Machine Learned Regularisation for Solving Inverse Problems

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- Dr Marcello Carioni
- Dr Christian Etmann
- Dr Julian Gilbey
- Dr Rihuan Ke
- Dr Yury Korolev
- Dr Madeleine Kotzagiannidis
- Dr Lisa-Maria Kreusser
- Dr Jonas Latz
- Dr Subhadip Mukherjee
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- Georgios Batzolis
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Main messages of this talk

- Machine learning and in particular deep learning offers interesting opportunities for inverse problems:
  - high quality solutions through data-adaptivity;
  - computationally efficient once trained.

- They only work in practice when combined with mathematical and statistical modelling.

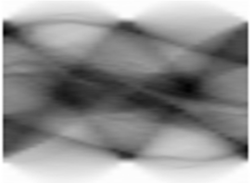
- In general, there is a lack of understanding of these approaches and a need for more mathematical scrutiny.

- Learned variational models are an example of hybrid methodologies that compromise between empirical and theoretical performance.

The talk is taking a lot of its ‘wisdom’ from this paper: Arridge, Maass, Öktem, CBS, Acta Numerica ’19

What is an inverse imaging problem?

In short: compute image $u \in X$ from $Y \ni y = Tu + n$, X, Y normed vector spaces. In computed tomography (CT) T is the Radon transform.

T  $+ n =$ 

Video clip from Samuli:

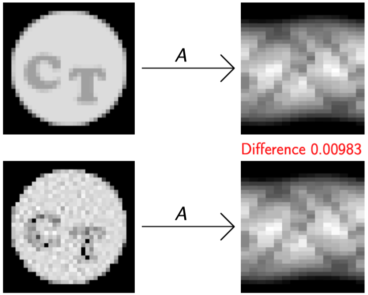
`https://www.youtube.com/watch?v=newxZbw7YAs`

Inverse problem: measuring (corrupted!) data y compute image u.

CT images from LUNA dataset `https://luna16.grand-challenge.org`.

Ill-posedness

Example: Sparse tomography: more unknowns than measured angles and intercepts.



Courtesy of Samuli Siltanen

Ill-posedness: T^{-1} is not invertible (unbounded or discontinuous)

Typical reasons: Undersampling, nonlinearity, noise, ...

Inverse problems are ill-posed $\rightarrow$ well-posedness through regularisation

The variational approach

General task: **restore** $\mathbf{u}$ from an **observed datum** $\mathbf{y}$ where

$$y = \underbrace{T(u)}_{\text{forward model}} + \underbrace{n}_{\text{noise}}.$$

Variational approach: Compute u as a minimizer of

$$\mathcal{J}(u) = \alpha \underbrace{R(u)}_{\text{regularisation}} + \underbrace{D(T(u), y)}_{\text{data fidelity}} \to \min_{u \in X},$$

where

- $R(u)$ is a prior/regulariser that models a-priori information on u weighted by positive α, e.g., $R(u) = \|\nabla u\|_1$ (in infinite dimensions $|Du|(\Omega)$)
- $D(\cdot, \cdot)$ is a distance function, e.g. $D(T(u), y) = \|T(u) - y\|_2^2$ and X suitable Banach space, e.g., $X = BV(\Omega)$.

Engl, Hanke, Neubauer '96; Rudin, Osher, Fatemi, Physica D '92; Natterer, Wübbeling '01; Candes, Romberg, Tao, IEEE Trans Inf Theory '06; Kaltenbacher, Neubauer, Scherzer '08; Schuster, Kaltenbacher, Hofmann, Kazimierski '12

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Example: Sparse-angle CT reconstruction: top row is based on mathematical/handcrafted models; bottom row is using novel deep learning based models.

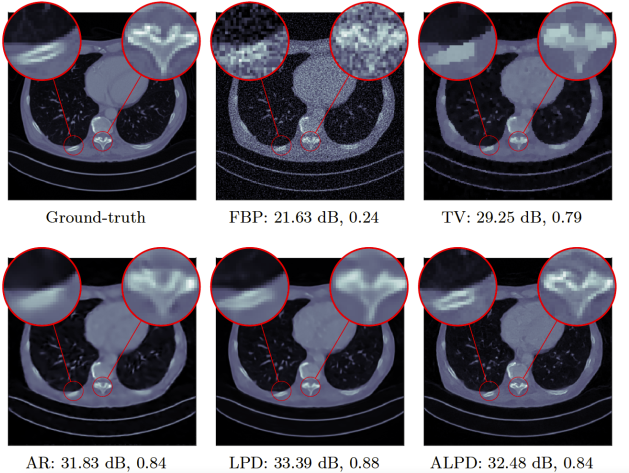


Photo courtesy of Subho Mukherjee

Deep learning for inverse imaging

Main paradigms:

- Fully Learned Models [1]
- Learned Post Processing [2]
- Learned Iterative Schemes [3]
- Learning the Regulariser [4]

Reviews: McCann, Jin, Unser, IEEE Signal Processing Magazine '17; Arridge, Maass, Öktem, CBS, Acta Numerica '19

[1] Zhu, Bo, Liu, Cauley, Rosen, Rosen, Nature '18.

[2] Jin, McCann, Froustey, Unser, IEEE TIP, '17; Kang, Min, Ye, Medical Physics '17.

[3] Yang, Sun, Li, Xu, NeurIPS '16; Meinhardt, Moeller Hazirbas, Cremers, ICCV '17; Putzky, Welling, arXiv:1706.04008; Adler, Öktem, Inverse Problems '17; Hammernik et al. MRM '18; Adler, Lunz, Verdier, CBS, Öktem, NeuIPS '18; Hauptmann et al., IEEE TMI '19; de Hoop, Lassas, Wong, arXiv:1912.11090; Gilton, Ongie, Willett, IEEE TCI '19; Mukherjee, Öktem, CBS, SSVM '21; Bubba et al., SIIMS '21.

[4] Lunz, Öktem, CBS, NeurIPS '18; Ye, Ravishankar, Long, Fessler, IEEE TMI '18; Li, Schwab, Antholzer, Haltmeier, Inverse Problems '20; Kobler, Effland, Kunisch, Pock, CVPR '20; Mukherjee, Dittmer, Shumaylov, Lunz, Öktem, CBS, arXiv:2008.02839; Pinetz et al., SIIMS '21.

Let Ψ_Θ be a neural network with parameters Θ.

- Postprocessing. Reconstruct via

$$u = \Psi_\Theta T^\dagger y$$

- Learned Iterative Reconstruction.

$$\begin{aligned} u_0 &= T^\dagger y \\ u_{n+1} &= \Psi_\Theta(u_n,\ \nabla_{u_n} \|Tu_n - y\|_2^2) \end{aligned}$$

Advantage: great performance; disadvantage: black box!

Variational formulation could resolve some shortcomings of existing algorithms (e.g., provable notion of stability of regularisation and data consistency of the solution.)

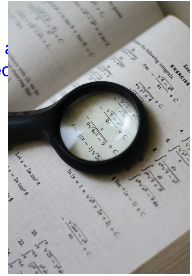
Deep learning challenges

Why is black box a problem?

No systematic way to design them

Identified as a 45mph speed sign

Safety danger



Lack of interpretation

Good recent reference: Berner, Grohs, Kutyniok, Petersen, The Modern Mathematics of Deep Learning, arXiv:2105.04026

Deep learning for inverse imaging

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[6] Jin, McCann, Froustey, Unser, IEEE TIP, '17; Kang, Min, Ye, Medical Physics '17.

[7] Yang, Sun, Li, Xu, NeurIPS '16; Meinhardt, Moeller Hazirbas, Cremers, ICCV '17; Putzky, Welling, arXiv:1706.04008; Adler, Öktem, Inverse Problems '17; Hammernik et al. MRM '18; Adler, Lunz, Verdier, CBS, Öktem, NeuIPS '18; Hauptmann et al., IEEE TMI '19; de Hoop, Lassas, Wong, arXiv:1912.11090; Gilton, Ongie, Willett, IEEE TCI '19; Mukherjee, Öktem, CBS, SSVM '21; Bubba et al., SIIMS '21.

[8] Lunz, Öktem, CBS, NeurIPS '18; Ye, Ravishankar, Long, Fessler, IEEE TMI '18; Li, Schwab, Antholzer, Haltmeier, Inverse Problems '20; Kobler, Effland, Kunisch, Pock, CVPR '20; Mukherjee, Dittmer, Shumaylov, Lunz, Öktem, CBS, arXiv:2008.02839; Pinetz et al., SIIMS '21.

Knowledge and data-driven hybrids

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- We have: rich range of mathematical image processing models, sourced from PDEs, variational calculus, functional analysis, numerical analysis and optimisation:
  - mathematical guarantees
  - interpretability
  - agnostic to dataset
  - limit in expressibility of models

- We use learning to: complement what we cannot model well, so that the resulting inversion model is mathematically sound and so that training is more feasible also in small data regimes.

Learning variational regularization

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Variational Problem: $y \in Y$ and $T : X \to Y$ linear and bounded, X, Y Banach spaces. Then, consider

$$\arg\min_u \|Tu - y\|_2^2 + \alpha R(u)$$

- Interpretability: explicit prior.
- Stability and convergence results.
- Regularisation parameter to adopt to noise level.
- Incorporates forward model explicitly.
- Incorporates noise statistics.

Stick to the variational problem and only learn the regulariser R.

Examples for learning regularisers

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- Sparse coding & dictionary learning '06–: Aharon, Allard, Binev, Bruckstein, Bruna, Chandrasekaran, DeVore, Elad, Fadili, Mallat, Mayral, Papyan, Peyre, Ponce, Sulam, . . . :

$$\min_{\gamma,\phi} \|T(\sum_i \gamma_i \phi_i) - y\|_2^2 + \|\gamma\|_1$$

- Black-box denoiser: Plug-and-Play Prior (P^3) method Venkatakrishnan, Bouman, Wohlberg, GlobalSIP '13; Wei, Aviles-Rivero, Liang, Fu, Huang, CBS, ICML '20 best paper award, Regularisation by Denoising (RED) Romano, Elad, Milanfar, SIIMS '17; Terris, Repetti, Pesquet, Wiaux, ICASSP '20,

$$\min_u D(T(u), y) + \alpha R(u), \quad \text{with } R(u) = \langle u, u - \Lambda(u)\rangle, \quad \Lambda : X \to X \text{ denoiser.}$$

- Bilevel optimisation '03–: Chung, De Los Reyes, Fonseca, Haber, Hintermüller, Horesh, Kunisch, Langer, Liu, Pock, Tappen, Tenorio, CBS, . . .

$$\min_\lambda F(u_\lambda) \quad \text{s.t. } u_\lambda = \mathrm{argmin}_v R(\lambda, u) + D(T(u), y)$$

- Deep neural networks as regularisers Lunz, Öktem, CBS, NeurIPS '18; Maass, Öktem, CBS, Acta Numerica '19; Li, Schwab, Antholzer, Haltmeier, Inverse Problems '20; Kobler, Effland, Kunisch, Pock, CVPR '20; Mukherjee, Dittmer, Shumaylov, Lunz, Öktem, CBS, arxiv 20

Learned adversarial regularisers

Joint work with

Marcello Carioni

Sören Dittmer

Sebastian Lunz

Subhadip Mukherjee

Ozan Öktem

Zak Shumaylov

S. Lunz, O. Öktem, CBS, Adversarial Regularizers in Inverse Problems, in NeurIPS 2018; S. Mukherjee, S. Dittmer, Z. Shumaylov, S. Lunz, O. Öktem, CBS, Learned convex regularizers for inverse problems, arXiv:2008.02839; Carioni, Mukherjee, CBS, End-to-end reconstruction meets data-driven regularization for inverse problems, arXiv:2106.03538

Train regulariser adversarially

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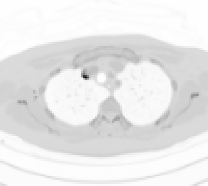
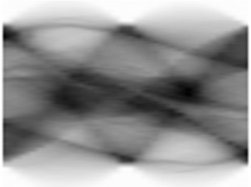
How to learn a regulariser for $\min_v \alpha\mathcal{R}(v) + \|Tv - y\|_2^2$?

'Good guys'



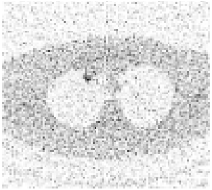
$U^* \sim \mathbb{P}_U$

Data



$Y \sim \mathbb{P}_Y$

'Bad guys'



$U \sim \mathbb{P}_n := T_\sharp^\dagger \mathbb{P}_Y$

Train regulariser in adversarial manner to be small for samples from $\mathbb{P}_U$ and large for samples from $\mathbb{P}_n$.

Lunz, Öktem, CBS, NeurIPS 2018; Arridge, Maass, Öktem, CBS, Acta Numerica 2019; Mukherjee, Dittmer, Shumaylov, Lunz, Öktem, CBS, arxiv 2020

Train regulariser adversarially

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- Idea from Wasserstein GANs [9]: use 1-Wasserstein distance as (unsupervised) loss for regulariser

$$\mathrm{Wass}(\mathbb{P}_n, \mathbb{P}_U) = \sup_{R \in 1-Lip} \mathcal{E}_{U \sim \mathbb{P}_n} R(U) - \mathcal{E}_{U \sim \mathbb{P}_U} R(U)$$

- Train the regulariser to learn image statistics – good and bad guys DO NOT need to be paired!
- Parametrization for R^*: $R_\Theta(u) = \Psi_\Theta(u) + \rho_0 \|u\|_2^2$, where $\Psi_\Theta(u)$ is a [convex[10]] convolutional NN and L-Lipschitz.
- Train the Network with the loss [11]

$$\min_\Theta \mathbb{E}_{U \sim \mathbb{P}_U} \left[\Psi_\Theta(U)\right] - \mathbb{E}_{U \sim \mathbb{P}_n} \left[\Psi_\Theta(U)\right] + \mu \cdot \mathbb{E}\left[\left(\|\nabla_u \Psi_\Theta(U)\|_* - 1\right)_+^2\right].$$

---

[9] Arjovsky, Chintala & Bottou, ’17

[10] Amos, Xu, Kolter ICML ’17; S. Mukherjee, S. Dittmer, Z. Shumaylov, S. Lunz, O. Öktem, CBS, arXiv:2008.02839

[11] Gulrajani et al., ’17

Algorithm summary

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- Create training data $\mathbb{P}_U$ (good guys) and $\mathbb{P}_n$ (bad guys) – do not need to be paired!
- Train regularizer in adversarial and unsupervised fashion by minimizing

$$\mathbb{E}_{U\sim\mathbb{P}_U}\left[\Psi_\Theta(U)\right] - \mathbb{E}_{U\sim\mathbb{P}_n}\left[\Psi_\Theta(U)\right] + \mu\,\mathbb{E}\left[\left(\|\nabla_u\Psi_\Theta(U)\|_* - 1\right)_+^2\right].$$

- Deploy the learned adversarial [convex] regularizer (A[C]R) into variational problem

$$\arg\min_u \|Tu - y\|_2^2 + \alpha\left(\Psi_\Theta(u) + \rho_0\|u\|_2^2\right)$$

- Solve the above via (sub)gradient descent.

This [convex] variational model is amenable to analysis! And we get well-posedness :)

Code available at `https://github.com/Subhadip-1`

Well-posedness of A[C]R problem

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AR

1. Existence: by Lipschitz continuity and coercivity
2. Stability: Let $y_n \to y$ in Y and

$$x_n \in \arg\min_{x \in X} \|Tx - y_n\|^2 + \alpha R_\Theta(x),$$

then x_n has weakly convergent subsequence with limit

$$\hat{x} \in \arg\min_{x \in X} \|Tx - y\|^2 + \alpha R_\Theta(x).$$

ACR

1. Existence and uniqueness: by strong-convexity
2. Stability: $\left\|\hat{x}_\alpha\left(y^{\delta_1}\right) - \hat{x}_\alpha\left(y\right)\right\|_2 \leq \frac{4\beta_1\delta_1}{\alpha\rho_0}$, if $\left\|y^{\delta_1} - y\right\|_2 \leq \delta_1$
3. Convergence: $\hat{x}_\alpha(y) \to x^\dagger$ if $\alpha \to 0$ and $\frac{\delta}{\alpha} \to 0$ when $\delta = \|\boldsymbol{e}\|_2 \to 0$, where

$$x^\dagger = \arg\min_{x \in X} R_\Theta(x) \text{ s.t. } Tx = y_0,$$

where y_0 is noise-free data.
4. Convergent sub-gradient algorithm

Lunz, CBS, Öktem, NeurIPS '18; Mukherjee, Dittmer, Shumaylov, Lunz, Öktem, CBS, arXiv:2008.02839

Unrolling AR: end-to-end meets variational regularisation

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- Data model: $U \sim \mathbb{P}_U$, $Y = TU + N \sim \mathbb{P}_Y$
- Learn two networks G_ϕ and R_θ adversarially:

$$\min_{\phi} \max_{\theta: R_\theta \in \mathbb{L}_1} \mathbb{E}_{\mathbb{P}_Y} \|Y - TG_\phi(Y)\|_2^2 + \lambda \left(\mathbb{E}_{\mathbb{P}_Y} \left[R_\theta(G_\phi(Y)) \right] - \mathbb{E}_{\mathbb{P}_U} \left[R_\theta(U) \right] \right)$$

- Equivalent to: $\min_{\phi} \mathbb{E}_{\mathbb{P}_Y} \|Y - TG_\phi(Y)\|_2^2 + \lambda \, \text{Wass}(\mathbb{P}_U, (G_\phi)_{\#}\mathbb{P}_Y)$
- Alt. min.: init. $\theta_0 \leftarrow \underset{\theta: R_\theta \in \mathbb{L}_1}{\arg\min} \mathbb{E}_{\mathbb{P}_U} \left[R_\theta(U) \right] - \mathbb{E}_{\mathbb{P}_Y} \left[R_\theta(T^\dagger Y) \right]$:
  1. $\phi_n \leftarrow \underset{\phi}{\arg\min} \, \mathbb{E}_{\mathbb{P}_Y} \left[\|Y - TG_\phi(Y)\|_2^2 + \lambda R_{\theta_n}(G_\phi(Y)) \right]$
  2. $\theta_{n+1} \leftarrow \underset{\theta: R_\theta \in \mathbb{L}_1}{\arg\min} \, \mathbb{E}\left[R_\theta(U) \right] - \mathbb{E}\left[R_\theta(G_{\phi_n}(Y)) \right]$.
- Returns a regularizer R_{θ^*} and a network G_{ϕ^*} that minimizes the corresponding variational loss
- Fits within the variational framework, yet offers a fast and efficient reconstruction.

Carioni, Mukherjee, CBS, End-to-end reconstruction meets data-driven regularization for inverse problems, arXiv:2106.03538

Computed tomography example

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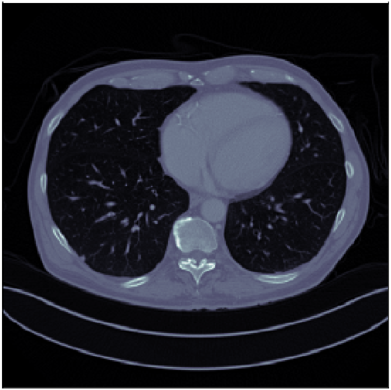
Dataset: Mayo clinic open CT data[12]

- Training data: 2250 slices extracted from 9 patients; test data: 128 slices from 1 patient
- Sparse-view geometry: parallel beam, 200 angles, 400 lines/angle, additive Gaussian noise with $\sigma = 2.0$
- Acronyms:
  - FBP: filtered back projection
  - TV: total variation regularisation Rudin, Osher, Fatemi, Physics D '92
  - AR: classical AR, minimized via SGD and with unrolled updating of $\mathbb{P}_n$ Carioni, Mukherjee, CBS, End-to-end reconstruction meets data-driven regularization for inverse problems, arXiv:2106.03538
  - ACR: adversarial convex regularizer Mukherjee, Dittmer, Shumaylov, Lunz, Öktem, CBS, arXiv:2008.02839
  - LPD: learned primal-dual (supervised) Adler, Öktem, IEEE TMI '18

[12] Chen, Baiyu, et al. "An open library of CT patient projection data." Medical Imaging 2016: Physics of Medical Imaging. Vol. 9783. International Society for Optics and Photonics, 2016.

Sparse-view CT



ground-truth

FBP: 21.6262 dB, 0.2435

Sparse-view CT

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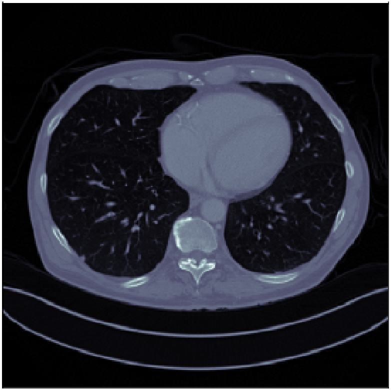
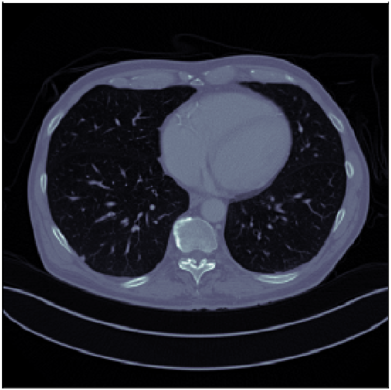


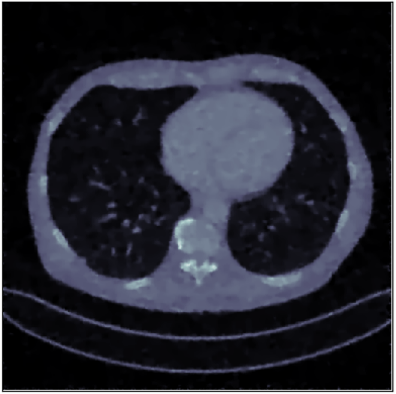
ground-truth

TV: 29.2506 dB, 0.7905

Sparse-view CT

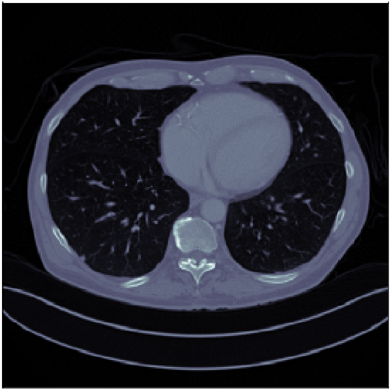


ground-truth

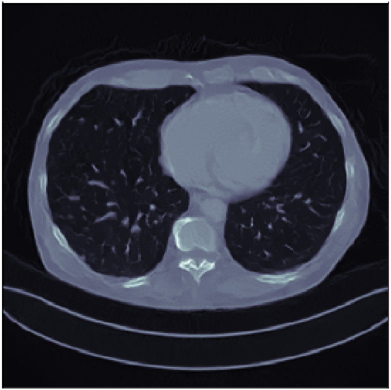


ACR: 30.0016 dB, 0.8246

Sparse-view CT



ground-truth



AR: 32.91 dB, 0.8942

Sparse-view CT

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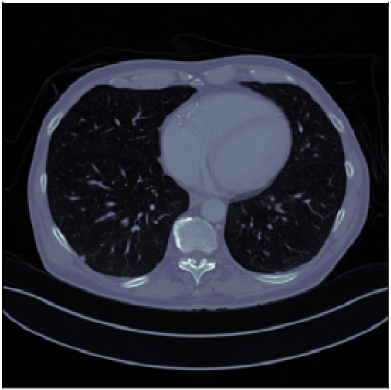


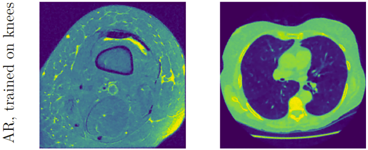
ground-truth

LPD: 33.6218 dB, 0.8871

Extensions and open problems

- Generalisability of machine learned regularisers – only empirical investigations so far, see PhD thesis of Sebastian Lunz
- Stronger constraints on learned regulariser (e.g., source condition joint with Martin Burger, Subho Mukherjee)
- Learned regularisers to fulfill certain qualitative properties (e.g. equivariant NNs for regularisers that are invariant to affine transformations joint with Ferdia Sherry, Elena Celledoni, Matthias Ehrhardt, Christian Etmann, Brynjulf Owren, arXiv:2102.11504
- Choice of optimality criteria (e.g., task-adapted inversion joint with Subhadip Mukherjee, Thomas Buddenkotte, Christian Etmann, Evis Sala and Ozan Öktem)[13]
- Training regularisers for large- and high-dimensional inverse problems invertible networks joint with Christian Etmann and Rihuan Ke
- Uncertainty quantification with learned convex regulariser – e.g. via proximal MCMC Pereyra, Statistics and Computing '16

Cross dataset experiments: left knee, right lung



[13] http://all-in-one.maths.cam.ac.uk

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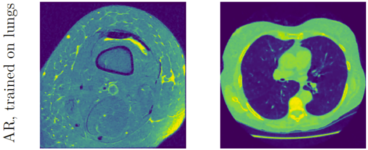

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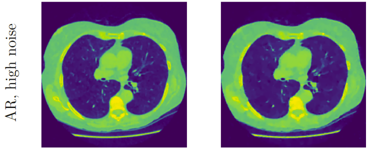
Cross noise experiments: left low noise, right high noise



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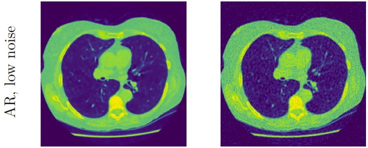
- Stronger constraints on learned regulariser (e.g., source condition joint with Martin Burger, Subho Mukherjee)
- Learned regularisers to fulfill certain qualitative properties (e.g. equivariant NNs for regularisers that are invariant to affine transformations joint with Ferdia Sherry, Elena Celledoni, Matthias Ehrhardt, Christian Etmann, Brynjulf Owren, arXiv:2102.11504
- Choice of optimality criteria (e.g., task-adapted inversion joint with Subhadip Mukherjee, Thomas Buddenkotte, Christian Etmann, Evis Sala and Ozan Öktem)[13]
- Training regularisers for large- and high-dimensional inverse problems invertible networks joint with Christian Etmann and Rihuan Ke
- Uncertainty quantification with learned convex regulariser – e.g. via proximal MCMC Pereyra, Statistics and Computing '16

Cross noise experiments: left low noise, right high noise



[13] http://all-in-one.maths.cam.ac.uk

Take Away Messages

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- The role of deep learning as a powerful image prior / regulariser for inverse problems
- Hybrid methods: rigorous mathematical methods with data-driven components
- Many open questions wrt generalisability/universality of learned regularisers, interpretability, uncertainty quantification etc.

Lunz, Öktem, CBS, Adversarial Regularizers in Inverse Problems, in NeurIPS 2018; Mukherjee, Dittmer, Shumaylov, Lunz, Öktem, CBS, arxiv 2020
Overview paper on data-driven inversion: Arridge, Maass, Öktem, CBS, Acta Numerica 2019.

Thank you very much for your attention!

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