Deep Learning

Lecture 0: Introduction

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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?

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Chihuahua or muffin?

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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.


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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 \bullet
- 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.

A person riding a notorcycle on a dirt road

Two dogs play in the grass

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.

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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 (NVIDIA, 2023)

How AI is advancing medicine (Google, 2023)

Building autonomous cars (Waymo, 2022)

The breakthrough

Attention Is All You Need Ashish Vaswani* Noam Shazeer* Niki Parmar* **Jakob Uszkoreit* Google Brain Google Brain Google Research Google Research** avaswani@google.com noam@google.com nikip@google.com usz@google.com **Llion Jones*** Aidan N. Gomez^{*} [†] Łukasz Kaiser* **Google Research University of Toronto Google Brain** llion@google.com aidan@cs.toronto.edu lukaszkaiser@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 Englishto 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.

Decoder

A brutal simplicity:

- The more data, the better the model.
- The more parameters, the better the model. \bullet
- 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.

Conversational AI assistants (Anthropic, 2024)

Code assistants (Cursor, 2024)

Not just text, but also images and sounds.

With great power comes great responsibility.

Risks

The report classifies risks associated with general-purpose AI into three categories:

- 1. Risks from **malicious use** (scams, manipulation, cyberattacks, biological/chemical attacks)
- 2. Risks from **malfunctions** (hallucinations, biases, loss of control)
- 3. **Systemic** risks (labour market risks, global R&D divide, power concentration)

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Environmental impacts

"AI is a moderate but rapidly growing contributor to global environmental impacts through energy use and greenhouse gas (GHG) emissions. Current estimates indicate that data centres and data transmission account for an estimated 1% of global energy-related GHG emissions, with AI consuming 10– **28% of data centre energy capacity**. Al energy demand is expected to grow substantially [...]"

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The Impact of Generative AI on Critical Thinking: Self-Reported **Reductions in Cognitive Effort and Confidence Effects From a Survey of Knowledge Workers**

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Abstract

The rise of Generative AI (GenAI) in knowledge workflows raises questions about its impact on critical thinking skills and practices. We survey 319 knowledge workers to investigate 1) when and how they perceive the enaction of critical thinking when using GenAI, and 2) when and why GenAI affects their effort to do so. Participants shared 936 first-hand examples of using GenAI in work tasks. Quantitatively, when considering both task- and user-specific factors, a user's task-specific self-confidence and confidence in GenAI are predictive of whether critical thinking is enacted and the effort of doing so in GenAI-assisted tasks. Specifically, higher confidence in GenAI is associated with less critical thinking, while higher self-confidence is associated with more critical thinking. Qualitatively, GenAI shifts the nature of critical thinking toward information verification, response integration, and task stewardship. Our insights reveal new design challenges and opportunities for developing GenAI tools for knowledge work.

Confidence Effects From a Survey of Knowledge Workers. In CHI Conference on Human Factors in Computing Systems (CHI '25), April 26-May 01, 2025,
Yokohama, Japan. ACM, New York, NY, USA, 23 pages. https://doi.org/10. 1145/3706598 3713778

1 Introduction

Generative AL(GenAI) tools, defined as any "end user tool L. Lyhose technical implementation includes a generative model based on deep learning".¹ are the latest in a long line of technologies that raise questions about their impact on the quality of human thought, a line that includes writing (objected to by Socrates), printing (objected to by Trithemius), calculators (objected to by teachers of arithmetic) and the Internet

Such consternation is not unfounded. Used improperly, technologies can and do result in the deterioration of cognitive faculties that ought to be preserved. As Bainbridge [7] noted, a key irony of automation is that by mechanising routine tasks and leaving

Dumb and dumber

"When people rely on generative AI, their effort shifts toward verifying that an AI's response is good enough to use, instead of using higher-order critical **thinking skills** like creating, evaluating, and analyzing information. If humans only intervene when AI responses are insufficient then workers are deprived of routine opportunities to practice their judgment and strengthen their cognitive musculature, leaving them atrophied and unprepared [...]."

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

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

nature

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Article | Open access | Published: 15 July 2021

Highly accurate protein structure prediction with **AlphaFold**

John Jumper¹, 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, Rishub Jain, Jonas Adler, Trevor Back, Stig Petersen, David Reiman, Ellen Clancy, Michal Zielinski, ... 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 $\frac{1,2,3,4}{2}$, 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' $\frac{8}{5}$ -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

AI for Science (Deepmind, AlphaFold, 2020)

Drug discovery with graph neural networks

Cell

A Deep Learning Approach to Antibiotic Discovery

Graphical Abstract

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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

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

Chris Bishop, 2020.

The end.