Networks for nonlinear diffusion problems

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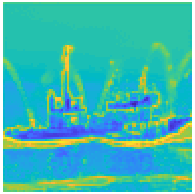

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Deep Learning in imaging

Find a non-linear mapping $A_\Theta : X \to Y$ parametrised by a finite set of parameters Θ, which need to be learned, such that

$$g = A_\Theta u$$

A few questions arise:

- how and to what extent can learned models replace physical models?
- what are appropriate architectures for the learned models, what is the size of the parameter set Θ that needs to be learned, and how can these be interpreted?

[Ye, Han, Cha; 2018], [Haber, Ruthotto; 2018], [Ruthotto,Haber; 2018]

Popular network architectures

The most popular network architectures are based on (discrete) convolutions.

We recall that the convolution of two functions $f, g \in L^1(\mathbb{R}^d)$ is defined by

$$(g * f)(x) = \int_{\mathbb{R}^d} g(x-y)f(y)\mathrm{d}y.$$

Two major question arise:

- Are convolutions suited to capture the physics for a large class of problems?
- Can we improve interpretability by using other underlying operations?

Considering general linear integral transforms

Consider mappings between images in dimension d, e.g. $X = Y = L^p(\Omega \subset \mathbb{R}^d)$.

For example a general linear integral transform such as

$$u^{\mathrm{obs}}(x) = \int_\Omega K(x, y) u^{\mathrm{true}}(y) \mathrm{d}y$$

includes stationary convolution as a special case if the kernel is translation invariant, i.e. $K(x, y) \equiv K(x - y)$.

Outline

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General diffusion processes

We consider the general diffusion process in $\mathbb{R}^d$. On a fixed time interval with some diffusivity $\gamma(u)$, we have

$$\begin{cases} \partial_t u = \nabla \cdot (\gamma(u)\nabla u) & \text{in } \mathbb{R}^d \times (0, T] \\ u(x,0) = u_0(x) & \text{in } \mathbb{R}^d. \end{cases}$$

We denote the spatial derivative by

$$\left(\mathcal{L}(\gamma)u\right)(x,t) := \nabla \cdot (\gamma(u)\nabla u(x,t)).$$

Stationary diffusion as convolution

For *isotropic diffusion* the differential operator becomes the spatial Laplacian $\mathcal{L}(\gamma = 1) = \Delta$.

In this case, the solution u at time T is given by convolution with a *Green's function*

$$u_T(x) = G_{\sqrt{2T}}(x) * u_0(x)$$

where $G_{\sqrt{2T}} = \frac{1}{(4\pi T)^{d/2}} \exp\left[-\frac{x^2}{4T}\right]$ in dimension d.

Nonlinear diffusion

In the general case for an *anisotropic diffusion flow* (ADF) we are interested in a scalar *diffusivity* $\gamma \in [0,1]$ that depends on u itself, i.e.

$$\partial_t u = \nabla \cdot (\gamma(u) \nabla u) \,.$$

This is an example of a non-linear evolution

$$u_T(x) = \mathcal{K}_T u_0 = \int_0^T \int_{\mathbb{R}^d} K^{\mathrm{ADF}}(x, y, u(y,t)) u_0(y) \mathrm{d}y \mathrm{d}t$$

where $K^{\mathrm{ADF}}(x, y, u(x,t))$ is now a non-stationary, non-linear and time-dependent kernel.

In general there is no explicit expression for K^{ADF} and numerical methods are required for the solution.

[Weickert, 1998]

Time discretisation

To establish a process between two states of the function u, denoted at time t_n by $u^{(n)} = u(x, t_n)$, then with $t_{n+1} = t_n + \delta t$:

$$u^{(n+1)} = u^{(n)} + \int_{t_n}^{t_{n+1}} \mathcal{L}(\gamma) u(x, t) \, \mathrm{d}t.$$

Consider a fixed diffusivity at each time instance $\gamma^{(n)} = \gamma(u(x, t = t_n))$, then the integral is approximated by

$$\delta t \mathcal{L}(\gamma^{(n)}) u^{(n)} = \delta t (\nabla \cdot \gamma^{(n)} \nabla u^{(n)}).$$

We obtain an approximate solution by iterating for time steps δt using either an *explicit* scheme

$$\mathcal{D}_{\delta t}^{\mathrm{Expl}}(\gamma^{(n)}) u^{(n)} = \left(Id + \delta t \mathcal{L}(\gamma^{(n)}) \right) u^{(n)} \, ,$$

or an *implicit* scheme

$$\mathcal{D}_{\delta t}^{\mathrm{Impl}}(\gamma^{(n)}) u^{(n)} = \left(Id - \delta t \mathcal{L}(\gamma^{(n)}) \right)^{-1} u^{(n)} \, .$$

Outline

Motivation: From continuum to discrete

We formulate a continuum network, where each layer is interpreted as time instance:

$$F_k = u(x, t_k)$$

Layers are then connected by diffusion layer operator, with learnable parameter $\Theta = \{\gamma, \delta t\}$, and given by the time stepping scheme

$$\mathcal{D}_\Theta F_{k-1} = \mathcal{D}_{\delta t}^{\mathrm{Expl}}(\gamma^{(k-1)})u^{(k-1)} = (Id + \delta t \mathcal{L}(\gamma^{(k)}))u^{(k-1)} = F_k.$$

Discretisation: Diffusion layer

Consider two-dimensional $n \times n$ images and denote the discrete vectorised layers as $\mathbf{F}_k \in \mathbb{R}^{n^2}$.

We consider the explicit diffusion layer operator

$$\mathcal{D}_{\delta t}^{\mathrm{Expl}}(\gamma^{(k-1)})u^{(k-1)} = (Id + \delta t \mathcal{L}(\gamma^{(k)}))u^{(k-1)}$$

.

Then the differential operator $\mathcal{L}(\gamma^{(k)}) = \nabla \cdot \gamma^{(k)} \nabla$ can be approximated by the stencil

$$\mathsf{L}_{\delta t}(\gamma^{(k)}) = \delta t \begin{pmatrix} & \gamma_1^{(k)} & \\ \gamma_2^{(k)} & -\sum_i \gamma_i^{(k)} & \gamma_4^{(k)} \\ & \gamma_3^{(k)} & \end{pmatrix}.$$

Linear diffusion network

The discrete diffusion layer is then given by

$$\mathbf{F}_k = (\mathrm{Id} + \mathrm{L}_{\delta t}(\gamma^{(k)}))\mathbf{F}_{k-1}.$$

The basis of learning a linear diffusion network is now given as estimating the diagonals of $\mathrm{L}_{\delta t}(\gamma^{(k)})$ and the time-step δt:

$$\begin{tikzcd}
\boxed{\mathbf{F}_0} \arrow[r, "\mathrm{L}_{\delta t}(\gamma^{(1)})"] \arrow[r, bend left, "+\mathrm{Id}"] & \boxed{\mathbf{F}_1} \arrow[r, "\mathrm{L}_{\delta t}(\gamma^{(2)})"] \arrow[r, bend left, "+\mathrm{Id}"] & \boxed{\mathbf{F}_2} \arrow[r, "\mathrm{L}_{\delta t}(\gamma^{(3)})"] \arrow[r, bend left, "+\mathrm{Id}"] & \boxed{\mathbf{F}_3}
\end{tikzcd}$$

Discretisation: Inverse filtering

For the inversion task we need to include regularisation.

Especially in the presence of noise, the inverse operator $\mathcal{E}_{\delta t}(\zeta)$ has to be regularised by addition of a smoothing operation $\mathcal{S}$:

$$\mathcal{E}_{\delta t}(\zeta) + \alpha\mathcal{S} \to \mathsf{Id} - \mathsf{L}_{\delta t}(\zeta) + \alpha\mathsf{S} =: \mathsf{Id} - \mathsf{W}_{\delta t}(\zeta)$$

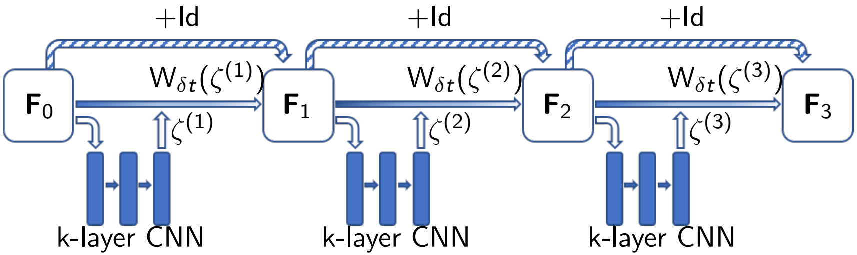
With the general filter matrix

$$\mathsf{W}_{\delta t}(\zeta) = \delta t \begin{pmatrix} & \zeta_1 & \\ \zeta_2 & -\zeta_5 & \zeta_4 \\ & \zeta_3 & \end{pmatrix}.$$

A nonlinear diffusion network: DiffNet

For nonlinear diffusion/filtering, the filters depend on the solution u
$\Rightarrow$ we can not learn the filters explicitly.

We rather estimate the filters ζ implicitly by a small k-layer convolutional neural network (CNN), which are then applied to the image in the filtering layer:



Outline

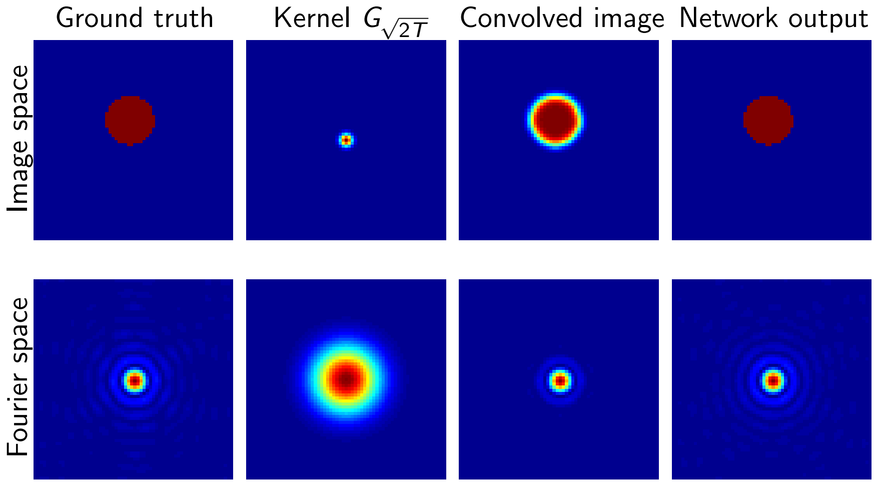
First experiment: Simple deconvolution

We first examine a simple deconvolution experiment to determine what features DiffNet learns in an inverse problem.
We consider:

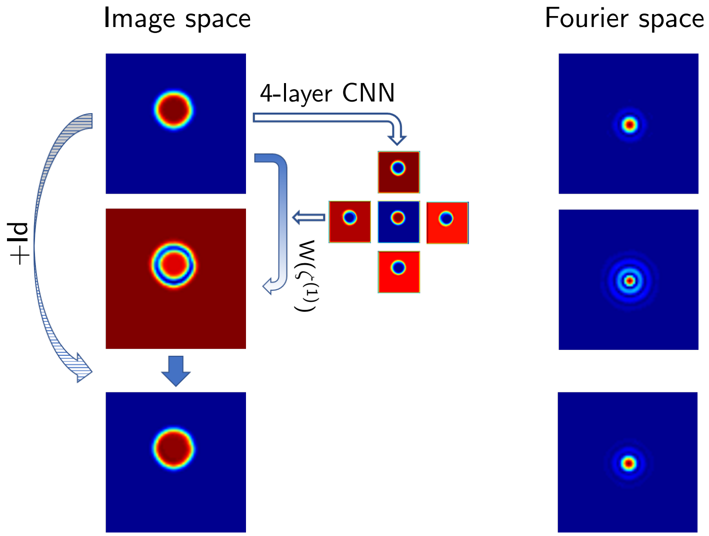
$$\begin{cases} \partial_t u = \nabla \cdot (\gamma \nabla u) & \text{in } \Omega^d \times (0, T] \\ \partial_\nu u = 0 & \text{on } \partial\Omega \times (0, T] \\ u(x,0) = u_0(x) & \text{in } \Omega^d. \end{cases}$$

With constant diffusivity $\gamma \equiv 1$ and $T = 1$.

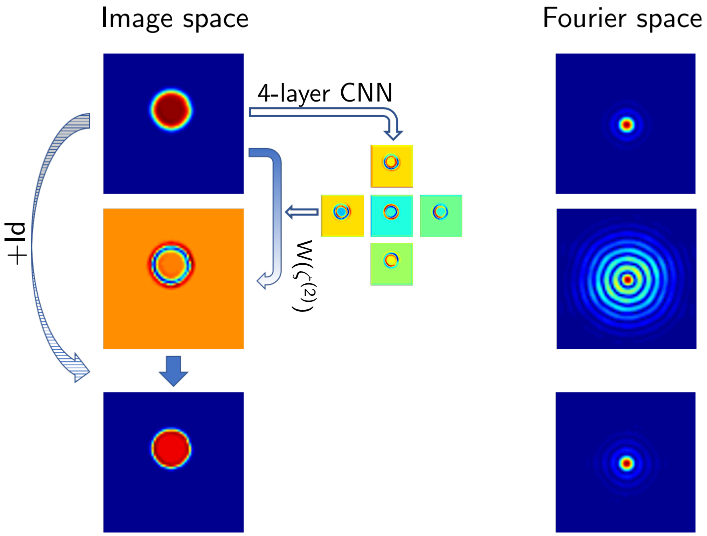
Illustration



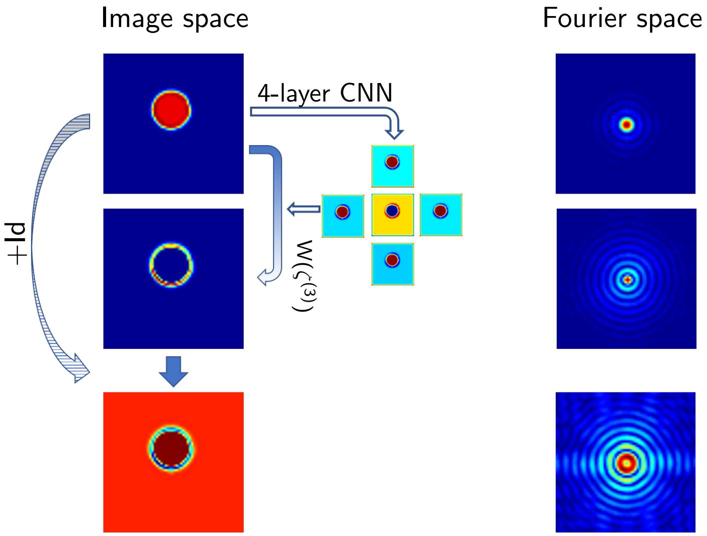
Break down of DiffNet: First layer



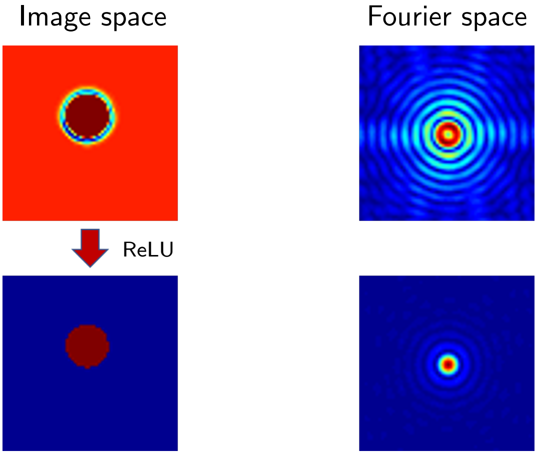
Break down of DiffNet: Second layer



Break down of DiffNet: Third layer



Break down of DiffNet: Output



Nonlinear diffusion

Let us now consider the nonlinear diffusion process with the Perona-Malik filter function [Perona & Malik, 1990], that is the diffusivity is given as a function of the gradient

$$\gamma(|\nabla u|^2) = \frac{1}{1 + |\nabla u|^2/\lambda^2}$$

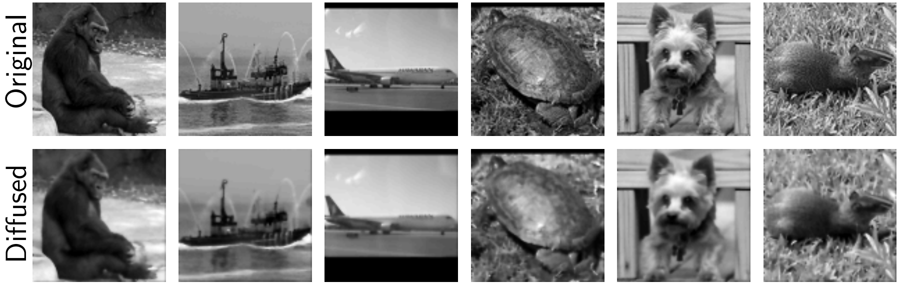
with contrast parameter $\lambda > 0$.

We concentrate on the inverse problem of restoring an image that has been diffused and contaminated by noise.

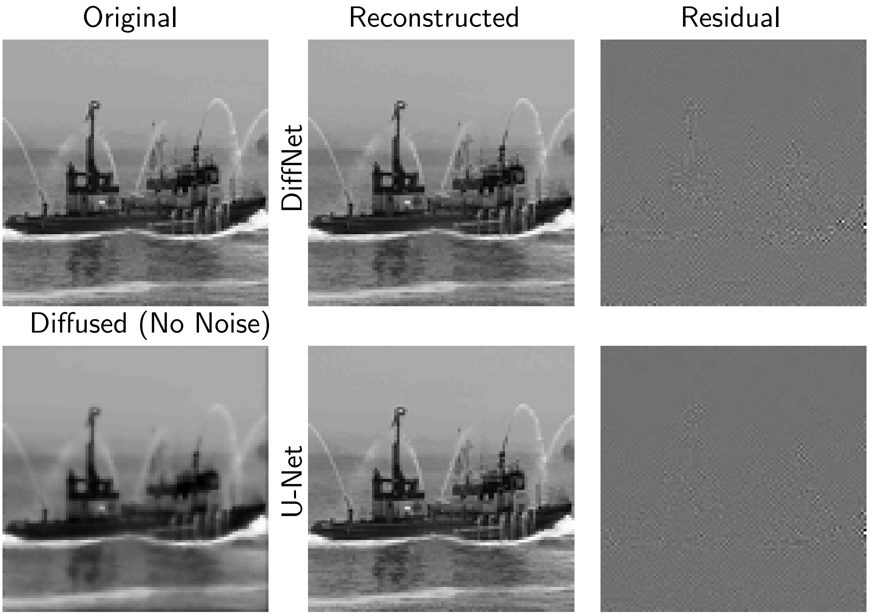
Training data

Data from the STL-10 database [Coates & Ng, 2011]: 100,000 images, resolution 96×96. (90,000 training, 10,000 test).

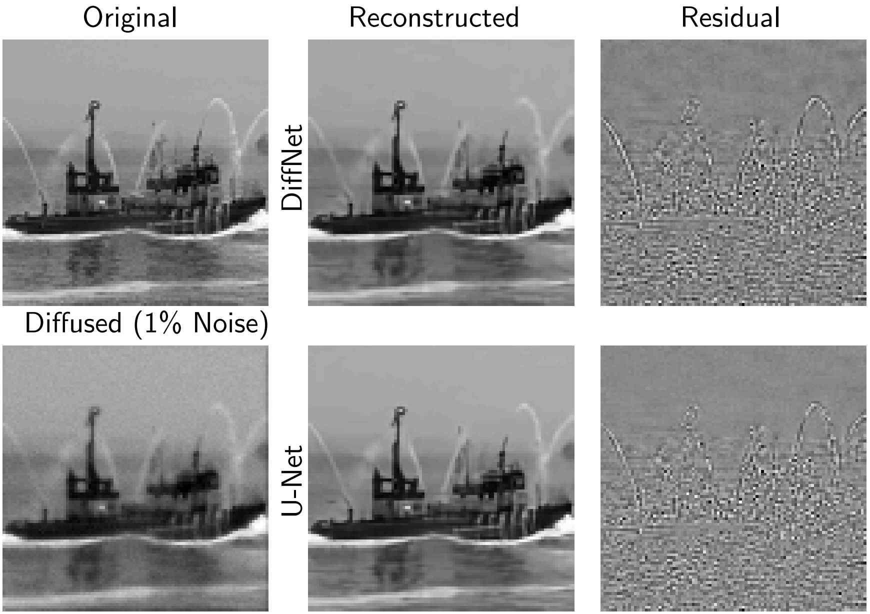
Diffused for 4 time steps with $\delta t = 0.1$ and $\lambda = 0.2$:



Comparison: Inversion (no noise)



Comparison: Inversion (1% noise)

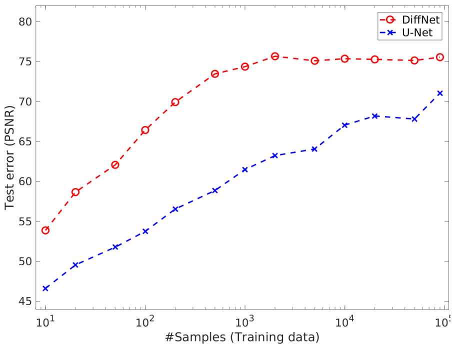


Some remarks

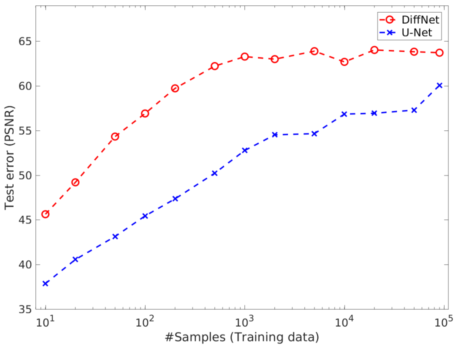
- Updates in DiffNet are performed explicitly and the CNN in the architecture is only used to produce the filters ζ.
- Hence DiffNet needs to learn a problem specific processing, in contrast to a purely data driven processing in a CNN.
- Amount of necessary learnable parameters is much lower:
  5-layer DiffNet: 101,310 parameters;
  U-Net with filter size 3×3: 34,512,705
- DiffNet uses only $\sim 0.3\%$ of parameters compared to U-Net.

Test error vs. training size

Forward Problem

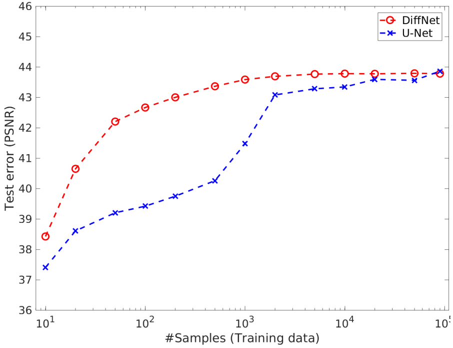


Inverse Problem (no Noise)

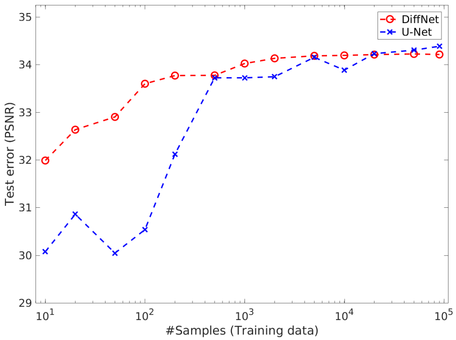


Test error vs. training size

Inverse Problem (0.1% noise)



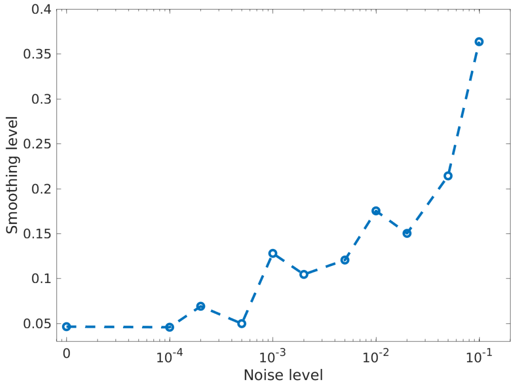
Inverse Problem (1% noise)



Increasing smoothing with noise level

We conjectured, that the learned update filters can be decomposed $W(\zeta) = L(\zeta) + \alpha S(\zeta)$. Thus, the magnitude α has to increase with higher noise.

We computed an estimate of S as $\sum_{i=1}^{4} \zeta_i - \zeta_5$ and interpret the smoothing level α as the mean of the absolute value of S.



Take home message

- By taking physics into account, we can obtain more expressive network architectures
- Reduction in necessary parameters and some interpretability

Reference: [Arridge, H, Journal of Mathematical Imaging and Vision (accepted)]

Acknowledgements

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Thank you for your attention