Physikalisch-Technische Bundesanstalt
Braunschweig and Berlin
National Metrology Institute

Data-Driven Regularization Methods in Imaging

Thematic Einstein Semester on

Mathematics of Imaging in Real-World Challenges

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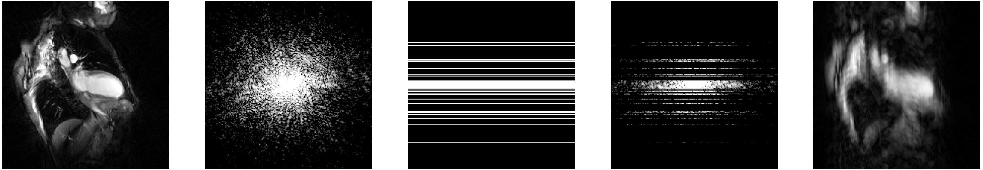
Problem: Measurements are **incomplete**.



$\mathbf{x}$	$\mathbf{y} := \mathbf{F}\mathbf{x}$	$\mathbf{S}_I$	$\mathbf{y}_I := (\mathbf{S}_I \circ \mathbf{F})\mathbf{x}$	$\mathbf{x}_I := \mathbf{F}_I^{\mathsf{H}}\mathbf{y}_I$
unknown image	fully-sampled k-space data (Cartesian)	binary mask	undersampled k-space data	initial reconstruction, $R \approx 8$

$\rightarrow$ scanning time $\sim \frac{1}{R}$

Machine Learning/Data-Driven Regularization

Regularization in the form of penalty terms:

$$F_{\mathcal{R}}(\mathbf{x}) = D(\mathbf{A}\mathbf{x}, \mathbf{y}) + \mathcal{R}(\mathbf{x}) \to \min_{\mathbf{x}}!$$

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$\rightarrow$ What is a good choice for the regularization $\mathcal{R}(\mathbf{x})$?

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$$F_{\mathcal{R}}(\mathbf{x}) = D(\mathbf{A}\mathbf{x}, \mathbf{y}) + \mathcal{R}(\mathbf{x}) \rightarrow \min_{\mathbf{x}}!$$

$\rightarrow$ What is a good choice for the regularization $\mathcal{R}(\mathbf{x})$?

Main Idea:
Let $\mathcal{R}(\mathbf{x})$ be learned from data, i.e. $\mathcal{R}(\mathbf{x}) = \mathcal{R}_{\Theta}(\mathbf{x})$, where Θ is a set of trainable parameters.

Conventions, Dataset, Code, . . .

In the following:

$$\mathbf{F}_I\mathbf{x} + \mathbf{e} = \mathbf{y}_I,$$

- $\mathbf{x} \in \mathbb{C}^N$, $N = N_x \cdot N_y \cdot N_t$, $\mathbf{y} \in \mathbb{C}^M$ with $M < N$ (underdetermined system)
- $\mathbf{F}_I = \mathbf{S}_I\mathbf{F}$, where $\mathbf{S}_I$ binary mask, $I \subset J = \{1, \ldots, N\}$
- $\mathbf{x}_I := \mathbf{F}_I^{\mathsf{H}}$ - zero-filled reconstruction
- dynamic cardiac MRI
- Cartesian sampling grid
- single-coil

Neural Networks in a Nutshell - Neural Networks

A neural network with L layers is typically a function f_Θ of the form

$$f_\Theta = (\sigma_L \circ f^L_{\Theta_L}) \circ \ldots \circ (\sigma_1 \circ f^1_{\Theta_1}),$$

where $\Theta := \cup_{l=1}^L \Theta_l$ are called the weights.

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Training a network on a dataset of pairs $\mathcal{D} := \{(x_i, y_i)_{i=1}^{M}\}$ refers to finding a set of weights such that

$$\Theta^* \in \arg\min_{\Theta} \mathcal{L}(\Theta) \quad \text{with} \quad \mathcal{L}(\Theta) := \frac{1}{M} \sum_{i=1}^{M} l(f_\Theta(x_i), y_i),$$

where $l(\cdot,\cdot)$ is an appropriate **Loss-Function**, e.g. the L_2-error.

Neural Networks in a Nutshell - Training/Validation/Test Sets

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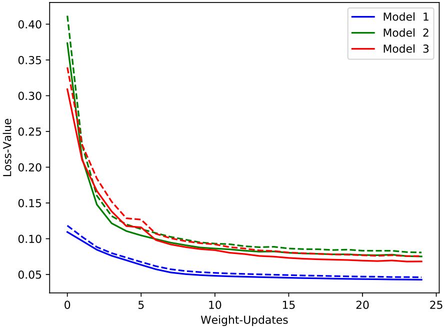
- Test Set: apply the model and report results

Remark: Never (EVER!) make decisions about the model on the test set!!

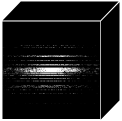
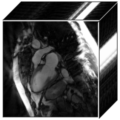


Types of Neural Networks for Image Reconstruction

Main different types of (supervised) NNs for image reconstruction

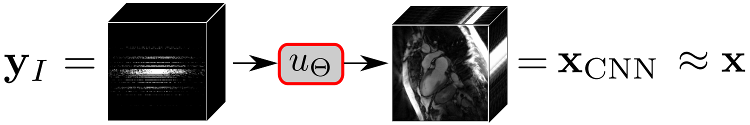
- Full inversion
- Post-Processing methods
- Decoupled methods
- Iterative/Cascaded networks

Learn the Full Inversion

$\mathbf{y}_I =$  $\longrightarrow \boxed{u_\Theta} \longrightarrow$  $= \mathbf{x}_{\mathrm{CNN}} \approx \mathbf{x}$

Idea: Learn to invert the forward model [13].

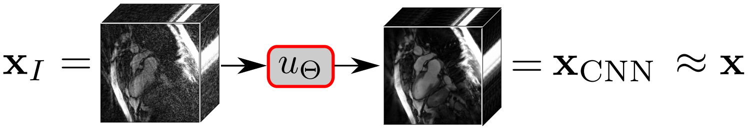
Learn the Full Inversion



Idea: Learn to invert the forward model [13].

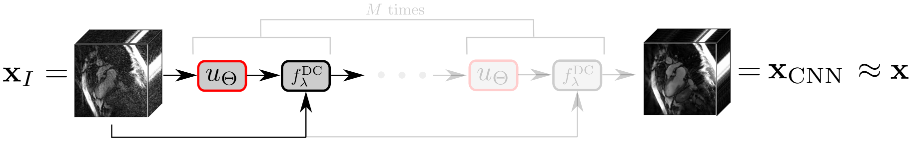
Remark: Typically, not recommended, as the physical model is (at least partially) known!

Post Processing



Idea: Train a network to reduce noise/artefacts from an initial image, see e.g. [6], [11], [3], [7].

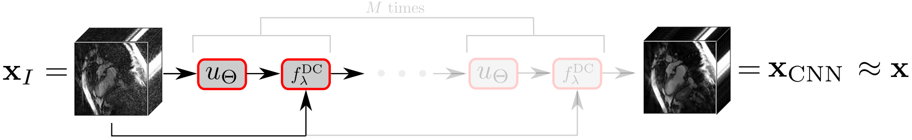
Decoupled Methods



Part of the network NOT Part of the network

u_Θ - Network f_λ^{DC} - Data-consistency block which contains $\mathbf{F}_I$, $\mathbf{F}_I^{\mathsf{H}}$

Idea: First learn, then reconstruct, e.g. [5], [4], [8].



Part of the network   NOT Part of the network

u_Θ - Network f_λ^{DC} - Data-consistency block which contains $\mathbf{F}_I$, $\mathbf{F}_I^{\mathsf{H}}$

Idea: Learn to reconstruct [1], [2], [12], [10], [9].

Outline

In this tutorial: **Iterative Neural Networks**

Consider the functional

$$\min_{\mathbf{x}} \frac{1}{2}\|\mathbf{F}_I\mathbf{x} - \mathbf{y}_I\|_2^2 + \frac{\lambda}{2}\|\mathbf{x}\|_2^2.$$

Tikhonov-Regularization

Consider the functional

$$\min_{\mathbf{x}} \frac{1}{2}\|\mathbf{F}_I\mathbf{x} - \mathbf{y}_I\|_2^2 + \frac{\lambda}{2}\|\mathbf{x}\|_2^2.$$

Calculate the derivative, set it to zero, re-arrange and obtain the system:

$$(\mathbf{F}_I^{\mathsf{H}}\mathbf{F}_I + \lambda\,\mathbf{I})\,\mathbf{x} = \mathbf{F}_I^{\mathsf{H}}\mathbf{y}_I,$$

which has a closed-form solution

$$\mathbf{x}^* = \mathbf{F}^{\mathsf{H}}\mathbf{M}\mathbf{F}\mathbf{x}_I,$$

where

$$\mathbf{M}_{k,k} = \begin{cases} 1/(1+\lambda) & \text{if } k \in I, \\ 1/\lambda & \text{if } k \notin I. \end{cases}$$

Generalized Tikhonov-Regularization

For some prior $\mathbf{x}_{\text{prior}}$, consider the functional

$$\min_{\mathbf{x}} \frac{1}{2}\|\mathbf{F}_I\mathbf{x} - \mathbf{y}_I\|_2^2 + \frac{\lambda}{2}\|\mathbf{x} - \mathbf{x}_{\text{prior}}\|_2^2.$$

Generalized Tikhonov-Regularization

For some prior $\color{red}{\mathbf{x}_{\text{prior}}}$, consider the functional

$$\min_{\mathbf{x}} \frac{1}{2}\|\mathbf{F}_I\mathbf{x} - \mathbf{y}_I\|_2^2 + \frac{\lambda}{2}\|\mathbf{x} - \color{red}{\mathbf{x}_{\text{prior}}}\|_2^2.$$

Calculate the derivative, set it to zero, re-arrange and obtain the system:

$$\left(\mathbf{F}_I^{\mathsf{H}}\mathbf{F}_I + \lambda\,\mathbf{I}\right)\mathbf{x} = \mathbf{F}_I^{\mathsf{H}}\mathbf{y}_I + \lambda\,\color{red}{\mathbf{x}_{\text{prior}}}$$

which has a closed-form solution

$$\mathbf{x}^* = \mathbf{F}^{\mathsf{H}}\left(\mathbf{\Lambda}\mathbf{F}\color{red}{\mathbf{x}_{\text{prior}}} + \frac{1}{1+\lambda}\mathbf{y}_I\right)$$

where

$$\mathbf{\Lambda}_{k,k} = \begin{cases} \lambda/(1+\lambda) & \text{if } k \in I, \\ 1 & \text{if } k \notin I. \end{cases}$$

Network Architecture

The network in [1] alternates between the following two steps for $1 \leq k \leq M$:

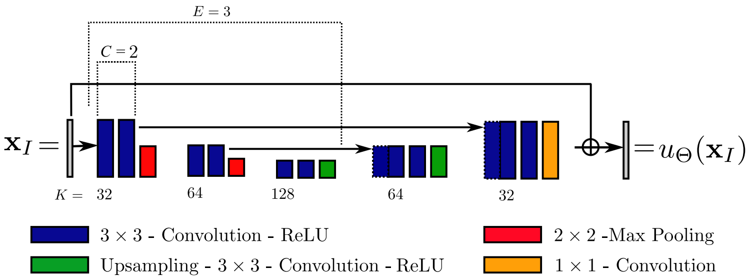
$$\begin{aligned} \mathbf{x}_{\mathrm{CNN}}^{k} &= u_{\Theta}(\mathbf{x}^{k}) \\ \mathbf{x}^{k+1} &= \arg\min_{\mathbf{x}} \|\mathbf{F}_{I}\mathbf{x} - \mathbf{y}_{I}\|_2^2 + \lambda \|\mathbf{x} - \mathbf{x}_{\mathrm{CNN}}^{k}\|_2^2 \end{aligned}$$

Network Architecture

The network in [1] alternates between the following two steps for $1 \leq k \leq M$:

$$
\begin{aligned}
\mathbf{x}_{\mathrm{CNN}}^{k} &= u_{\Theta}(\mathbf{x}^{k}) \\
\mathbf{x}^{k+1} &= \arg\min_{\mathbf{x}} \|\mathbf{F}_I \mathbf{x} - \mathbf{y}_I\|_2^2 + \lambda \|\mathbf{x} - \mathbf{x}_{\mathrm{CNN}}^{k}\|_2^2 \\
&= \mathbf{F}^{\mathsf{H}}(\boldsymbol{\Lambda}\mathbf{F}\mathbf{x}_{\mathrm{CNN}}^{k} + \frac{1}{1+\lambda}\mathbf{y}_I)
\end{aligned}
$$

with $\mathbf{x}^0 := \mathbf{F}_I^{\mathsf{H}}\mathbf{y}_I$ and $\boldsymbol{\Lambda}$ as before.



Hyper-parameters:

- E - number of encoding stages
- C - number of convolutional layers per stage
- K - initial number of filters

Let's begin! ;)

https://github.com/ckolbPTB/TES_21_22_Tutorials/

Questions:

- In the code `tutorial1_data_driven_reg_methods_apply_cnn_modl.ipynp`, try to vary the regularization parameter λ, the CNN-block for the MODL architecture, the length of the network, etc... What are your observations?
- Do the networks work for all different λ and different acceleration factors?
- Which of thee provided pre-trained networks seems to be better?
- Following the recipe on page 13 in this presentation, what would the data-consistency block look like for the following denoising problem

$$\min_{\mathbf{x}} \frac{1}{2}\|\mathbf{x} - \mathbf{y}_I\|_2^2 + \frac{\lambda}{2}\|\mathbf{x} - \mathbf{x}_{\text{prior}}\|_2^2\,?$$

Thank you for your attention.

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