An introduction to physics-informed neural networks

A hands on approach

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August 18, 2025

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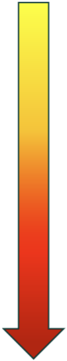
Neural networks: groundwork → breakthrough

- **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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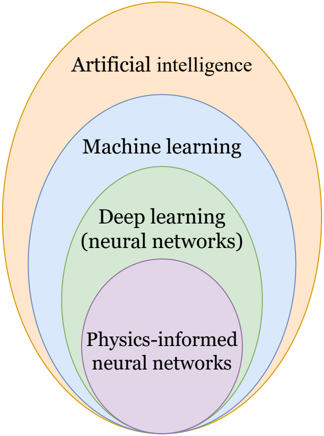

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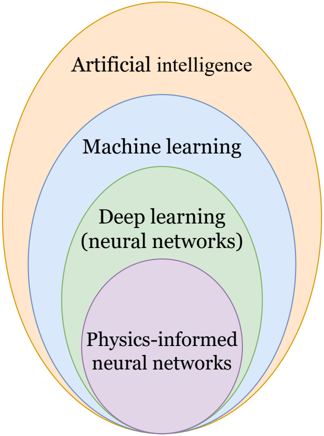

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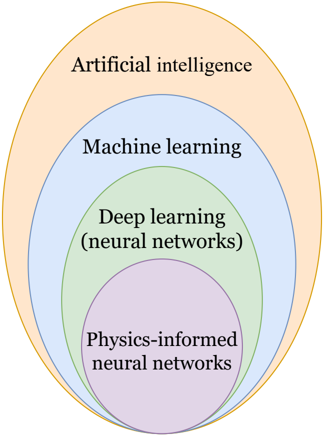
- Historically, AI research started with rule-based and symbolic approaches (GOFAI), well before machine learning became dominant. Today, machine learning/deep learning is almost synonymous with AI due to its dominance.



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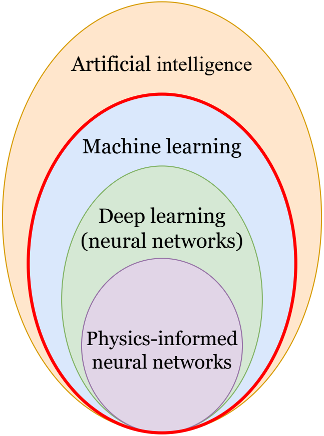

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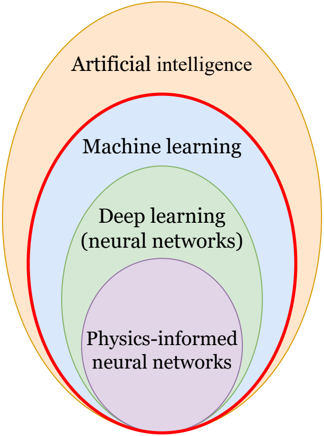

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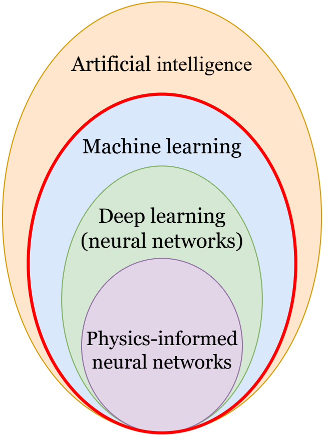
- Physics-informed neural networks (PINNs): an extension of neural networks tailored to analyzing differential equations



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

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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.

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

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- The gradient gives is a vector operation that gives the direction of steepest ascent.
- Update our parameters in the opposite (negative) direction $\rightarrow$ one step toward minimizing the loss function $\rightarrow$ improves our parametric model

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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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- 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.

Example: 1D Poisson problem

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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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- Backpropagate $\nabla_\theta \mathcal{L}$ and update θ with (stochastic) gradient descent.
- Monitor physics and boundary losses; visualize $f_\theta(x)$ against a reference when available.

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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.

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 PDEs 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`