



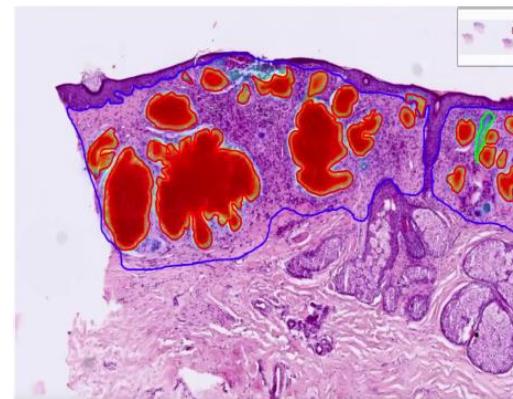
Prof. Dr. Dr. h.c. Peter Maass

Basics of Deep Learning

From Mathematical Research to
Technology

KoMSO Academy 2024
Berlin, Nov. 14 2024

AI beyond Computer Vision



Industrial applications

VW, Ariane Airbus, Siemens, DB,

Digital pathology

1st clinical installations

CT tomography

Academic example

PDE models

$$u_t + \textcolor{red}{v}^t \nabla u + \operatorname{div}((1 - \textcolor{red}{D}) \nabla u) = \textcolor{red}{f}$$

given measured u , determine $(\textcolor{red}{v}, \textcolor{red}{D}, \textcolor{red}{f})$

Outline

1 Neural networks

- Network architecture
- Data manifold
- Regularization by architecture

2 An industrial CT application

3 PDE based applications

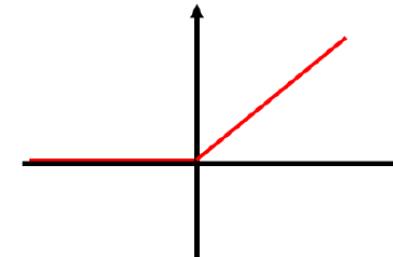
- Limitations of present DL concepts
- Topology optimization, Ariane

Neural networks for function approximation

Parameterized function systems: trigonometric functions, splines, wavelets, neural nets...

$$\Phi_{\Theta}(x) = \varphi(W_3 \cdot \varphi(W_2 \cdot \varphi(W_1 x + b_1) + b_2) + b_3)$$

- Parameters: $W_j, b_j, j = 1, M$
e.g. $W_j \in \mathbb{R}^{n_j \times m_j}$ fully connected, MLP
Toeplitz matrices, CNN
 - Activation function $\varphi : \mathbb{R} \rightarrow \mathbb{R}$
e.g. φ chosen as tanh, ReLu, ...
 - Accuracy, complexity
Number of parameters Unet: $\sim 8 \cdot 10^6$



Neural networks for function approximation

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$$\varphi_{\Theta}(x) = \varphi(W_3 \varphi(W_2 \varphi(W_1 x + b_1) + b_2) + b_3)$$

- Least squares regression for given data $(x_i, y_i), i = 1, \dots, N$

$$\Theta_{opt} = \operatorname{argmin}_{\Theta} \sum_i^N \|\varphi_{\Theta}(x_i) - y_i\|^2$$

Training: costly minimization, stochastic gradient descent

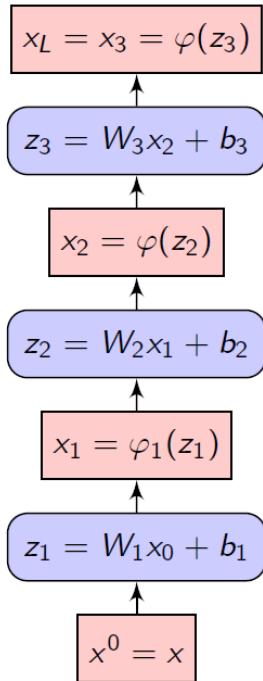
- Application of trained network with fixed Θ_{opt}

$$\varphi_{\Theta_{opt}}(x_{new}) = \varphi(W_3 \varphi(W_2 \varphi(W_1 x_{new} + b_1) + b_2) + b_3)$$

Linear operations, pointwise non-linearities, very efficient

Feedforward Neural Network

Feedforward neural network with L layers:



input: x_0

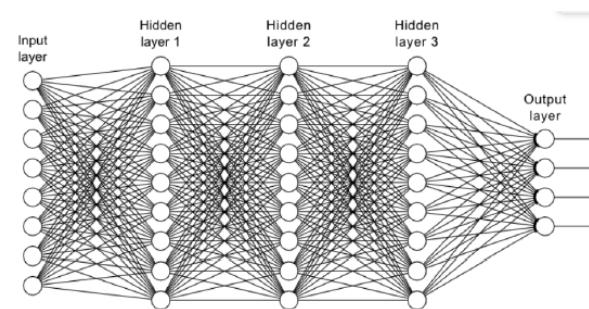
$$z_k = W_k x_{k-1} + b_k$$

$$x_k = \varphi(z_k)$$

output: x_L

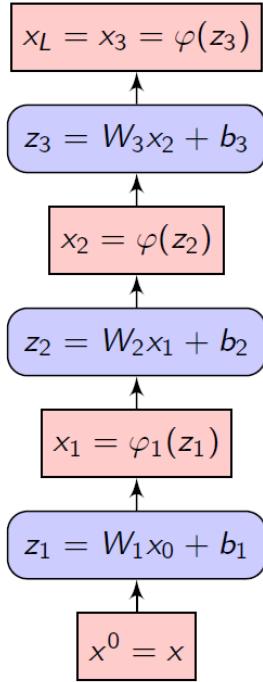
φ non-linear, componentwise, network parameters $\Theta = \{W_k, b_k\}$

$$\varphi_\Theta(x_0) = x_L = \varphi(W_3 \varphi(W_2 \varphi(W_1 x + b_1) + b_2) + b_3)$$



Feedforward Neural Network

Feedforward neural network with L layers:



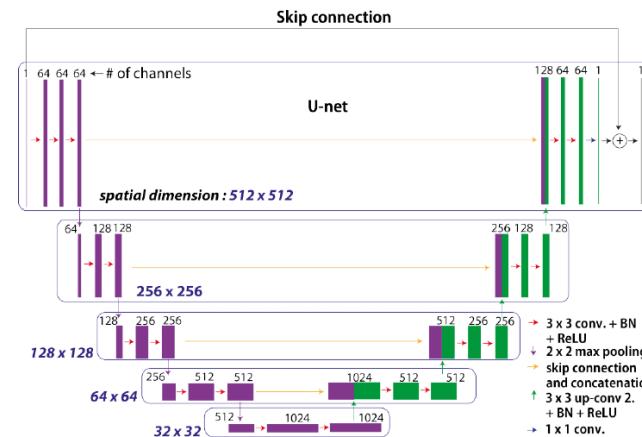
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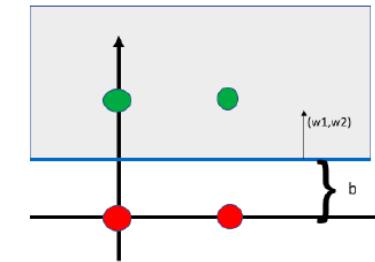
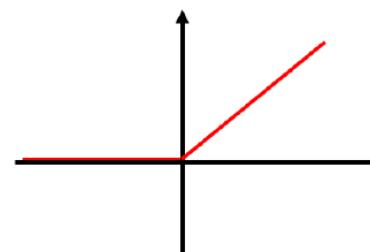
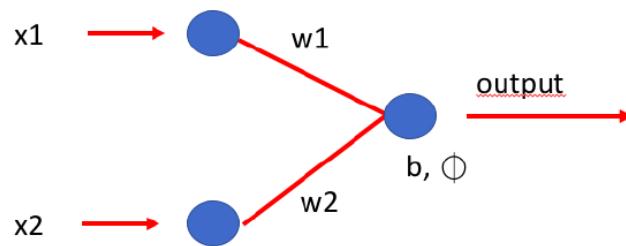
output: x_L

$$\varphi_\Theta(x_0) = x_L = \varphi(W_3 \varphi(W_2 \varphi(W_1 x + b_1) + b_2) + b_3)$$



Trivial Network

- Network without inner layer, *ReLU*- activation
- Multiplikationsnetzwerk, Input (x, y) , Output xy (Produkt)
- Matrix-Vektor-Multiplikation

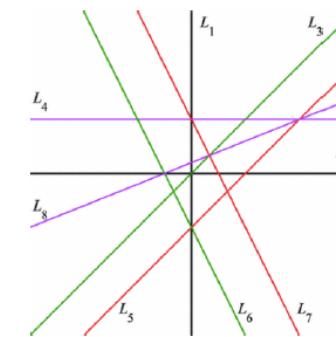
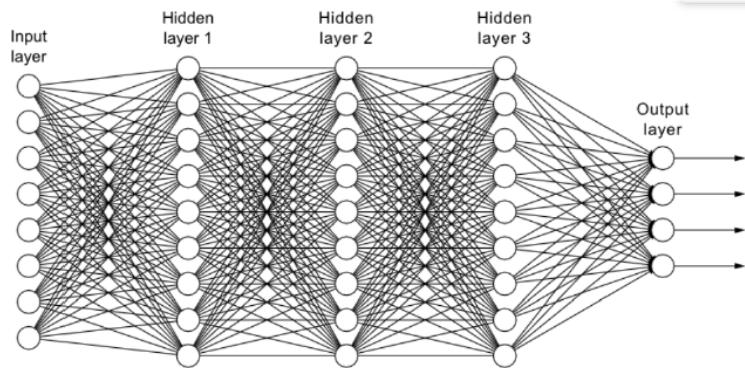


$$\text{output } z = \varphi(w_1 * x_1 + w_2 * x_2 - b)$$

$$w_1 * x_1 + w_2 * x_2 - b \geq 0$$

Arrangement of hyperplanes

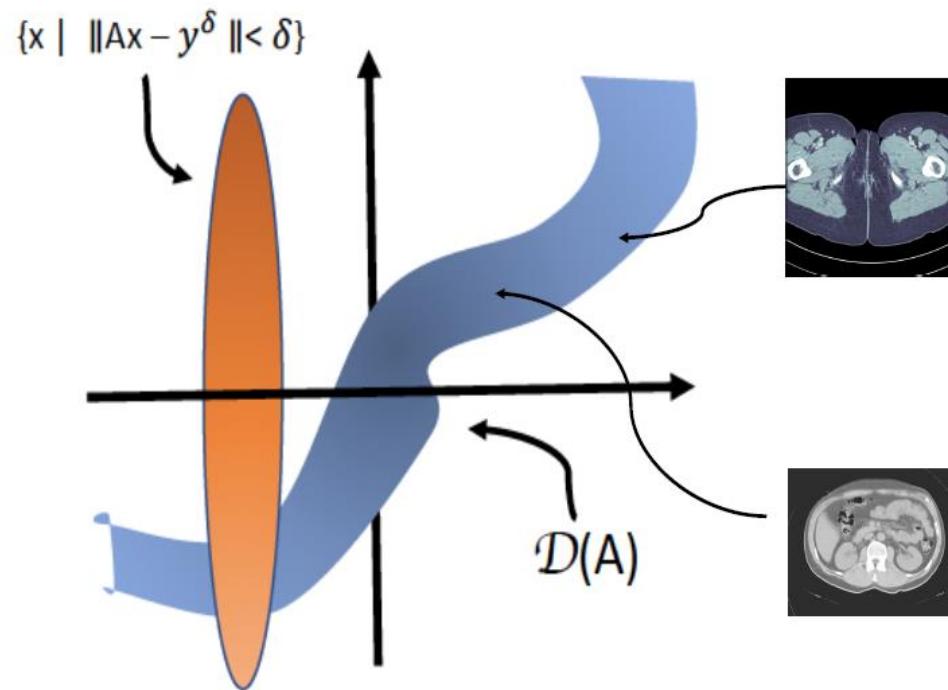
- Adaptive segmentation of input space
- Exponentially increasing complexity
- piecewise linear function



Approximation of complex functions by adaptive, linear cells

Exploiting the data manifold

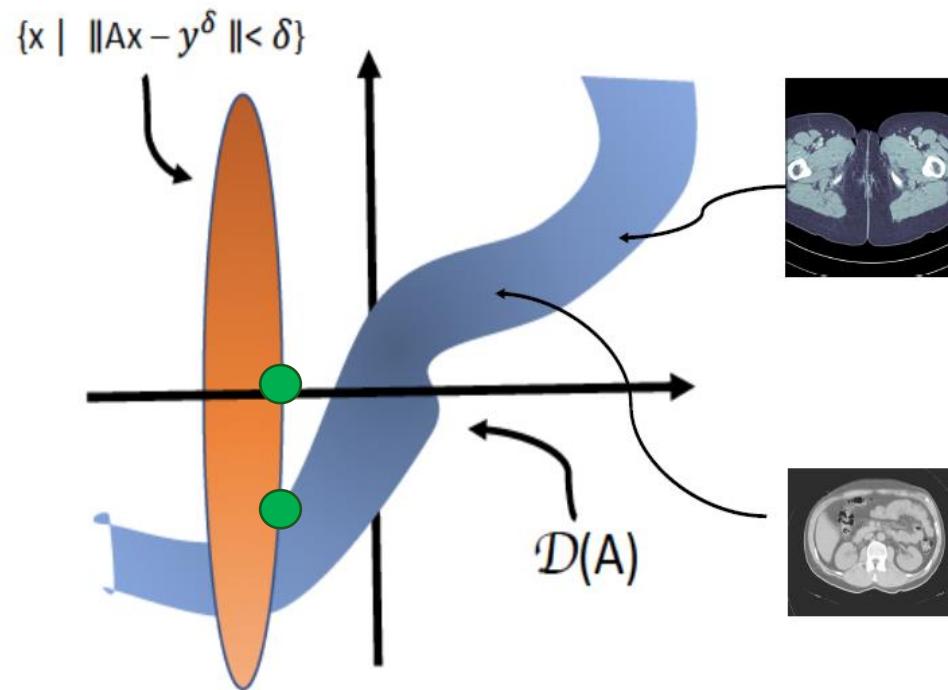
$Ax \sim y^\delta$, "No model is perfect" , "Not every matrix is an image"



Mallat, Haltmeier, Adler, Öktem, Lunz, Schönlieb, Arridge, Hauptmann, Grasmaier, Harrach, Dittmer, Otero,

Exploiting the data manifold

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Mallat, Haltmeier, Adler, Öktem, Lunz, Schönlieb, Arridge, Hauptmann, Grasmaier, Harrach, Dittmer, Otero,

Advantages of deep learning concepts

“No model is perfect”, “Not every matrix is an image”

Postprocessing of analytic reconstructions

- Learned projection

$$\varphi : X \rightarrow \mathcal{D}(A)$$

$$y^\delta \rightarrow x \rightarrow \varphi(x)$$

Learned prior distribution

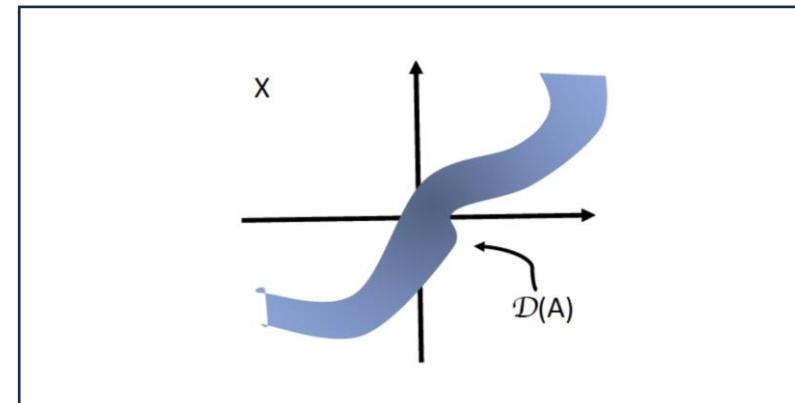
- probability for $x \in \mathcal{D}(A)$

$$\min_x \|Ax - y^\delta\|^2 - \log(\varphi(x))$$

Learning operator updates

- Residual data $(x^{(d)}, y^{(d)} - Ax^{(d)})$

$$\min_x \|Ax + \varphi(x) - y^\delta\|^2 + \alpha R(x)$$



Theoretical results

■ Complexity and Approximation

Cybenko (1989), Hornik, Stinchcombe, White (1989), Chen, Chen (1995),
Yarotsky (2017), Grohs, Petersen, et al. (2019), Karniadakis et al. (2021),
Gribonval, Kutyniok, Nielsen, Voigtländer (2021), Langer, Ay (2021), Shen, Yang, Zhang (2021)....

■ Stability of network architectures

Gregor, LeCun (2010), Kunisch, Pock (2013), Chen, Liu, Wang, Yin (2018),
Li, Schwab, Antholzer, Haltmeier (2018), Jin, Lu (2018), Lunz, Schönlieb (2018),
Arridge, PM, Öktem, Schönlieb (2019), Jacobsen, Behrmann, Zemel, Bethge (2020),
Ruiz, Gama, Ribeiro (2020), Baguer, Leuschner, et al (2020), Ruthotto, Steidl (2023)....

■ Neural networks and PDEs

Weinan E (2020), Kutyniok, Petersen, Raslan, Schneider (2019), Aarset, Holler, Nguyen (2022),
Bhattacharya, Hosseini, Kovachi, Stuart (2020), Lanthaler, Mishra (2021), Jiang, Willet (2021),
Lu, Jin, Karniadakis (2019), De Hoop, Huang, Qian, Stuart (2022), Tanyu, PM et al. (2023)....

III-posed inverse problem

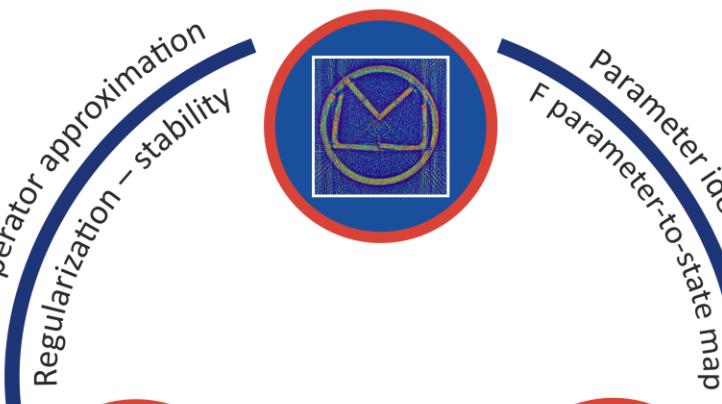
$$\text{given } y^\delta = F(x) + \eta$$

$$\min_x \|F(x) - y^\delta\|^2 + \alpha R(x)$$

**Data driven
neural network**

Θ network parameters

$$\min_{\Theta} \sum_i \|\varphi_{\Theta}(x_i) - y_i\|^2 + \alpha R(\Theta)$$



**Partial differential
equation**

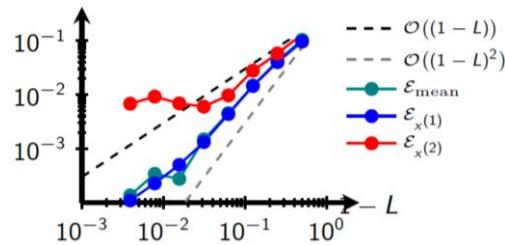
$$-\nabla (\lambda \nabla u) = f$$

given u^δ determine λ

Regularization by architecture

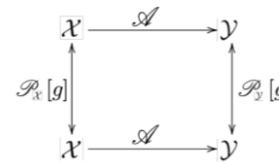
Network architectures for inverse problems

Operator approximation



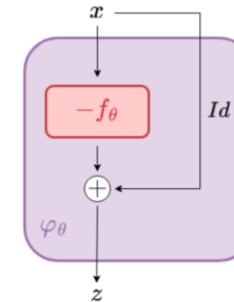
Janek Gödeke
quantifiable approx.
general activation

Equivariance



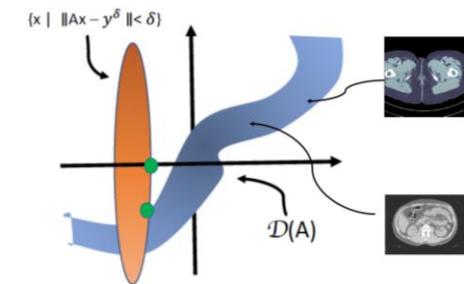
generalized CNN
group transform
stability

Invertible networks



iResNet architecture
 $y_{j+1} = y_j + \Phi_\Theta(y_j)$
Optimal convergence

Deep prior concepts



$\min \|A\Phi_\Theta(z) - y^\delta\|^2$
no training data
bi-level optimization

D. Nganyu Tanyu, J. Ning, T. Freudenberg, N. Heilenkötter, A. Rademacher, U. Iben, P. Maaß. Deep learning methods for partial differential equations and related parameter identification problems. *Inverse Problems*, 39(10), 2023.

C. Arndt, A. Denker, S. Dittmer, N. Heilenkötter, M. Iske, T. Kluth, P. Maaß, J. Nickel. Invertible residual networks in the context of regularization theory for linear inverse problems. Submitted for publication, 2023.

M. Beckmann, N. Heilenkötter. Equivariant Neural Networks for Indirect Measurements. Submitted for publication, 2023.

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- Limitations of present DL concepts
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X-Ray technology for in-process quality monitoring



SIKORA
Technology To Perfection

03/2021 – 09/2022

Simulation of measurement process, off-line computation
Co-operation funded by WFB (local business development fund, EFRE)

10/2022-12/2022

Sikora in-house evaluation

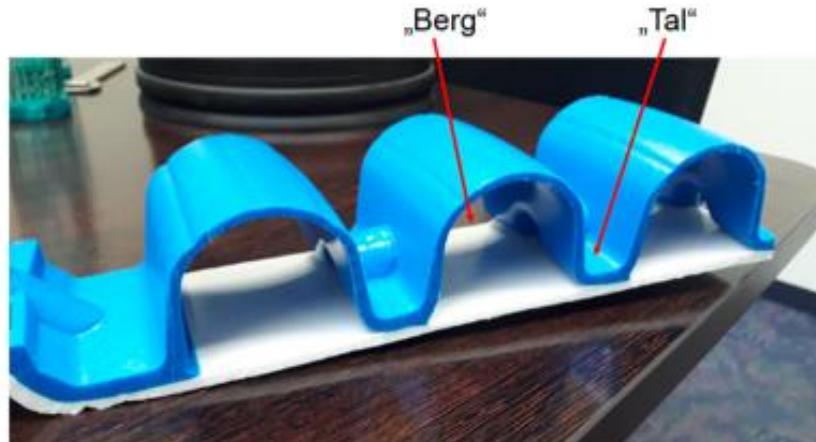
03/2023-07/2023

DLL development (WFB)

14/2024

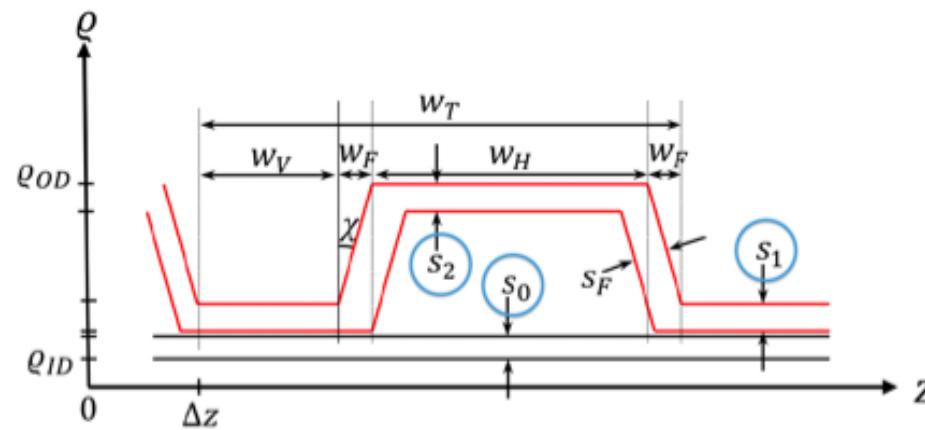
product release

WELLROHRE



Structure

- Innenhaut (weiß)
- Wellschicht (blau)
- Mono-Layer
- Single-Layer
- Multi-Layer



Parameters

- S_0
- S_2
- S_0+S_1

Online production monitoring

- Inprecise positioning
- Motion blur (< 9 m/s)



Kühlung & Trocknung



Basic X-Ray technology

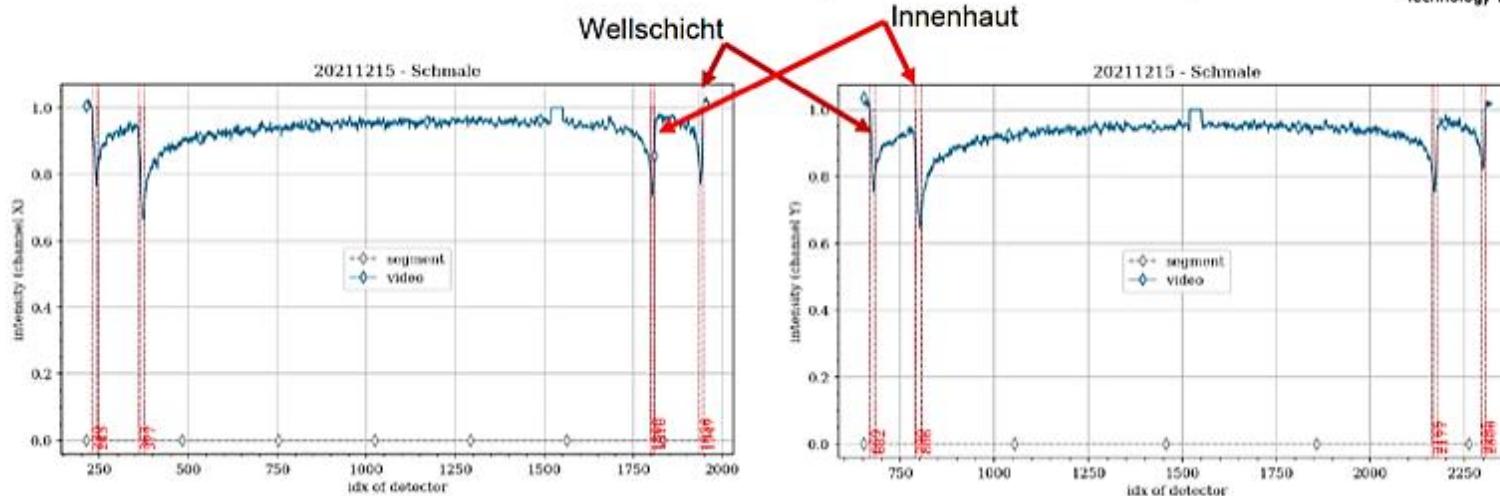
- 2 directions
- Limited angle
- $3 \mu\text{s}$ for each scan
- Significant ray widening
- Low compute power



Abschneider

AI-MODELL ZUR FEATURE-DETEKTION (SEGMENTIERUNG)

SIKORA
Technology To Perfection



Math Theorie:

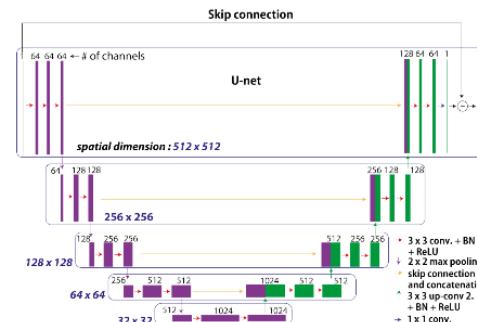
Range characterization for data calibration
Papers on equivariance

Machine Learning

Standard U-Net for segmentation

Implementation

Forward model for data generation
Dynamic link library



3-4 month mathematical research
(mainly reading papers)

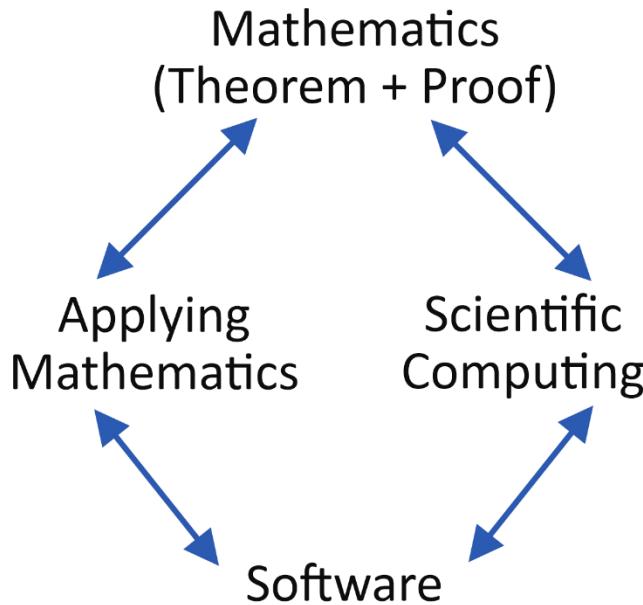
6 month math-inspired implementation
6 month testing, adaptation

6 month DLL programming

24 month at industrial partner

From Mathematical Research to Innovation

Novelty with relevance for society/economy



University

Research Papers
Patent
Open IP
Innovation Office
Law Office
Non-profit Qualification



Steinbeis

GmbH

Company

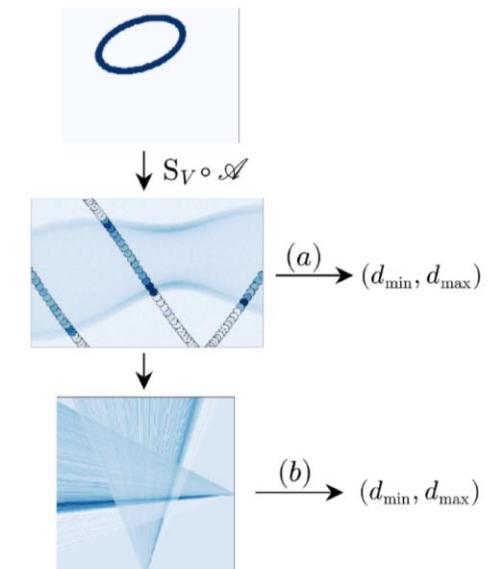
Problem solving
Patent
Proprietary IP
Software
Warranty Updates
Time to market

TRL: Mathematics needed for TRL 1-2, Mathematicians are needed on all levels

Equivariant NN for Indirect Measurements

Numerical Insights

- experiments on regression and classification tasks,
e.g. tube thickness measurements
- NN with equivariance towards the induced
symmetries of rotation and translation on \mathcal{Y} $\rightsquigarrow (a)$
- comparison to classical group-equivariant CNN $\rightsquigarrow (b)$
- first results:
 - improved generalization for small training data sets
 - increased robustness towards noise



Beckmann, N. Heilenkötter. Equivariant Neural Networks for Indirect Measurements. Submitted for publication, 2023.

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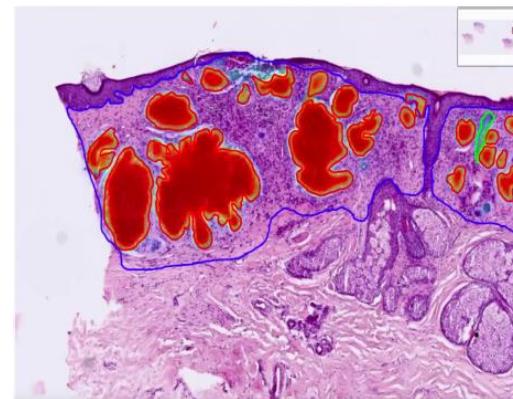
3 PDE based applications

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AI beyond Computer Vision



Industrial applications
VW, Ariane Airbus, Siemens, DB,



Digital pathology
1st clinical installation



CT tomography
Academic example

PDE models $u_t + \textcolor{red}{v}^t \nabla u + \operatorname{div}((1 - \textcolor{red}{D}) \nabla u) = \textcolor{red}{f}$
given measured u , determine $(\textcolor{red}{v}, \textcolor{red}{D}, \textcolor{red}{f})$

Poisson problem

$$\Delta u = \lambda \quad \text{on} \quad \Omega \subset \mathbb{R}^2$$

$$u = g \quad \text{on} \quad \partial\Omega$$

Parameter-to-state operator

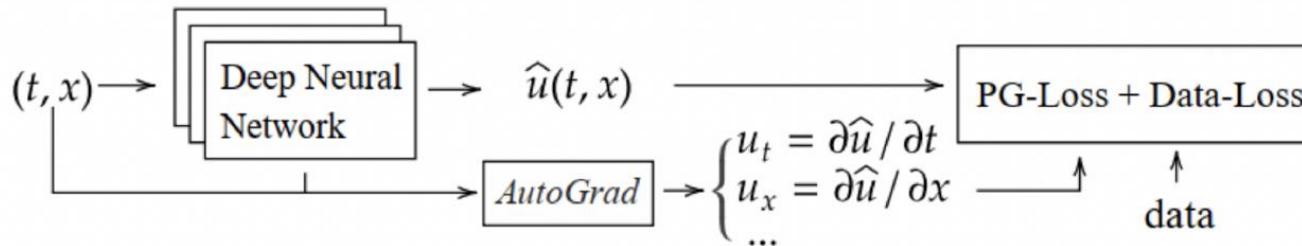
$$F : \mathcal{X} \rightarrow \mathcal{Y}$$

$$\lambda \mapsto u$$

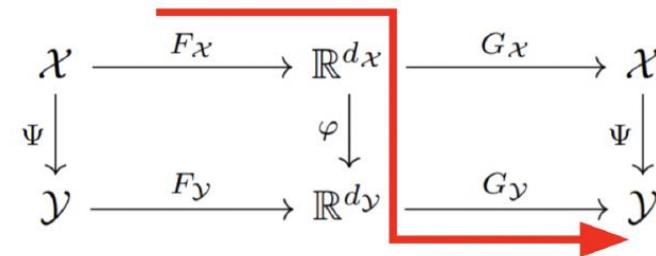
- Forward problem: evaluation of F for a single parameter λ
- Parametric studies: evaluation of F for many parameters λ
- Inverse problem: given measured u^δ or Pu , solve $F(\lambda) \sim u^\delta$

Deep learning concepts for PDE forward solvers, e.g. PINN

- function evaluation, neural network $\Phi_\Theta(t, x)$



- operator evaluation, neural network $\Phi_\Theta(\lambda)$, e.g. PCANN



$$\lambda = \sum c_k b_k \in \mathcal{X}, \quad \phi_\Theta : \mathbf{c} \mapsto \tilde{\mathbf{c}}, \quad u = \sum_\ell \tilde{c}_\ell \tilde{b}_\ell$$

Numerical Results – PCANN

Resolution	33×33	65×65	129×129	257×257	513×513
Poisson (μ_G)	4.02×10^{-2}	3.43×10^{-2}	4.62×10^{-2}	5.43×10^{-2}	4.32×10^{-2}
Darcy Flow (μ_P)	2.40×10^{-2}	1.63×10^{-2}	1.05×10^{-2}	1.08×10^{-2}	1.04×10^{-2}

Table: Relative L2 Errors for PCANN

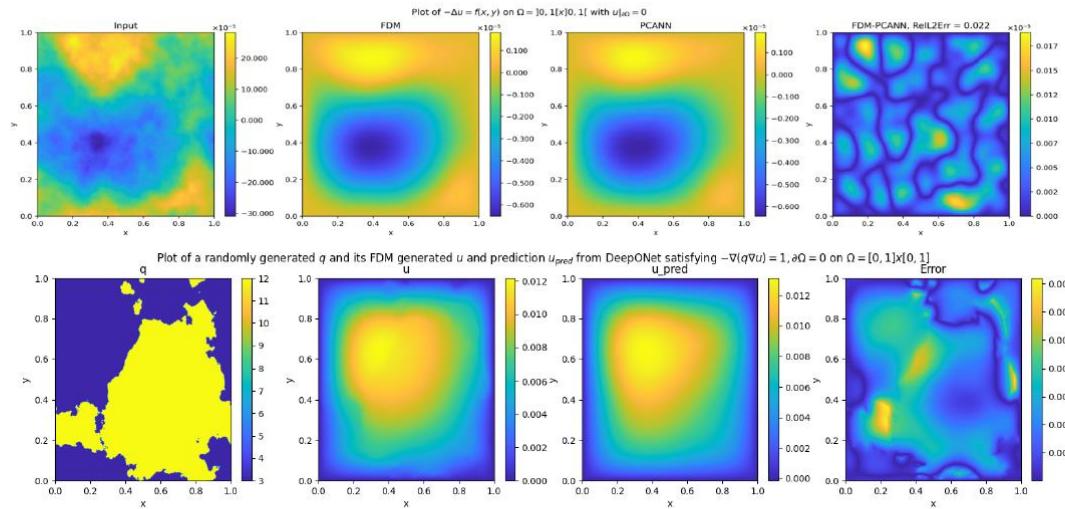


Figure: Parameter functions are Gaussian fields $\mu_G = \mathcal{N}(0, (-\Delta + 9I)^{-2})$ and $\mu_P = T_\sharp \mu_G$, details see K. Bhattacharya, A.M. Stuart, et al. , 2020

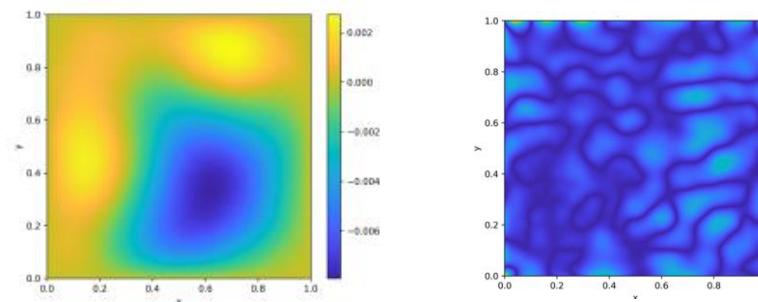
Numerical results inverse Darcy problem

$$\begin{aligned}-\nabla \cdot (\lambda(s) \nabla u(s)) &= f(s) \\ u(s) &= 0\end{aligned}$$

- Embedded Tikhonov
- Operator evaluation
- Very efficient
- Sufficient accuracy

- Parameter studies
- Rapid prototyping

	0%	0.1%	1%	5%	10%
PCANN	0.4684	0.4692	0.4680	0.4828	0.5148
PCALin	0.3157	0.3157	0.3159	0.3163	0.3183
FNO	0.1764	0.1764	0.1823	0.2143	0.2402
U-FNO	0.2140	0.2205	0.2017	0.2371	0.2734
MWT	0.1287	0.1250	0.1435	0.1880	0.2209
DeepONet	0.2484	0.2483	0.2469	0.2547	0.2691
PINO	0.1559	0.1549	0.1607	0.1932	0.2244
PI-DeepONet	0.2792	0.2801	0.2820	0.2822	0.2861

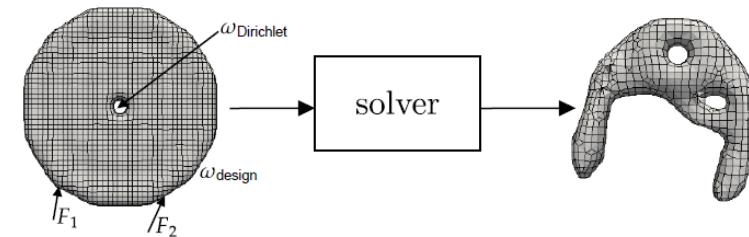


Deep Learning Methods for Partial Differential Equations and Related Parameter Identification Problems
Derick Nganyu Tanyu, Jianfeng Ning, Tom Freudenberg, Nick Heilenkötter, Andreas Rademacher, Uwe Iben, PM

Inverse design



Figure: Ariane 6 (Source ESA)



Problem:

forces F ,
Dirichlet boundary $\omega_{\text{Dirichlet}}$,
design space ω_{Design} ,
material properties

Solution:

optimized structure
density distribution

\min
density
subject to
compliance
physics,
weight constraints,
binary density.

Iterative method + PDE solver =



$$\min_{\rho} L(\rho)$$

$$L(K(\rho)) = \langle f, u(\rho) \rangle + \lambda \|\rho\|_1$$

- Density: $\rho(\cdot) \in [0, 1]$
- Displacement: $u(\cdot) \in \mathbb{R}^3$
- Compliance: $\langle f, u(\rho) \rangle \in \mathbb{R}_{\geq 0}$

Linear elasticity:

$$\epsilon = \frac{1}{2} [\nabla u + \nabla u^T]$$

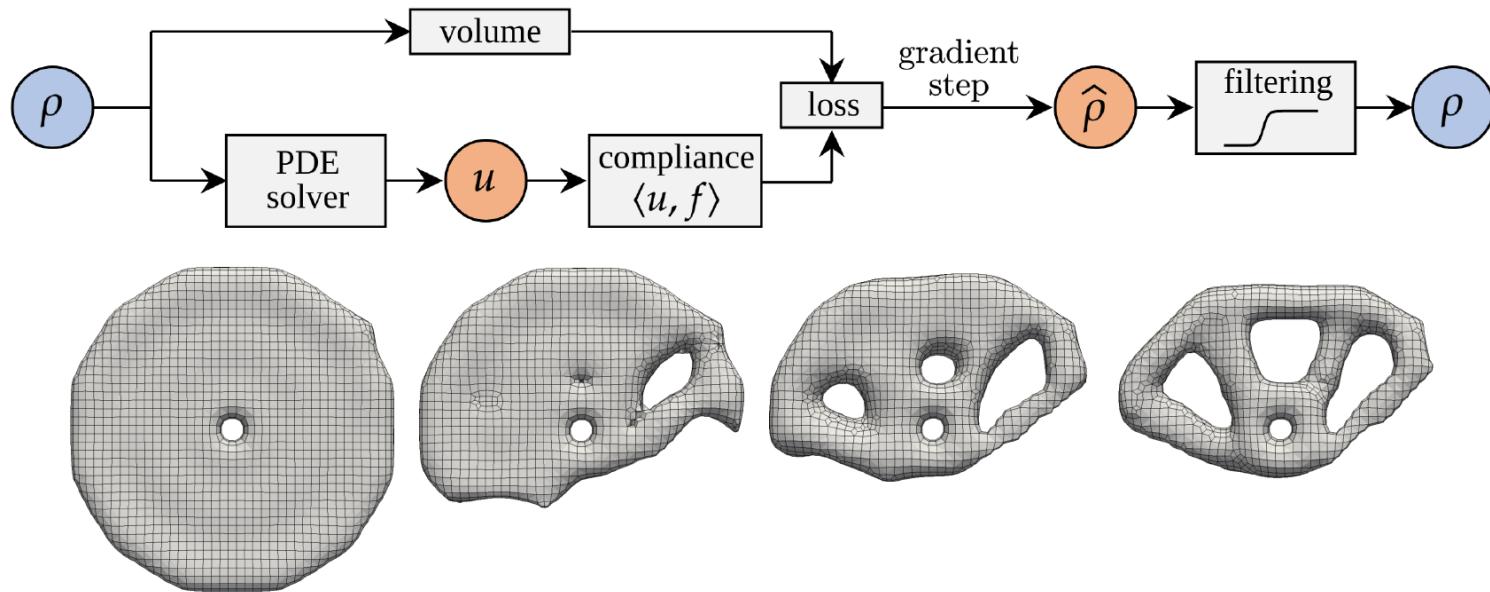
$$\nabla \cdot \sigma = -f$$

$$\sigma = C(\rho(\cdot)) : \epsilon$$

Iterative method + PDE solver =

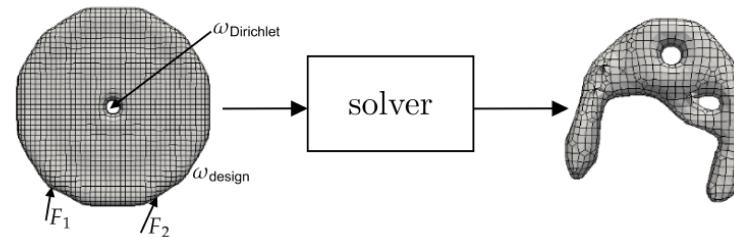


SIMP method (sketch):

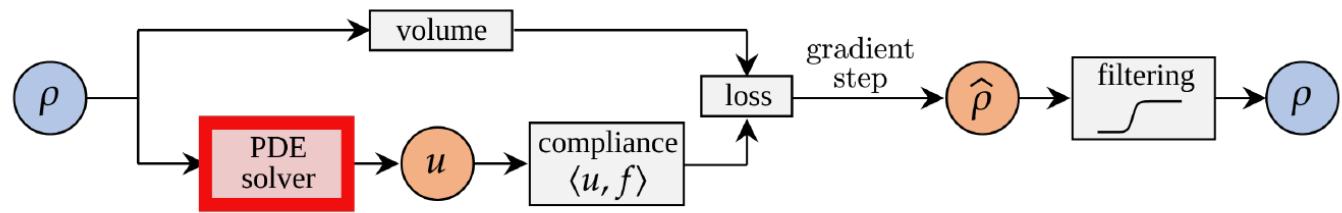


Deep learning approaches

1 End-to-end learning

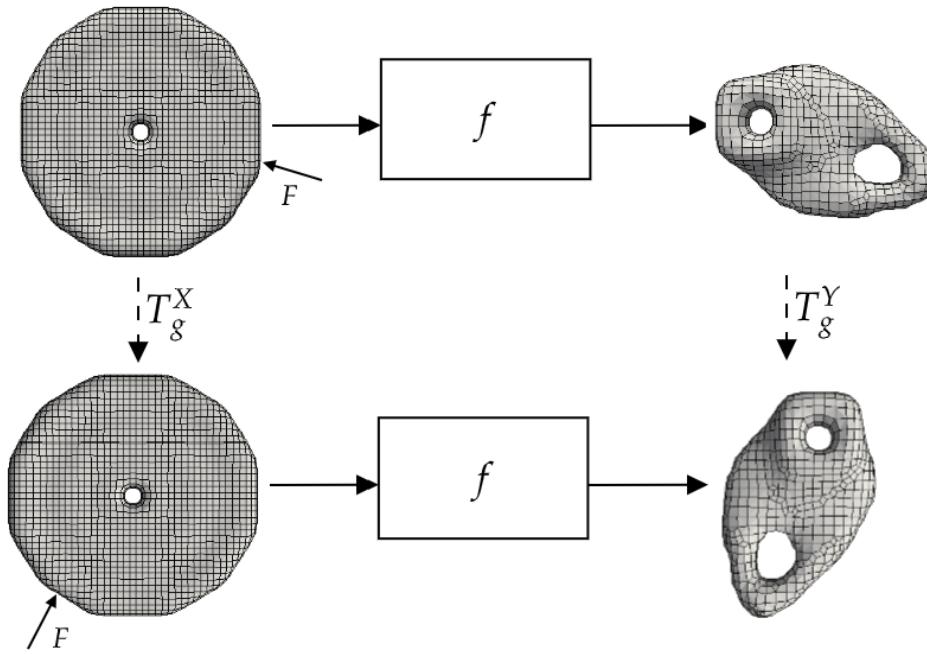


2 Learn substitute for PDE solver



3 Neural reparameterization, ∞ -resolution

Equivariance



$$f : X \rightarrow Y$$

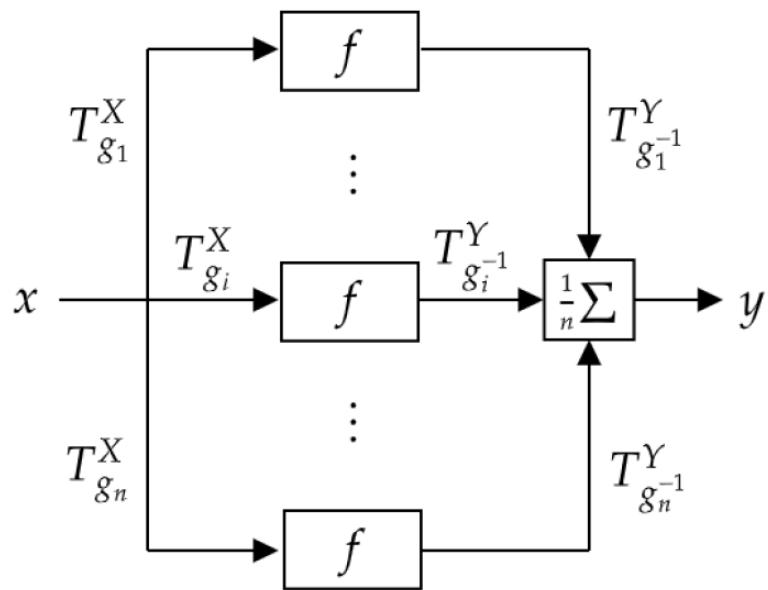
is G -equivariant¹ if

$$f(T_g^X x) = T_g^Y f(x)$$

$$\forall g \in G, x \in X.$$

¹Cohen and Welling (2016) – Group equivariant convolutional networks

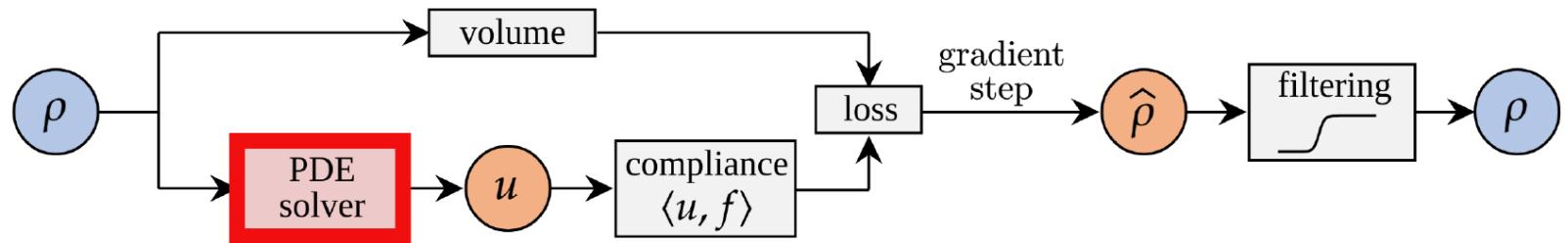
Group averaging¹



$$F_G^f(x) := \frac{1}{|G|} \sum_{g \in G} T_{g^{-1}}^Y [f(T_g^X(x))]$$

¹Puny et al. (2021) – Frame averaging for invariant and equivariant network design

SIMP trajectory learning



- Learn PDE solver

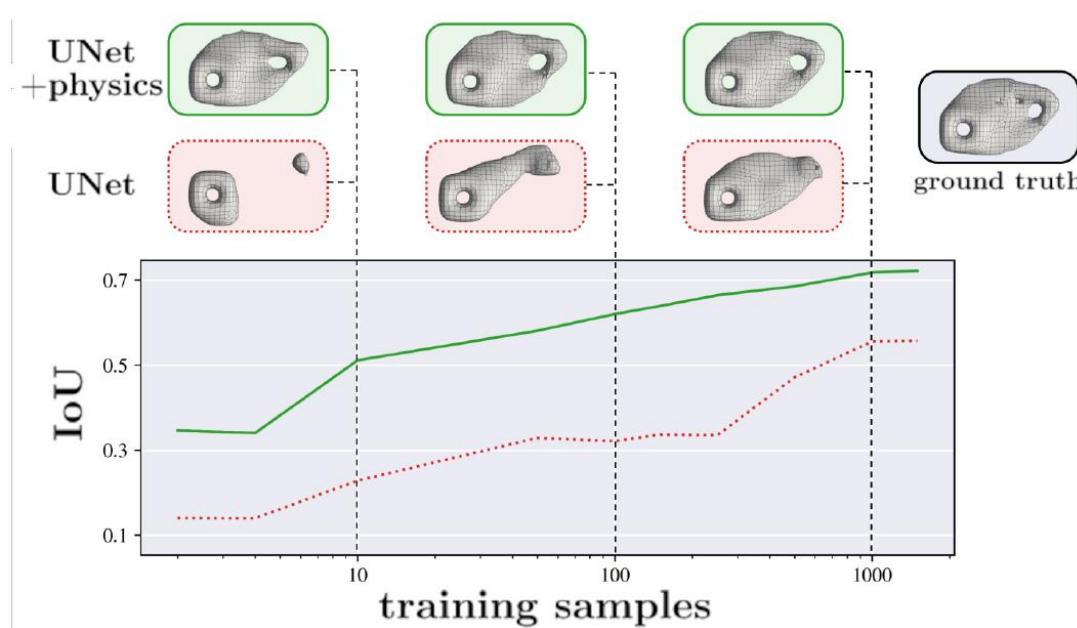
$$(\rho, f) \longmapsto u$$

- Supervised training via

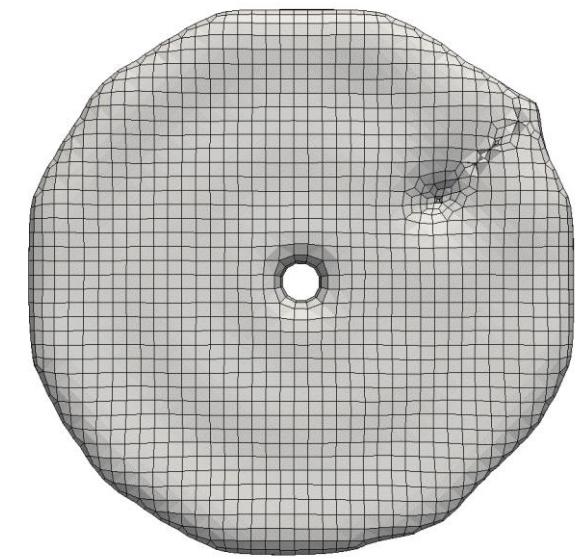
$$\mathcal{L}(u_{\text{pred}}, u) := \|u_{\text{pred}} - u\|_2^2 + \alpha \|\partial_\rho \langle u_{\text{pred}}, f \rangle - \partial_\rho \langle u, f \rangle\|_2^2$$

compliance

Results



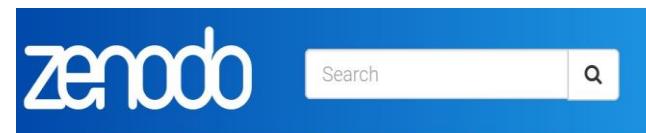
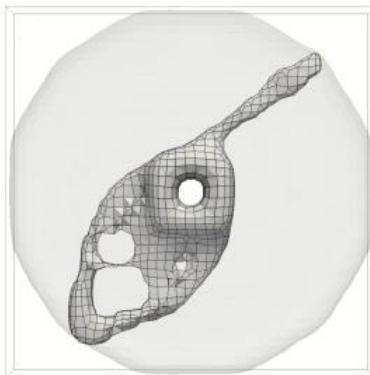
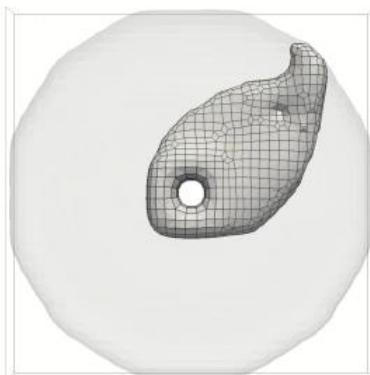
- "Physics:" Preprocessing includes von Mises stresses as input channel + Equivariance



 DL4TO

Inverse design of mechanical structures

Sören Dittmer, David Erzmann



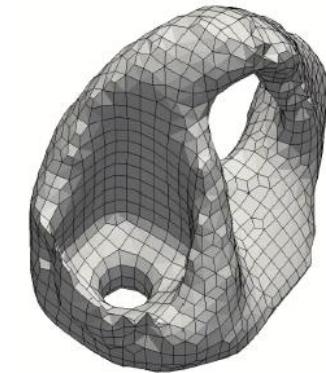
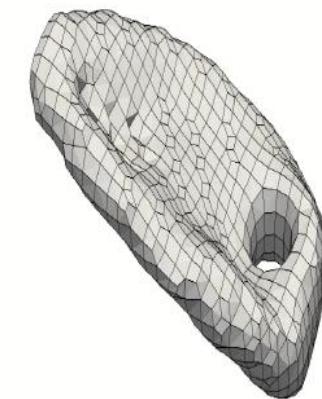
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Dataset Open Access

SELTO Dataset

Dittmer, Sören; Erzmann, David; Harms, Henrik; Falck, Rielson; Gosch, Marco

A Benchmark Dataset for Deep Learning-based Methods for 3D Topology Optimization.



Working group

