

Learning data-driven priors for image reconstruction: From bilevel optimisation to neural network-based unrolled schemes

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Inverse problems in imaging – General framework

We are given data \mathbf{z} that satisfy

$$\mathbf{z} = \mathbf{A}\mathbf{x}_{true} + \mathbf{e}$$

\mathbf{x}_{true} ground truth image

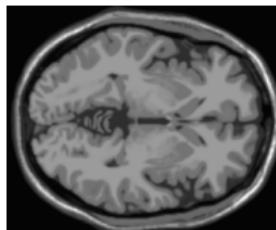
\mathbf{e} random noise

$\mathbf{A} : V^n \rightarrow V^m$ bounded linear operator, $V = \{\mathbb{R}, \mathbb{C}\}$

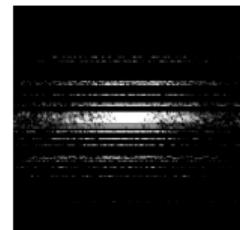
Identity



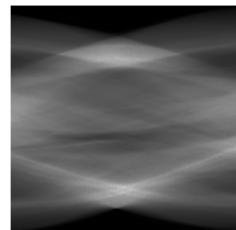
Convolution



Fourier coefficients



Radon transform



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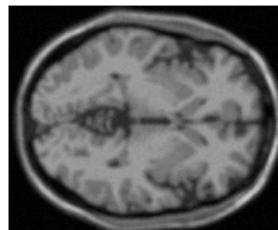
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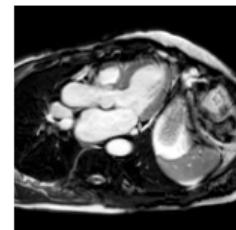
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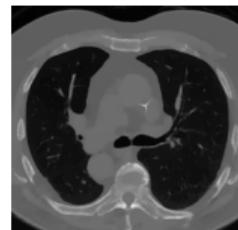
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Model-based regularisation methods

Variational regularisation approach

$$\min_{\mathbf{x} \in X} \underbrace{d(\mathbf{Ax}, \mathbf{z})}_{\text{data discrepancy}} + \underbrace{\mathcal{R}_\lambda(\mathbf{x})}_{\text{regularisation with weight } \lambda}$$

\mathcal{R}_λ : regularisation, imposes regularity, makes problem well-posed

d : ensures reconstruction close to the data

(its choice is dictated by the statistics of the noise, e.g. L^2 for Gaussian)

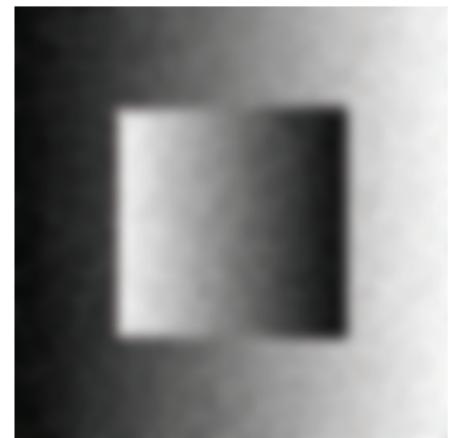
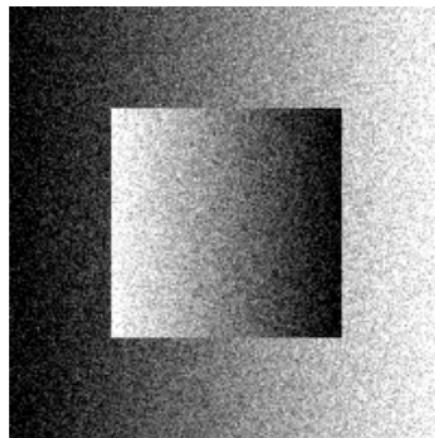
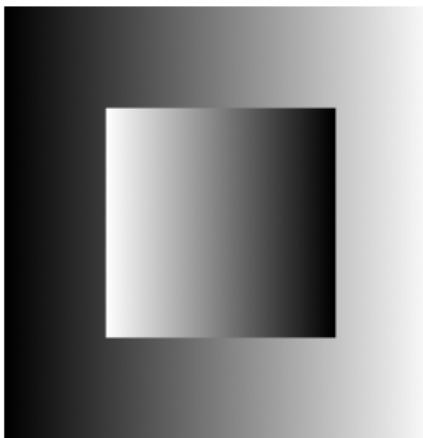
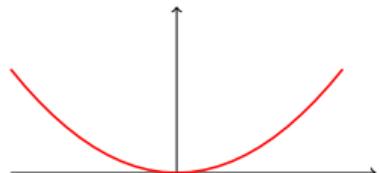
λ : balances the effect of data discrepancy and regularisation

Regularisation functionals

Tikhonov:

[Tikhonov (1963)]

$$\mathcal{R}_\lambda(\mathbf{x}) = \frac{\lambda}{2} \|\nabla \mathbf{x}\|_2^2$$

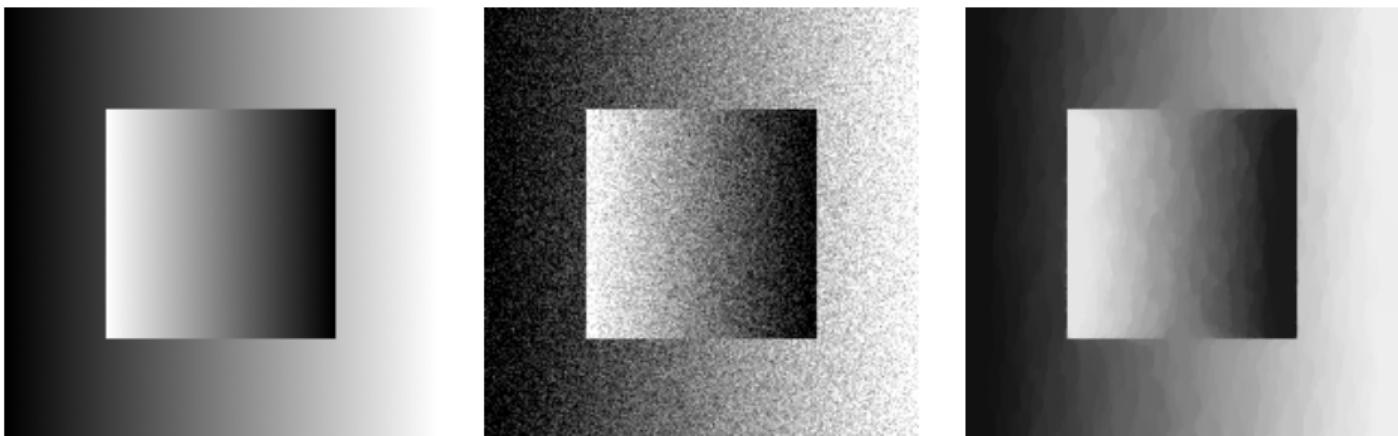
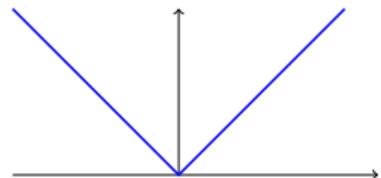


Regularisation functionals

Total Variation:

[Rudin, Osher, Fatemi (1992)]

$$\mathcal{R}_\lambda(\mathbf{x}) = \text{TV}(\mathbf{x}) = \lambda \|\nabla \mathbf{x}\|_1$$



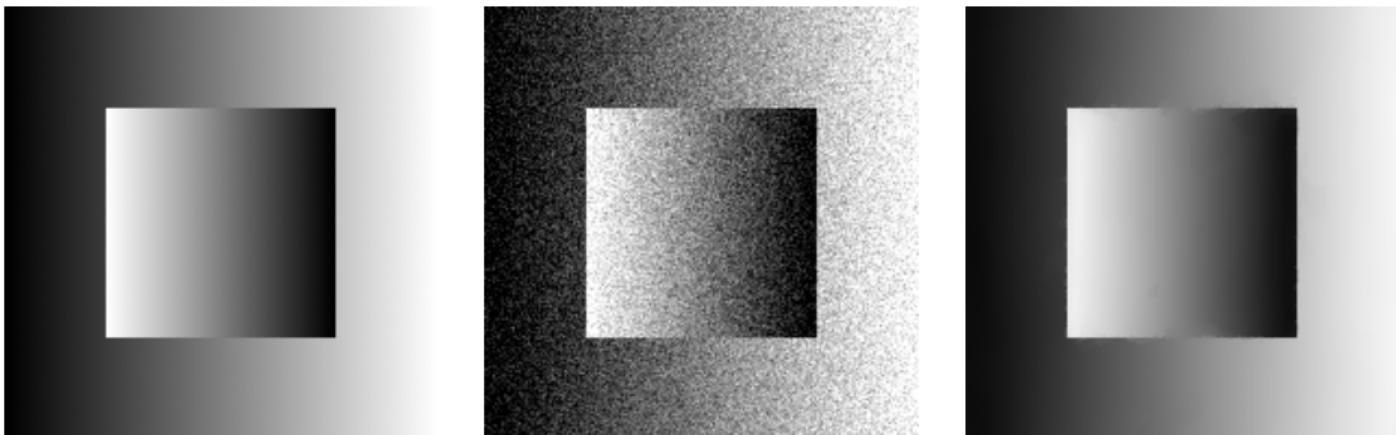
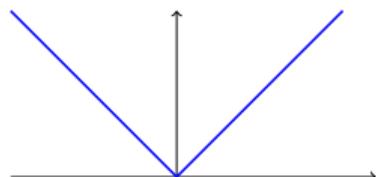
Regularisation functionals

Total Generalised Variation:

[Bredies, Kunisch, Pock (2010)]

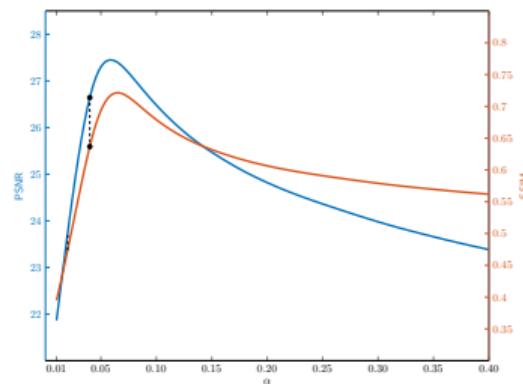
$$\text{TGV}(\mathbf{x}) = \min_{\mathbf{w}} \lambda_1 \|\nabla \mathbf{x} - \mathbf{w}\|_1 + \lambda_2 \|\mathcal{E} \mathbf{w}\|_1$$

$\mathcal{E} \mathbf{w}$: symmetrised gradient, $\left(\frac{\nabla \mathbf{w} + (\nabla \mathbf{w})^T}{2} \right)$



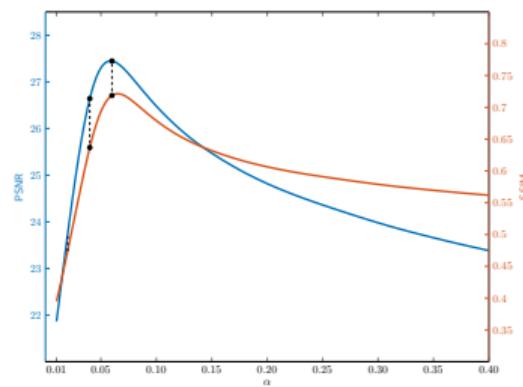
The influence of regularisation parameters

$$\min_{\mathbf{x}} \frac{1}{2} \|\mathbf{Ax} - \mathbf{z}\|_2^2 + \lambda \|\nabla \mathbf{x}\|_1, \quad \lambda > 0$$



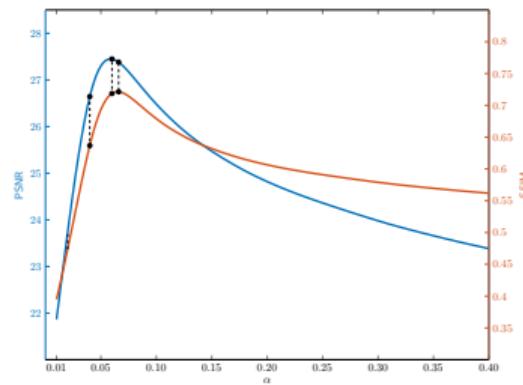
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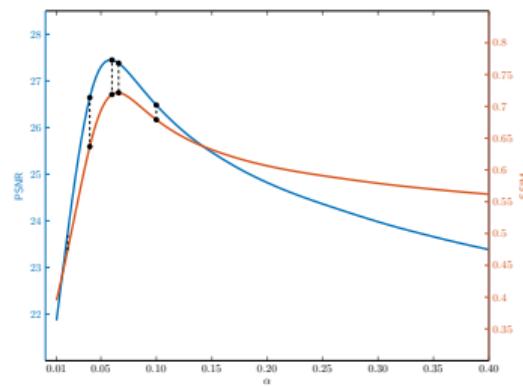
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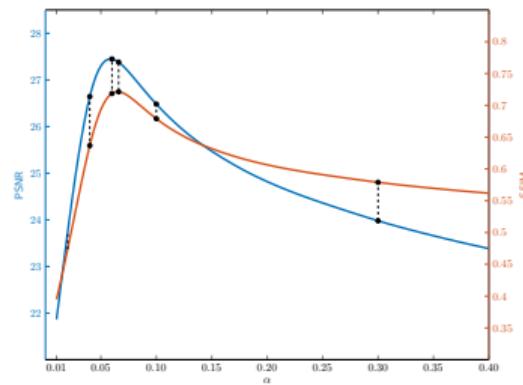
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Regularisation functionals with spatially varying parameters

Scalar Total Variation

$$\lambda \in \mathbb{R}, \lambda > 0$$

$$TV(\mathbf{x}) = \lambda \|\mathbf{x}\|_1$$

Regularisation functionals with spatially varying parameters

Spatially varying Total Variation:

$$\Lambda \in \mathbb{R}^{qn}, \Lambda > 0$$

$$TV(\mathbf{x}) = \|\Lambda \nabla \mathbf{x}\|_1$$

Regularisation functionals with spatially varying parameters

Spatially varying Total Variation:

$$\Lambda \in \mathbb{R}^{qn}, \Lambda > 0$$

$$TV(\mathbf{x}) = \|\Lambda \nabla \mathbf{x}\|_1$$

[Strong, Chan, 2005]

[Dong, Hintermüller, Rincon-Camacho, 2011]

[Jalalzai, 2014]

[Calatroni, Cao, De los Reyes, Schönlieb, Valkonen, 2017]

[Hintermüller, Rautenberg, Wu, Langer, 2017]

[Hintermüller, Papafitsoros, Rautenberg, 2017]

[Dong, Schönlieb, 2020]

[De los Reyes, Villacís, 2022]

[Pragliola, Calatroni, Lanza, Sgallari, 2021-22]

→ Mostly for denoising and static 2D inverse problems...

How to choose the parameters λ , Λ ?

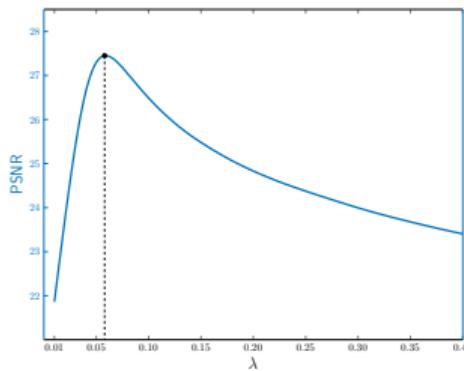
Bilevel optimization – supervised learning

“Supervised learning” approach using ground truth-degraded data pairs:

[De los Reyes, Schönlieb, Pock, Kunisch, Calatroni, Valkonen, Villacis... (2013-)]

$$\min_{\mathbf{x}, \lambda, (\text{or } \Lambda)} \frac{1}{2} \|\mathbf{x} - \mathbf{x}_{true}\|_2^2$$

s.t. \mathbf{x} solves the TV (or TGV) problem with parameters λ (or Λ)

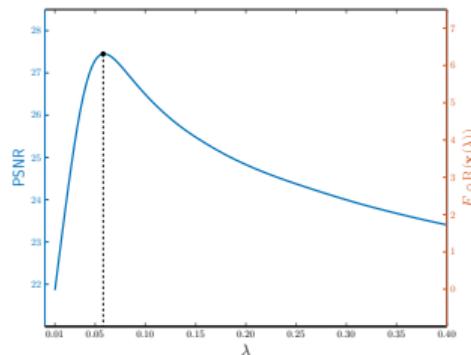


How to choose the parameters without using u_{true} ?

Bilevel optimisation – supervised learning

$$\min_{\mathbf{x}, \lambda, (\text{or } \Lambda)} \frac{1}{2} \|\mathbf{x} - \mathbf{x}_{true}\|_{L^2(\Omega)}^2$$

s.t. \mathbf{x} solves the TV (or TGV) problem with parameters λ (or Λ)



How to choose the parameters without using u_{true} ?

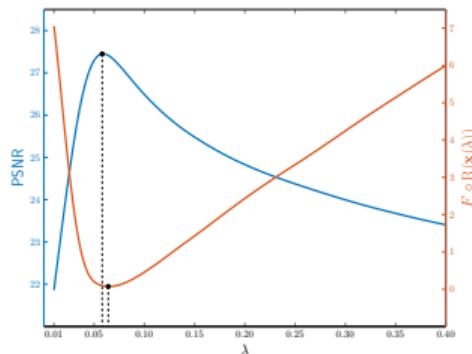
Bilevel optimisation – unsupervised learning

“Unsupervised learning” without using ground truth-degraded data pairs:

[Hintermüller, Papafitsoros, Rautenberg, Wu, Langer, Sun,...(2017-)]

$$\min_{\mathbf{x}, \lambda, (\text{or } \Lambda)} F(R\mathbf{x}) := \frac{1}{2} \|\max(R\mathbf{x} - \bar{\sigma}^2, 0)\|_2^2 + \frac{1}{2} \|\min(R\mathbf{x} - \underline{\sigma}^2, 0)\|_2^2$$

s.t. \mathbf{x} solves the TV (or TGV) problem with parameters λ (or Λ)

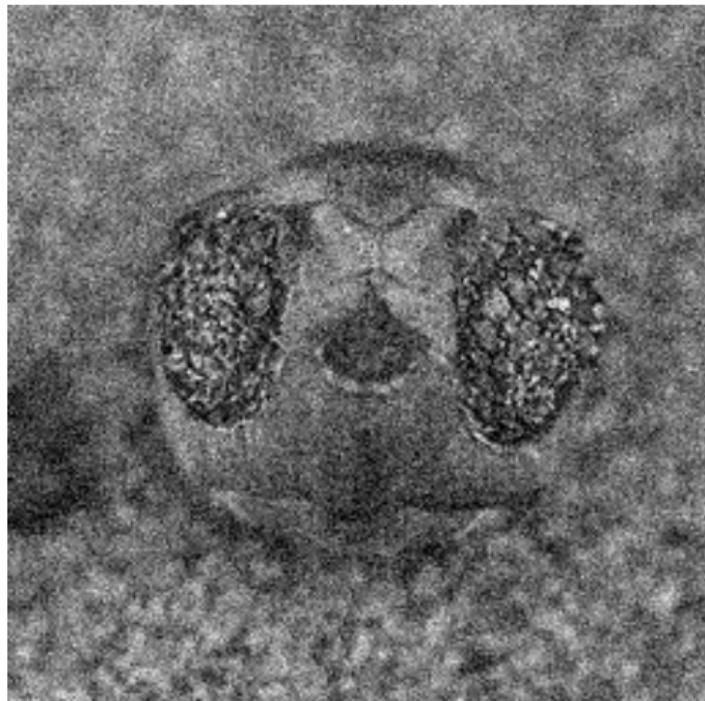


Numerical results: bilevel TV unsupervised learning



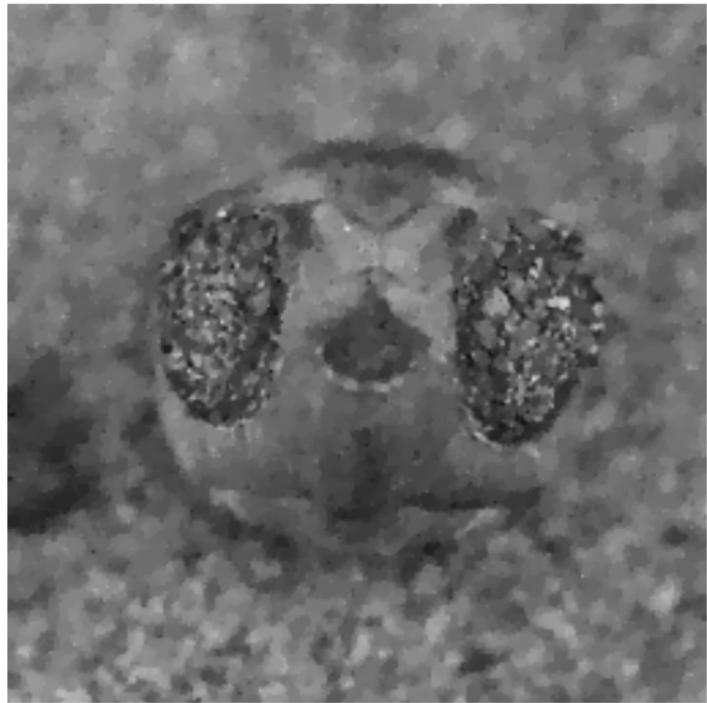
scalar TV, PSNR=27.75, SSIM=0.7701
bilevel TV, PSNR=27.52, SSIM=0.7722

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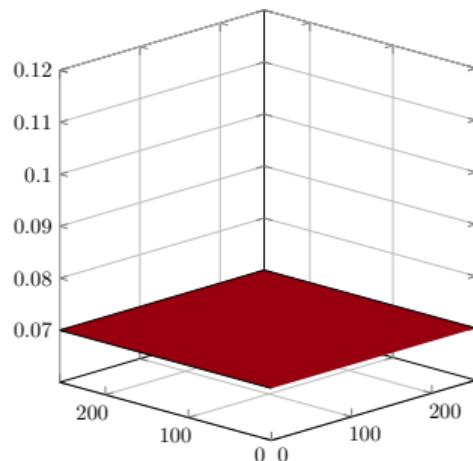


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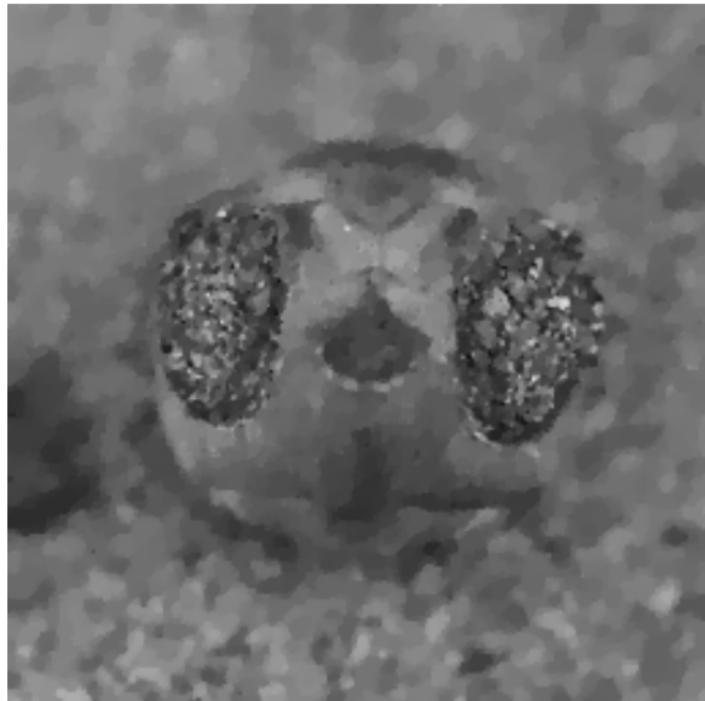
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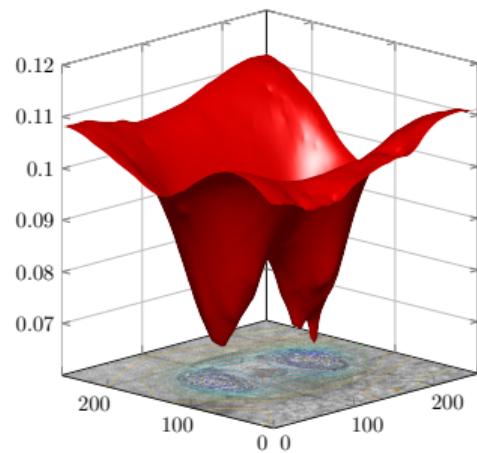
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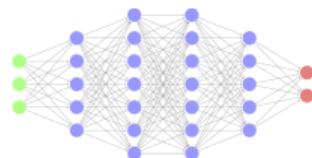
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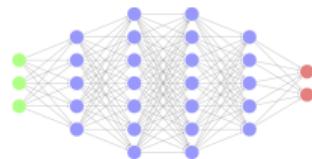
Deep learning-based methods



$$\underset{\Theta}{\text{minimize}} \quad \frac{1}{M} \sum_{i=1}^M l(\mathcal{N}_{\Theta}(\mathbf{z}^i), \mathbf{x}_{true}^i) + r(\Theta)$$

- Application of deep learning to inverse problems and mathematical imaging has seen a tremendous development over the last years
[\[Arridge, Maass, Öktem, Schönlieb, 2019\]](#)
- Fewer theoretical underpinnings; instabilities; challenging interpretation
[\[Antun, Renna, Poon, Adcock, Hansen, 2020\]](#)

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Combine

*Interpretability of
model-based methods*

*Flexibility and adaptability
of deep learning*

Combining deep learning and model-based methods

- Learning the regularization functional \mathcal{R} from data and embed it into a variational data fitting/regularisation functional scheme
[Lunz, Öktem, Schönlieb, 2018]
[Li, Schwab, Antholzer, Haltmeier, 2020]
- Enforcing the reconstruction to be close to an output of a network via \mathcal{R} , e.g.
 $\mathcal{R}(\cdot) = \|\cdot - u_\Theta(s)\|_2^2$ for some network with trainable parameters Θ and input s
[Duff, Campbell, Ehrhardt, 2021]
[Kofler, Haltmeier, Schaeffter, Kachelriess, Dewey, Wald, Kolbitsch, 2020]
- Substituting proximal operators in classical iterativeschemes by learned NN denoisers (in a "plug-and-play" fashion)
[Meinhardt, Moller, Hazirbas, Cremers, 2017]
[Romano, Elad, and Milanfar, 2017]
- Using learned iterative schemes
[Adler, Öktem, 2017-18]
[Hammernik, Klatzer, Kobler, Recht, Sodickson, Pock, Knoll, 2018]

Reviews:

[Arridge, Maass, Öktem, Schönlieb, 2019], [Monga, Li, Eldar, 2021], [Mukherjee, Hauptmann, Öktem, Pereyra, Schönlieb, 2023], [Kamilov, Bouman, Buzzard, Wohlberg, 2023]

Deep learning-based parameter learning

[Afkham, Chung, Chung, 2019], [Nekhili, Descombes, Calatroni, 2022]

Offline phase

- Given $(\mathbf{z}_i, \mathbf{x}_{true}^i)_{i=1}^M$ employ, e.g., a bilevel scheme to compute optimal $(\lambda_i)_{i=1}^M$
- Use training data $(\lambda_i, \mathbf{z}_i)_{i=1}^M$ to train a neural network \mathcal{N}_Θ

$$\min_{\Theta} \mathcal{L}(\Theta) := \frac{1}{M} \sum_{i=1}^M l(\mathcal{N}_\Theta(\mathbf{z}_i), \lambda_i)$$

Online phase

- Given some new data \mathbf{z}_{test} compute $\lambda_\Theta = \mathcal{N}_\Theta(\mathbf{z}_{test})$ and solve

$$\min_{\mathbf{x}} \frac{1}{2} \|\mathbf{Ax} - \mathbf{z}_{test}\|_2^2 + \lambda_\Theta \|\nabla \mathbf{x}\|_1$$

Deep learning-based parameter learning

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Offline phase

- Given $(\mathbf{z}_i, \mathbf{x}_{true}^i)_{i=1}^M$ employ, e.g., a bilevel scheme to compute optimal $(\lambda_i)_{i=1}^M$
Computationally intensive, esp. 3D and dynamic, not generalisable...
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$$\min_{\mathbf{x}} \frac{1}{2} \|\mathbf{Ax} - \mathbf{z}_{test}\|_2^2 + \lambda_\Theta \|\nabla \mathbf{x}\|_1$$

A deep unrolled scheme

$$\mathbf{z} = \mathbf{A}\mathbf{x}_{true} + \mathbf{e}$$

$$\min_{\mathbf{x}} \frac{1}{2} \|\mathbf{A}\mathbf{x} - \mathbf{z}\|_2^2 + \|\mathbf{\Lambda}\nabla\mathbf{x}\|_1, \quad (P)$$

NET_Θ : overparameterised CNN with parameters Θ , e.g. U-net

S : an iterative scheme that solves (P) , e.g. PDHG [Chambolle, Pock, 2011]

$$\mathbf{x}_T = S^T(\mathbf{x}_0, \mathbf{z}, \mathbf{\Lambda}, \mathbf{A}), \quad \mathbf{x}_T \rightarrow S^*(\mathbf{z}, \mathbf{\Lambda}, \mathbf{A}) \text{ as } T \rightarrow \infty$$

Fix $T \in \mathbb{N}$

$$\left\{ \begin{array}{l} \mathbf{\Lambda}_\Theta = \text{NET}_\Theta(\mathbf{x}_0) \\ \mathbf{x}_1 = S^1(\mathbf{x}_0, \mathbf{z}, \mathbf{\Lambda}_\Theta, \mathbf{A}) \\ \mathbf{x}_2 = S^2(\mathbf{x}_0, \mathbf{z}, \mathbf{\Lambda}_\Theta, \mathbf{A}) \\ \vdots \\ \mathbf{x}_T = S^T(\mathbf{x}_0, \mathbf{z}, \mathbf{\Lambda}_\Theta, \mathbf{A}) \end{array} \right.$$

$$\mathbf{x}_T = \mathcal{N}_\Theta^T(\mathbf{x}_0)$$

A deep unrolled scheme

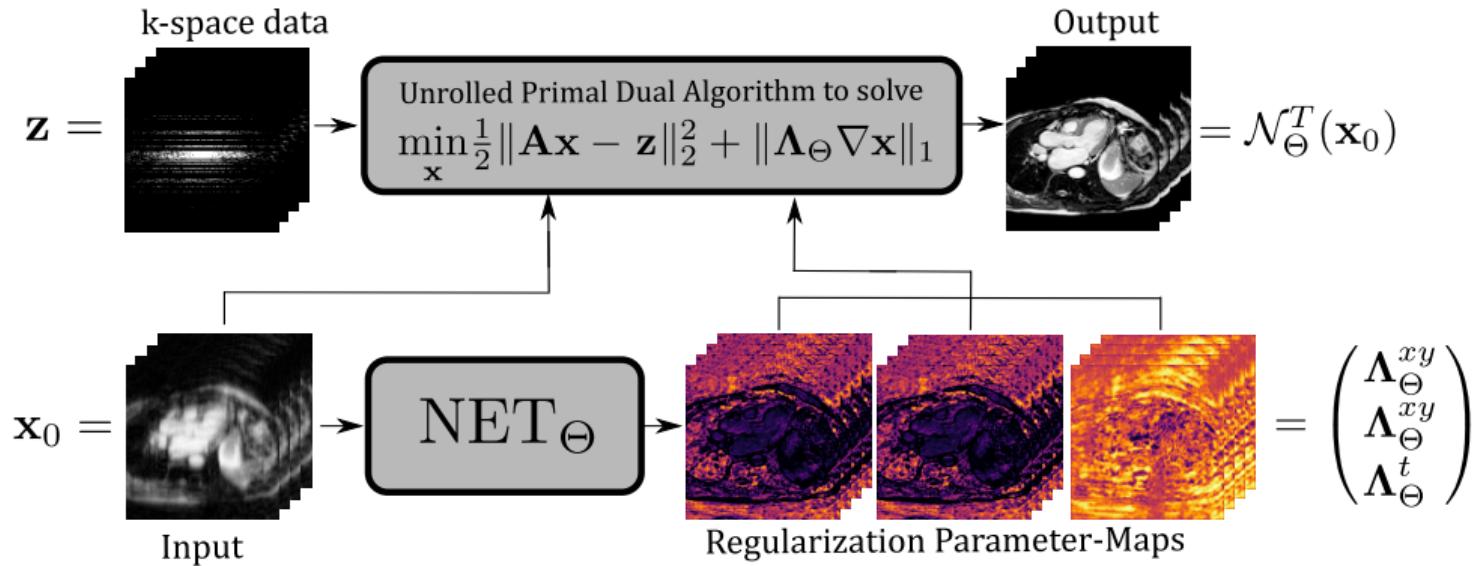
$$\begin{aligned}\mathcal{N}_\Theta^T(\mathbf{x}_0) &= S^T(\mathbf{x}_0, \mathbf{z}, \boldsymbol{\Lambda}_\Theta, \mathbf{A}) \\ &= S^T(\mathbf{x}_0, \mathbf{z}, \text{NET}_\Theta(\mathbf{x}_0), \mathbf{A})\end{aligned}$$

End-to-end training

Set of training pairs $\mathcal{D} = \{(\mathbf{x}_0^i, \mathbf{x}_{\text{true}}^i)_{i=1}^M : \mathbf{x}_0^i = A^* \mathbf{z}_i, \mathbf{z}_i := \mathbf{A} \mathbf{z}_{\text{true}}^i + \mathbf{e}_i\}$

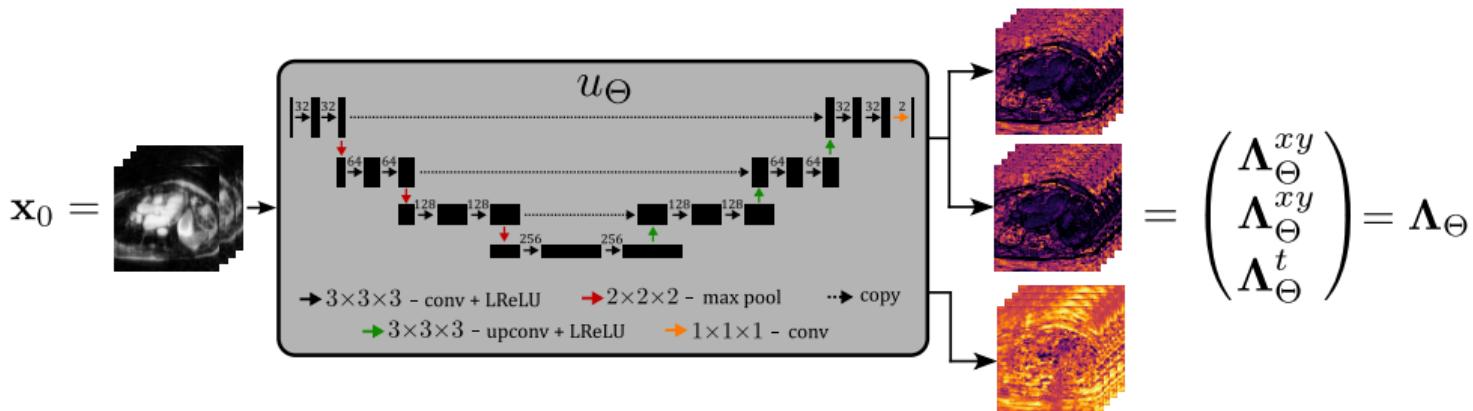
$$\min_\Theta \mathcal{L}(\Theta) := \frac{1}{M} \sum_{i=1}^M l(\mathcal{N}_\Theta^T(\mathbf{x}_0^i), \mathbf{x}_{\text{true}}^i) + r(\Theta)$$

A deep unrolled scheme



$$\text{TV}_{\Lambda^{xy,t}}(\mathbf{x}) := \sum_z \Lambda^{xy}(z) |\nabla_x \mathbf{x}(z)| + \Lambda^{xy}(z) |\nabla_y \mathbf{x}(z)| + \Lambda^t(z) |\nabla_t \mathbf{x}(z)|$$

A deep unrolled scheme



$$\text{TV}_{\Lambda^{xy,t}}(\mathbf{x}) := \sum_z \Lambda^{xy}(z) |\nabla_x \mathbf{x}(z)| + \Lambda^{xy}(z) |\nabla_y \mathbf{x}(z)| + \Lambda^t(z) |\nabla_t \mathbf{x}(z)|$$

A deep unrolled scheme: Consistency analysis

$$\min_{\Theta \in \mathbb{R}^\ell} \mathcal{L}^T(\Theta) := \frac{1}{M} \sum_{i=1}^M l(\mathcal{N}_\Theta^T(\mathbf{x}_0^i), \mathbf{x}_{true}^i) + r(\Theta)$$

$$\mathcal{N}_\Theta^T(\mathbf{x}_0) := S^T(\mathbf{x}_0, \mathbf{z}, \boldsymbol{\Lambda}_\Theta(\mathbf{x}_0))$$

$$\min_{\Theta \in \mathbb{R}^\ell} \mathcal{L}^*(\Theta) := \frac{1}{M} \sum_{i=1}^M l(\mathcal{N}_\Theta^*(\mathbf{x}_0^i), \mathbf{x}_{true}^i) + r(\Theta)$$

$$\mathcal{N}_\Theta^*(\mathbf{x}_0) := S^*(\mathbf{z}, \boldsymbol{\Lambda}_\Theta(\mathbf{x}_0))$$

A deep unrolled scheme: Consistency analysis

Unrolled PDHG algorithm [Chambolle, Pock, 2011]

Input: $L = \|\mathbf{K}\|$, $\tau\sigma \leq 1/L^2$, $\theta = 1$, initial guess \mathbf{x}_0

Parameters: number of iterations $T > 0$

Output: reconstructed image \mathbf{x}_T

- 1: $\bar{\mathbf{x}}_0 = \mathbf{x}_0$
- 2: $\mathbf{y}_0 = \mathbf{0}$
- 3: **for** $k < T$ **do**
- 4: $\mathbf{y}_{k+1} = \text{prox}_{\sigma f^*}(\mathbf{y}_k + \sigma \mathbf{K} \bar{\mathbf{x}}_k)$
- 5: $\mathbf{x}_{k+1} = \text{prox}_{\tau g}(\mathbf{x}_k - \tau \mathbf{K}^\top \mathbf{y}_{k+1})$
- 6: $\bar{\mathbf{x}}_{k+1} = \mathbf{x}_{k+1} + \theta(\mathbf{x}_{k+1} - \mathbf{x}_k)$
- 7: **end for**

$$\min_{\mathbf{x} \in X} f(\mathbf{Kx}) + g(\mathbf{x})$$

$$f(\mathbf{y}) = f(\mathbf{p}, \mathbf{q}) := f_1(\mathbf{p}) + f_2(\mathbf{q}) = \frac{1}{2} \|\mathbf{p} - \mathbf{z}\|_2^2 + \|\Lambda_\Theta \mathbf{q}\|_1, \quad \mathbf{K} := \begin{bmatrix} \mathbf{A} \\ \nabla \end{bmatrix}, \quad g(\mathbf{x}) := \mathbf{0}$$

A deep unrolled scheme: Consistency analysis

Assumptions:

- (i) The operator $\mathbf{A} : X \rightarrow Z$ is injective
- (ii) The fidelity term $d(\cdot, \mathbf{z})$ is $\mu_{\mathbf{z}}$ -strongly convex and Lipschitz continuously differentiable for every $\mathbf{z} \in Z$
- (iii) The parameters $\sigma, \tau > 0$ in PDHG are small enough such that the matrix

$$\mathbf{M} = \begin{pmatrix} \frac{1}{\tau} \mathbf{I} & -\mathbf{K}^T \\ -\mathbf{K} & \frac{1}{\sigma} \mathbf{I} \end{pmatrix}$$

is symmetric, positive definite, defining a norm $\|\cdot\|_{\mathbf{M}}$

- (iv) The regularization function $r : \mathbb{R}^\ell \rightarrow \overline{\mathbb{R}} := \mathbb{R} \cup \{+\infty\}$ is proper and lower semicontinuous.
- (v) The loss function $l : X \times X \rightarrow \mathbb{R}$ is continuous.
- (vi) The activation functions in the NET_{Θ} are continuous.

A deep unrolled scheme: Consistency analysis

Proposition. The following statements hold:

- (i) The solution map $\Lambda \mapsto S^*(\mathbf{z}, \Lambda)$ is Lipschitz for every $\mathbf{z} \in Z$. In particular the following bound holds for every $\Lambda_1, \Lambda_2 \in \mathbb{R}_+^{qn}$,

$$\|S^*(\Lambda_1, \mathbf{z}) - S^*(\Lambda_2, \mathbf{z})\|_2 \leq \frac{2\|\nabla\|}{\lambda_{\min}(\mathbf{A}^\top \mathbf{A})\mu_{\mathbf{z}}} \|\Lambda_1 - \Lambda_2\|_2.$$

- (ii) The map $\Lambda \mapsto S^T(\mathbf{x}_0, \mathbf{z}, \Lambda)$ is Lipschitz for every $\mathbf{z} \in Z$, $\mathbf{x}_0 \in X$ and $T \in \mathbb{N}$.
- (iii) For $\|\Lambda\|_2 \leq \bar{\Lambda}$ we obtain the following sub-linear rate, for $\mathbf{v}_0 := (\mathbf{x}_0, \mathbf{y}_0)$

$$\|S^T(\mathbf{x}_0, \mathbf{z}, \Lambda) - S^*(\mathbf{z}, \Lambda)\|_2 \leq \frac{3C_{\mathbf{z}, \mathbf{A}}}{T^{1/4}} (1 + \|\mathbf{v}_0 - \mathbf{v}^*(\Lambda, \mathbf{z})\|_{\mathbf{M}}),$$

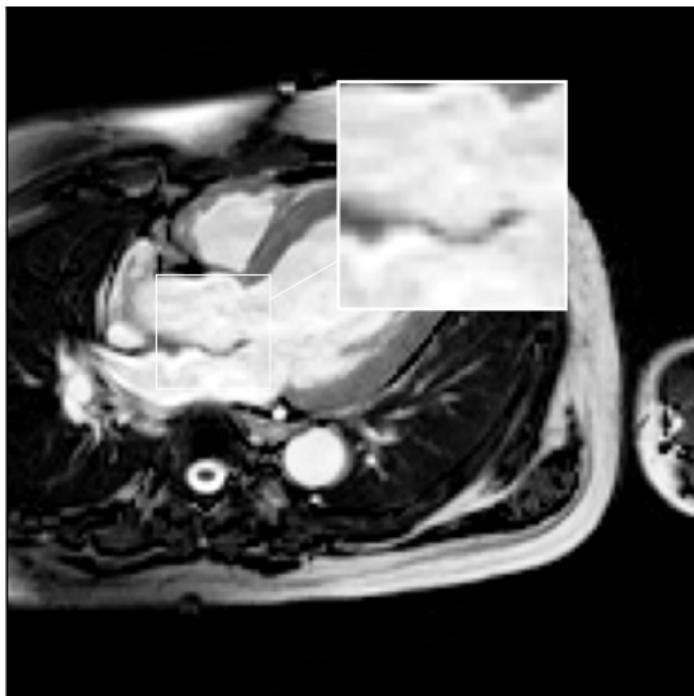
- (iv) Whenever $\Lambda_T \rightarrow \Lambda$ as $T \rightarrow \infty$, it holds $S^T(\mathbf{x}_0, \mathbf{z}, \Lambda_T) \rightarrow S^*(\mathbf{z}, \Lambda)$ for every $\mathbf{x}_0 \in X$, $\mathbf{z} \in Z$.

Theorem

Let the training set \mathcal{D} be fixed and consider the sequence of functions $\mathcal{L}^T : \mathbb{R}^\ell \rightarrow \overline{\mathbb{R}}$, $T \in \mathbb{N}$, as well as $\mathcal{L}^* : \mathbb{R}^\ell \rightarrow \overline{\mathbb{R}}$ defined as before. Then we have that \mathcal{L}^T Γ -converges to \mathcal{L}^* as $T \rightarrow \infty$.

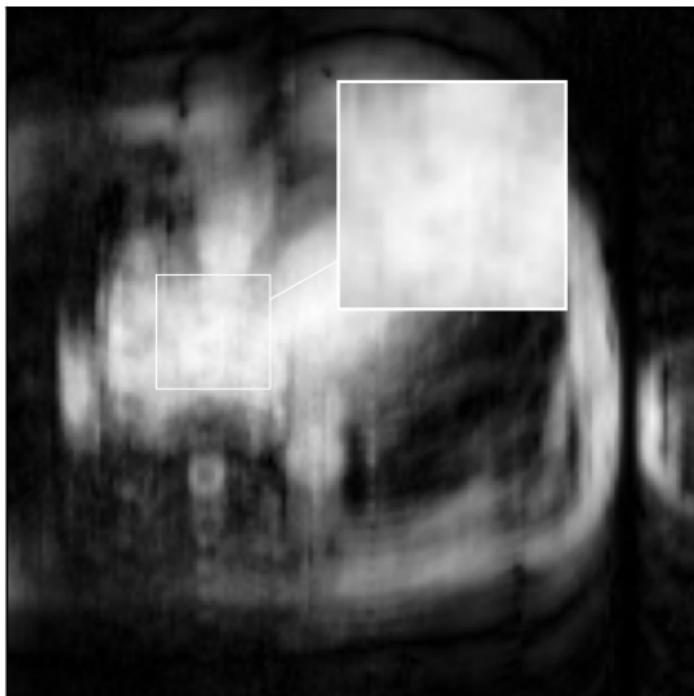
Let $\epsilon_T \rightarrow 0$. Suppose that Θ_T is an ϵ_T -minimizer of \mathcal{L}^T i.e. $\mathcal{L}^T(\Theta_T) \leq \inf_{\Theta \in \mathbb{R}^\ell} \mathcal{L}^T(\Theta) + \epsilon_T$. Then, if Θ is an accumulation point of $(\Theta_T)_{T \in \mathbb{N}}$ it is a minimizer of \mathcal{L}^* and $\mathcal{L}^*(\Theta) = \limsup_{T \rightarrow \infty} \mathcal{L}^T(\Theta_T)$.

Application to dynamic MRI



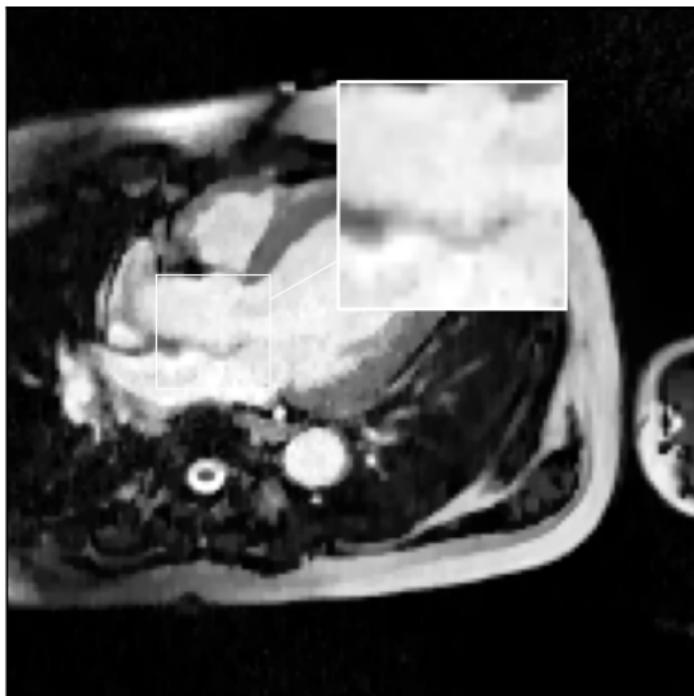
Ground truth

Application to dynamic MRI

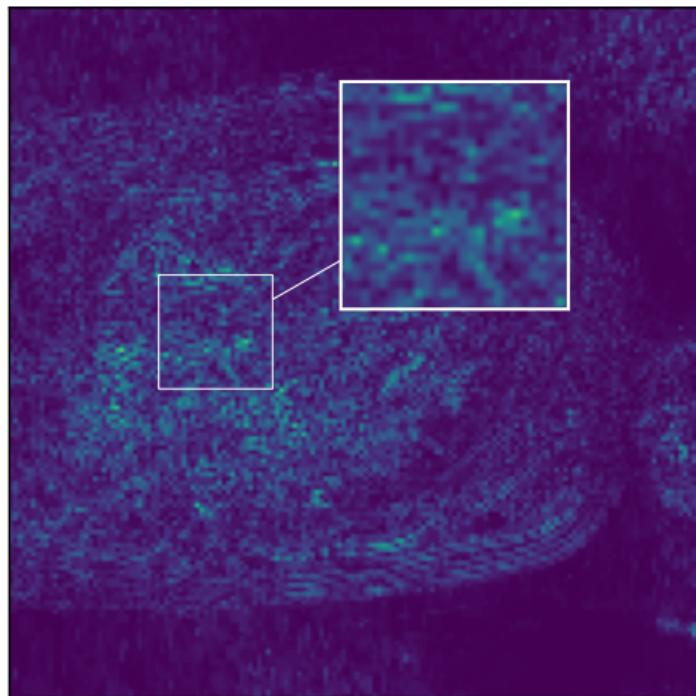


zero filled

Application to dynamic MRI

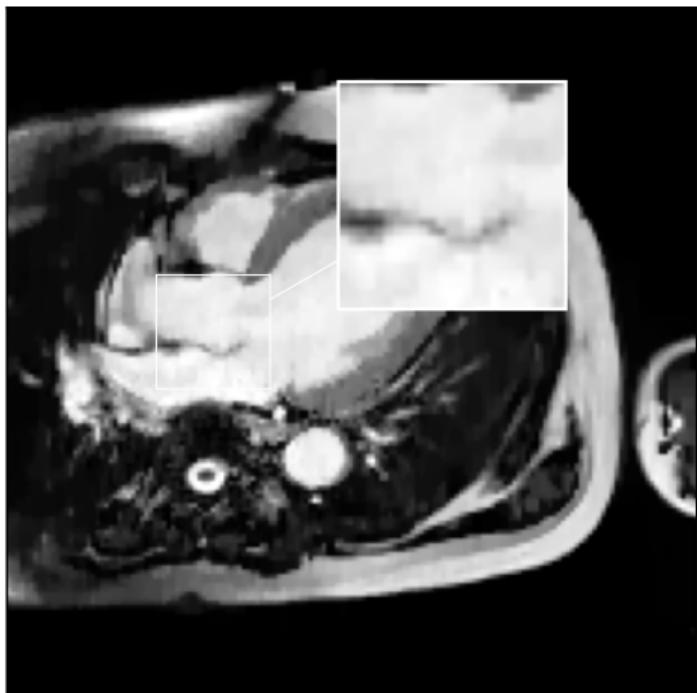


Reconstruction, best scalar λ w.r.t. PSNR

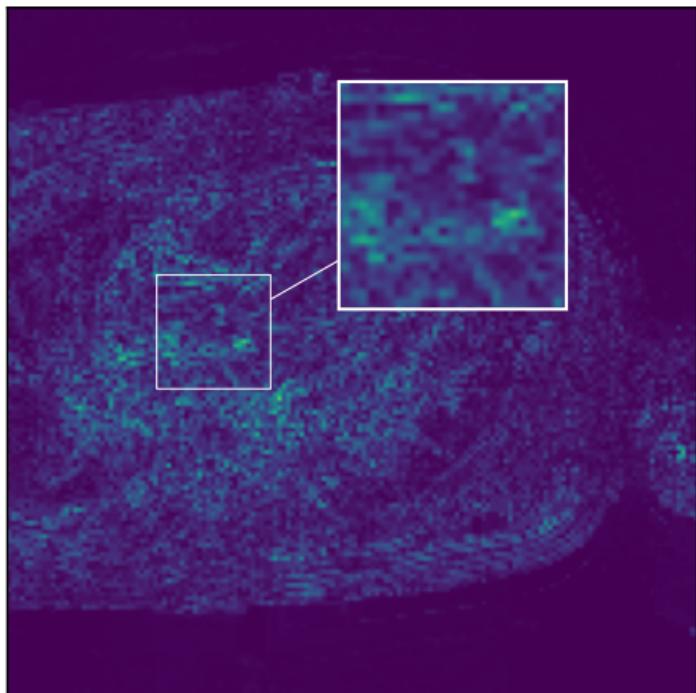


Difference to the ground truth

Application to dynamic MRI

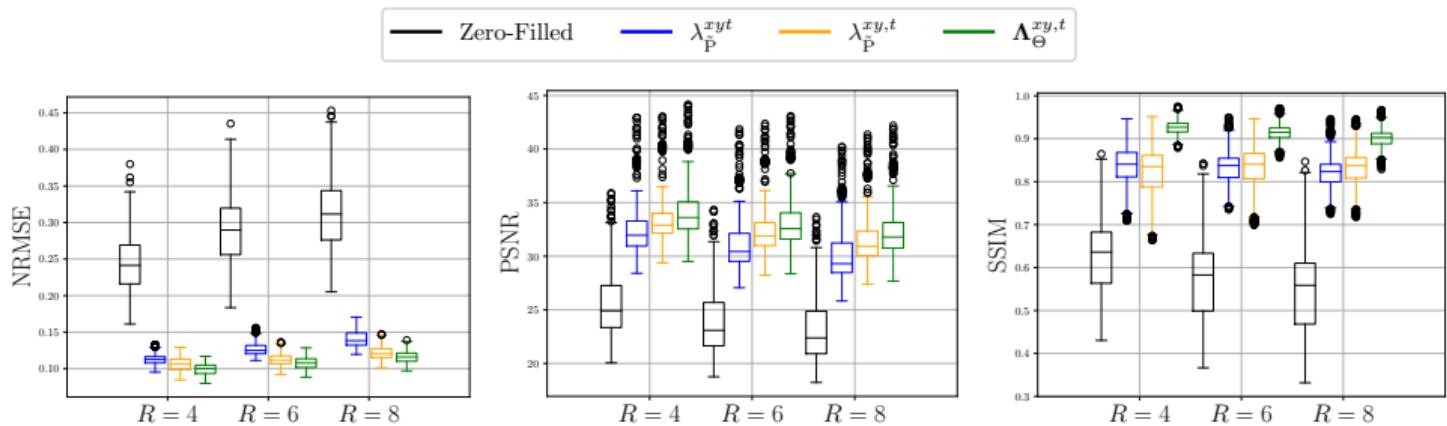


Reconstruction with Λ_Θ



Difference to the ground truth

Application to dynamic MRI



Application to dynamic MRI

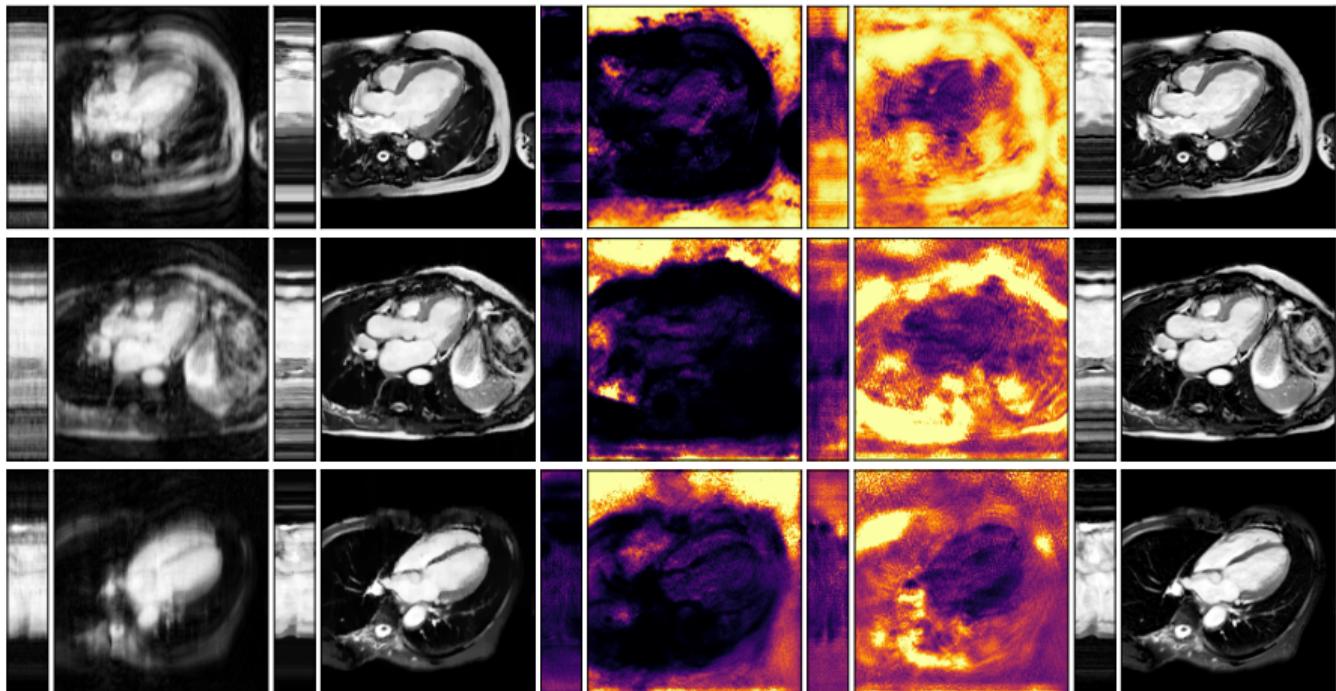
Zero-Filled

PDHG $\Lambda_{\Theta}^{xy,t}$

Λ_{Θ}^{xy}

Λ_{Θ}^t

Target



0.00

0.05

0.10

0.15

0.20

0.25

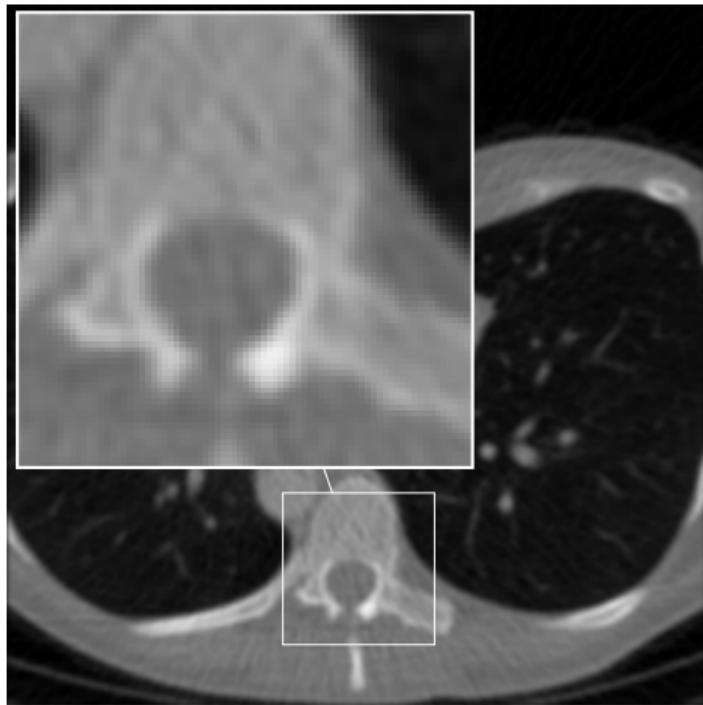
Application to dynamic MRI

Application to Computerized Tomography



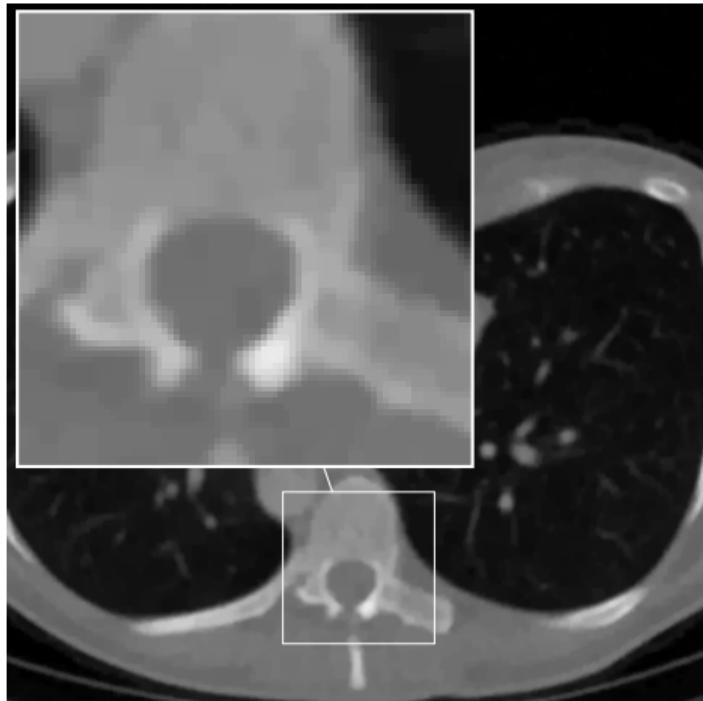
Ground truth

Application to Computerized Tomography

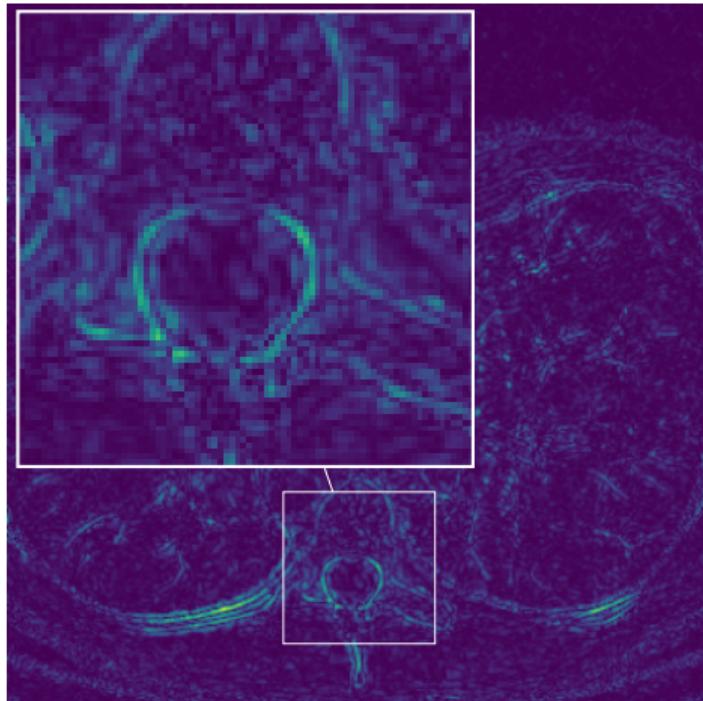


FBP

Application to Computerized Tomography



Reconstruction, best scalar λ w.r.t. PSNR

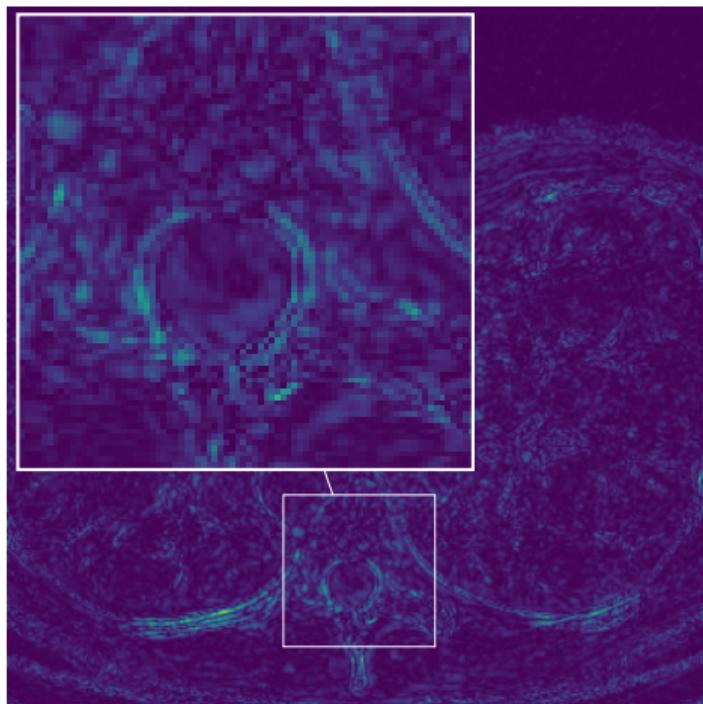


Difference to the ground truth

Application to Computerized Tomography

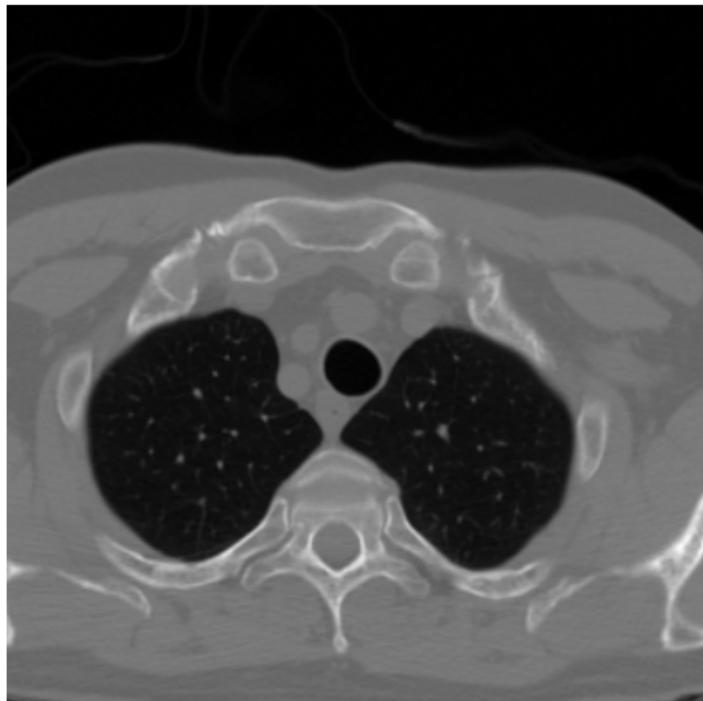


Reconstruction with Λ_Θ

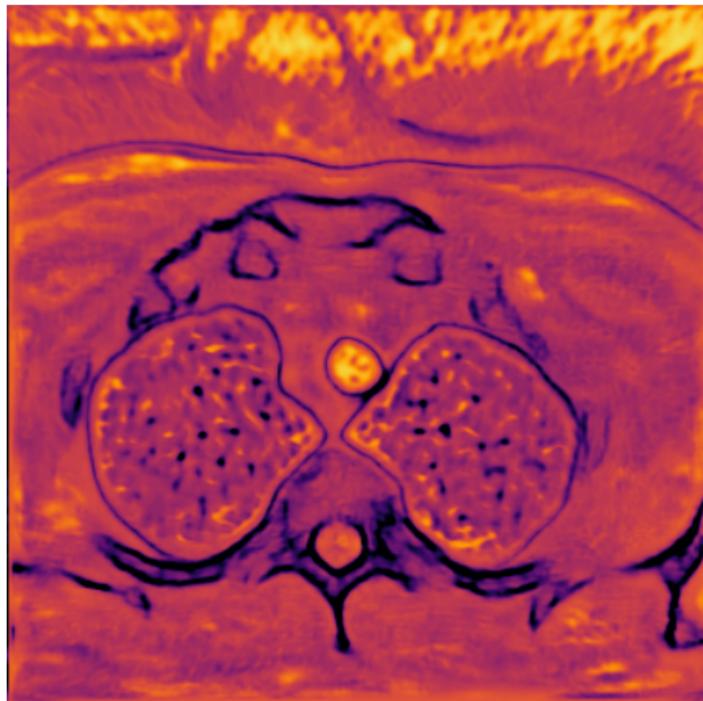


Difference to the ground truth

Application to Computerized Tomography



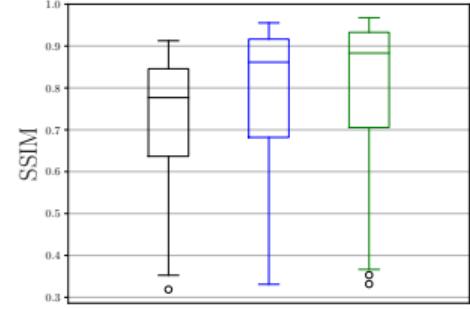
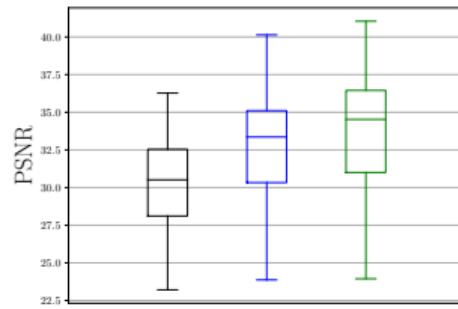
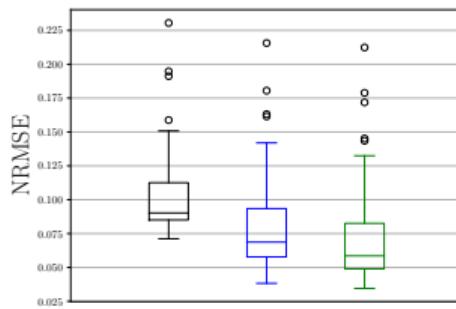
Reconstruction with Λ_Θ



Λ_Θ produced by unrolled scheme

Application to Computerized Tomography

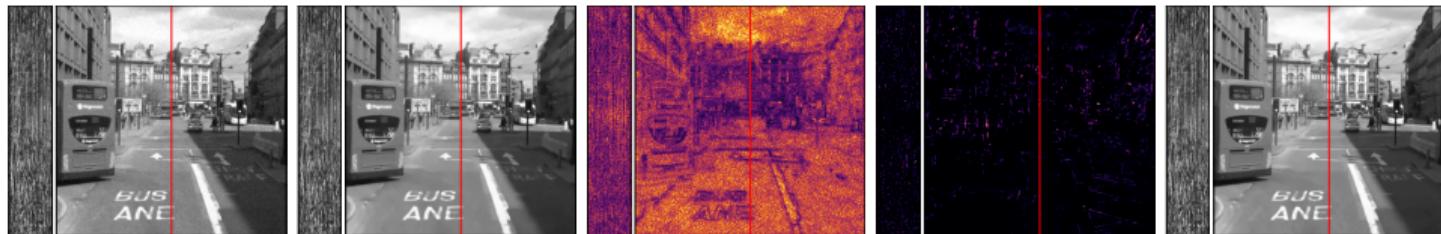
— FBP — λ_P^{xy} — Λ_Θ^{xy}



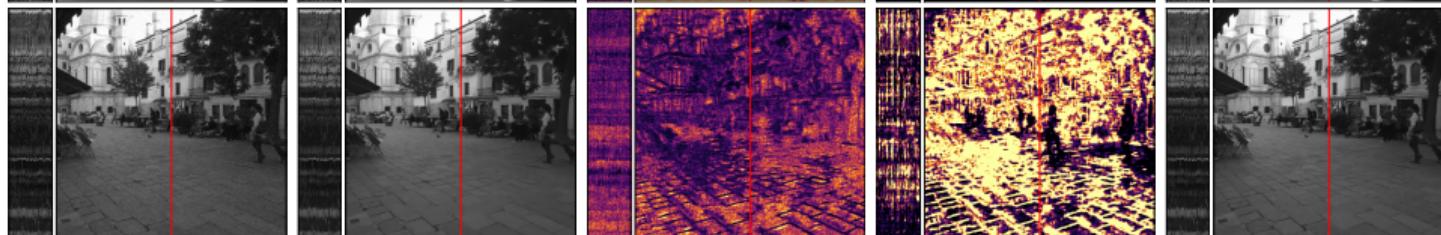
Application to dynamic denoising

Moving camera

Noisy PDHG $\Lambda_{\Theta}^{xy,t}$ Λ_{Θ}^{xy} Λ_{Θ}^t Target



Static camera



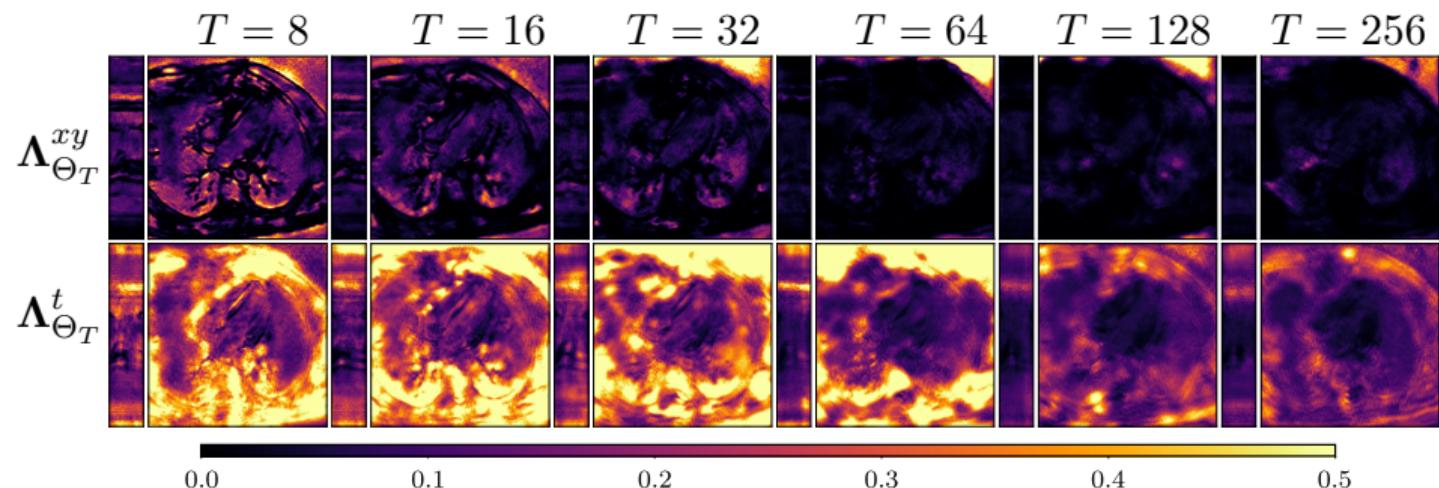
$$\Lambda_{\Theta}^{xy}$$



$$\Lambda_{\Theta}^t$$



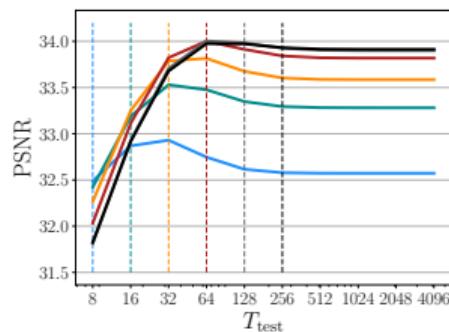
Choosing T at training and test times



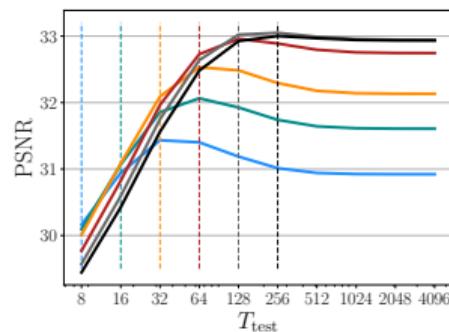
Choosing T at training and test times

Legend: $T_{\text{train}} = 8$ (blue), $T_{\text{train}} = 16$ (teal), $T_{\text{train}} = 32$ (orange), $T_{\text{train}} = 64$ (red), $T_{\text{train}} = 128$ (dark grey), $T_{\text{train}} = 256$ (black)

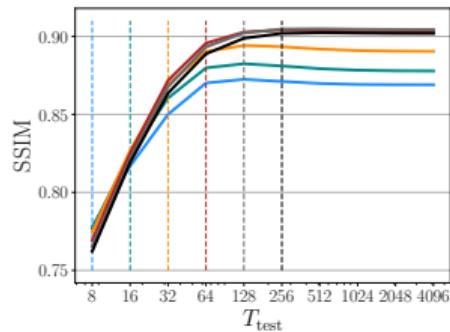
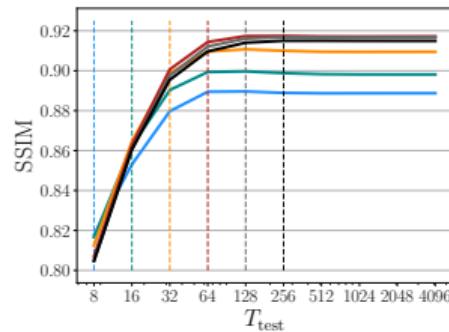
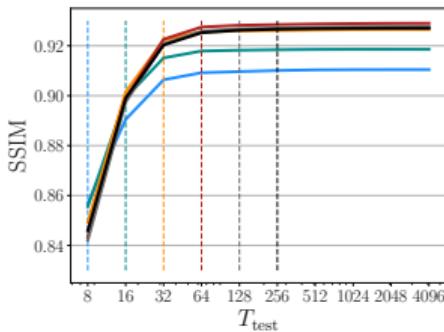
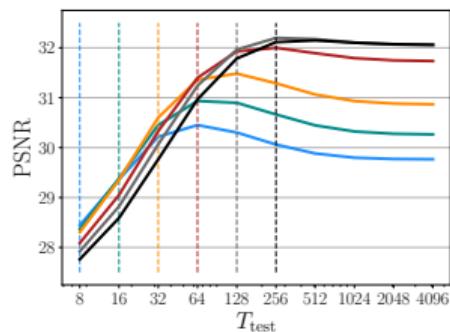
$R = 4$



$R = 6$



$R = 8$



Summary

- Simple yet efficient data-driven approach to automatically select *spatio-temporal* dependent regularization parameter-maps for the variational image reconstruction
- Interpretable algorithm since the “black-box” nature of the CNN is placed entirely on the regularization parameter and not to the image itself
- Consistency analysis in terms of ϵ -minimizers

Open questions:

- Consistency results in terms of stationary points....?
- Investigate theoretically in what degree CNN-produced artefacts in the parameter-maps can affect or create artefacts to the corresponding reconstructions
- Avoid using large T , computing hyper-gradients, deep equilibrium models...

A highly collaborative effort!

- Learning regularization parameter-maps for variational image reconstruction using deep neural networks and algorithm unrolling, submitted, arXiv:2301.05888, 2023
- Unrolled three-operator splitting for parameter-map learning in low dose X-ray CT reconstruction, Fully3D, 2023
- CNN-based estimation of spatio-temporal regularization parameter-maps for TV-reconstruction in dynamic cardiac MRI, ISMRM, 2023

Andreas Kofler, Fabian Alteküger, Fatima Antarou Ba, Christoph Kolbitsch, Evangelos Papoutsellis, David Schote, Clemens Sirotenko, Felix Zimmermann, Kostas Papafitsoros

MATHS MEETS IMAGE

Hackathon on image reconstruction,
segmentation and shape analysis

17 – 19 March 2022 at The Classroom, Berlin



Thank you for your attention

<http://kostaspapafitsoros.weebly.com>