

# Machine Learning I – FALL 2025

**Jian Tang**

HEC Montreal

Mila-Quebec AI Institute

CIFAR AI Research Chair

Email: [jian.tang@hec.ca](mailto:jian.tang@hec.ca)



# Course Information

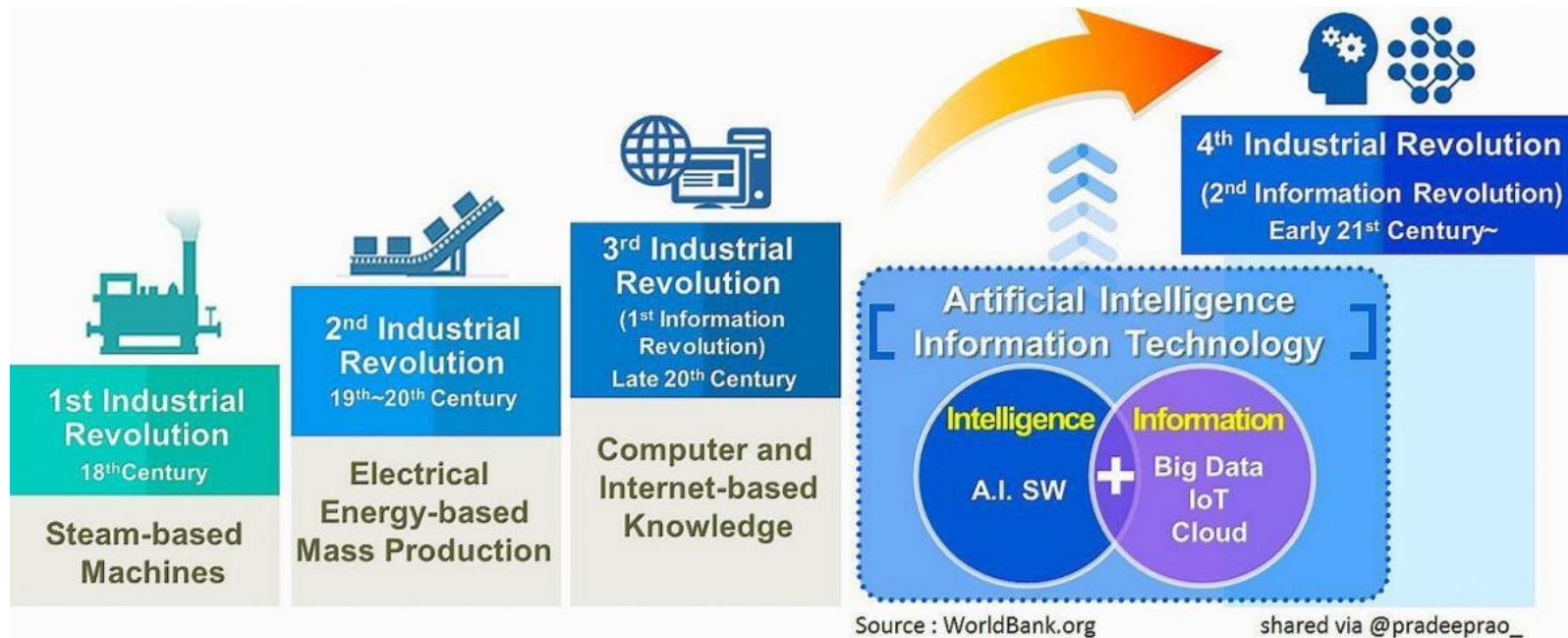
- Website:
  - [https://deepgraphlearning.github.io/MATH60629A\\_2025A/main.html](https://deepgraphlearning.github.io/MATH60629A_2025A/main.html)
- Instructor: **Jian Tang**
  - Associate Professor, Department of Decision Science, HEC Montreal
  - Homepage: [www.jian-tang.com](http://www.jian-tang.com)
  - Email: [jian.tang@hec.ca](mailto:jian.tang@hec.ca)
- Teaching Assistants: Xinyu Yuan, Zhihao Zhan
  - Ph.D at Mila and University of Montreal
  - Email: [xinyu.yuan@mila.quebec](mailto:xinyu.yuan@mila.quebec), [zhihao.zhan@mila.quebec](mailto:zhihao.zhan@mila.quebec)
- Join discord for discussion through this link:
  - Discord: <https://discord.gg/Jz8pX45g>

**"Artificial Intelligence** is the most revolutionary technology in decades, on par with **computers, cellphones** and the **internet.**"



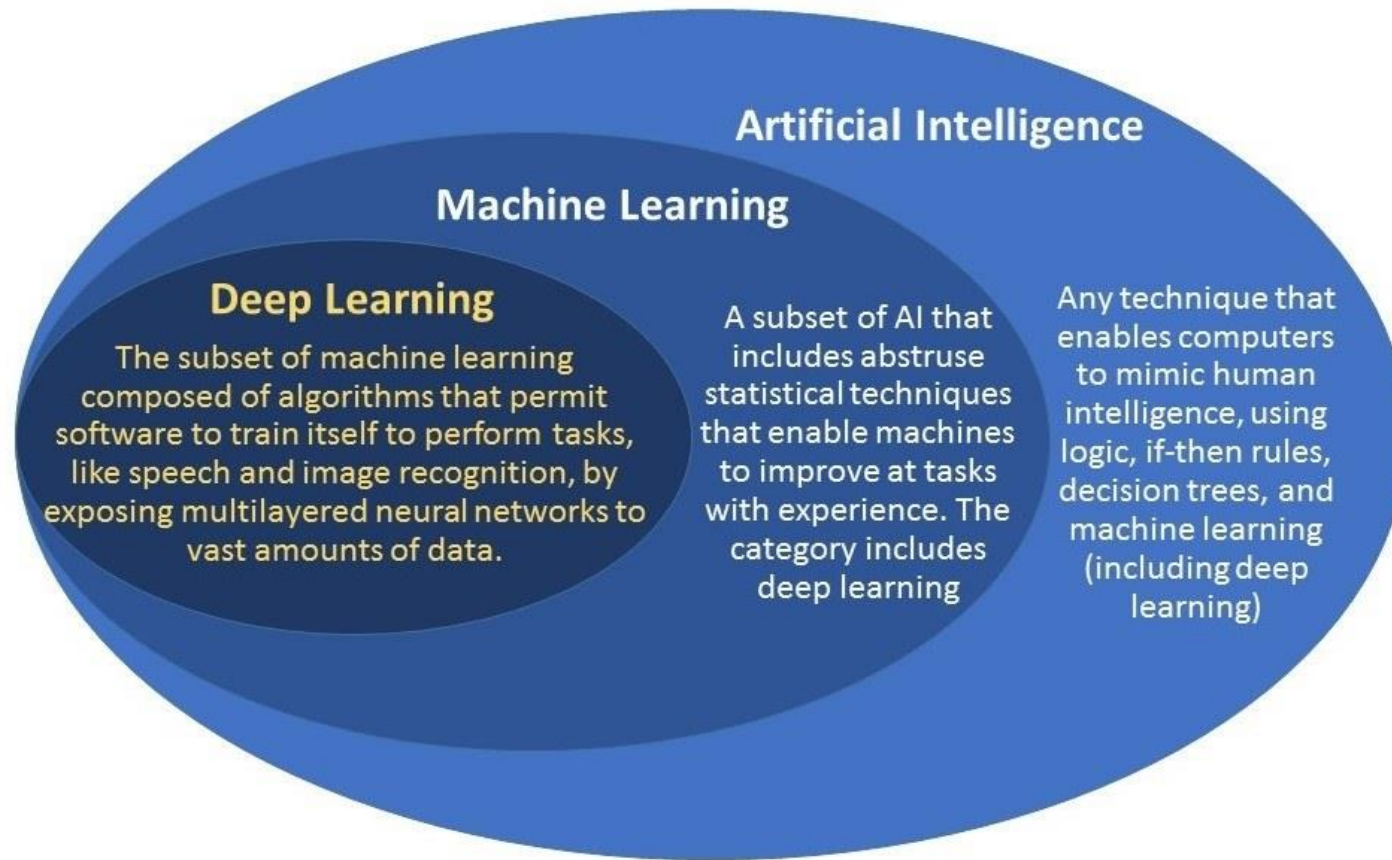
# Artificial Intelligence: the Fourth Industrial Revolution

- Artificial Intelligence
  - “the term is often used to describe machines (or computers) that mimic “cognitive” functions that humans associate with the [human mind](#), such as “learning” and “problem solving“.” -- Wikipedia



-image from Internet

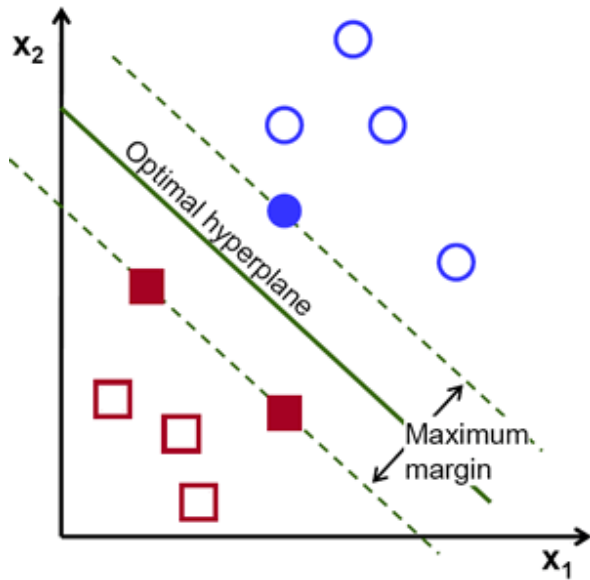
# Artificial Intelligence v.s. Machine Learning v.s. Deep Learning



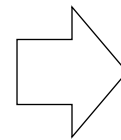
# Machine Learning

- “**Machine learning** is a field of [computer science](#) that uses statistical techniques to give [computer systems](#) the ability to "learn" (i.e., progressively improve performance on a specific task) with [data](#), without being explicitly programmed.”

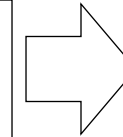
-Wikipedia



Support vector machines



**Hand-crafted**  
Feature Extractor



Simple Trainable Classifier  
e.g., SVM, LR

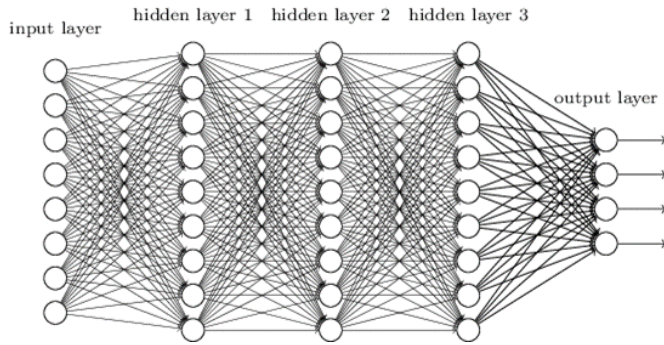


Domain experts

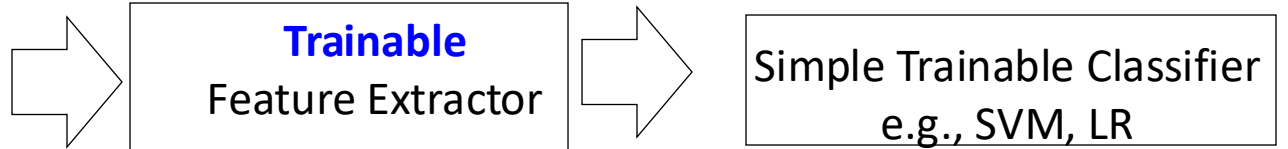


# Deep Learning = Feature Representation Learning

- Algorithms that allow to learn features from data (a.k.a, End-to-end learning)



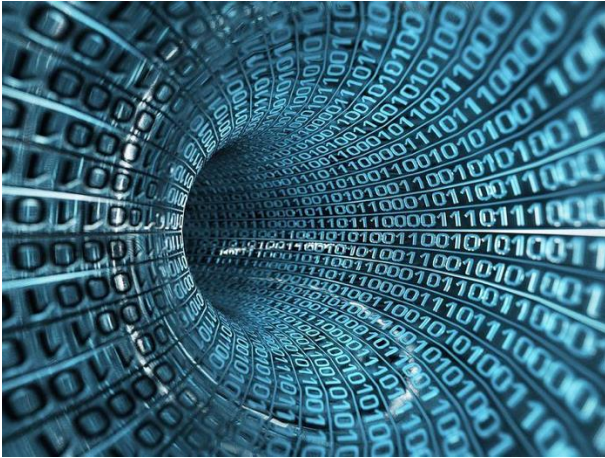
Deep Neural Networks



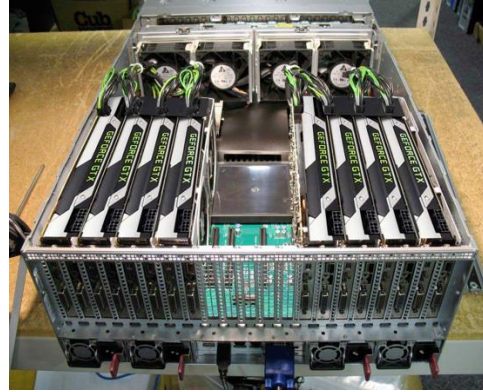
Domain experts



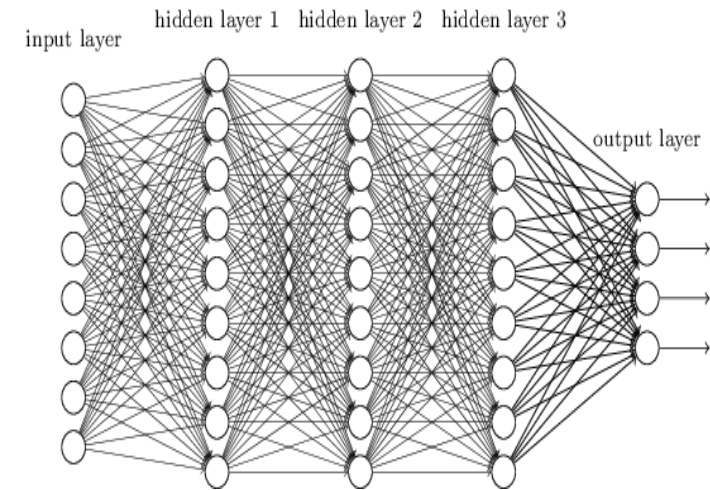
# Why Deep Learning Now?



Big Data



Big Computation



Big Model



# AlphaGo/AlphaZero

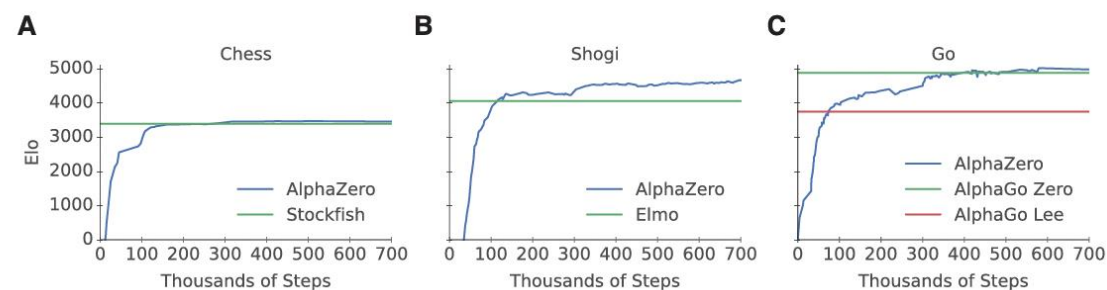


Figure 1: **Training AlphaZero for 700,000 steps.** Elo ratings were computed from games between different players where each player was given one second per move. **(A)** Performance of AlphaZero in chess, compared with the 2016 TCEC world-champion program Stockfish. **(B)** Performance of AlphaZero in shogi, compared with the 2017 CSA world-champion program Elmo. **(C)** Performance of AlphaZero in Go, compared with AlphaGo Lee and AlphaGo Zero (20 blocks over 3 days).

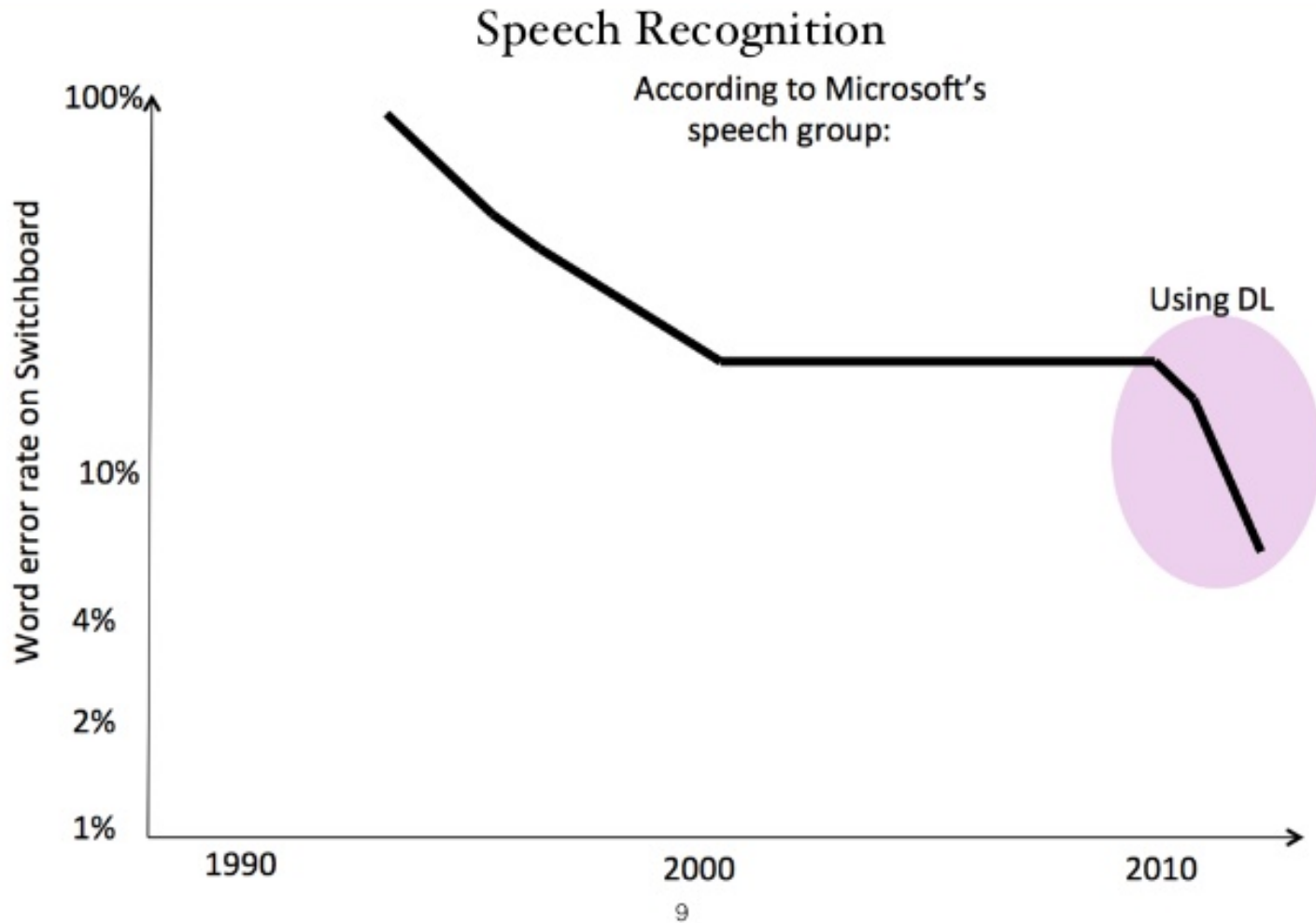
# Speech Recognition



Skype to get 'real-time' translator

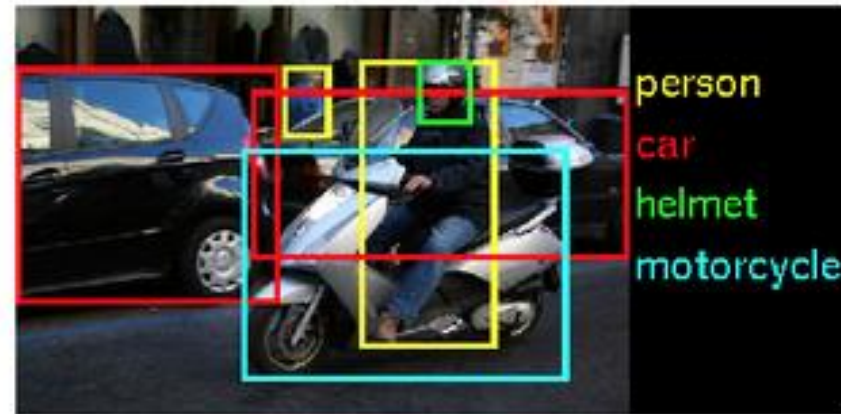
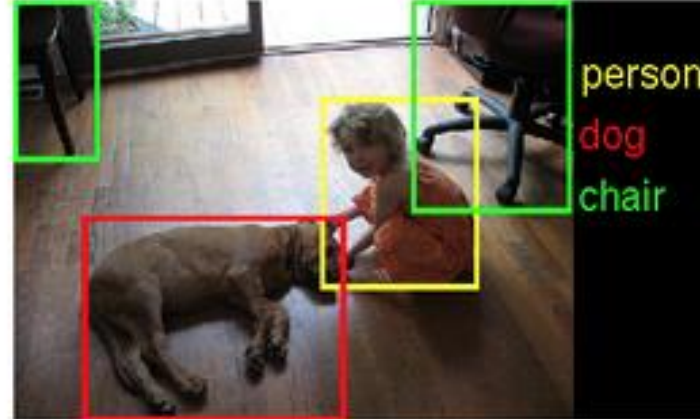
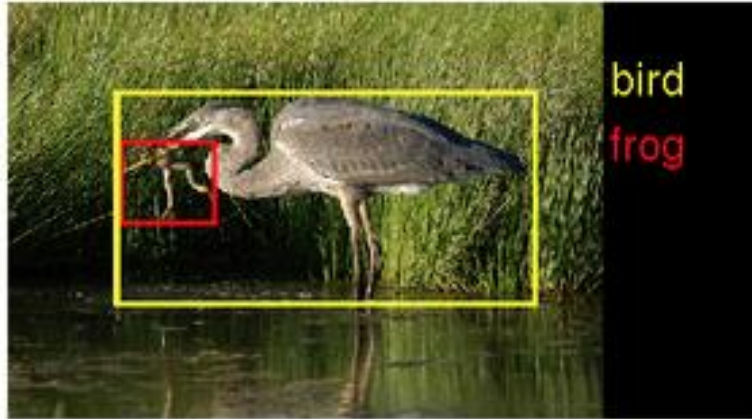


# Speech Recognition Results

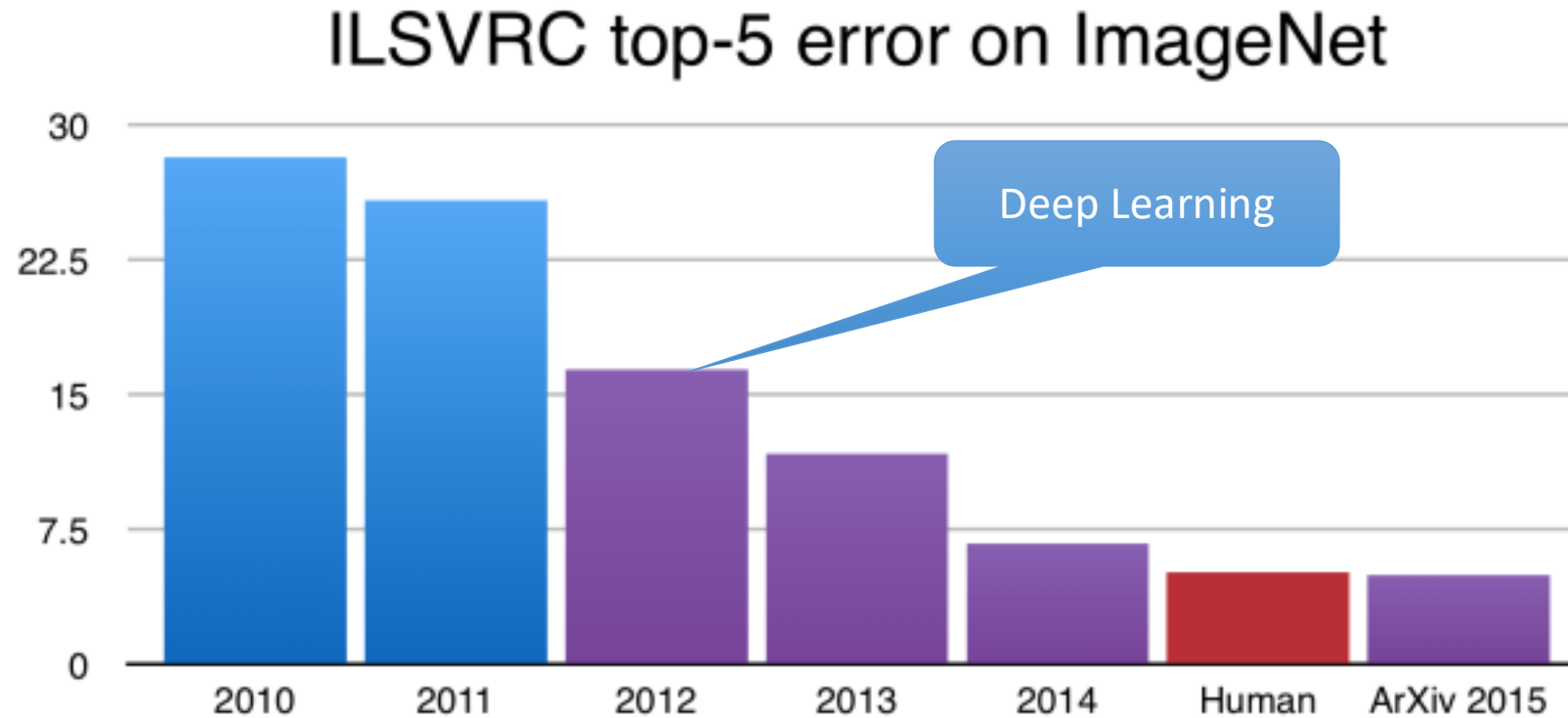


( Figure from Microsoft's speech Group)

# Image Recognition

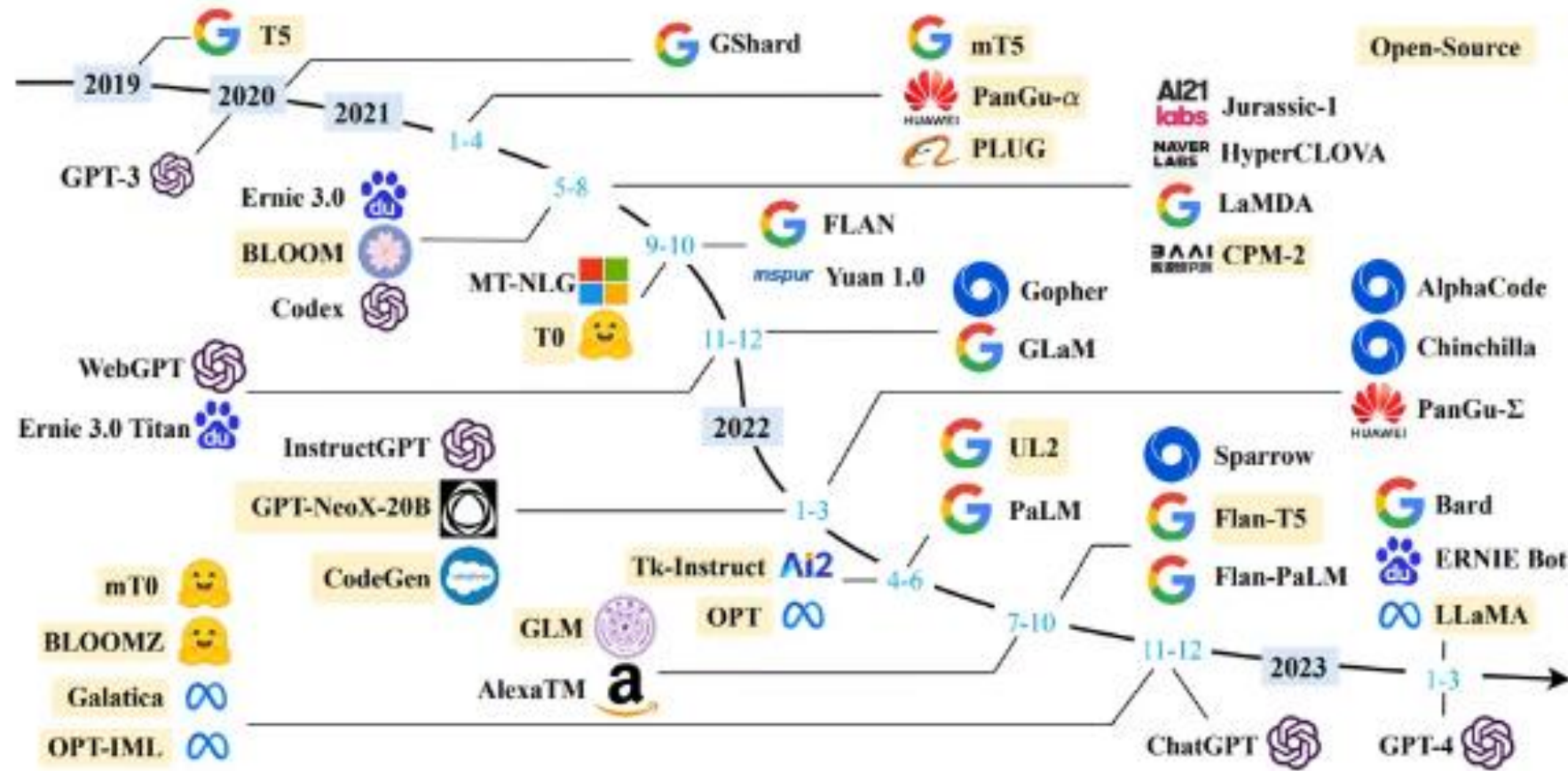


# Results on ImageNet





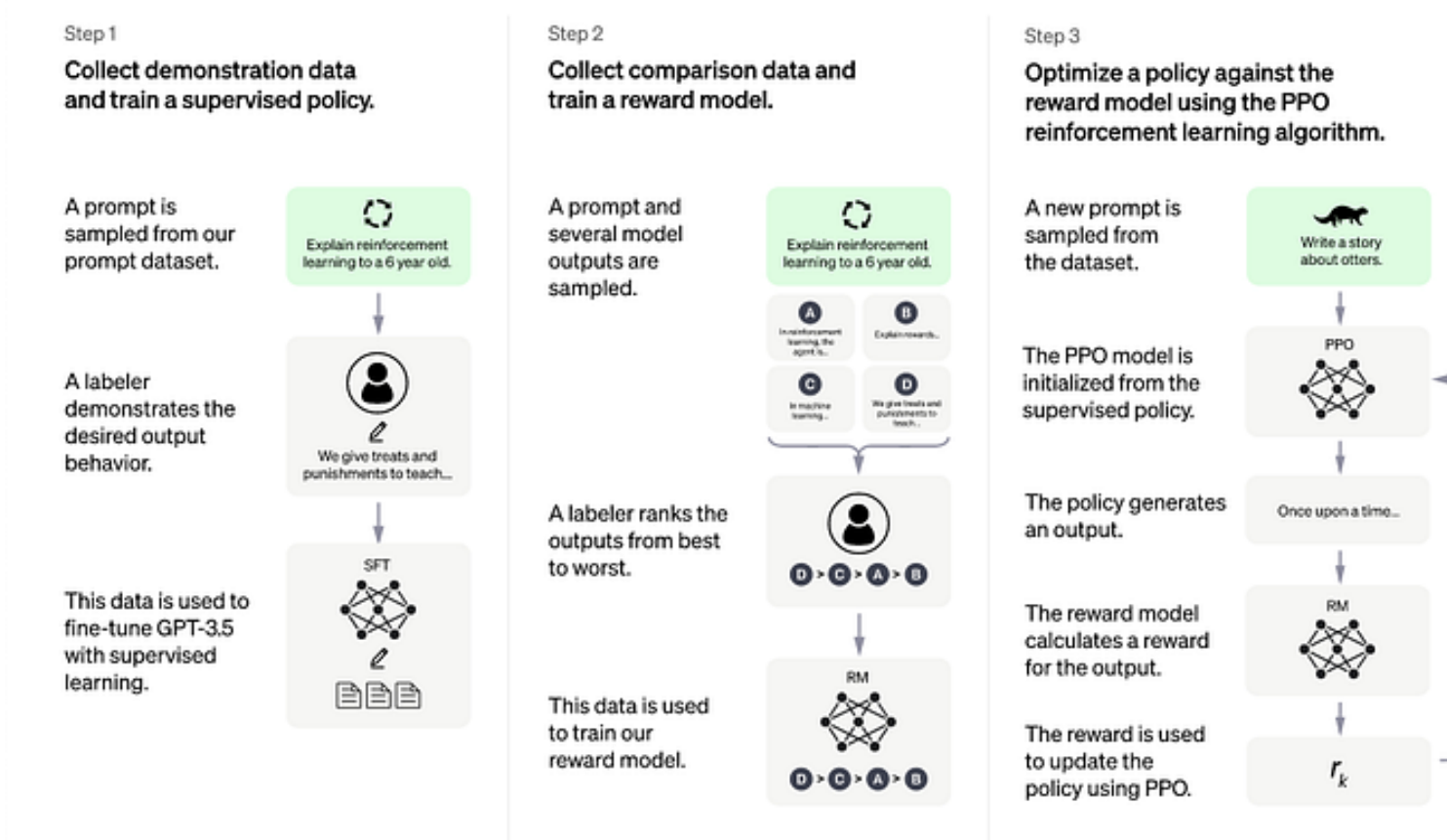
# Large Language Models





# ChatGPT/GPT-4

“**ChatGPT** (Generative Pre-trained Transformer)<sup>[1]</sup> is a [chatbot](#) launched by [OpenAI](#) in November 2022. It is built on top of OpenAI’s [GPT-3.5](#) family of [large language models](#), and is [fine-tuned](#) with both [supervised](#) and [reinforcement learning](#) techniques.” --Wikipedia



# From Text to Image

- DALL·E3: Creating Images from Text by OpenAI
- <https://openai.com/index/dall-e-3/>



DALL·E 3

A Dutch still life of an arrangement of tulips in a fluted vase. The lighting is subtle, casting gentle highlights on the flowers and emphasizing their delicate details and natural beauty.

# GPT-4o: Multi-modality Learning across Audio, Vision, and Text



<https://vimeo.com/945586717>

# From Text to Video

- Open AI Sora: <https://openai.com/index/sora/>



Prompt: A stylish woman walks down a Tokyo street filled with warm glowing neon and animated city signage. She wears a black leather jacket, a long red dress, and black boots, and carries a black purse. She wears sunglasses and red lipstick. She... +

- Kling AI: <https://kling.kuaishou.com/en>

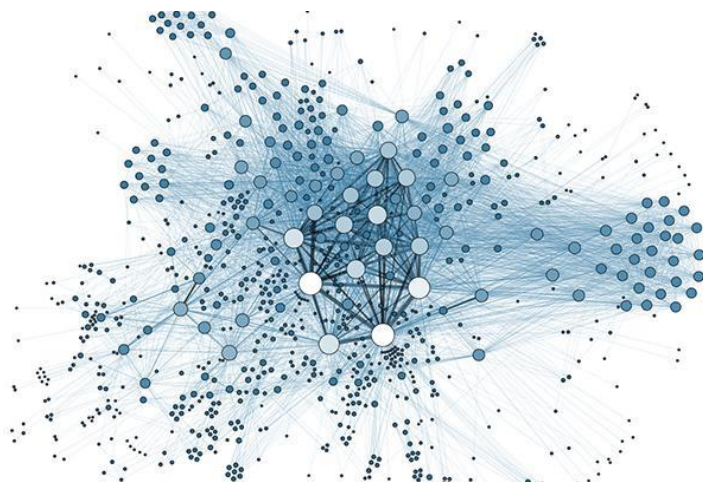


# Robotics

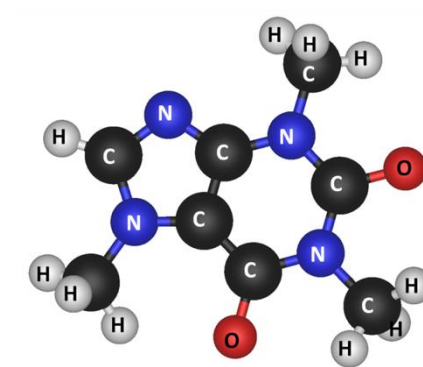


# Graph/Networks Analysis

- Social networks, World Wide Web
- Molecules



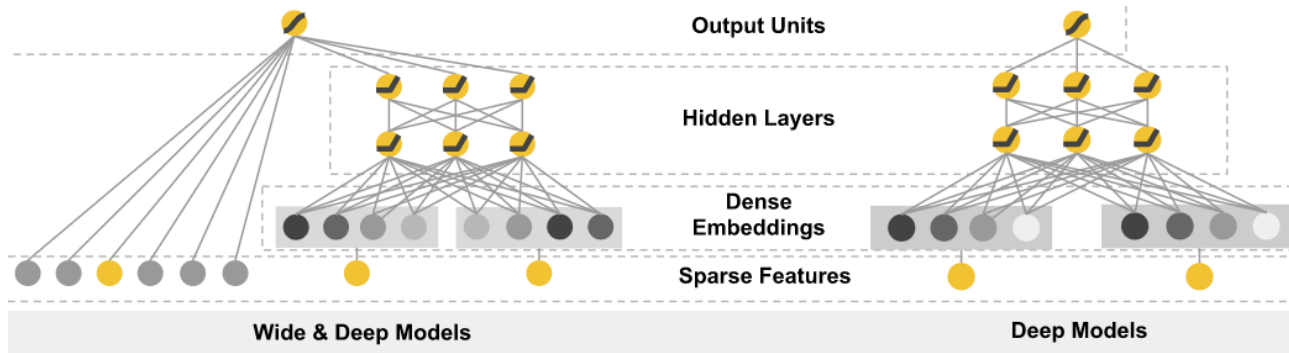
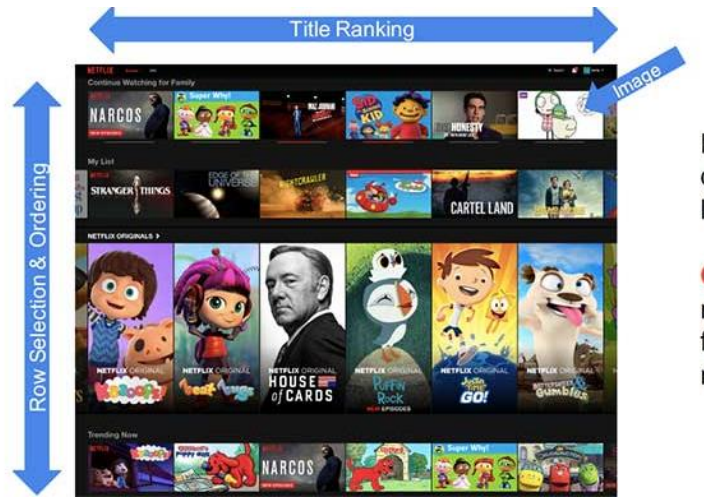
Social Networks



Molecules



# Recommender Systems



Wide & deep learning for  
recommender systems (Google 2016)

## The ACM Conference Series on Recommender Systems

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RECSYS 2018

PAST CONFERENCES

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### Workshop on Deep Learning for Recommender Systems

The workshop centers around the use of Deep Learning technology in Recommender Systems and algorithms. DLRS 2017 builds upon the positively received traits of DLRS 2016. DLRS 2017 is a fast paced half-day workshop with a focus on high quality paper presentations and keynote. We welcome original research using deep learning technology for solving recommender systems related problems. [Deep Learning is one of the next big things in Recommendation Systems](#)

RECSYS 2017 (COMO)

[About the Conference](#)

[Call for Contributions](#)

## Workshops on Deep Learning for Recommender Systems

# AI for Math

Recently, the IMO has also become an aspirational challenge for AI systems as a test of their advanced mathematical problem-solving and reasoning capabilities. Last year, Google DeepMind's combined AlphaProof and AlphaGeometry 2 systems [achieved the silver-medal standard](#), solving four out of the six problems and scoring 28 points. Making use of specialist formal languages, this breakthrough demonstrated that AI was beginning to approach elite human mathematical reasoning.

This year, we were amongst an inaugural cohort to have our model results officially graded and certified by IMO coordinators using the same criteria as for student solutions. Recognizing the significant accomplishments of this year's student-participants, we're now excited to share the news of Gemini's breakthrough performance.

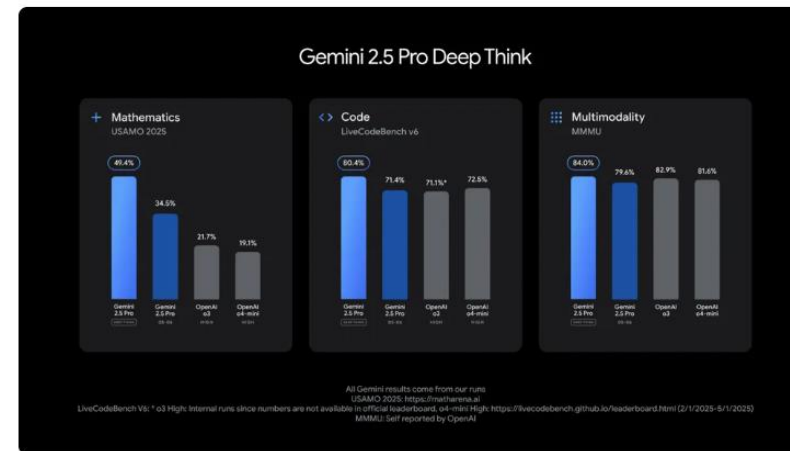
## Breakthrough Performance at IMO 2025 with Gemini Deep Think

An advanced version of Gemini [Deep Think](#) solved five out of the six IMO problems perfectly, earning 35 total points, and achieving gold-medal level performance. The solutions can be found online [here](#).

## Deep Think

Through exploring the frontiers of Gemini's thinking capabilities, we're starting to test an enhanced reasoning mode called [Deep Think](#) that uses new research techniques enabling the model to consider multiple hypotheses before responding.

2.5 Pro Deep Think gets an impressive score on [2025 USAMO](#), currently one of the hardest math benchmarks. It also leads on [LiveCodeBench](#), a difficult benchmark for competition-level coding, and scores 84.0% on [MMMU](#), which tests multimodal reasoning.



<https://deepmind.google/discover/blog/advanced-version-of-gemini-with-deep-think-officially-achieves-gold-medal-standard-at-the-international-mathematical-olympiad/>

# AI for Material Discovery

nature

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Article | [Open access](#) | Published: 29 November 2023

## Scaling deep learning for materials discovery

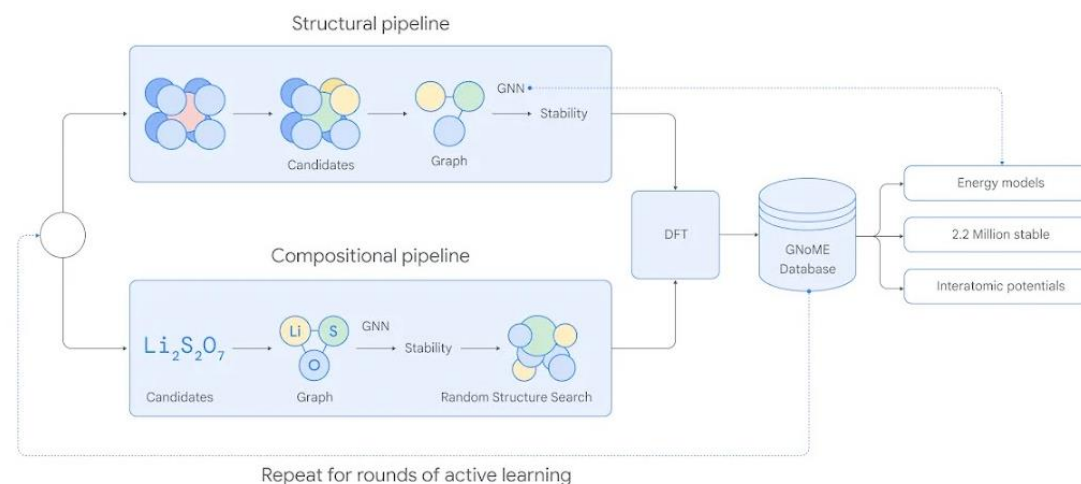
[Amil Merchant](#) , [Simon Batzner](#), [Samuel S. Schoenholz](#), [Muratahan Aykol](#), [Gowoon Cheon](#) & [Ekin Dogus Cubuk](#) 

[Nature](#) **624**, 80–85 (2023) | [Cite this article](#)

**297k** Accesses | **657** Citations | **1079** Altmetric | [Metrics](#)

### Abstract

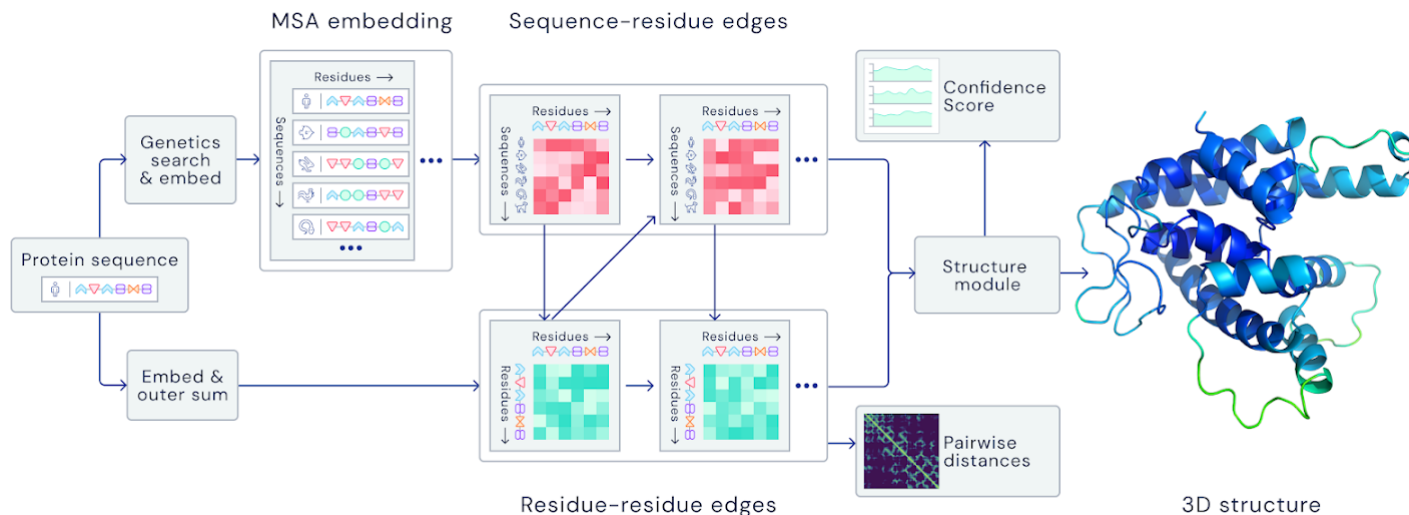
Novel functional materials enable fundamental breakthroughs across technological applications from clean energy to information processing<sup>1,2,3,4,5,6,7,8,9,10,11</sup>. From microchips to batteries and photovoltaics, discovery of inorganic crystals has been bottlenecked by expensive trial-and-error approaches. Concurrently, deep-learning models for language, vision and biology have showcased emergent predictive capabilities with increasing data and computation<sup>12,13,14</sup>. Here we show that graph networks trained at scale can reach unprecedented levels of generalization, improving the efficiency of materials discovery by an order of magnitude. Building on 48,000 stable crystals identified in continuing studies<sup>15,16,17</sup>, improved efficiency enables the discovery of 2.2 million structures below the current convex hull, many of which escaped previous human chemical intuition. Our work represents an order-of-magnitude expansion in stable materials known to humanity. Stable discoveries that are on the final convex hull will be made available to screen for technological applications, as we demonstrate for layered materials and solid-electrolyte candidates. Of the stable structures, 736 have already been independently experimentally realized. The scale and diversity of hundreds of millions of first-principles calculations also unlock modelling capabilities for downstream applications, leading in particular to highly accurate and robust learned interatomic potentials that can be used in condensed-phase molecular-dynamics simulations and high-fidelity zero-shot prediction of ionic conductivity.



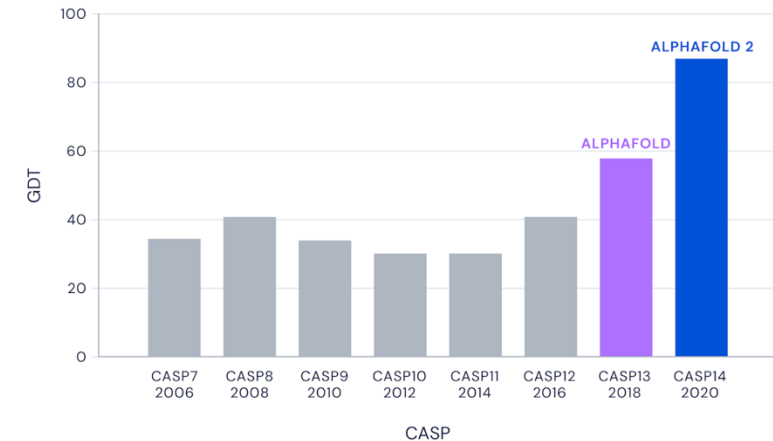
GNoME: Harnessing graph networks for materials exploration

# AI for Protein Structure Prediction

- Protein Structure Prediction: a fundamental problem in biology
  - Predict the 3D structures of proteins from their amino acid sequences
  - <https://deepmind.com/blog/article/alphafold-a-solution-to-a-50-year-old-grand-challenge-in-biology>
- A breakthrough of protein structure prediction by deep learning (December, 2020)



Median Free-Modelling Accuracy



# Flipped Classroom

- Every week:
- Class preparation (Offline):
  - Watching capsules (60-90 minutes)
  - Background reading (60 minutes)
- Class time (In person):
  - Summary, Q&A, problem solving (90-180 minutes)

# Suggestions for navigating a flipped classroom

- In class: Come prepared
  - Watch the capsules ahead of time: Stay active while watching the capsules (e.g., take notes, pause, think of how it fits in the broader context)
  - Do the readings
  - **Write down your questions**
  - Turn off notifications (emails, social networks, texts, etc).
  - **Post questions in Discord**



# Lab Sessions

- Most weeks, we have a hands-on session
- We also have one practical lab sessions for Python and ML on Week #4

# Evaluation

- Your final score for the course will be computed using the following weights:
  - Homework (20%)
  - Capsule summaries (10%)
  - Project (30%)
  - Final Exam (40%)

# Homework (20%)

- Two assignments
  - Two programming exercises

# Capsule Summaries (10%)

- Provide a short summary (10 to 15 lines of text in the form) of 10 capsules throughout the semester.
- The summary of a capsule must be provided before its class (e.g., a summary of capsule on “Learning Problems” must be submitted by 09/02).

# Course Projects (30%)

- Working in groups
  - Each group should have 2-3 students
- Step 1: Group Registration
- Step 2: Project proposal
- Step 3: Poster session (last class)
- Step 4: Submit a project report
  - One week after the poster session
- More instruction details on this will arrive

# Final Exam (40%)

- Open book exam
- No computers or LLMs



# Homework Late Policy

- Each student should hand in your homework or project report on time
  - 50% grade reduction (within 2 days after the deadline)
  - 0 points (more than 2 days passed after the deadline)

# Course Outline

- Week 2: ML Fundamentals
- Week 3&4: Supervised Learning
- Week 5&7: Deep learning
- Week 8: Unsupervised Learning
- Week 10: Project Meetings
- Week 11: Large scale computing
- Week 12: Recommender Systems
- Week 13: Attention
- Week 14: Transformers and Pretraining
- Week 15: Poster Session

# Getting Help

- Post your questions in Discord. The TAs and me will respond.
  - Join Discord through: <https://discord.gg/Jz8pX45g>
- My office hour:
  - 2-3pm Tuesday
  - Office: 4.805, CSC Building
- My email:
  - [Jian.tang@hec.ca](mailto:Jian.tang@hec.ca)
  - tangjian@mila.quebec

# Questions?