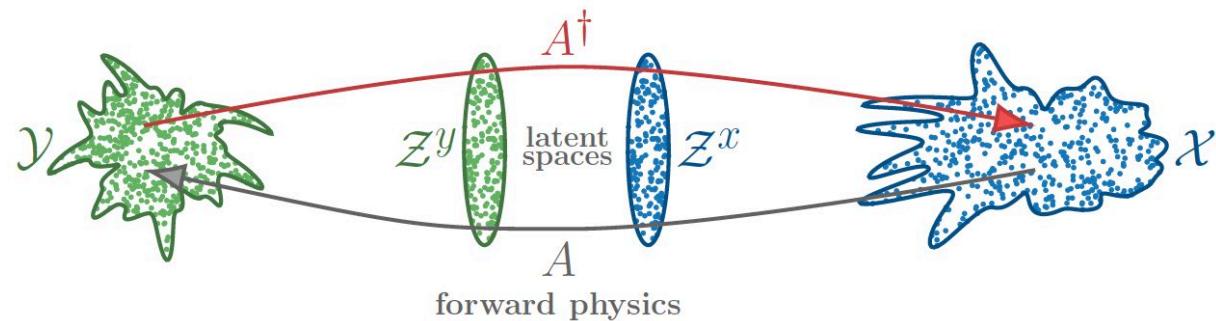


Learned SVD

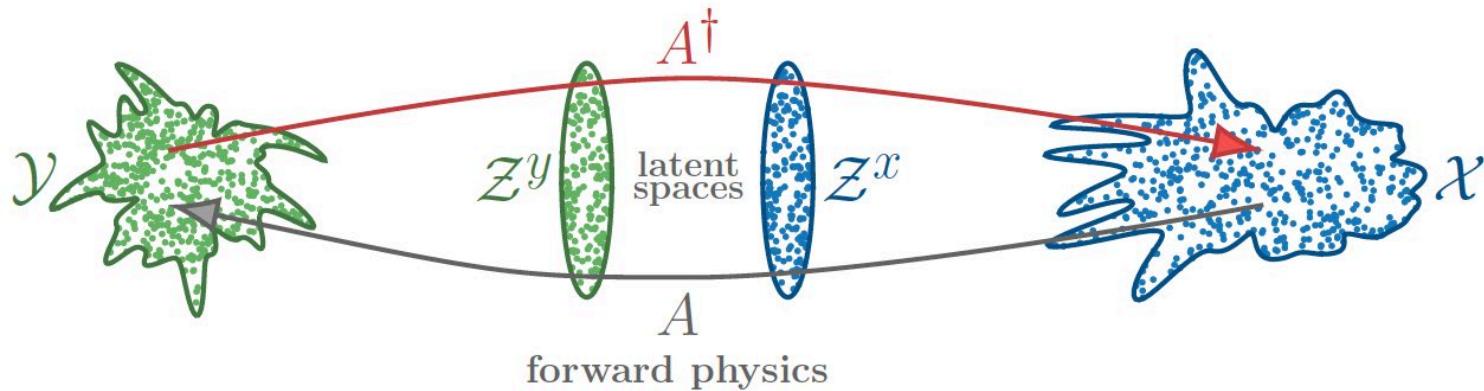
Deep Learning Decomposition for Inverse Problems

Yoeri Boink, Srirang Manohar, Stephan van Gils, Christoph Brune

Applied Analysis, SACS cluster
Applied Mathematics



WHAT IS A MEANINGFUL MAP?



- Well-posed (existence, uniqueness, stability)?
- Robust inversion / parameter estimation?
- Structure preserving?
- Understandable decomposition?
- Expressive?
- Generalizable?



$$\varphi(x) := \tau(W_L \tau(W_{L-1} \dots \tau(W_1 x) \dots))$$

INVERSE PROBLEMS

- Given measurements of the form

$$y^\delta = Ax + \eta^\delta$$

with x, y in appropriate Banach spaces and A (linear) operator between these spaces.

- Noise distribution η^δ known
- If pseudo-inverse A^\dagger available, it is typically **ill-posed (following Hadamard)**
- Example: A Radon transform (CT)

- Classical solution:** Tikhonov regularization

$$x_\alpha = (A^*A + \alpha \text{Id})^{-1} A^* y^\delta = V \underbrace{(S^2 + \alpha \text{Id})^{-1} S}_{S_\alpha^{-1}} U^* y^\delta$$

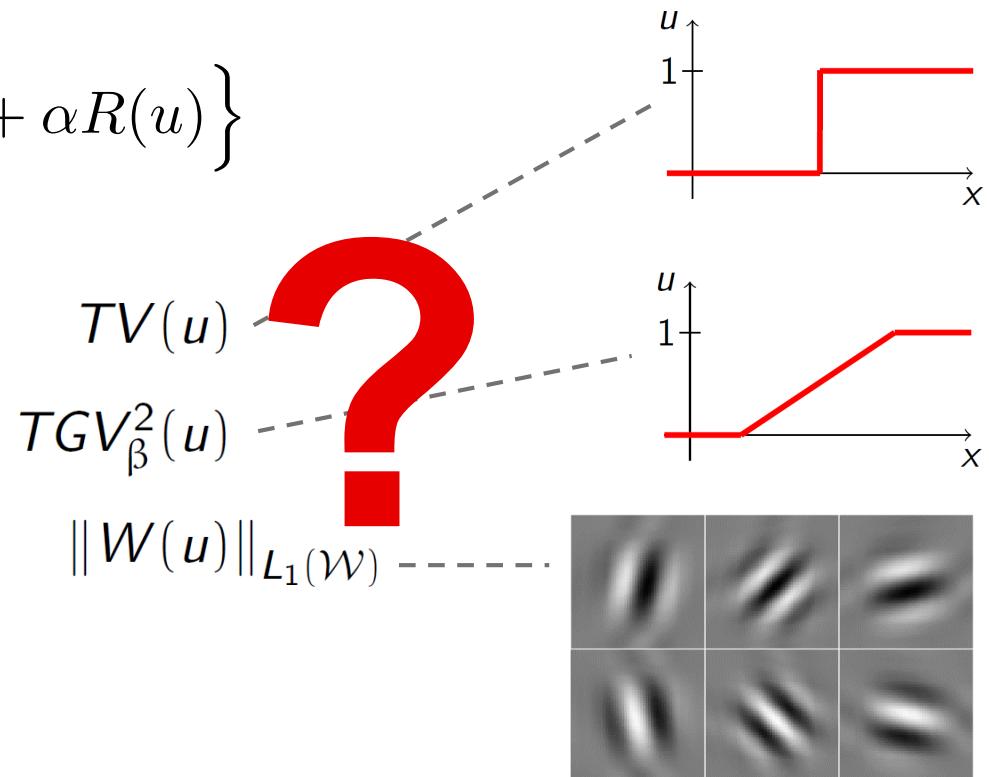
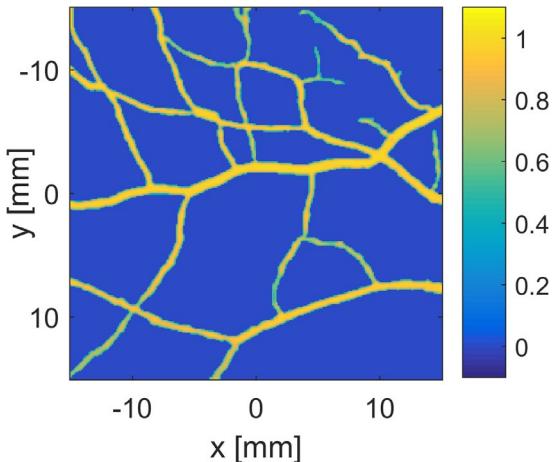
AN ILLUSTRATIVE GUIDE TO THE ART OF SHADOWS



ZAMCO & SONS, LLC. EDUCATIONAL LETTERPRESS, LANCASTER, PA

VARIATIONAL REGULARIZATION - CHOOSING FUNCTION SPACES

$$\min_{u \in L^2(\Omega)} \left\{ \|Au - f\|_{L^2(\Sigma)}^2 + \alpha R(u) \right\}$$



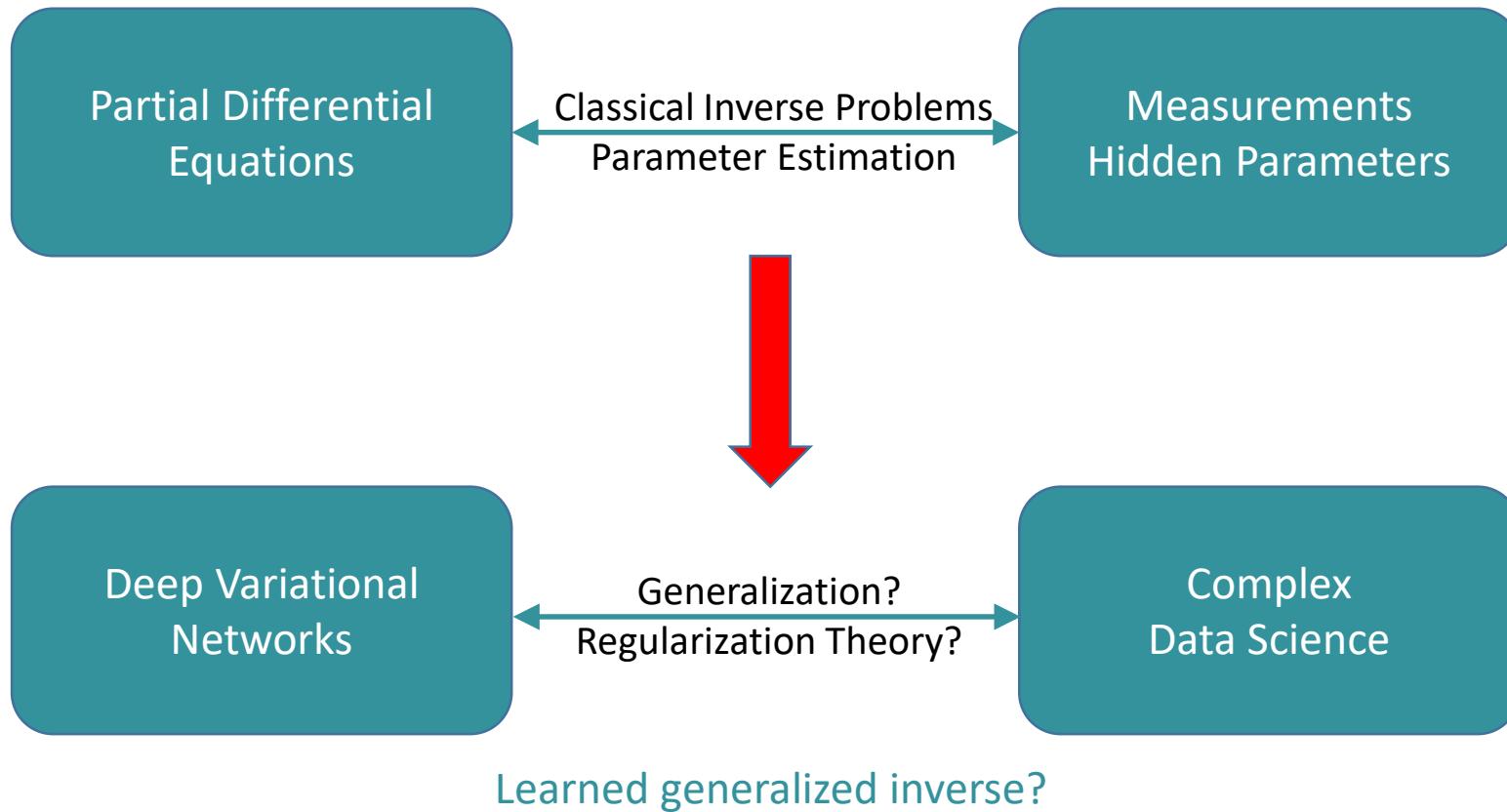
- Engl, Hanke, Neubauer (1996)
- Natterer, Wübbeling (2001)
- Candes, Romberg, Tao (2006)

- Kaltenbacher, Neubauer, Scherzer (2008)
- Schuster et al (2008)
- Osher, Burger, Goldfarb, Xu, Yin (2005)

- Rudin, Osher, Fatemi - Nonlinear total variation based noise removal algorithms (1992)
- Bredies, Kunisch, Pock - Total Generalised Variation (2010)

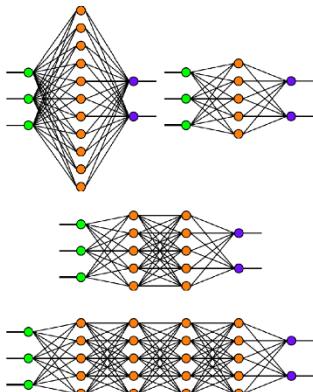
VARIATIONAL METHODS AND DEEP LEARNING

$$\min_{u \in L^2(\Omega)} \left\{ \|Au - f\|_{L^2(\Sigma)}^2 + \alpha R(u) \right\}$$



MATHEMATICS OF DEEP LEARNING

Architecture Design



uncertainty,
parameters

bi-level,
non-convex

accurate,
stable,
reproducible

training data,
generalization

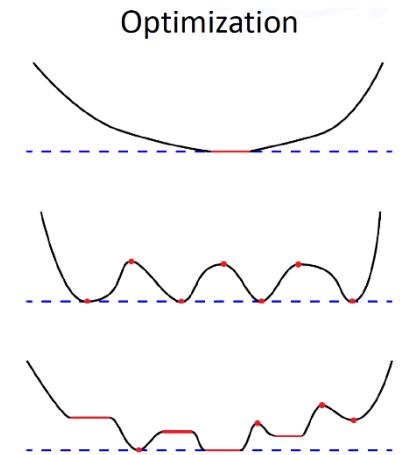
Architecture

Optimization

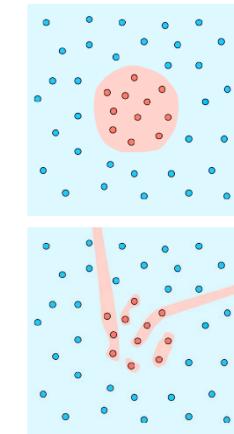
Modeling

Regularization

DL



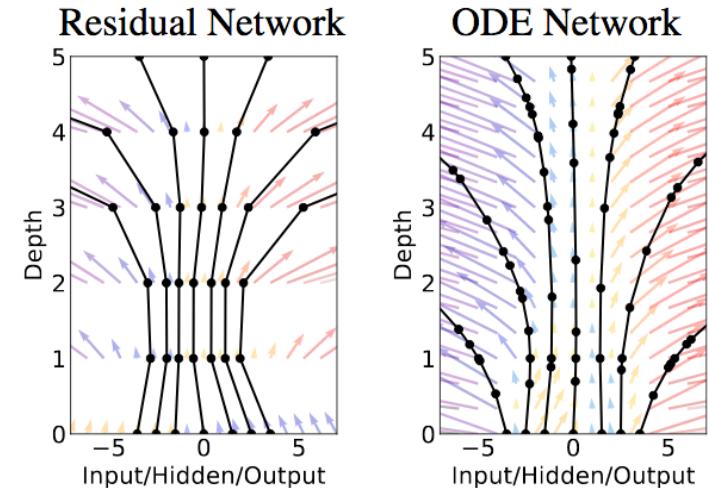
Generalization



Vidal et al. Mathematics of Deep Learning, 2018

VARIATIONAL METHODS AND DEEP LEARNING

Deep Residual Neural Networks
are connected to
Partial Differential Equations



Variational methods

	Norms nonconvex	Differential operators	Scale-space, Harmonic analysis	Regularization theory	Inverse problems	Vector fields, multimodality	Time dependent modeling
Deep networks	Activation functions ReLU, sigmoid	Convolutions functions per layer	Scattering networks	Generalization properties	AEs GANs	Multiple populations?	Residual? Skip connections?



Chen, Pock - Trainable Nonlinear Reaction Diffusion, 2016



Mallat - Understanding deep convolutional networks, 2016



Chen et al - Neural Ordinary Differential Equations, 2018



Ciccone et al - Stable Deep Networks from Non-Autonomous DEs, 2018



Haber, Ruthotto - Stable architectures for deep neural networks, 2017

DEEP LEARNING FOR INVERSE PROBLEMS

■ Fully Learned Models

$$x = \varphi_\theta(y)$$



Zhu et al – Image reconstruction by domain-transform manifold learning (Nature, 2018)

■ Post Processing

$$x = \varphi_\theta(A^\dagger(y))$$



Jin, McCann, Froustey, Unser – Deep Convolutional Neural Network for Inverse Problems in Imaging (2018)

■ Iterative Schemes

$$x_0 = A^\dagger(y)$$



Putzky, Welling - Recurrent Inference Machines for Solving Inverse Problems (2017)



Meinhardt, Möller, Hazirbas, Cremers - Learning Proximal Operators (2017)



Banert, Ringh, Adler, Karlsson, Öktem – Data-driven nonsmooth optimization (2018)

■ Learning a Regularizer



Li, Schwab, Antholzer, Haltmeier - NETT Solving Inverse Problems with Deep Neural Networks (2018)



Lunz, Öktem, Schönlieb – Adversarial Regularizers in Inverse Problems (2018)



Arridge et al – Solving inverse problems using data-driven models (Acta Numerica, 2019)

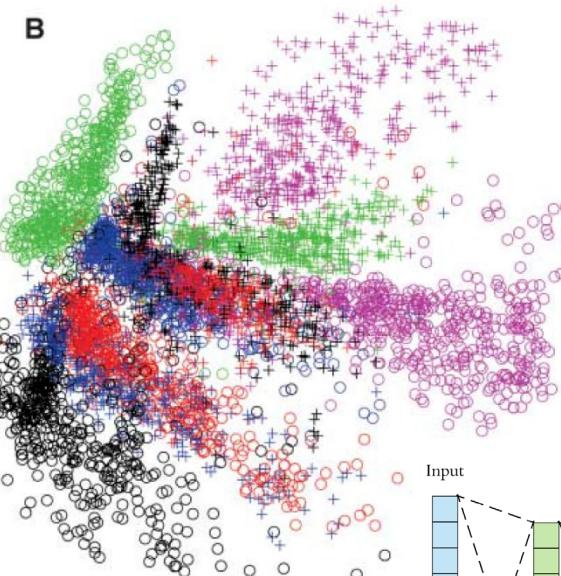
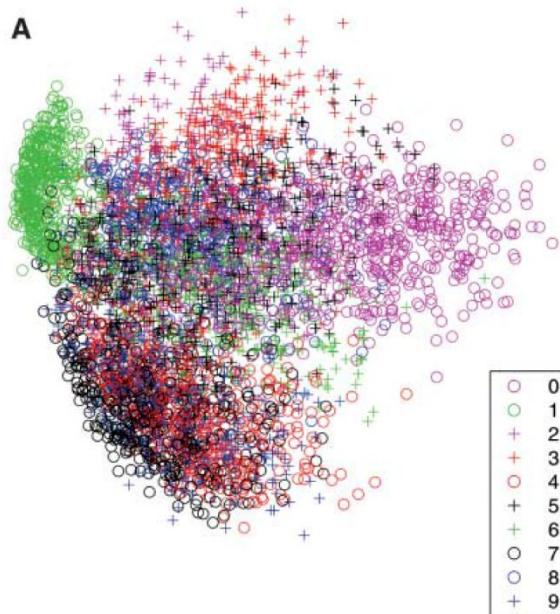
■ Review

DATA DIMENSIONALITY REDUCTION

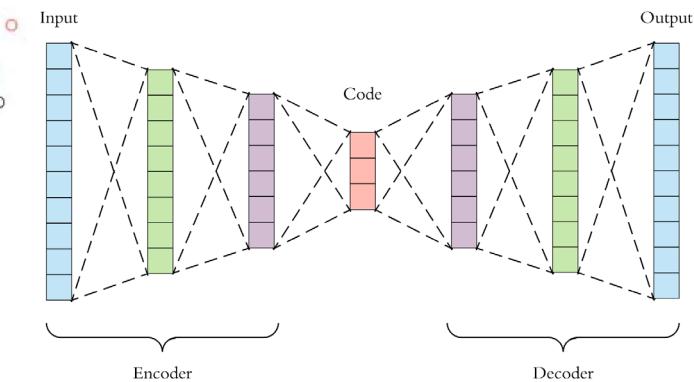
STRUCTURE, SCALE AND INTERPOLATION OF DATA

SVD
linear

$$\begin{aligned} M &= U \Sigma V^* \\ m \times n &\quad m \times m \quad m \times n \quad n \times n \\ U &\quad U^* = I_m \\ V &\quad V^* = I_n \end{aligned}$$

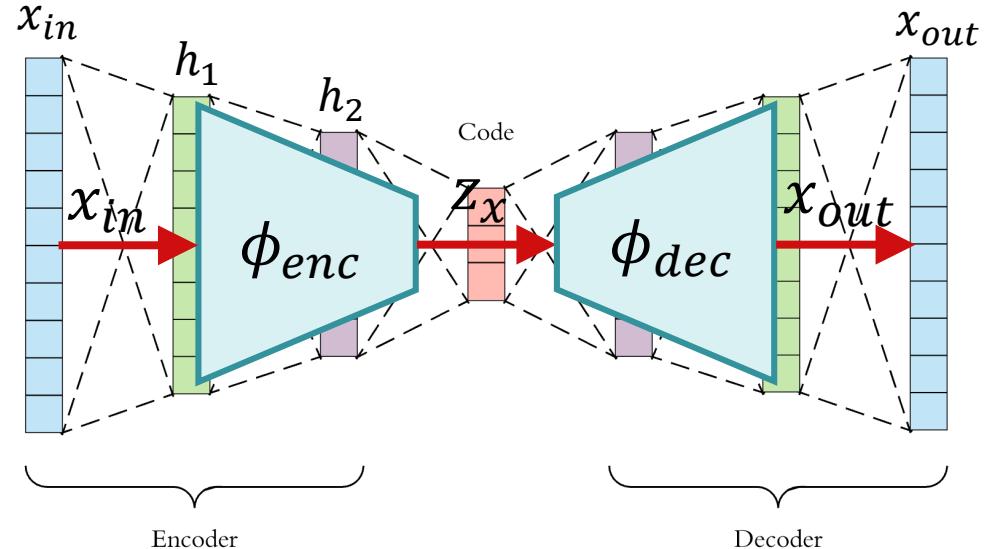
Autoencoder
nonlinear



Hinton - Reducing the Dimensionality of Data with Neural Networks (Science, 2006)

AUTOENCODERS (AE)

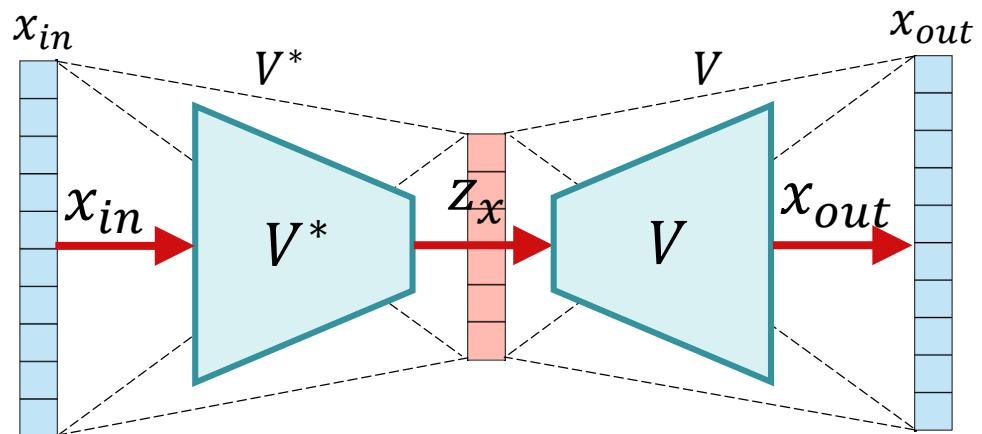
$$\left. \begin{array}{l} h_1 = \sigma(W_1 x_{in} + b_1) \\ h_2 = \sigma(W_2 h_1 + b_2) \\ \vdots \end{array} \right\} \quad x_{out} = \phi_{dec}(\phi_{enc}(x_{in}))$$



SVD: 2 connected AE

- 1 layer
- no nonlinearities σ
- no bias b

$$\begin{aligned} M &= U \Sigma V^* \\ m \times n &\qquad m \times m \qquad m \times n \qquad n \times n \\ U & \qquad U^* = I_m \\ V & \qquad V^* = I_n \end{aligned}$$



AUTOENCODERS AND GRADIENT FLOWS

- Assume we have a trained AE with tied weights, i.e. $f(x) = W^\top \phi(Wx)$
- x and $f(x)$ live in the same vector space, i.e.

$$G(x) = f(x) - x$$

is a vector field pointing from x to reconstructed $f(x)$

- Under assumptions, $G(x)$ is the gradient field of an energy $E(x)$

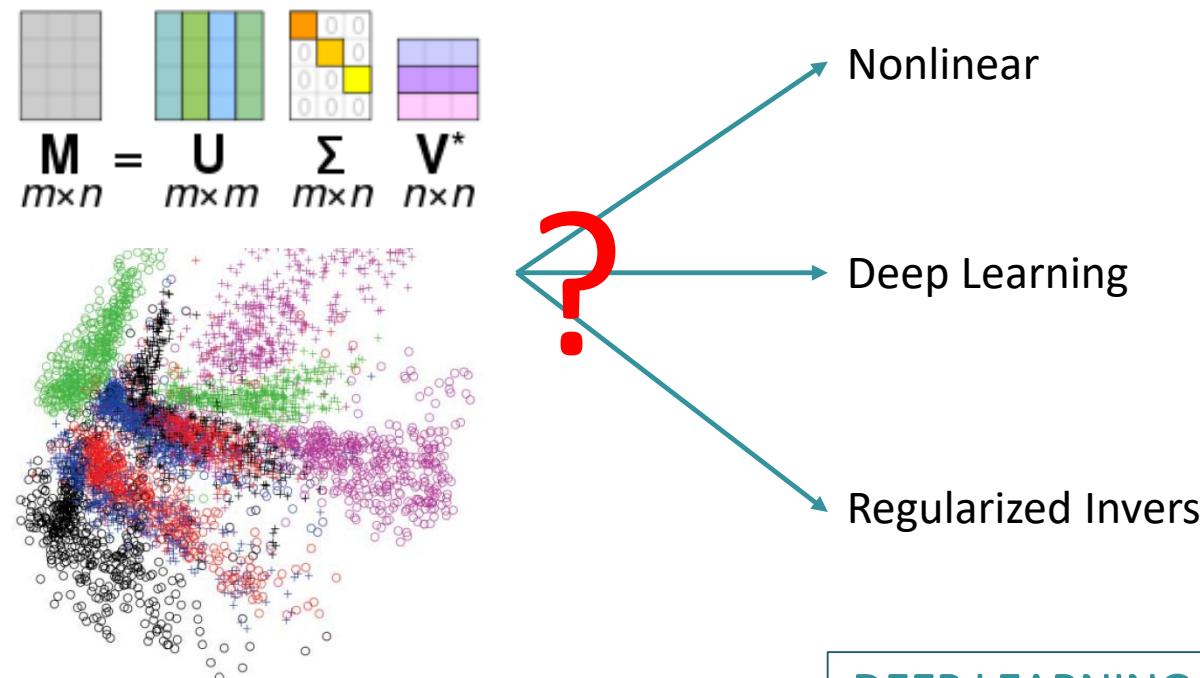
$$G(x) = f(x) - x \sim -\partial_x E$$

$$\Rightarrow \exists \text{ energy } E(x; W) \text{ with } f(x) = W^\top \phi(Wx) = x - \partial_x E(x; W)$$

$$E(x) = \sum_{i=1}^{N^2} \Phi((Wx)_i) + \frac{1}{2} \|x\|_2^2 \quad \text{with} \quad \phi(x) = -\Phi'(x)$$

NEW FRAMEWORK LEARNED SVD

DEEP LEARNING DECOMPOSITION FOR INVERSE PROBLEMS

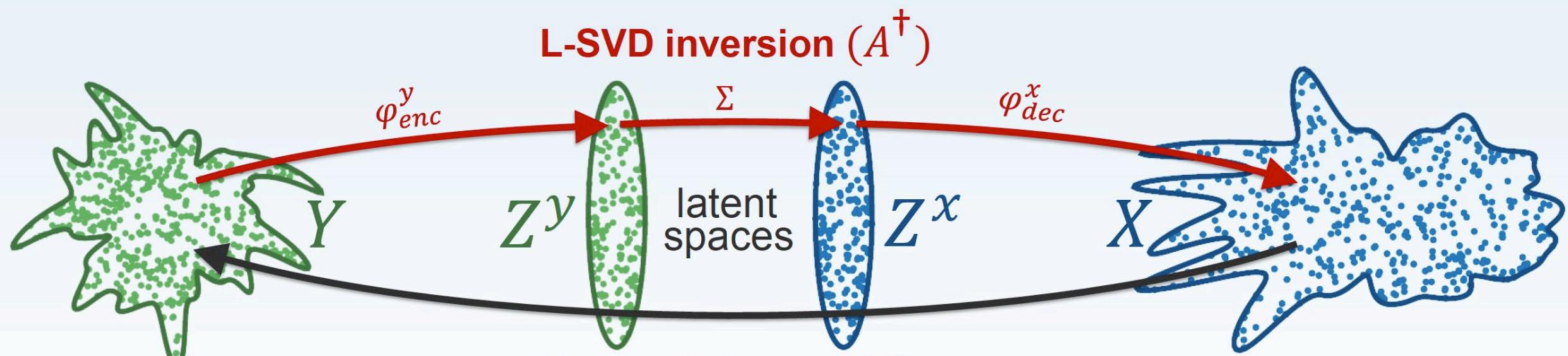


DEEP LEARNING MODEL

STRUCTURE, INTERPOLATION AND SCALE?

LEARNED SINGULAR VALUE DECOMPOSITION (L-SVD)

- Truncated SVD for linear inverse problems $y^\delta = Ax + \eta^\delta, A = USV^* \Rightarrow \tilde{x} = V_K S_K^{-1} U_K^* y^\delta$
- Propose nonlinear, learned SVD $\hat{x}^\Sigma = \varphi_{dec}^x (\Sigma \varphi_{enc}^y (y^\delta))$



- From model-driven to data-driven
- From linear to nonlinear encoding
- Regularization by hybrid autoencoding

LEARNED SINGULAR VALUE DECOMPOSITION (L-SVD)

We define the nonlinear functions

$$\varphi_{enc}^y : Y \mapsto Z^y, \quad \varphi_{dec}^y : Z^y \mapsto Y, \quad \varphi_{enc}^x : X \mapsto Z^x, \quad \varphi_{dec}^x : Z^x \mapsto X$$

and we define the square matrix $\Sigma \in \mathbb{R}^{k \times k}$. Moreover we define the variables

$$\begin{aligned} z_y &:= \varphi_{enc}^y(y^\delta), & z_x^{AE} &:= \varphi_{enc}^x(x), & z_x^\Sigma &:= \Sigma z_y, \\ \hat{y}^{AE} &:= \varphi_{dec}^y(z_y), & \hat{x}^{AE} &:= \varphi_{dec}^x(z_x^{AE}), & \hat{x}^\Sigma &= \varphi_{dec}^x(z_x^\Sigma). \end{aligned}$$

$$\min_{\text{par}_{\text{NN}}} \left\{ \sum_{i=1}^{\#\text{train}} \underbrace{D_1(\hat{x}_{(i)}^\Sigma, x_{(i)})}_{\text{reconstruction}} + \alpha_y \underbrace{D_2(\hat{y}_{(i)}^{AE}, y_{(i)})}_{\text{autoencoder}} + \alpha_x \underbrace{D_3(\hat{x}_{(i)}^{AE}, x_{(i)})}_{\text{autoencoder}} \right\}$$

LEARNED SINGULAR VALUE DECOMPOSITION (L-SVD)

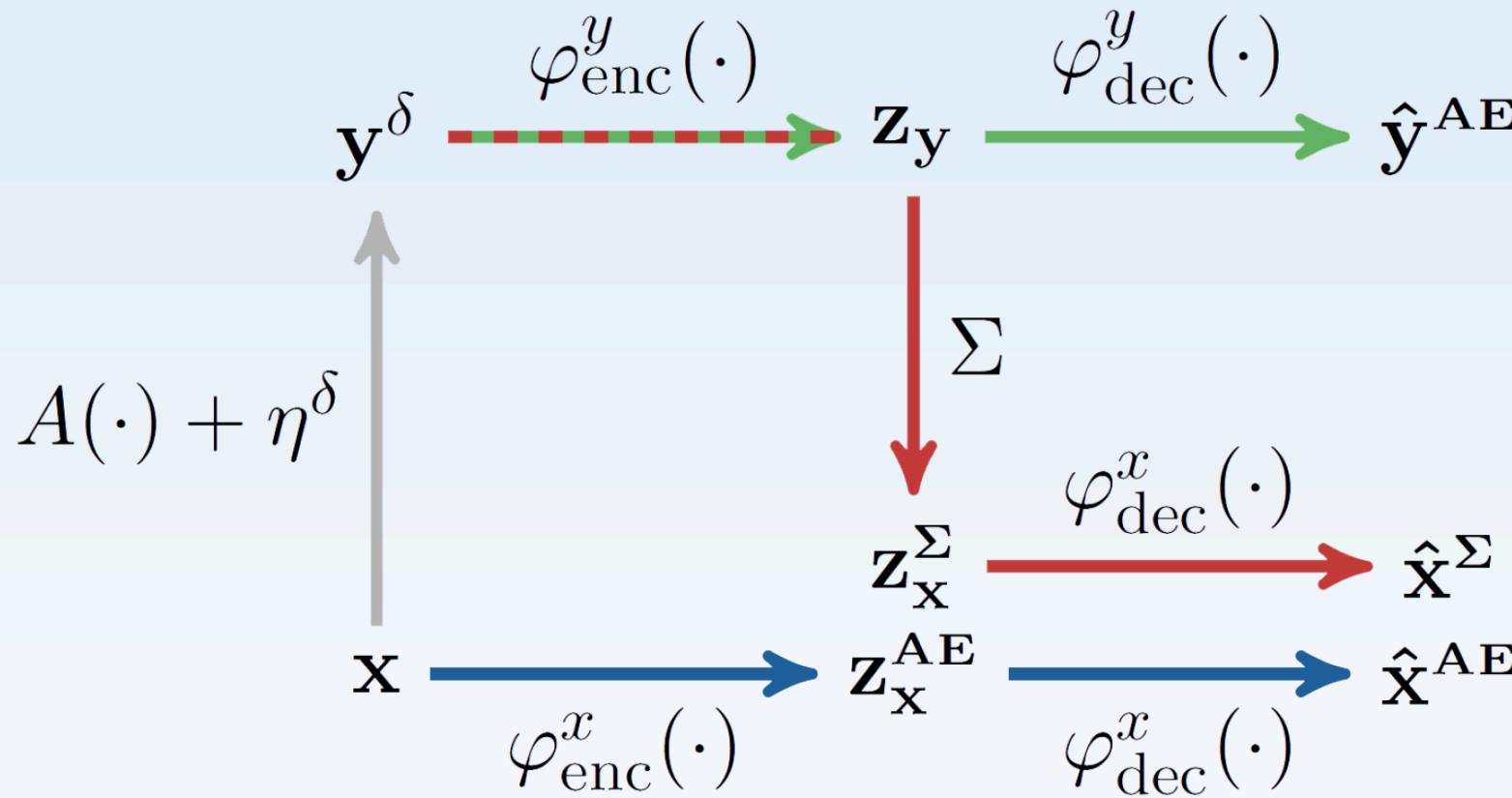
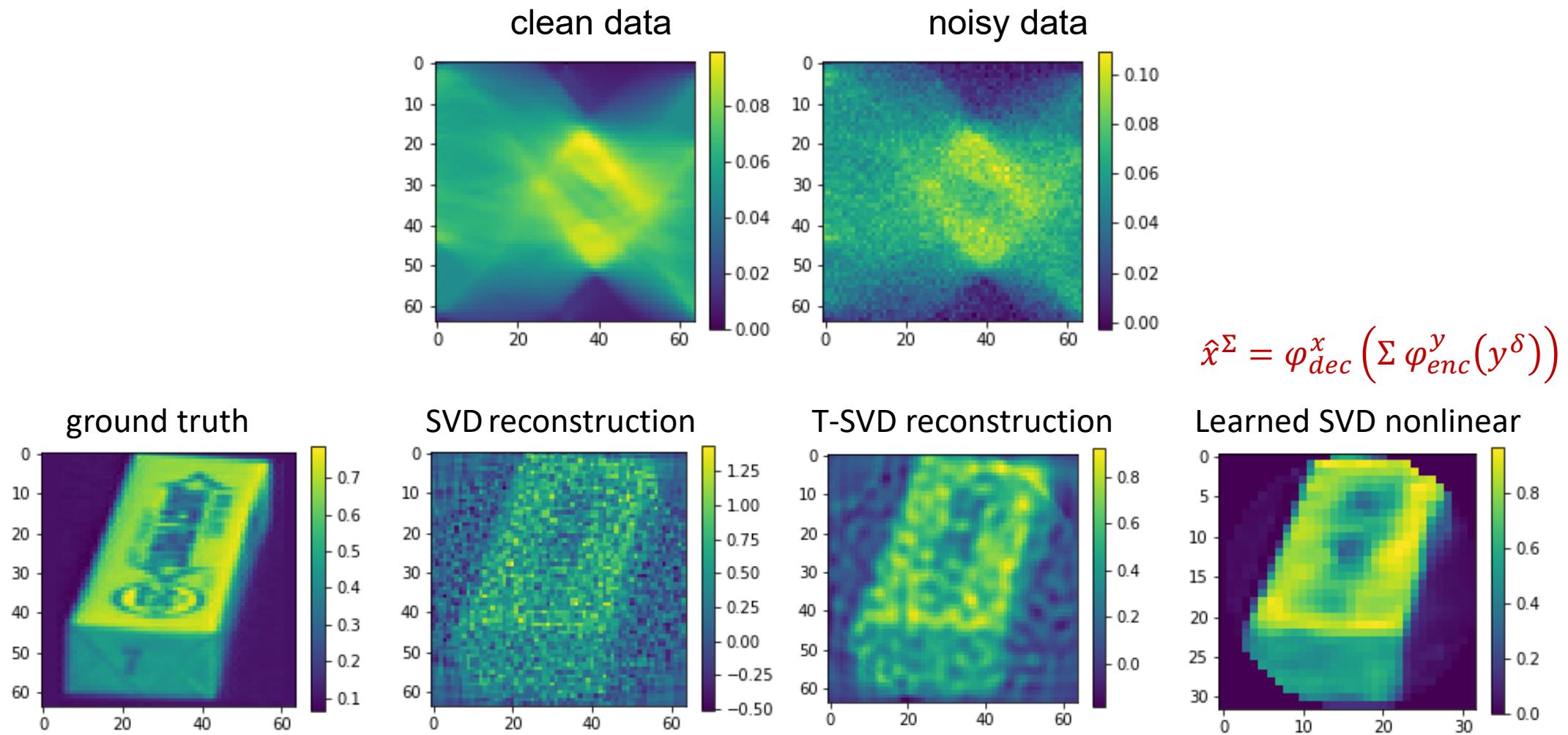


Figure 1: in **green** the autoencoder for data y^δ ; in **blue** the autoencoder for signal x ; in **red** the reconstruction procedure.

SOLVING THE INVERSE PROBLEM



SIMULATION EXPERIMENTS

- Simulation experiments for CT-reconstruction (A is Radon transform).
- Trained on rescaled MNIST dataset (64x64 pixels).
- Two scenarios were tested:
 - 1) linear L-SVD, ‘full-angle’ (64 angles), no bottleneck latent space ($Y = Z^y = Z^x = X = \mathbb{R}^{4096}$);
 - 2) nonlinear L-SVD, limited-angle (8 angles), bottleneck latent space ($Y = \mathbb{R}^{256}$, $Z^y = Z^x = \mathbb{R}^{64}$, $X = \mathbb{R}^{4096}$).
- Gaussian noise on data with standard deviation $\delta = 0.05$.
- Fully-connected networks, 4 layers in AE_X , 1 layer in AE_Y .
- No biases.
- Leaky ReLU with parameter 0.1 in autoencoders.
- Adam optimiser with learning rate 0.001.

MODEL-DRIVEN TO DATA-DRIVEN

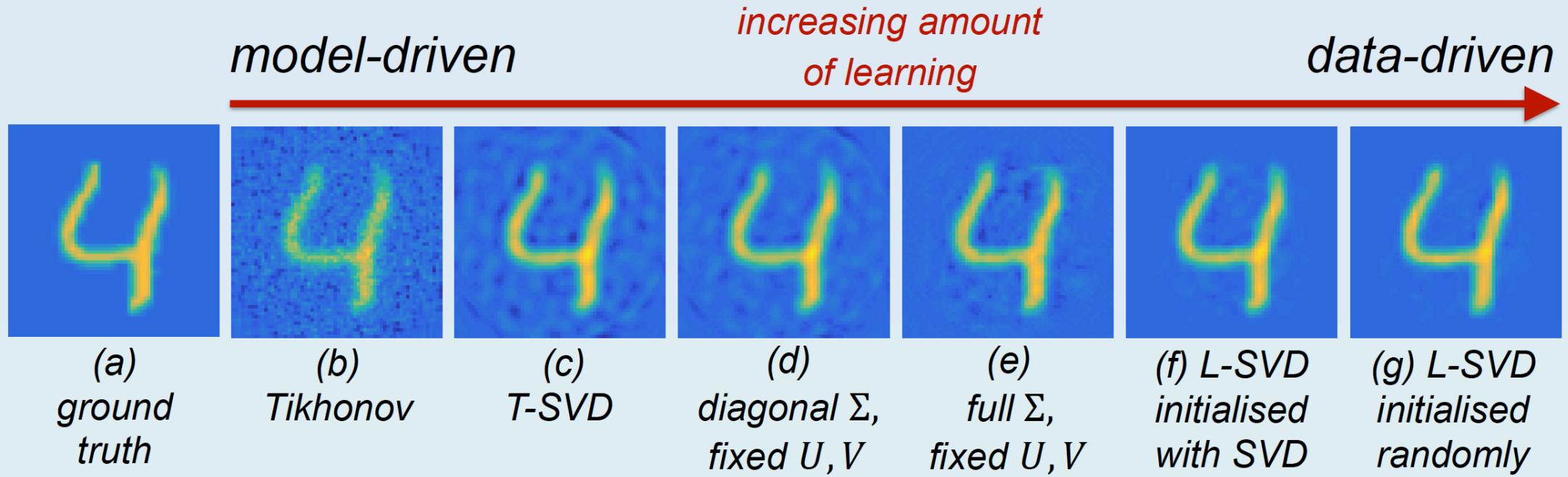


Figure 2: linear reconstruction methods with increasing amount of learning. Linear L-SVD provides better results than methods that are less data-driven.

HYBRID DICTIONARY LEARNING

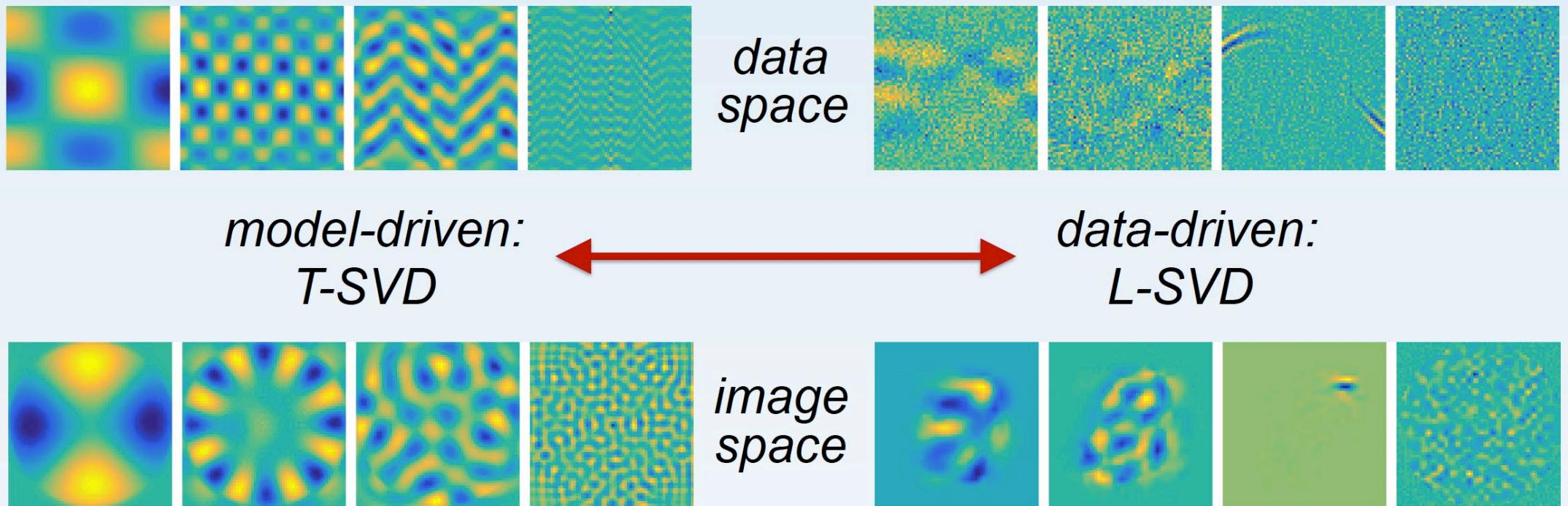
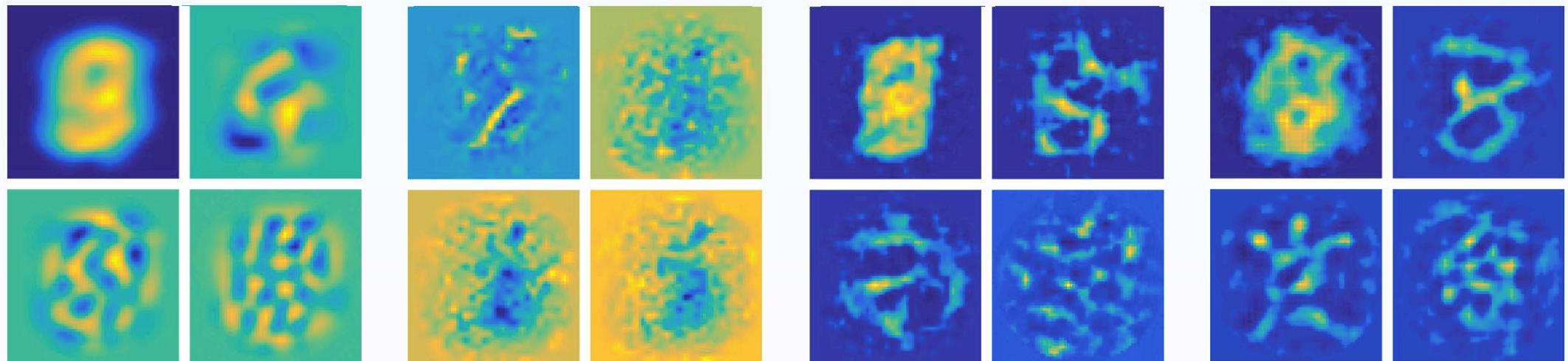


Figure 3: selected ‘dictionary elements’ from T-SVD and linear L-SVD. L-SVD shows similar structures (harmonics) as T-SVD, but with a stronger focus on the specific data.

HYBRID LATENT SPACE REPRESENTATION



(a) *linear AE/L-SVD*

(b) *nonlinear AE*

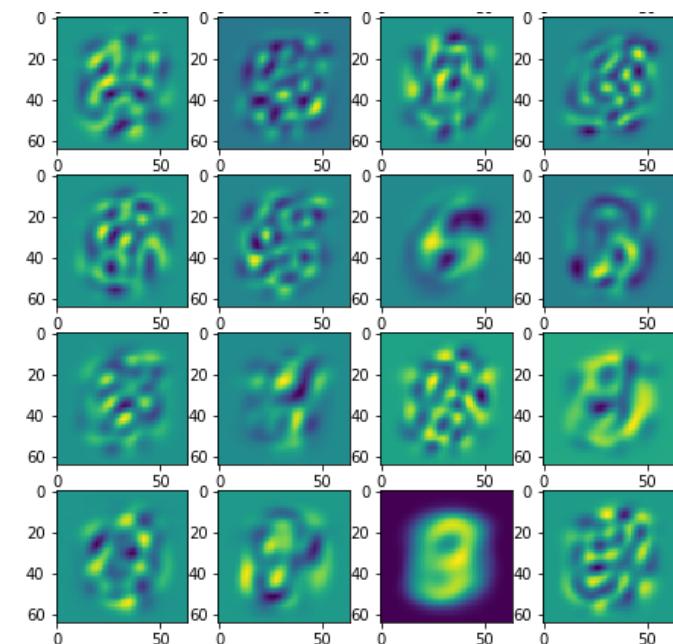
(c) *L-SVD without
AE branches*

(d) *L-SVD*

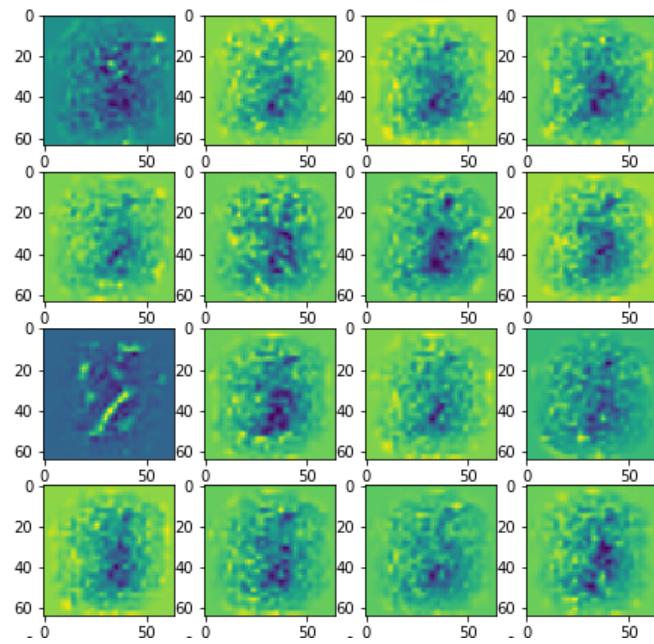
- Selected unit vectors from latent space decoded to image space
- Nonlinear L-SVD learns more interpretable representation
- Combines features from data space, image space and operator
- Autoencoder provides ‘smoother’ and better connected structures

STRUCTURE: LATENT REPRESENTATIONS

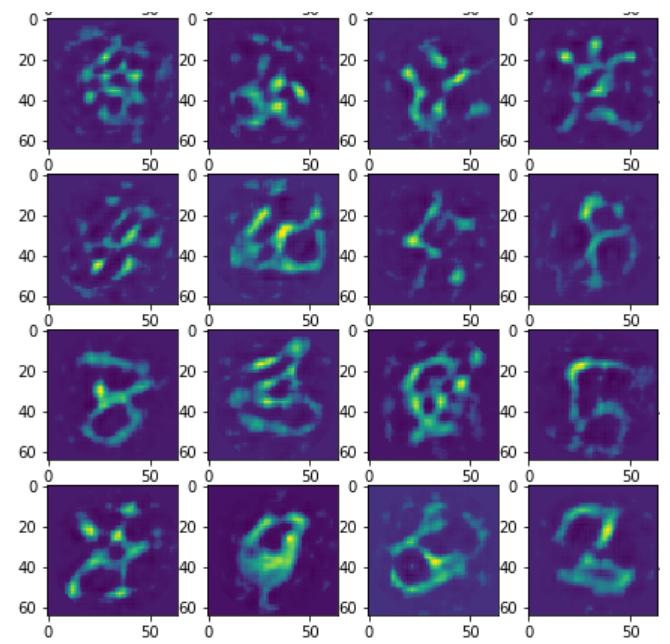
linear AE/L-SVD



nonlinear AE

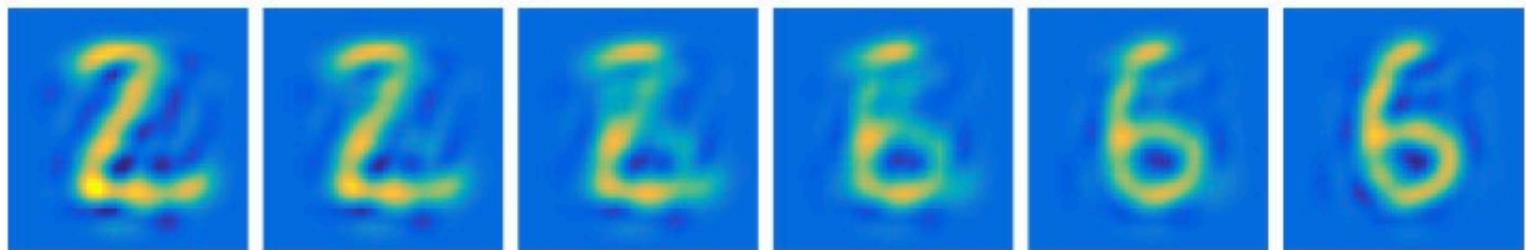


L-SVD

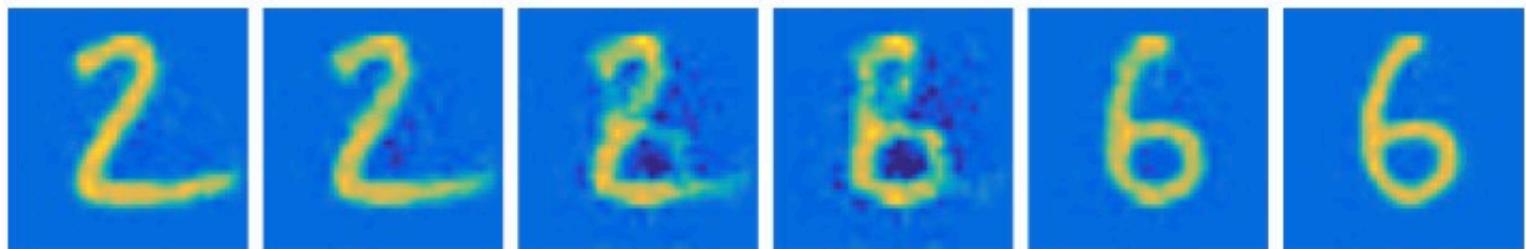


INTERPOLATION

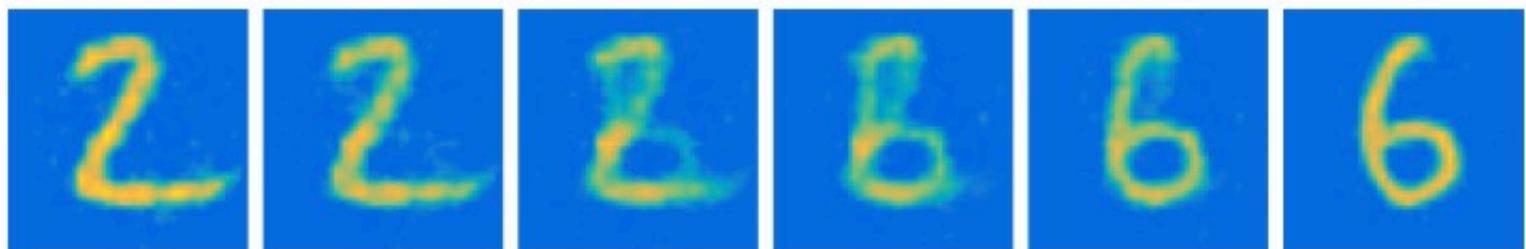
linear L-SVD



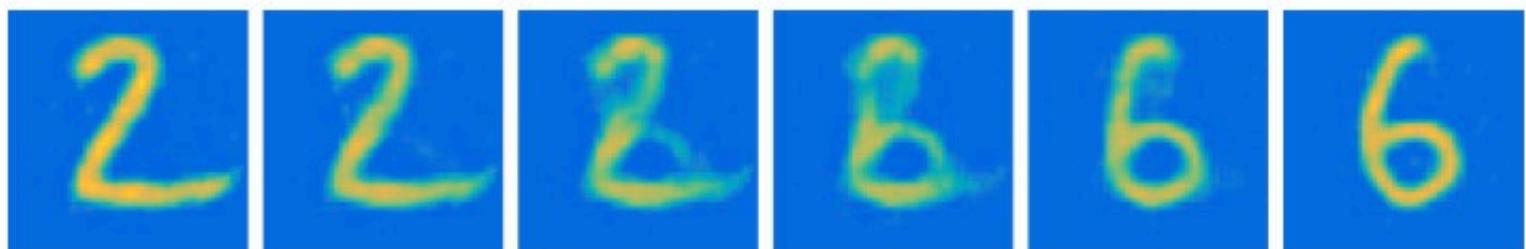
nonlinear AE



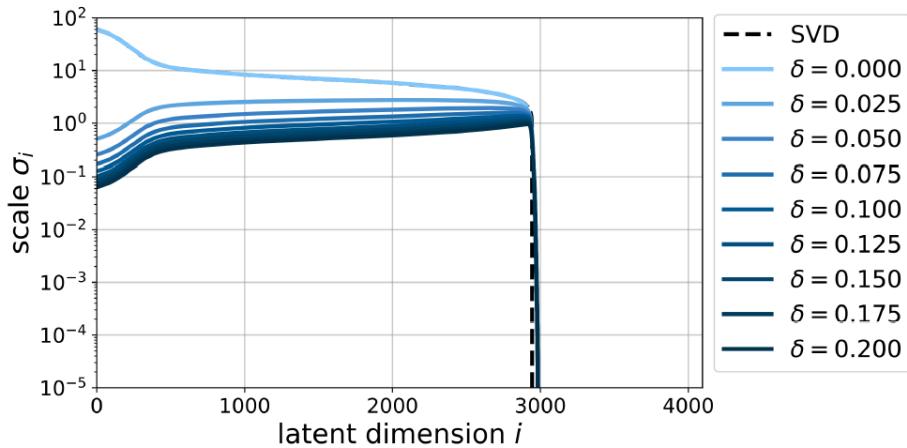
nonlinear RecNet



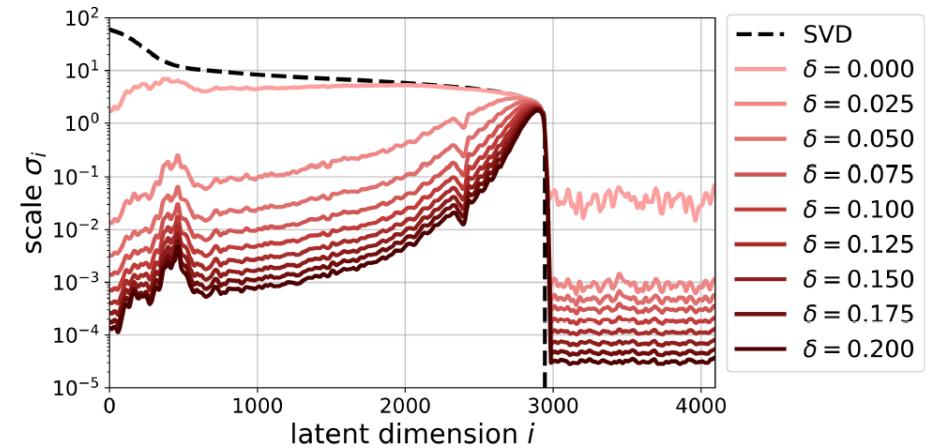
nonlinear L-SVD



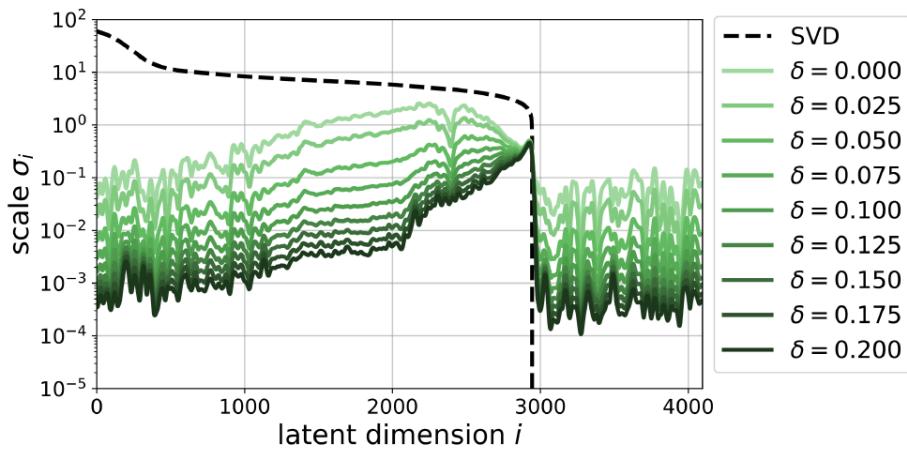
LEARNED REGULARIZATION (SCALES FROM NOISE)



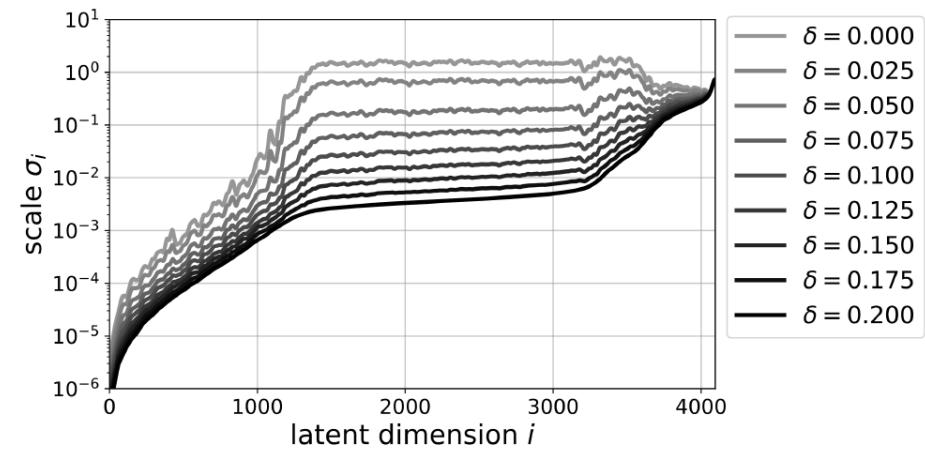
(a) Tikhonov regularisation



(b) only scales learned: U, V fixed



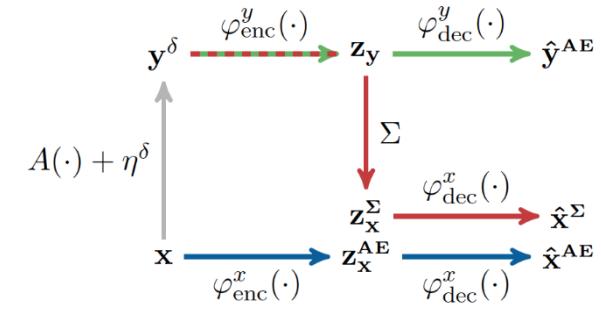
(c) L-SVD with SVD initialisation



(d) L-SVD with random initialisation

STABILITY ESTIMATE

$$\begin{aligned}
\|\hat{x}_{(1)}^\Sigma - \hat{x}_{(2)}^\Sigma\|_{\ell^2} &\leq \|\varphi_{\text{dec}}^x\|_{\text{op}} \|\hat{z}_{x,(1)} - \hat{z}_{x,(2)}\|_{\ell^2} \\
&\leq |\sigma_{\max}| \|\varphi_{\text{dec}}^x\|_{\text{op}} \|\hat{z}_{y,(1)} - \hat{z}_{f,(2)}\|_{\ell^2} \\
&\leq \|\varphi_{\text{enc}}^y\|_{\text{op}} |\sigma_{\max}| \|\varphi_{\text{dec}}^x\|_{\text{op}} \|y_{(1)} - y_{(2)}\|_{\ell^2}
\end{aligned}$$



RECONSTRUCTION ERROR ESTIMATE

Theorem 3.3. Consider the L-SVD network as defined in section 3.1. Assume that for some $0 < \varepsilon_z < 1$ we have that for all $\tilde{z}_x \in B_1$, $\|\tilde{z}_x - z_x^\Sigma\|_{\ell^2} < \varepsilon_z$. Then there exists a $C > 0$ s.t. for all $\tilde{z}_x \in B_1$, $\|\varphi_{\text{dec}}^x(\tilde{z}_x) - \varphi_{\text{dec}}^x(\Sigma \varphi_{\text{enc}}^y(A \varphi_{\text{dec}}^x(\tilde{z}_x)))\|_{\ell^2} < C$. Moreover, for all $x \in \mathbb{R}^n$ for which $\varphi_{\text{enc}}^x(x) \in B_{1-\varepsilon_z}$, we have the error estimate $\|x - \varphi_{\text{dec}}^x(\Sigma \varphi_{\text{enc}}^y(Ax))\|_{\ell^2} < C$.



Y.E. Boink, C. Brune - Learned SVD: Solving Inverse Problems via Hybrid Autoencoding (arXiv preprint, Nov 2019)

RESEARCH CONTEXT

MANIFOLD LEARNING, INVERSE PROBLEMS

-  Zhu et al – Image reconstruction by domain-transform manifold learning (Nature, 2018)
-  Lunz et al – Adversarial Regularizers in Inverse Problems (Neurips, 2018)
-  Angles, Mallat – Generative networks as inverse problems with scattering transforms (ICLR, 2018)
-  Wong et al – Training Auto-encoder-based Optimizers for Terahertz Image Reconstruction (arXiv, 2019)

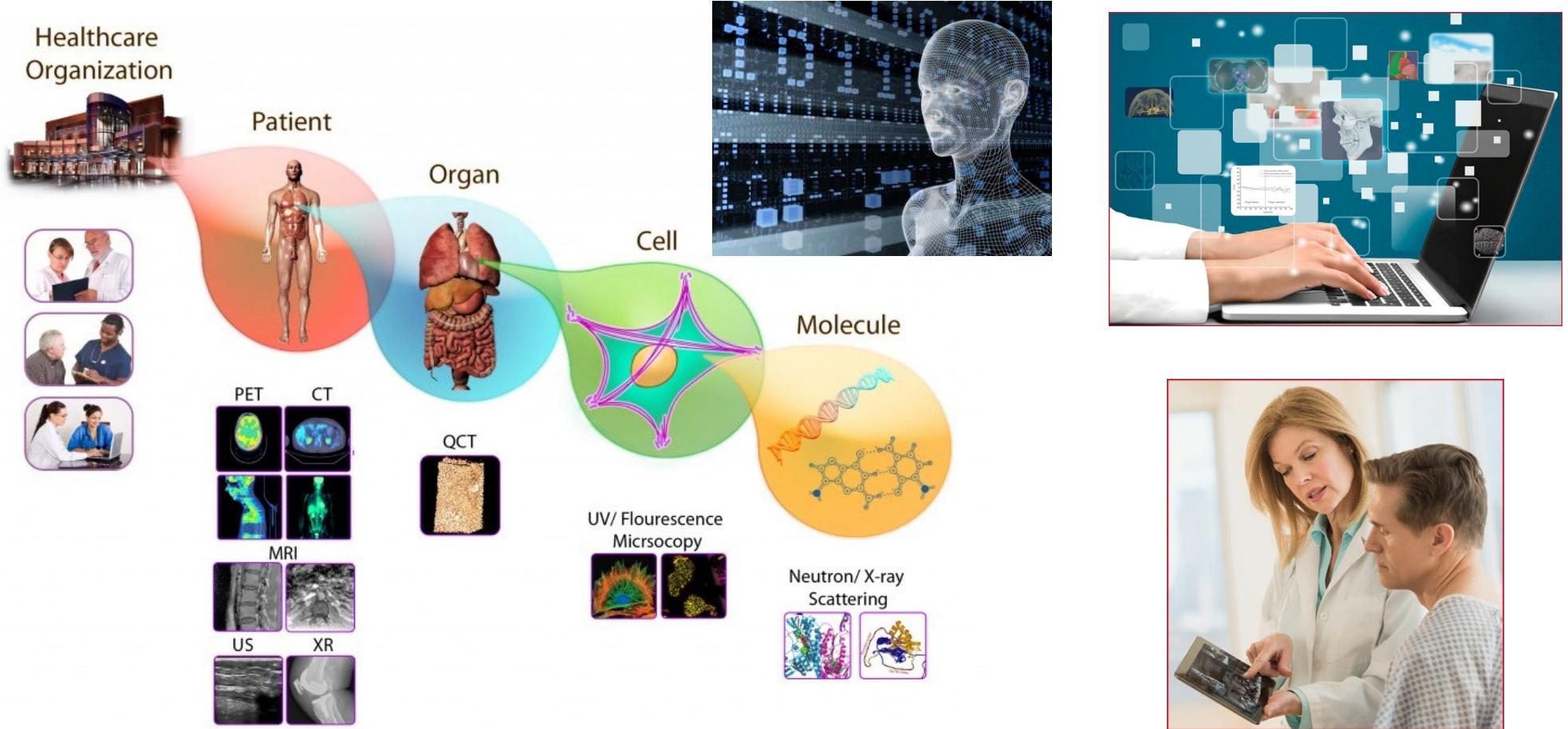
SEMI-SUPERVISED AUTOENCODERS

-  Ye et al – Understanding Geometry of Encoder-Decoder CNNs (ICML, 2019)
-  Le et al – Supervised autoencoders: Improving generalization performance with unsupervised regularizers (NeurIPS, 2018)
-  Epstein et al – Generalization bounds for unsupervised and semi-supervised learning with AutoEncoders (arXiv, 2019)

MODEL REDUCTION AND LEARNING

BAYESIAN INVERSION AND SPARSITY

Deep Learning for Inverse Problems in Medical Imaging



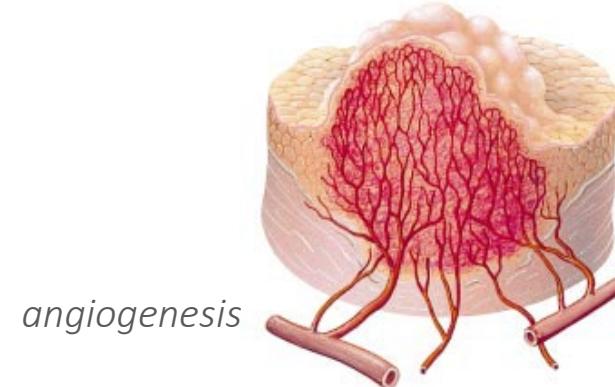
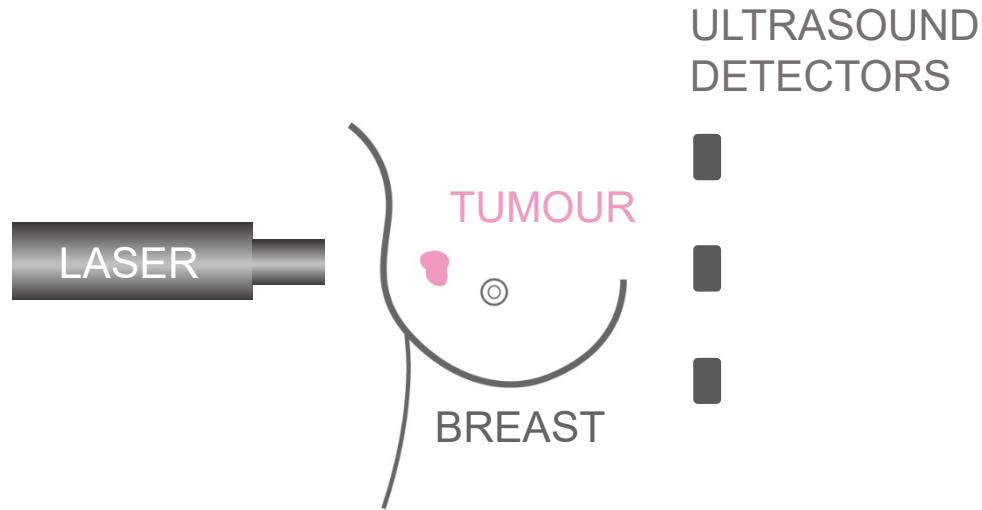
Multimodality, multiscale, multidimension, big data, mobile...

Deep Learning in Medical Imaging: Overview and Future Promise of an Exciting New Technique, IEEE Trans Med Imag, 2016

PHOTOACOUSTIC BREAST IMAGING

Folkman, 1996

(ILLUSTRATIONS MADE BY SJOUKJE SCHOUSTRA – BMPI GROUP, UNI TWENTE)

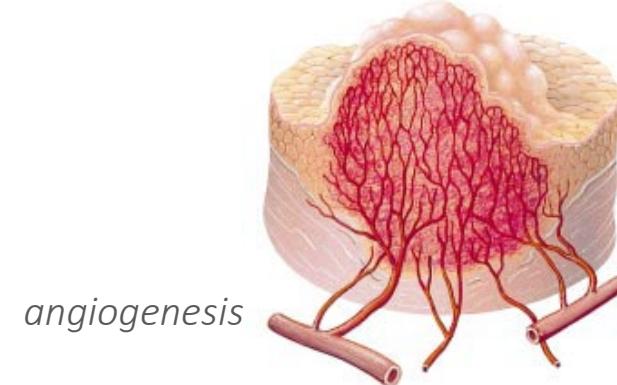
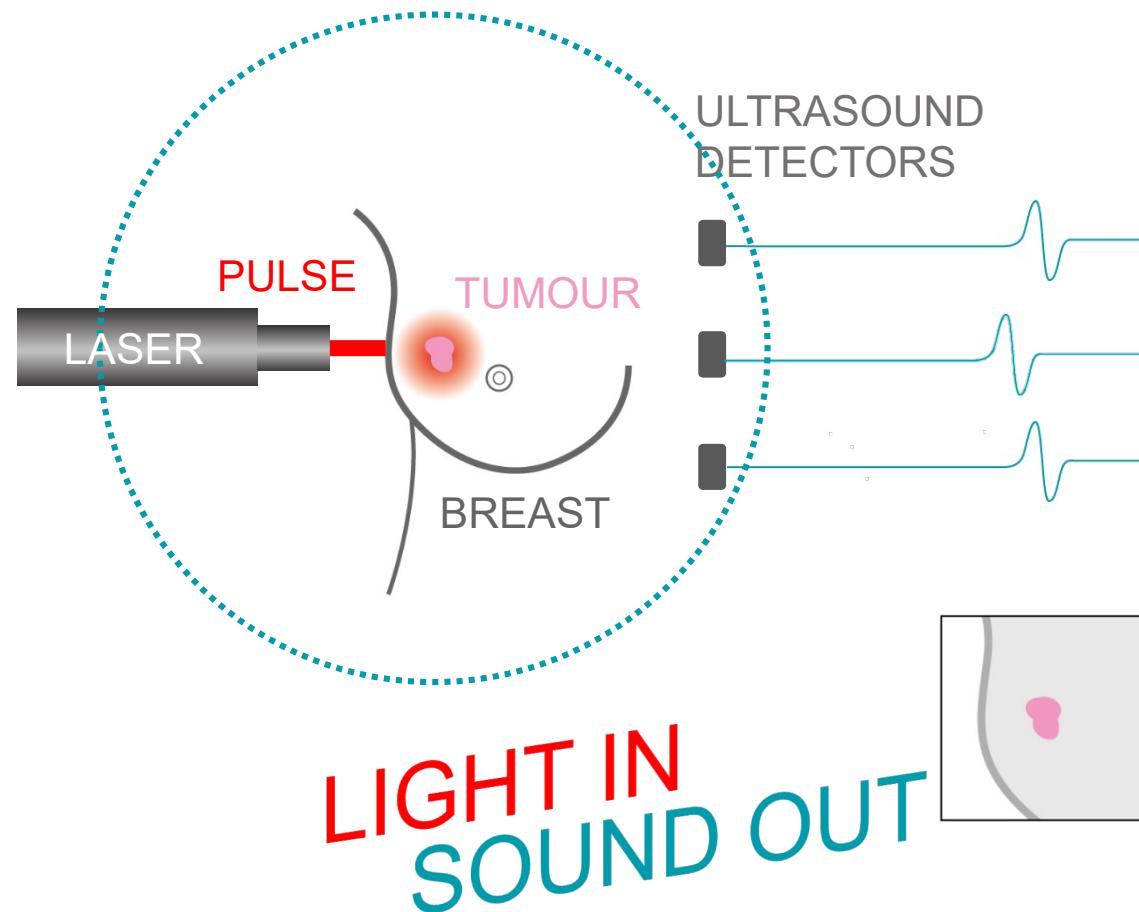


**LIGHT IN
SOUND OUT**

PHOTOACOUSTIC BREAST IMAGING

(ILLUSTRATIONS MADE BY SJOUKJE SCHOUSTRA – BMPI GROUP, UNI TWENTE)

Folkman, 1996



PHOTOACOUSTIC EFFECT

- LIGHT ABSORPTION
- TEMPERATURE RISE
- EXPANSION
- PRESSURE RISE
- ULTRASOUND WAVE
- SIGNALS
- RECONSTRUCTION

PHOTOACOUSTIC TOMOGRAPHY

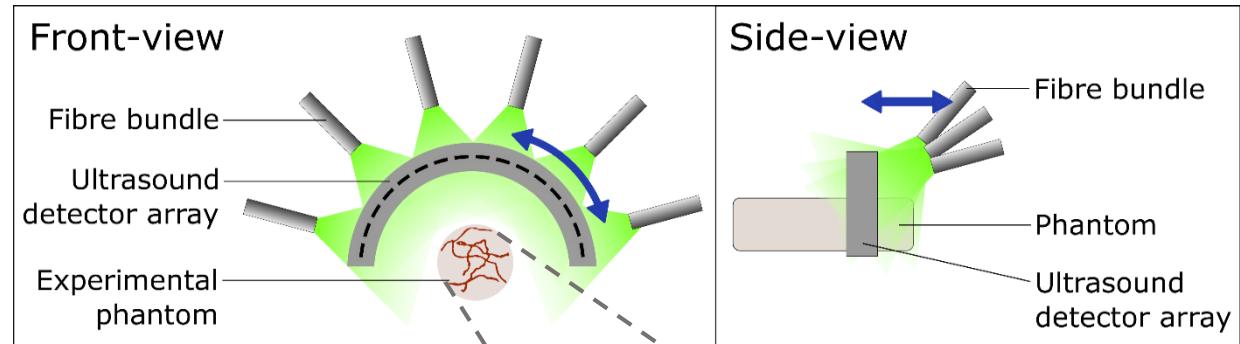
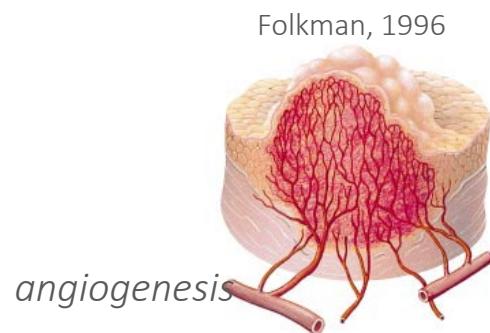


Figure: 2D slice-based imaging with rotating fibres and sensor array.¹

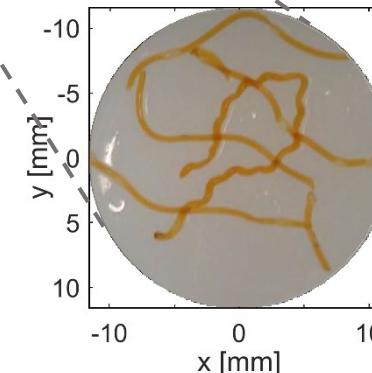
We make use of a projection model with calibration²:

$$\tilde{p}(x, t) = \left(\frac{1}{t} \iint_{|x-\tilde{x}|=ct} u(\tilde{x}) d\tilde{x} \right) *_t \frac{\partial I(t)}{\partial t} *_t h_{IR}(t),$$

$$\tilde{p}(x, t) = \left(\frac{1}{t} \iint_{|x-\tilde{x}|=ct} u(\tilde{x}) d\tilde{x} \right) *_t p_{cal}(t),$$

$$f = Au := \iint_{|x-\tilde{x}|=ct} u(\tilde{x}) d\tilde{x}$$

↓
PAT-operator



¹ Van Es, Vlieg, Biswas, Hondebrink, Van Hespen, Moens, Steenbergen, Manohar - Coregistered photoacoustic and ultrasound tomography of healthy and inflamed human interphalangeal joints (2015)

² Wang, Xing, Zeng, Chen - Photoacoustic imaging with deconvolution (2004)

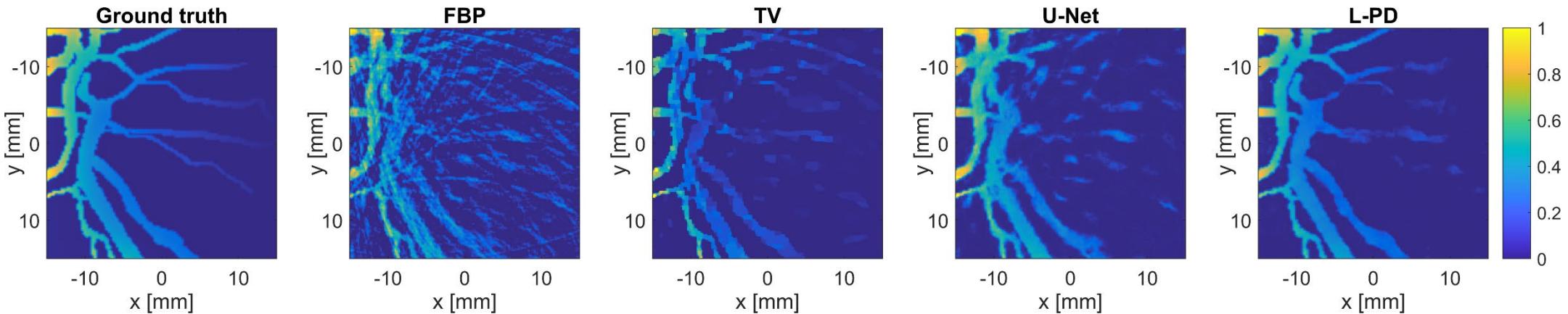
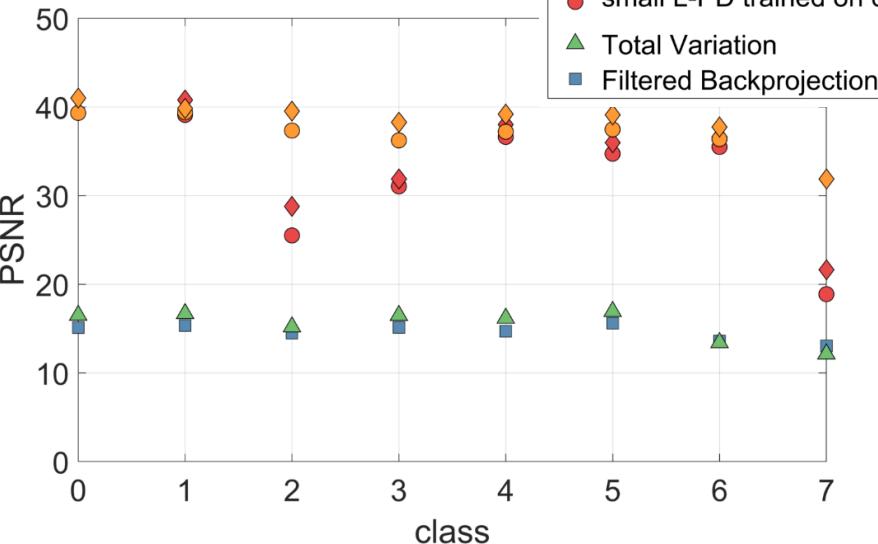
DEEP LEARNING PHOTOACOUSTIC TOMOGRAPHY

for $n \leftarrow 1$ to N **do**

$$q_{\{1,\dots,k\}}^{n+1} = q_{\{1,\dots,k\}}^n + \Gamma_{\Theta_n} \left(q_{\{1,\dots,k\}}^n, Au_1^n, f \right),$$

$$u_{\{1,\dots,k\}}^{n+1} = u_{\{1,\dots,k\}}^n + \Lambda_{\Theta_n} \left(u_{\{1,\dots,k\}}^n, A^* q_1^{n+1} \right).$$

end for

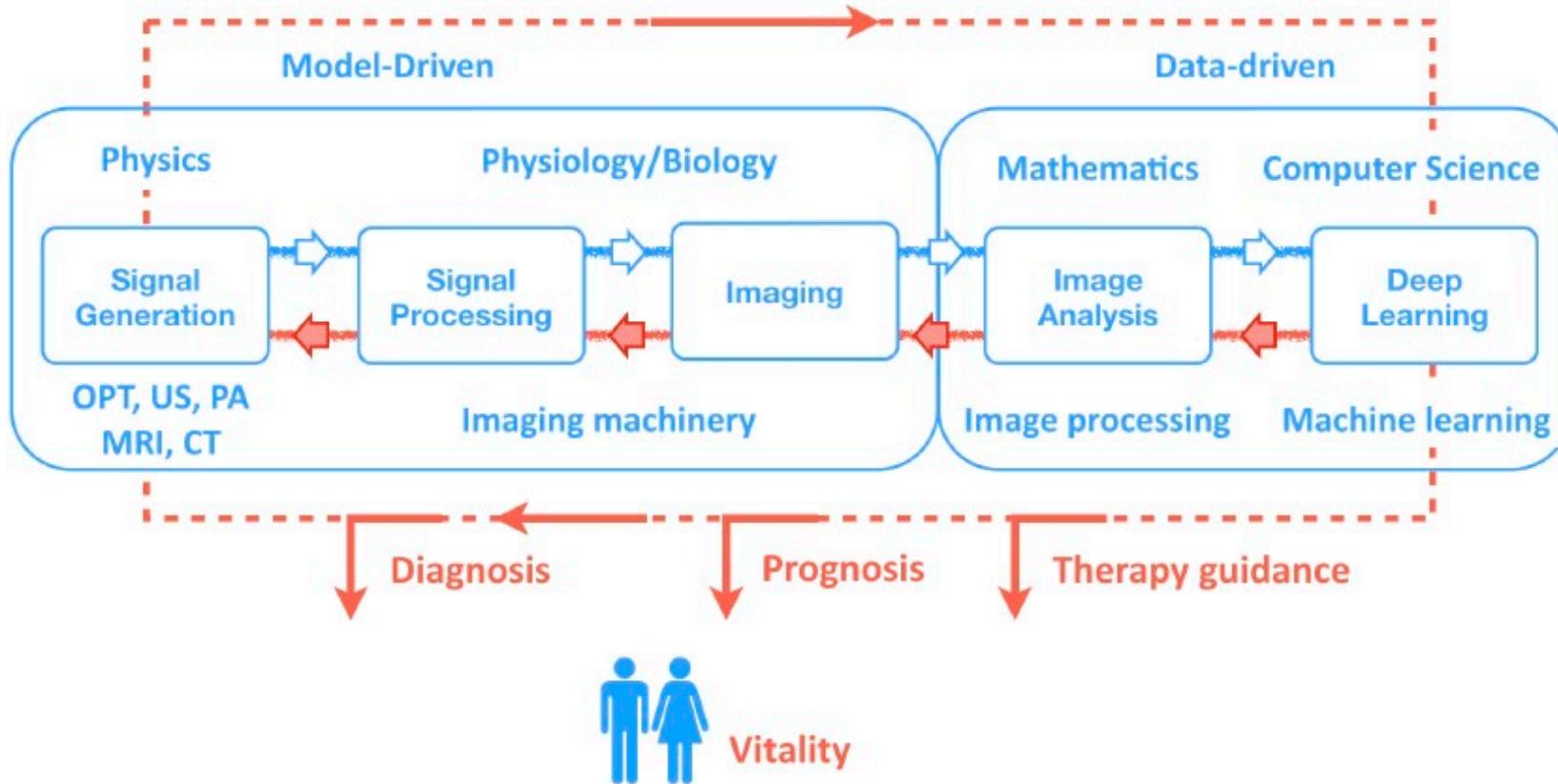


Boink, van Gils, Manohar, Brune - Sensitivity of a partially learned model-based reconstruction algorithm (PAMM 2018)



Boink, Manohar, Brune - A Partially Learned Algorithm for Joint Photoacoustic Reconstruction and Segmentation (IEEE 2019)

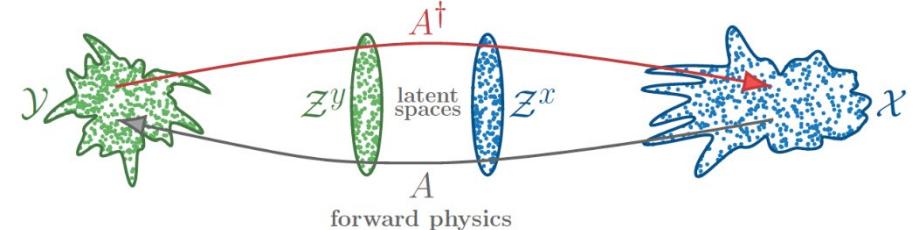
4TU Precision Medicine



Deep learning for model-driven imaging

- ➡ “classical” physics-based reconstruction enriched by deep learning
- ⬅ “black-box” deep learning enriched by physical constraints

CONCLUSIONS AND FUTURE WORK



Learned SVD framework for nonlinear decomposition and inversion

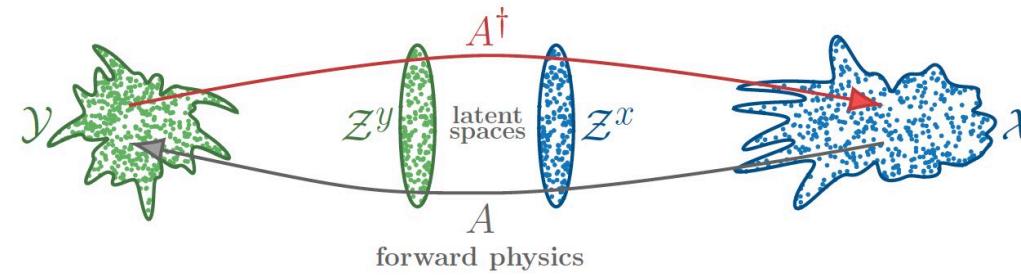
- L-SVD connects data and signal manifold in a straightforward manner with a linear layer
- Via nonlinear AE, L-SVD has superior performance with interpretable results
- Hybrid autoencoding provides regularization for reconstruction
- L-SVD has a lot of freedom in the exact architecture chosen. Future work will investigate more advanced autoencoders for larger-scale inverse problems. (GANs, VAEs)



Y.E. Boink, C. Brune - Learned SVD: Solving Inverse Problems via Hybrid Autoencoding (arXiv preprint, Nov 2019)



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