

Physics-Informed Machine Learning -in a nutshell-

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About me ...



Researcher @TUHH

Founder @tensorDynamic GmbH

Head of Machine Learning Dynamics Group (M-14)



Data analytics for physical systems.
Turning dark data into value.

www.tuhh.de/dyn

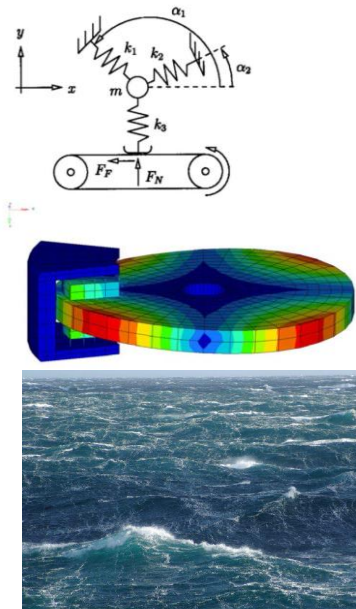
www.tensordynamic.com

Feel free to get in contact!

Our mission

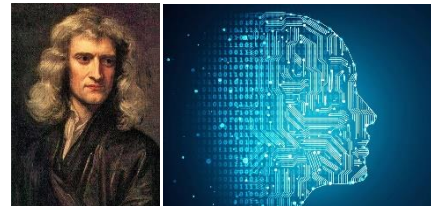
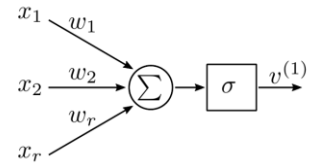
Physics

- Waves and vibrations
- Analytical modeling
- Numerical simulations



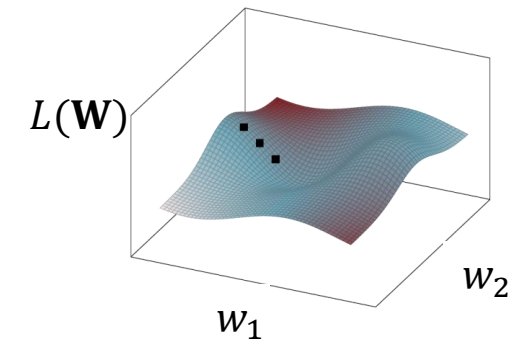
Data Science

- Data management and analytics
- Machine Learning, Deep Learning
- Explainable Artificial Intelligence



Physics-Informed Machine Learning

Digital Twins



Today: more than buzz-words ...

Physics-Consistent Learning

Physics-Informed Learning

Physics-Informed Neural Networks

Physics-Constrained Neural Networks

Videos: Machine Learning for Physicists 2019

Physics-Assisted Neural Networks

Physics-Guided Neural Networks

[Submitted on 10 Jun 2020]
Physics informed deep learning for computational elastodynamics without labeled data
Chengping Rao, Hao Sun, Yang Liu

A New Deep Learning Model for Fault Analysis with Good Anti-Noise Adaptation Ability in Vibration Signals

deep learning dynamics

Scholar Ungefähr 4.170.000 Ergebnisse (0,10 S)

Deep learning in fluid dynamics
J.N. Kutz - Journal of Fluid Mechanics, 2017 - cambridge.org
It was only a matter of time before **deep** neural networks (DNNs)—**deep learning**—made their mark in turbulence modelling, or more broadly, in the general area of high-dimensional, complex dynamical systems. In the last decade, DNNs have become a dominant data ...
☆ 99 Zitiert von: 274 Ähnliche Artikel Alle 5 Versionen

Exact solutions to the nonlinear dynamics of learning in deep linear neural networks
A.M. Saxe, J.L. McClelland, S. Ganguli - arXiv preprint arXiv:1312.6120, © 2013 - arxiv.org
Despite the widespread practical success of **deep learning** methods, our theoretical understanding of the **dynamics of learning** in **deep** neural networks remains quite sparse. We attempt to bridge the gap between the theory and practice of **deep learning** by ...
☆ 99 Zitiert von: 1070 Ähnliche Artikel Alle 12 Versionen »

Svcca: Singular vector canonical correlation analysis for deep learning dynamics and interpretability
M. Raghu, J. Gilmer, J. Yosinski, ... - arXiv preprint arXiv: ..., 2017 - arxiv.org
We propose a new technique, Singular Vector Canonical Correlation Analysis (SVCCA), a tool for quickly comparing two representations in a way that is both invariant to affine

Figure 2. Newton and the machine. Image of sir Isaac Newton alongside a schematic of a 10-layer deep neural network. In each layer (apart from the input layer), a node takes the weighted input from the previous layer's nodes (plus a bias) and then applies an activation function before passing data to the next node. The weights (and bias) are free parameters which are updated during training.

Physics Informed Deep Learning: Data-driven Solutions and Discovery of Nonlinear Partial Differential Equations

Code About

20 45

3 years ago

3 years ago

8 months ago

maziarraissi.github.io/pinns

Readme

MIT License

Physics-informed machine learning for predictive turbulence modeling: Toward a complete

Conference Paper Full-text available December 2016 · Proceedings of the 2016 Summer

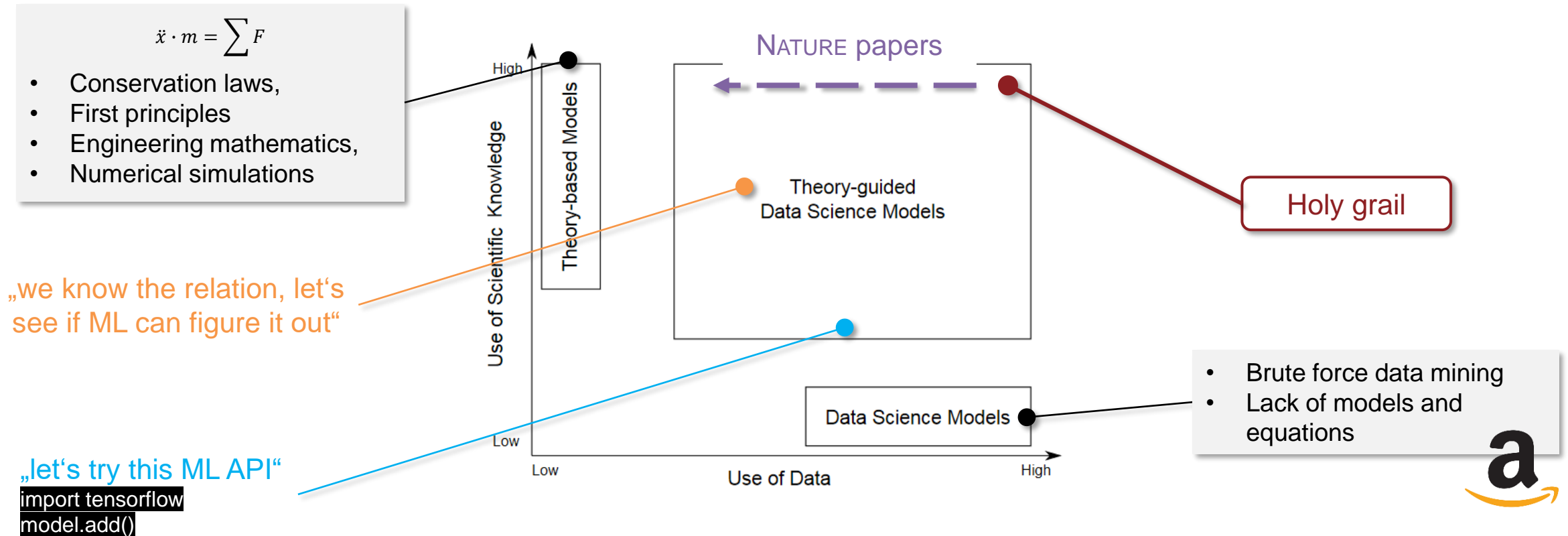
Jian-Xun Wang · Jinlong Wu · Julia Ling · [...] · Heng Xiao

913 Reads · 23 Citations

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Data and Scientific Knowledge: the big picture

How to achieve **knowledge conservation** *and* **data-driven discovery**?



Karpatne et al. (NIPS 2017): How Can Physics Inform Deep Learning Methods in Scientific Problems?

Challenges in physical data (opposed to www data streams)

1. **Availability** & cost of acquisition
2. **Sparsity**
 - a) Time
 - b) Space
 - c) Hidden variables
3. **Labels**
4. **Non-stationarity**



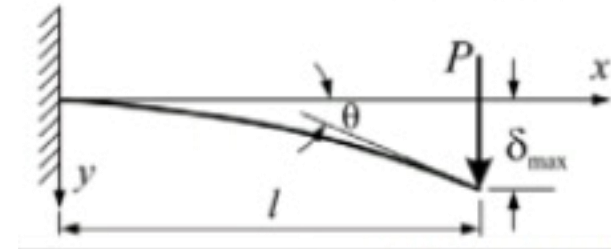
Vattenfall / REVE

First principles vs. universal function approximators

- Foundation of (deep) neural networks: **Universal function approximation theorem** Cybenko, G. (1989)

“Given a sufficiently complex architecture, a neural network with sigmoid activations can approximate any function”
(a non-mathematical summary)

- Learning the bending beam problem** $f_{\theta}(P) = \hat{\delta}$
 - Provide many load-deflection pairs $[P, \delta]$
 - Train a NN $f_{\theta}(P) = \hat{\delta}$ optimizing weights θ
 - Be happy if $|\hat{\delta} - \delta| < \text{tol}$ 😊



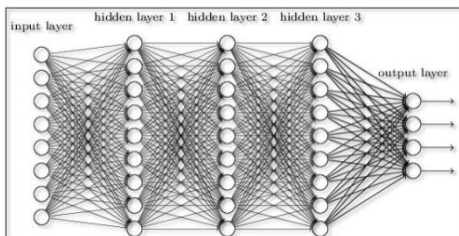
- But ...**
 - How to ensure generalization for out-of-sample predictions?*
 - How to make predictions for a beam of different material / length / cross-section?*

$$y = \frac{px^2}{6EI} (3l - x)$$

How to constrain universal function approximators to learn solely physically correct relations?

- Complex pattern recognition
- Highly nonlinear relationships
- High dimensionality
- Generality, adaptivity

Models featuring millions of parameters for learning some correlations



- Mass/energy/... conservation
- Determinism, continuity
- Structure, symmetries
- Underlying principles

(mostly) Simplistic equations explaining highly complex processes



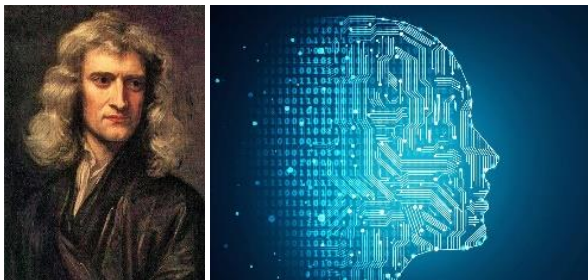
$$\rho \left(\frac{\partial \vec{v}}{\partial t} + (\vec{v} \cdot \nabla) \vec{v} \right) = -\nabla p + \mu \Delta \vec{v} + \vec{f}$$

How can we even dream about finding physics-constrained models?

Some ideas to encode physics into NNs



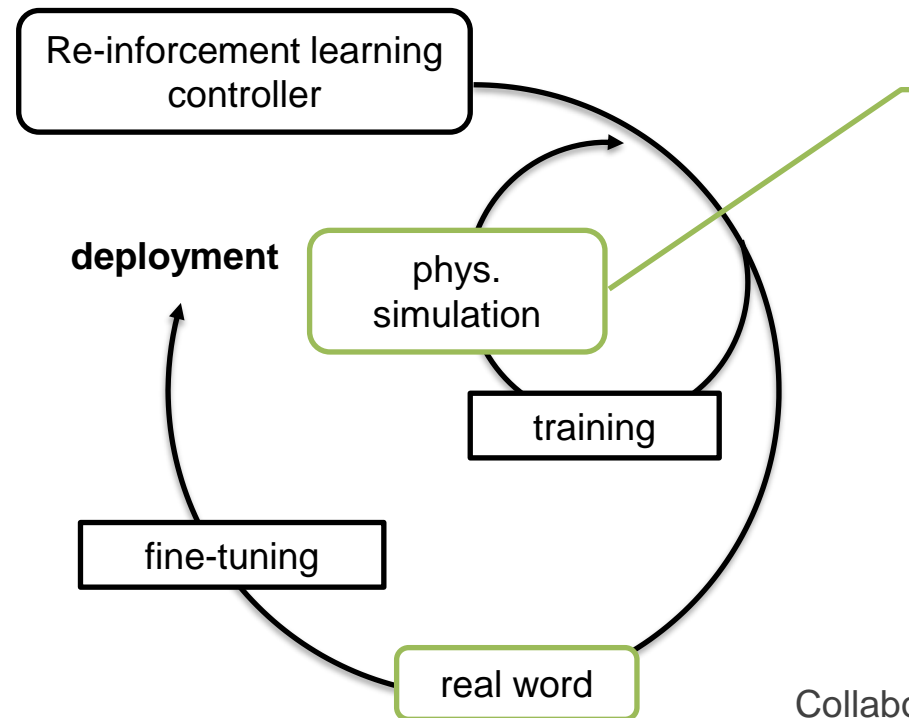
- **Light** (*Physics-assisted learning, physics-guided NNs*)
 - Training data from well-controlled physical process / numerical simulation with minimal noise corruption
 - Discrepancy models
- **Medium** (*Physics-informed learning*)
 - Physical NN regularizers
- **Deep** (*Physics-constrained learning*)
 - Physics-conform activation functions?
 - Completely new neural architectures / models?
 - ???



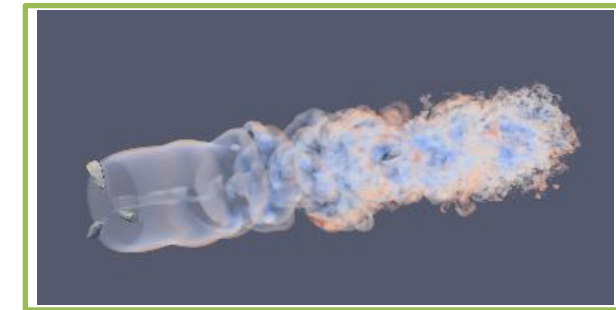
Physics-guided learning

■ Training data from simulations

- Pre-training using handcrafted data (many)
- Transfer learning / fine tuning on real/experimental data (few!)



High-fidelity simulations
(Lattice-Boltzmann)



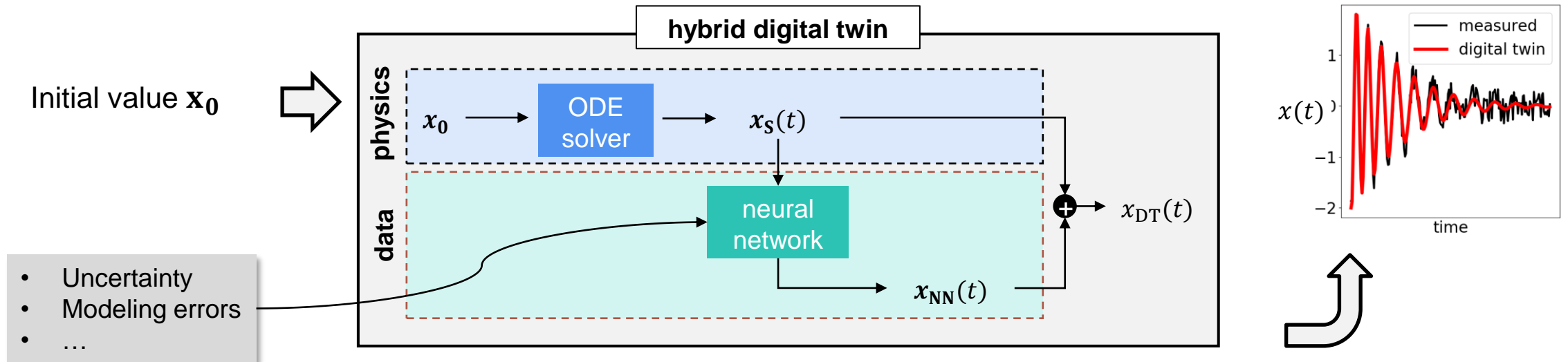
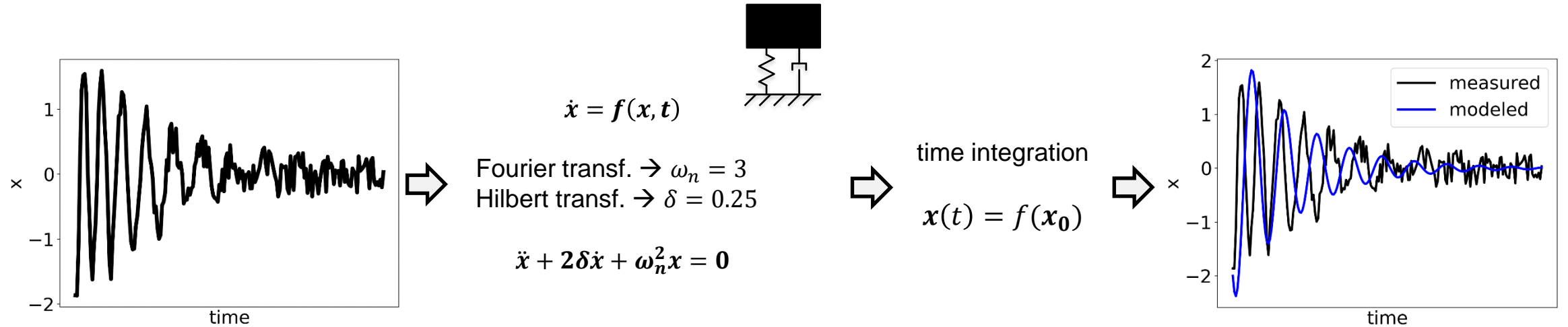
Collaboration with Uppsala Universitet
Wind Energy Group (Stefan Ivanell)
Henrik Asmuth, Henry Korb



UPPSALA
UNIVERSITET

Physics-assisted learning: Discrepancy models

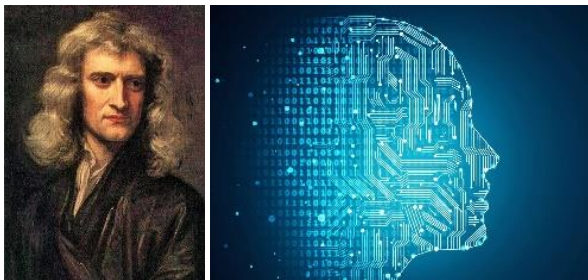
https://github.com/TUHH-DYN/DigitalTwin_Tutorial



Some ideas to encode physics into NNs



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Physics-informed learning (1)

Conventional formulation of the loss function:

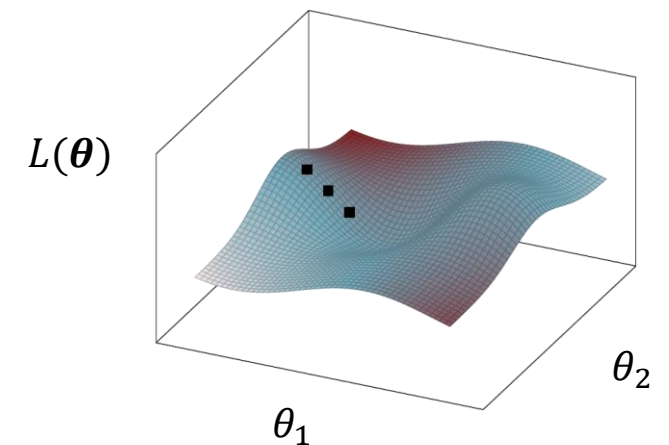
$$L(\theta, x, \hat{y}) = \|\hat{y} - y\| \text{ (some norm)} \rightarrow \text{MAE, MSE, ...}$$

▪ Soft regularization:

- Loss function $L(\theta, x, \hat{y})$ formulated with respect to physical quantities derived from predictions \hat{y} and ground truth y
- e.g. emphasizing spectral properties $L(\theta, x, \hat{y}) = |\text{FFT}(\hat{y}) - \text{FFT}(y)|$
- Can be tricky! Non-convex / non-smooth loss functionals, ... !

Overall goal:

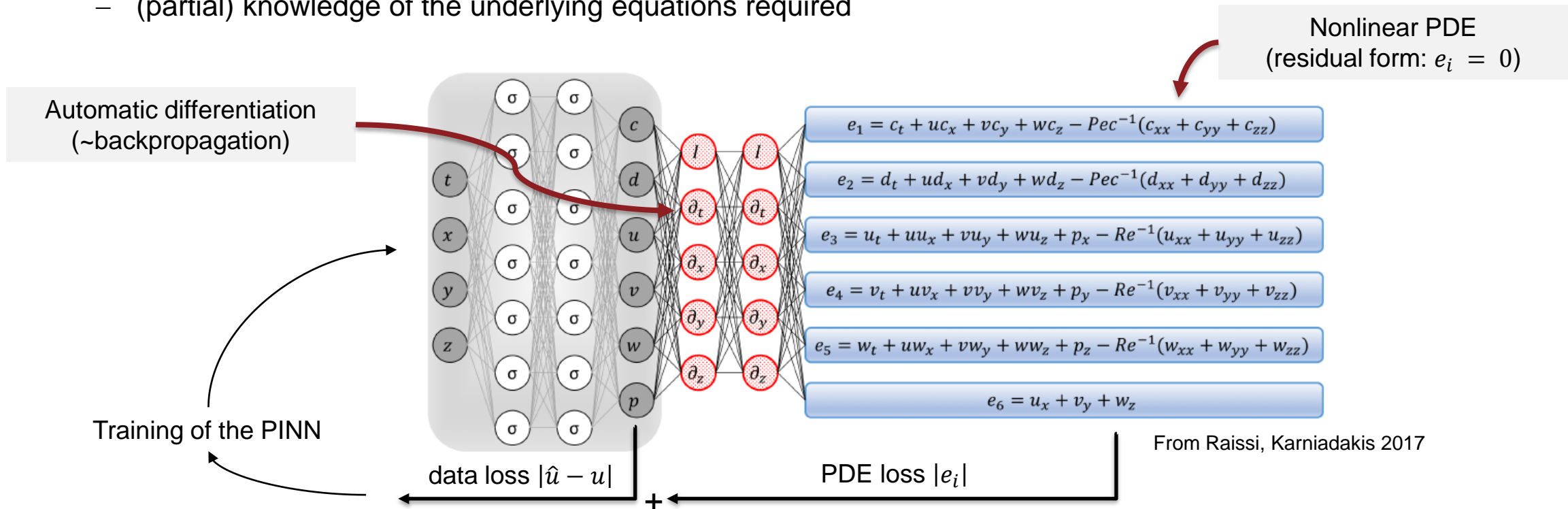
Engineer gradients that point into directions that promote function approximators with minimal prediction error w.r.t. physical aspects



Physics-informed learning (2)

Data-driven solution of nonlinear PDEs

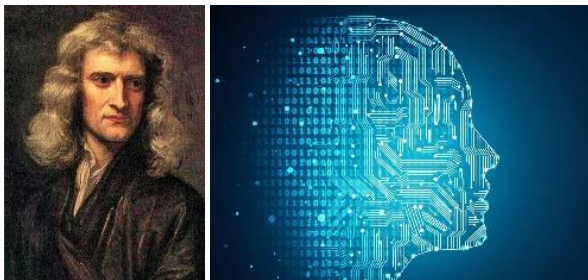
- **Strict regularization:** PINNs [Raissi, Karniadakis 2017]
 - Loss function $L(\theta, x, \hat{y})$ formulated with respect to governing equations
 - Governing equations ~exactly fulfilled at sample points
 - (partial) knowledge of the underlying equations required



Some ideas to encode physics into NNs

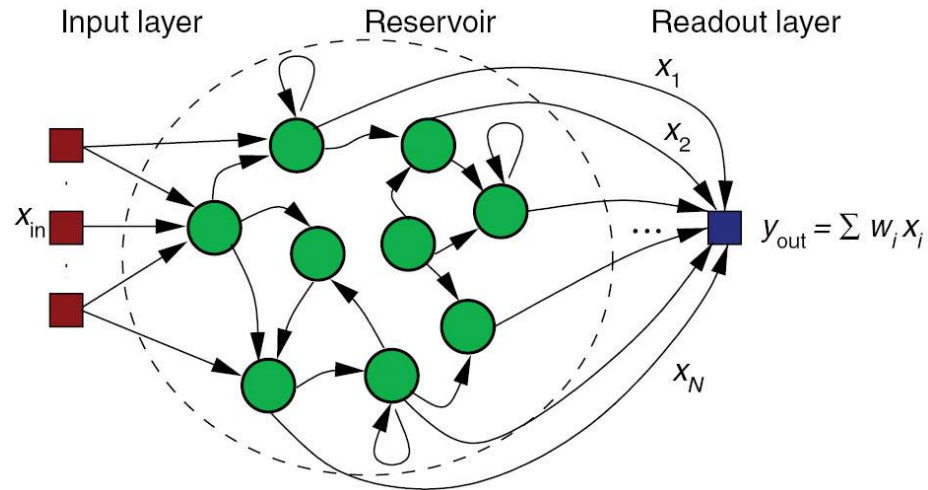


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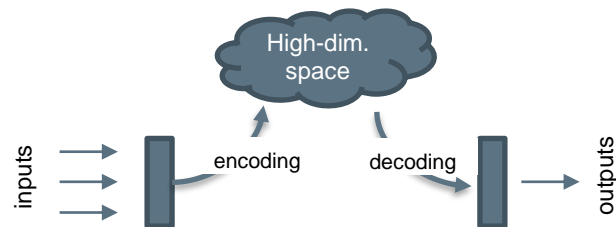


Physical reservoir computing

Reservoir computing



<https://julien-vitay.net/project/reservoircomputing/>



- Nonlinear mapping in high-dim. feature space
- Read observations from that space
- Fixed weights in reservoir! → hardware design

Physical reservoirs



Tanaka, Gouhei, et al. "Recent advances in physical reservoir computing: A review." *Neural Networks* 115 (2019): 100-123.

Reservoir: water basin

Input: droplets falling into the water

Decoding: surface elevation measurement

- Raissi, Maziar; Karniadakis, George Em (2018): Hidden physics models. Machine learning of nonlinear partial differential equations. In: Journal of Computational Physics 357, S. 125–141. DOI: 10.1016/j.jcp.2017.11.039.
- Raissi, M.; Perdikaris, P.; Karniadakis, G. E. (2019): Physics-informed neural networks: A deep learning framework for solving forward and inverse problems involving nonlinear partial differential equations. In: Journal of Computational Physics 378, S. 686–707. DOI: 10.1016/j.jcp.2018.10.045.
- Raissi, Maziar; Yazdani, Alireza; Karniadakis, George Em (2020): Hidden fluid mechanics: Learning velocity and pressure fields from flow visualizations. In: Science (New York, N.Y.) 367 (6481), S. 1026–1030. DOI: 10.1126/science.aaw4741.
- Rudy, Samuel H.; Brunton, Steven L.; Proctor, Joshua L.; Kutz, J. Nathan (2017): Data-driven discovery of partial differential equations. In: Science advances 3 (4), e1602614. DOI: 10.1126/sciadv.1602614.
- Rudy, Samuel; Alla, Alessandro; Brunton, Steven L.; Kutz, J. Nathan (2019): Data-Driven Identification of Parametric Partial Differential Equations. In: SIAM J. Appl. Dyn. Syst. 18 (2), S. 643–660. DOI: 10.1137/18M1191944.
- Brunton, Steven L.; Proctor, Joshua L.; Kutz, J. Nathan (2016): Discovering governing equations from data by sparse identification of nonlinear dynamical systems. In: Proceedings of the National Academy of Sciences of the United States of America 113 (15), S. 3932–3937.

- Interested in collaborations / networking / discussing?
- Methods / application cases for Physics-Informed Learning?

Thank you!

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