Regularization by architecture: A deep prior approach for inverse problems

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24.01.2019
Stockholm, Sweden

Paper:

https://export.arxiv.org/abs/1812.03889

Code:

https://github.com/otero-baguer/analytic-deep-prior

Outline

Section 1

Introduction

Preliminaries

Consider an operator $A : X \to Y$ between Hilbert spaces X and Y.

Inverse Problem (General task)

Given measured noisy data

$$y^\delta = Ax^\dagger + \tau, \tag{1}$$

obtain an approximation $\hat{x}$ for $x^\dagger$, where τ, with $\|\tau\| \leq \delta$, describes the noise in the measurement.

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Classical approach: Variational regularization

$$\hat{x}_\alpha = \arg\min \frac{1}{2}\|Ax - y^\delta\|^2 + \alpha\mathcal{R}(x) \tag{2}$$

Examples of hand-crafted priors:

- $\|x\|^2$
- $\|x\|_1$
- $TV(x)$

Remark: α selection

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Deep learning and inverse problems

- Primal-Dual reconstructions
- Learned gradient descent
- Learned post-processing: $\mathcal{F}_\theta \circ A^\dagger$
- Learned regularizers: $\mathcal{R}_\theta$
- Learned priors and generative networks (GAN, VAE)

Drawbacks:

- Need a lot of data. How to get the ground-truths?
- Real data noise might be different from the one present on the training samples.

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Is it possible to solve inverse problems using deep learning without any training data?

Generative Networks

Let's consider a generative Neural Network $\varphi_W(z)$ previously trained.

- W is fixed after the training phase.
- We can obtain images by sampling $\mathbf{z}$.

For solving inverse problems:

- $\hat{z} = \arg\min_z \|\varphi_W(z) - y^\delta\|$
- $\hat{x} = \varphi_W(\hat{z})$

Can we obtain images by sampling $\mathbf{W}$ for a fixed z using the same network architecture (without training)?

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Section 2

Deep Image Prior (DIP)

Basic Idea[1]

Given measured noisy data

$$y^\delta = Ax^\dagger + \tau, \tag{3}$$

train a neural network $\varphi_W(z)$ with parameters W by minimizing the loss function

$$\|A\varphi_W(z) - y^\delta\|^2 \tag{4}$$

with respect to W, for a single fixed input z and output y^δ.

Then compute $\hat{x} = \varphi_W(z)$

[1] Dmitry Ulyanov, Andrea Vedaldi, and Victor S. Lempitsky. "Deep Image Prior". In: *CoRR* (2017). arXiv: 1711.10925.

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Some insights

- The network $\varphi_W(z)$ has a standard U-Net-like architecture.
- It has enough expressive power to reproduce some noise.
- Optimization method with early stopping plays an important role.
- Solving each instance requires training the network.
- It takes a lot of time.

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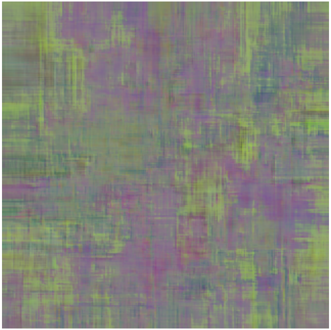
Example

(a) Data (y^δ)



(b) Iteration 0

Example

(a) Data (y^δ)

(b) Iteration 50

Example

(a) Data (y^δ)

(b) Iteration 100

Example

(a) Data (y^δ)

(b) Iteration 150

Example

(a) Data (y^δ)

(b) Iteration 200

Example

(a) Data (y^δ)

(b) Iteration 250

Example

(a) Data (y^δ)

(b) Iteration 300

Example

(a) Data (y^δ)

(b) Iteration 350

Example

(a) Data (y^δ)

(b) Iteration 400

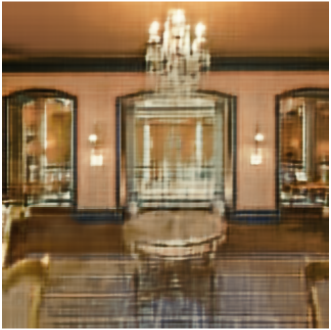
Example

(a) Data (y^δ)

(b) Iteration 450

Example

(a) Data (y^δ)



(b) Iteration 500

Example

(a) Data (y^δ)

(b) Iteration 550

Example

(a) Data (y^δ)

(b) Iteration 600

Example

(a) Data (y^δ)

(b) Iteration 650

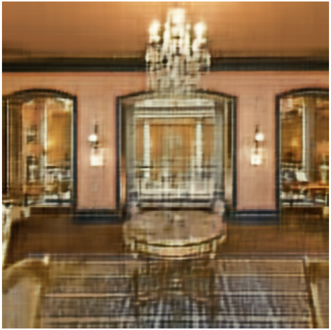
Example

(a) Data (y^δ)

(b) Iteration 700

Example

(a) Data (y^δ)



(b) Iteration 750

Example

(a) Data (y^δ)

(b) Iteration 800

Example

(a) Data (y^δ)

(b) Iteration 850

Example

(a) Data (y^δ)

(b) Iteration 900

Example

(a) Data (y^δ)

(b) Iteration 950

Example

(a) Data (y^δ)

(b) Iteration 1000

Example

(a) Data (y^δ)

(b) Iteration 1050

Example

(a) Data (y^δ)

(b) Iteration 1100

Example

(a) Data (y^δ)

(b) Iteration 1150

Example

(a) Data (y^δ)

(b) Iteration 1200

Example

(a) Data (y^δ)

(b) Iteration 1250

Example

(a) Data (y^δ)

(b) Iteration 1300

Example

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(b) Iteration 1350

Example

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(b) Iteration 1400

Example

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Example

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Example

(a) Data (y^δ)

(b) Iteration 1550

Example

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Example

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(b) Iteration 1650

Example

(a) Data (y^δ)

(b) Iteration 1700

Example

(a) Data (y^δ)

(b) Iteration 1750

Example

(a) Data (y^δ)

(b) Iteration 1800

Example

(a) Data (y^δ)

(b) Iteration 1850

Example

(a) Data (y^δ)

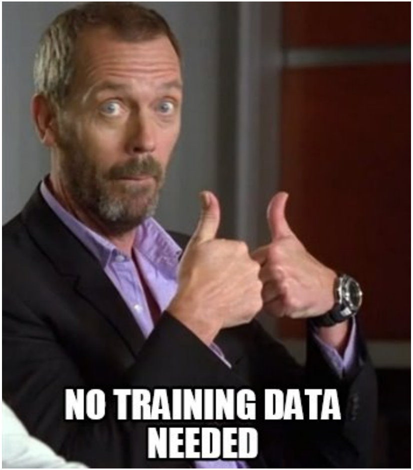
(b) Iteration 1900

DIP vs Global-Local GAN[2]

(a) Iteration 1900

(b) Global-Local GAN

[2] Satoshi Iizuka, Edgar Simo-Serra, and Hiroshi Ishikawa. "Globally and Locally Consistent Image Completion". In: *ACM Transactions on Graphics (Proc. of SIGGRAPH 2017)* 36.4 (2017).


NO TRAINING DATA
NEEDED

Section 3

Analytic Deep Prior

Trivial remark

Can the DIP approach be used to solve ill-posed inverse problems?

Consider a trivial network $\varphi_W(z) = W$, and that W corresponds to elements in X.

$\Longrightarrow$ The approximate solution to the inverse problem is given by $\hat{x} = \varphi_W(z) = W$.

$\Longrightarrow$ Minimizing $\|A\varphi_W(z) - y^\delta\|^2 = \|AW - y^\delta\|$ by gradient descent with respect to W is equivalent to the classical Landweber iteration.

$$\alpha \sim \frac{1}{n} \tag{5}$$

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Convex optimization reminder

In the variational approach we usually minimize:

$$J(x) = \frac{1}{2}\|Ax - y^\delta\|^2 + \alpha\mathcal{R}(x). \tag{6}$$

where $\mathcal{R}$ is convex but not differentiable.

The necessary first order condition for a minimizer is given by

$$0 \in A^*(Ax - y^\delta) + \alpha\partial\mathcal{R}(x) \tag{7}$$

$$x \in x + \lambda A^*(Ax - y^\delta) + \lambda\alpha\partial\mathcal{R}(x) \tag{8}$$

$$x - \lambda A^*(Ax - y^\delta) \in x + \lambda\alpha\partial\mathcal{R}(x). \tag{9}$$

which is equivalent to

$$\operatorname*{Prox}_{\lambda\alpha\mathcal{R}}\left(x - \lambda A^*(Ax - y^\delta)\right) = x. \tag{10}$$

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Turning the fixed point condition into an iteration scheme yields

$$\begin{aligned} x^{k+1} &= \operatorname*{Prox}_{\lambda\alpha\mathcal{R}}\left(x^k - \lambda A^*(Ax^k - y^\delta)\right) && (11)\\ &= \operatorname*{Prox}_{\lambda\alpha\mathcal{R}}\left((I - \lambda A^*A)x^k + \lambda A^* y^\delta\right) \ . && (12) \end{aligned}$$

Rewriting $W = I - \lambda A^*A$, $b = \lambda A^*$ and $\phi(\cdot) = \mathrm{Prox}_{\lambda\alpha\mathcal{R}}(\cdot)$ yields

$$x^{k+1} = \phi\left(Wx^k + b\right) \tag{13}$$

Convex optimization reminder

Example

Consider $\mathcal{R}(x) = I_+(x)$ (indicator function for non-negative numbers)

$$\operatorname*{Prox}_{\lambda\alpha\mathcal{R}}(x) = \mathbf{ReLu}(x) \tag{14}$$

The iteration scheme $x^{k+1} = \phi\left(Wx^k + b\right)$ is quite similar to a Neural Network.

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Analytic Deep Prior

Now we consider the particular architecture of a fully connected feed-forward iterative network with L identical layers

$$\varphi_W(z) = x^L, \tag{15}$$

where

$$x^{k+1} = \phi\left(Wx^k + b\right) \tag{16}$$

for $k = 0, .., L-1$ and $x^0 = z$.

- ϕ is the proximal mapping of a regularizing functional $\lambda\alpha R$
- W is such that $I - W = \lambda B^* B$ for some B
- $b = \lambda B^* y^\delta$

Analytic Deep Prior

In this setting, $\varphi_W(z)$ is identical to the L-th iterate of the PG method for minimizing

$$J_B(x) = \frac{1}{2}\|Bx - y^\delta\|^2 + \alpha\mathcal{R}(x), \tag{17}$$

If $\varphi_W(z) = x(B) = \arg\min\ J_B(x)$: Updating W, i.e. B, changes the discrepancy term in the Tikhonov functional.

Definition

We call this setting an **analytic deep prior** if B is trained from a single data point y^δ by gradient descent applied to

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Training/Optimization

The training of B for given data y^δ is achieved by a gradient descent method applied to

$$F(B) = \frac{1}{2}\|Ax(B) - y^\delta\|^2 \tag{19}$$

$$\text{s.t.} \quad x(B) = \arg\min_x \; J_B(x). \tag{20}$$

The stationary points are characterized by $\partial F(B) = 0$ and gradient descent iterations with stepsize η are given by

$$B^{\ell+1} = B^\ell - \eta \partial F(B^\ell). \tag{21}$$

Hence we need to compute the derivative of F with respect to B.

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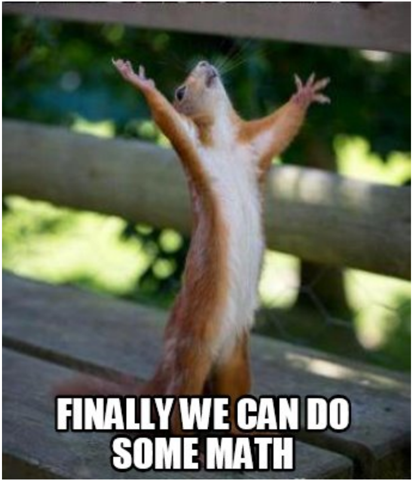
FINALLY WE CAN DO
SOME MATH

Example

Consider $\mathcal{R}(x) = \frac{1}{2}\|x\|^2$.

In this case $x(B) = \arg\min J_B(x) = (B^*B + \alpha I)^{-1}B^*y^\delta$.

For illustration we consider the rather unrealistic case $x^\dagger = u$, where u is a singular function of A ($Au = \sigma v$)

$$y^\delta = Au + \delta v = (\sigma + \delta)v \tag{22}$$

A lengthy computation exploiting $B^0 = A$ and $\beta_0 = \sigma$ shows that

$$B^{\ell+1} = B^\ell - c_\ell v u^* \tag{23}$$

Implementation

Goal: Find optimal B, to minimize the loss function

$$\frac{1}{2}\|Ax(B) - y^\delta\|^2 \tag{24}$$

Equivalent to train the network $\varphi_W(z)$ for the single data point (z, y^δ) updating B by back-propagation.

How many layers should the network have in order to ensure that $\varphi_W(z) = x(B) = \arg\min J_B$?

Thousands of layers! (slow convergence of the PG method).

Prohibitive!

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Solution:

- Consider only a reduced network with a small number, $L = 10$, of layers
- Set the input to be the network's output after the previous iteration.

Figure: The implicit network with $(k+1)L$ layers. Here $\varphi^L_{W_k}$ refers to a block of L identical fully connected layers with weights $W_k = I - \lambda B_k^T B_k$ and $b_k = \lambda B_k^T y^\delta$.

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$$z \to \underbrace{\boxed{\varphi^L_{W_0}} \to \boxed{\varphi^L_{W_1}} \to \boxed{\varphi^L_{W_2}} \to \cdots \to \boxed{\varphi^L_{W_k}}}_{k+1} \to x_k$$

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Section 4

Academic Example

Setup

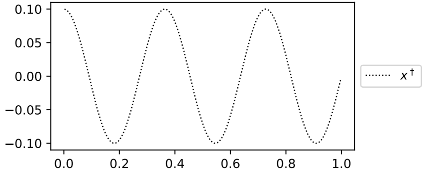
Consider the integration operator $A: \; L^2\left([0,1]\right) \; \rightarrow \; L^2\left([0,1]\right)$

$$(Ax)\left(t\right) = \int_0^t x(s)ds. \tag{25}$$

and

- $A_n \in \mathbb{R}^{n\times n}$: discretization of A.
- $x^\dagger \in \mathbb{R}^n$: one of the singular vectors u of A.
- $y^\delta = A_n x^\dagger + \tau$ with $\tau \sim \mathcal{N}(0, \sigma^2 \mathbb{1}_n)$

Ground-truth and data



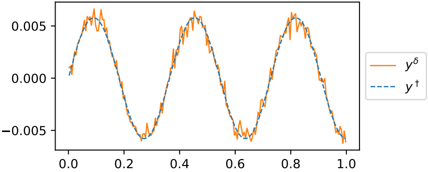
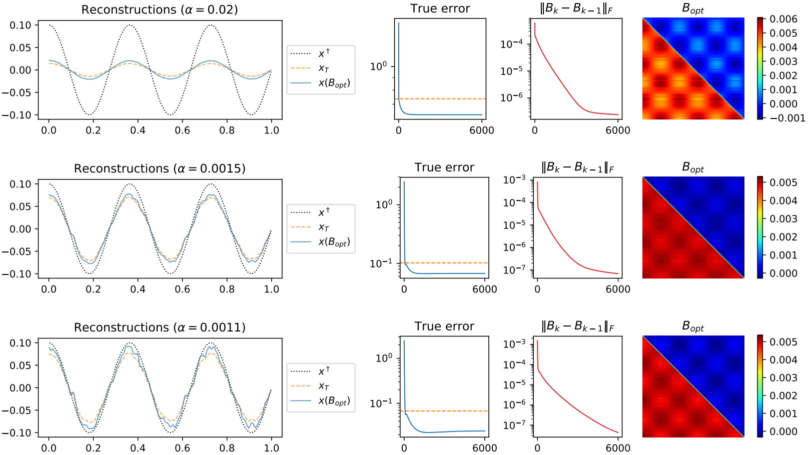


Figure: $x^\dagger = u_5$ and y^δ with $n = 200$ and 10% of noise.

Results $\left(R(\cdot) = \frac{1}{2}\|\cdot\|^2\right)$



Ground-truth and data

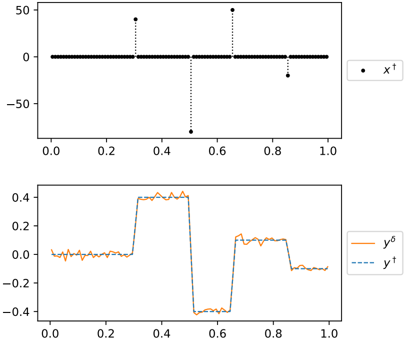
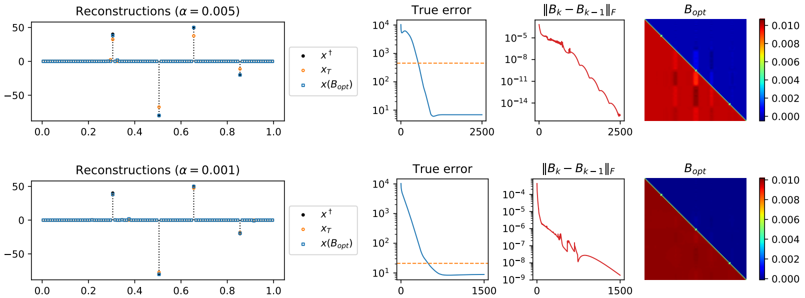


Figure: $x^\dagger$: sparse and y^δ with $n = 200$ and 10% of noise.

Results $(R(\cdot) = \|\cdot\|_1)$



Network convergence

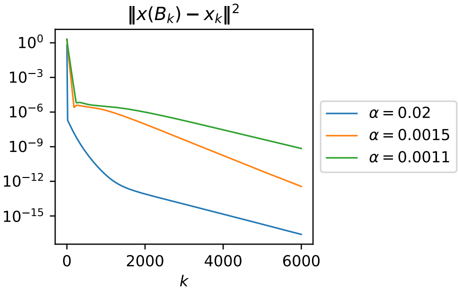
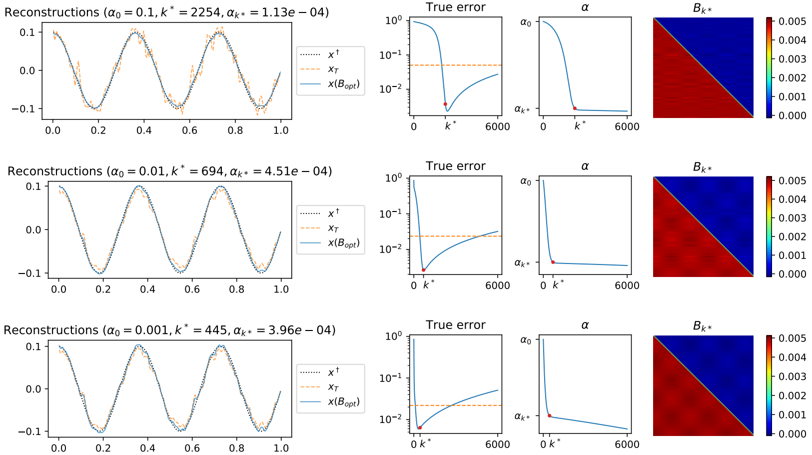


Figure: Difference between x_k and $x(B_k)$ after each training iteration k.

Results (adaptive α)



DFG Universität Bremen

Section 5

Magnetic Particle Imaging (MPI)

What is MPI?

Imaging modality based on injecting ferromagnetic nanoparticles which are consequently transported by the blood flow.

Goal: Measure the 3-D location and concentration of the nanoparticles.

Advantages:

- High spacial resolution (< 1mm)
- Measurement time (< 0.1 s)
- No harmful radiation

Figure: Magnetic particles developed in Lübeck

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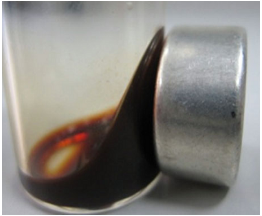

Figure: Magnetic particles developed in Lübeck

How it works?

- A magnetic field is applied, which is a superposition of:
  - static gradient field, which generates a field-free-point (FFP)
  - highly dynamic spatially homogeneous field, which moves the FFP in space.
- Mean magnetic moment of the nanoparticles in the neighborhood of the FFP generates an electro-magnetic field.
- Voltages are measured by so-called receive coils.
- The time-dependent measurements $v_\ell(t)$ in the receive coils constitute the data for reconstructing $c(x)$.

Inverse Problem

Linear Fredholm integral equation of the first kind describes the forward operator.

- Precisely modeling MPI is still an unsolved problem[3].
- The integral kernel is commonly determined in a time-consuming calibration procedure.

After discretization we end up with a linear system:

$$Sc = v \tag{26}$$

Goal: Reconstruct c from measured noisy data $v^\delta = Sc + \tau$.

[3] Tobias Kluth, Bangti Jin, and Guanglian Li. "On the degree of ill-posedness of multi-dimensional magnetic particle imaging". In: *Inverse Problems* 34.9 (2018).

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Experimental setup

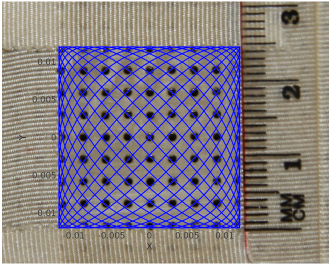
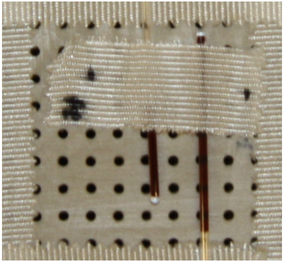


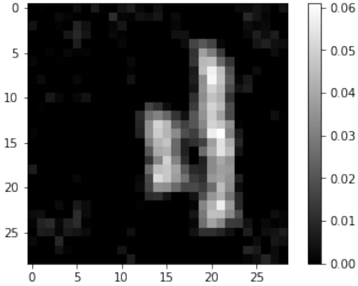
Figure: Used experimental platform with the FFP trajectory in blue. [4]

[4] Photo taken at University Medical Center Hamburg-Eppendorf by T. Kluth.

Results

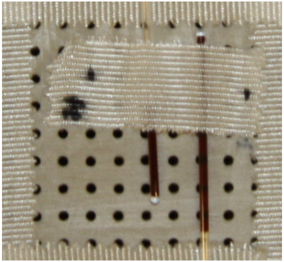


(a) Phantom (4mm)



(b) Kacmarz reconstruction ($\alpha = 5 \cdot 10^{-4}$)

Results



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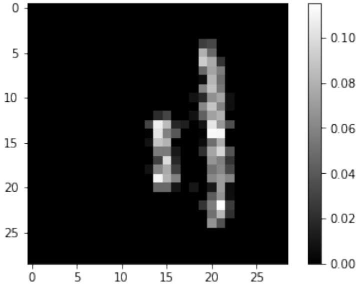
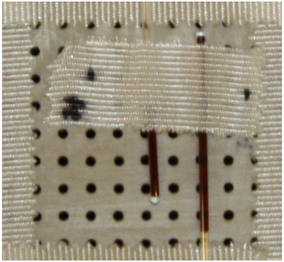


(b) l_1 reconstruction ($\alpha = 5 \cdot 10^{-3}$)

Results



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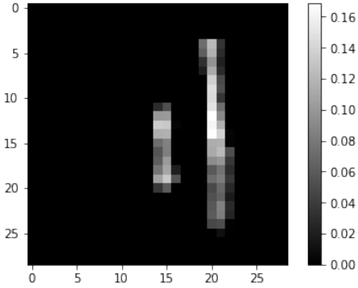
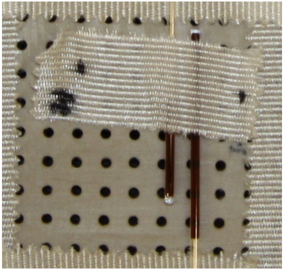
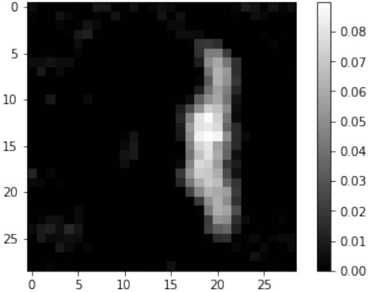


(b) DIP reconstruction ($lr = 5 \cdot 10^{-5}$)

Results

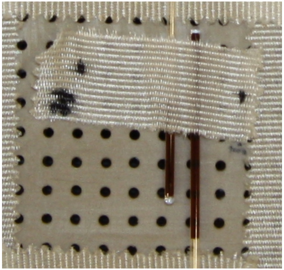


(a) Phantom (2mm)



(b) Kacmarz reconstruction ($\alpha = 5 \cdot 10^{-4}$)

Results



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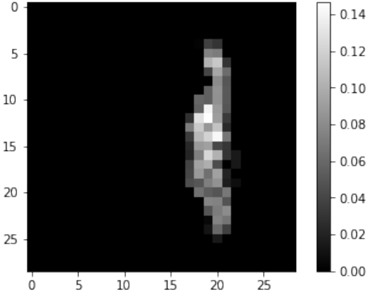

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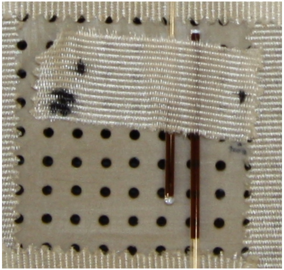
Results



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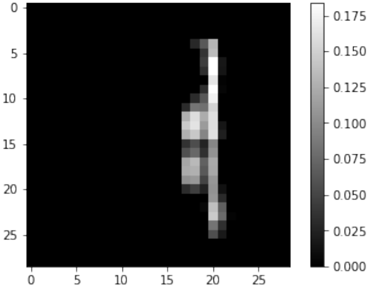

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Thanks!