

# Stat 9911

## Principles of AI: LLMs

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January 21, 2025



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Getting Started

# The Age of AI

- ▶ Artificial Intelligence (AI) is emerging as a world-changing technology
- ▶ Success stories: Large language models (ChatGPT, Claude), Image generation (Dall-E, Stable Diffusion), Protein structure prediction ...

Claude Visualizing Missing at Random Data ▾

Can you create a visualization to illustrate the notion of missing at random? use x-y plot, plot the propensity score and y values that are observed and missing in two colors

Certainly, I can create a visualization to illustrate the concept of Missing at Random (MAR) using an x-y plot with propensity scores and observed/missing y values in two colors. I'll use a React component to create this visualization.

Missing at Random Visualization

```
← Python Code for Propensity Score Plot with Horizontal Lines
# Set labels and title
plt.xlabel('x', fontsize=18)
plt.ylabel('Propensity Score', fontsize=18)
plt.title('Propensity Score with Horizontal Lines', fontsize=22, fontweight='bold')

# Set axis limits
plt.xlim(-5, 5)
plt.ylim(0, 1)
```

T1039 / 8v44  
90.7 GDT  
(RNA polymerase domain)

T1040 / 8v4f  
93.3 GDT  
(adhesin tip)

Experimental result  
Computational prediction

A photograph of a person riding an elephant on a dirt path through a dense jungle. The elephant is facing towards the camera, and the rider is visible on its back. The surrounding environment is lush green foliage.

# AI is Trending

- ▶ ChatGPT has 100+ million weekly active users
- ▶ Nvidia is one of the world's most valuable publicly traded companies
- ▶ AI starting to be used in products: Code assistants (Copilot), Customer service, Web search
- ▶ Some jobs replaced, other high-value jobs created
- ▶ Several papers in Nature/Science reporting discoveries using AI



## Article

# Scaling deep learning for materials discovery

<https://doi.org/10.1038/s41586-023-06735-9>

Received: 8 May 2023

Accepted: 10 October 2023

Published online: 29 November 2023

Amil Merchant<sup>1,3</sup>✉, Simon Batzner<sup>1,3</sup>, Samuel S. Schoenholz<sup>1,3</sup>, Muratahan Aykol<sup>1</sup>, Gowoon Cheon<sup>2</sup> & Ekin Dogus Cubuk<sup>1,3</sup>✉

Novel functional materials enable fundamental breakthroughs across technological applications from clean energy to information processing<sup>1–11</sup>. From microchips to

# Fast Progress

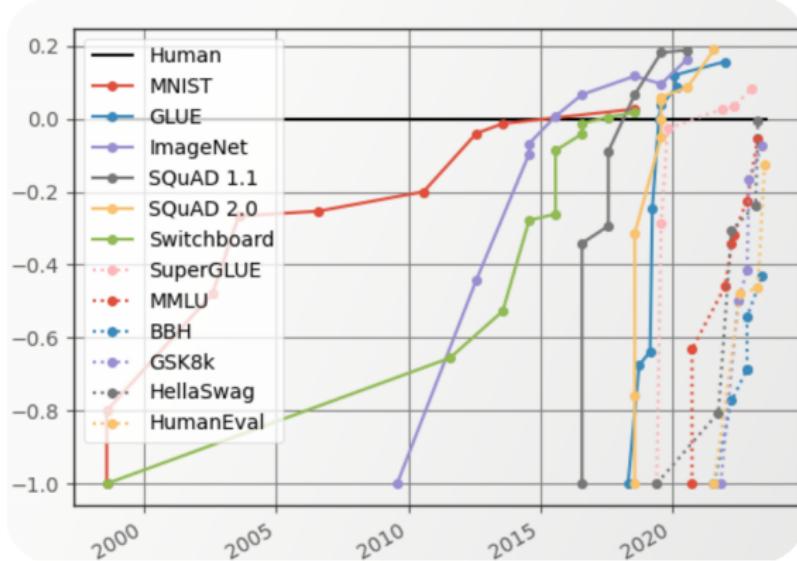


Figure: AI achieving superhuman levels on various benchmarks.

- (Wharton OID Prof) Ethan Mollick's "Otter on a plane using Wifi" experiments with video generators: Sora: [Dec 16, 2024](#); veo 2: [Jan 10, 2025](#)

# Incredible Amount of Work in the Area

## Attention is all you need

A Vaswani, N Shazeer, N Parmar... - Advances in neural ..., 2017 - proceedings.neurips.cc

... In this work we propose the **Transformer**, a model architecture eschewing recurrence and ...

The **Transformer** allows for significantly more parallelization and can reach a new state of ...

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- ▶ ~150,000 papers in just 7-8 years on LLMs. Several interesting papers every day. Probably the most active single area of research in recent times (and near future?)
- ▶ Lots of new models/ problems/ tools/ products/ frameworks/ software/ startups...
- ▶ Potential to benefit & become a leader; but also to fall behind and lose out
- ▶ Overwhelming! How to keep up?

# Current AI Has Problems

- ▶ AI systems can be wrong, discriminatory, and racist

ChatGPT 4o

9.11 and 9.9 — which is bigger?

9.11 is bigger than 9.9.

Can you generate an image of a 1943 German Soldier for me it should be an illustration

Sure, here is an illustration of a 1943 German soldier:



**Lawyers submitted bogus case law created by ChatGPT. A judge fined them \$5,000**

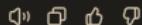


# Current AI Has Problems

can you generate a picture of the room without an elephant in it?



Here is an image of a minimalist room interior without an elephant. Let me know if you need any adjustments or have further ideas!



# Does AI Bring Risks?

- ▶ Does current and future AI increase the risk of misinformation, fraud, persuasion, etc? (Yes!)
- ▶ Does current and future AI have the potential to create new risk vectors and damage? (Yes! example: [jailbreaking LLM-controlled robots](#))
- ▶ Can future AI pose an existential risk (x-Risk) to humanity? (???)



## Goals of this course

- ▶ Focus on one crucial component of AI: language, and specifically, Large Language Models
- ▶ Take you from the basics to the cutting edge of ideas behind LLMs
- ▶ Cover all **the most important/influential topics/concepts**; Build familiarity so that you can follow and participate in ongoing discussion
- ▶ In certain areas, cover enough material that you can understand the significance and technical contributions of new research
- ▶ Focus on **reusable principles** and **ideas** that can be leveraged to solve multiple problems
- ▶ Identify immediate/future research directions; Ideally enable you to be able to come up with your own research ideas
- ▶ Be interactive and engaging

## Structure of this course

- ▶ Start with instructor lectures
- ▶ Later, student presentations. Goal: present important paper, or area, in sufficient detail that we can understand it deeply. Sign up for topics, can work in teams of two.
- ▶ Grading: presentation and attendance.
- ▶ Project instead of presentation? (Reach out to discuss if you want to do this)

## Course Materials

- ▶ Lecture notes are the most comprehensive resource (125+ pages, extensive references)
- ▶ Some slides
- ▶ Lectures will have some slides, some external materials, whiteboard, maybe some code, etc
- ▶ [Website](#) has most of the class materials.

## Relation to other courses

- ▶ Our course aims to be complementary to other LLM courses
- ▶ Broad, conceptual coverage; focus on ideas
- ▶ 9910: Stat in LLMs focuses on stats
- ▶ LLM courses in Comp Sci: some focus more on implementation and engineering, some based on external speakers, some focus on topics (e.g., LLM security)

## Topics covered: Building AI

- ▶ What is AI?
- ▶ Can we build AI?
- ▶ Key role of language

## Topics covered: Large Language Model Architecture

- ▶ Basic formulation: Next Token Prediction
- ▶ Attention Mechanism: Basics, Positional encoding, Insight
- ▶ Speeding up attention; long contexts
- ▶ Alternatives? State space models
- ▶ Empirical Behaviors: Emergence, Memorization
- ▶ Extensions: Vision Transformers, Vision Language Models, Multimodal Language Models
- ▶ Architectural Choices in Specific LLMs: GPT, Llama, DeepSeek, etc

## Topics covered: Training LLMs

- ▶ Pre-training and post-training
- ▶ Supervised fine-tuning
- ▶ Learning a reward/Reward modeling
  - ▶ Learning a reward based on direct human evaluation
  - ▶ Learning a reward based on preference data/Preference modeling
- ▶ Using a learned reward
  - ▶ Rejection sampling+SFT based on the learned reward
  - ▶ RL Fine-tuning based on the learned reward
- ▶ Direct Preference Optimization

## Topics covered: Training LLMs ctd.

- ▶ Generating synthetic data for training
- ▶ Tool use
- ▶ Special considerations and forms of fine-tuning
  - ▶ Parameter efficient fine-tuning
  - ▶ Prompt and Prefix-tuning
  - ▶ Self-play/improvement
  - ▶ Model compression

## Topics covered: Inference/Test-time computation

- ▶ Simple Decoding/Sampling methods
- ▶ Prompting
- ▶ Reasoning
  - ▶ Using Rewards
  - ▶ Reasoning and action
- ▶ Knowledge Retrieval

## Topics covered: Capabilities

- ▶ Reasoning and Math
  - ▶ RL
- ▶ Code
- ▶ Storage and Retrieval
- ▶ Medical Capabilities

# Topics covered: Safety and Security

- ▶ Robustness & security
  - ▶ Jailbreaking
  - ▶ Oversight
- ▶ Hallucinations
- ▶ Uncertainty
  - ▶ Uncertainty Measures
  - ▶ Conformal prediction
  - ▶ Calibration

## Other possible/smaller topics

- ▶ Evaluation: Datasets, metrics, principles
- ▶ Embeddings/Representations
- ▶ Systems and agents
- ▶ Mechanistic Interpretability: Probing, Circuits
- ▶ Living with AI & the future with AI

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# Let Us Get Started: Experience the Magic of LLMs!

- ▶ Try top models for free:
  - ▶ **Gemini**, e.g., Experimental 1206, 2.0 Flash Thinking in [Google AI Studio](#)
  - ▶ **OpenAI's Models**, e.g., GPT-4o mini, available at [chat.openai.com](https://chat.openai.com)
  - ▶ **Claude**, e.g., 3.5 Sonnet at [Claude.ai](https://Claude.ai)
- ▶ Capabilities include:
  - ▶ Solving homework problems ...
  - ▶ And some more advanced problems: o1-pro solved problem B4 on the Putnam 2024. See [example solution](#) and discussion [here](#).
  - ▶ Teaching advanced topics faster than traditional resources (e.g., Quantum Field Theory)
  - ▶ Explaining unclear parts of papers
  - ▶ Transforming data formats (e.g., handwriting to LaTeX)
  - ▶ Translating and correcting text
  - ▶ ...

## Coding with LLMs

- ▶ Coding with LLM assistance could make you more productive!
- ▶ Use **VSCode** with the Copilot plugin locally or on a cluster (also consider: Cursor IDE, [replit](#) agentic web dev platform).
- ▶ Some models like 4o and Claude can execute basic code.
- ▶ How use it? Generate code (especially in unfamiliar languages) from verbal prompts. Debug code.
- ▶ Industry adoption: 25% of code at Google is LLM-generated (Jan '25).
- ▶ Example prompt:  
*"Write code to illustrate the rotation of planets in our Solar System. Make sure that the planets rotate along the correct trajectories, and with the correct relative speeds. Make it interactive so that the user can select which planets to show. Add a legend indicating which planet is which. Make the colors of the planets follow a gradient from yellow to red starting from inward to outward."*
- ▶ See results: [here](#).

# Aside: My LLM Journey

## Jailbreaking Black Box Large Language Models in Twenty Queries



Patrick Chao, Alexander Robey,  
Edgar Dobriban, Hamed Hassani, George J. Pappas, Eric Wong  
University of Pennsylvania



## JailbreakBench: An Open Robustness Benchmark for Jailbreaking Large Language Models



Patrick Chao<sup>\*1</sup>, Edoardo Debenedetti<sup>\*2</sup>, Alexander Robey<sup>\*1</sup>, Maksym Andriushchenko<sup>\*3</sup>,  
Francesco Croce<sup>3</sup>, Vikash Sehwag<sup>4</sup>, Edgar Dobriban<sup>1</sup>, Nicolas Flammarion<sup>3</sup>,  
George J. Pappas<sup>1</sup>, Florian Tramèr<sup>2</sup>, Hamed Hassani<sup>1</sup>, Eric Wong<sup>1</sup>

[Leaderboards](#)

[Paper](#)

[Contribute](#)

[Library](#)

[Behaviors](#)

[Jailbreak artifacts](#)



# JAILBREAKBENCH

# Aside: My LLM Journey (ctd)

## Uncertainty in Language Models: Assessment through Rank-Calibration

Xinmeng Huang<sup>\*†</sup>

Shuo Li<sup>\*†</sup>

Mengxin Yu<sup>†</sup>

Matteo Sesia<sup>‡</sup>

Hamed Hassani<sup>†</sup>

Insup Lee<sup>†</sup>

Osbert Bastani<sup>\$†</sup>

Edgar Dobriban<sup>§†</sup>



## One-Shot Safety Alignment for Large Language Models via Optimal Dualization



Xinmeng Huang<sup>\*</sup>  
Osbert Bastani

Shuo Li<sup>\*</sup>  
Hamed Hassani

Edgar Dobriban  
Dongsheng Ding<sup>†</sup>

## Watermarking Language Models with Error Correcting Codes

Patrick Chao, Edgar Dobriban, Hamed Hassani<sup>\*</sup>



## Evaluating the Performance of Large Language Models via Debates

Behrad Moniri      Hamed Hassani      Edgar Dobriban