Weck Laboratories

Artificial Intelligence and the Lab

Agustin Pierri, Ph.D.

August 6, 2024

EMS

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Artificial Intelligence and the Lab
or:
How I Learned to Stop Worrying and Love the AI

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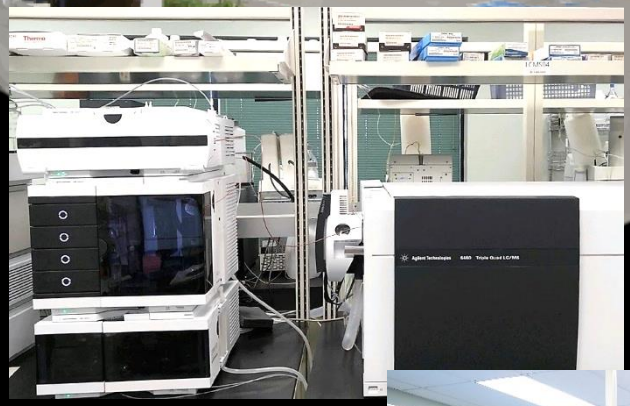
EMS

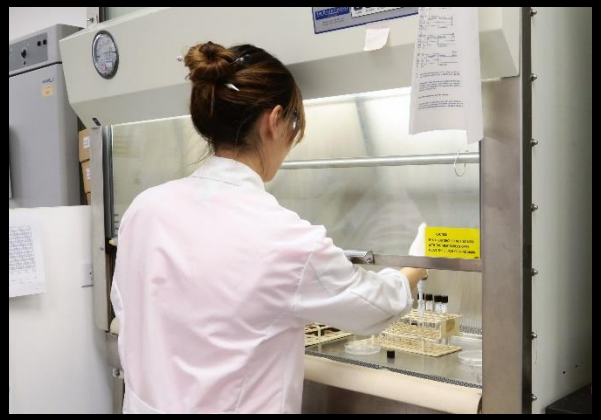
Introduction

About our laboratory

A full-service evironmental lab

- Organics
- Inorganics
- Microbiology
- Radiochemistry
- POPs
- Emerging contaminants





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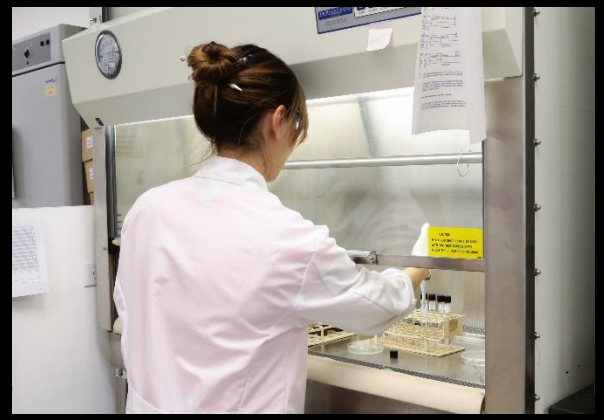
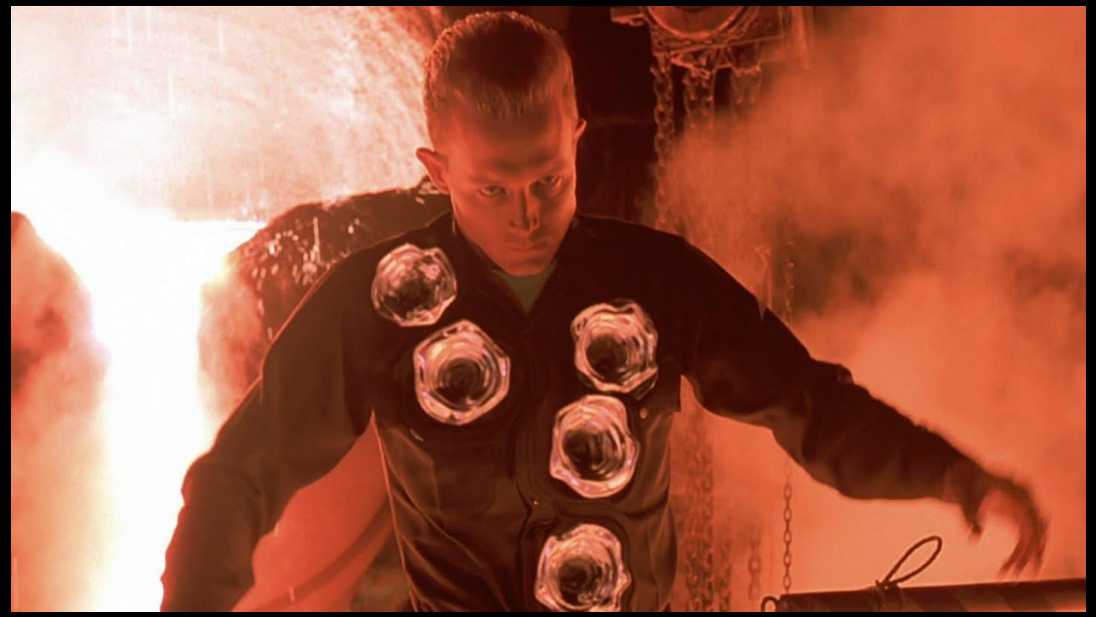
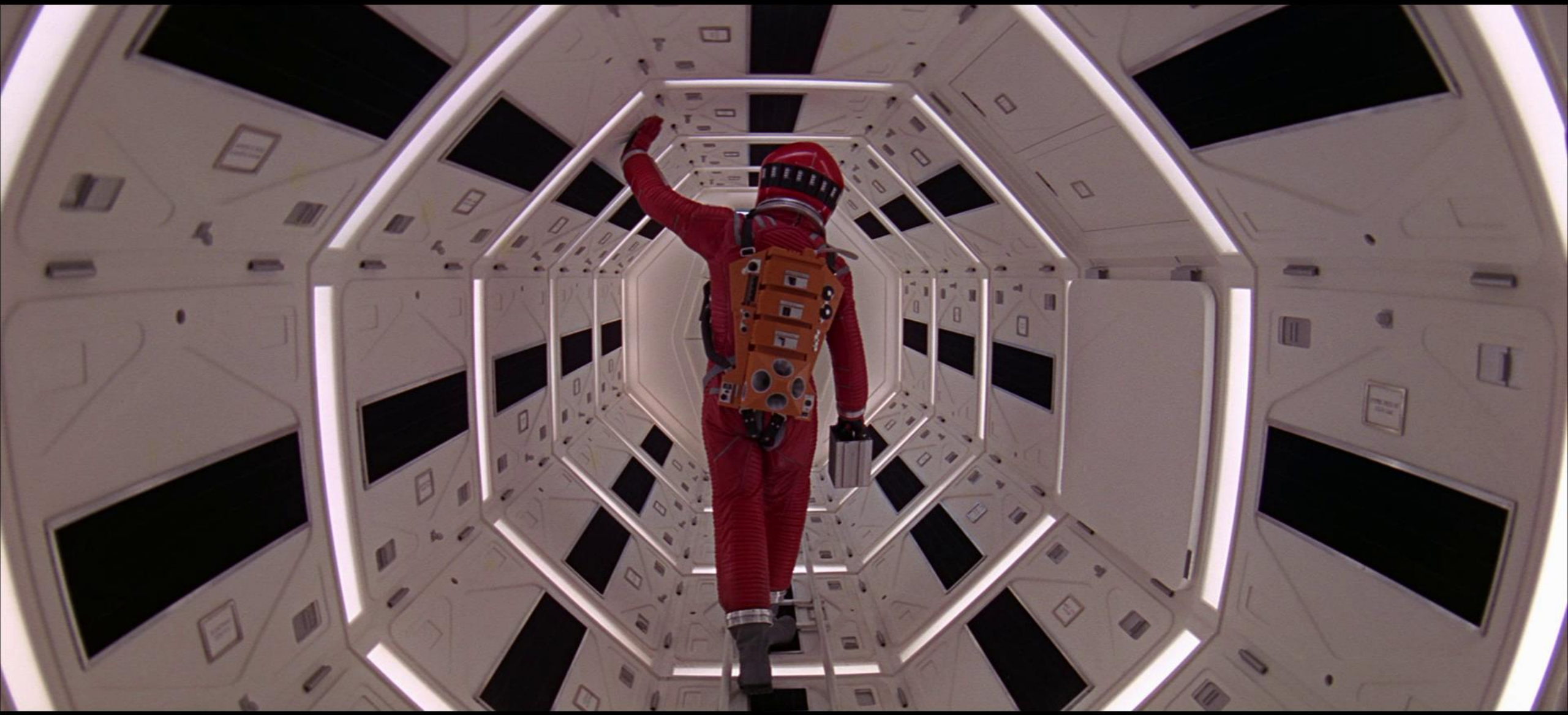
- Emerging technologies



Artificial Intelligence

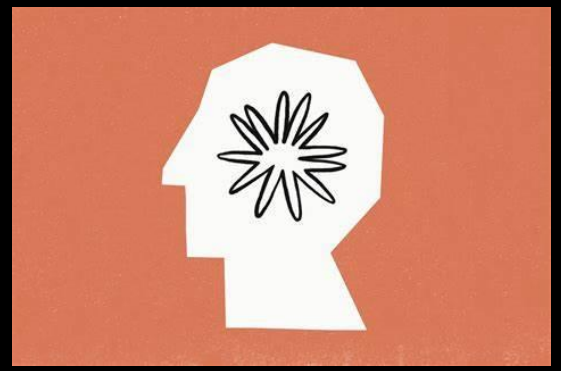
What is artificial intelligence?





Artificial intelligence today

OpenAI – ChatGPT
Microsoft – Copilot
Google – Gemini
Anthropic – Claude
Meta – Llama
Apple – Apple Intelligence
Samsung – Galaxy AI
X – Grok



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Who uses AI?

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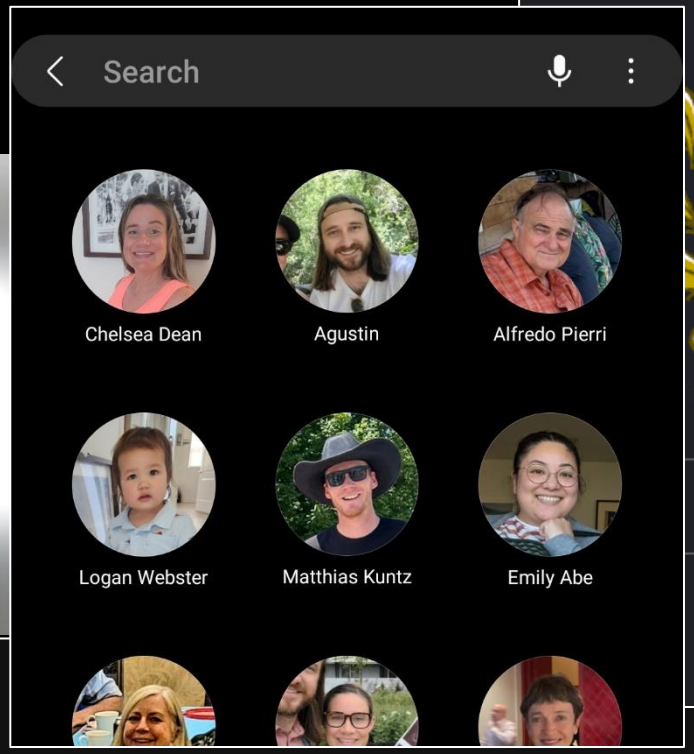

Your top mixes

Country Mix
Zach Bryan, Dasha, George Strait and more

Pop Mix
Chappell Roan, Billie Eilish, Olivia Rodrigo an...

Kendrick Lamar Mix
Outkast, Tommy Richman and The...

90s Mix
blink-182, Sublime, Green Day and more

Upbeat Mix
Beyoncé, Taylor Swift, Miley Cyrus and more

Chill Mix
Taylor Swift, Billie Eilish, Tracy Chapman and more

Hip Hop Mix
2Pac, JAY-Z, Outkast and more

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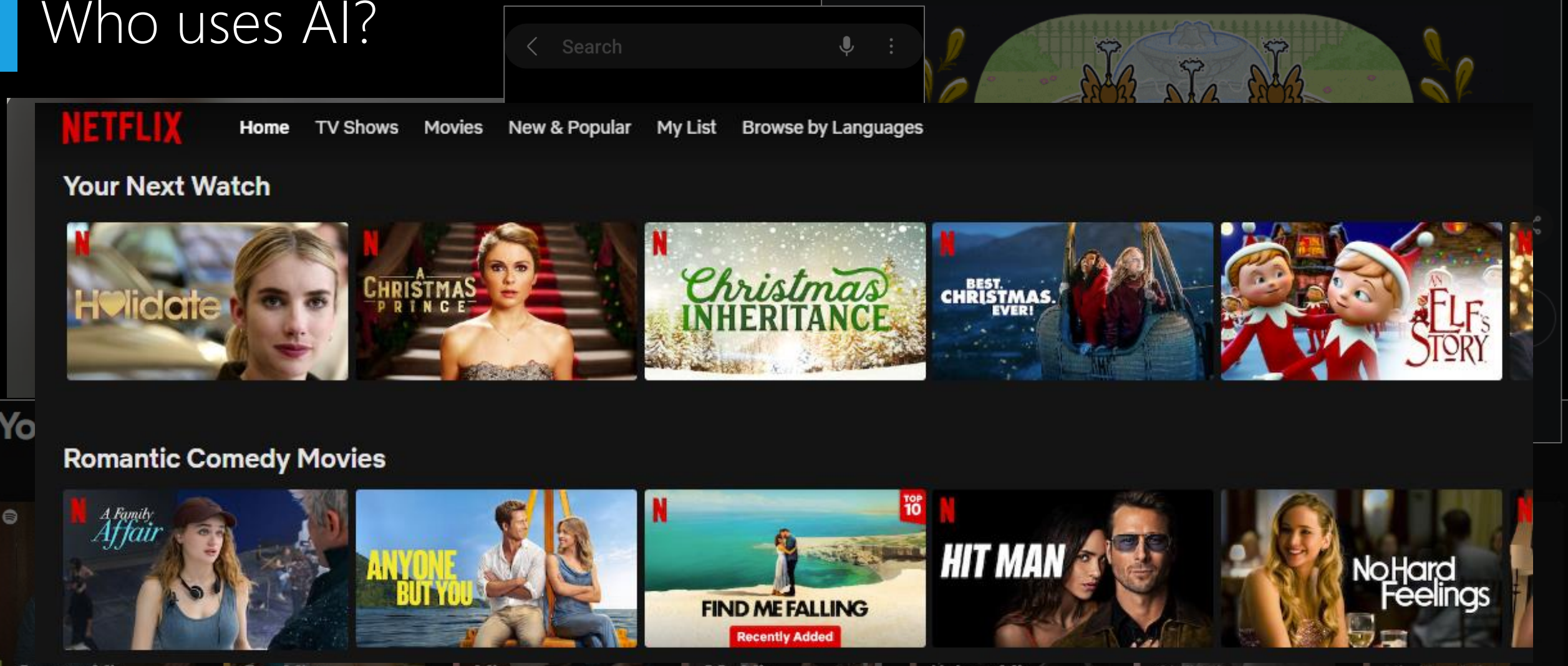
Search
NETFLIX
Home
TV Shows
Movies
New & Popular
My List
Browse by Languages
Your Next Watch
Holidate
A Christmas Prince
Christmas Inheritance
Best Christmas. Ever!
An Elf's Story
Romantic Comedy Movies
A Family Affair
Anyone But You
Top 10
Find Me Falling
Recently Added
Hit Man
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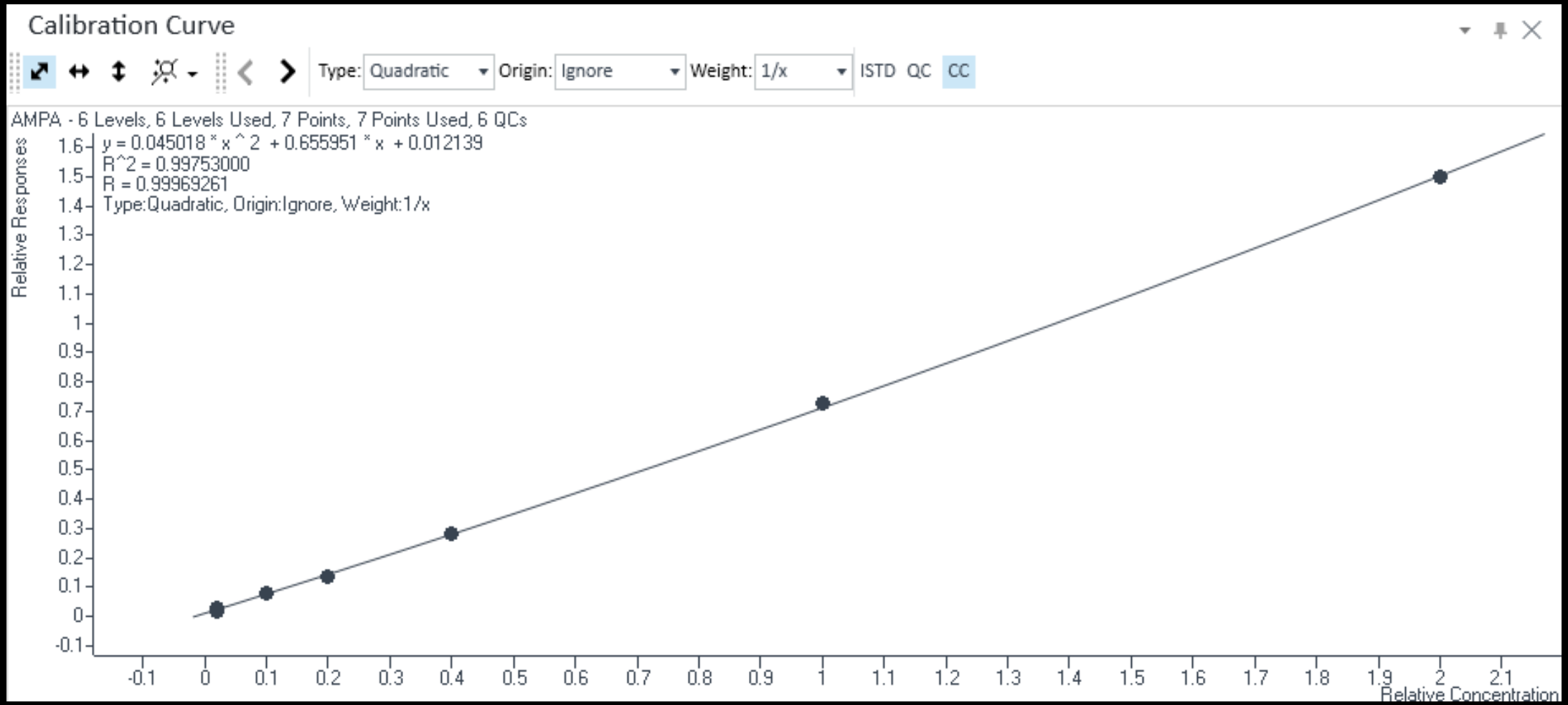
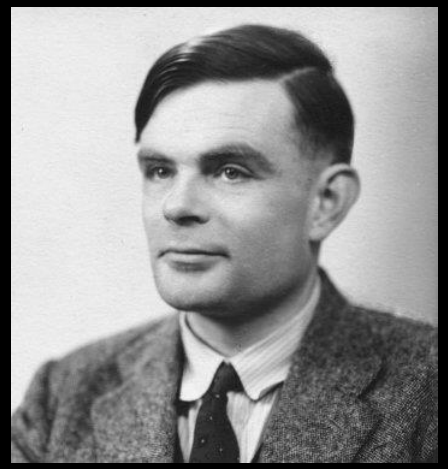
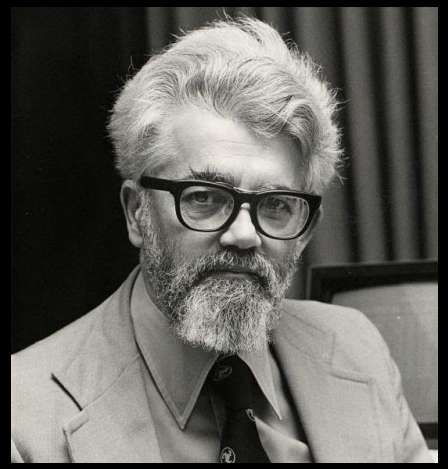

Calibration Curve
Type: Quadratic
Origin: Ignore
Weight: 1/x
ISTD QC CC
AMPA - 6 Levels, 6 Levels Used, 7 Points, 7 Points Used, 6 QCs
y = 0.045018 * x ^ 2 + 0.655951 * x + 0.012139
R^2 = 0.99753000
R = 0.99969261
Type:Quadratic, Origin:Ignore, Weight:1/x
Relative Responses
Relative Concentration

History of AI





Attention Is All You Need

Ashish Vaswani* Google Brain avaswani@google.com

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Llion Jones* Google Research llion@google.com

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

Łukasz Kaiser* Google Brain lukaszkaiser@google.com

Illia Polosukhin* ‡ illia.polosukhin@gmail.com

1950s-1960s: Industrial robots

1997: Deep Blue

2011: Siri and IBM Watson

2016: AlphaGo

2017: "Attention Is All You Need"

2022: ChatGPT-3.5

What is AI?

Artificial Intelligence:

"Machines that mimic human intelligence and cognitive functions and can be used for human tasks like problem-solving and image recognition."

Artificial Narrow Intelligence (ANI)

Artificial General Intelligence (AGI)

Artificial Super Intelligence (ASI)

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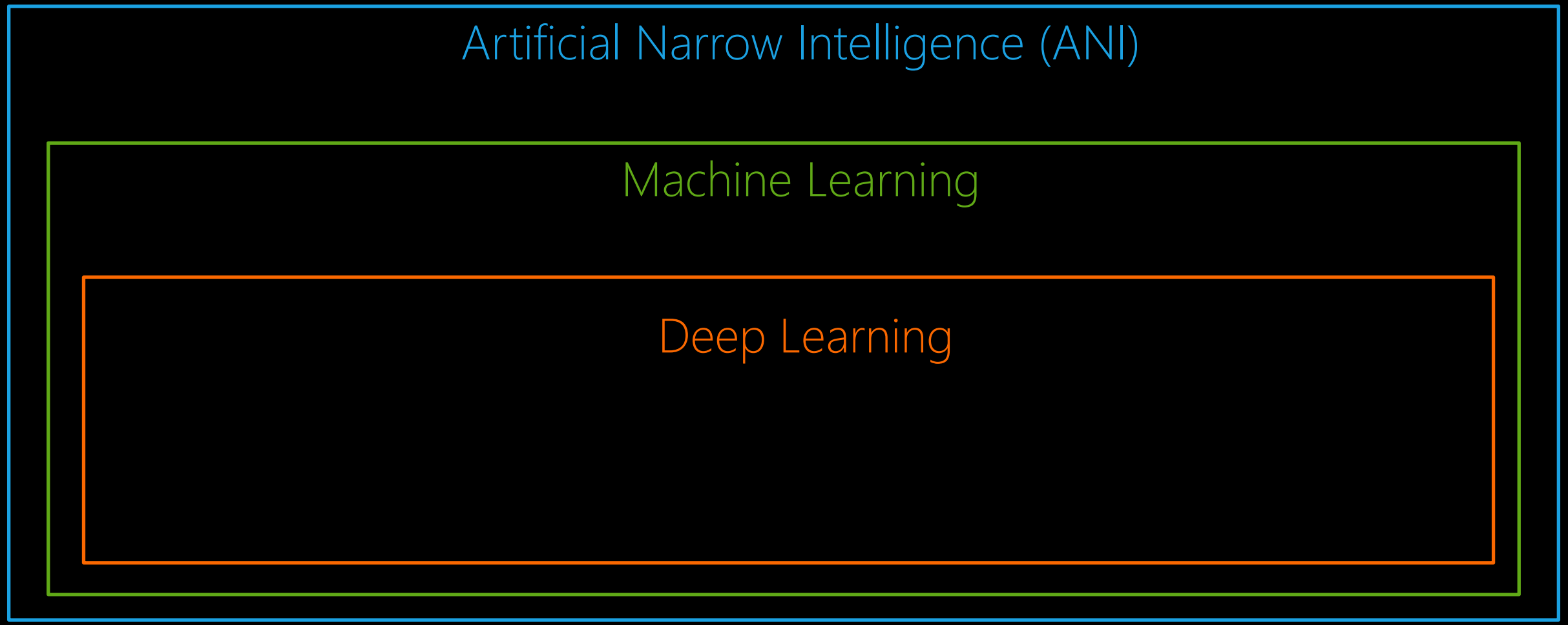
Artificial Narrow Intelligence (ANI)
Machine Learning
Deep Learning

Some key terms

Generative AI (GenAI):

AI model:

Large Language/Action Models (LLMs/LAMs):

Training:

Prompt/Inference:

Some key terms

Generative AI (GenAI): AI technology that uses ML to generate new content

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Prompt/Inference: The input and output of GenAI models

Some (more) key terms

Retrieval Augmented Generation (RAG):

Neural network:

Computer vision:

Transformer:

Hallucinations and bias:

Some (more) key terms

Retrieval Augmented Generation (RAG): Using external sources to augment inferences

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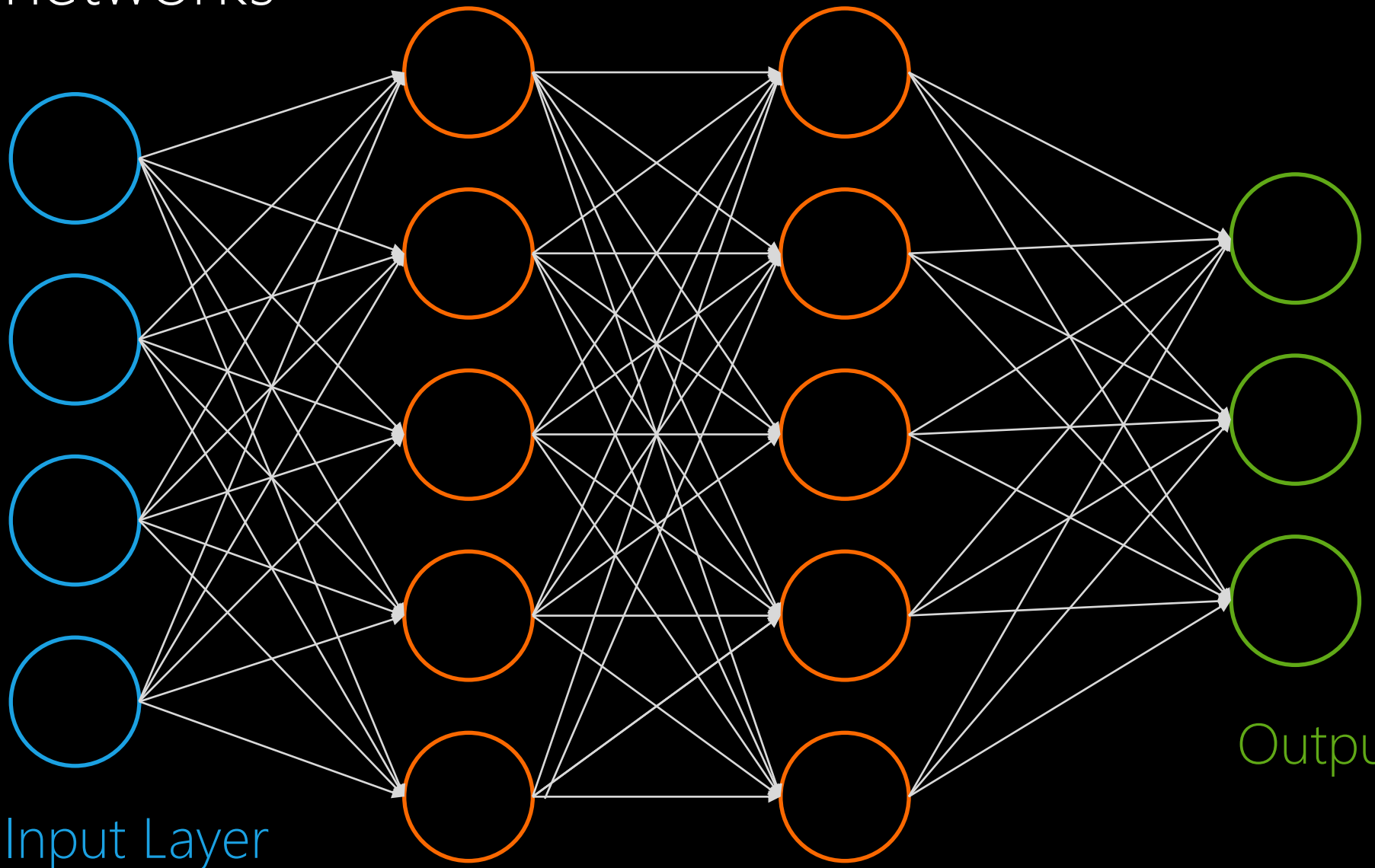
Hallucinations and bias: Incorrect responses and bias based on training data

Neural networks



What is AI good for?

AI case studies

Legal “copilot” for law firms

Harvey.

Scientific discovery

Examples of machine learning in materials discovery

Researchers	Result
Lyngby et. al.[282]	Predicted 11,630 new, stable 2D materials.
Yao et. al.[283]	Found 2 new 'invar alloys' which have a low thermal expansion and can be useful for several applications.
Vasylenko et. al.[284]	Identified 4 new materials, including materials that have desirable properties for use in solid state batteries.
Sun et. al.[285]	An approach for pre-screening for new organic photovoltaic materials.
Stanev et. al.[286]	Identified >30 potential high-temperature superconducting materials.

Moderna mRNA vaccine development

J&J drug discovery and clinical trial recruitment

Johnson&Johnson

Applications of AI in environmental monitoring

What can AI do in a lab?

Anything a human can do…

What can AI do in a lab?

Anything a human can do…

…kind of.

What can AI do in a lab?

Less human replacement, more virtual assistant to simplify laboratory tasks.

What can AI do in a lab?

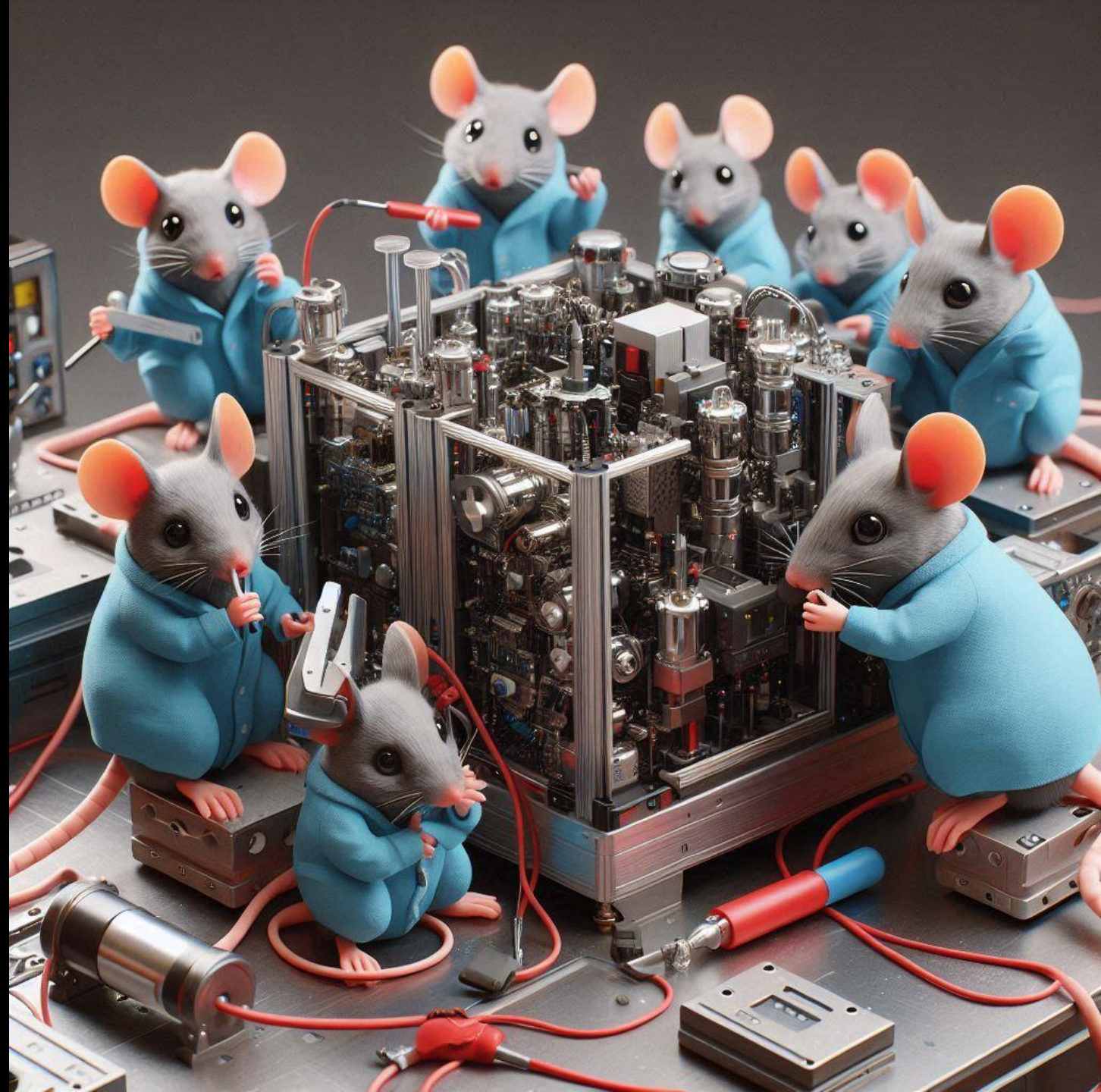
Use computer vision for automated storage and retrieval systems.

What can AI do in a lab?

Use computer vision to automatically track and log every sample container.

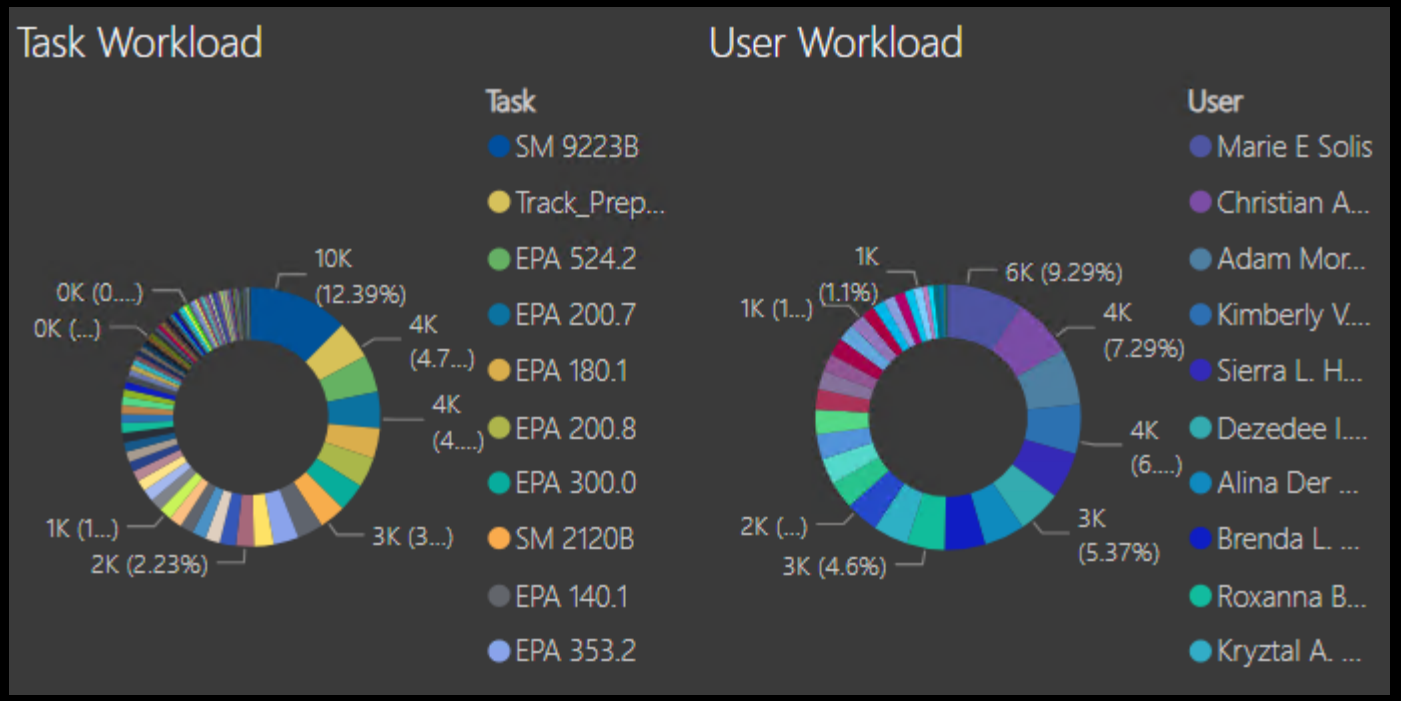
What can AI do in a lab?

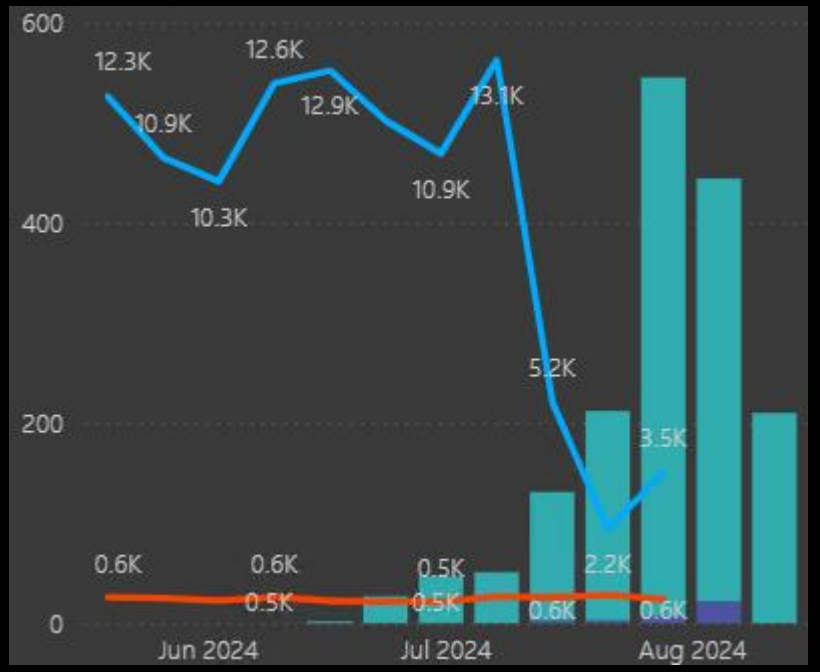
Use in-lab generated data sets to predict instrument maintenance intervals.

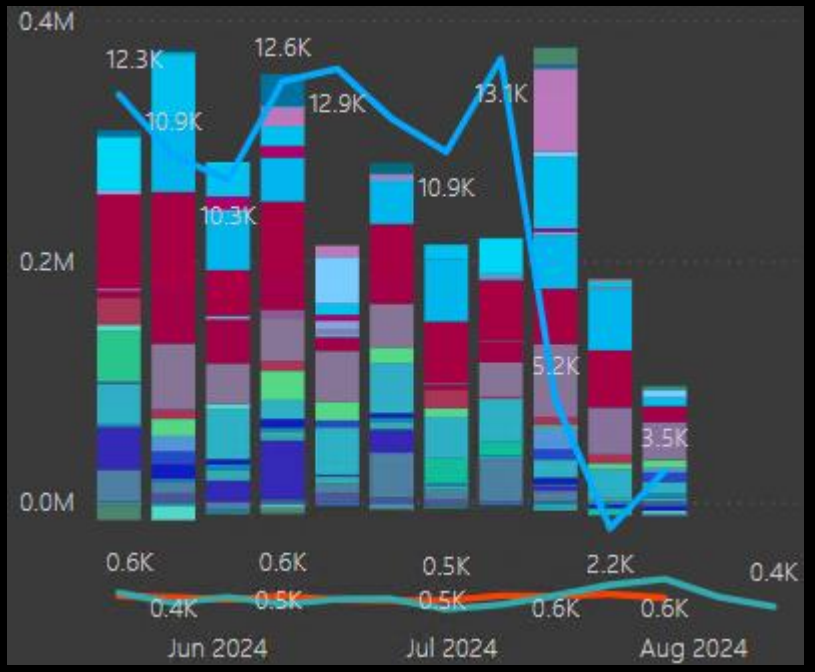


What can AI do in a lab?

Evaluate performance metrics to optimize instrument and analyst capacity.

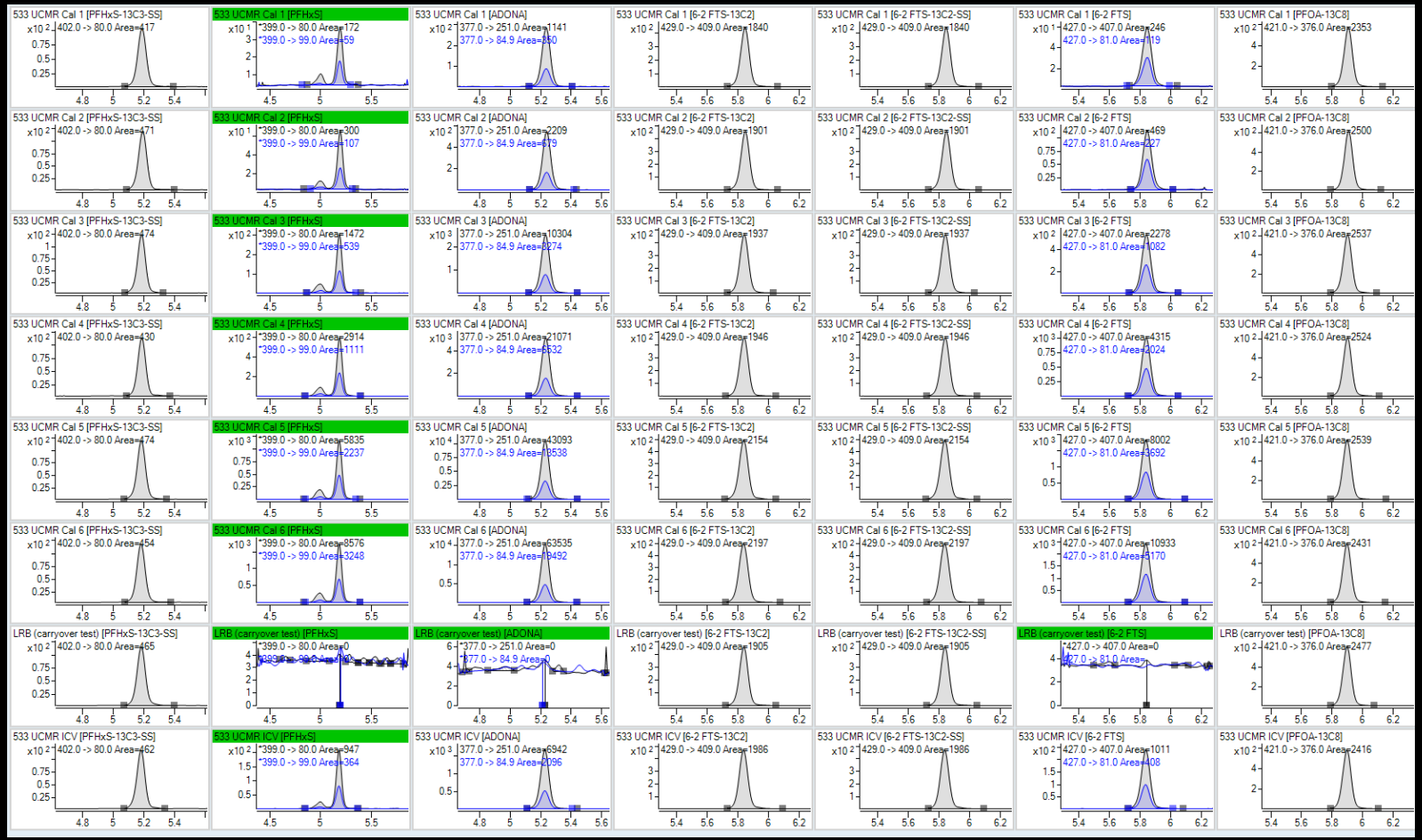


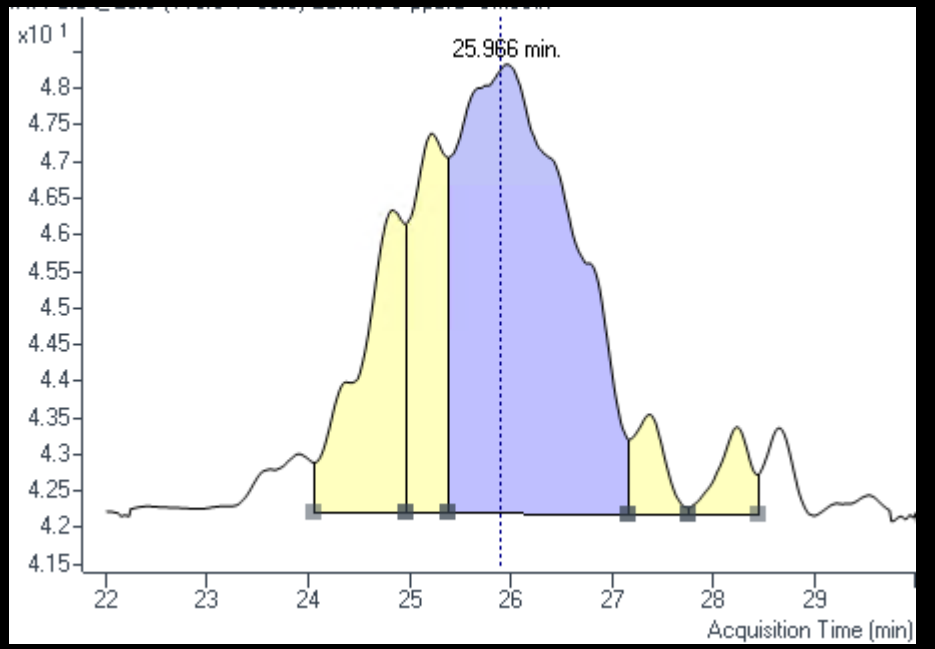


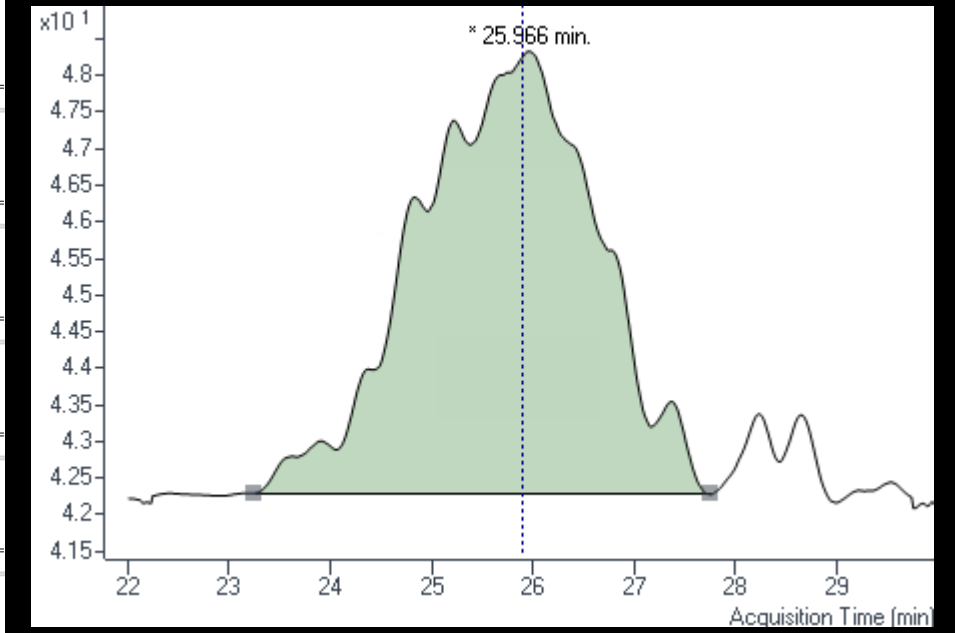


What can AI do in a lab?

Assist analysts with evaluating chromatograms and complex peak integrations.

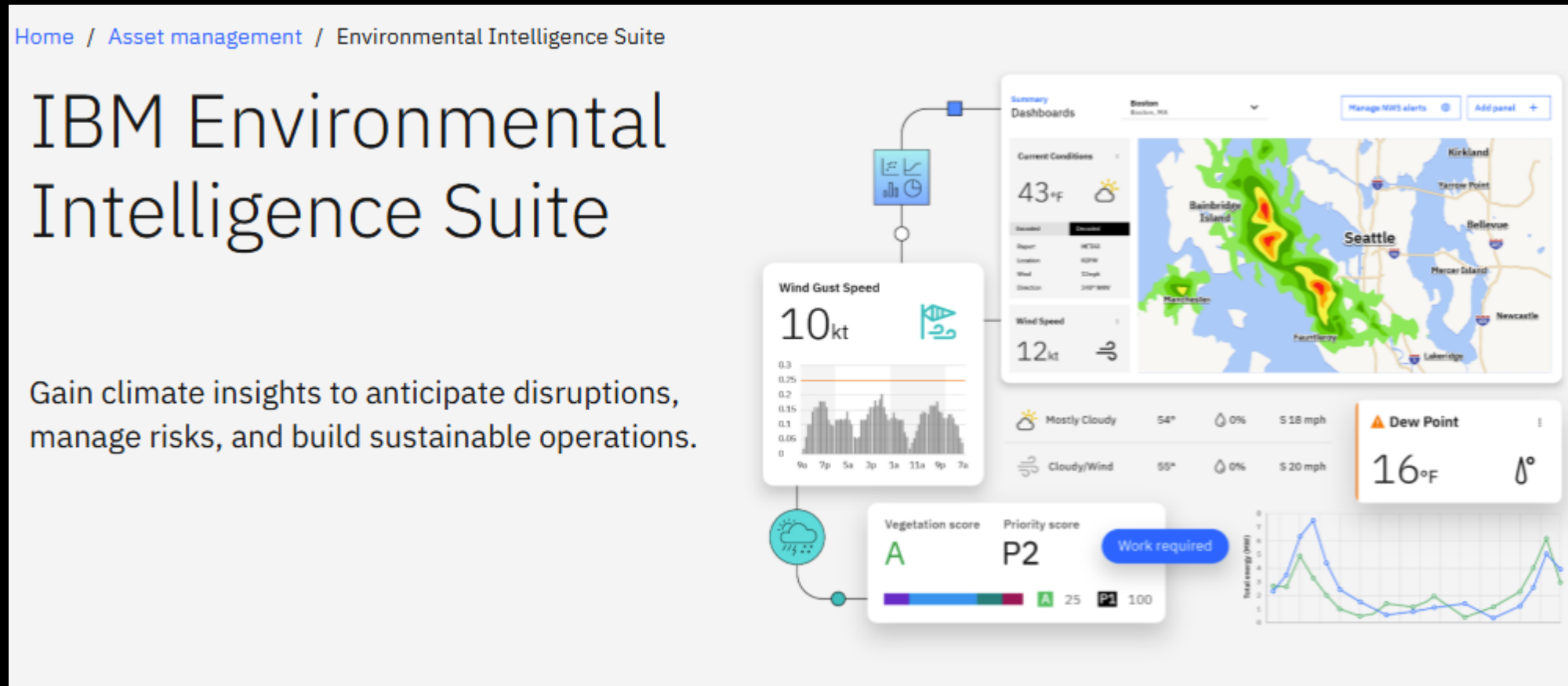






What can AI do in a lab?

Evaluate large data sets to identify trends in environmental pollution data.



What can AI do in a lab?

Assist secondary data reviewers while evaluating laboratory data.

What can AI do in a lab?

Identify low resources by monitoring supplies, instrument capacity, and analyst availability with respect to incoming sample load.

What can AI do in a lab?

Create and train a custom GPT for internal and external chatbots.

Weck
Intelligent
Support
Entity

Drawbacks

Drawbacks of AI

Hallucinations

Drawbacks of AI

Hallucinations

Ethics

Drawbacks of AI

Hallucinations

Ethics

Environmental costs

Drawbacks of AI

Hallucinations

Ethics

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Data privacy

Drawbacks of AI

Hallucinations

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Data privacy

Balancing AI + humans

AI has limitless potential, but needs to be used responsibly

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Thank you