

Deep Learning

Lecture 0: Introduction

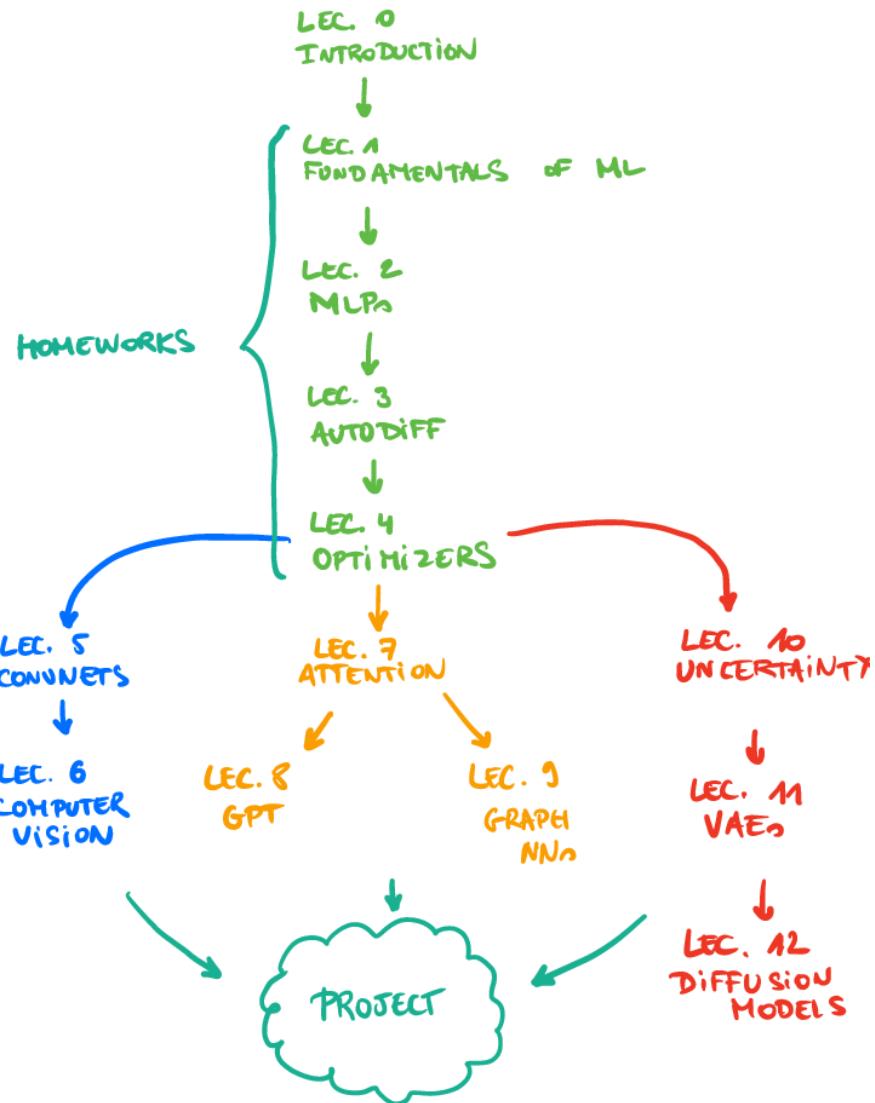
Prof. Gilles Louppe
g.louppe@uliege.be

Today

- Course outline
- Introduction to deep learning
- Fundamentals of machine learning

Outline

- Lecture 1: Fundamentals of machine learning
- Lecture 2: Multi-layer perceptron
- Lecture 3: Automatic differentiation
- Lecture 4: Training neural networks
- Lecture 5: Convolutional neural networks
- Lecture 6: Computer vision
- Lecture 7: Attention and transformer networks
- Lecture 8: GPT
- Lecture 9: Graph neural networks
- Lecture 10: Uncertainty
- Lecture 11: Auto-encoders and variational auto-encoders
- Lecture 12: Score-based diffusion models



My mission

By the end of this course, you will have a strong and comprehensive understanding of deep learning.

You will learn how to design deep neural networks for various advanced probabilistic inference tasks and how to train them.

The models covered in this course have broad applications in artificial intelligence, engineering, and science.

Why learning?



What do you see?



Sheepdog or mop?



Chihuahua or muffin?

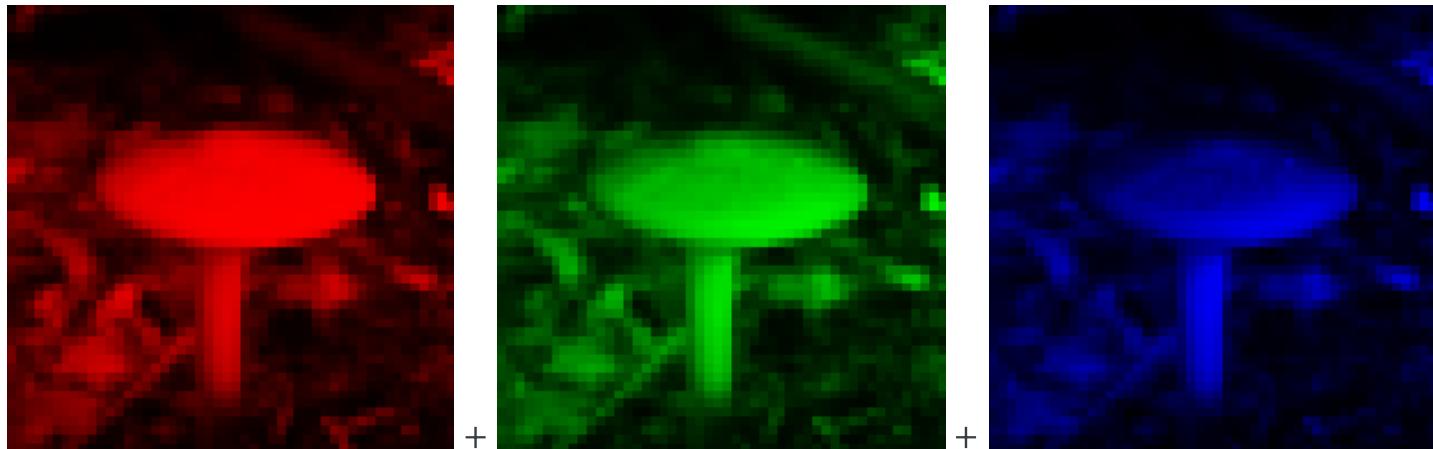
The (human) brain is so good at interpreting visual information that the gap between raw data and its semantic interpretation is difficult to assess intuitively.



This is a mushroom.



This is a mushroom.



This is a mushroom.

```
array([[[0.03921569, 0.03529412, 0.02352941, 1.          ],
       [0.2509804 , 0.1882353 , 0.20392157, 1.          ],
       [0.4117647 , 0.34117648, 0.37254903, 1.          ],
       ...,
       [0.20392157, 0.23529412, 0.17254902, 1.          ],
       [0.16470589, 0.18039216, 0.12156863, 1.          ],
       [0.18039216, 0.18039216, 0.14117648, 1.          ]],

      [[0.1254902 , 0.11372549, 0.09411765, 1.          ],
       [0.2901961 , 0.2509804 , 0.24705882, 1.          ],
       [0.21176471, 0.2        , 0.20392157, 1.          ],
       ...,
       [0.1764706 , 0.24705882, 0.12156863, 1.          ],
       [0.10980392, 0.15686275, 0.07843138, 1.          ],
       [0.16470589, 0.20784314, 0.11764706, 1.          ]],

      [[0.14117648, 0.12941177, 0.10980392, 1.          ],
       [0.21176471, 0.1882353 , 0.16862746, 1.          ],
       [0.14117648, 0.13725491, 0.12941177, 1.          ],
       ...,
       [0.10980392, 0.15686275, 0.08627451, 1.          ],
       [0.0627451 , 0.08235294, 0.05098039, 1.          ],
       [0.14117648, 0.2        , 0.09803922, 1.          ]],

      ...]
```

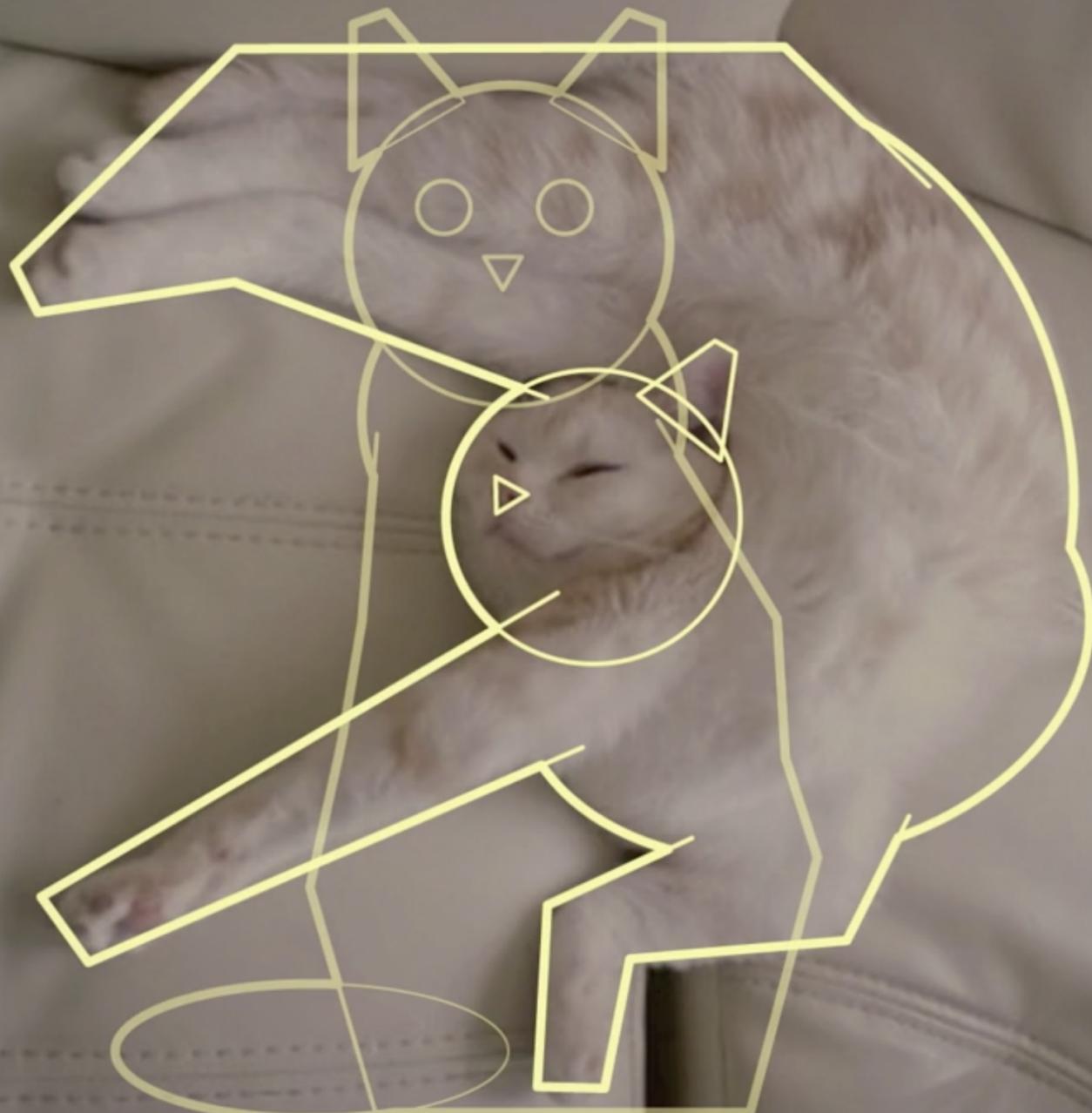
This is a mushroom.

Writing a computer program that sees?









To extract semantic information, we need models with high complexity **that cannot be manually designed.**

However, we can write a program that learns the task of extracting semantic information.



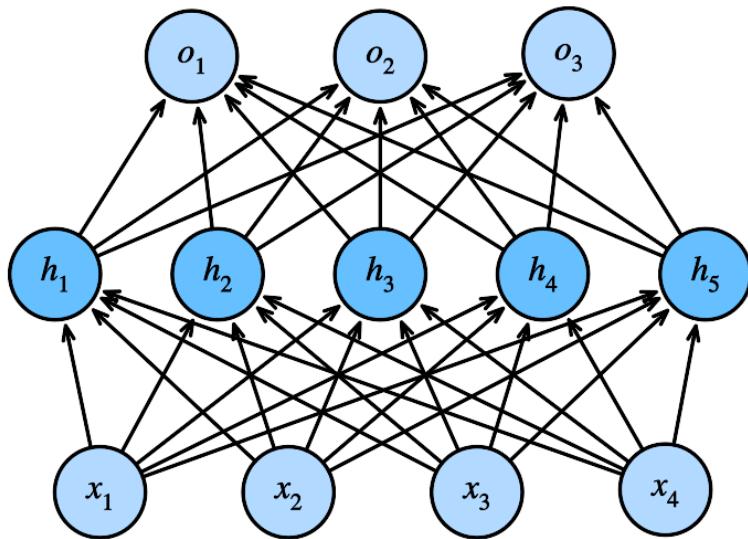
The **machine learning approach** consists in:

- defining a parametric model
- optimizing its parameters, by "making it work" on the training data.

The deep learning revolution

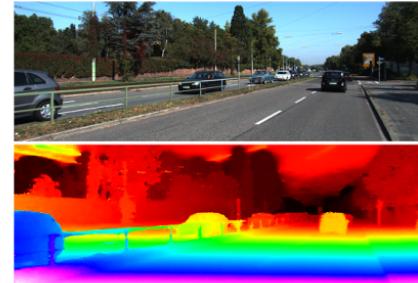
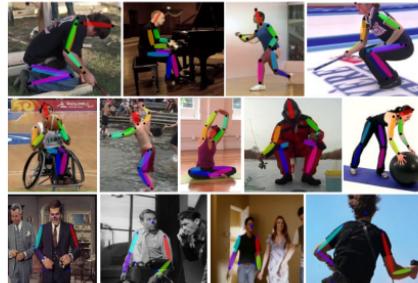
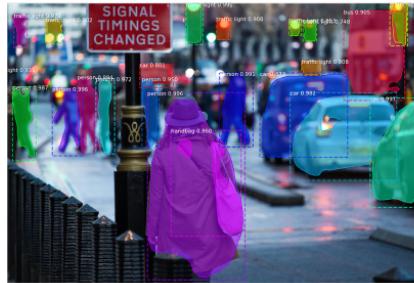
Deep learning **scales up** the statistical and machine learning approaches by

- using larger models known as neural networks,
- training on larger datasets,
- using more compute resources.





Specialized neural networks can be trained achieve super-human performance on many complex tasks that were previously thought to be out of reach for machines.

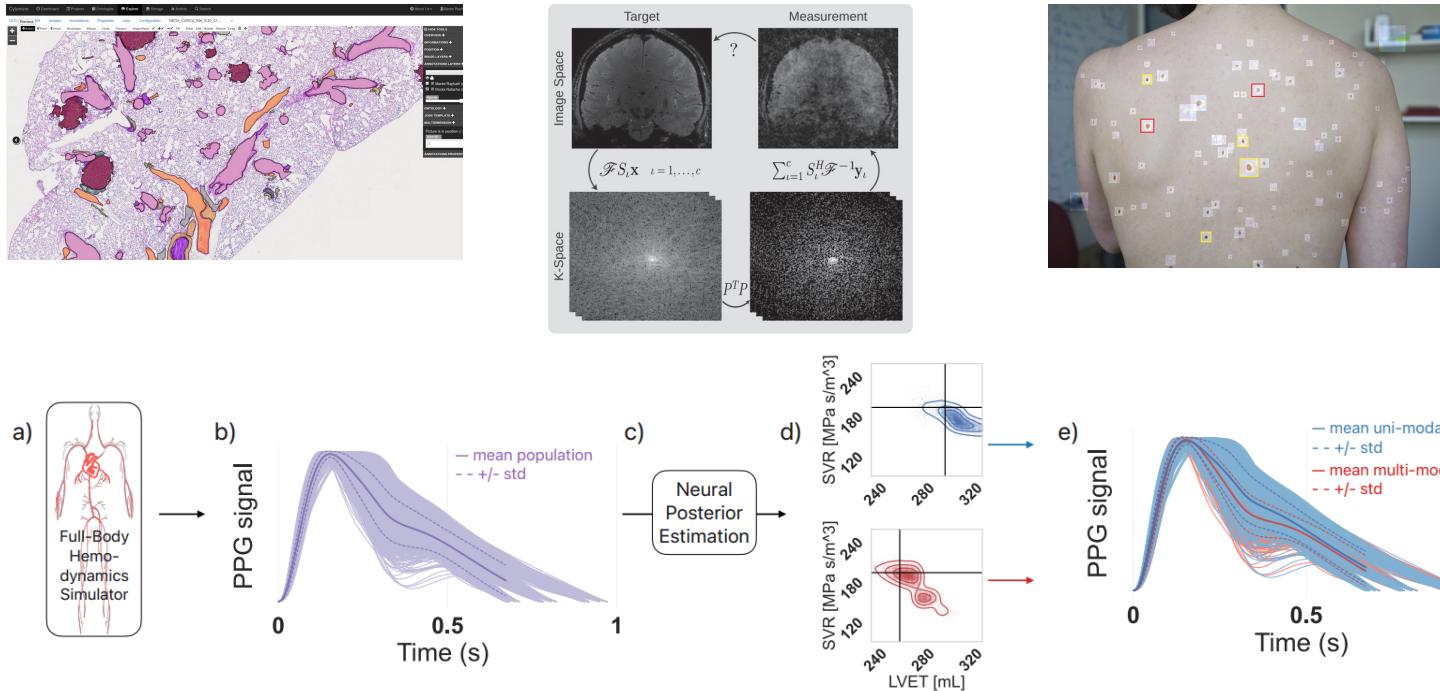


- I: Jane went to the hallway.
I: Mary walked to the bathroom.
I: Sandra went to the garden.
I: Daniel went back to the garden.
I: Sandra took the milk there.
Q: Where is the milk?
A: garden

(Top) Scene understanding, pose estimation, geometric reasoning.

(Bottom) Planning, Image captioning, Question answering.

Neural networks form **primitives** that can be transferred to many domains.



(Top) Analysis of histological slides, denoising of MRI images, nevus detection.

(Bottom) Whole-body hemodynamics reconstruction from PPG signals.



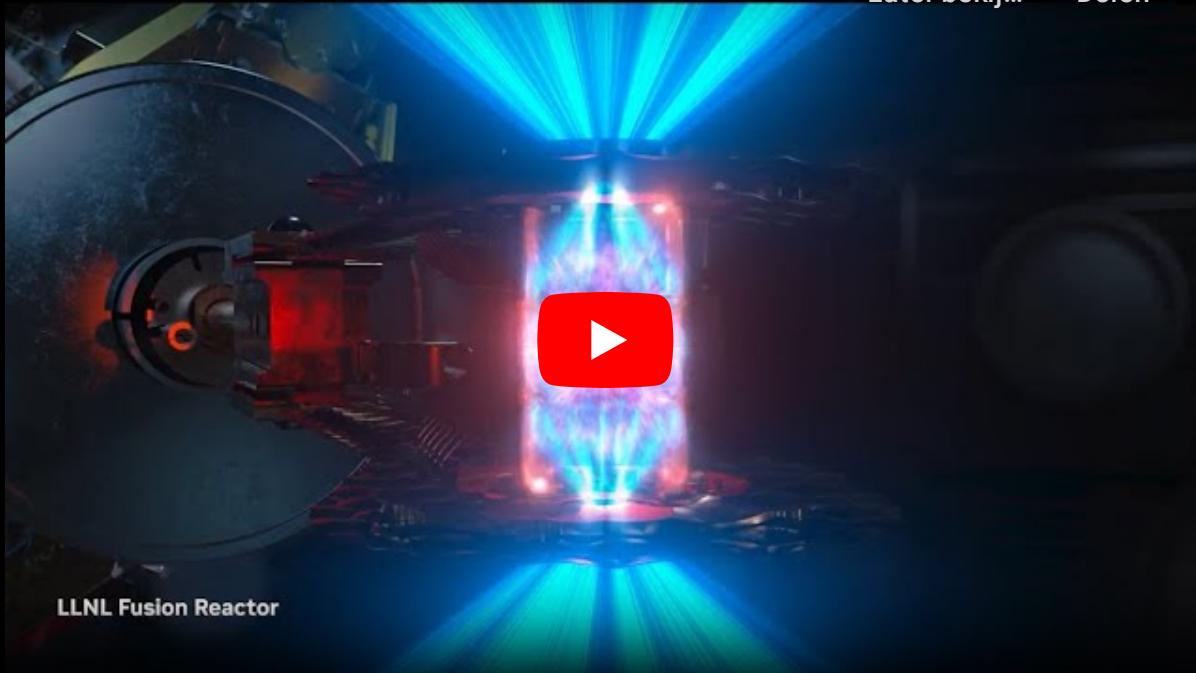
Powering the Future of Clean Energy | I AM ...



Later bekij...
Later bekijken



Delen



Powering the future of clean energy (NVIDIA, 2023)



Camels, Code & Lab Coats: How AI Is Advancing Medicine



Later bekijk...



Delen



How AI is advancing medicine (Google, 2023)



Sense, Solve, and Go: The Magic of the Wa...



Later bekij...



Delen



Building autonomous cars (Waymo, 2022)

The breakthrough

Attention Is All You Need

Ashish Vaswani*
Google Brain
avaswani@google.com

Noam Shazeer*
Google Brain
noam@google.com

Niki Parmar*
Google Research
nikip@google.com

Jakob Uszkoreit*
Google Research
usz@google.com

Llion Jones*
Google Research
llion@google.com

Aidan N. Gomez* †
University of Toronto
aidan@cs.toronto.edu

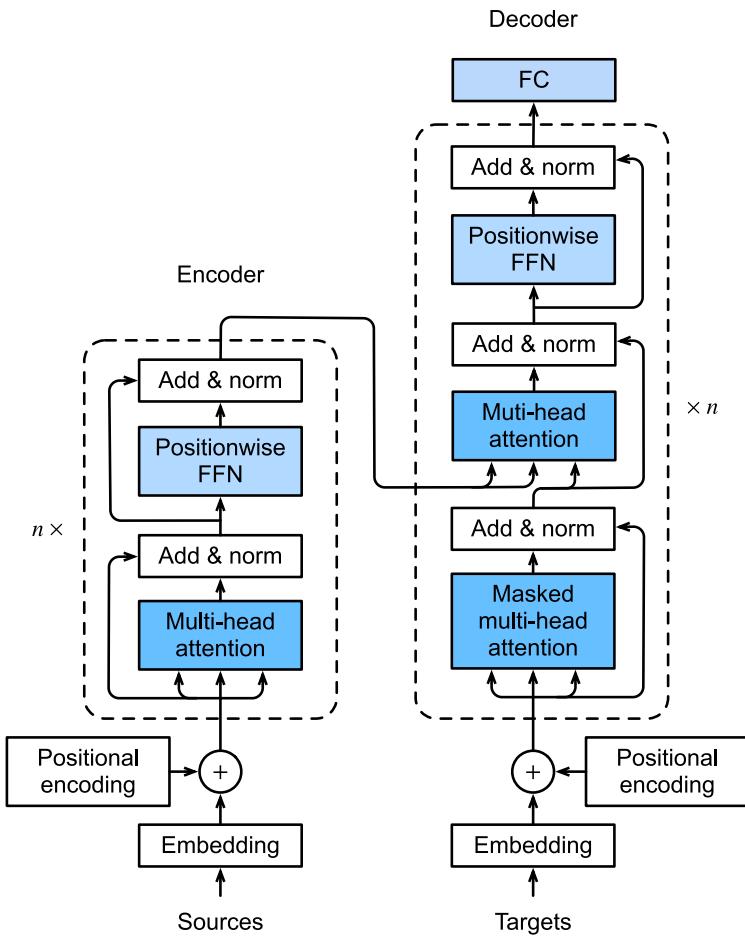
Lukasz Kaiser*
Google Brain
lukasz.kaiser@google.com

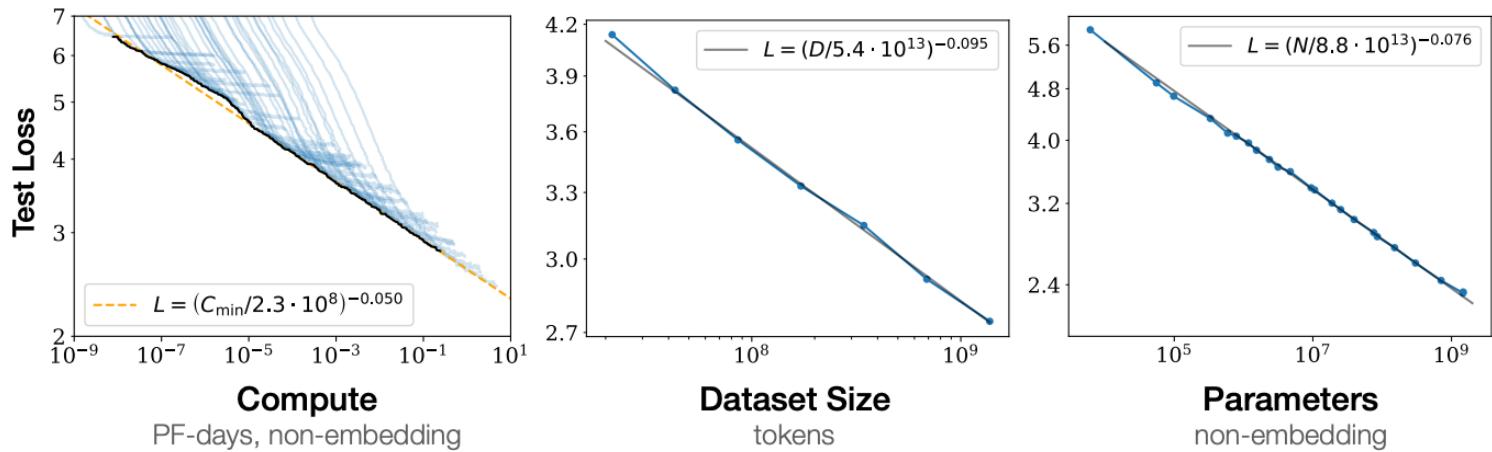
Illia Polosukhin* ‡
illia.polosukhin@gmail.com

Abstract

The dominant sequence transduction models are based on complex recurrent or convolutional neural networks that include an encoder and a decoder. The best performing models also connect the encoder and decoder through an attention mechanism. We propose a new simple network architecture, the Transformer, based solely on attention mechanisms, dispensing with recurrence and convolutions entirely. Experiments on two machine translation tasks show these models to be superior in quality while being more parallelizable and requiring significantly less time to train. Our model achieves 28.4 BLEU on the WMT 2014 English-to-German translation task, improving over the existing best results, including ensembles, by over 2 BLEU. On the WMT 2014 English-to-French translation task, our model establishes a new single-model state-of-the-art BLEU score of 41.8 after training for 3.5 days on eight GPUs, a small fraction of the training costs of the best models from the literature. We show that the Transformer generalizes well to other tasks by applying it successfully to English constituency parsing both with large and limited training data.

Vaswani et al., 2017.





A brutal simplicity:

- The more data, the better the model.
- The more parameters, the better the model.
- The more compute, the better the model.

Scaling up further to gigantic models, datasets, and compute resources keeps pushing the boundaries of what is possible, **with no sign of slowing down**.



Claude 3.5 Sonnet as a writing partner



Later bekij...

Delen

The screenshot shows a conversational interface with two main panels. On the left, a user message is shown:

AI: *...knowing how their families' histories intertwine and potentially influence their current relationship and work together. It adds depth to the story by suggesting multiple avenues for backstory and character development.*

User: *Would you like me to explain any part of the genogram in more detail or explore how these family connections might influence the story?*

AI: *Fantastic. I'm curious how best to showcase the arthropod <-> human interaction. Could you ideate on a sample of the translation?*

User: *Certainly! Let's explore a sample of how the arthropod-human interaction and translation might work between Claw'd and Dr. Wave. I'll create a brief dialogue that demonstrates this unique communication system.*

AI: *[Performs a series of rapid claw clicks, antennae vibrations, and releases a pattern of small bubbles]*

JustAI (Translation Interface): *Analyzing crab communication patterns... Processing...*

AI: *Translated output: "Hey doc,*

Below the main interface, there is a sidebar titled "Sample Dialogue: Claw'd and Dr. Wave's Translated Interaction". It contains the following text:

Setting: *An underwater research station. Dr. Wave is analyzing data on a holographic display. Claw'd approaches, his movements captured by an array of advanced sensors.*

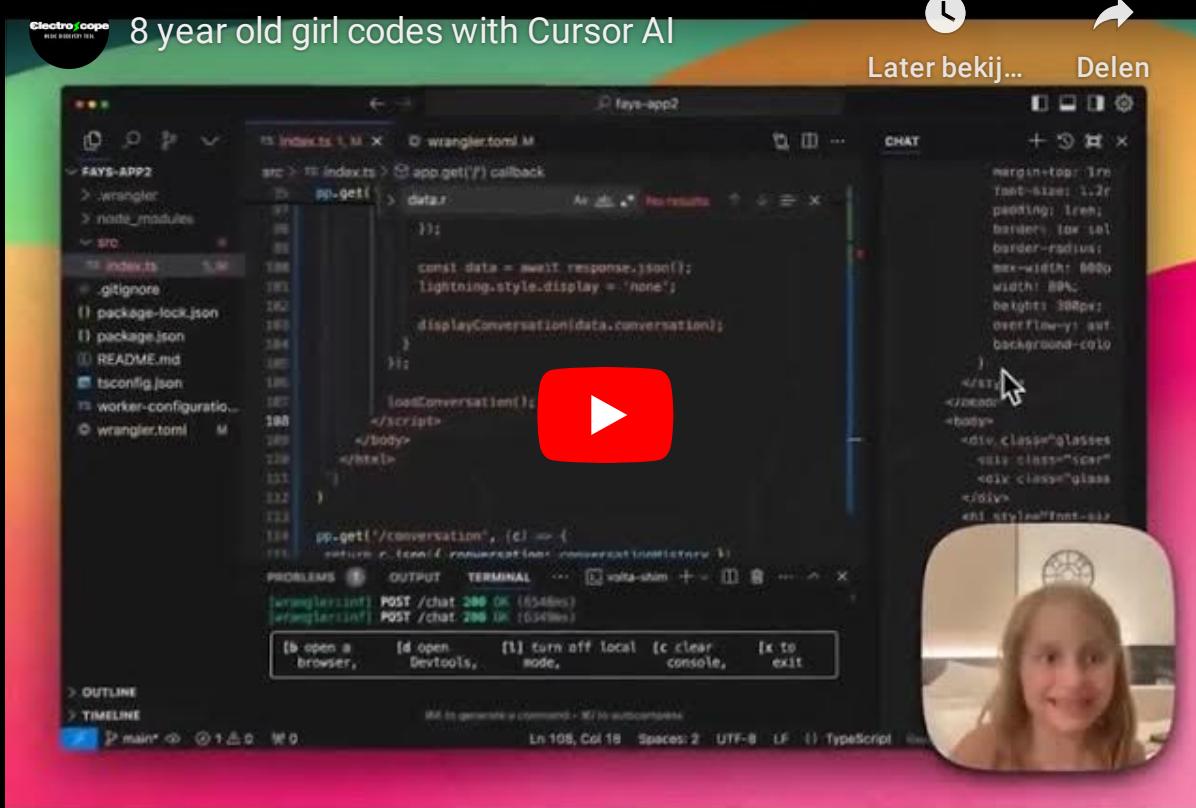
Claw'd: *[Performs a series of rapid claw clicks, antennae vibrations, and releases a pattern of small bubbles]*

JustAI (Translation Interface): *Analyzing crab communication patterns... Processing...*

AI: *Translated output: "Hey doc,*

At the bottom of the sidebar, it says "Last edited just now" and has a "Copy" button.

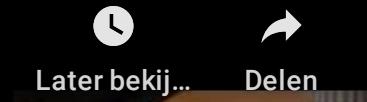
Conversational AI assistants (Anthropic, 2024)



Code assistants (Cursor, 2024)



Rock, Paper, Scissors with GPT-4o



Not just text, but also images and sounds.

Deep learning can also **solve problems that no one could solve before**.

AlphaFold: From a sequence of amino acids to a 3D structure

nature

Explore content ▾ About the journal ▾ Publish with us ▾

nature > articles > article

Article | [Open access](#) | Published: 15 July 2021

Highly accurate protein structure prediction with AlphaFold

John Jumper , Richard Evans, Alexander Pritzel, Tim Green, Michael Figurnov, Olaf Ronneberger, Kathryn Tunyasuvunakool, Russ Bates, Augustin Žídek, Anna Potapenko, Alex Bridgland, Clemens Meyer, Simon A. A. Kohl, Andrew J. Ballard, Andrew Cowie, Bernardino Romera-Paredes, Stanislav Nikolov, Rishabh Jain, Jonas Adler, Trevor Back, Stig Petersen, David Reiman, Ellen Clancy, Michał Zieliński, ... Demis Hassabis 

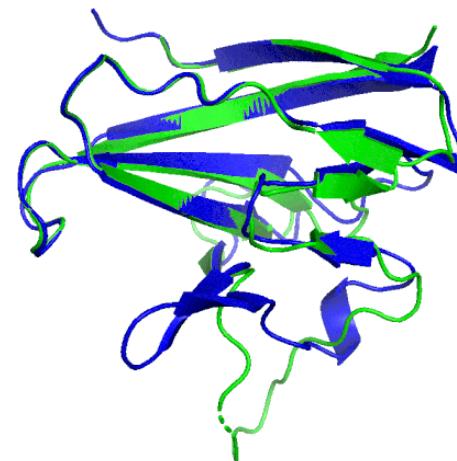
+ Show authors

[Nature](#) 596, 583–589 (2021) | [Cite this article](#)

1.42m Accesses | 12k Citations | 3493 Altmetric | [Metrics](#)

Abstract

Proteins are essential to life, and understanding their structure can facilitate a mechanistic understanding of their function. Through an enormous experimental effort^{1,2,3,4}, the structures of around 100,000 unique proteins have been determined⁵, but this represents a small fraction of the billions of known protein sequences^{6,7}. Structural coverage is bottlenecked by the months to years of painstaking effort required to determine a single protein structure. Accurate computational approaches are needed to address this gap and to enable large-scale structural bioinformatics. Predicting the three-dimensional structure that a protein will adopt based solely on its amino acid sequence—the structure prediction component of the ‘protein folding problem’⁸—has been an important open research problem for more than 50 years⁹. Despite recent progress^{10,11,12,13,14}, existing methods fall far short of atomic accuracy, especially when no homologous structure is available. Here we provide the





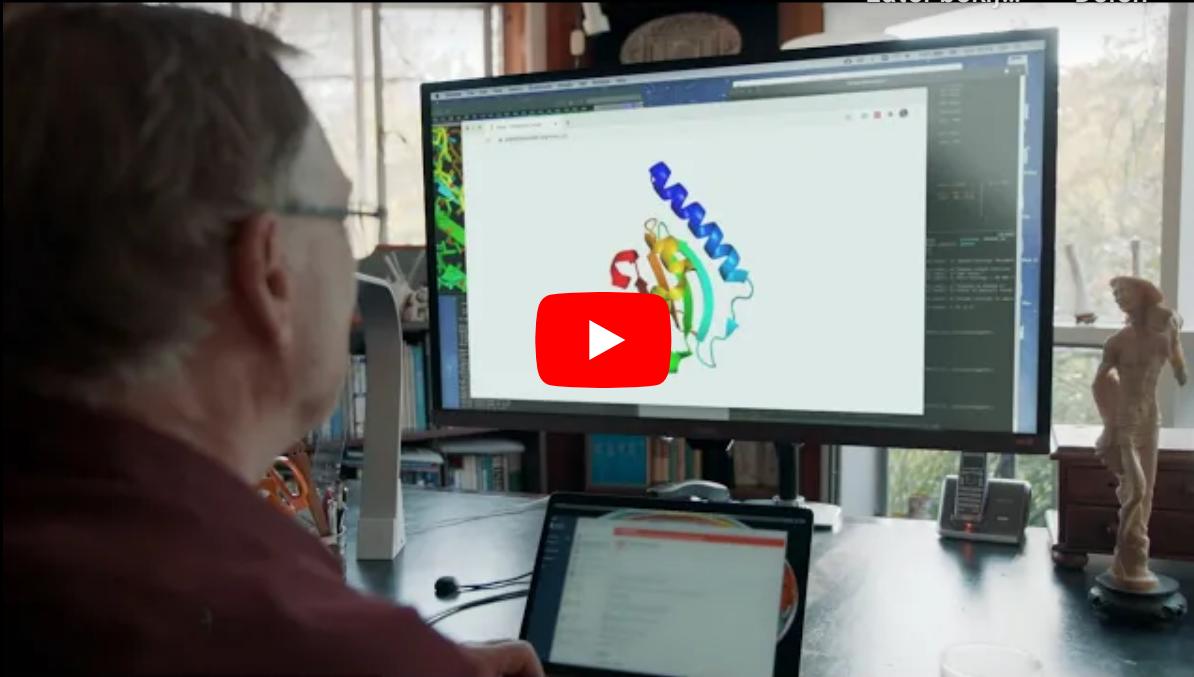
AlphaFold: The making of a scientific break...



Later bekij...



Delen



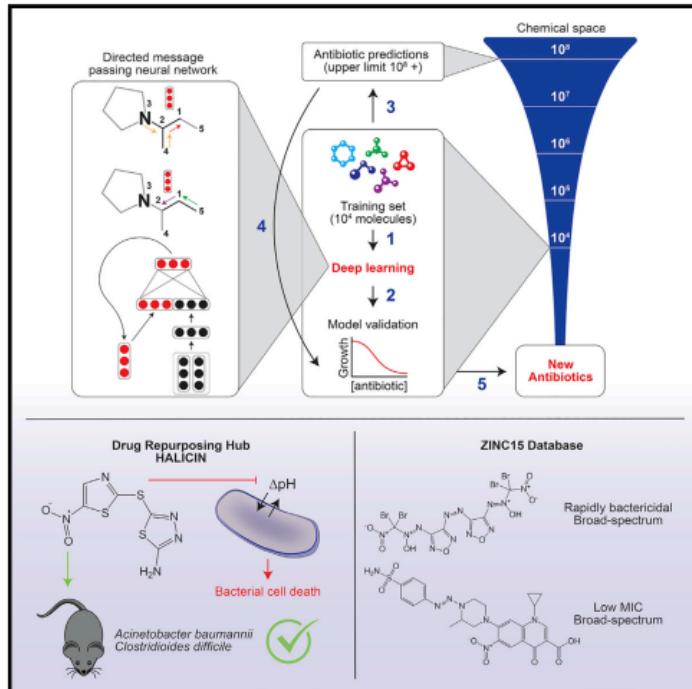
AI for Science (Deepmind, AlphaFold, 2020)

Drug discovery with graph neural networks

Cell

A Deep Learning Approach to Antibiotic Discovery

Graphical Abstract



Authors

Jonathan M. Stokes, Kevin Yang,
Kyle Swanson, ..., Tommi S. Jaakkola,
Regina Barzilay, James J. Collins

Correspondence

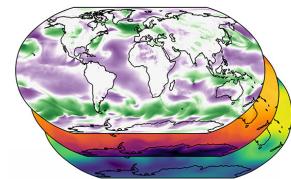
regina@csail.mit.edu (R.B.),
jimjc@mit.edu (J.J.C.)

In Brief

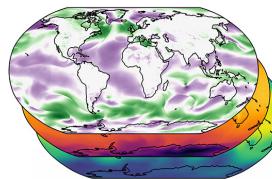
A trained deep neural network predicts antibiotic activity in molecules that are structurally different from known antibiotics, among which Halicin exhibits efficacy against broad-spectrum bacterial infections in mice.

GraphCast: fast and accurate weather forecasts

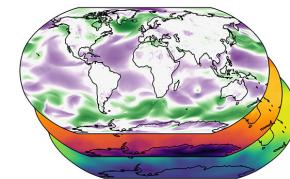
a) Input weather state



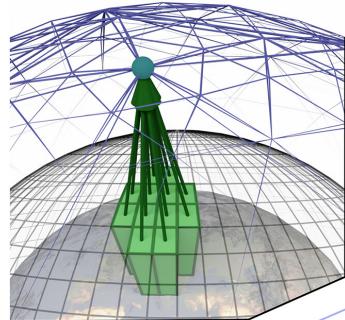
b) Predict the next state



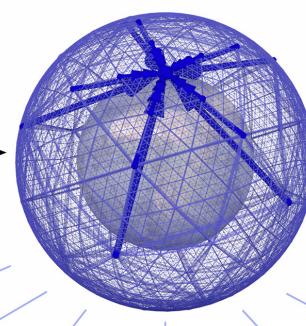
c) Roll out a forecast



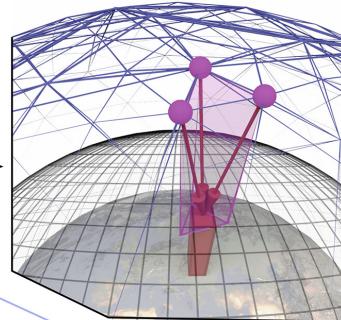
d) Encoder



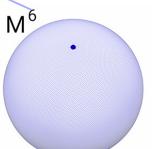
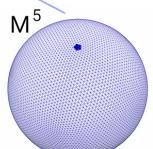
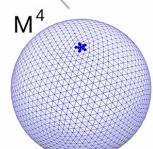
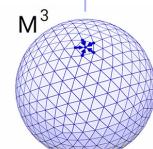
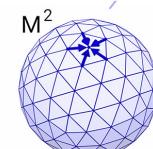
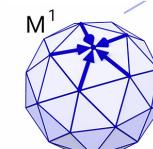
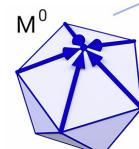
e) Processor



f) Decoder



g) Simultaneous multi-mesh message-passing





For the last forty years we have programmed computers; for the next forty years we will train them.

Chris Bishop, 2020.

