An introduction to physics-informed neural networks

A hands on approach

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CHALMERS

Agenda

What we will do

- Take an abstract look at the PINN framework and how it evolves from supervised learning
- Show simple examples
- Provide the audience with a Jupyter notebook available in Google Colab to experiment with code

What we will not do

- Explain neural networks (weights, biases, activation functions, backpropagation,...)
- Look at complicated systems of differential equations trained on big datasets
- Explain all the code (do it at your own pace afterwards if you're interested, can use ChatGPT to help explain,...)

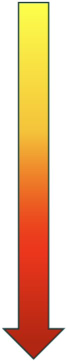
Neural networks: groundwork → breakthrough

- **1940s–2000s: Groundwork.** From early perceptrons to backprop and convolutional neural networks. Good ideas, limited by data, compute, and training issues.
- **2006–2011: Pieces click.** Better activations (ReLU), big labeled datasets, and GPUs make deep nets practical.
- **2012: AlexNet.** Scales the recipe and wins ImageNet by a large margin. Sets off an AI takeoff that is still ongoing.

Neural networks: 2012-onward

Some notable events

- 2012–2016: AlexNet wins ImageNet. DQN hits "human-level" Atari. ResNet becomes a default backbone for vision tasks. AlphaGo beats the world champion at Go.
- 2017-2020: Transformer architecture ("Attention Is All You Need"). BERT uses self-supervised pretraining for language understanding. GPT-3. Diffusion models. AlphaFold (protein folding).
- 2020–onward: AlphaFold2 protein structures at near experimental accuracy. Stable diffusion, text-to-image goes mainstream. ChatGPT. GPT-4. LLama, Sora, DeepSeek, ...



General interest in artificial intelligence (research, public discourse, etc...)

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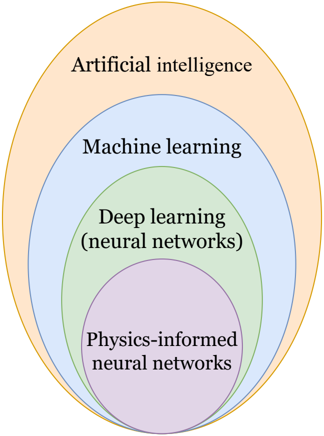

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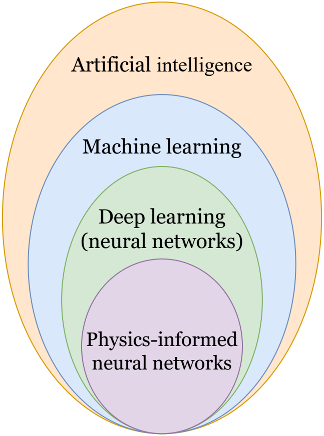

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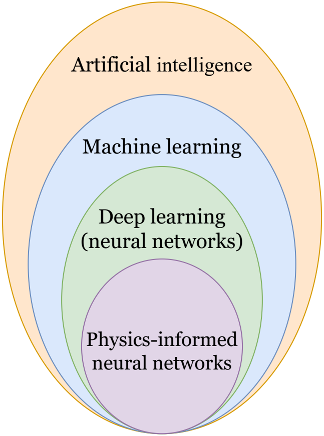
- Historically, AI research started with rule-based and symbolic approaches (GOFAI), well before machine learning became dominant. Today, machine learning/deep learning is almost synonymous with AI due to its dominance.



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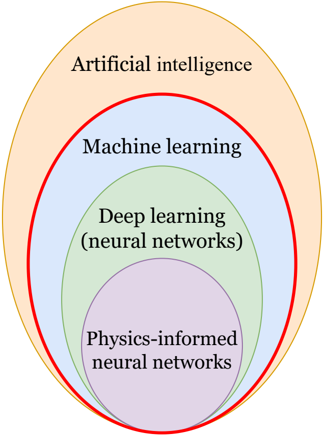

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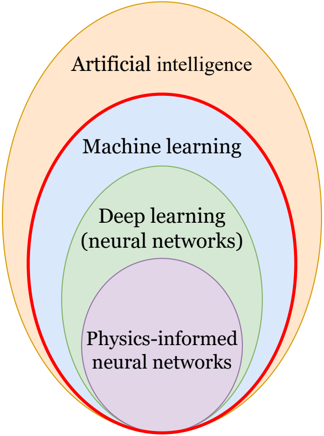

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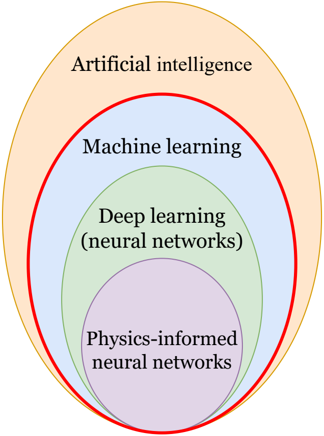
- Physics-informed neural networks (PINNs): an extension of neural networks tailored to analyzing differential equations



Machine learning: supervised learning for regression tasks with parametric models

Today's focus, looking at a subfield of machine learning

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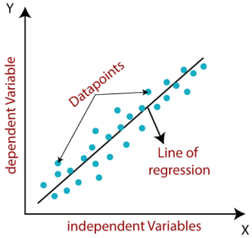
  - **Non-parametric models**: doesn't assume a fixed set of parameters, typically more flexible models that scale with data size. Not covered here.

Supervised learning for regression: problem setup

- Data: pairs $\mathcal{D} = \{(x_i, y_i)\}_{i=1}^{N}$, with $x_i \in \mathbb{R}^d$, $y_i \in \mathbb{R}$.



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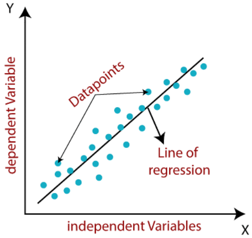

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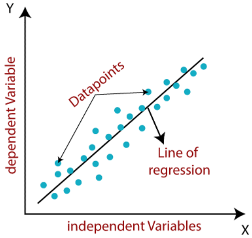
- Curve–fitting view: assume $y_i = g(x_i) + \varepsilon_i$ (unknown function g plus noise ε_i).



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- Prediction for an input x: $\hat{y} = f_\theta(x)$.
- Training (curve-fitting) = find θ that makes $\hat{y}_i = f_\theta(x_i)$ fit the data well.

Loss function: Mean Squared Error (MSE)

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- Why MSE? Smooth and differentiable, heavily penalizes large errors.

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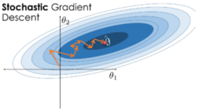
- Update our parameters in the opposite (negative) direction $\rightarrow$ one step toward minimizing the loss function $\rightarrow$ improves our parametric model

Training with (stochastic) gradient descent

- Initialize θ (e.g., randomly).



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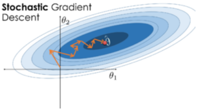

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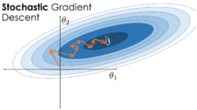

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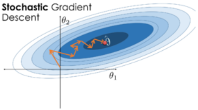

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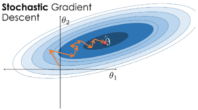

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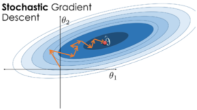

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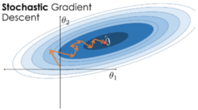
- Next: a short Python demo training such a network to fit noisy data and plotting predictions and MSE over epochs.



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- Experimental data can be noisy, sparse, or not cover the full domain.
- We often know physics a priori (differential equations, boundary/initial conditions).
- Idea of PINNs: keep NN regression and add MSE-style penalties that encode the physics.

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$$\mathcal{L}(\theta) = \underbrace{\frac{1}{N_{\text{data}}} \sum_i \big(f_\theta(x_i) - y_i\big)^2}_{\text{data MSE (optional)}} + \underbrace{\frac{1}{N_{\text{col}}} \sum_j r_\theta(x_j)^2}_{\text{ODE residual MSE}} + \underbrace{\frac{1}{N_{\text{bc}}} \sum_k b_\theta(z_k)^2}_{\text{BC/IC MSE}}.$$

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- Train with gradient descent as before; derivatives inside r_θ come from automatic differentiation.

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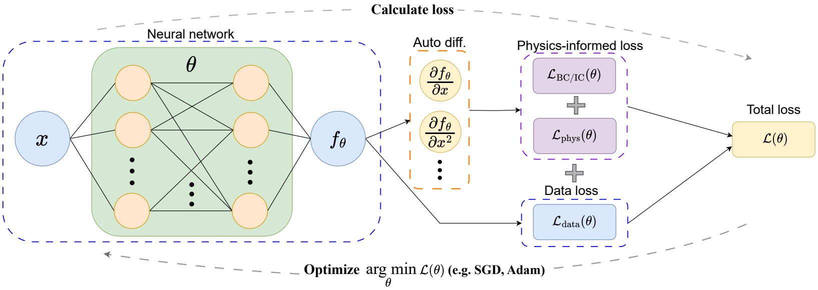
- If measurements (x_i, y_i) exist, add the usual data MSE.

Schematic of a PINN



Example: 1D Poisson problem

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- Use $f_\theta(x)$ for the solution; via autodiff compute $f''_\theta(x)$.

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- (Optional) With noisy samples (x_i, y_i), include $\mathcal{L}_{\text{data}} = \frac{1}{N_{\text{data}}} \sum_i \Big(f_\theta(x_i) - y_i\Big)^2$.

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- Monitor physics and boundary losses; visualize $f_\theta(x)$ against a reference when available.

Next: PINN code demo (1D Poisson)

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- Build MSE-style losses for the ODE residual and boundary conditions using f_θ.
- Train with gradient descent; plot predictions and the loss over iterations.

Code example

Code example

When should you consider PINNs?

- **Scarce or noisy data:** PINNs shine when measurement data is limited but governing equations are well known.
- **Hybrid scenarios:** Combine experimental data with simulation-based physics constraints.
- **Forward & inverse problems:**
  - Forward: approximate the solution of DEs directly.
  - Inverse: infer hidden parameters (e.g., material properties) from partial observations.

PINNs in research

- **Engineering:** fluid dynamics, structural mechanics, heat transfer, power systems.
- **Physics:** quantum mechanics, plasma physics, electromagnetics.
- **Biology/medicine:** blood flow modeling, tumor growth, protein folding.
- **Energy systems:** battery modeling, renewable energy integration, smart grids.
- Rapidly growing community: papers, workshops, benchmark suites, open-source libraries (DeepXDE, JAX/torch PINN frameworks).

Thank you & Resources

Thank you!

Source code and presentation available at:

`github.com/emiresenov/SESBC-Webinar`