

# Solving Inverse Problems with Deep Learning

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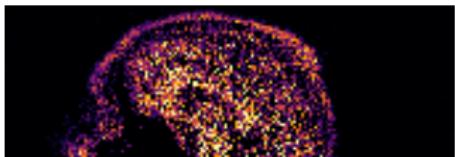


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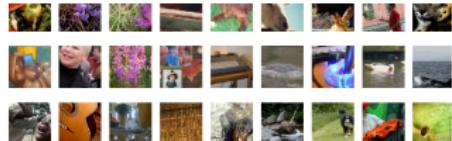


# Outline

**1)** Inverse Problems  
and how to solve them



**2)** Learning from examples:  
Machine Learning meets Inverse  
Problems



## **Inverse Problems and how to solve them**

## Inverse problems

$$A\textcolor{red}{u} = \textcolor{blue}{b}$$

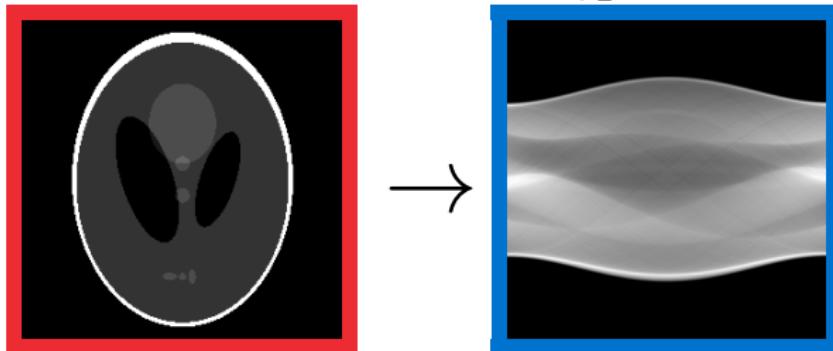
$\textcolor{red}{u}$  : desired solution

$\textcolor{blue}{b}$  : observed data

$A$  : mathematical model

**Goal:** recover  $\textcolor{red}{u}$  given  $\textcolor{blue}{b}$

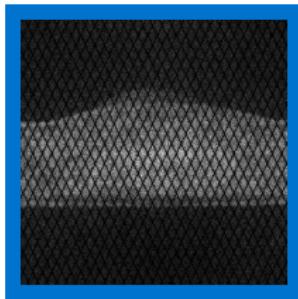
- CT: Radon / X-ray transform  $\textcolor{red}{A}\textcolor{red}{u}(L) = \int_L u(x)dx$



# What is the problem with Inverse Problems?

A solution may

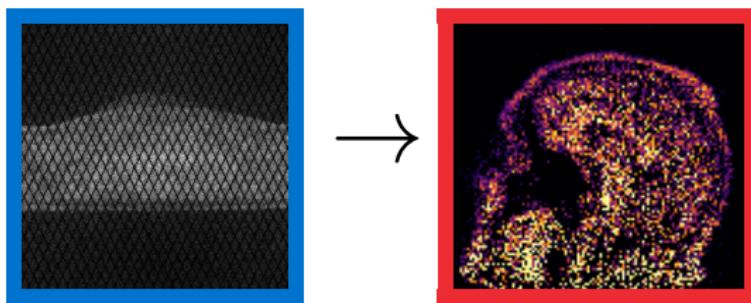
- ▶ **not exist:** define generalized solution (e.g. least squares)
- ▶ **not be unique:** select one via a-priori information
- ▶ **be sensitive to noise:**
  - Positron Emission Tomography (PET)
  - Data: PET scanner in London
  - Model: ray transform,  $\mathbf{A}u(L) = \int_L u(r)dr$
  - Find  $u$  such that  $\mathbf{A}u = b$



# What is the problem with Inverse Problems?

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# How to solve Inverse Problems?

$$A\textcolor{red}{u} = \textcolor{blue}{b}$$

$\textcolor{red}{u}$  : desired solution

$\textcolor{blue}{b}$  : observed data

$A$  : mathematical model

**Goal:** recover  $\textcolor{red}{u}$  given  $\textcolor{blue}{b}$

- ▶ Option 1: Analytical methods
- ▶ Option 2: Variational regularization
- ▶ Option 3: Iterative regularization
- ▶ Option 4\*: Bayesian methods

## Option 1: Analytical methods

$$A\mathbf{u} = \mathbf{b}, \quad \Phi_\lambda : \mathbf{b} \mapsto \mathbf{u}$$

- ▶ Find formula  $\Phi_\lambda$ , e.g. in MRI zero-filled reconstruction, sum-of-squares, in CT or PET filtered backprojection
- ▶ Often:  $\Phi_0 = A^\dagger$

### Pros:

- ▶ very fast!

### Cons:

- ▶ limited modelling options: forward operator
- ▶ need high-quality data: e.g. (close to) injective
- ▶ difficult to use a-priori information: e.g. nonnegativity or smoothness

Hardly used when image quality is important (except CT)

## Option 2: Variational regularization

$$\Phi_\lambda(\mathbf{b}) = \arg \min_{\mathbf{u}} \left\{ \mathcal{D}(A\mathbf{u}, \mathbf{b}) + \lambda \mathcal{R}(\mathbf{u}) \right\}$$

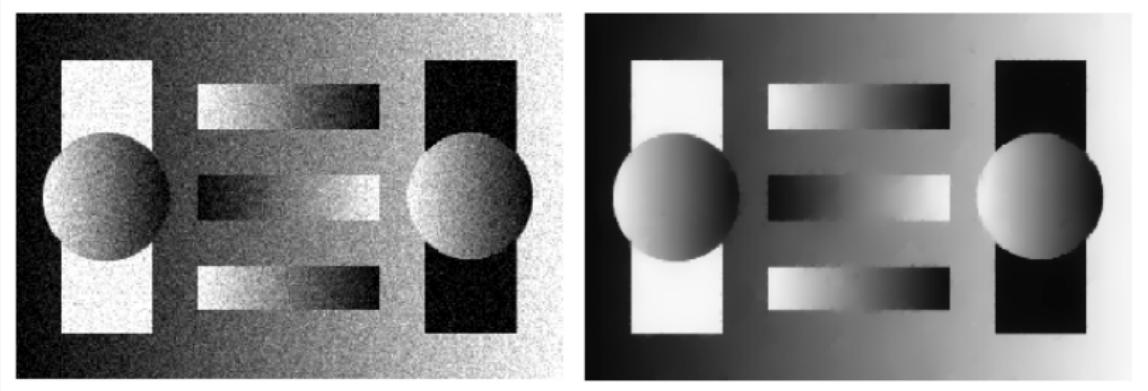
$\mathcal{D}$  measures **fidelity** between  $A\mathbf{u}$  and  $\mathbf{b}$ , related to noise statistics

$\mathcal{R}$  **regularizer** penalizes unwanted features and ensures stability;

e.g. TV Rudin, Osher, Fatimi '92  $\mathcal{R}(\mathbf{u}) = \|\nabla \mathbf{u}\|_1$ ,

TGV Bredies, Kunisch, Pock '10  $\mathcal{R}(\mathbf{u}) = \inf_v \|\nabla \mathbf{u} - v\|_1 + \beta \|\nabla v\|_1$

$\lambda \geq 0$  **regularization parameter** balances fidelity and regularization



## Option 2: Variational regularization (cont 2)

$$\Phi_\lambda(\mathbf{b}) = \arg \min_{\mathbf{u}} \{ \mathcal{D}(A\mathbf{u}, \mathbf{b}) + \lambda \mathcal{R}(\mathbf{u}) \}$$

- ▶ Only theoretical. Need to find algorithm  $(u^k)$  such that

$$\Phi_\lambda(\mathbf{b}) := \lim_{k \rightarrow \infty} u^k$$

- ▶ Proximal Gradient Descent / Forward-Backward Splitting

Bauschke and Combettes '11, Beck '17 ...

$$u^{k+1} = \text{prox}_{\tau_k \lambda \mathcal{R}}(u^k - \tau_k \nabla \mathcal{E}(u^k))$$

$$\mathcal{E}(u) = \mathcal{D}(Au, \mathbf{b})$$

proximal operator Moreau '62

$$\text{prox}_f(z) := \arg \min_u \left\{ \frac{1}{2} \|u - z\|^2 + f(u) \right\}$$

Iterate: fit data, denoise

## Option 2: Variational regularization (cont)

$$\Phi_\lambda(\mathbf{b}) = \arg \min_{\mathbf{u}} \left\{ \mathcal{D}(A\mathbf{u}, \mathbf{b}) + \lambda \mathcal{R}(\mathbf{u}) \right\}$$

### Pros:

- ▶ good modelling: forward operator, data fit and regularizer provide a lot of freedom
- ▶ data quality can be poor if exploiting a-priori knowledge
- ▶ a lot of theory available

### Cons:

- ▶ difficult to choose regularisation parameter  $\lambda$
- ▶ slow: many evaluations of  $A$  and  $A^*$  **ongoing research**
- ▶ modelling simple: TV, TGV work great on geometric phantoms, room for improvement for real data

## Option 3: Iterative regularization

**Idea:** take algorithm ( $u^k$ ) which converges to solution of  $Au = b$ .

For noisy data, stop early. Choose number of iterations  $K(\delta)$ :

$$\Phi_{K(\delta)}(b^\delta) = u_{K(\delta)}$$

### Examples:

- ▶ Landweber iteration:  $u^{k+1} = u^k - \tau_k \nabla \mathcal{E}(u^k)$  Landweber '51
- ▶ Linerised Bregman iteration:  
$$u_{k+1} = \arg \min_u \{\tau_k \langle u, \nabla \mathcal{E}(u^k) \rangle + D_J(u, u^k)\}$$
 Yin et al. '08

### Pros:

- ▶ modelling and data similar to variational regularization
- ▶ some theory available

### Cons:

- ▶ slower than analytical methods, typically faster than variational regularization
- ▶ difficult to determine when to stop
- ▶ as variational regularization most modelling rather simple

# Comparison: Pros and Cons

## Analytical

- ++ fast
- + good theory
- tailored to very specific setting
- too simple

## Variational

- ++ rich theory
- + good applicability
- + modelling simple
- slow

## Iterative

- + good applicability
- + modelling simple
- medium speed
- some theory

- ▶ variational and iterative regularization state-of-the-art prior to deep learning
- ▶ good **modelling** options: make use of some domain knowledge
- ▶ a lot of **theory**: well understood

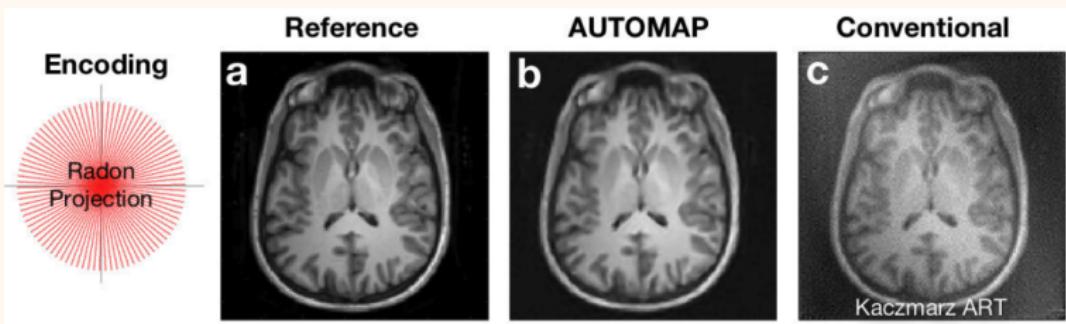
difficult to include more data: what does a **typical** reconstruction look like?

# Machine Learning meets Inverse Problems (i.e. mostly deep learning)

# “Analytic methods” meet Deep Learning

- ▶ automap [Zhu et al. '18](#), Nature paper with 1600+ citations
  - ▶ ignore physical modelling (i.e.  $A$ )

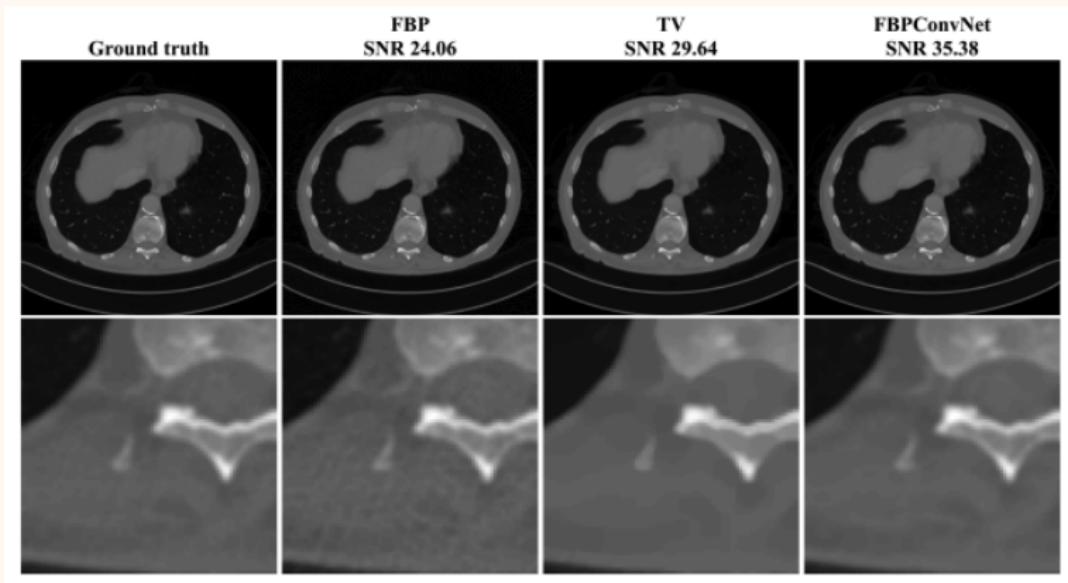
$$\Phi(\mathbf{b}) = \mathcal{N}_\theta(\mathbf{b})$$



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  - ▶ rough recon with physical model, then apply neural network

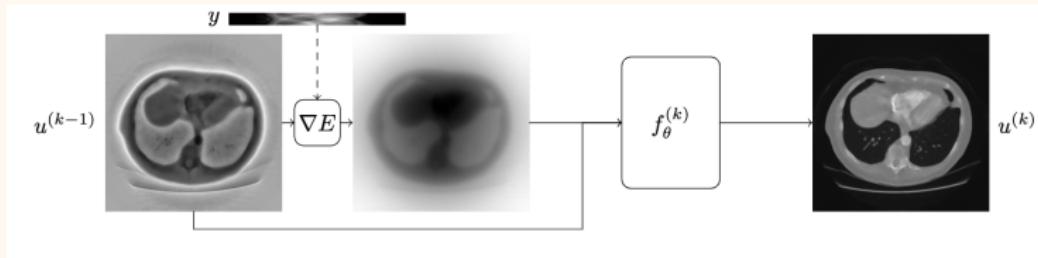
$$\Phi(\mathbf{b}) = \mathcal{N}_\theta(A^\dagger \mathbf{b})$$



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 $\Phi(\mathbf{b}) = \mathcal{N}_\theta(A^\dagger \mathbf{b})$
- ▶ unrolling, e.g. [Gregor and Le Cun '10](#), [Adler and Öktem '17](#)
  - ▶ take few iterations of algorithm and replace prox with neural network

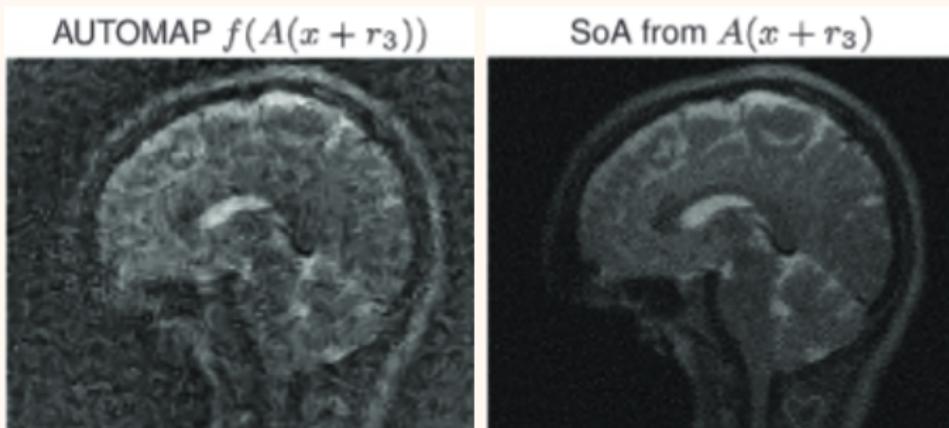
$$\Phi(\mathbf{b}) = u^K, \quad u^{k+1} = \mathcal{N}_\theta^{\textcolor{red}{k}}(u^k - \tau_k \nabla \mathcal{E}(u^k))$$



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Not as stable as pre-deep learning approaches [Antun et al. '19](#)



# Variational regularization meets Deep Learning

Idea: learn a regularizer  $R_\theta$  for variational regularization

- ▶ based on **generative model** [Bora et al. '17](#),  $G_\theta$ : e.g. VAE, GAN  
Learn  $G_\theta$  from a set of images ( $u_k$ )      Image by [Hu et al. '20](#)



Solve inverse problem via

$$z^* \in \arg \min_z \|AG_\theta(z) - b\|^2, \quad u^* = G_\theta(z^*)$$

Notice that  $u^*$  can also be found via

$$\min_u \|Au - b\|^2 + R(u), \quad R(u) = \inf_z \iota_{\{0\}}(u - G_\theta(z))$$

Other options might be suitable [Duff et al. JMIV '23](#), e.g.

$$R(u) = \inf_z \|u - G_\theta(z)\|_2^2$$

# Variational regularization meets Deep Learning

**Idea:** learn a regularizer  $R_\theta$  for variational regularization

- ▶ based on **generative model** [Bora et al. '17](#)
- ▶ based on **denoiser** [Romano et al. '17](#)

$$R(u) = \frac{1}{2} u^T (u - \mathcal{N}_\theta(u))$$

# Variational regularization meets Deep Learning

**Idea:** learn a regularizer  $R_\theta$  for variational regularization

- ▶ based on **generative model** [Bora et al. '17](#)
- ▶ based on **denoiser** [Romano et al. '17](#)
- ▶ train **directly**
  - ▶ if “good” images ( $u_k$ ) and “bad” images ( $v_k$ ) are available [Benning et al. '17](#), choose parameters  $\theta$  to minimize

$$\mathbb{E}_u R_\theta(u) - \mathbb{E}_v R_\theta(v)$$

- ▶ if  $R_\theta$  is also constrained to be 1-Lipschitz, this computes Wasserstein distance between distributions of  $(u_k)$  and  $(v_k)$ . Used in [Lunz et al. '19](#) with  $v = A^\dagger b$ .
- ▶ train  $R_\theta$  using **bilevel learning**:

$$\min_{\theta} \mathbb{E}_{u^*, b} \|\Phi_\theta(b) - u^*\|^2$$

$$\Phi_\theta(b) = \arg \min_u D(Au, b) + R_\theta(u)$$

- ▶ input-convex neural networks [Mukherjee et al. '20](#)

# Iterative regularization meets Deep Learning

- ▶ **Plug and play methods:** Take learned denoiser  $\mathcal{N}_\theta$  and replace prox operator [Venkatakrishnan et al. '13](#), e.g.

$$u^{k+1} = \mathcal{N}_\theta(u^k - \tau_k \nabla \mathcal{E}(u^k))$$

Stop when  $\mathcal{E}(u^k) < \delta$ . Not well behaved. Difficult to choose parameters, when to stop etc.

- ▶ difficult to guarantee this terminates
- ▶ difficult to train end-to-end: no formula available when the iterations will stop, likely discontinuous

## Methods that don't fit into these boxes:

- ▶ deep equilibrium [Gilton et al. '21](#)
  - ▶ use single network but iterate infinitely

$$\Phi(\textcolor{blue}{b}) = \lim_{k \rightarrow \infty} u^k, u^{k+1} = \mathcal{N}_\theta(u^k - \tau_k \nabla \mathcal{E}(u^k))$$

- ▶ score-based diffusion [Song et al. '21'](#)

# Summary

## What to learn? I.e. network architecture

- ▶ deep learning and inverse problems can be combined in **various ways**
- ▶ directly using the network (“analytic” methods) can be **unstable**
- ▶ incorporating **more structure** (e.g. variational regularization) or information (e.g.  $A$ ) makes the approach **more stable and needs less data**

## What to learn from? I.e. training data

- ▶ Supervised: end-to-end, bilevel learning ( $u_i^*, b_i$ ), potentially using  $A$
- ▶ Unsupervised: ( $u_i^*$ ), negative examples ( $v_i$ )
- ▶ Semi-Supervised: ( $u_i^*$ ), ( $b_i$ ), potentially using  $A$

# Towards Reliable Solutions of Inverse Problems with Deep Learning

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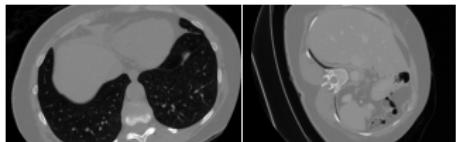


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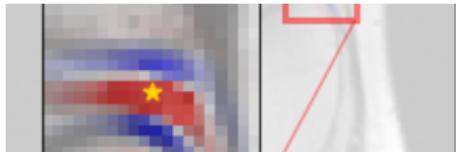


# Outline

1) Equivariance and Inverse Problems



2) Regularization with Generative Models



3) Inexact algorithms for Bilevel Learning



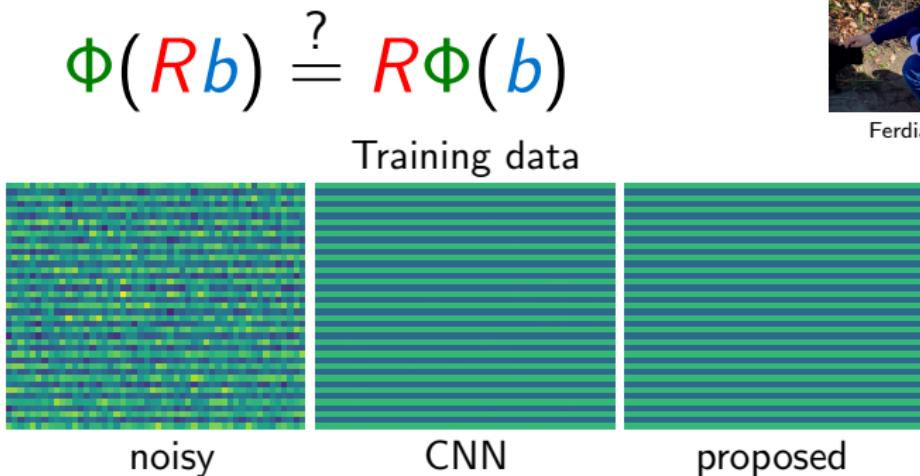
# Equivariance and Inverse Problems

# What happens when data is rotated?

Example:  $R$  rotation,  $\Phi$  denoising network



Ferdia Sherry



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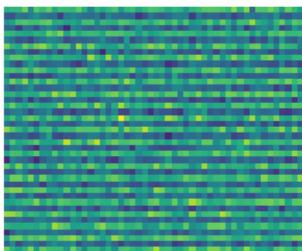
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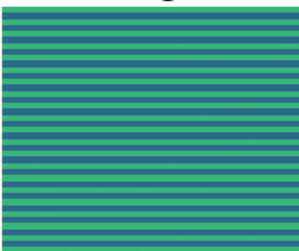
Ferdia Sherry

$$\Phi(Rb) \stackrel{?}{=} R\Phi(b)$$

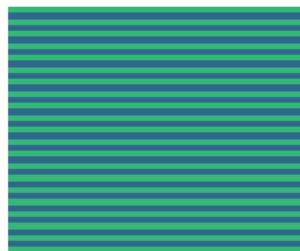
Training data



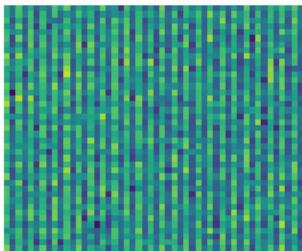
noisy



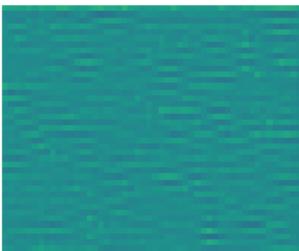
CNN  
Test data



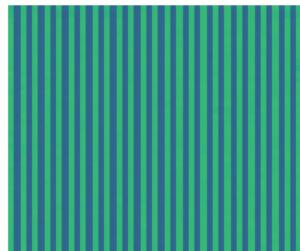
proposed



noisy



CNN



proposed

## How to get “equivariant” mappings?

$$\Phi(Rb) = R\Phi(b)$$

- ▶ **equivariance by learning**: e.g. data augmentation  $(b_i, u_i)_i$  becomes  $(R_i b_i, R_i u_i)_i$ 
  - ✓ **simple to implement** for image-based tasks (e.g. denoising, image segmentation etc)
  - ✗ **potentially computationally costly**: larger training data
  - ✗ **no guarantees** to generalize to test data
  - ✗ **not always easy/possible** (for inverse problems only viable in simulations or if data is not paired)

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  - ✗ **not always easy/possible** (for inverse problems only viable in simulations or if data is not paired)
- ▶ **equivariance by design**
  - ✓ **mathematical guarantees**
  - ✗ **not trivial** to do

Provable equivariant neural networks have been studied a lot for segmentation, classification, denoising etc

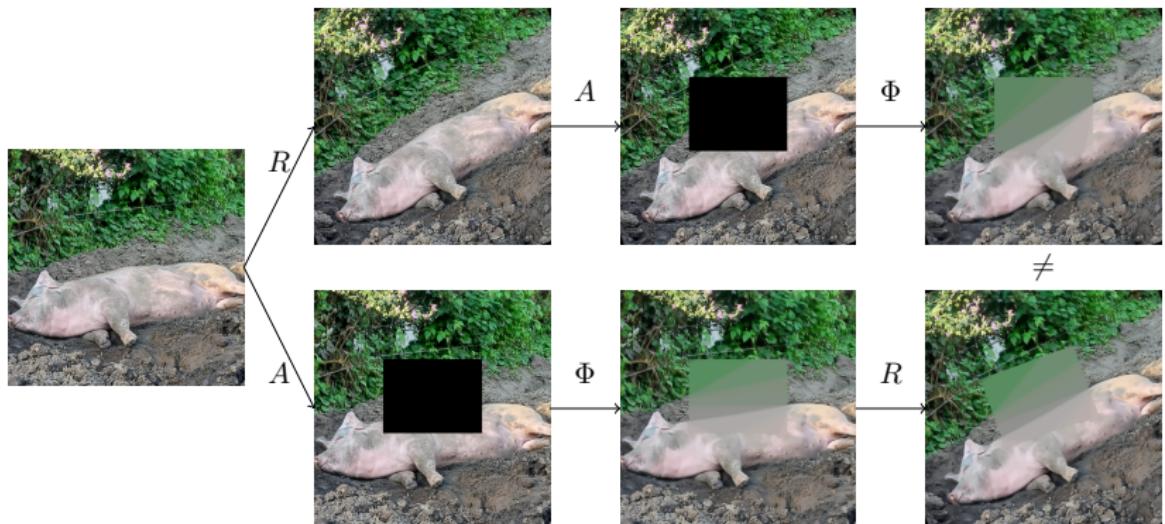
Bekkers et al. '18, Weiler and Cesa '19, Cohen and Welling '16, Dieleman et al. '16, Sosnovid et al. '19, Worall and Welling '19, ...

## Equivariance and inverse problems

- ▶ inverse problem  $Au = b$ , solution operator:  $\Phi : Y \rightarrow X$
- ▶ **Hope**  $\Phi \circ A$  is equivariant, e.g.  $R \circ \Phi \circ A = \Phi \circ A \circ R$

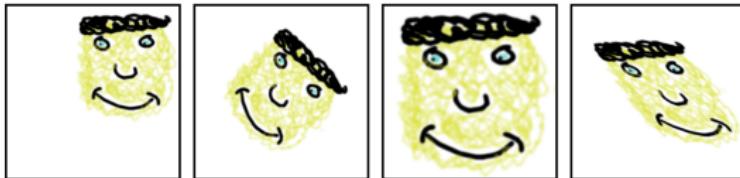
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- ▶  $\Phi \circ A$  generally **not equivariant**. TV inpainting



# Group acting on images

- ▶ Example groups (image from [Chen et al. '23](#)):



- ▶  $\overline{G} = \mathbb{R}^n \rtimes H$ ,  $H$  subgroup of the general linear group  $\text{GL}(n)$
- ▶  $g \cdot x = Rx + t, g = (t, R) \in \overline{G}, t \in \mathbb{R}^n, R \in H$
- ▶  $(\textcolor{red}{g} \cdot \textcolor{blue}{u})(x) = \textcolor{blue}{u}(\textcolor{red}{R}^{-1}(x - \textcolor{red}{t}))$

This includes [Weiler and Cesa '19](#)

- ▶ **Translations:**  $H = \{e\}$
- ▶ **Roto-Translations:**  $H = \text{SO}(n)$
- ▶ **Finite Roto-Translations**  $H = Z_M$  (finite subgroup of  $\text{SO}(n)$ )

## Invariant functional implies equivariant prox

**Theorem** Celledoni et al. '21

Let  $X = L^2(\Omega)$ ,  $J$  **invariant**:  $J(gu) = J(u)$ . Then  $\text{prox}_J$  is **equivariant**, i.e. for all  $u \in X$

$$\text{prox}_J(g \cdot u) = g \cdot \text{prox}_J(u).$$

- ▶ Total variation (and higher order variants) is invariant to rigid motion
- ▶ Natural condition on networks for unrolled algorithms
- ▶ Easily generalized to other groups Celledoni et al. '21
- ▶ Proof does **generalize** to variational regularization with  $L^2$ -datafit **if  $A$  is equivariant**

# How to construct equivariant networks?

**Proposition** Let  $G$  be any group and  $\Phi$  and  $\Psi$  equivariant.

- ▶ The **composition**  $\Phi \circ \Psi$  is equivariant.
- ▶ The **sum**  $\Phi + \Psi$  is equivariant.
- ▶ The **identity**  $u \mapsto u$  is equivariant.

**Next slide** There are non-trivial  $\overline{G}$ -equivariant linear operators.

**Proposition** Let  $G$  be any group and  $(\Phi u)(x) = u(x) + b(x)$ .  $\Phi$  is equivariant if  $b$  is **invariant**, i.e.  $g \cdot b = b$ .

**Proposition** There are  $\overline{G}$ -equivariant nonlinearities.

Construct  $\overline{G}$ -equivariant neural networks the usual way:

- ▶ layers  $\Phi = \Phi_n \circ \dots \circ \Phi_1$
- ▶  $\Phi(u) = \sigma(Au + b)$
- ▶ ResNet  $\Phi(u) = u + \sigma(Au + b)$

## Equivariant linear functions ( $\pi_X \equiv id$ )

**In a nutshell:** Linear  $\overline{G}$ -equivariant operators are convolutions with a kernel satisfying an additional constraint.

**Theorem** paraphrasing e.g. Weiler and Cesa '19

Let  $X, Y$  be function spaces, e.g.  $X = L^2(\mathbb{R}^n, \mathbb{R}^m)$ ,  $Y = L^2(\mathbb{R}^n, \mathbb{R}^M)$ . The linear operator  $\Phi : X \rightarrow Y$ ,

$$\Phi f(x) = \int K(x, y) f(y) dy$$

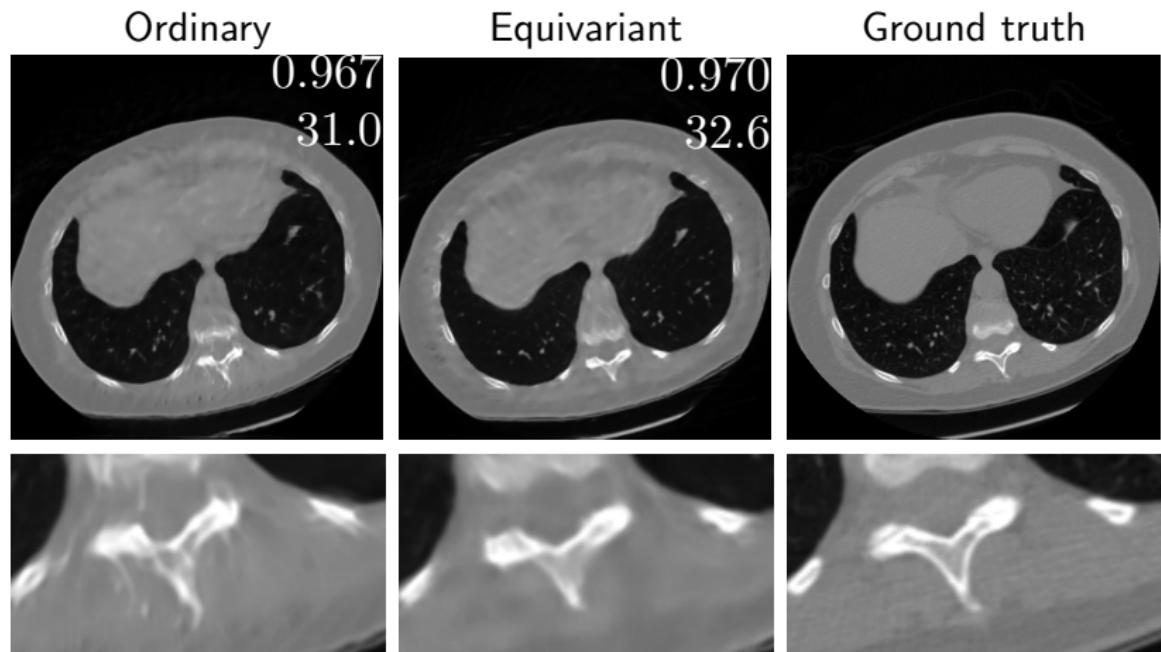
with  $K : \mathbb{R}^n \rightarrow \mathbb{R}^{M \times m}$  is  $\overline{G}$ -equivariant iff there is a  $k$  such that

$$\Phi f(x) = \int k(x - y) f(y) dy$$

and  $k$  is  $H$ -invariant, i.e. for all  $R \in H$ ,  $x \in \mathbb{R}^n$ :  $k(Rx) = k(x)$ .

## CT Results

- ▶ LIDC-IDRI data set, 5000+200+1000 images, 50 views
- ▶ Equivariant = roto-translations; Ordinary = translations



- ▶ **higher** SSIM and PSNR
- ▶ **fewer** artefacts and **finer** details

# CT Results

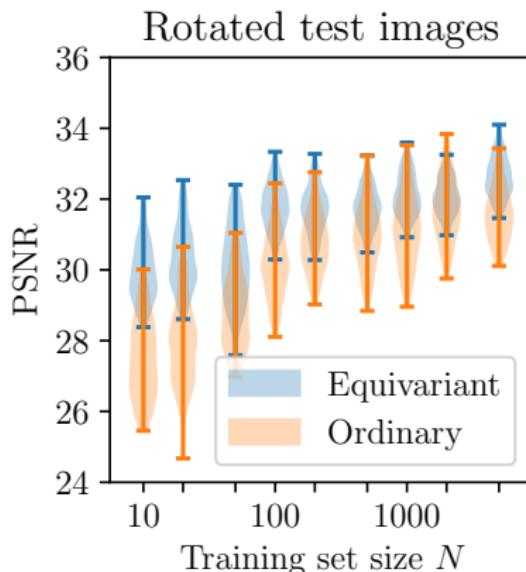
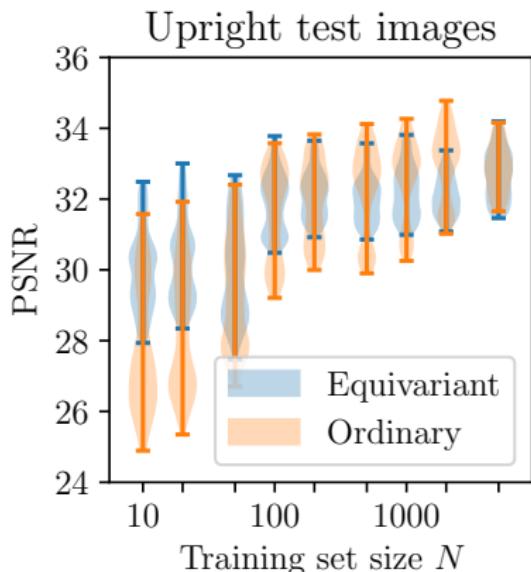
Celledoni et al., Inverse Problems, '21.

Equivariant = roto-translations; Ordinary = translations

Equivariant improves upon Ordinary:

- ▶ **small** training sets
- ▶ **unseen** orientations

Generalisation performance of the learned methods



## Regularization with Generative Models

# Generative Regularizers



Image by [Hu et al. '20](#)

- ▶ Given a generative model  $G_\theta : Z \rightarrow U$  (e.g. AE, VAE, GAN), one can define a **generative regularizer** [Duff et al. JMIV '23](#), e.g.

$$R(u) = \inf_z \left\{ \frac{1}{2} \|u - G_\theta(z)\|_2^2 + S(z) \right\}$$

- ▶ A variant with **hard constraints** has been used in [Bora et al. '17](#)

$$R(u) = \inf_z \iota_{\{0\}}(u - G_\theta(z))$$

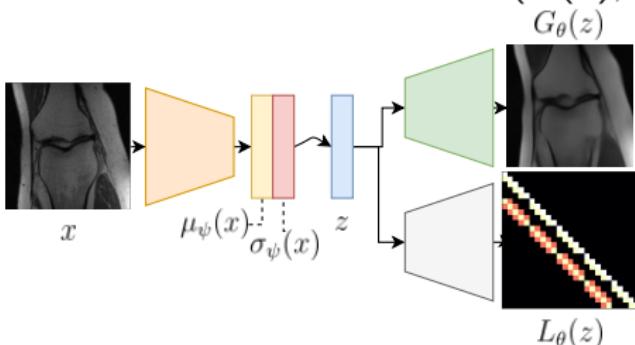
- ▶ In both cases: **only the mean** is modelled

# Modelling the Covariance Duff et al. PMB '23

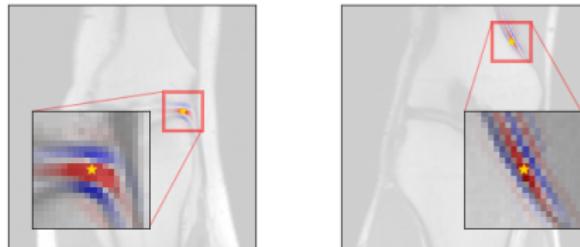
- Motivated by Dorta et al. '18, we use the regularizer

$$R(u) = \inf_z \left\{ \log \det(\Sigma(z)) + \frac{1}{2} \|u - G(z)\|_{\Sigma^{-1}(z)}^2 + \frac{1}{2} \|z\|_2^2 \right\}$$

This is related to  $u \propto \mathcal{N}(G(z), \Sigma(z))$  and  $z \propto \mathcal{N}(0, I)$ .



- Visualization of learned **positive** and **negative** covariance.



# Example: Magnetic Resonance Imaging (MRI)

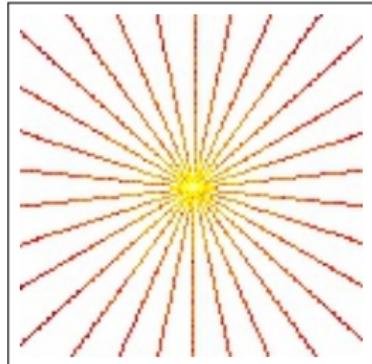
## MRI Reconstruction

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

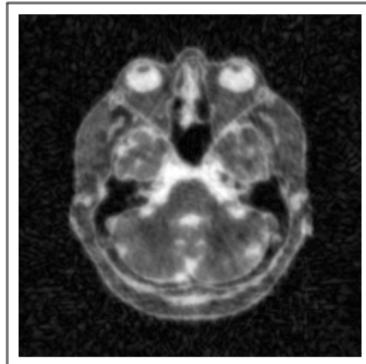
$$\min_{\textcolor{red}{u}} \left\{ \sum_{i \in \Omega} |(\mathcal{F}\textcolor{red}{u})_i - \textcolor{blue}{b}_i|^2 \right\}$$



MRI scanner



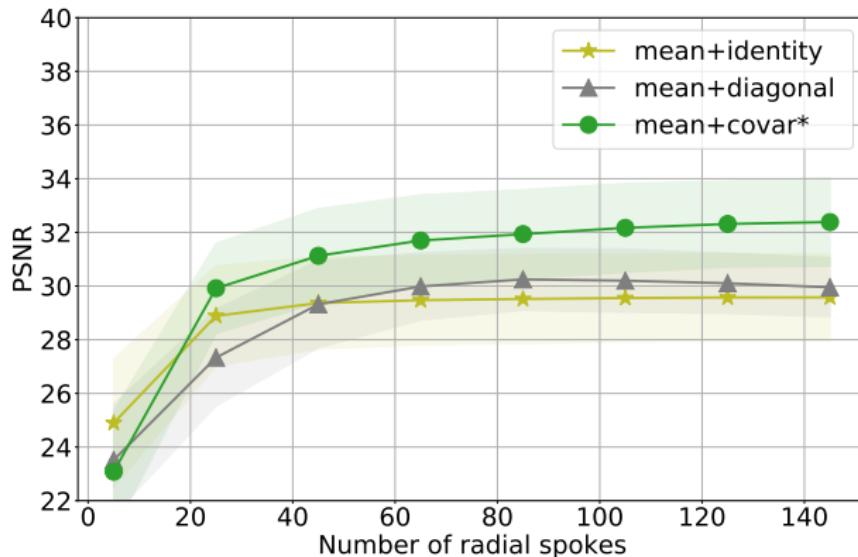
sampling  $\mathcal{S}^*y$



minimizer

## Comparison: Covariance Models

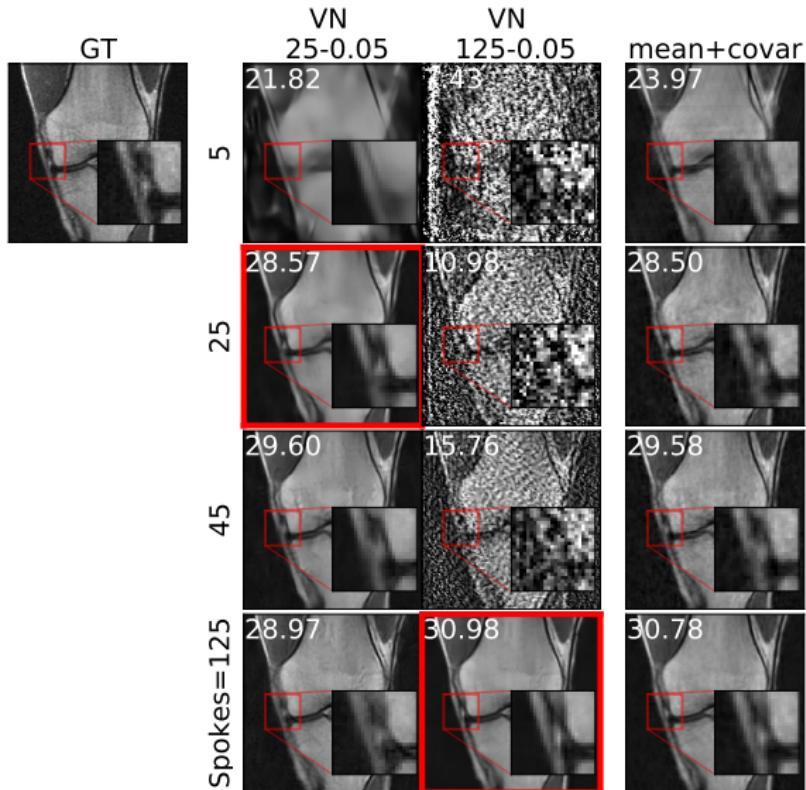
- ▶ constant diagonal (identity)
- ▶ varying diagonal (diagonal)
- ▶ proposed (covar)



- ▶ In any case, the proposed model appears superior.

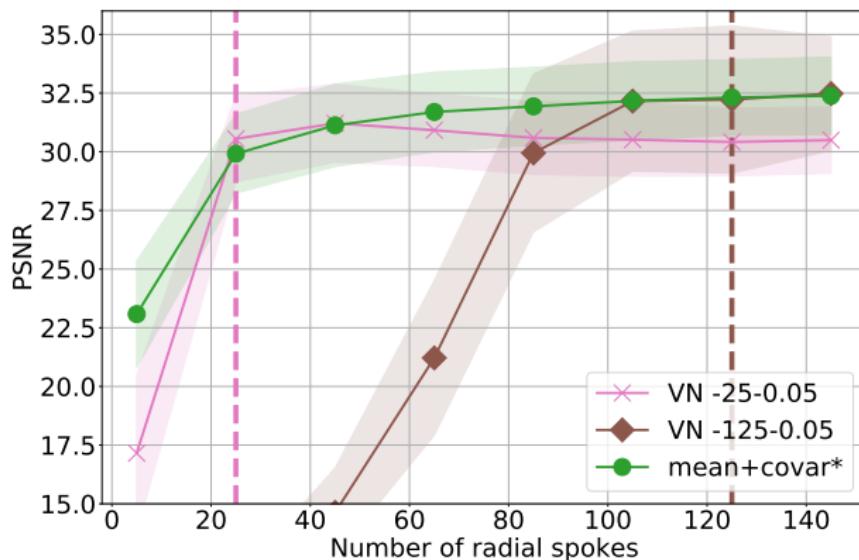
# Comparison: End-to-end Learning

- ▶ Compare to Variational Network (VN) [Hammernik et al. '18](#)  
trained for specific sampling and noise (indicated in red).



## Comparison: End-to-end Learning (cont)

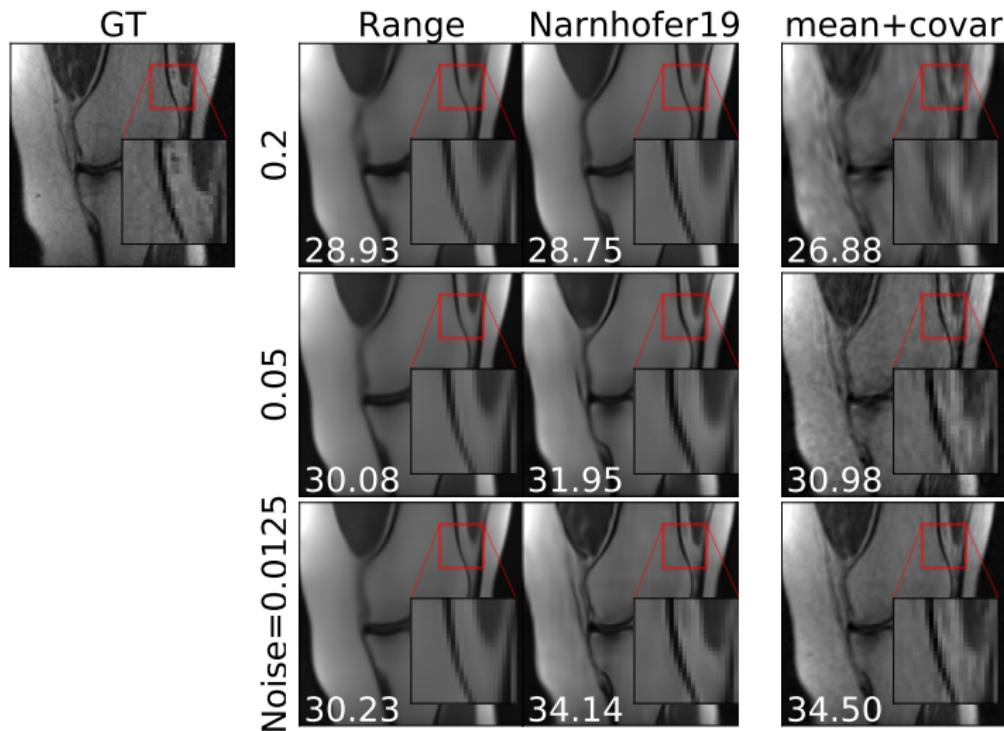
Compare to Variational Network (VN) Hammernik et al. '18 trained for specific sampling and noise (dashed lines).



- ▶ Similar peak performance but proposed model **generalizes better** to unseen settings.

## Comparison: Other unsupervised methods

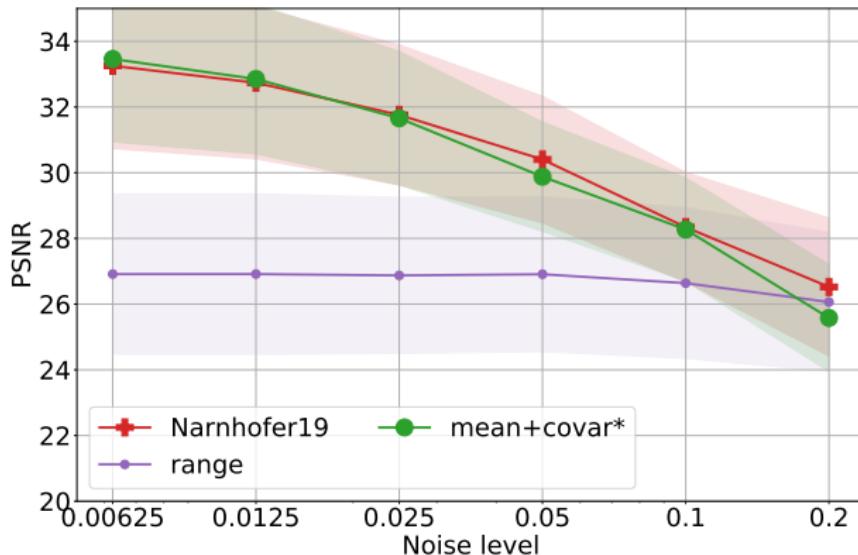
- ▶ Compare to [Bora et al. '17](#) (Range) which restricts to the range.
- ▶ Compare to [Narnhofer et al. '19](#) which uses an Inverse GAN.



- ▶ [Bora et al. '17](#), [Narnhofer et al. '19](#) produce **smoother solutions**.

## Comparison: Other unsupervised methods (cont)

- ▶ Compare to [Bora et al. '17](#) (Range) which restricts to the range.
- ▶ Compare to [Narnhofer et al. '19](#) which uses an Inverse GAN.



- ▶ Better than [Bora et al. '17](#). Similar to [Narnhofer et al. '19](#).

# Inexact Algorithms for Bilevel Learning

# Bilevel learning for inverse problems

**Upper level** (learning):

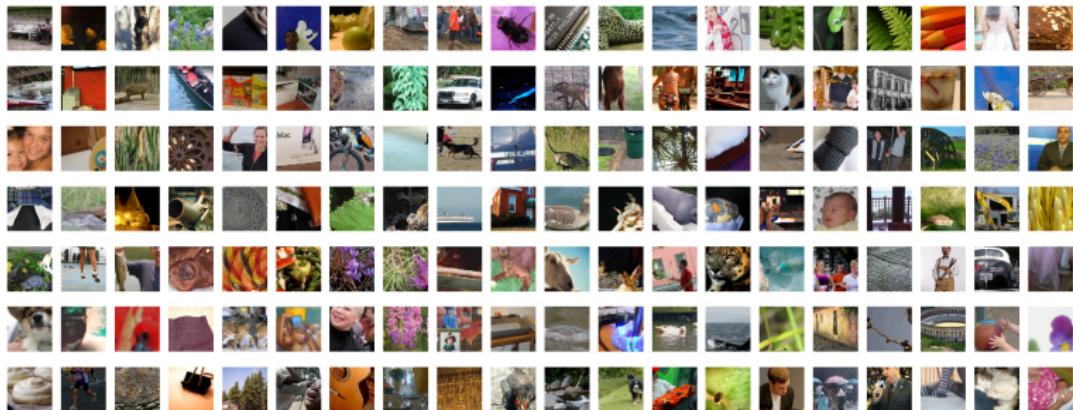
Given  $(u_i^*, b_i)_{i=1}^n$ ,  $b_i = Au_i^* + \varepsilon_i$ , solve

$$\min_{\theta, \hat{u}_i} \frac{1}{n} \sum_{i=1}^n \|\hat{u}_i - u_i^*\|_2^2$$

**Lower level** (solve inverse problem):

$$\hat{u}_i \in \arg \min_u \{\mathcal{D}(Au, b_i) + \mathcal{R}_\theta(u)\}$$

von Stackelberg 1934, Kunisch and Pock '13, De los Reyes and Schönlieb '13



# How to solve bilevel learning?

**Bilevel problem:**

$$\min_{\theta, \hat{u}} U(\hat{u}) \quad \text{s.t.} \quad \hat{u}(\theta) = \arg \min_u L(u, \theta)$$

- ▶ Reduced formulation:  $\tilde{U}(\theta) := U(\hat{u}(\theta))$
- ▶ Implicit function theorem:  $\nabla \tilde{U}(\theta) = -B^T q$ , with
  - ▶  $q$  solves  $Aq = \nabla U(\hat{u}(\theta))$
  - ▶  $A = \partial_u^2 L(\hat{u}(\theta), \theta)$
  - ▶  $B = \partial_\theta \partial_u L(\hat{u}(\theta), \theta)$

# Algorithm for Bilevel learning

**Reduced formulation:**  $\min_{\theta} \tilde{U}(\theta)$

- ▶ Compute gradients: Given  $\theta$ 
  - (1) **Optimization:**  $\hat{u}(\theta)$ , e.g. via L-BFGS [Nocedal and Wright '00](#)
  - (2) **Linear system:**  $Aq = \nabla U(\hat{u}(\theta))$ , e.g. via CG
  - (3) Matrix-vector product:  $\nabla \tilde{U}(\theta) = -B^T q$
- ▶ Solve reduced formulation via L-BFGS-B

# Algorithm for Bilevel learning

**Reduced formulation:**  $\min_{\theta} \tilde{U}(\theta)$

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  - (3) Matrix-vector product:  $\nabla \tilde{U}(\theta) = -B^T q$
- ▶ Solve reduced formulation via L-BFGS-B

**This approach has a number of problems:**

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

# How to solve Bilevel Learning Problems?

- ▶ Ignore “problems”, just compute it. e.g. Sherry et al. '20
- ▶ Semi-smooth Newton: similar problems Kunisch and Pock '13
- ▶ Replace lower level by finite number of iterations of algorithm: not bilevel anymore Ochs et al. '15

**Use algorithm that acknowledges difficulties:**

e.g. **inexact DFO** Ehrhardt and Roberts '21

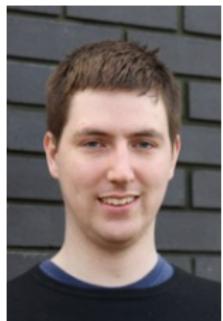
$$\min_{\theta} f(\theta)$$

**Key idea:** Use  $f_\epsilon : |f(\theta) - f_\epsilon(\theta)| < \epsilon$

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

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



Lindon Roberts

# Dynamic Accuracy Derivative Free Optimization

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

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

- 1) Sample  $f_{\epsilon^k}$  in a neighbourhood of  $\theta_k$
- 2) Build model  $m_k(\theta) \approx f_{\epsilon^k}$
- 3) Minimise  $m_k$  around  $\theta_k$  to get  $\theta_{k+1}$
- 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  $\gamma_{\text{inc}} < 1 < \gamma_{\text{dec}}$ ,  $\eta_1 \leq \eta_2 < 1$ , and  $\eta'_1 < \min(\eta_1, 1 - \eta_2)/2$ .

- 1: Select an arbitrary interpolation set and construct  $m^0$  (26).
- 2: for  $k = 0, 1, 2, \dots$  do
- 3:   repeat
- 4:     Evaluate  $\tilde{f}(\theta^k)$  to sufficient accuracy that (32) holds with  $\eta'_1$  (using  $s^k$  from the previous iteration of this inner repeat/until loop). Do nothing in the first iteration of this repeat/until loop.
- 5:     if  $\|x^k\| \leq \epsilon$  then
- 6:       By replacing  $\Delta^k$  with  $\gamma'_{\text{dec}} \Delta^k$  for  $i = 0, 1, 2, \dots$ , find  $m^k$  and  $\Delta^k$  such that  $m^k$  is fully linear in  $B(\theta^k, \Delta^k)$  and  $\Delta^k \leq \|s^k\|$ . *[criticality phase]*
- 7:       end if
- 8:       Calculate  $s^k$  by (approximately) solving (27).
- 9:     until the accuracy in the evaluation of  $\tilde{f}(\theta^k)$  satisfies (32) with  $\eta'_1$  *[accuracy phase]*
- 10:   Evaluate  $\tilde{f}(\theta^k + s^k)$  so that (32) is satisfied with  $\eta'_1$  for  $\tilde{f}(\theta^k + s^k)$ , and calculate  $\hat{\rho}^k$  (29).
- 11:   Set  $\theta^{k+1}$  and  $\Delta^{k+1}$  as:
 
$$\theta^{k+1} = \begin{cases} \theta^k + s^k, & \hat{\rho}^k \geq \eta_2, \text{ or } \hat{\rho}^k \geq \eta_1 \text{ and } m^k \\ & \text{fully linear in } B(\theta^k, \Delta^k), \\ \theta^k, & \text{otherwise,} \end{cases} \quad (33)$$
- 12:   and
 
$$\Delta^{k+1} = \begin{cases} \min(\gamma_{\text{inc}} \Delta^k, \Delta_{\max}), & \hat{\rho}^k \geq \eta_2, \\ \Delta^k, & \hat{\rho}^k < \eta_2 \text{ and } m^k \text{ not} \\ & \text{fully linear in } B(\theta^k, \Delta^k), \\ \gamma_{\text{dec}} \Delta^k, & \text{otherwise.} \end{cases} \quad (34)$$
- 13: end for

## Theorem Ehrhardt and Roberts '21

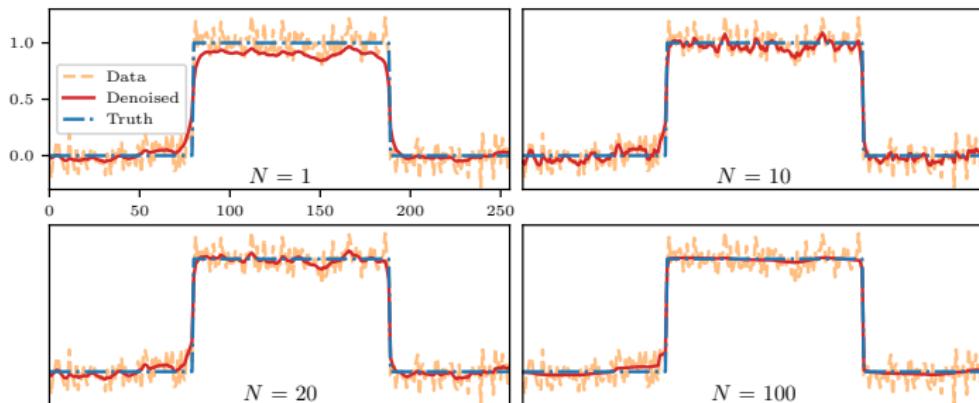
If  $f$  is sufficiently smooth and bounded below, then the algorithm is globally convergent in the sense that

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

# Parametric regularizer Ehrhardt and Roberts '21

$$\min_{\theta=(\alpha,\nu,\xi)} \left\{ \frac{1}{2} \sum_i \|\hat{u}_i(\theta) - u_i\|_2^2 + \beta \kappa^2(\theta) \right\}, \quad \kappa(\theta) = 1 + \frac{\alpha \|\nabla\|^2}{\nu(1+\xi)}$$

$$\hat{u}_i(\theta) = \arg \min_u \left\{ \frac{1}{2} \|u - b_i\|_2^2 + \alpha \left( \sum_j \sqrt{\|(\nabla u)_j\|_2^2 + \nu^2} + \frac{\xi}{2} \|u\|_2^2 \right) \right\}$$

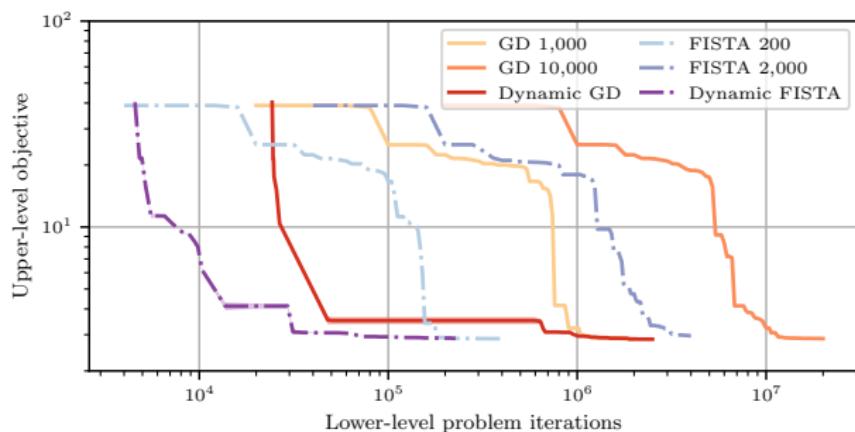


**Reconstruction of  $\hat{u}_1$  after  $N$  evaluations of  $f(\theta)$**

# Dynamic Accuracy v Fixed Unrolling

Compare:

- ▶ proposed dynamic accuracy approach [Ehrhardt and Roberts '21](#)
- ▶ lower-level solution  $\approx$  fixed number of iterations [Ochs et al. '15](#)



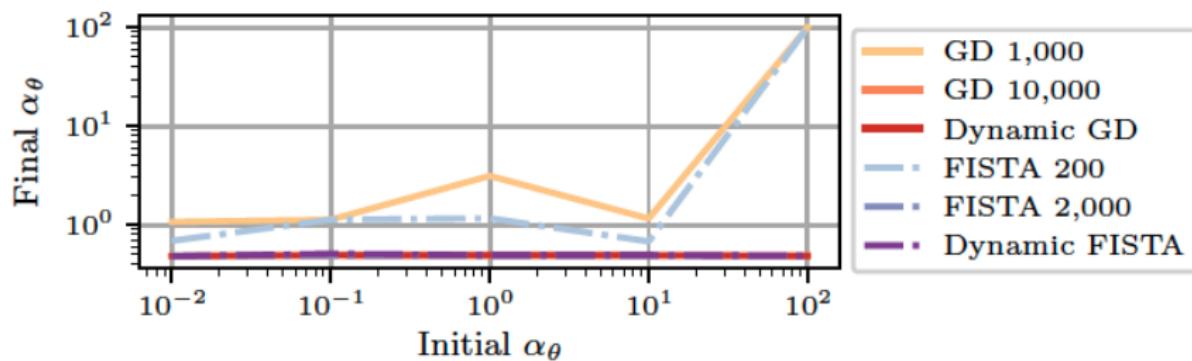
**Objective value  $f(\theta)$  vs. computational effort**

Dynamic accuracy is faster: **10x speedup**

# Robustness to initialization etc

Compare:

- ▶ proposed dynamic accuracy approach [Ehrhardt and Roberts '21](#)
- ▶ approximate lower-level solution by fixed number of iterations, similar to [Ochs et al. '15](#) (Fixed)



- ▶ Fixed **not robust to number of iterations**
- ▶ Fixed with large number of iterations and dynamic accuracy are **robust to initialization**

# Conclusions

- ▶ Exploiting **equivariance**
  - ▶ natural condition when **proximal operators** are replaced
  - ▶ needs **less data**
  - ▶ **no extra computational cost** at test time
- ▶ **Generative regularizers**: modelling of prior correlations
  - ▶ Unsupervised model: **no paired data** required
  - ▶ Learning independent of inverse problem: **generalization**
- ▶ **Bilevel learning** computationally challenging: requires **novel solutions**
  - ▶ Next step: Inexact first-order algorithms for bilevel learning