



Stop Chatting, Start Scanning

AI's Visual Takeover in Pharma for Data
Extraction with the Power of LLMs

Ercan Şükür



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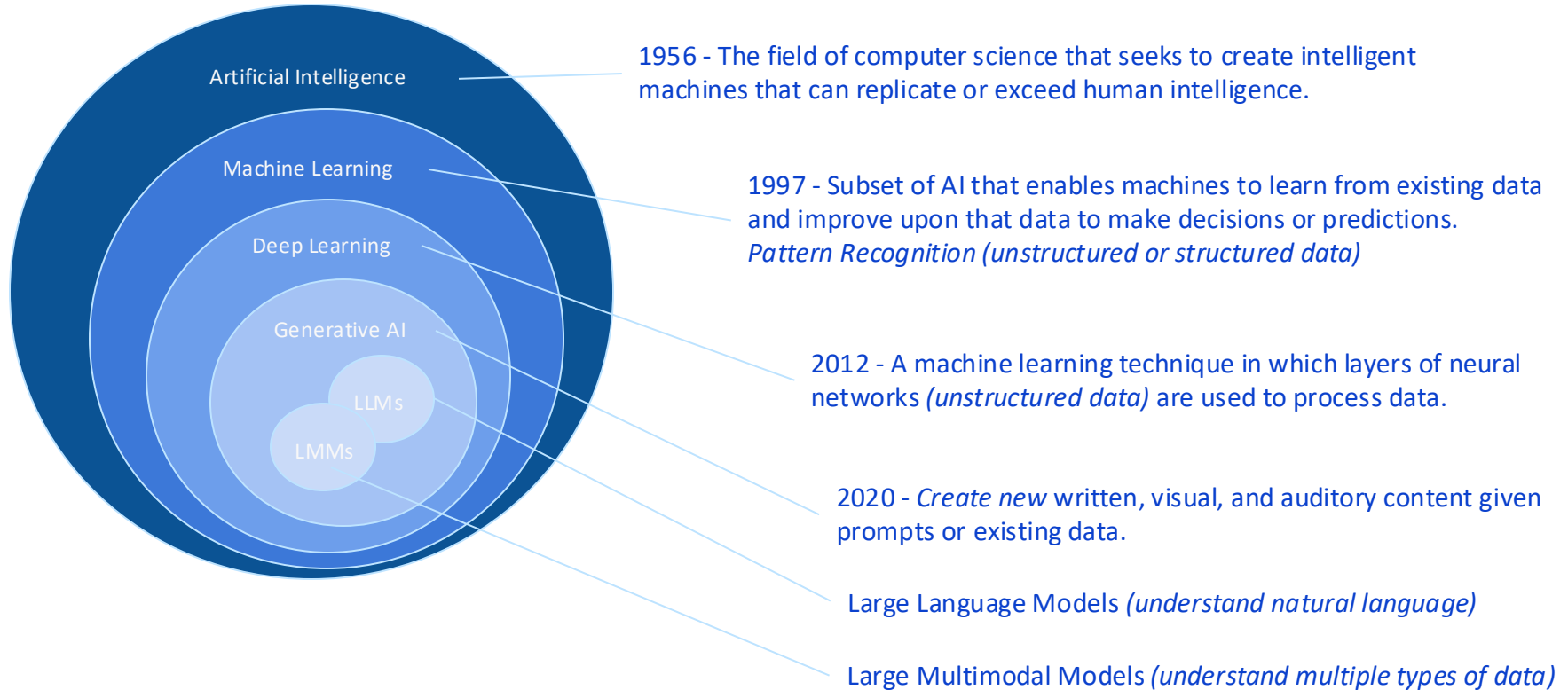
12.11.2024 | PHUSE EU Connect 2024



What is Generative AI and a LLM/LMM?

What is Generative AI (GenAI)?

Or: Who will soon be at the top of evolution?



What is a Large Language Model (LLM)?

Demystifying LLMs

Previous words
(context)

The boy went to the

The word that has
the highest
probability is
chosen.

What is a Large Multimodal Model (LMM)?

Demystifying LMMs

Input (Multimodal Context*)

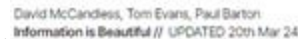
*text, images, video, audio, or even sensor data

"a cat playing in the park."



LMM
(DALL E3)

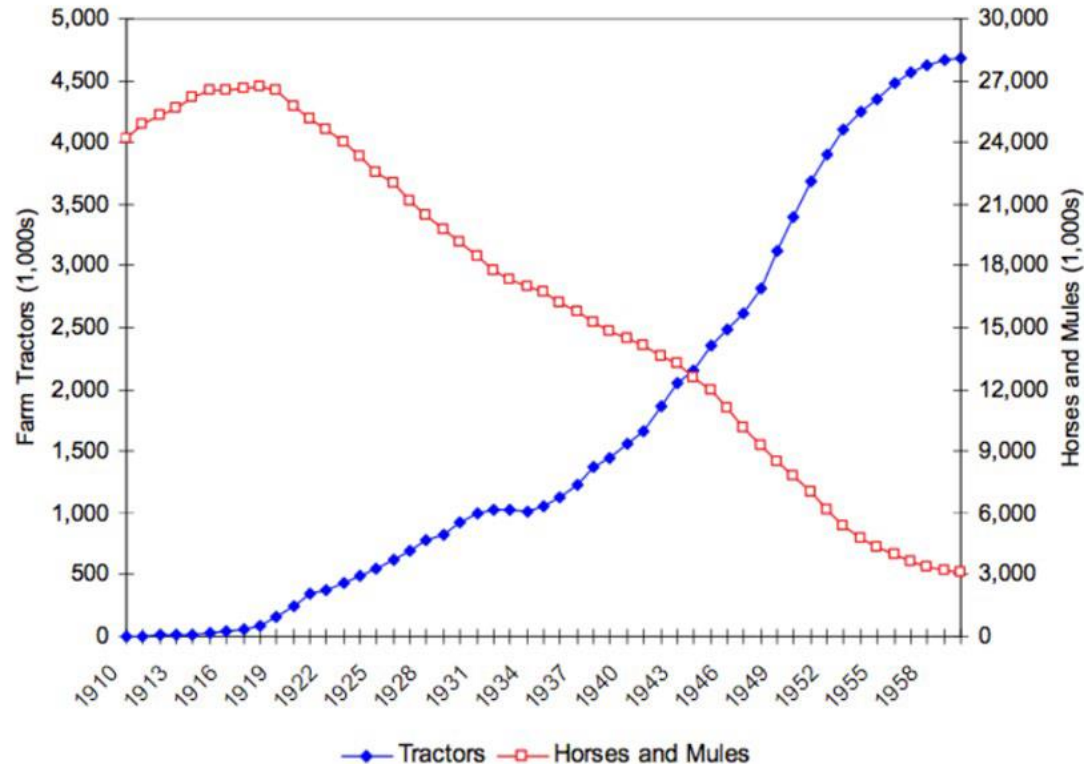




* = parameters undisclosed // see the data

The Shift from Tradition to Technology

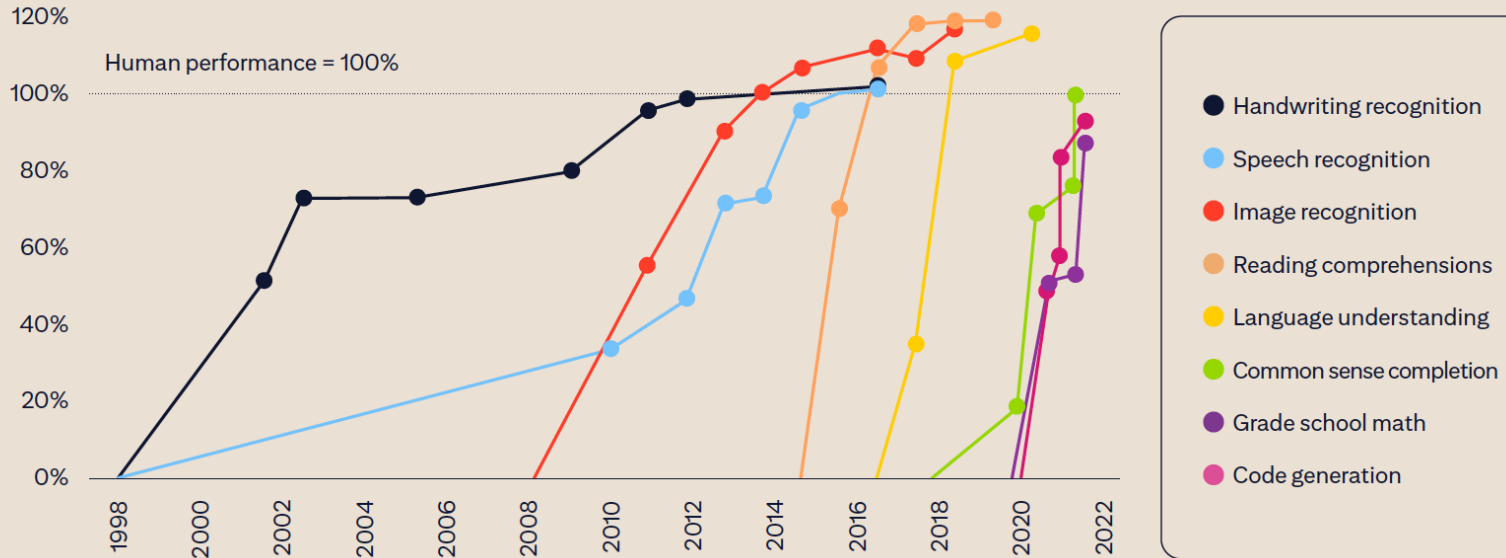
The Rise of Machines and the Decline of Tradition



Source: US Dept of Commerce

The Rise of A.I. LLMs & how they surpassed humans

AI has surpassed humans at a number of tasks



Source: Contextual AI, Will Henshall for TIME

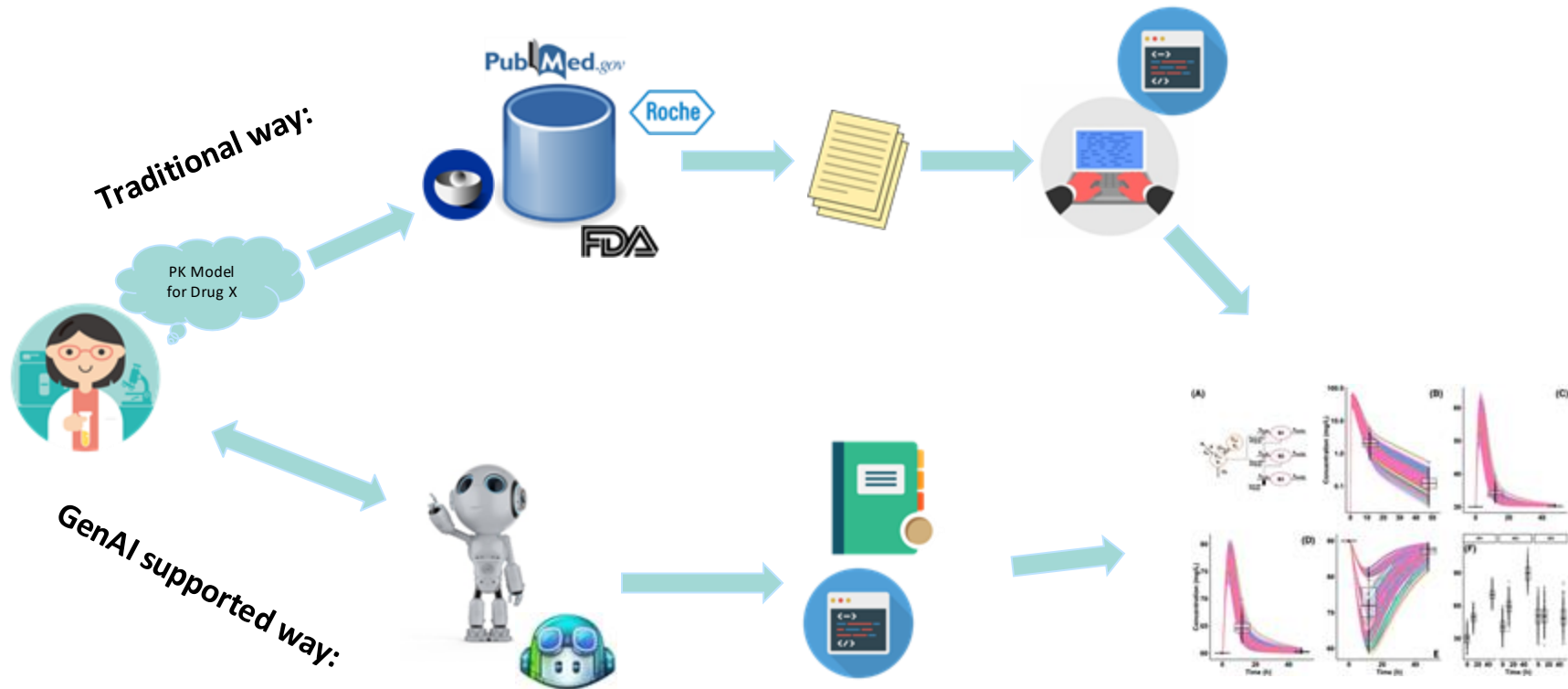
PMx-Bot

PMx = Pharmacometrics*

Pharmacometrics is the science of quantifying drug efficacy, safety, and pharmacokinetics through mathematical models to optimize drug development, dosing, and therapeutic decision-making

Traditional Way vs AI supported

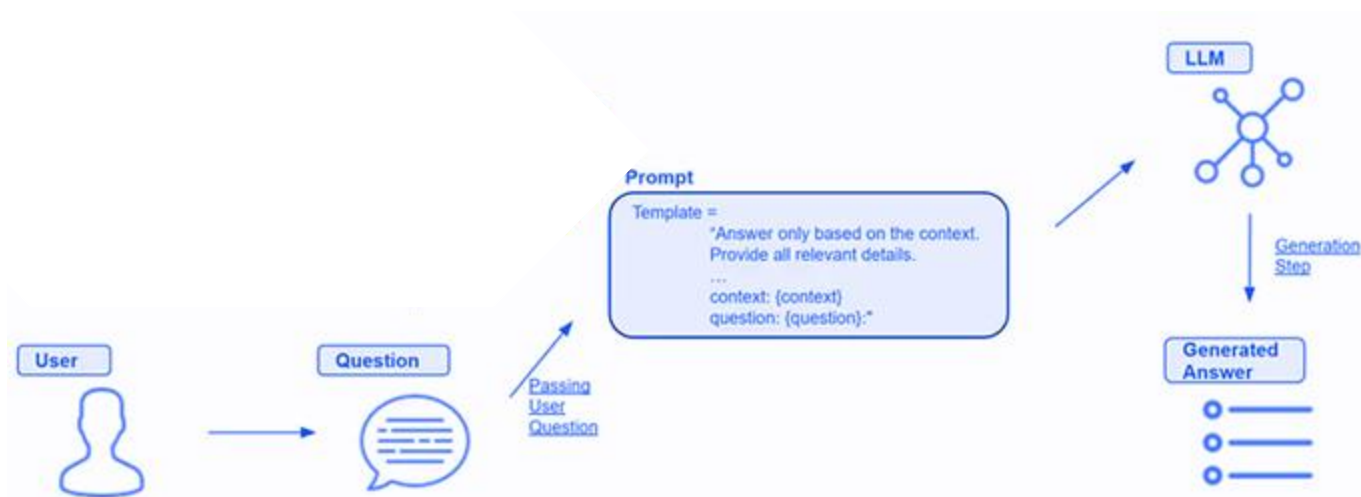
Being more efficient to make decisions faster



Architecture

Bringing our domain expertise

- Problem:
LLMs are trained to generate human-like text, not true text.
- Idea:
We need to 'ground' them in reality so that they don't make things up.



Demo

[Home](#) > [Journal of Pharmacokinetics and Pharmacodynamics](#) > [Article](#)

Pharmacokinetic Modelling of 5-FU Production from Capecitabine—A Population Study in 40 Adult Patients with Metastatic Cancer

Published: December 2005

Volume 32, pages 817–833, (2005) [Cite this article](#)[Download PDF](#)  Access provided by F. Hoffmann – La Roche Ltd.

[Journal of Pharmacokinetics and Pharmacodynamics](#)

[Aims and scope](#) →[Submit manuscript](#) →[Saik Urien](#)  [Keyvan Rezaei](#) & [François Lokiec](#) 459 Accesses  28 Citations [Explore all metrics](#) →

Abstract

Aims: To model the biotransformation steps of 5-FU production from capecitabine and identify patient characteristics that may influence the drug disposition. **Methods:** Blood samples and demographic data were collected from two phase I studies in which adult patients received oral capecitabine for various malignancies. Capecitabine, 5'-deoxy-5-fluorocytidine (5'-DFCR), 5'-deoxy-5-fluorouridine (5'-DFUR) and 5-fluorouracile (5-FU) concentration–time data were analysed via a population approach using NONMEM.

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Avoid common mistakes on your manuscript.



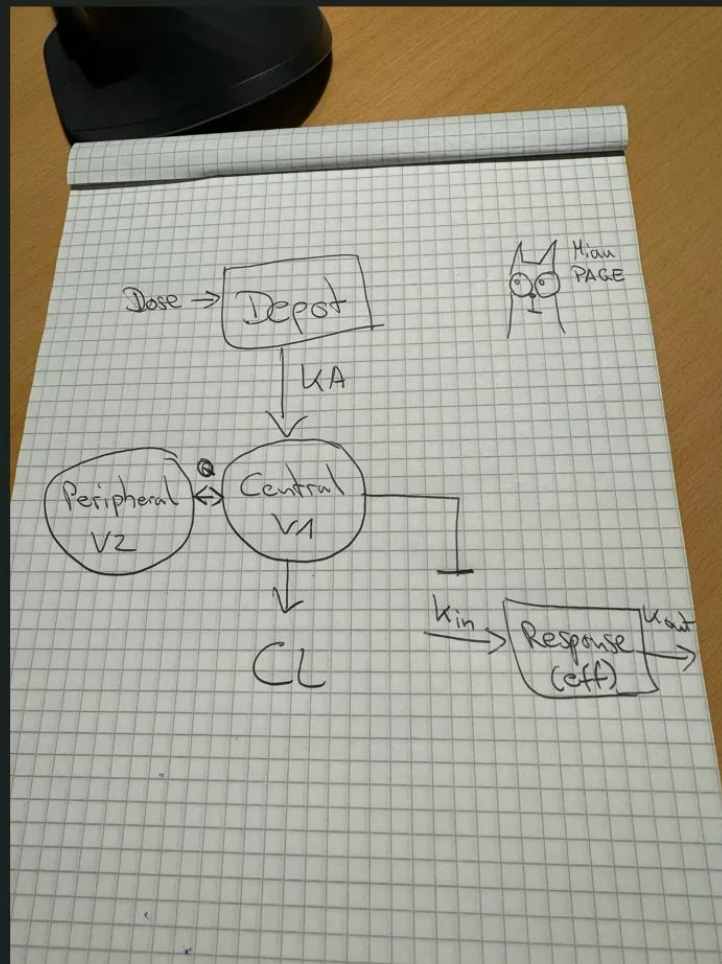
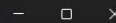
Sections

References

[Abstract](#)[Article PDF](#)[References](#)[Author information](#)[Rights and permissions](#)



sketch_miau_00.jpeg



Demo

Reproducing a Paper

Pharmacokinetics and safety of candidate toci blind, single-dose phase I study

Kyung-Sang Yu, Byungwook Kim, Dongseong Shin, Min Kyu Park, Jun Gi Hwang, Min-Gul Kim, Hy Edward Keystone

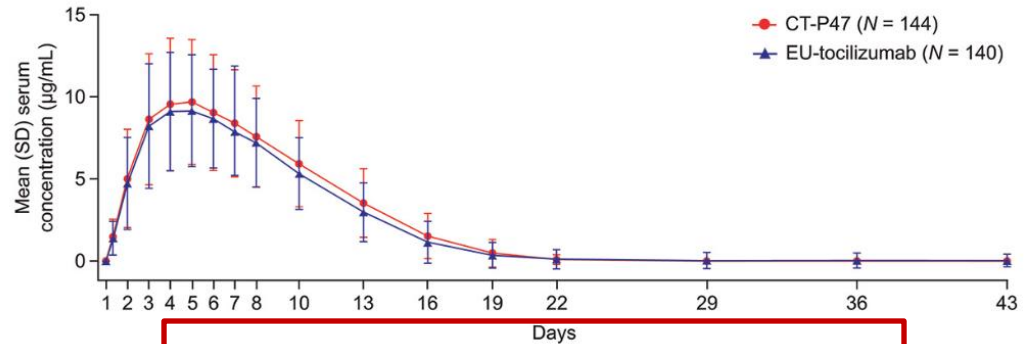
<https://doi.org/10.1080/13543784.2023.2212155>

Figure 2 of 2

Figure 2. Mean (SD) serum concentrations of CT-P47 and EU-tocilizumab

Note: Values below the lower limit of quantification were set to

EU-tocilizumab = European Union-approved reference tocilizumab



Study Day	Mean (SD) serum concentration (µg/mL)	
	CT-P47 (N = 144)	EU-tocilizumab (N = 140)
1 (pre-dose)	0	0
1 (8 h post-dose)	1.47 (1.06)	1.40 (1.03)
2	5.02 (3.00)	4.72 (2.80)
3	8.61 (4.00)	8.20 (3.78)
4	9.54 (4.01)	9.08 (3.60)
5	9.66 (3.79)	9.14 (3.39)
6	9.02 (3.51)	8.65 (3.00)
7	8.39 (3.24)	7.86 (2.65)
8	7.57 (3.08)	7.20 (2.68)
10	5.92 (2.62)	5.31 (2.18)
13	3.54 (2.09)	2.97 (1.79)
16	1.52 (1.37)	1.14 (1.27)
19	0.47 (0.84)	0.36 (0.78)
22	0.09 (0.27)	0.11 (0.58)
29	0.00 (0.01)	0.04 (0.48)
36	0	0.04 (0.46)
43	0	0.03 (0.39)

Demo

Reproducing a Paper

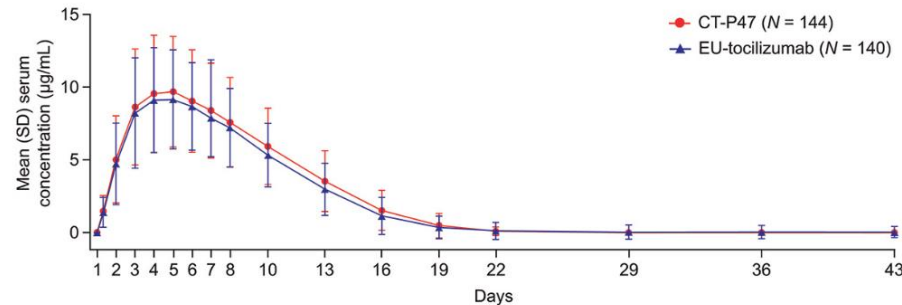


Table 2 of 4
Table 2. Summary of PK variables (PK set; Part 2).

	CT-P47 (N = 144)	EU-tocilizumab (N = 140)
AUC _{0-∞} (day*µg/mL)		
n	138 ^a	136 ^{a,b}
Mean (SD)	94.34 (40.95)	85.98 (36.23)

94.34 (40.95)

85.98 (36.23)

<https://doi.org/10.1080/13543784.2023.2212155>



PMx-Bot

By Ercan Suekuer

Your guide for pharmacometrics modeling and data interpretation.

How do I model a two-compartment PK model?

What are common issues with nonlinear mixed-...

Can you help interpret these PK/PD results?

What are some best practices for parameter...



Message PMx-Bot



Demo

My little Data Scientist Assistant



PMx-Bot

By Ercan Suekuer 

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Impact on Programming

AI Coding

Exploring Top Tools Accelerating

Top 3 AI coding bots:



```
macbook:~/tmp/demo 12:45
Aider v0.51.2-dev
Main model: gpt-4o-2024-08-06 with diff edit format
Weak model: gpt-4o-mini
Git repo: none
Repo-map: disabled
Use /help <question> for help, run "aider --help" to see cmd line args
> 
```

Google's AI-Driven Code Revolution

Over 25% of Google's Code Now Written by AI



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Over 25% of Google's code is now written by AI—and CEO Sundar Pichai says it's just the start

BY GREG MCKENNA

October 30, 2024 at 4:14 PM GMT+1



Alphabet CEO Sundar Pichai.

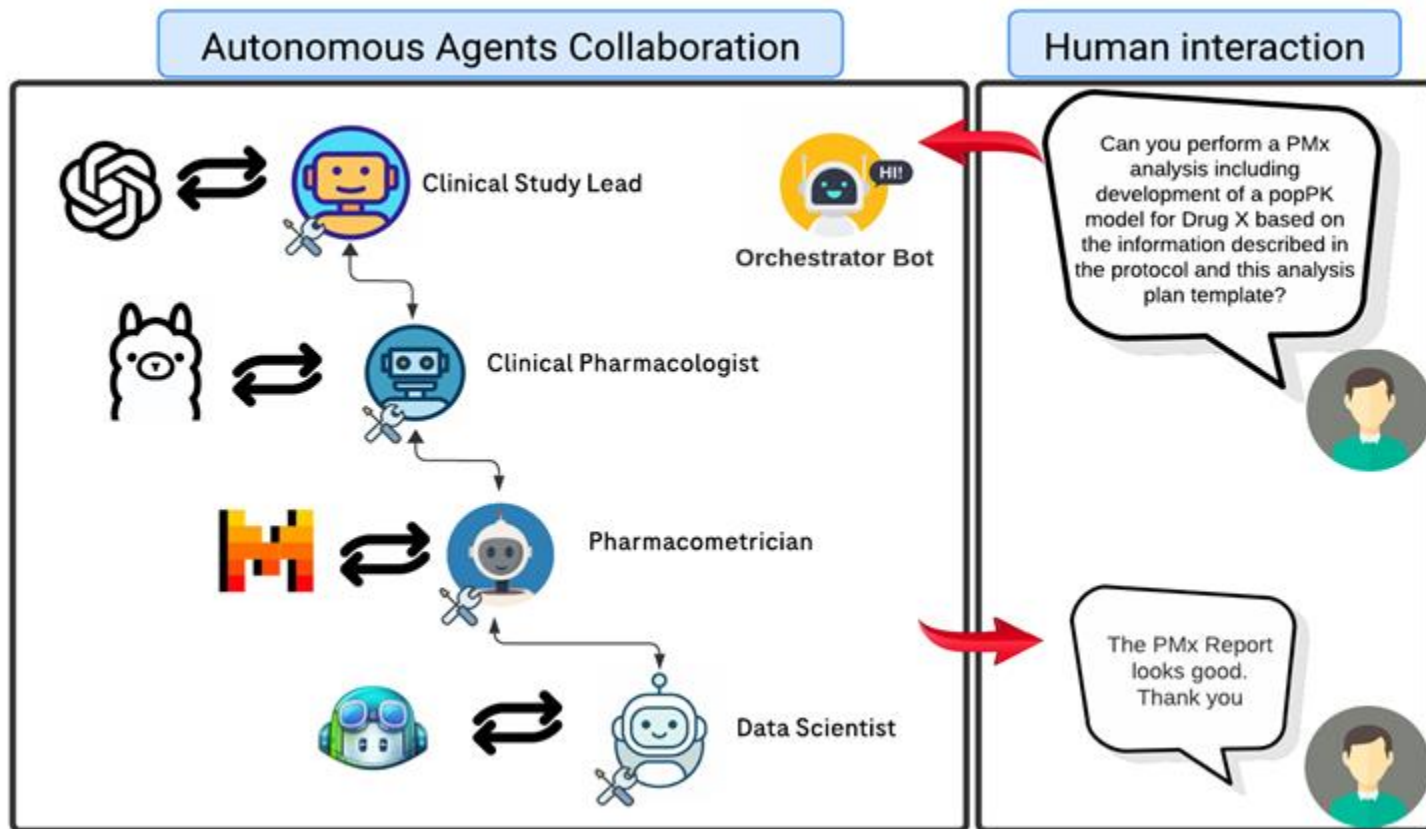
JEENAH MOON—BLOOMBERG/GETTY IMAGES

Future Horizon

~~Future~~ Future Horizon

Autonomous Agents

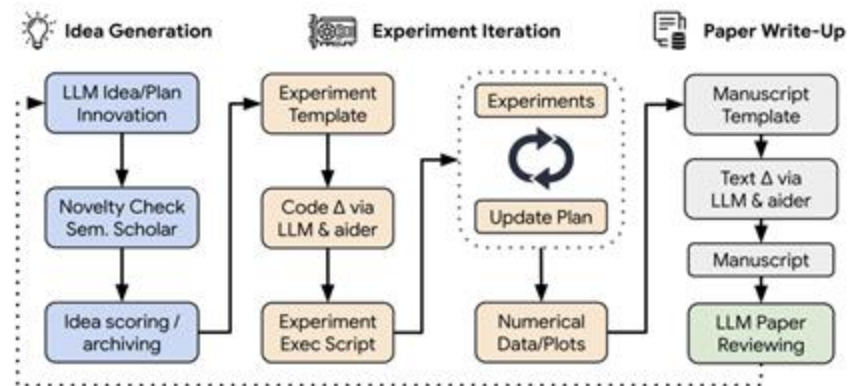
AI Bots by their own



Agent based approaches are making waves in the scientific community

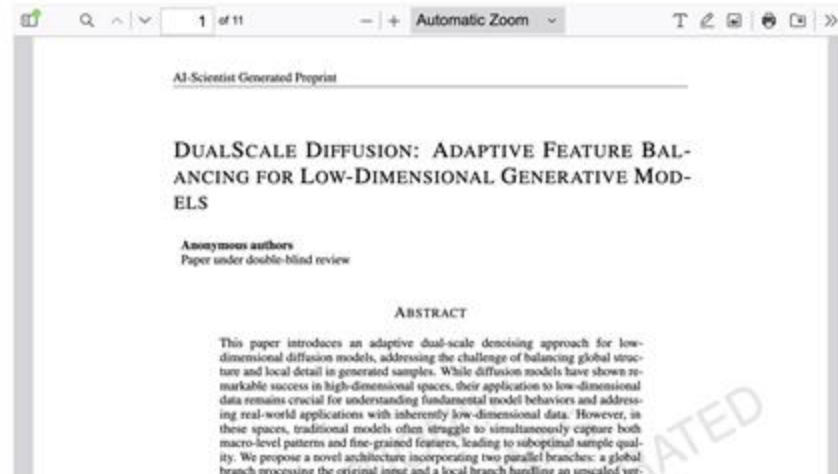
The AI Scientist: Towards Fully Automated Open-Ended Scientific Discovery

August 13, 2024



Conceptual illustration of The AI Scientist. The AI Scientist first brainstorms a set of ideas and then evaluates their novelty. Next, it edits a codebase powered by recent advances in automated code generation to implement the novel algorithms. The Scientist then runs experiments to gather results consisting of both numerical data and visual summaries. It crafts a scientific report, explaining and contextualizing the results. Finally, the AI Scientist generates an automated peer review based on top-tier machine learning conference standards. This review helps refine the current project and informs future generations of open-ended ideation.

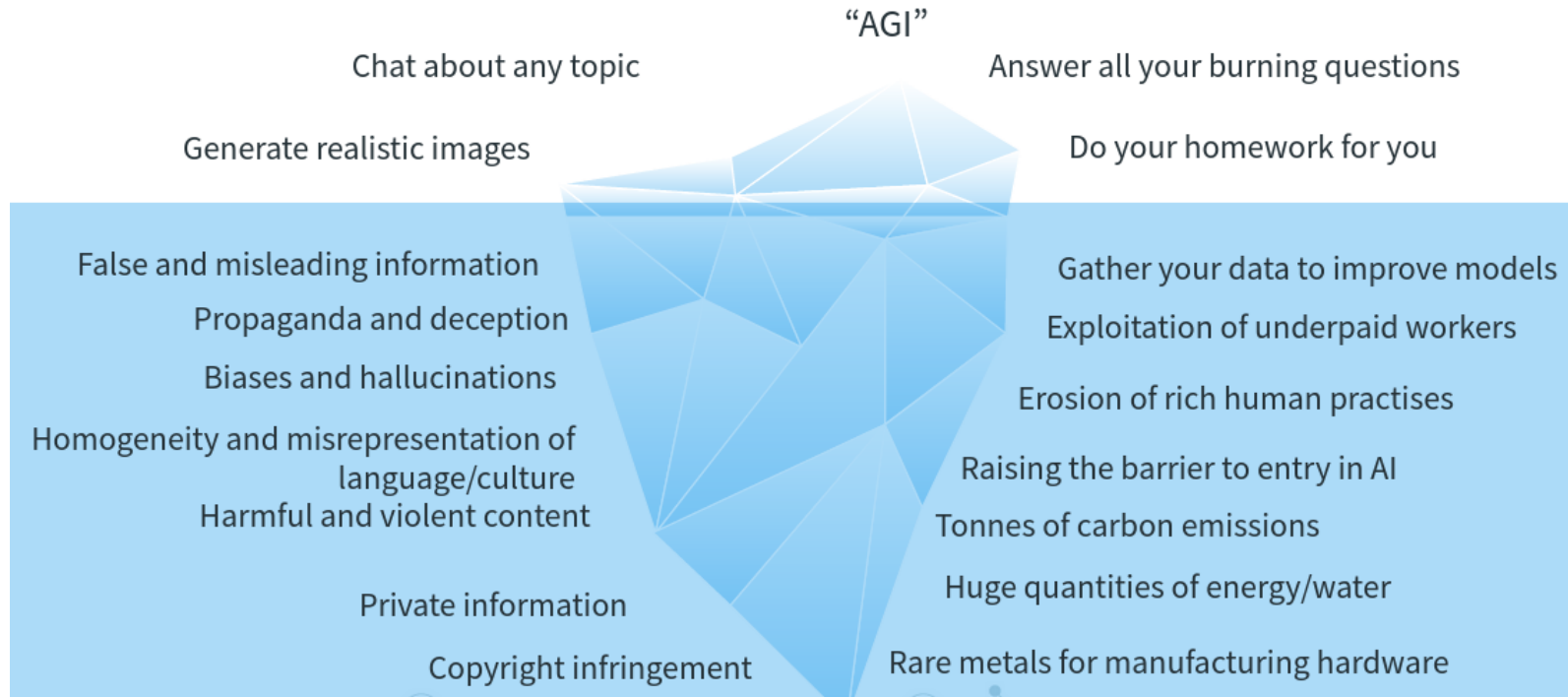
Diffusion Modeling



DualScale Diffusion: Adaptive Feature Balancing for Low-Dimensional Generative Models

further notes...

The Mounting Environmental & Human Costs of Generative AI



Conclusion & Call to Action

Conclusion & Call to Action

We need a mindset change - asap

Rejection



Positive



Panic





Doing now what patients need next