Bilevel Learning for Inverse Problems

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Joint work with:

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The Leverhulme Trust

Engineering and Physical Sciences Research Council

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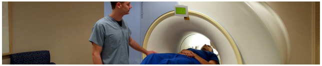
Outline

1) Motivation



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

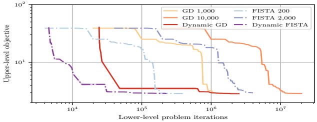
$$\min_{x,y} f(x,y)$$

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

2) Efficient solution?

Yes, e.g. inexact DFO algorithms

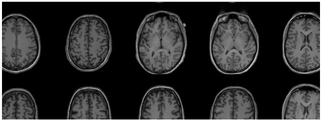
Ehrhardt and Roberts JMIV '21



3) High-dimensional learning?

Yes, e.g. learn MRI sampling

Sherry et al. IEEE TMI '20



Inverse problems and Variational Regularization

$$Ax = y$$

- x : desired solution
- y : observed data
- A : mathematical model

Goal: recover x given y

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x : desired solution

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Goal: recover x given y

Variational regularization

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, stability

$\lambda \geq 0$ **regularization parameter**: weights data and regularizer

Scherzer et al. '08, Ito and Jin '15, Benning and Burger '18

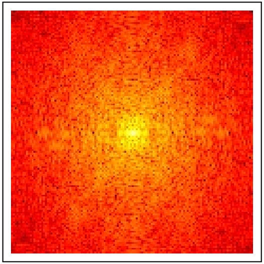
Example: Magnetic Resonance Imaging (MRI)

MRI Reconstruction Lustig et al. '07

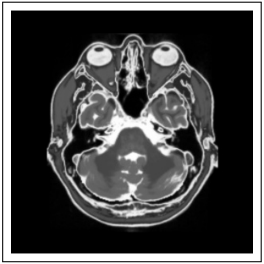
Fourier transform F, sampling $Sw = (w_i)_{i\in\Omega}$

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

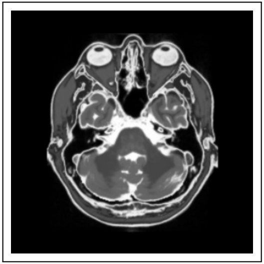
MRI scanner



sampling S^*y



$\lambda = 0$



$\lambda = 1$

Example: Magnetic Resonance Imaging (MRI)

MRI Reconstruction Lustig et al. '07

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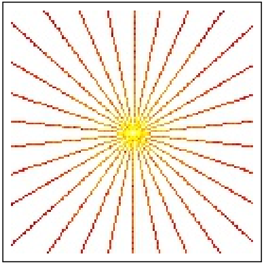
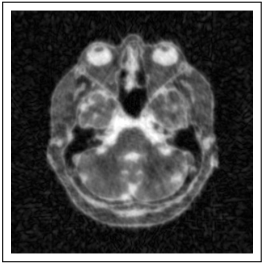
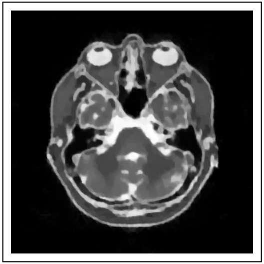


sampling S^*y



$\lambda = 0$



$\lambda = 10^{-4}$

Example: Magnetic Resonance Imaging (MRI)

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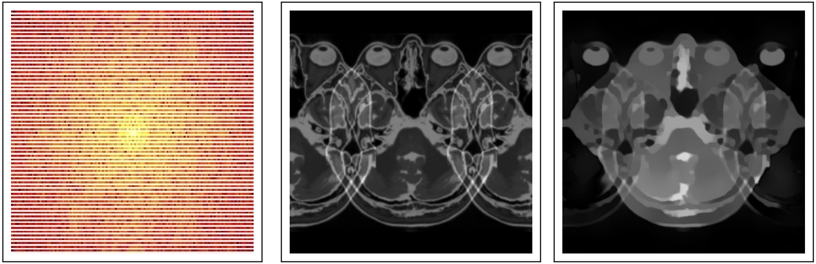
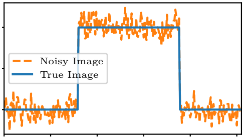


sampling $S^* y$ | $\lambda = 0$ | $\lambda = 10^{-3}$

How to choose the sampling Ω? Should it depend on $\mathcal{R}$ and λ?

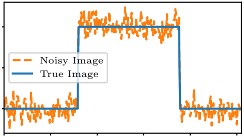
More "complicated" regularizers

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



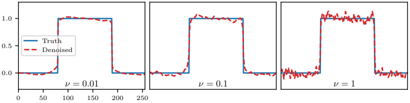
More "complicated" regularizers

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

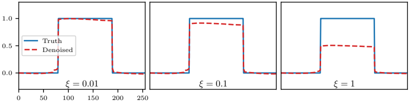


- Smooth and strongly convex
- Solution depends on choices of α, ν and ξ

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



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



How to choose all these parameters?

Motivation

- Solve inverse problems via **variational regularization**
- **Many parameters**
  - Low level: regularization parameter, smoothness, strong convexity, ...
  - High level: sampling, regularizer, ...
- Some parameters have underlying theory and heuristics but generally **difficult to choose** in practice

Bilevel learning for inverse problems

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

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

Lower level (solve inverse problem):

$$\hat{x} \in \arg\min_z \{\mathcal{D}(Az, y) + \lambda \mathcal{R}(z)\}$$

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

Bilevel learning for inverse problems

Upper level (learning):

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

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

Lower level (solve inverse problem):

$$\hat{x}_i \in \arg\min_z \{\mathcal{D}(Az, y_i) + \lambda \mathcal{R}(z)\}$$

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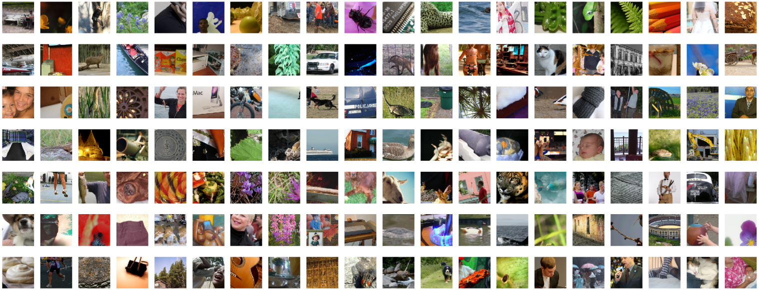

Inexact Algorithms for Bilevel Learning

Bilevel learning: Reduced formulation

Upper level:

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

Lower level:

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

Bilevel learning: Reduced formulation

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

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

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

Bilevel learning: Reduced formulation

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

Lower level:
$$\hat{x}(\lambda) := \hat{x} = \arg\min_z L(z, \lambda)$$

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

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

$$\nabla \tilde{U}(\lambda) = (\hat{x}'(\lambda))^* \nabla U(\hat{x}(\lambda)) = -A^* w$$

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

Algorithm for Bilevel learning

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

- Compute gradients: Given λ
  (1) Compute $\hat{x}(\lambda)$, e.g. via PDHG Chambolle and Pock '11
  (2) Solve $Bw = \nabla U(\hat{x}(\lambda))$, $B := \partial_x^2 L(\hat{x}(\lambda), \lambda)$ e.g. via CG
  (3) Compute $\nabla \tilde{U}(\lambda) = -A^* w$, $A := \partial_\lambda \partial_x L(\hat{x}(\lambda), \lambda)$
- Solve reduced formulation via L-BFGS-B Nocedal and Wright '00

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This approach has a number of problems:

- $\hat{x}(\lambda)$ has to be computed
- Derivative assumes $\hat{x}(\lambda)$ 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 problem by finite number of iterations of algorithms: not bilevel anymore Ochs et al. '15

Use algorithm that acknowledges difficulties:
e.g. inexact DFO Ehrhardt and Roberts '21

Lindon Roberts

Dynamic Accuracy Derivative Free Optimization

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

Key idea: Use f_ϵ:

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

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

E.g. if

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

then

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

Dynamic Accuracy Derivative Free Optimization

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

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

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

Algorithm 1 Dynamic accuracy DFO algorithm for (22).

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

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

Select an arbitrary interpolation set and construct m^0 (26).
for $k = 0, 1, 2, \dots$ **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 $i = 0, 1, 2, \dots$, find m^k and Δ^k such that m^k is fully linear in $B(\theta^k, \Delta^k)$ and $\Delta^k \leq \|g^k\|$. *[criticality phase]*
    end if
    Calculate s^k by (approximately) solving (27).
  until the accuracy in the evaluation of $\widetilde{f}(\theta^k)$ satisfies (32) with η_1' *[accuracy phase]*
  Evaluate $\widetilde{r}(\theta^k + s^k)$ so that (32) is satisfied with η_1' for $\widetilde{f}(\theta^k + s^k)$, and calculate $\widetilde{\rho}^k$ (29).
  Set θ^{k+1} and Δ^{k+1} as:

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

and

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

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

Theorem Ehrhardt and Roberts '21

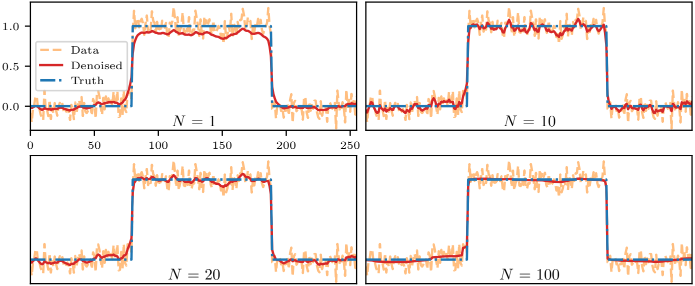
If f is sufficiently smooth and bounded below, then the algorithm is globally convergent in the sense that

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

Denoising (learn α, ν and ξ) Ehrhardt and Roberts '21

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

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



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

Robustness to initialization etc

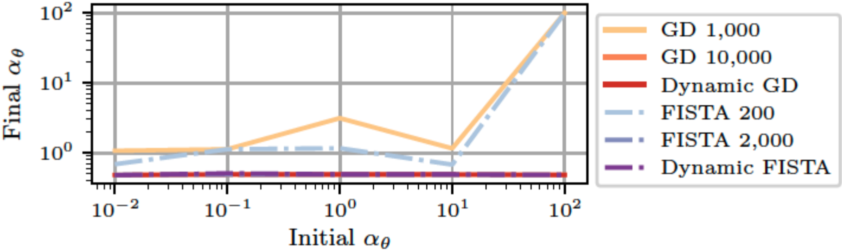
Compare:

- proposed dynamic accuracy approach Ehrhardt and Roberts '21
- unrolling: lower-level solution $\approx$ fixed number of iterations Ochs et al. '15

Robustness to initialization etc

Compare:

- proposed dynamic accuracy approach Ehrhardt and Roberts '21
- unrolling: lower-level solution ≈ fixed number of iterations Ochs et al. '15

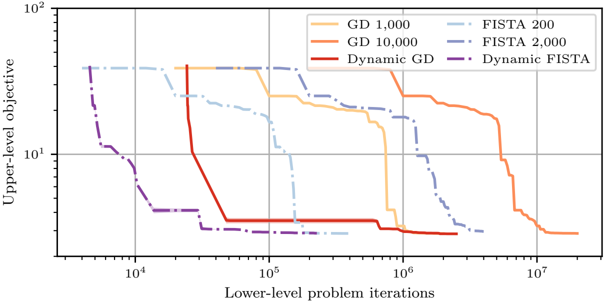


- unrolling not robust to number of iterations
- unrolling with large number of iterations and dynamic accuracy are robust to initialization

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. '16'



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

Dynamic accuracy is faster: 10x speedup

Learn sampling pattern in MRI

Learn sampling pattern in MRI

Ferdia Sherry

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

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

Lower level (MRI reconstruction):

$$\hat{x}_i(\lambda, s) = \arg\min_z \left\{ \sum_{j=1}^{N} s_j^2 |(Fz - y_i)_j|^2 + \lambda \mathcal{R}(z) \right\} \quad s_j \in \{0,1\}$$

Sherry et al. '20

Learn sampling pattern in MRI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Lower level (MRI reconstruction):

$$\hat{x}_i(\lambda, s) = \arg\min_z \left\{ \sum_{j=1}^N s_j^2 |(Fz - y_i)_j|^2 + \lambda \mathcal{R}(z) \right\} \quad s_j \in [0, 1]$$

Sherry et al. '20

Warm up

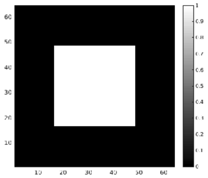
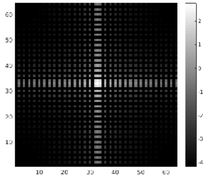
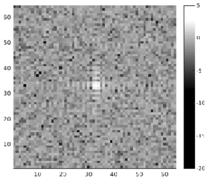


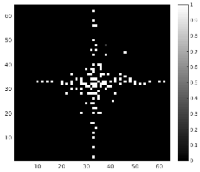
Figure: Discrete 2d bump



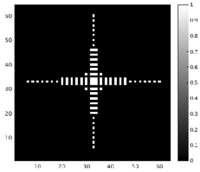
(a) Original data: $\log |y|$



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



(c) Learned sampling pattern



(d) Largest 2.76% Fourier Coefficients

Warm up

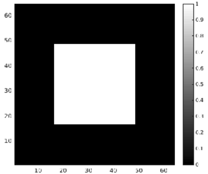
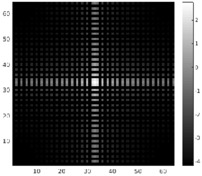


Figure: Discrete 2d bump



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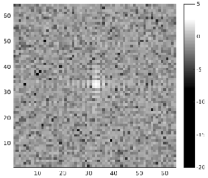

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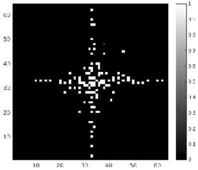
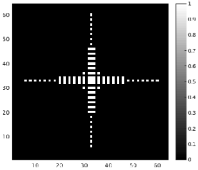


(c) Learned sampling pattern



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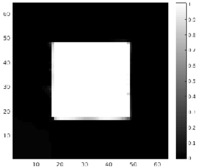
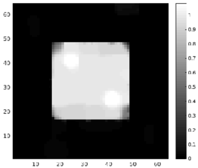
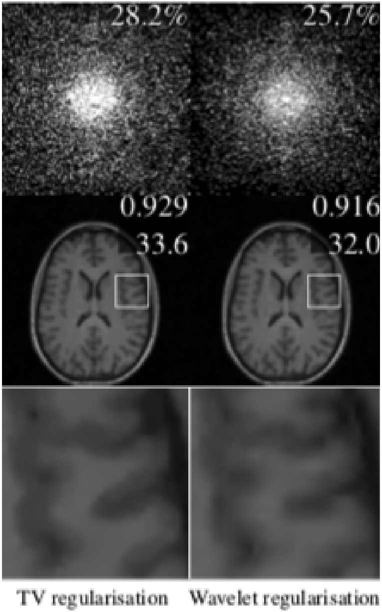


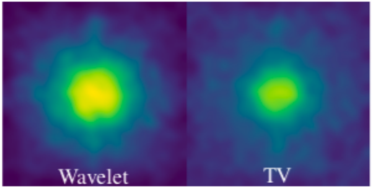
(e) Learned sampling pattern

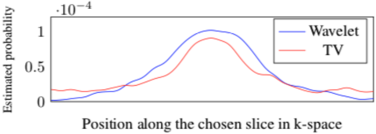


(f) Largest 2.76% Fourier Coefficients

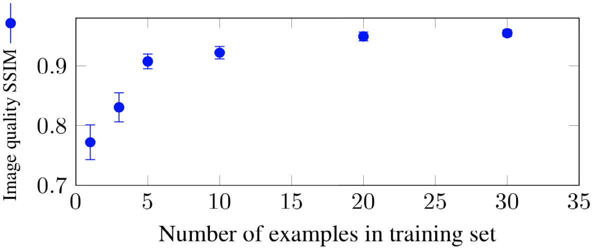
Compare regularizers Sherry et al. '20



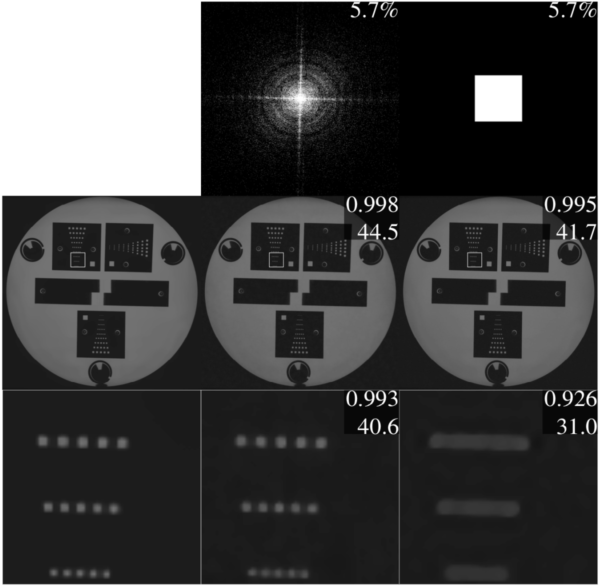




More insights: sampling and number of data Sherry et al. '20



High resolution imaging: 1024^2 Sherry et al. '20



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PostDoc Vacancy
$\approx$ 3 year position, starting in September 2022 or soon after
deadline tomorrow!

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