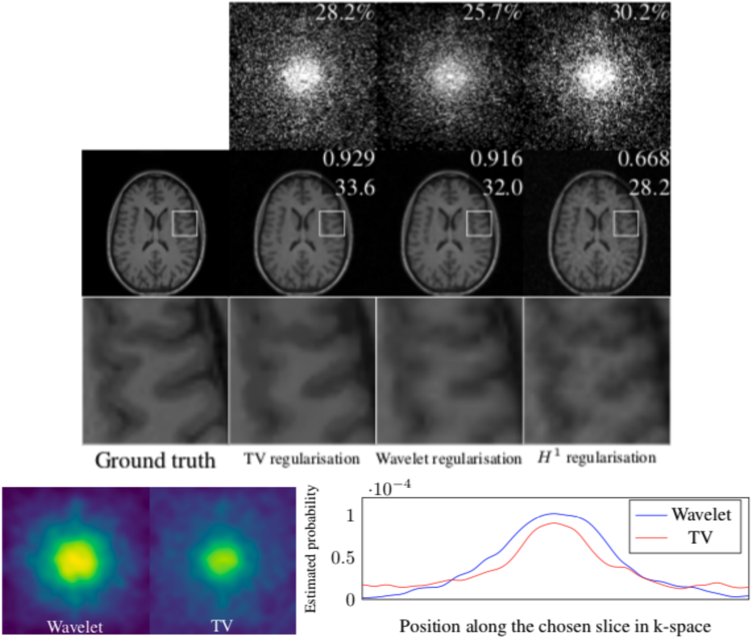
Reminder: **Upper level** (learning)

$$\min_{\lambda\geq 0, s\in[0,1]^m} \frac{1}{n}\sum_{i=1}^{n} \|R(\lambda, s, y_i) - x_i\|_2^2 + \beta_1\|s\|_1 + \beta_2\|s(1-s)\|_1$$

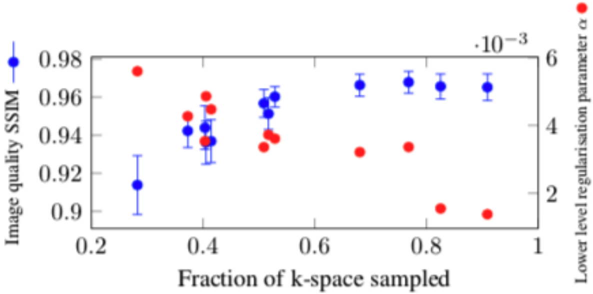
$$\beta = \beta_1 = \beta_2$$

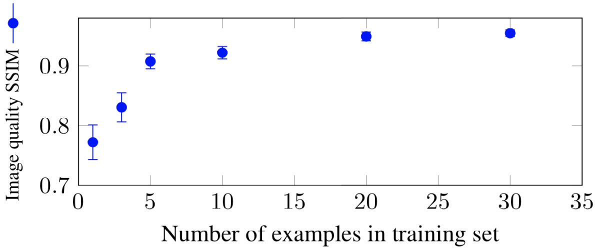


Compare regularizers Sherry et al. 2020

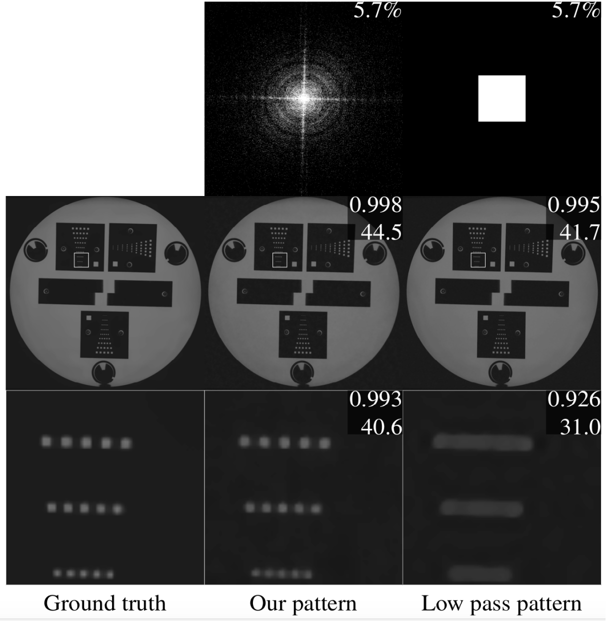


More insights: sampling and number of data Sherry et al. 2020





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



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

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Bilevel learning: Reduced formulation

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

Lower level:

$$x_\lambda := \hat{x} = \arg\min_x L(x, \lambda) \quad \Leftrightarrow \quad \partial_x L(x_\lambda, \lambda) = 0$$

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

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$$\nabla \tilde{U}(\lambda) = (\partial_\lambda x_\lambda)^* \nabla U(x_\lambda)$$

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

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_λ, 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 $\nabla \tilde{U}(\lambda) = -A^* w$, $A := \partial_\theta \partial_x L(x_\lambda, \lambda)$

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This approach has a number of problems:

- x_λ has to be computed
- Derivative assumes x_λ is exact minimizer
- Large system of linear equations has to be solved

How to solve Bilevel Problem?

- 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

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

Ehrhardt and Roberts 2021

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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

Ehrhardt and Roberts 2021

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

Theoretical Guarantees

Algorithm converges with inexact evaluations of $\hat{x}_i(\theta)$:

Theorem Ehrhardt and Roberts 2021

If f is sufficiently smooth and bounded below, then:

- The Dynamic Accuracy DFO algorithm is globally convergent in the sense that $\lim_{k\to\infty} \|\nabla f(\theta_k)\| = 0$.
- All evaluations of $\hat{x}_i(\theta)$ together require at most $\mathcal{O}(\epsilon^{-2}|\log \epsilon|)$ iterations (of gradient descent, FISTA etc.)

Numerical Results

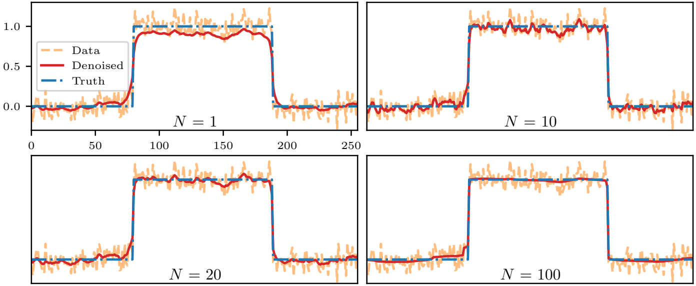
- Dynamic Accuracy DFO
  github.com/lindonroberts/inexact_dfo_bilevel_learning
- Compare to regular DFO with "fixed accuracy" lower-level solutions (constant # iterations of GD/FISTA)
  - In practice, have to guess appropriate # iterations
- Measure decrease in $f(\theta)$ as function of total GD/FISTA iterations

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

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

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

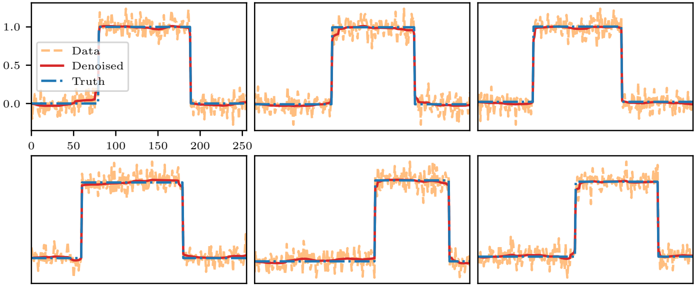
With more evaluations of $f(\theta)$, the parameter choices give better reconstructions:



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

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

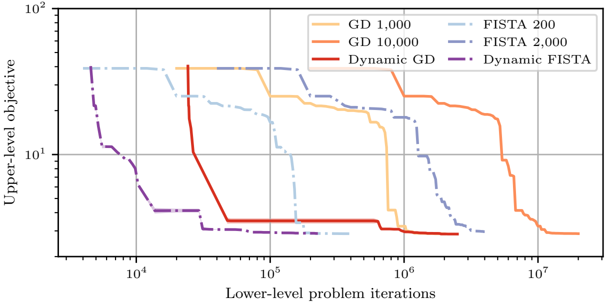
Final learned parameters give good reconstructions of all training data:



Final reconstructions after 100 **evaluations of** $f(\theta)$

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

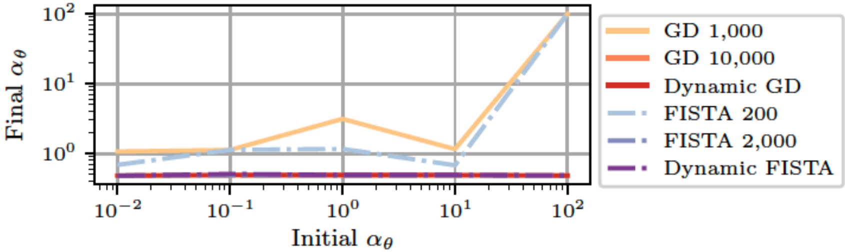
Dynamic accuracy is faster than "fixed accuracy" (at least 10x speedup):



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

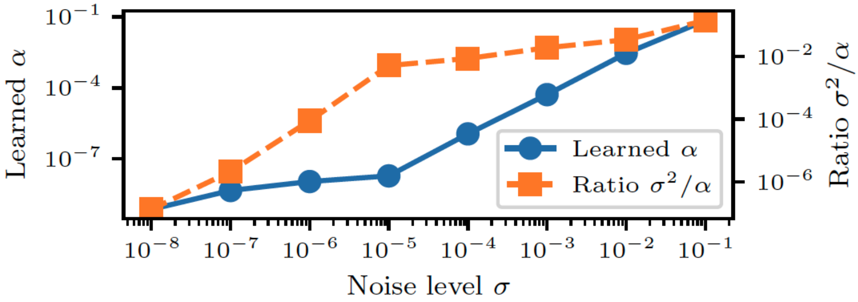
1D Denoising Problem Ehrhardt and Roberts 2021

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?

MRI Sampling revisited

MRIs measure a subset of Fourier coefficients of an image: reconstruct using

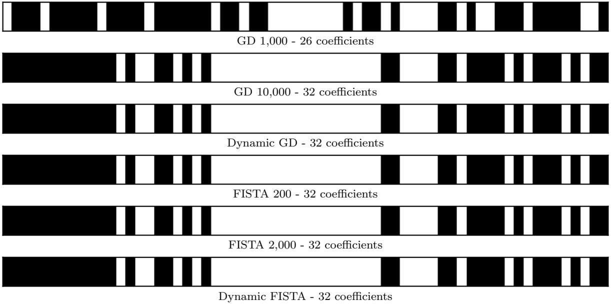
$$\min_x \frac{1}{2}\|S(Fx - y)\|^2 + \mathcal{R}(x)$$

where sampling pattern $S = \mathrm{diag}(s_1, \ldots, s_d)$.

- Use same smoothed TV regulariser $\mathcal{R}$ (with fixed α, ν, ξ)
- Learn $s_j(\theta) := \sqrt{\theta_j/(1-\theta_j)}$ Chen et al. 2014
- Promote sparsity: $\mathcal{J}(\theta) = \|\theta\|_1$.

Learning MRI Sampling Patterns

All variants learn 50% sparse sampling patterns:

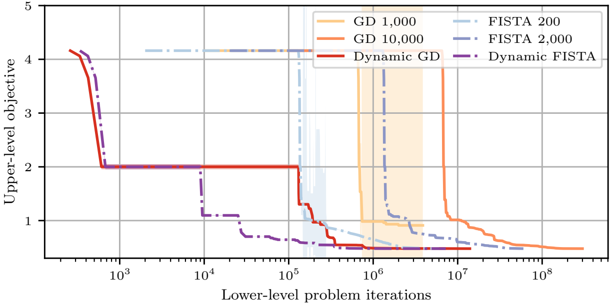


Learned sampling patterns (white = active)

Robustness to lower-level solver with "enough" accuracy

Learning MRI Sampling Patterns

... and dynamic accuracy is still substantially faster than fixed accuracy:



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

Conclusions and Outlook

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- **Bilevel learning**: supervised learning framework to learn parameters in variational regularization
- **Learned sampling** better than generic sampling
  - "Optimal" sampling **depends on regularizer**
  - **Very little data** needed
- **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**

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Future work

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