Deep convolutional framelets: application to diffuse optical tomography

: learning based approach for inverse scattering problems

Jaejun Yoo

NAVER Clova ML

OUTLINE (bottom up!)

I. INTRODUCTION

II. EXPERIMENTS

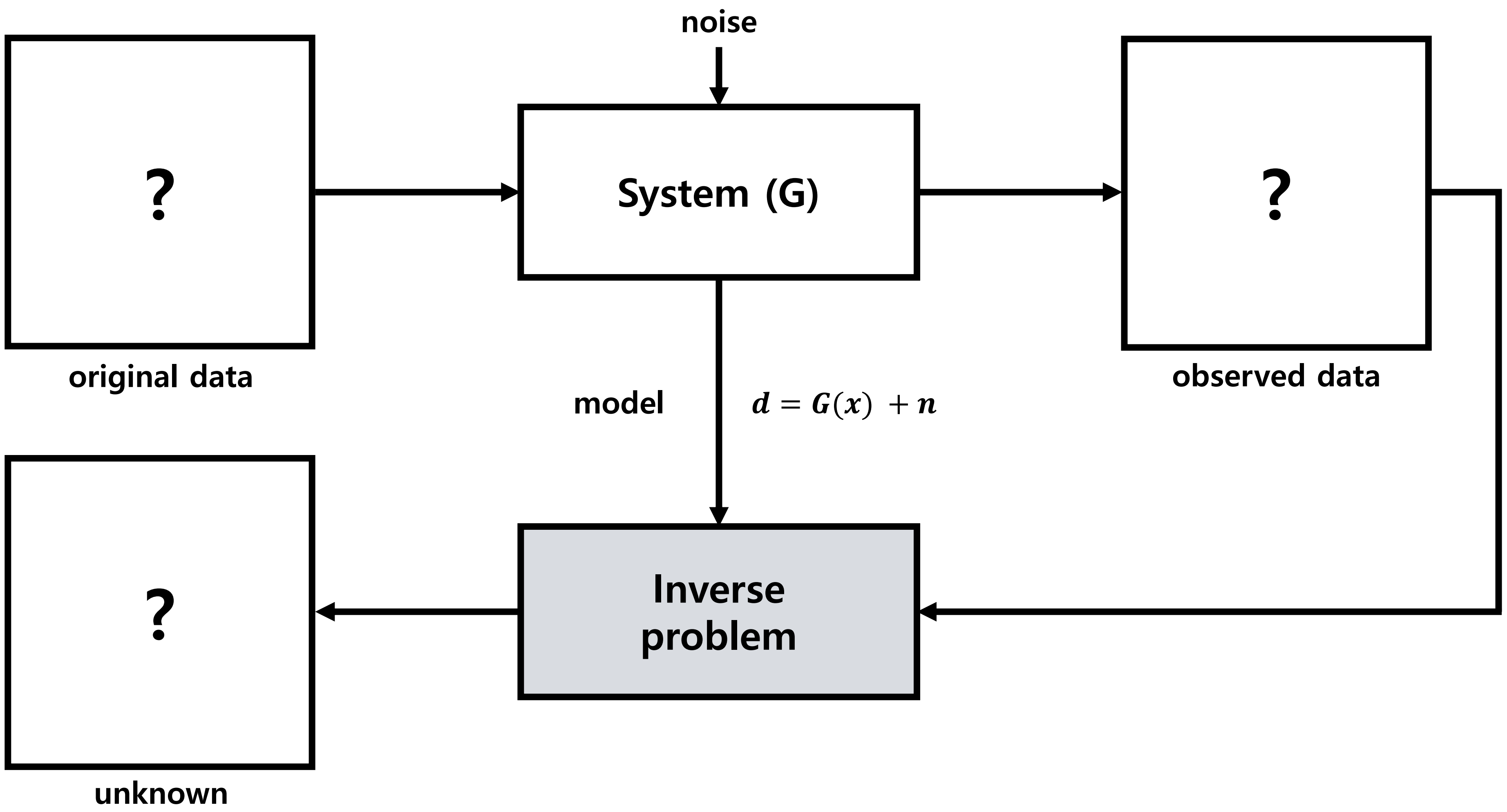
III. THEORY

- NETWORK DESIGN FRAMEWORK

IV. CONCLUSION

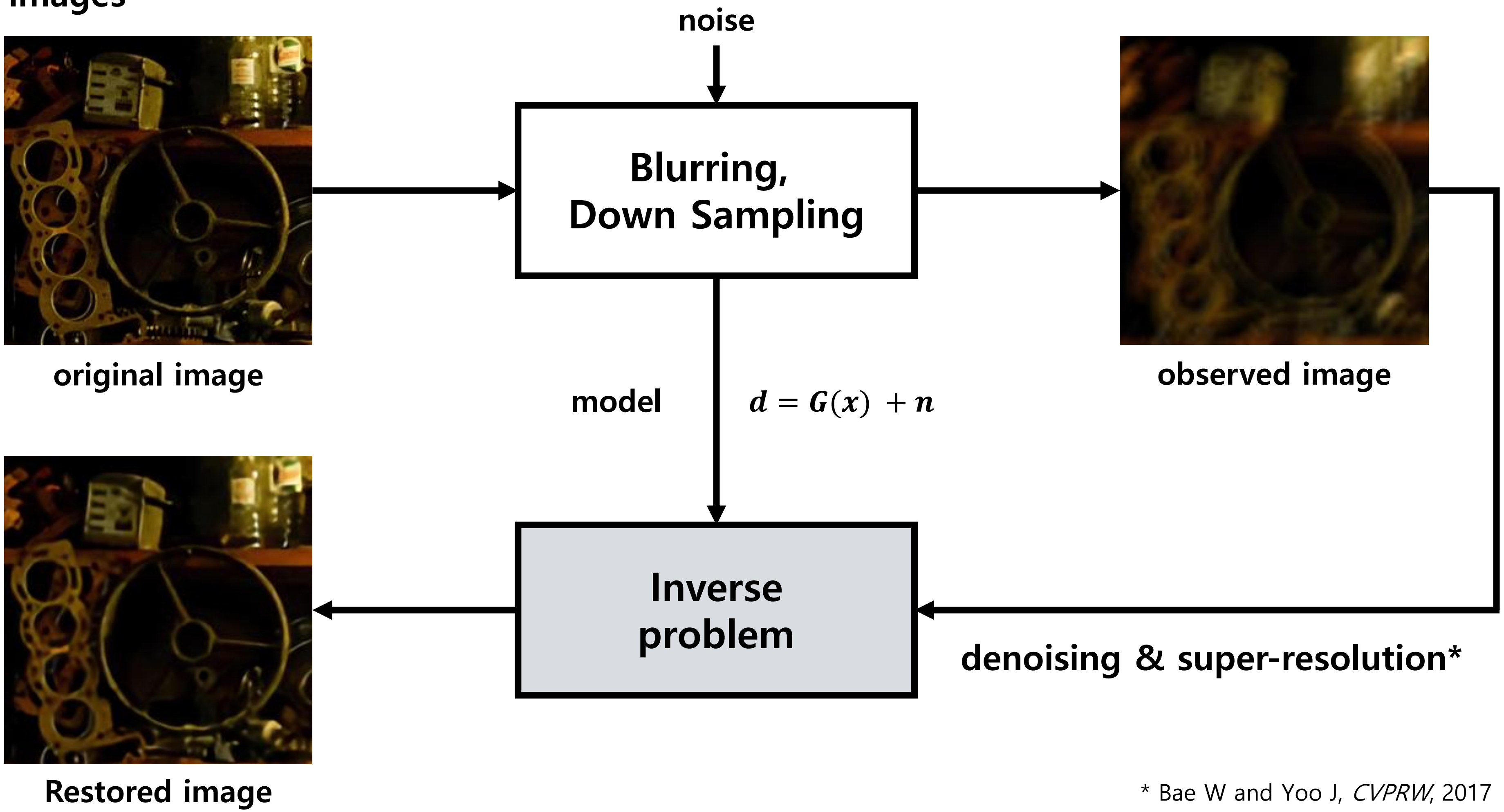
0. AGENDA SETUP

INVERSE PROBLEMS



INVERSE PROBLEMS

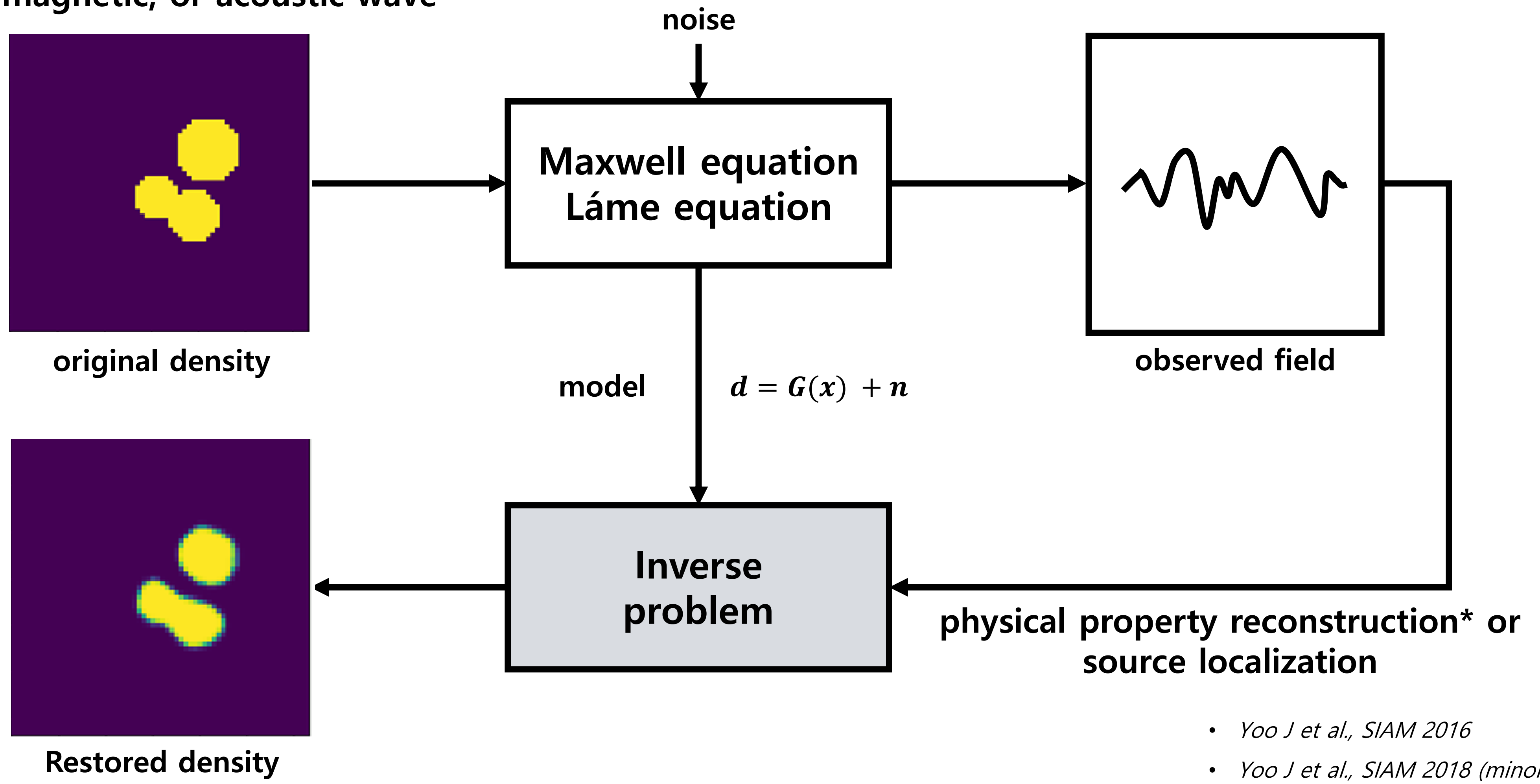
e.g. natural images



* Bae W and Yoo J, *CVPRW*, 2017

INVERSE PROBLEMS

e.g. electromagnetic, or acoustic wave



- *Yoo J et al., SIAM 2016*
- *Yoo J et al., SIAM 2018 (minor revision)*

INVERSE PROBLEMS

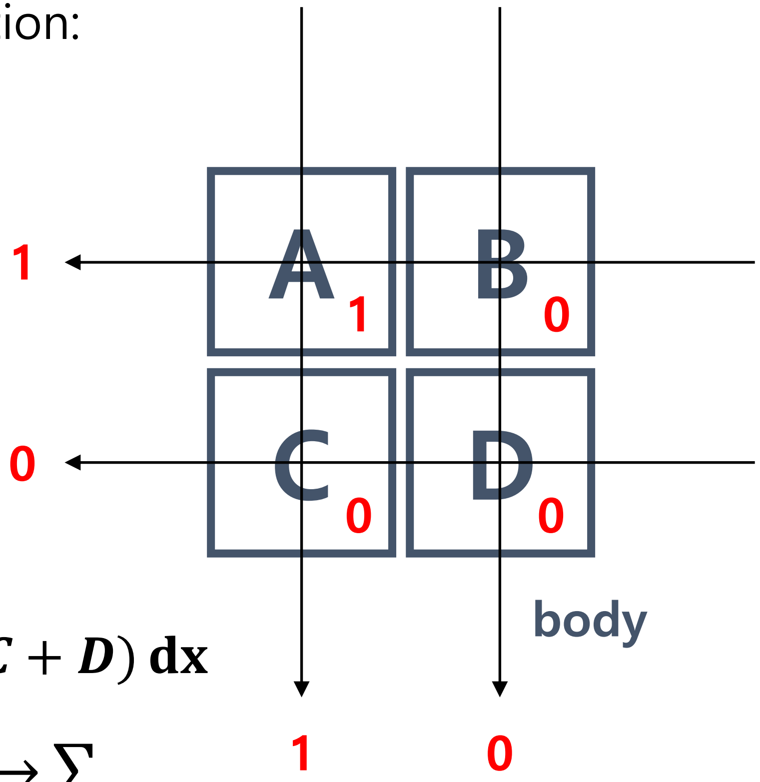
General statement of the problem

- To find the best model such that $\boldsymbol{d} = \boldsymbol{G}(\boldsymbol{x})$
- In linear system, e.g. **X-ray CT**, we minimize the following cost function:

$$\mathbf{d} = \mathbf{Gx}, \qquad \boldsymbol{\phi} = \|\boldsymbol{d} - \boldsymbol{Gx}\|_2^2$$

- In **signal processing** society:

$$\boldsymbol{Gx} = \begin{bmatrix} 1,0,1,0 \\ 0,1,0,1 \\ 1,1,0,0 \\ 0,0,1\ 1 \end{bmatrix} \begin{bmatrix} A \\ B \\ C \\ D \end{bmatrix}, \qquad \boldsymbol{rank}(\boldsymbol{G}) = 4$$



$$\int \boldsymbol{G}(\boldsymbol{C}+\boldsymbol{D})\,\mathbf{dx}$$

$$\boxed{\boldsymbol{well - posed\ problem}, \qquad \exists \boldsymbol{G}^{-1}}$$

$$\int \rightarrow \sum$$

more constraints, assumptions, regularization, iterative methods, etc.

INVERSE PROBLEMS

General statement of the problem

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$$\mathbf{d} = \mathbf{Gx}, \qquad \boldsymbol{\phi} = \|\boldsymbol{d} - \boldsymbol{Gx}\|_2^2$$

- In **machine learning** society:

$\rightarrow$ **CNN** $\rightarrow$

Conv, ReLU, pooling, etc.

$\boldsymbol{d}$ $\qquad$ $\widetilde{\boldsymbol{G}}^{\boldsymbol{T}}$, **where** $\widetilde{\boldsymbol{G}}^{\boldsymbol{T}}\boldsymbol{G} = \boldsymbol{I}$ $\qquad$ $\boldsymbol{x}$

AGENDA

Deep learning works extremely well… but why?

- Sometimes blind application of these techniques provides even better performance than mathematically driven classical signal processing approaches.
- The more we observe impressive empirical results in image reconstruction problems, the more unanswered questions we encounter:

  "Why convolution? Why do we need a pooling and unpooling in some architectures? etc."
- What is the link between the classical signal processing theory and deep learning?

Can deep learning go beyond?

- Would it be possible to train the network learn the complicated non-linear physics?
- How?

I. INTRODUCTION

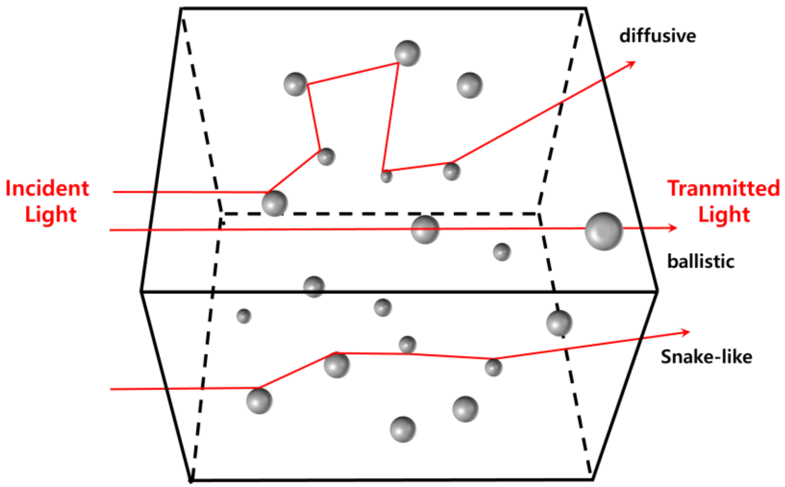
A. Inverse scattering problem (DOT)

B. What to solve? & How to solve?

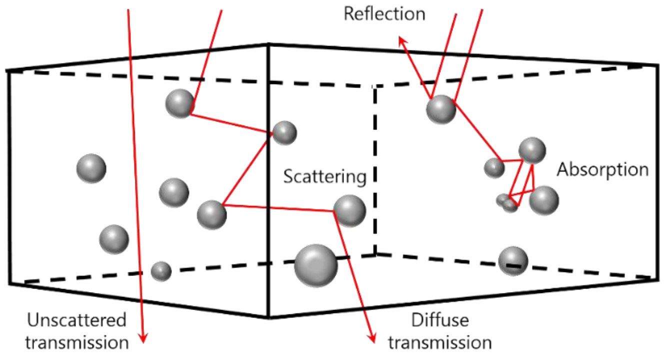
INVERSE SCATTERING PROBLEMS

Photon/Wave scattering in a turbid media (Very ***non-linear, ill-posed***)

- Trajectories/Interactions (absorption, scattering, reflection, etc.)
- Electromagnetic, Elastic, Optical, Acoustic waves : $\boldsymbol{d} = \boldsymbol{G}(\boldsymbol{x}) \leftarrow$ *more generalized model*



photon trajectories



Light interaction with matter

INVERSE SCATTERING PROBLEMS

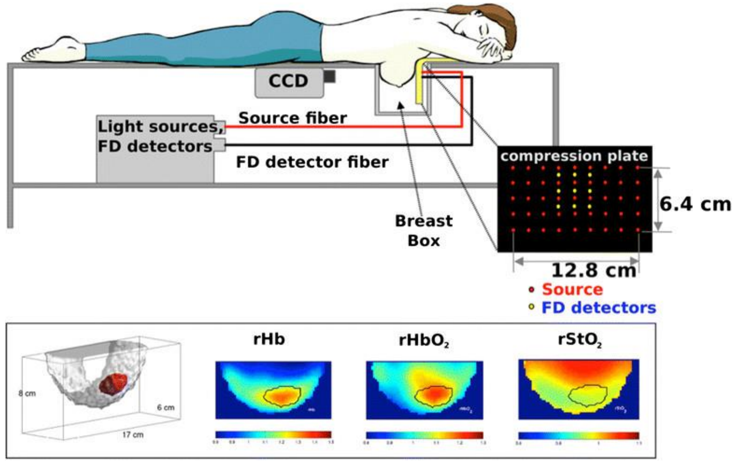
Inverse Scattering Problems in Medical Imaging

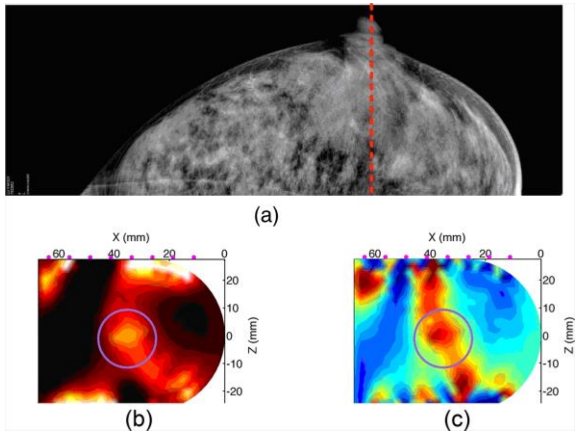
- Applications

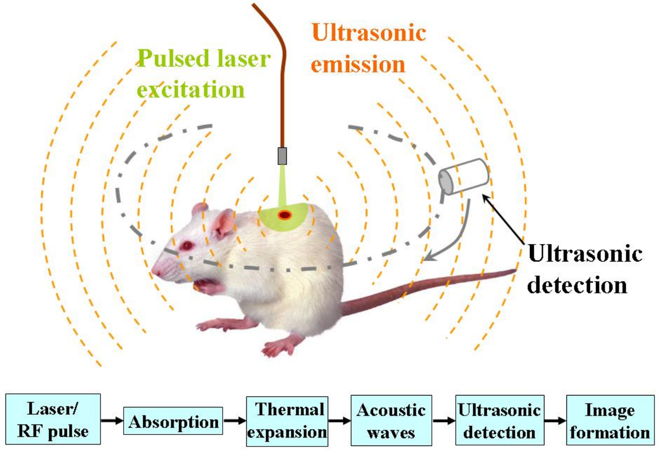
  Near Infra-Red (NIR), Ultrasound, Photo-acoustic, EEG, etc.

  Non-invasive, non-destructive examination

  Fast, cheap, and portable machine





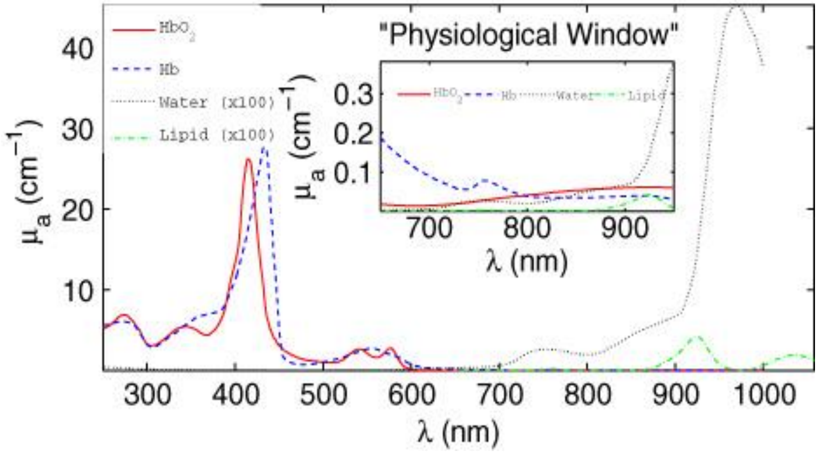


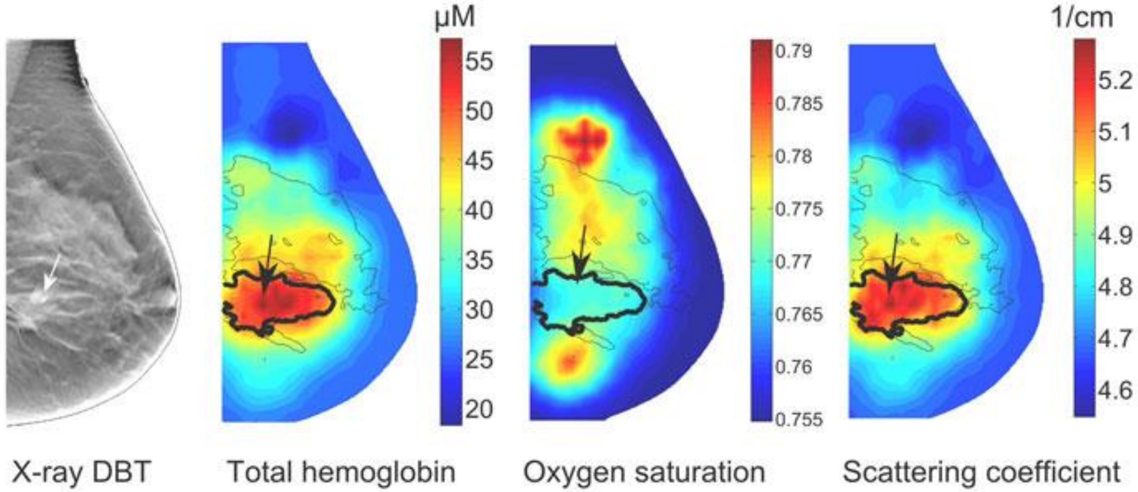
INVERSE SCATTERING PROBLEMS

Near-infrared (NIR, ~650-950 nm)

Near-infrared light can travel deep in tissue, as a result of the relatively small absorption of water and hemoglobin.

*** Durduran et al., MICCAI, 2010**



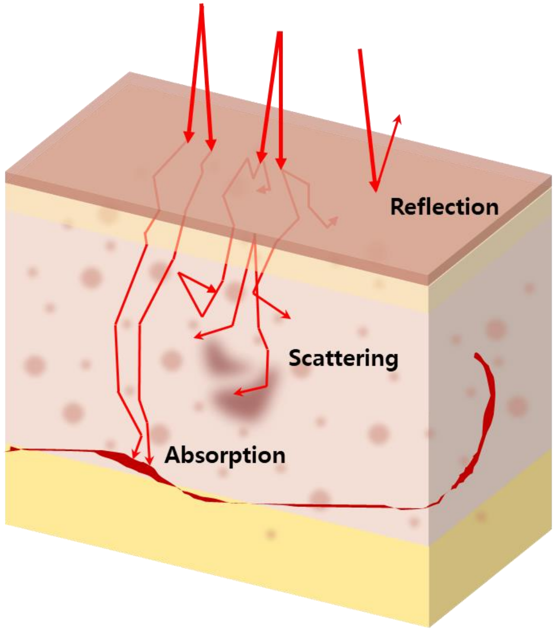


The goal of DOT is to reconstruct the spatial distribution of optical/physiological properties at each point (or volume element) in the tissue from measurements of fluence rate on the tissue surface.

INVERSE SCATTERING PROBLEMS

Lipmann-Schwinger Equation

- Mapping between the 3D distribution of optical properties f and the measurements g



1) 광센서로부터 광학 계수 분포 f 에 대한 측정 데이터 g를 얻습니다.

$$g := u_m^s(\mathbf{x}) = \mathcal{M}_m[f](\mathbf{x})$$

$$f = \mathcal{T} g$$

3D distribution $f \rightarrow$ Measurement g

(f comes from a smoothly varying perturbation $\delta\mu$)

3D distribution f → Measurement g

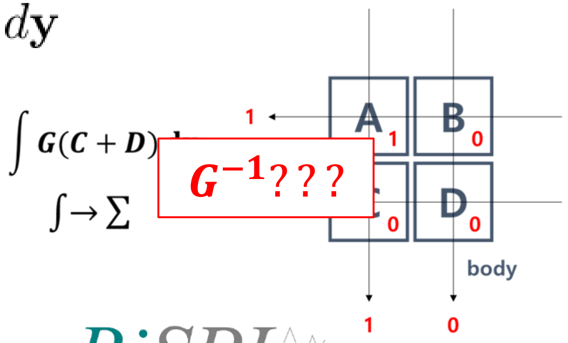
(f comes from a smoothly varying perturbation $\delta\mu$)

2) 이 때, 둘 사이의 관계는 적분 방정식으로 표현할 수 있습니다.

$$\mathcal{M}_m[f](\mathbf{x}) := -\frac{1}{D_0}\int_{\cup_{n=1}^{N}\Omega_n} G(\mathbf{x},\mathbf{y})u_m^t(\mathbf{y})f(\mathbf{y})d\mathbf{y}$$

Measurement g → 3D distribution f ???

non-linear, ill-posed



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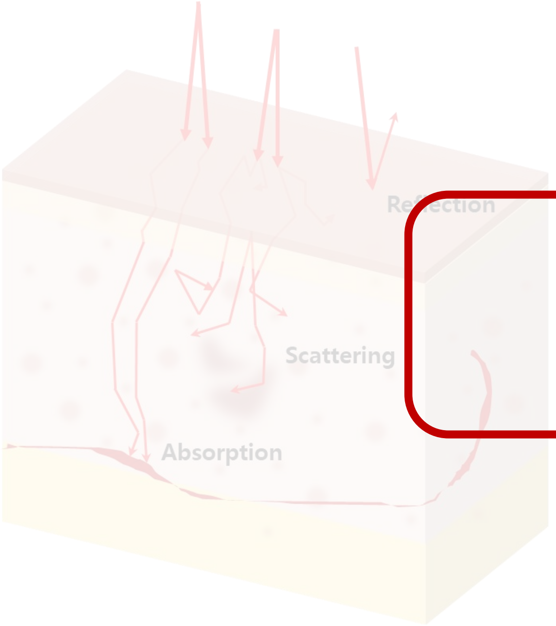

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DEEP LEARNING !!!....??

2) 이 때, 둘 사이의 관계는 적분 방정식으로 표현할 수 있습니다.

OKAY.....

$$\mathcal{M}_m[f](\mathbf{x}) := -\frac{1}{D_0}\int_{\cup_{n=1}^N \Omega_n} G(\mathbf{x},\mathbf{y})u^t_m(\mathbf{y})f(\mathbf{y})d\mathbf{y}$$

Measurement g → 3D distribution f ???

non-linear, ill-posed

ISSUES TO OVERCOME

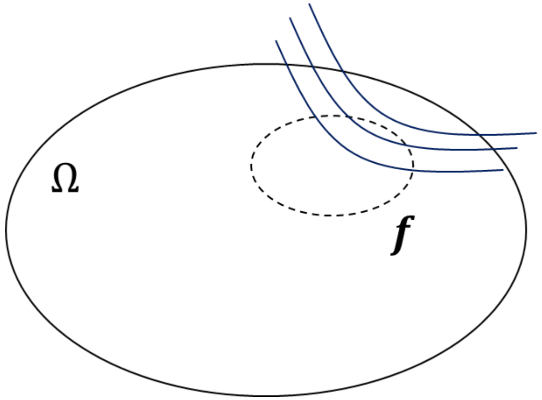
1. Lack of good conventional algorithms

- Applying conventional inversion algorithms and denoising the artifacts using the CNNs are unsatisfactory since they rely on heavy assumptions and linearization.

e.g. Born approximation

$$\mathcal{M}_m[f](\mathbf{x}) \quad := \quad -\frac{1}{D_0}\int_{\cup_{n=1}^{N}\Omega_n} G(\mathbf{x},\mathbf{y})u_m^i(\mathbf{y})f(\mathbf{y})d\mathbf{y}$$

$$u_m^i(\boldsymbol{x}) \gg u_m^s(\boldsymbol{x})$$



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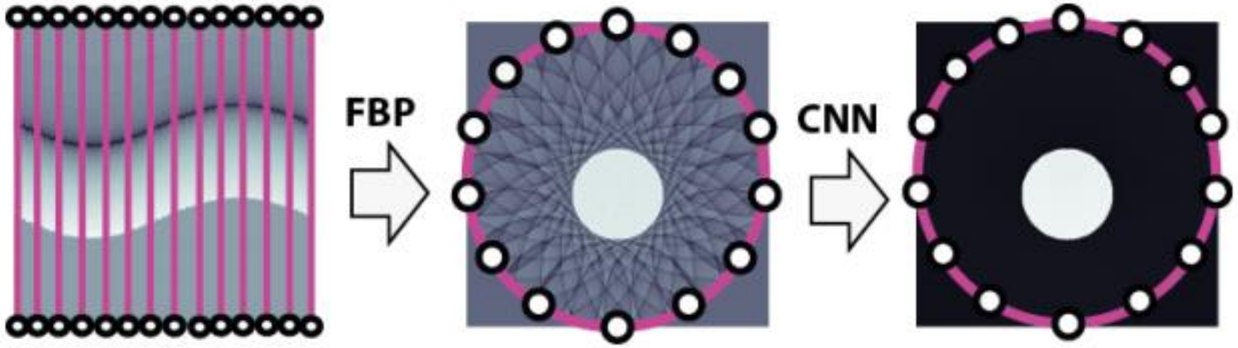

Photoacoustic tomography (PAT)[3]

[1] ODT, Kamilov et al., Optica, 2015

[2] Electron scattering, Broek and Koch, *Physical review letter*

[3] PAT, Antholzer et al. *arXiv*, 2017

ISSUES TO OVERCOME

1. **Lack of good conventional algorithms**
    - Applying conventional inversion algorithms and denoising the artifacts using the CNNs are unsatisfactory since they rely on heavy assumptions and linearization.
2. **Domain & dimension mismatch (How to design the network???)**
    - The measurements $\boldsymbol{g}$ and optical distribution image $\boldsymbol{f}$ live in different domain with different dimension (1D → 3D, severely ill-posed).
3. **Commercial device was not available.**
    - Still laboratory or research level usage.
    - **Proto-type device** available (not calibrated or validated).
4. **Lack of real data**
    - At the early stage, **only a single data** measured by **proto-type device** were available

ISSUES TO OVERCOME

1. Lack of good conventional algorithms
   - Applying conventional inversion algorithms and denoising the artifacts using the CNNs are unsatisfactory since they rely on heavy assumptions and linearization.

DCNN is certainly the trend of this era …

2. Domain & dimension mismatch (How to design the network???)
   - The measurements g and optical distribution image f live in different domain with different dimension (1D → 3D, severely ill-posed).

We need a new design of network architecture

3. Commercial device was not available.
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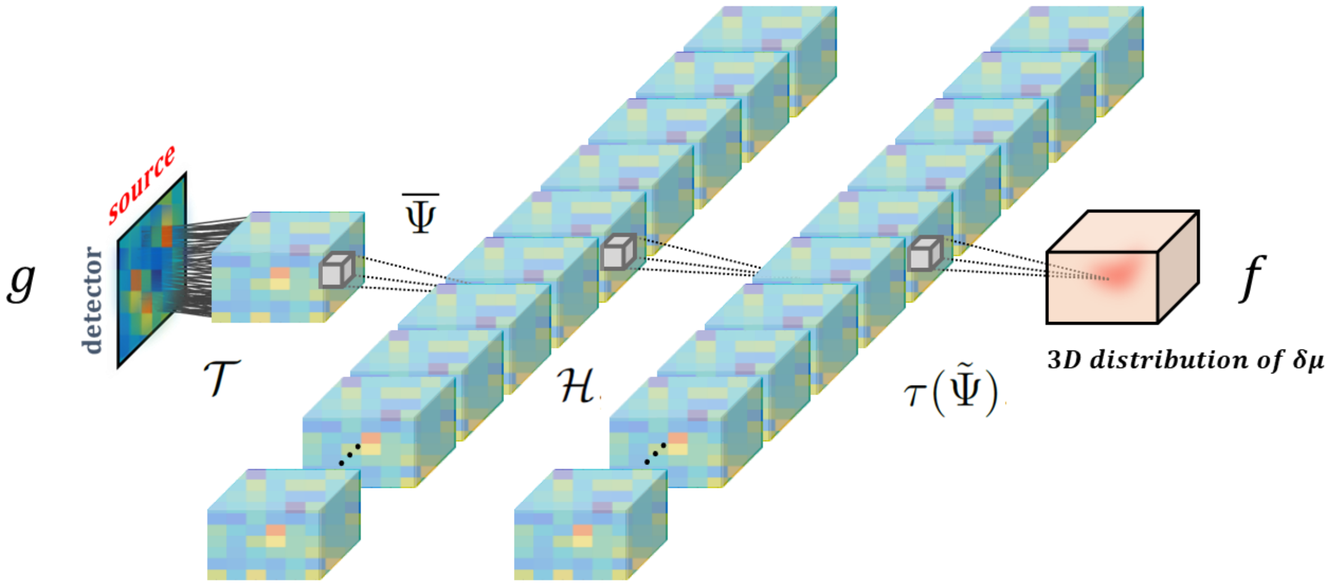
ISSUES #1,2 : SOLUTION

Neural network for inverting Lipmann-Schwinger Equation

- $f = \mathcal{T} g \quad , \quad \mathcal{T} := \mathcal{M}^{-1}$



$$C = (\mathcal{T} g) \circledast \overline{\Psi}, \quad \hat{C} = \mathcal{C} \circledast \mathcal{H}, \quad f = \left(\hat{C}\right) \circledast \tau(\tilde{\Psi})$$

- The inverting operator is naturally found during the training phase.
- Achieve a denoised signal with a good signal representation which is trained via data without any assumption.

ISSUES #1,2 : SOLUTION

Table 2. Network architecture specifications. Here, NM is the number of filtered measurement pairs (Polypropylene: $NM = 538$, Biomimic: $NM = 466$, Mouse (normal): $NM = 470$, Mouse (with tumor): $NM = 1533$).

Type	Polypropylene			Biomimic			Animal		
	patch size /stride	output size	depth	patch size /stride	output size	depth	patch size /stride	output size	depth
Gaussian noise	-	$1 \times 1 \times NM$	-	-	$1 \times 1 \times NM$	-	-	$1 \times 1 \times NM$	-
fully connected	-	$1 \times 1 \times 40,960$	1	-	$1 \times 1 \times 53,760$	1	-	$1 \times 1 \times 12,288 \times 2$	2
dropout	-	-	-	-	-	-	-	-	-
reshape	-	$32 \times 64 \times 20 \times 1$	-	-	$48 \times 70 \times 16 \times 1$	-	-	$32 \times 32 \times 12 \times 2$	-
3D convolution	$3 \times 3 \times 3/1$	$32 \times 64 \times 20 \times 16$	16	$3 \times 3 \times 3/1$	$48 \times 70 \times 16 \times 64$	64	$3 \times 3 \times 3/1$	$32 \times 32 \times 12 \times 128$	128
3D convolution	$3 \times 3 \times 3/1$	$32 \times 64 \times 20 \times 1$	1	$3 \times 3 \times 3/1$	$48 \times 70 \times 16 \times 64$	64	$3 \times 3 \times 3/1$	$32 \times 32 \times 12 \times 128$	128
3D convolution	-	-	-	$3 \times 3 \times 3/1$	$48 \times 70 \times 16 \times 1$	1	$3 \times 3 \times 3/1$	$32 \times 32 \times 12 \times 1$	1

- The overall structure of the networks is remained same across different set of experiment data
- The number of convolution layers and their filters vary dependent on the data but this is chosen to show the best performance not due to the failure of the network
- Note that the rest of parameters such as Gaussian noise variance and dropout rate are remained same for every case

ISSUES TO OVERCOME

~~1. Lack of good conventional algorithms~~ **BUSTED**

- Applying conventional inversion algorithms and denoising the artifacts using the CNNs are unsatisfactory since they rely on heavy assumptions and linearization.

~~2. Domain & dimension mismatch~~ **BUSTED**

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- Still laboratory or research level usage.
- **Proto-type device** available (not calibrated or validated).

Make your hands dirty. Start from the system.

4. Lack of real data

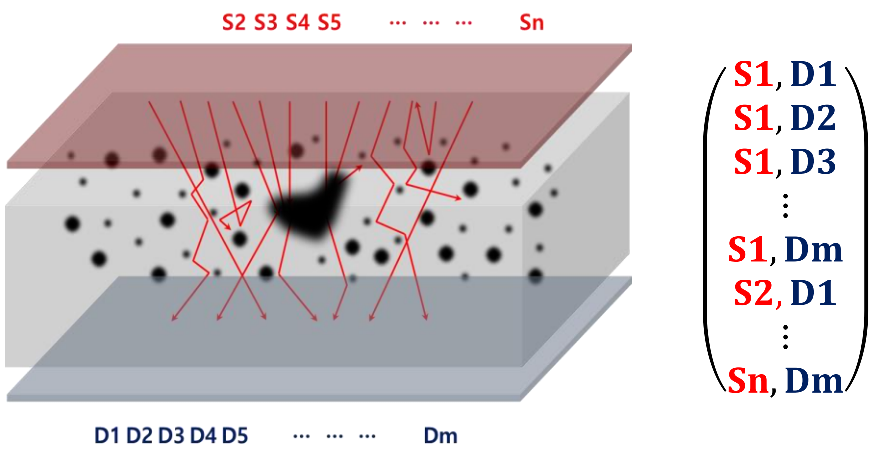
- At the early stage, **only a single data** measured by **proto-type device** were available

If you don't have the data. Make it up.

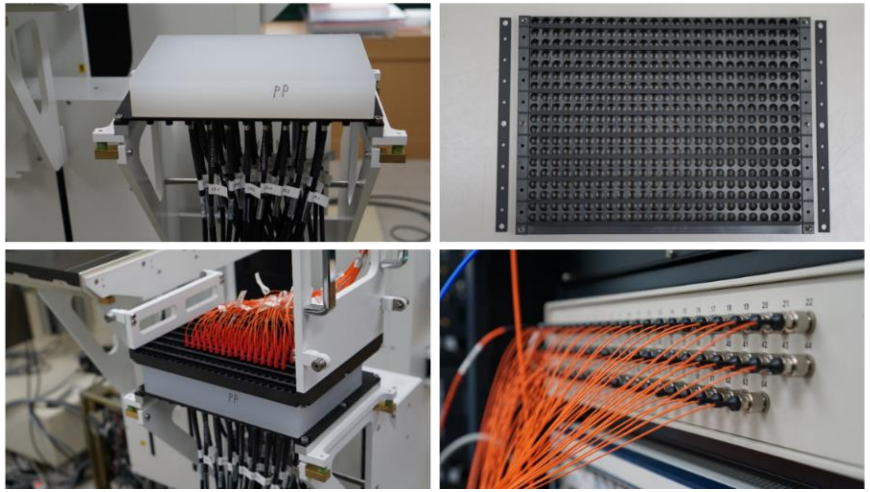
ISSUES #3,4 : SOLUTION

System calibration and data acquisition

- Based on the data from hardware system (KERI), performed the signal analysis to calibrate the hardware system.
- Phantom with known optical values are used.



Schematic illustration of DOT system



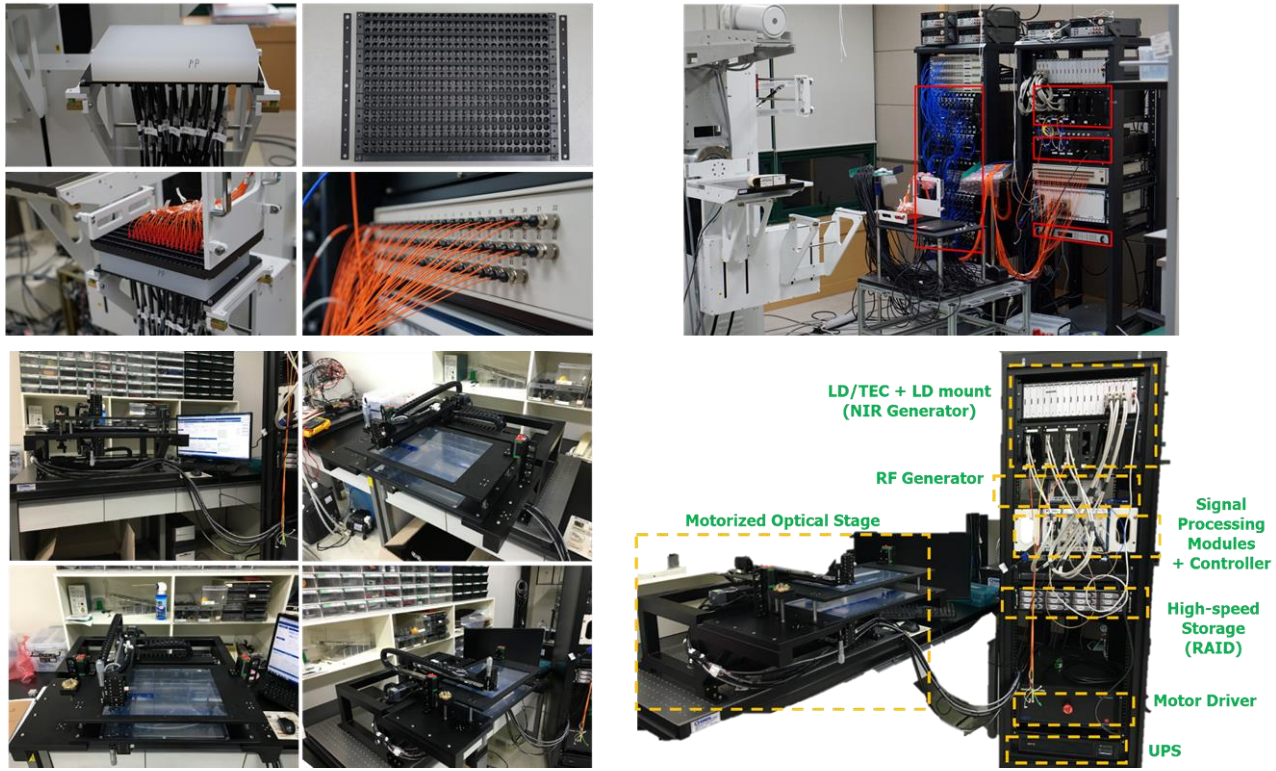
DOT system (KERI)

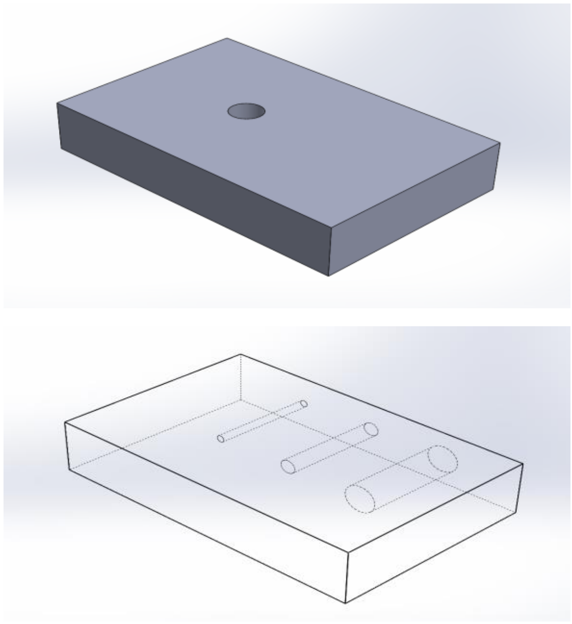
ISSUES #3,4 : SOLUTION

System calibration and data acquisition

(a)

(b)

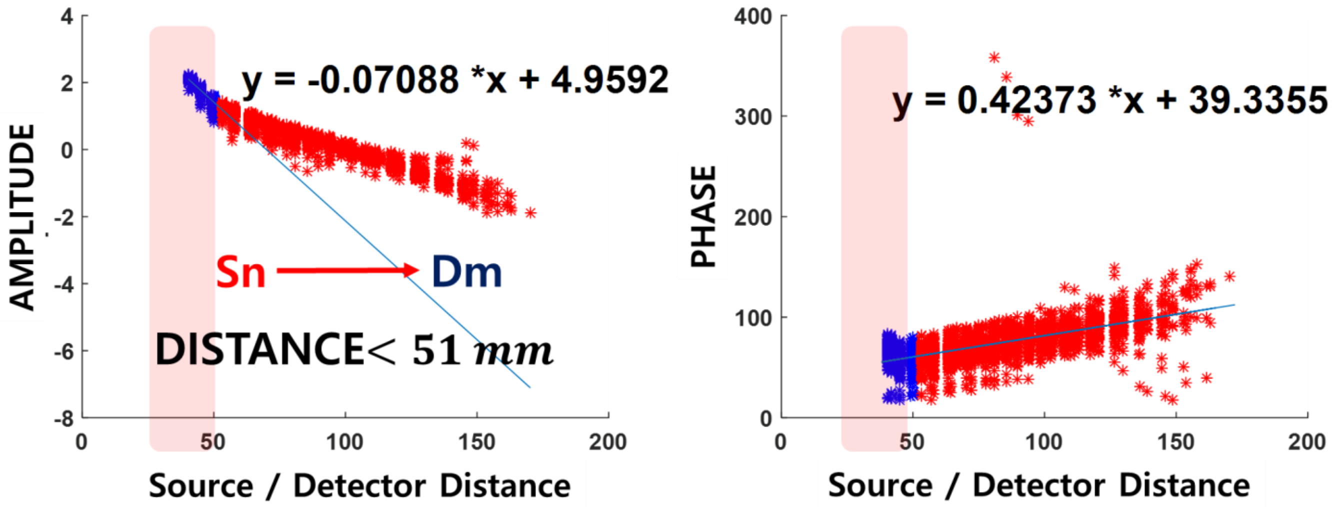




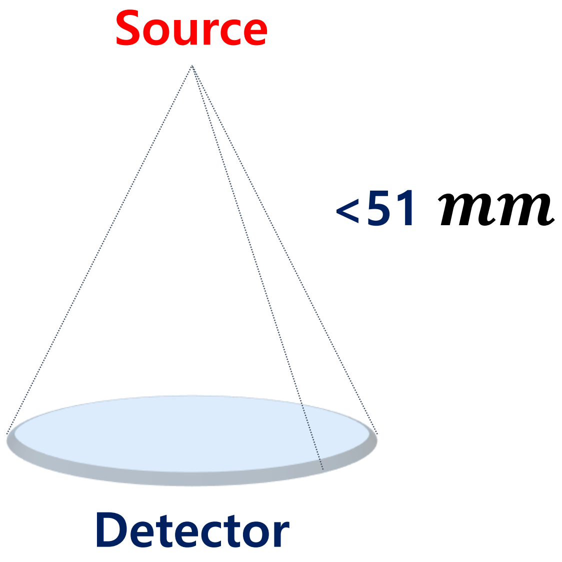
ISSUES #3,4 : SOLUTION

Data preprocessing

- Discard the measurement pairs over the src-det distance limit ($51\ mm$)
- Find the optical coefficients based on the homogeneous model



Data preprocessing based on src-det distance



ISSUES #3,4 : SOLUTION

Simulation data generation

- Using the finite element method (FEM) based solver *NIRFAST*
- Mesh data are re-gridded to matrix form
- Up to three anomalies with different size ($\text{radius: } 2\,mm \sim 13\,mm$) and optical properties at various position (x, y, z)
- Anomaly has two to five times bigger optical properties than the homogeneous background (similar to tumor compared to the normal tissue).
- 1500 data (1000 for training / 500 for validation)

NIRFAST Slicer

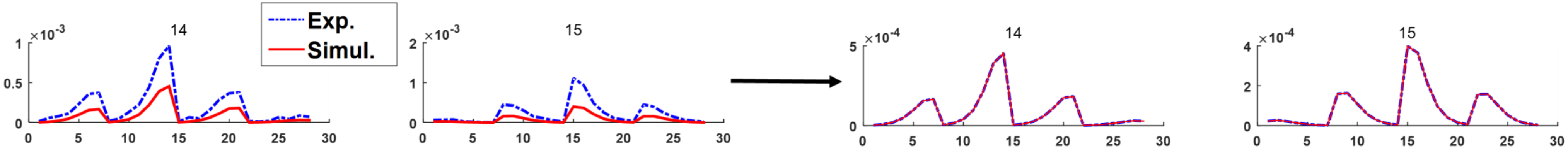
THAYER SCHOOL OF ENGINEERING AT DARTMOUTH   UNIVERSITY OF BIRMINGHAM   3DSlicer   Kitware

ISSUES #3,4 : SOLUTION

Data preprocessing

- Discard the measurement pairs over the src-det distance limit $(51\,mm)$
- Find the optical coefficients based on the homogeneous model
- Domain adaptation from real to simulation data

  (matching the signal envelope, amplitudes, etc.)



Matching the signal envelop

$$C = u^{i}_{simul}(\boldsymbol{x})./u^{i}_{exp}(\boldsymbol{x})$$

ISSUES #3,4 : SOLUTION

Data preprocessing

- Discard the measurement pairs over the src-det distance limit (51 mm)
- Find the optical coefficients based on the homogeneous model
- Domain adaptation from real to simulation data
  (matching the signal envelope, amplitudes, etc.)

EXPERIMENT DESIGN, DEVICE CALIBRATION, DATA PREPROCESSING, UNDERSTANING PHYSICS, DATA GENERATION, EXPERIMENT, EXPERIMENT, EXPERIMENT … TRIALS AND ERRORS	DL MODEL DESIGN

This took 80% of the research

Matching the signal envelop

$$C = u^i_{simul}(x)./u^i_{exp}(x)$$

ISSUES TO OVERCOME

~~1. Lack of good conventional algorithms~~ BUSTED

- Applying conventional inversion algorithms and denoising the artifacts using the CNNs are unsatisfactory since they rely on heavy assumptions and linearization.

~~2. Domain & dimension mismatch~~ BUSTED

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- Still laboratory or research level usage.
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~~4. Lack of real data~~ BUSTED

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II. EXPERIMENTS

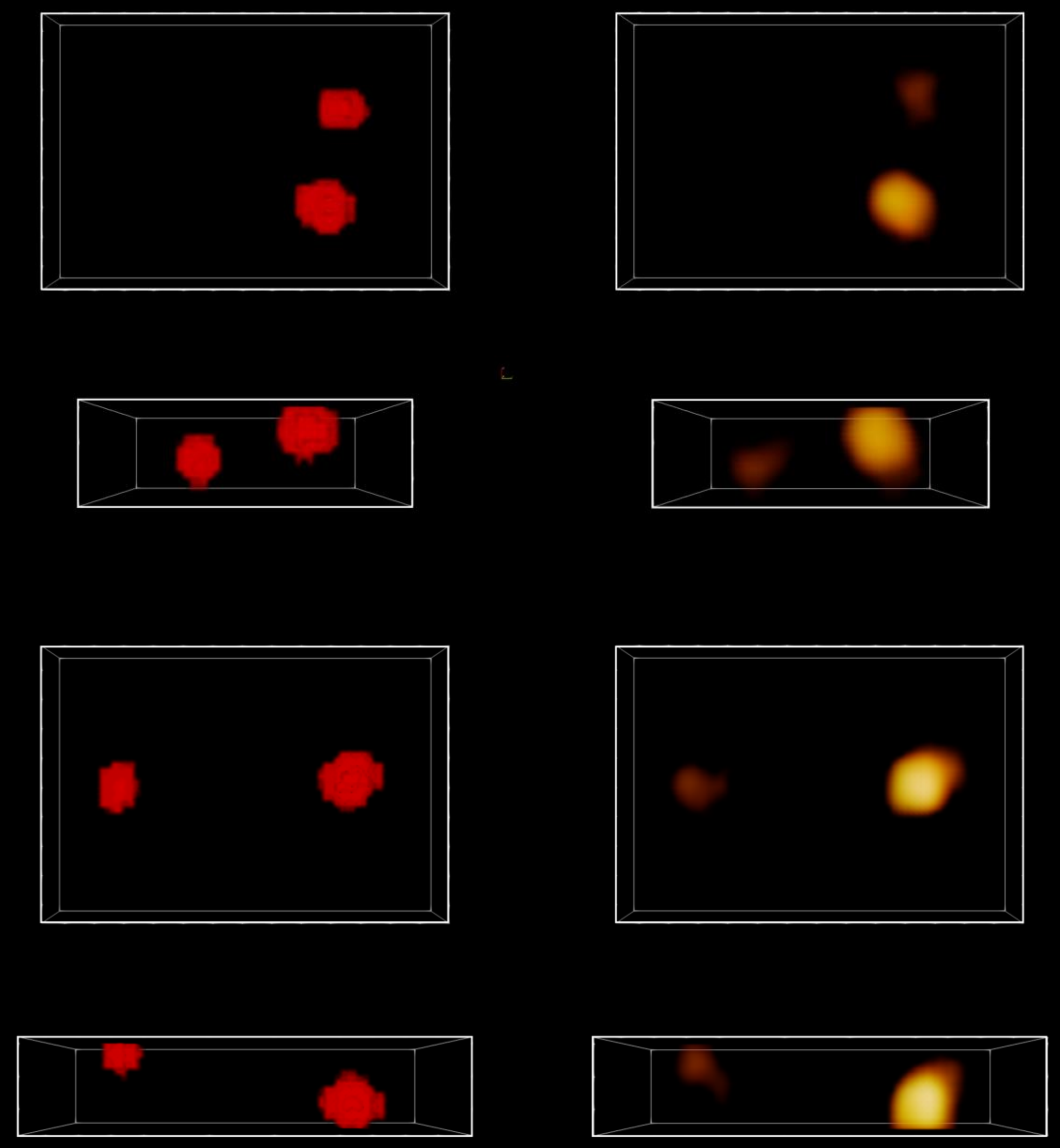
A. Results

B. Take home messages

SIMULATION

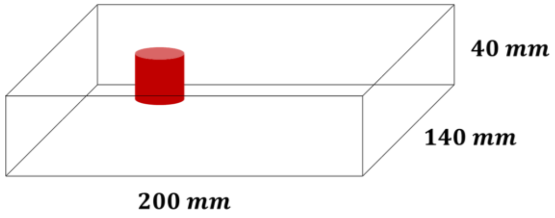
TRAINING

- Additive Gaussian noise ($\sigma = 0.2$)
- Dropout ($p = 0.7$) for FC layer
- Background μ_a values are subtracted
- Data is centered and normalized to range between (-1,1)
- MSE loss
- ADAM optimizer (default setup)
- Batch size: 64
- Early stoppling (no improvement in validation loss for 10 epochs)
- Training time: ~380 SEC

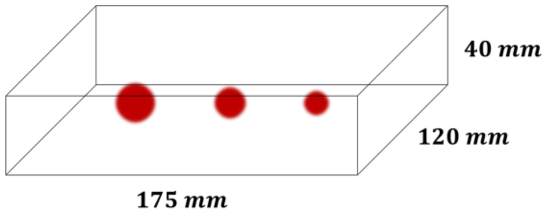


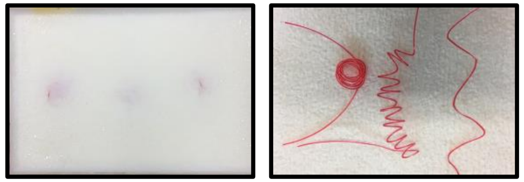
PHANTOM

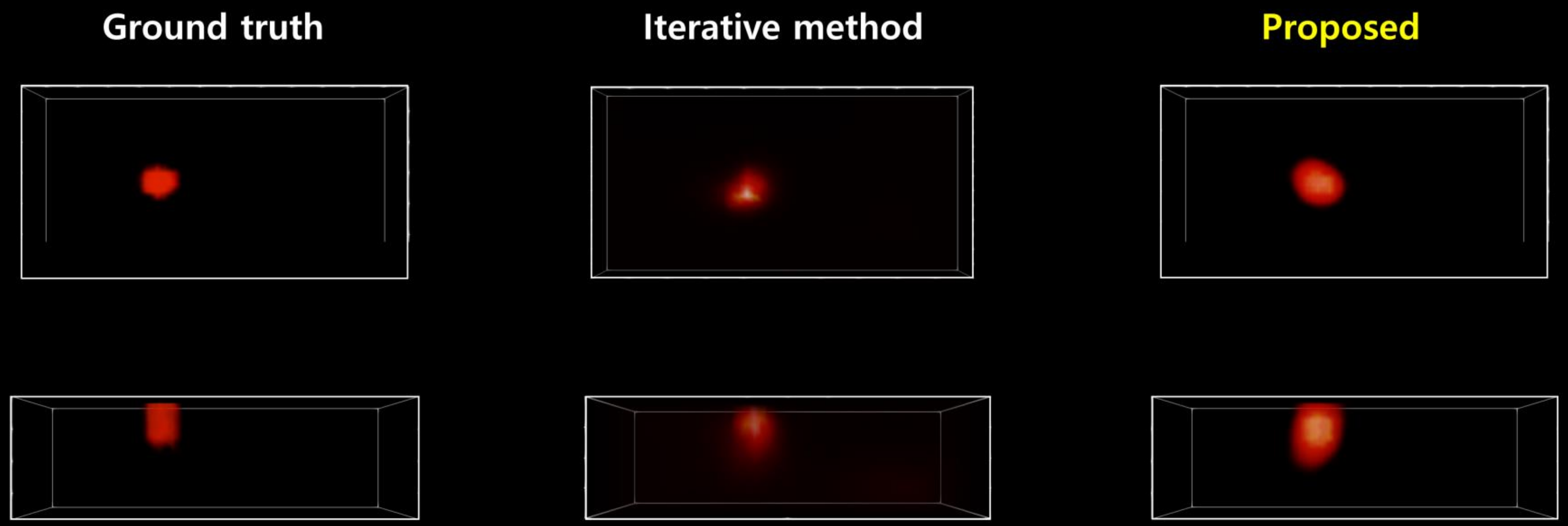
Polyprophylene phantom
($200\ mm \times 140\ mm \times 40\ mm$)

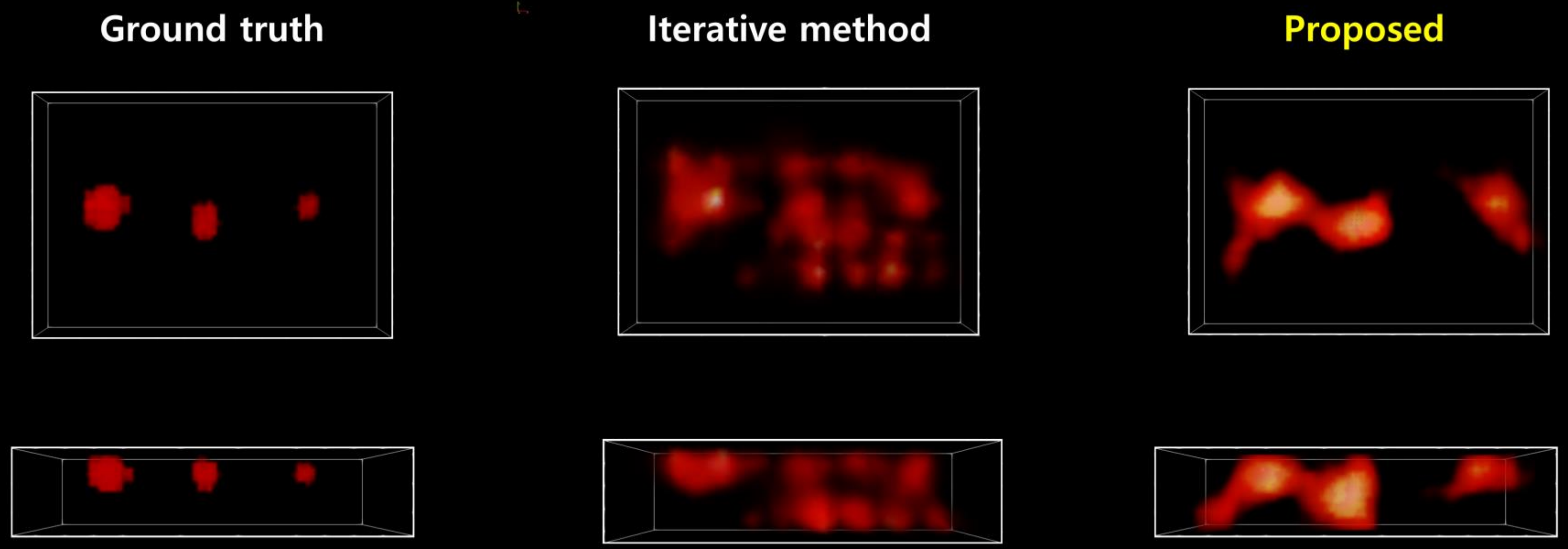


Biomimic phantom
($175\ mm \times 120\ mm \times 40\ mm$)









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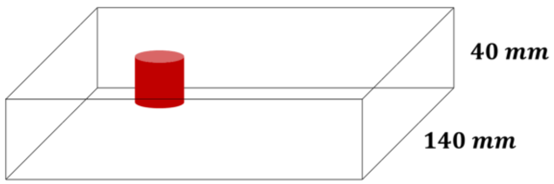

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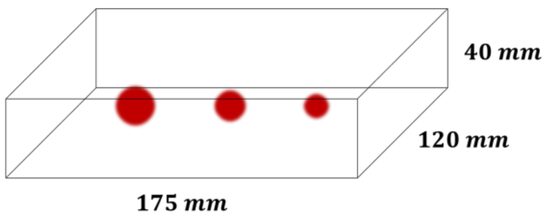

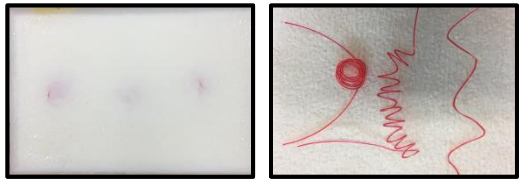

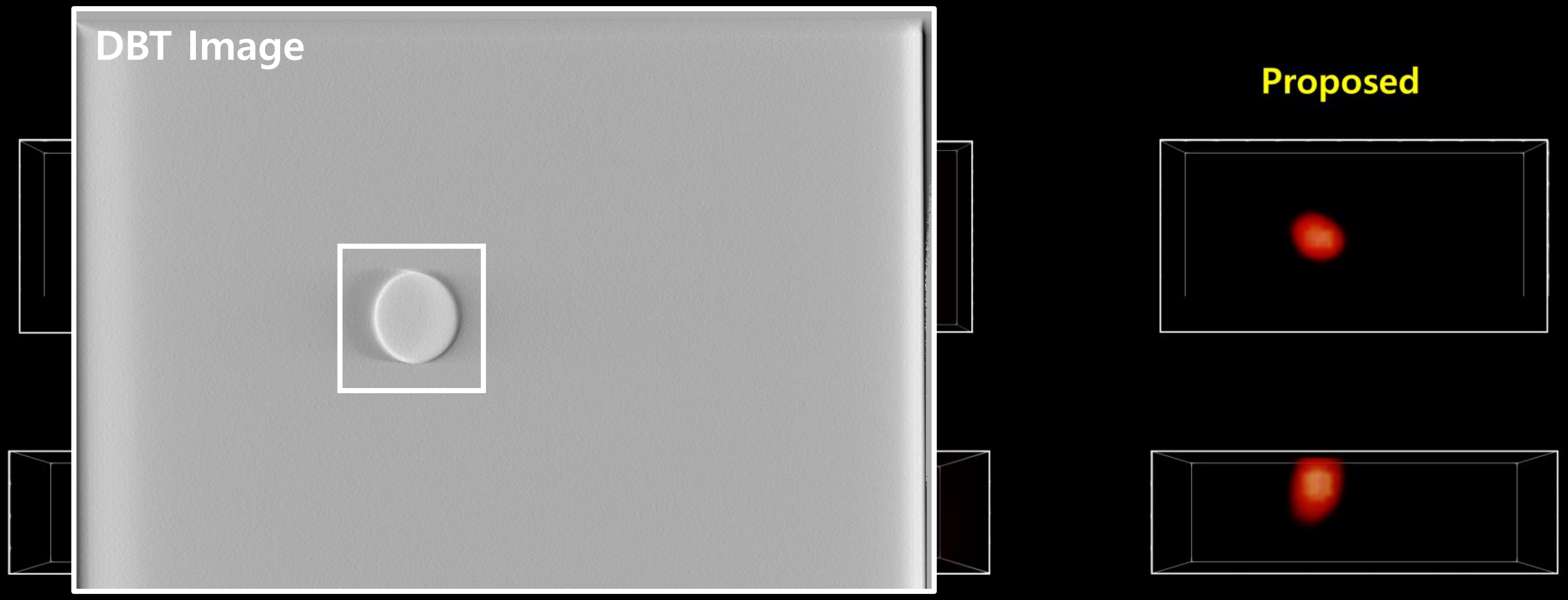

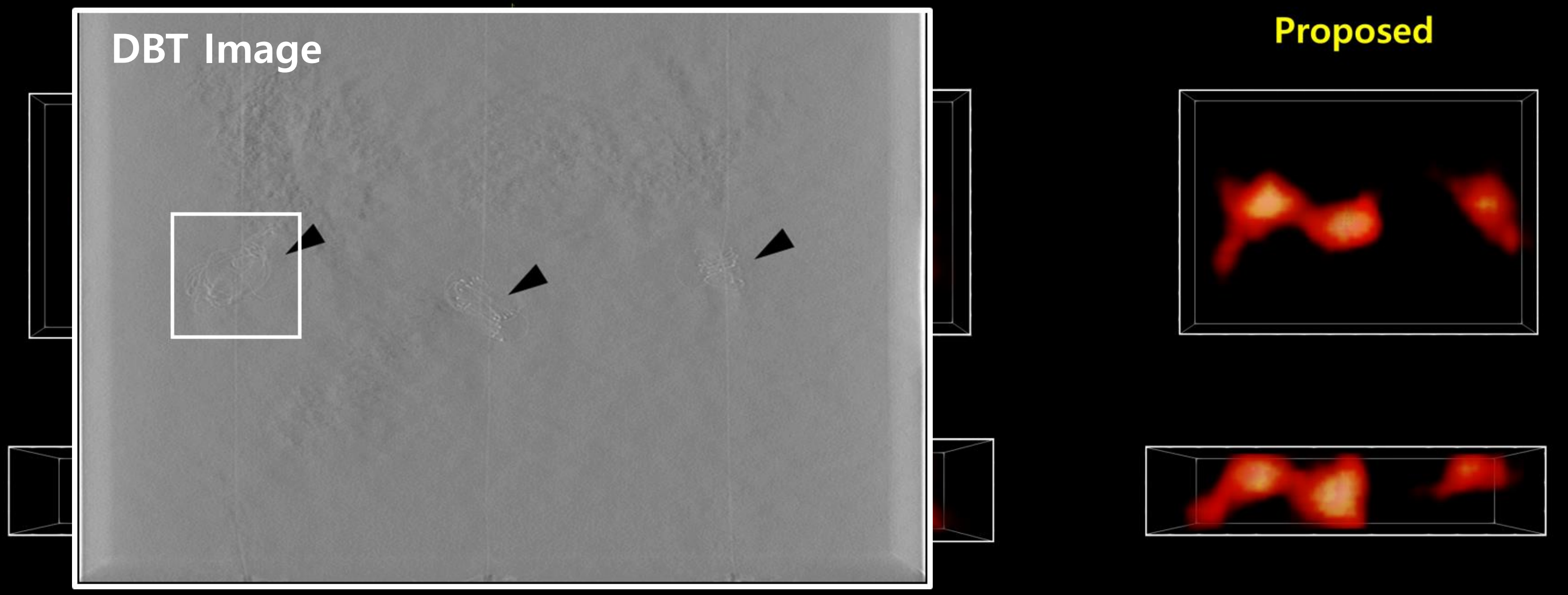

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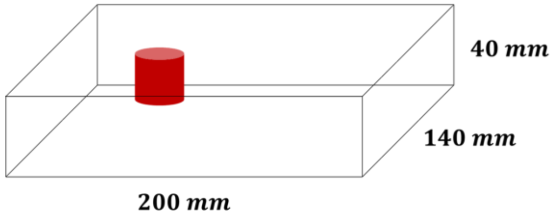
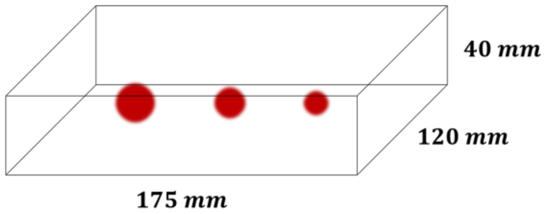
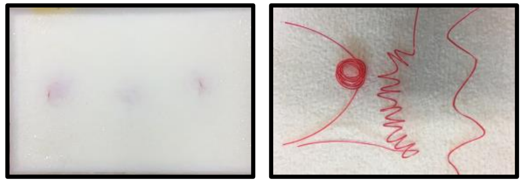
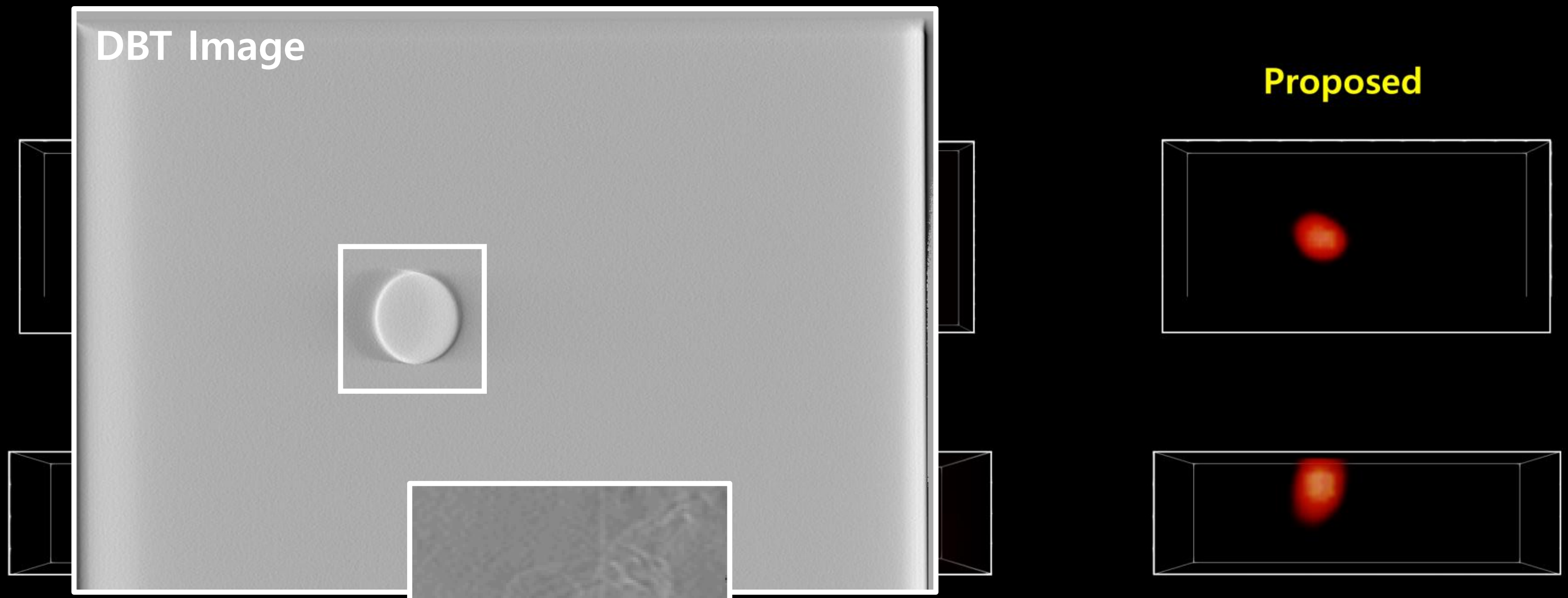
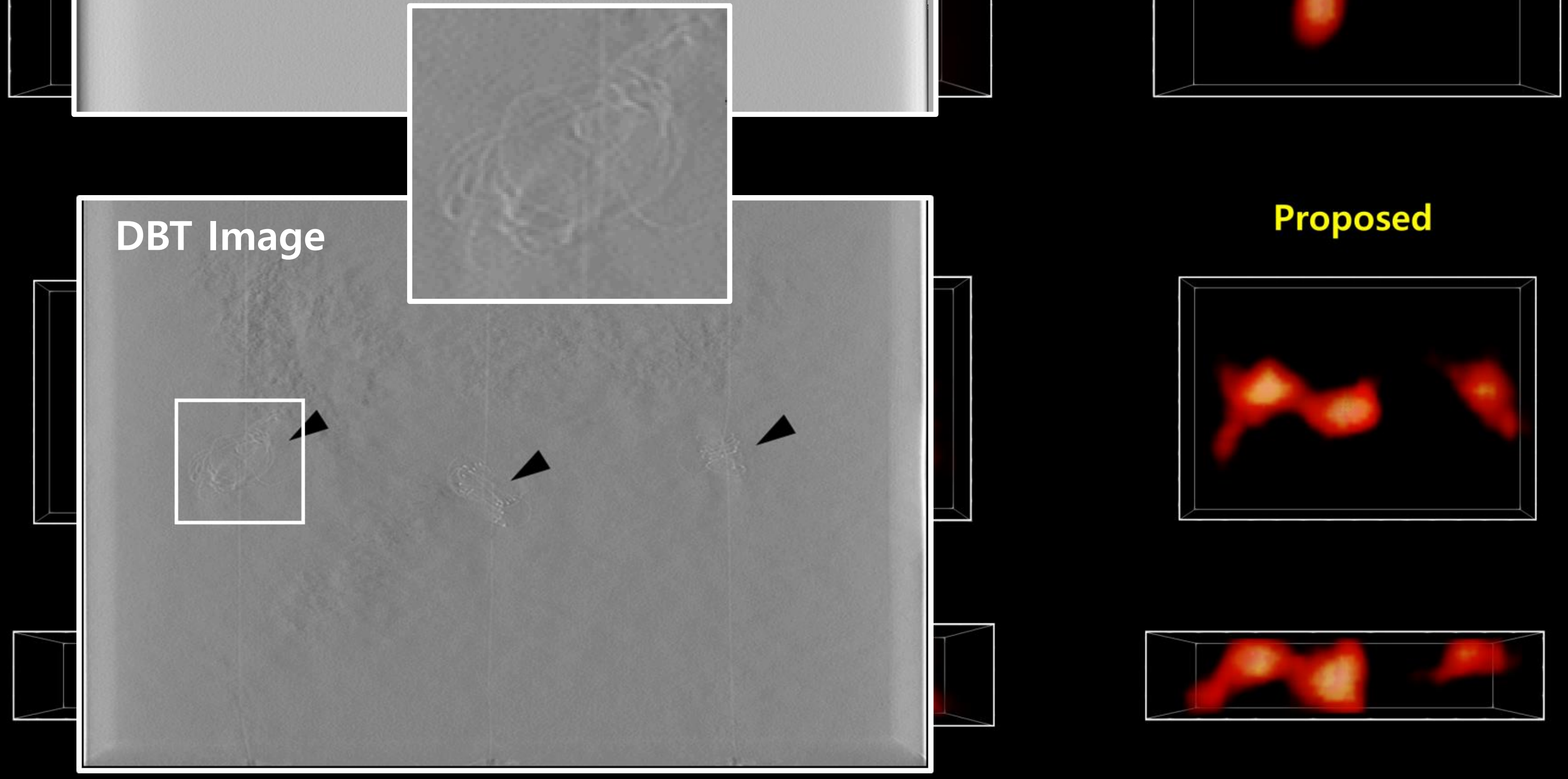


Biomimic phantom
$(175\ mm \times 120\ mm \times 40\ mm)$

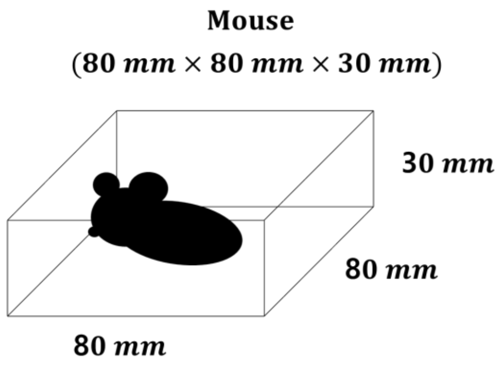


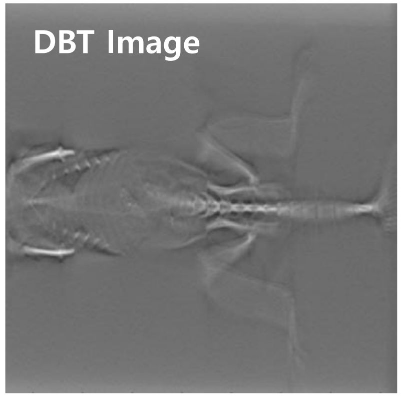


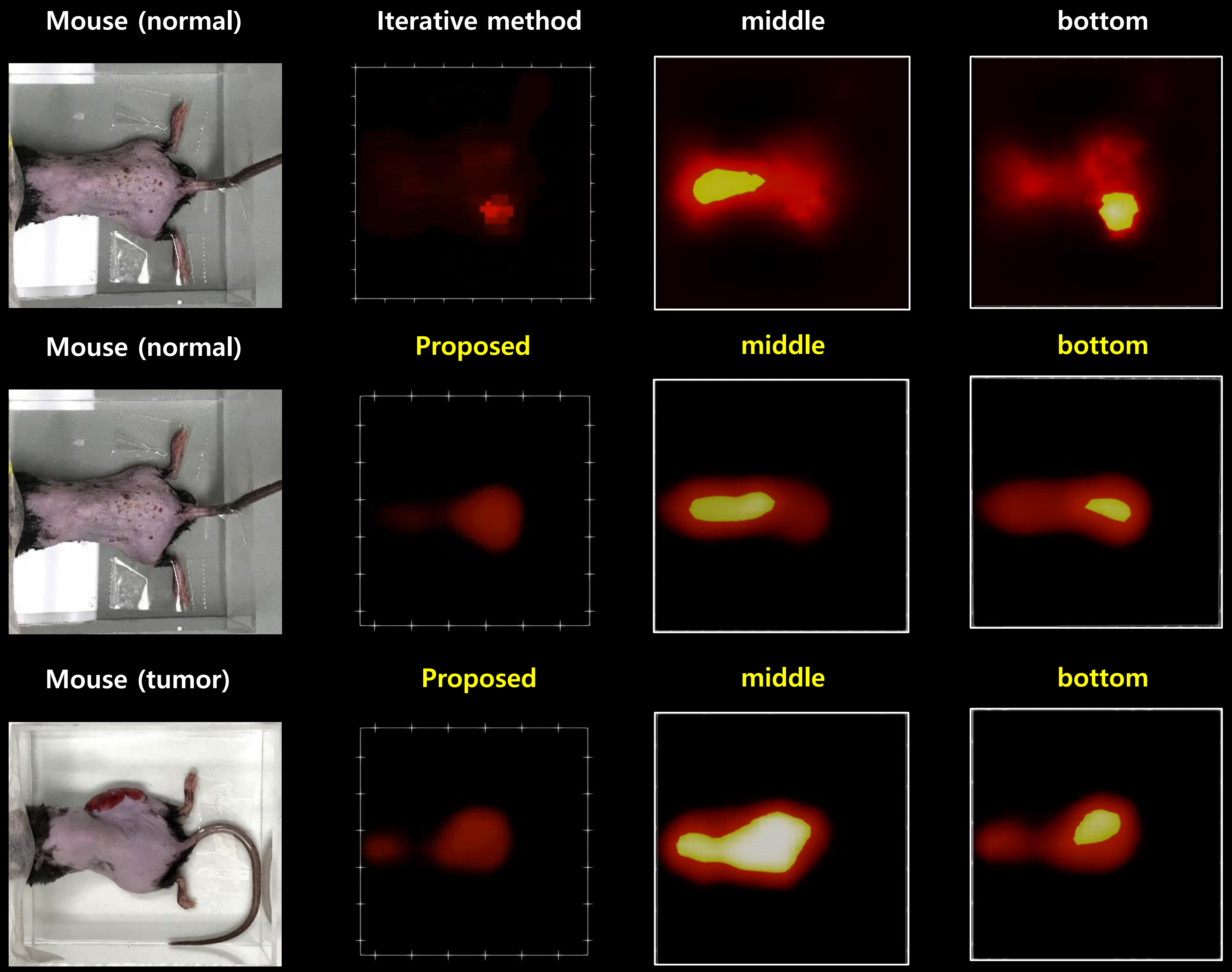




IN VIVO

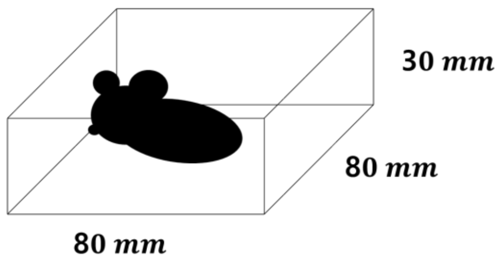

Mouse
(80 mm × 80 mm × 30 mm)
30 mm
80 mm
80 mm

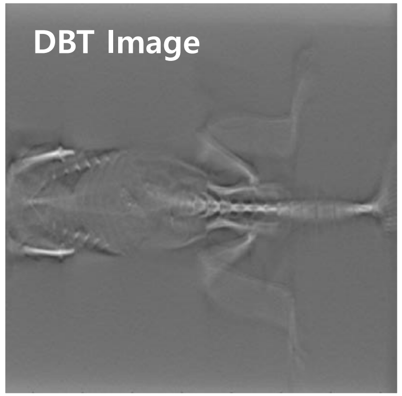

DBT Image

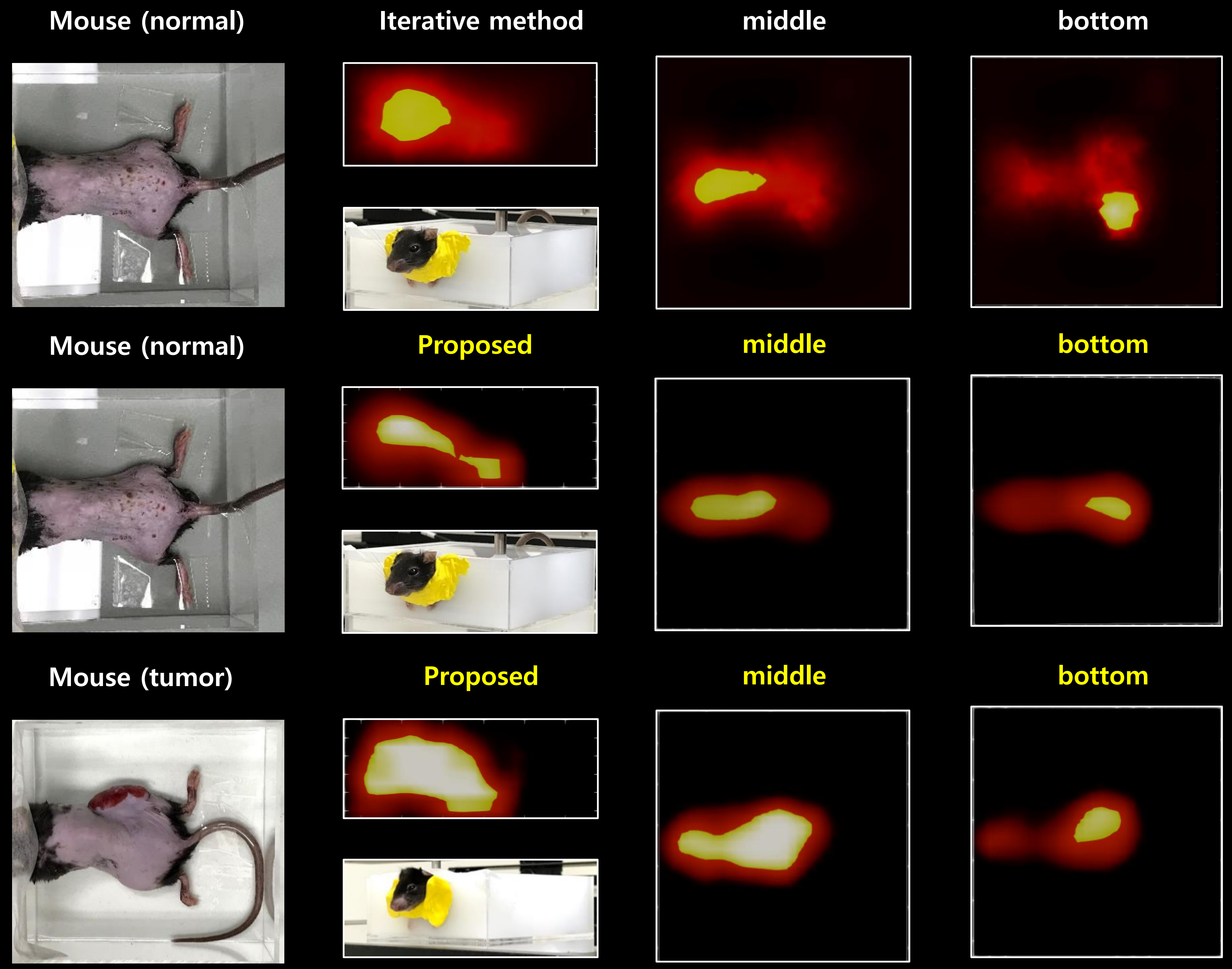

Mouse (normal)
Iterative method
middle
bottom
Mouse (normal)
Proposed
middle
bottom
Mouse (tumor)
Proposed
middle
bottom

IN VIVO

Mouse
(80 mm × 80 mm × 30 mm)







TAKE HOME MESSAGE

1) Domain knowledge matters

2) Data preprocessing is important

* DL NEEDS BABYSITTING A LOT!

- GARBAGE IN → GARBAGE OUT
- 측정 신호에 대한 이해(DOMAIN KNOWLEDGE)를 바탕으로 충분한 PREPROCESSING 필요하다.

3) Do not afraid to make your hands dirty

4) Quick trial and errors

* MAKE YOUR WORKING ENVIRONMENT

- IDEA가 생겼을 때 바로 실험을 해볼 수 있는 환경을 만드는 것이 중요하다.

EXPERIMENT DESIGN, DEVICE CALIBRATION, DATA PREPROCESSING, UNDERSTANING PHYSICS, DATA GENERATION, EXPERIMENT, EXPERIMENT, EXPERIMENT … TRIALS AND ERRORS	DL MODEL DESIGN

This took 80% of the research

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20%가 20%일 수 있었던 이유

EXPERIMENT DESIGN, DEVICE CALIBRATION, DATA PREPROCESSING, UNDERSTANING PHYSICS, DATA GENERATION, EXPERIMENT, EXPERIMENT, EXPERIMENT … TRIALS AND ERRORS	DL MODEL DESIGN

OKAY THAT WORKS...BUT WHY?

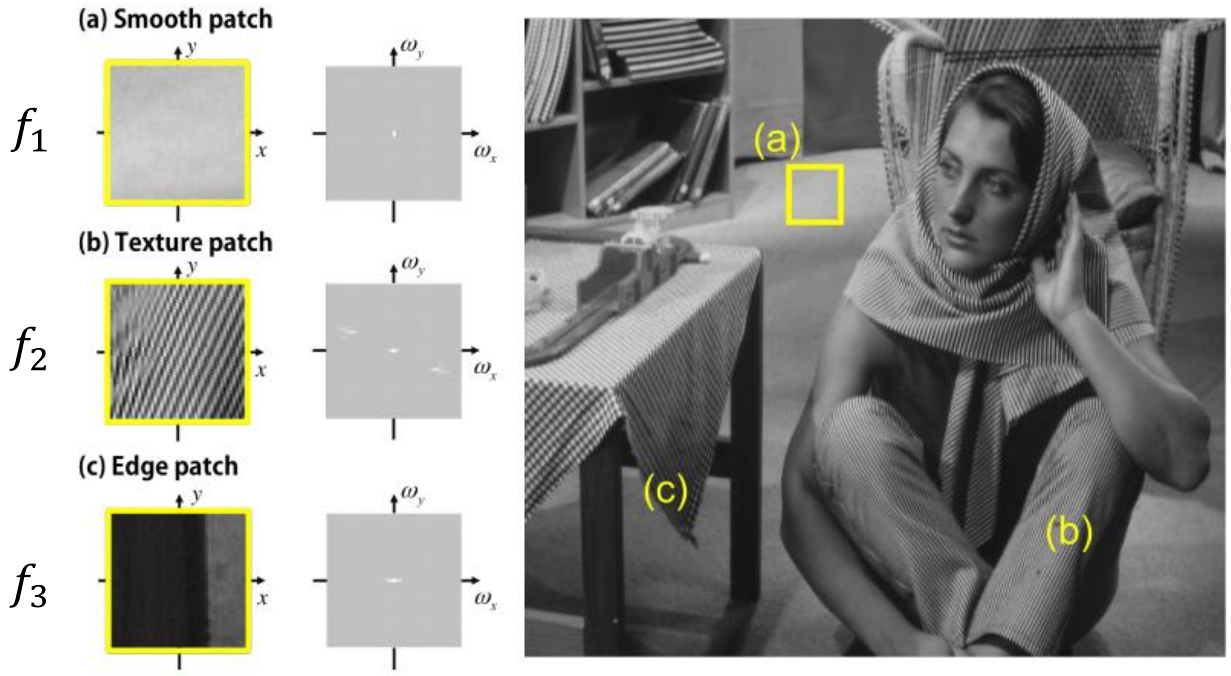
IV. THEORY

A. Deep Convolutional Framelets

DEEP CONVOLUTIONAL FRAMELETS

OBSERVATION 1

"Lifted **Hankel matrix** of noiseless signal f is often low-ranked whereas that of noise ϵ is usually full-ranked" [1-3]



Ye JC et al., 2017

For an image patch f, smooth or structured signals has a sparse coefficients in Fourier domain.

Let $f \in \mathbb{R}^n$ be a vectorized patch with n number of pixels. Here,

$\mathbb{H}_d(\boldsymbol{f})$ is a **Hankel matrix** of signal f with size d.

$$f: \begin{bmatrix} 1 \\ 2 \\ 3 \end{bmatrix} \Rightarrow \mathbb{H}_d(\boldsymbol{f}) \begin{bmatrix} 1 & 2 & 3 \\ 2 & 3 & 1 \\ 3 & 1 & 2 \end{bmatrix}$$

DEEP CONVOLUTIONAL FRAMELETS

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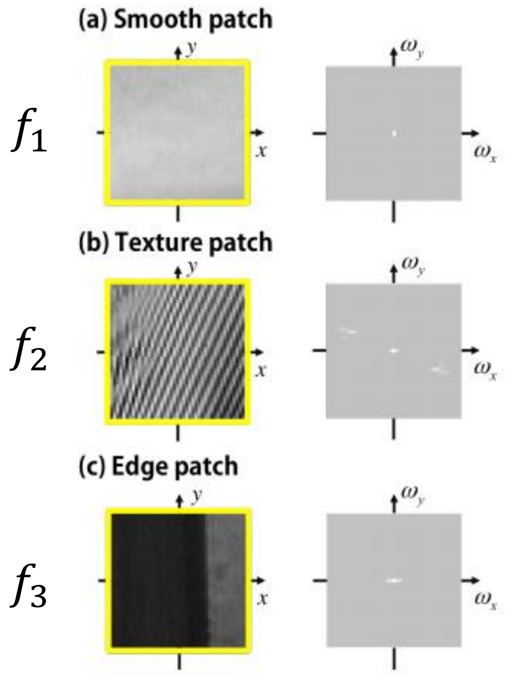
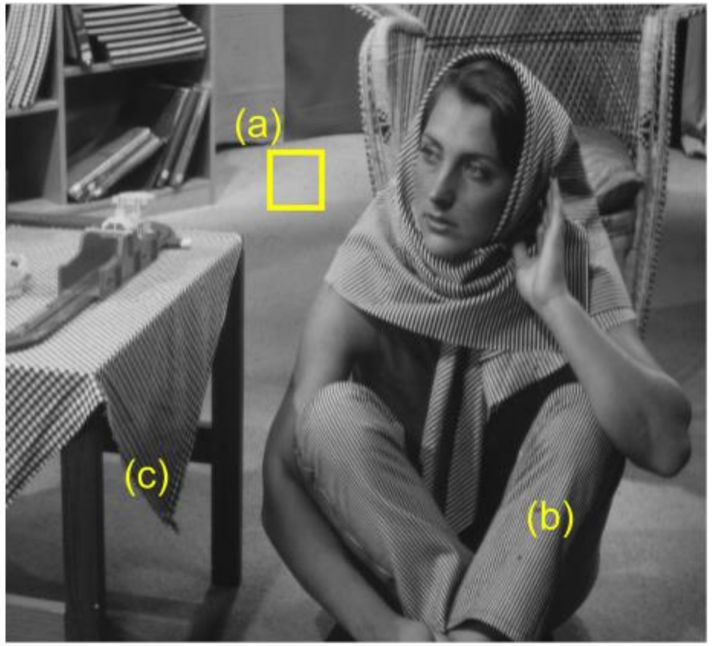


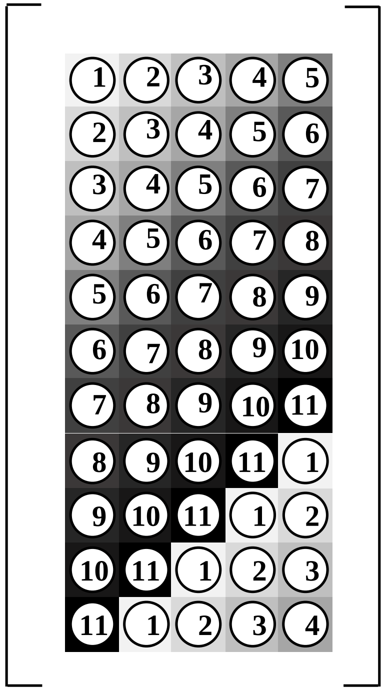


Ye JC et al., 2017

For an image patch f,

$$\hat{f} \in \mathbb{R}^n = f + \epsilon$$

$$\mathbb{H}_d(\hat{\boldsymbol{f}}) = \mathbb{H}_d(\boldsymbol{f}) + \mathbb{H}_d(\boldsymbol{\epsilon}) =$$



$\mathbb{R}^{n \times d}$

Matrix factorization

: low-ranked

: full-ranked (or sparse)

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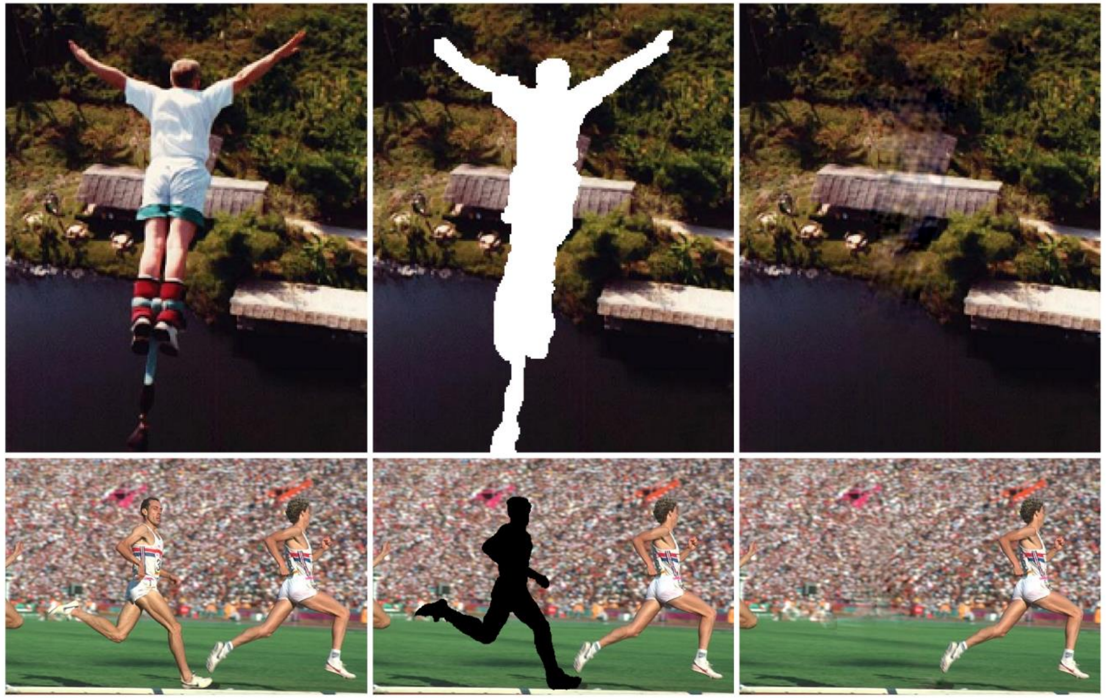
"Lifted **Hankel matrix** of noiseless signal f is often low-ranked whereas that of noise ϵ is usually full-ranked" [1-3]

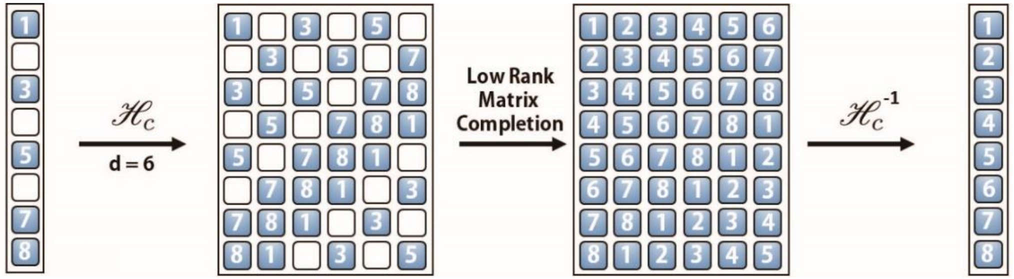


Jin et al., *IEEE TIP*, 2015

For an image patch with missing pixels $f \in \mathbb{R}^n$,

$\mathbb{H}_d(\boldsymbol{f}) \in \mathbb{R}^{n \times d}$ is a rank-deficient Hankel matrix,

Matrix completion, or Netflix problem

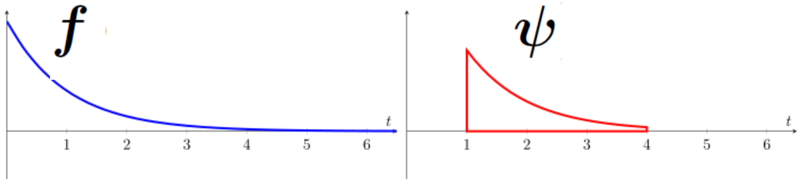


OBSERVATION 2

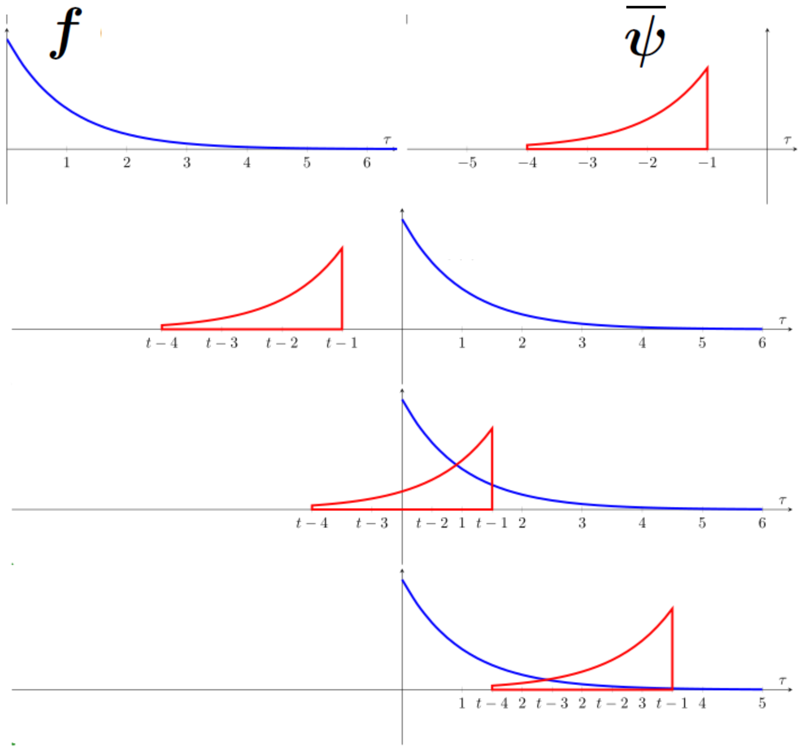
"There is a close relationship between **Hankel matrix** and **convolution operation**, which leads us to CNN."

Convolution

$$(f \circledast \psi)(t) = \int_{-\infty}^{\infty} f(\tau)\psi(t-\tau)d\tau$$



"convolution", WiKipedia



DEEP CONVOLUTIONAL FRAMELETS

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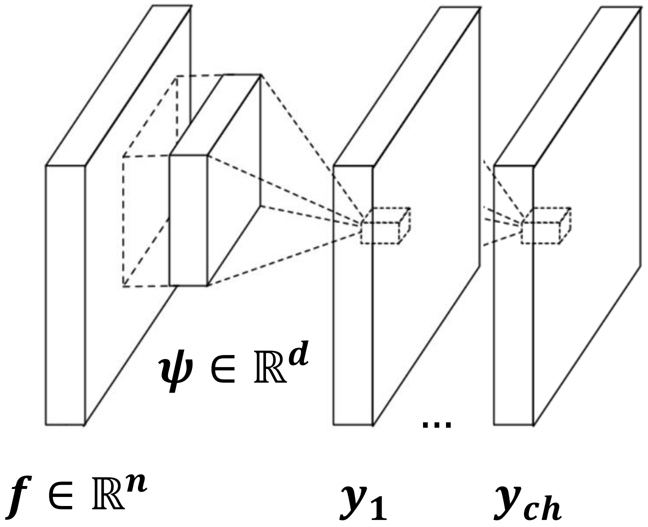
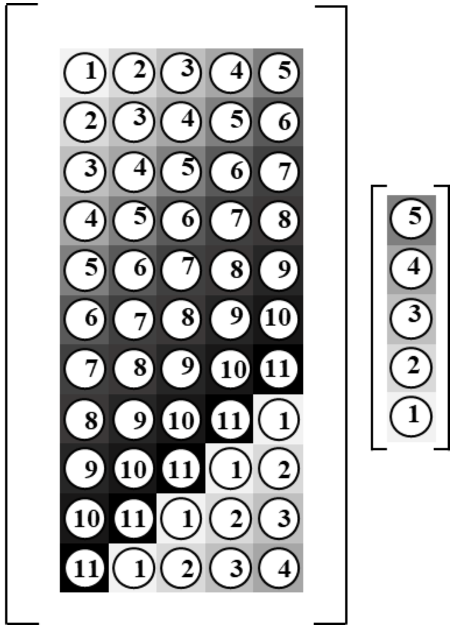


$\Longleftrightarrow$ $\mathscr{H}(\hat{f})\,\bar{\psi} =$



$$Y = f \circledast \Psi = \mathbb{H}_d(f)\overline{\Psi} \qquad \mathbb{H}_d(f) = U\Sigma V^\top$$

DEEP CONVOLUTIONAL FRAMELETS

OBSERVATION 2

"There is a close relationship between **Hankel matrix** and **convolution operation**, which leads us to CNN."

$$\tilde{\Phi}\Phi^\top = I_{n\times n} \quad , \quad \Psi\tilde{\Psi}^\top = P_{R(V)}$$

$$\mathbb{H}_d(f) \quad = \quad \tilde{\Phi}\Phi^\top \mathbb{H}_d(f)\Psi\tilde{\Psi}^\top = \tilde{\Phi}C\Psi^\top$$

$$C \quad = \quad \Phi^\top \mathbb{H}_d(f)\Psi = \Phi^\top \left(f \circledast \overline{\Psi}\right)$$

Single-input multi-output (SIMO)

$$f = \mathbb{H}_d^\dagger\left(\mathbb{H}_d(f)\right) \quad = \quad \left(\tilde{\Phi}C\right) \circledast \tau(\tilde{\Psi}),$$

Multi-input single-output (MISO)

c.f.

$$\tau(\tilde{\Psi}) := \frac{1}{d}\begin{bmatrix} \tilde{\psi}_1 \\ \vdots \\ \tilde{\psi}_r \end{bmatrix} \in \mathbb{R}^{dr}$$

DEEP CONVOLUTIONAL FRAMELETS

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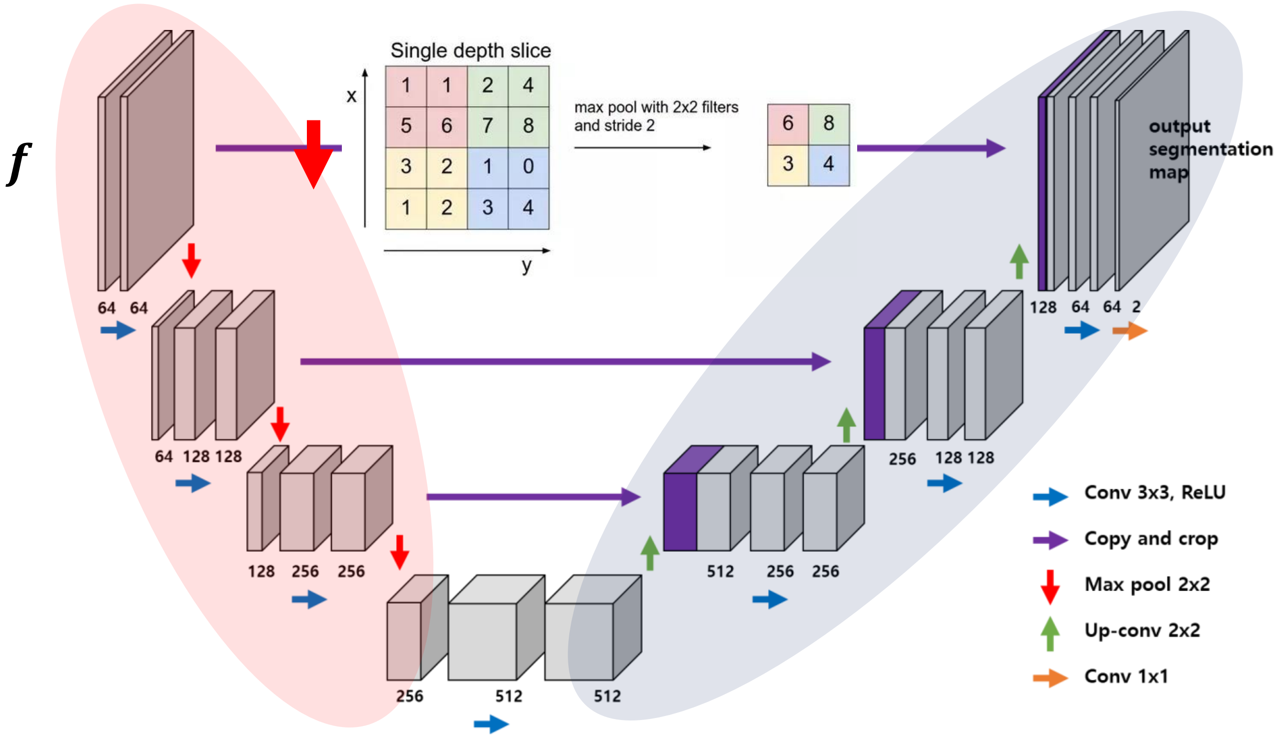


encoder

$$C = \Phi^\top \left(f \circledast \overline{\Psi}\right)$$

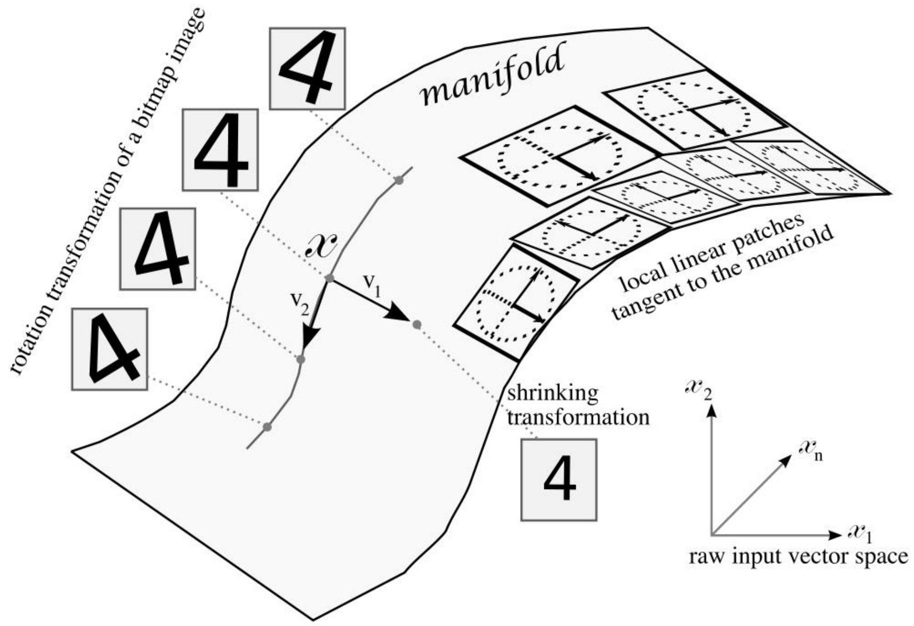
decoder

$$f = \mathbb{H}_d^\dagger(\mathbb{H}_d(f)) = \left(\tilde{\Phi} C\right) \circledast \tau(\tilde{\Psi}),$$

DEEP CONVOLUTIONAL FRAMELETS

OBSERVATION 3

"In the signal processing point of view, what CNNs are doing is to **find an energy-compacting signal representations** (low-ranked) by training a set of local bases $\boldsymbol{\Psi}$ for a given non-local bases $\boldsymbol{\Phi}$."



Yoshua Bengio's slides, 2013

encoder

$$C = \Phi^\top \left(f \circledast \overline{\Psi} \right)$$

decoder

$$f = \mathbb{H}_d^\dagger \left(\mathbb{H}_d(f) \right) \quad = \quad \left(\tilde{\Phi} C \right) \circledast \tau(\tilde{\Psi}),$$

SUMMARY SO FAR

Observation 1

Lifted **Hankel matrix of noiseless signal** f is often **low-ranked** whereas that of noise ϵ is usually full-ranked [1-3].

Observation 2

There is a close relationship between **Hankel matrix** and **Convolution**.

Observation 3

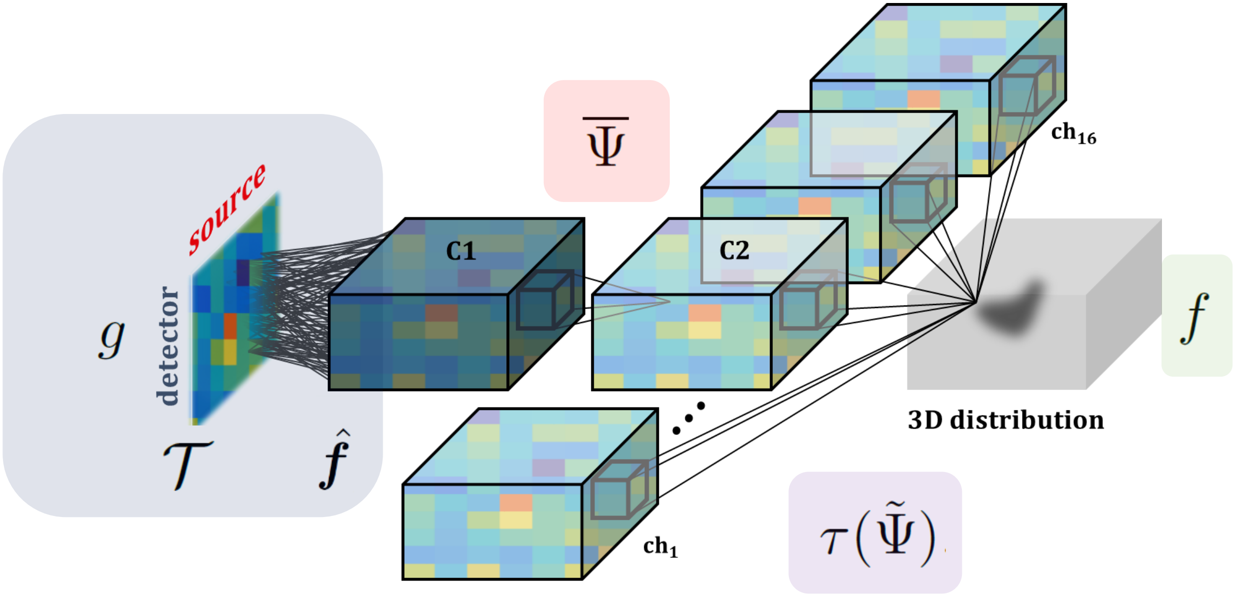
In signal processing perspective, what CNN actually does is **to find a new signal representation** by learning a set of local bases from the data while the global bases are fixed.

[1] Ye JC et al., *IEEE TIT*, 2017
[2] Yin et al., *SIAM*, 2017
[3] Ye and han, 2017

PROPOSED FRAMEWORK

Neural network for inverting Lipmann-Schwinger Equation

- $f = \mathcal{T} g$, $\mathcal{T} := \mathcal{M}^{-1}$



*** Deep Convolutional Framelets**

$$f = \mathbb{H}_d^{\dagger}(\mathbb{H}_d(f)) = \left(\tilde{\Phi} C\right) \circledast \tau(\tilde{\Psi}),$$

$$C = \Phi^{\top} \mathbb{H}_d(f) \Psi$$

$$\Phi = \tilde{\Phi} = I \ ,$$

$$C = (\mathcal{T} g) \circledast \overline{\Psi} \ , \quad f = (C) \circledast \tau(\tilde{\Psi})$$

- The inverting operator is naturally found during the training phase.
- Achieve a denoised signal with a good signal representation which is trained via data without any assumption.

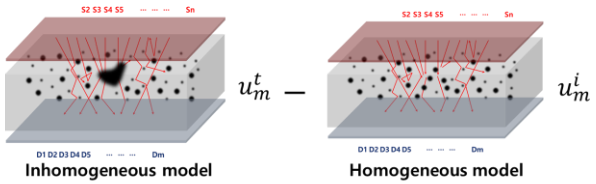
CONCLUSION

PROPOSED A NOVEL DEEP LEARNING FRAMEWORK FOR INVERSE SCATTERING PROBLEMS

Developed deep learning framework inverting Lippmann-Schwinger equation

Showed that the physical intuition is directly mapped to each layer of network

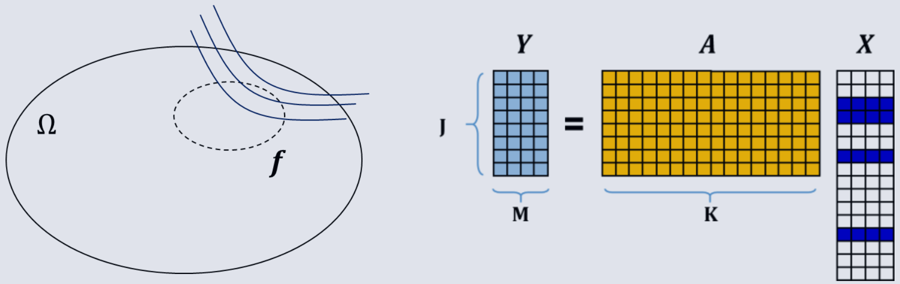
Showed that the framework successfully works in various examples



ADVANTAGES OVER THE OTHER APPROACHES

1. **end-to-end system / simple architecture**
   - no explicit modeling and boundary conditions
   - data-driven (benefit from the data set)
   - fast and efficient learning and inference
   - no post-processing for parameter tuning

conventional analytic approaches



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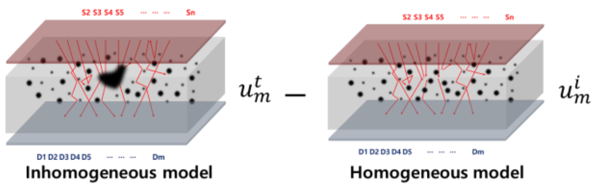

ADVANTAGES OVER THE OTHER APPROACHES

2. **extensibility / practicality**
   - for different modalities and final image sizes
   - for different experimental conditions
   - trainable with numerical data

     (learning the signal representation)