1 Computational Mechanics Meets Artificial Intelligence

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Chair of Data Engineering in Construction

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Deep Learning in Computational Mechanics – an introductory course, Herrmann et al. 2025

website

book

Contents

What is Artificial Intelligence?

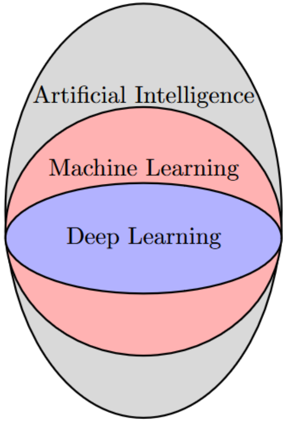
Artificial Intelligence: A Modern Approach, Norvig et al. 2020

Artificial Intelligence
- "Intelligence exhibited by machines/computers"
- (Total) Turing test requires: natural language processing, knowledge representation, automated reasoning, machine learning, (computer vision, robotics)

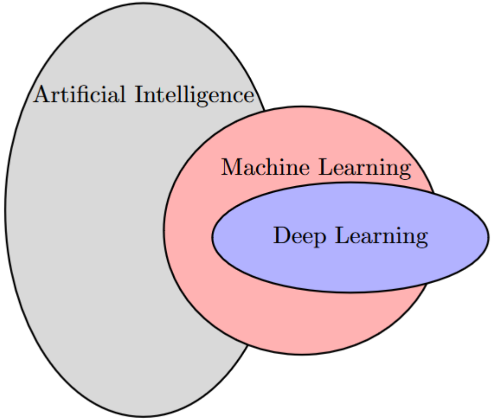
Intelligence
- Human or rational?
- Intelligent thoughts or intelligent behavior?

Machine Learning
- "Learn from data & generalize to unseen data (without explicit instructions)"

Deep Learning
- "Training (deep) neural networks"



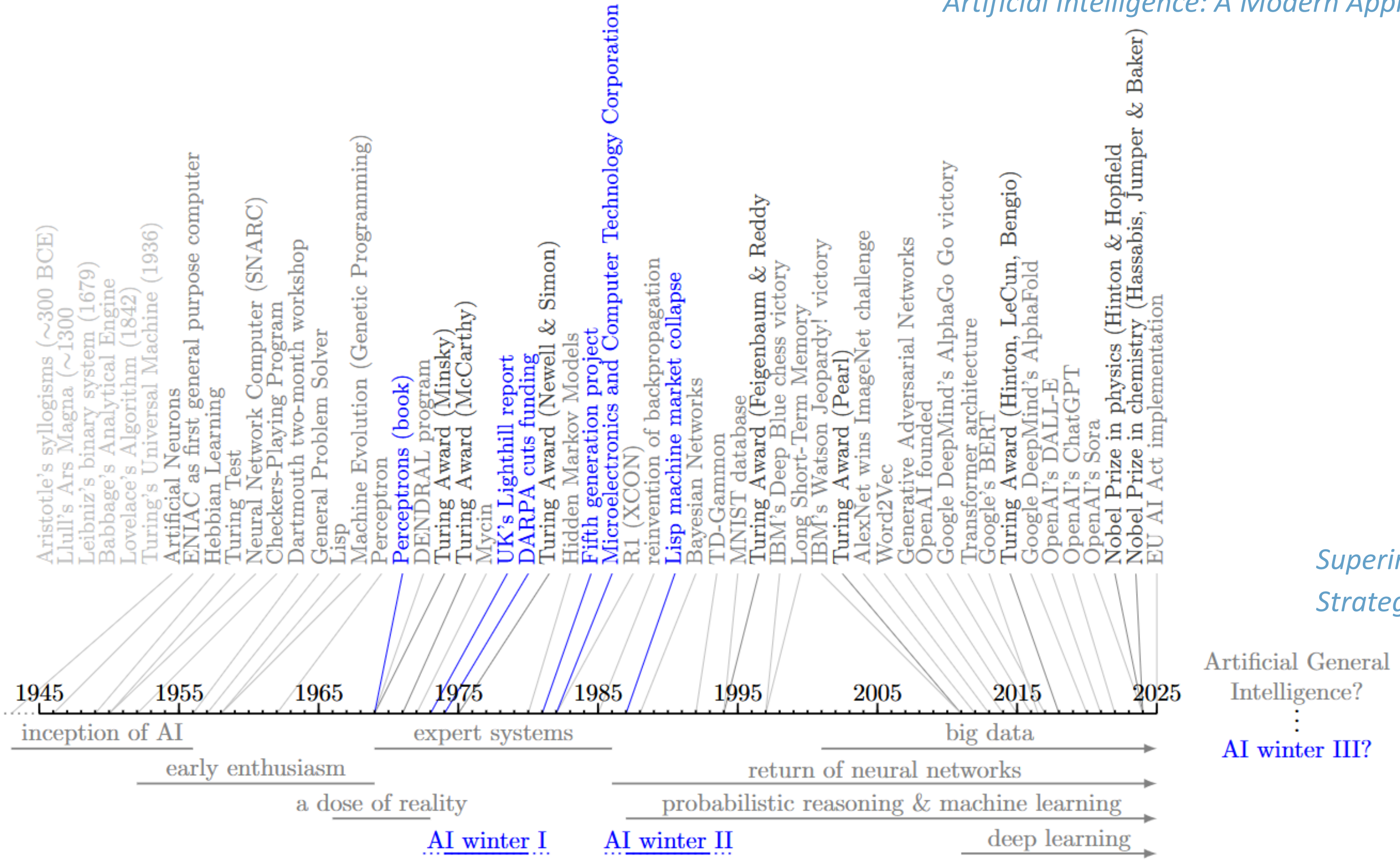
Or?



Inspired by Rebekka Woldseth, author of "On the use of artificial neural networks in topology optimisation"

History of Artificial Intelligence

Artificial Intelligence: A Modern Approach, Norvig et al. 2020



Superintelligence: Paths, Dangers, Strategies, Bostrom 2014

History of Artificial Intelligence

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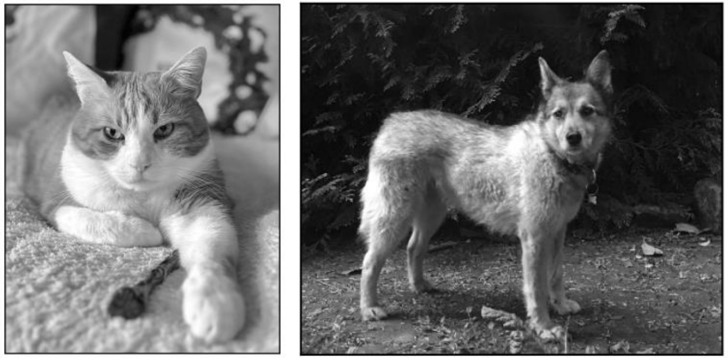
Artificial Intelligence: A Modern Approach, Norvig et al. 2020

- **The inception of artificial intelligence** (1943-1956)
  - Basic physiology of the brain → artificial neurons (on/off); updating rule as Hebbian Learning; SNARC
- **Early enthusiasm, great expectations** (1952-1969)
  - Turing "a machine can never do X"; models were based on logic and symbolic reasoning; (GPS, Lisp, perceptron)
- **A dose of reality** (1966-1973)
  - Overconfidence: models based on "informed introspection" & "intractability of attempted problems"; Lighthill
- **Expert systems** (1969-1986)
  - Instead of general-purpose tools; domain-specific knowledge; (DENDRAL, Mycin, R1); Fifth Generation Project
- **The return of neural networks** (1986-)
  - Reinvention of backpropagation
- **Probabilistic reasoning and machine learning** (1987-)
  - Reaction to failure of expert systems; learn from experience → adaptable & incorporation of uncertainty
  - Hidden Markov Models (Reinforcement Learning); Bayesian Networks; TD-Gammon
- **Big data** (2001-)
  - World Wide Web: large datasets (billions-trillions of samples); ImageNet (challenge), IBM's Watson
- **Deep learning** (2011-)
  - Hardware improvements (GPU: $10^{14} - 10^{17}$ vs CPU: $10^9 - 10^{10}$ Flops); (Deep CNNs in AlexNet); AlphaGo

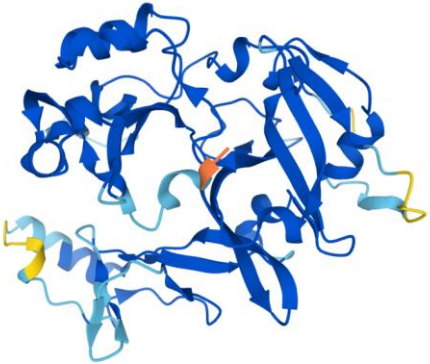
Recent Achievements in Artificial Intelligence

https://media.freemalaysiatoday.com/wp-content/uploads/2022/05/lifestyle-garry-emel-pic-110522.jpg

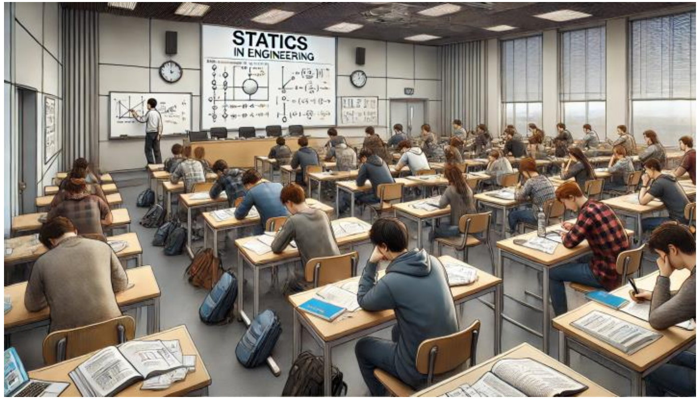


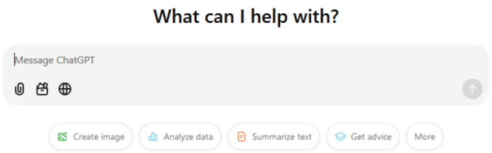
Cats versus dogs

https://media.freemalaysiatoday.com/wp-content/uploads/2016/03/AlphaGo.jpg



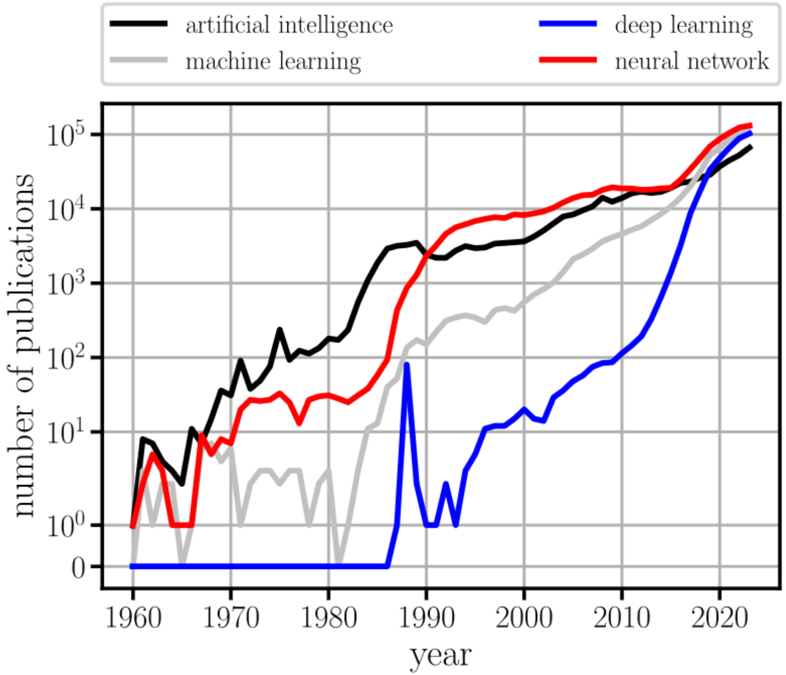
https://commons.wikimedia.org/wiki/File:C12orf29_AlphaFold.png



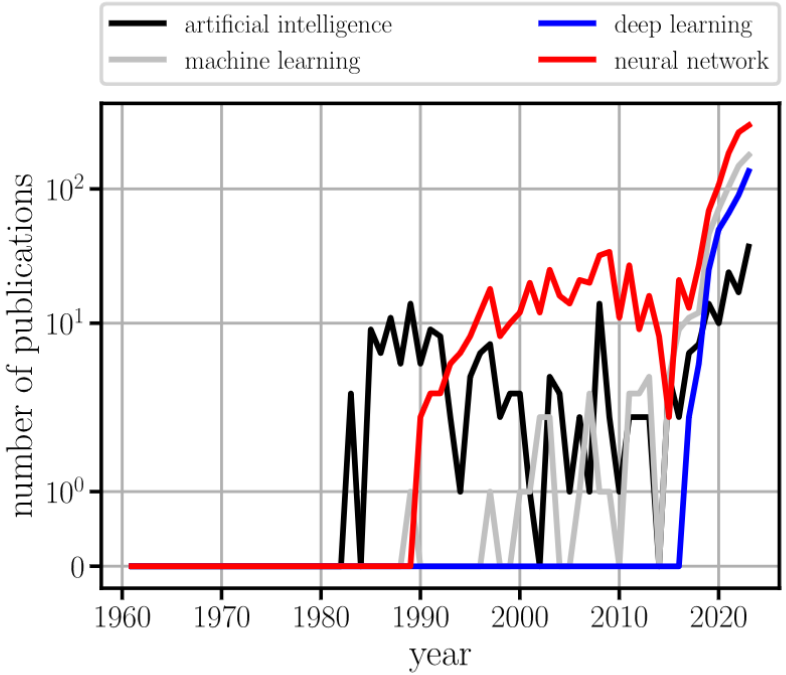


Artificial Intelligence in Science

Check www.aitracker.org for other trends



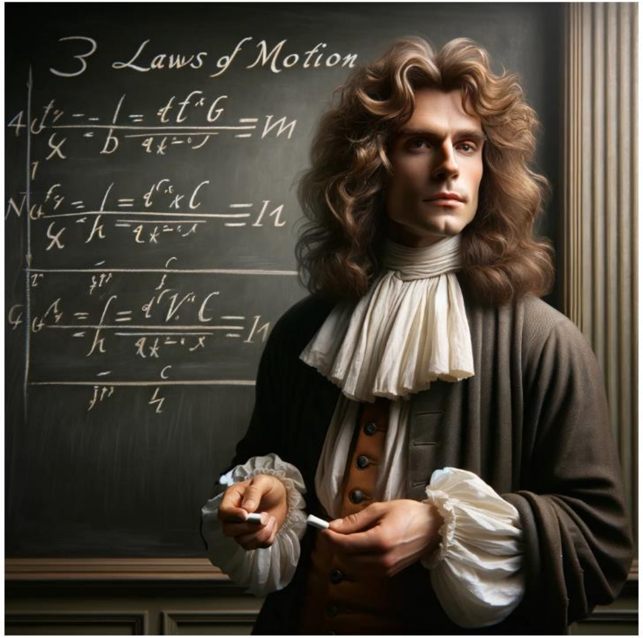
Publications in all fields

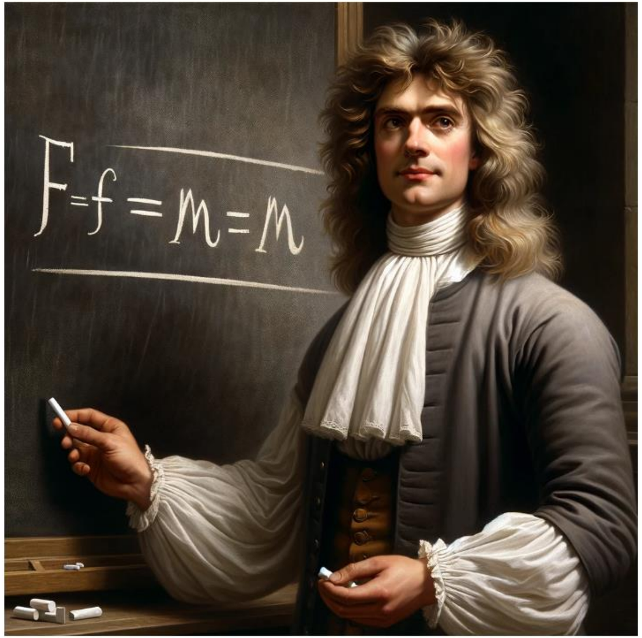


Publications in computational mechanics

Challenges

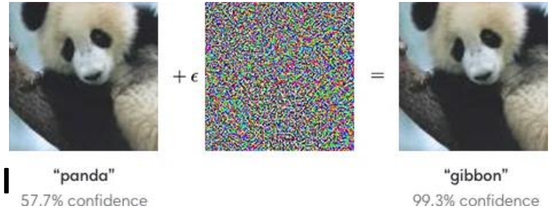
- “Generate an image of Isaac Newton in front of a blackboard on which his three laws are written in mathematical notation and chalk.“
- Follow-up: “The laws on the blackboard are incorrect. Please add the correct formulations. If you are unable to do so, simply focus on the second law, which is F=m*a.”





Generated with DALL-E-3

Challenges



https://openai.com/index/attacking-machine-learning-with-adversarial-examples/

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Limitations in deep learning in general

- Neural networks break in unpredictable ways → can be consistently fooled
- Deep learning is not robust due to sensitivity to hyperparameters → requires extensive tuning
- Neural networks are uninterpretable, i.e., limited explainability → limits reliability

See chapter 11 for details

Problems in deep learning in computational mechanics

- Reproducibility crisis (bias towards positive results, sensitivity, transparency)
- Fair evaluation metrics are disregarded (breakeven threshold, meaningful metrics, statistical assesements)
- State-of-the-art is not considered

$$\tau = \frac{T_{\text{data}} + T_{\text{train}}}{T_{\text{simulation}} - T_{\text{surrogate}}}$$

Good scientific practice for deep learning in computational mechanics

- Honest assessments & explanations (consider the state-of-the-art & proper metrics)
- Proposed methods should be robust towards hyperparameters (no extensive tuning for a novel problem)
- Careful & narrower selection of problem types (not general-purpose solution)
  - → domain-specific improvements

Towards a meaningful integration of neural networks in computational solid mechanics, Herrmann 2025

Example from topology optimization

The mean squared error

$$MSE = \frac{1}{m}\sum_{i=1}^{m}\left(x_{\mathrm{left}_i} - x_{\mathrm{right}_i}\right)^2$$

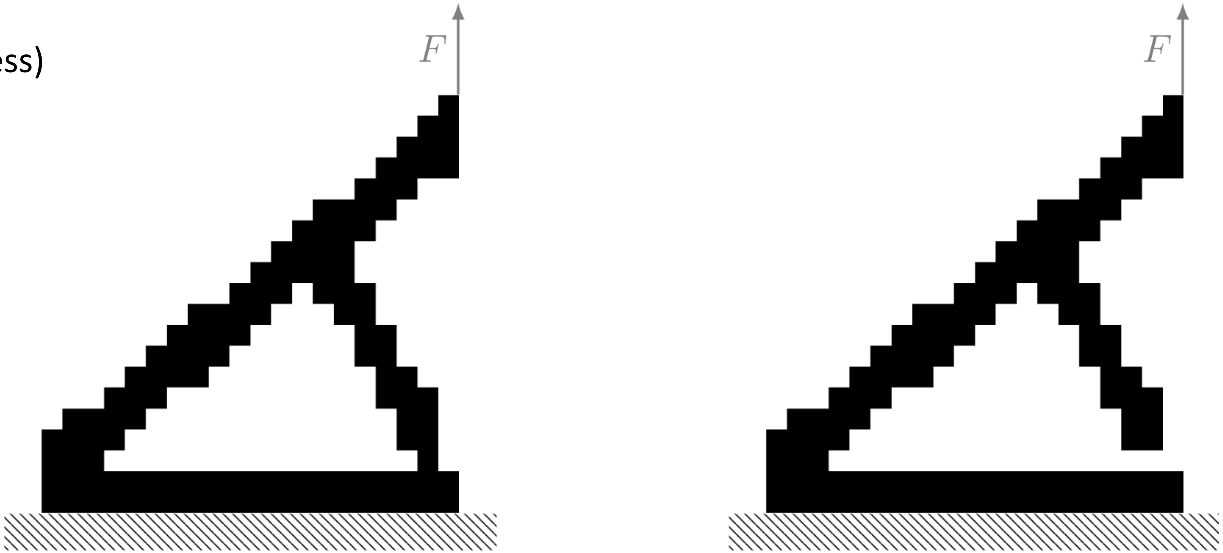
between the two structures is very small ($2.5 \cdot 10^{-3}$), due to one pixel difference.

Structural compliance (inverse of stiffness)

$c = \boldsymbol{F}^T \boldsymbol{u}$

Is different by one order of magnitude

For more details, see Chapter 9



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Computational Mechanics Meets Artificial Intelligence

Computational Mechanics

Abstraction of physical systems (reality) through simplified mathematical models (often differential equations), which are discretized and solved numerically for insight into real-world behavior

Exemplary tasks

- Efficient solutions techniques for forward problems, e.g., finite element, difference, and volume
- Identification tasks (inverse problems), e.g., inferring material distribution/properties from measurements
- Optimization, e.g., finding the optimal material distribution that maximizes stiffness

Machine Learning

Machine Learning, Mitchell 1997

”a computer program is said to learn from experience E with respect to some class of tasks T and performance measure P, if its performance at tasks T, as measured by P, improves with experience E”

Where can machine learning be applied in computational mechanics?

- Identification of mathematical models from data (instead of relying on hand-crafted models)
- Acceleration of forward solvers and optimizers
- Streamlining of pipelines to avoid human experts within the processes

Computational Mechanics Meets Artificial Intelligence

Deep learning in computational mechanics: a review, Herrmann et al. 2024

- **Simulation substitution**
  - Data-driven modelling — Simulation with graph neural networks; DMD; Transfer learning
  - Physics-informed learning — Hamiltonian/Lagrangian neural networks; SINDy; (PINNs)
- **Simulation enhancement** — Input-convex neural networks for material modeling; EUCLID; Neural networks as ansatz function of inverse quantities; Superresolution; Differentiable physics
- **Discretizations as neural networks** — Hardware acceleration with GPUs; (HiDeNN)
- **Generative approaches** — Generative design; Realistic data generation; Anomaly detection; Transformers for natural language processing
- **Deep reinforcement learning** — Control engineering tasks: autonomous flight; robots; Alternative gradient-free optimizer

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