

AstroMLab

Expediting Discoveries in Astronomy with LLM

Yuan-Sen Ting (丁源森)

The Ohio State University



NSF awarded over \$200 million for *AI Research Institutes*

Biological Sciences
~ 2 centers

Physical Sciences
~ 3 centers

Environmental Sciences
~ 2 centers

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Environmental Sciences
~ 2 centers

6 centers x
15M ~ 100M

Hype, myth, or real deal?

[nature](#) > [articles](#) > [article](#)

Article | [Open access](#) | Published: 15 July 2021

Highly accurate protein structure prediction with **AlphaFold**

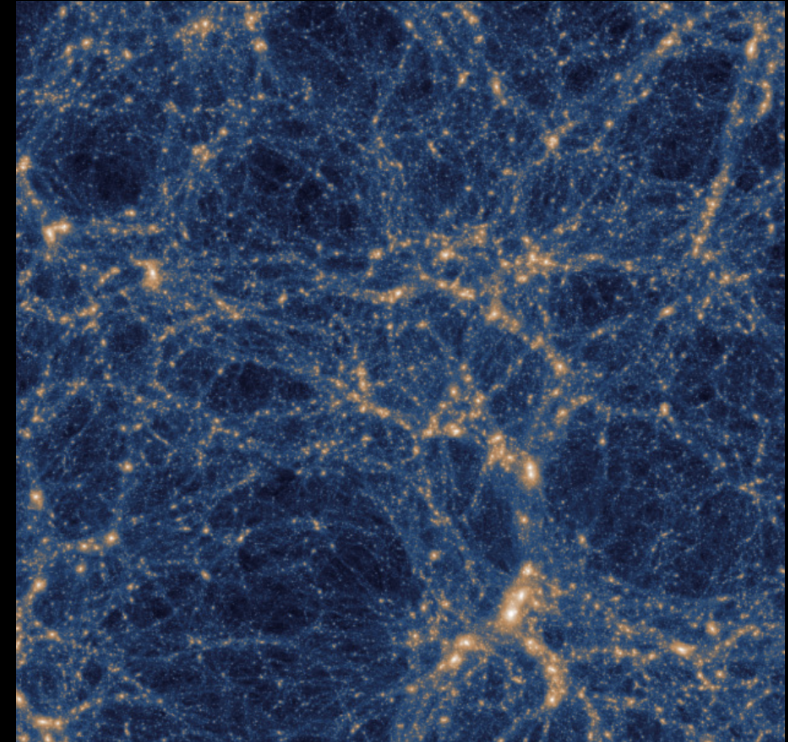
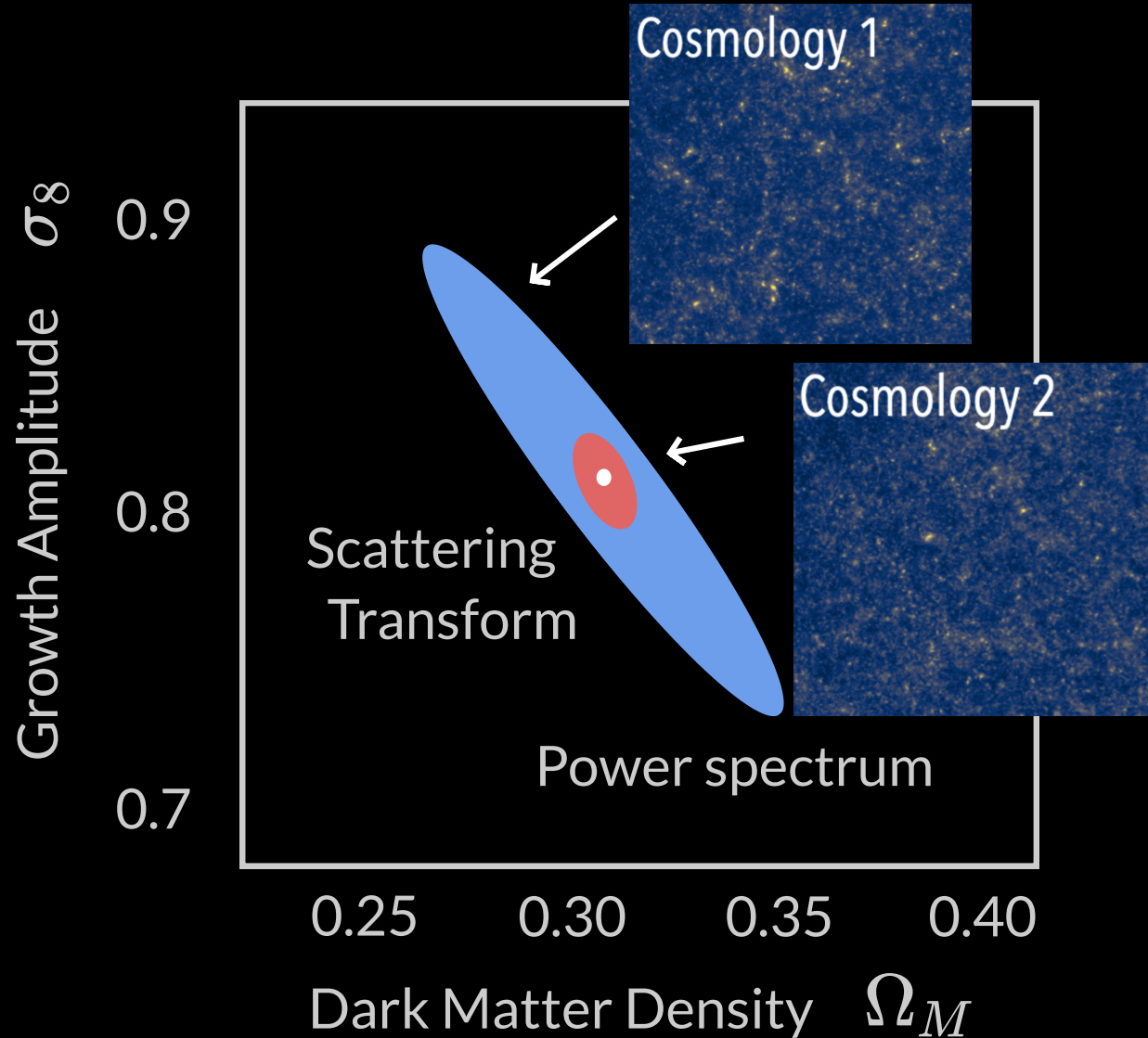
[John Jumper](#) , [Richard Evans](#), [Alexander Pritzel](#), [Tim Green](#), [Michael Figurnov](#), [Olaf Ronneberger](#), [Kathryn Tunyasuvunakool](#), [Russ Bates](#), [Augustin Žídek](#), [Anna Potapenko](#), [Alex Bridgland](#), [Clemens Meyer](#), [Simon A. A. Kohl](#), [Andrew J. Ballard](#), [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](#)

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1.60m Accesses | **13k** Citations | **3592** Altmetric | [Metrics](#)

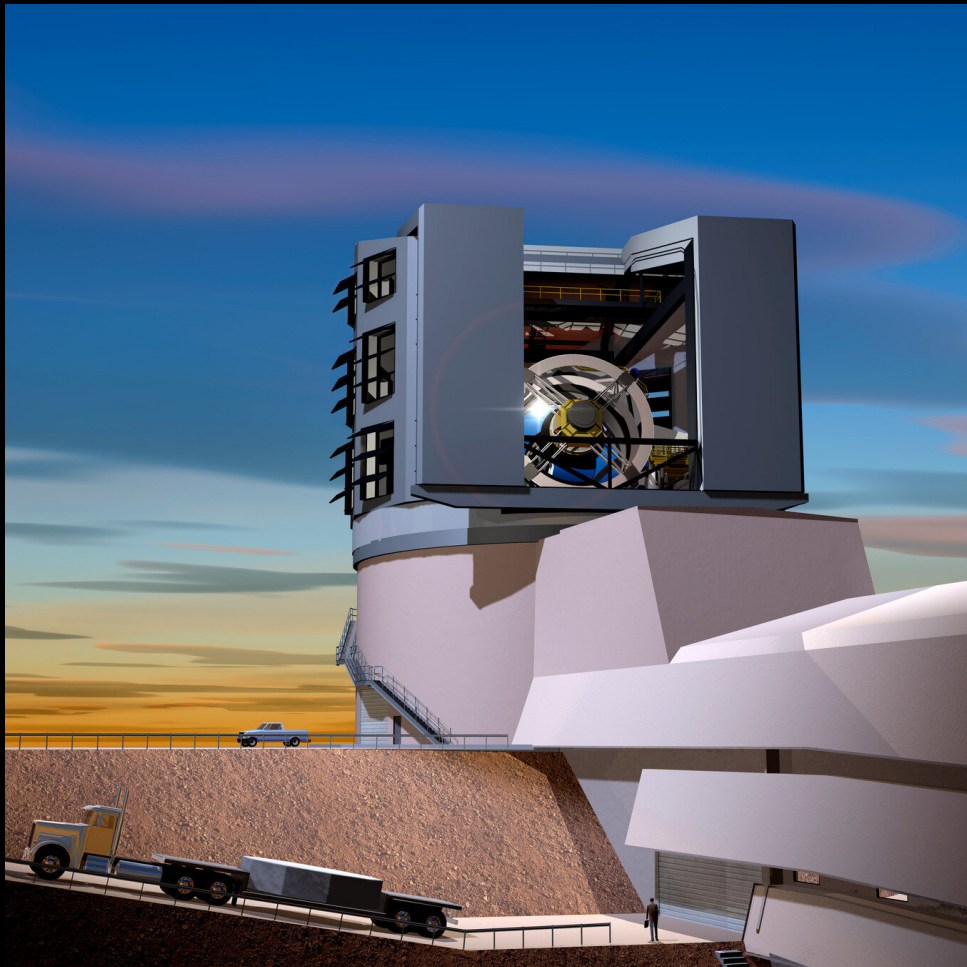
Why hasn't astronomy had its
"AlphaFold" moment yet?"

Most AI in Astronomy focuses on *extending* statistical methods



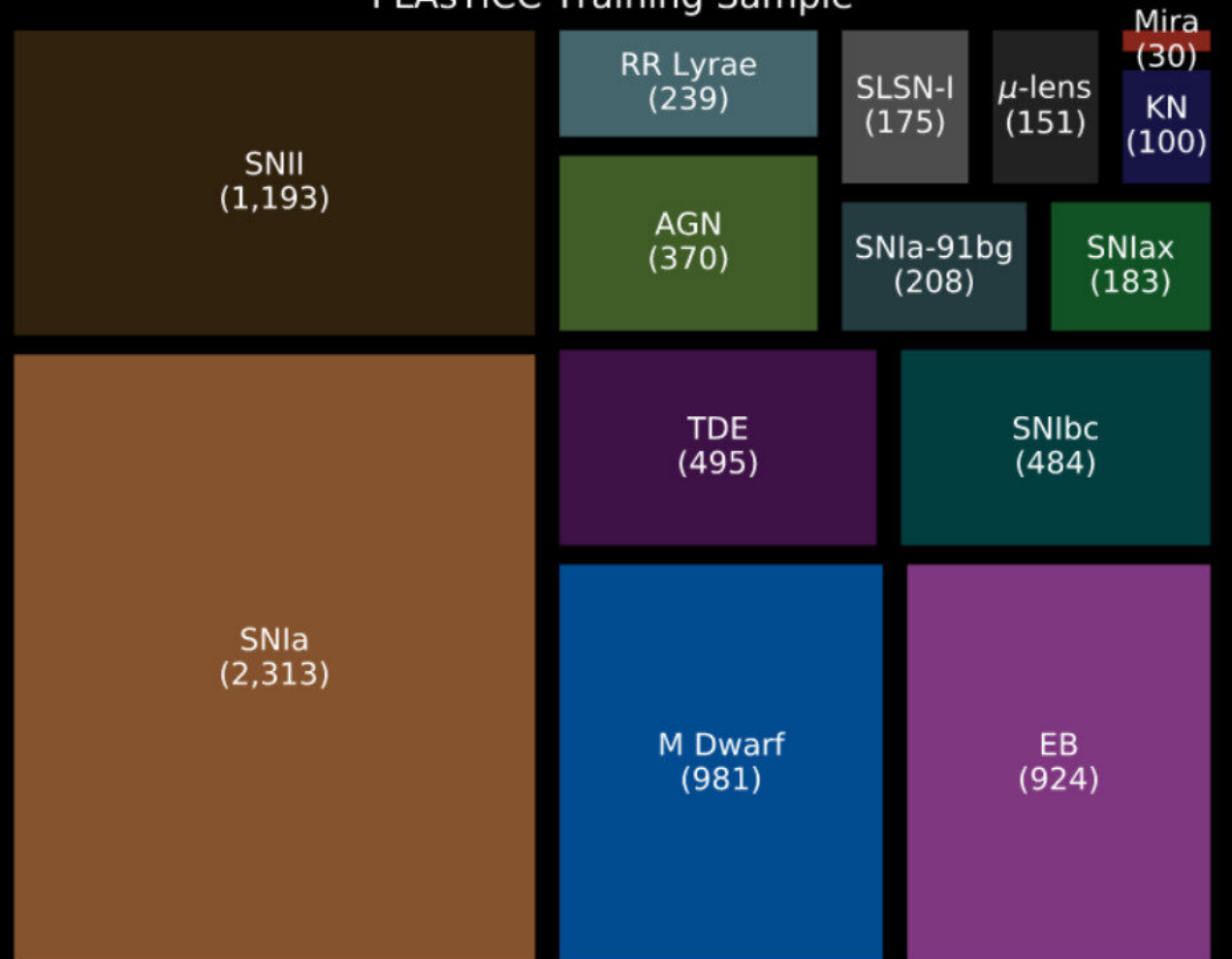
International Astrostatistics Association Award
Cheng, YST, Menard & Bruna + 20

or building effective brokers / *classifiers*



Rubin Observatory

PLAsTiCC Training Sample



Improving *individual* downstream tasks with annotated data in a confined setting will *not* revolutionize astronomy

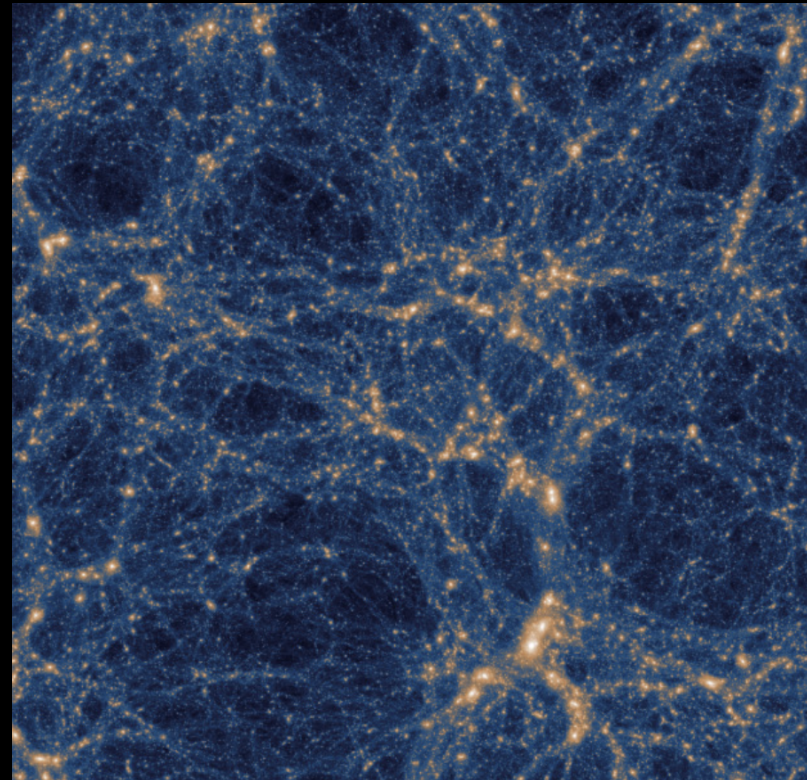
The *complexity* of astronomy is *too low* for AI

Highly non-Gaussian



My niece

Weakly non-Gaussian



Cosmic large-scale structure

Astronomy is *not* biology

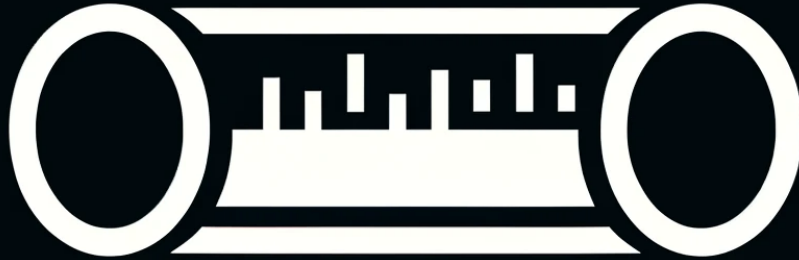
Data /
Observation

Theory /
Hypothesis

Astronomy is *not* biology

Data /
Observation

Theory /
Hypothesis

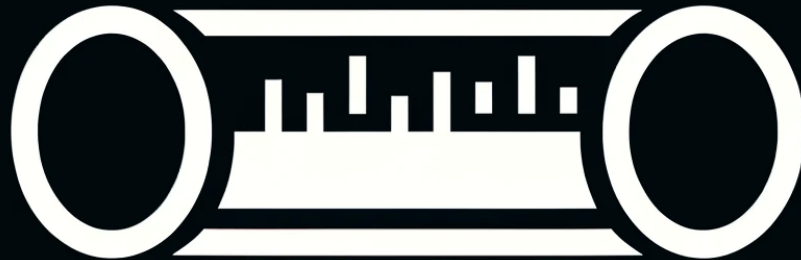


Analysis
Pipelines

Astronomy is *not* biology

Data /
Observation

Theory /
Hypothesis



Analysis
Pipelines



True

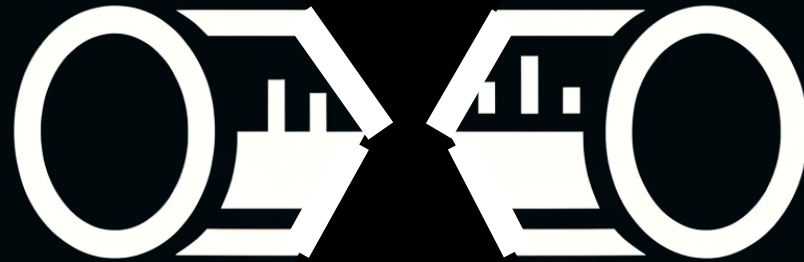


False

Biology faced a fundamental *bottleneck*

Data /
Observation

Theory /
Hypothesis



Analysis
Pipelines



True



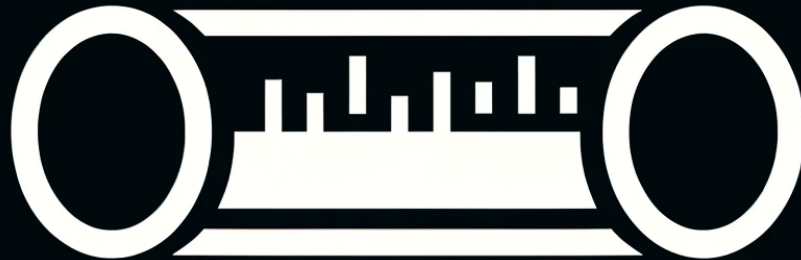
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Biology faced a fundamental *bottleneck*

Data /
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AlphaFold



Analysis
Pipelines



True

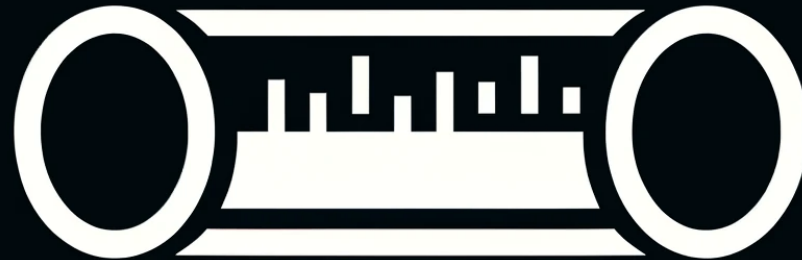


False

Astronomy already has a successful *standard model*

Data /
Observation

Theory /
Hypothesis



LambdaCDM



True



False



The Bitter Lesson - Rich Sutton, 2019

The Bitter Lesson - Rich Sutton, 2019

"We should build in only the *meta-methods* that can find and capture this arbitrary complexity.

Essential to these methods is that they can find good approximations, but the search for them should be *by our methods, not by us.*

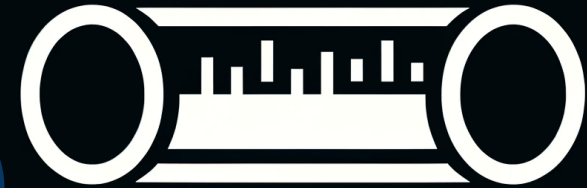
We want AI agents that can *discover like we can*, not which contain what we have discovered."

Toward an *AI Astronomer*

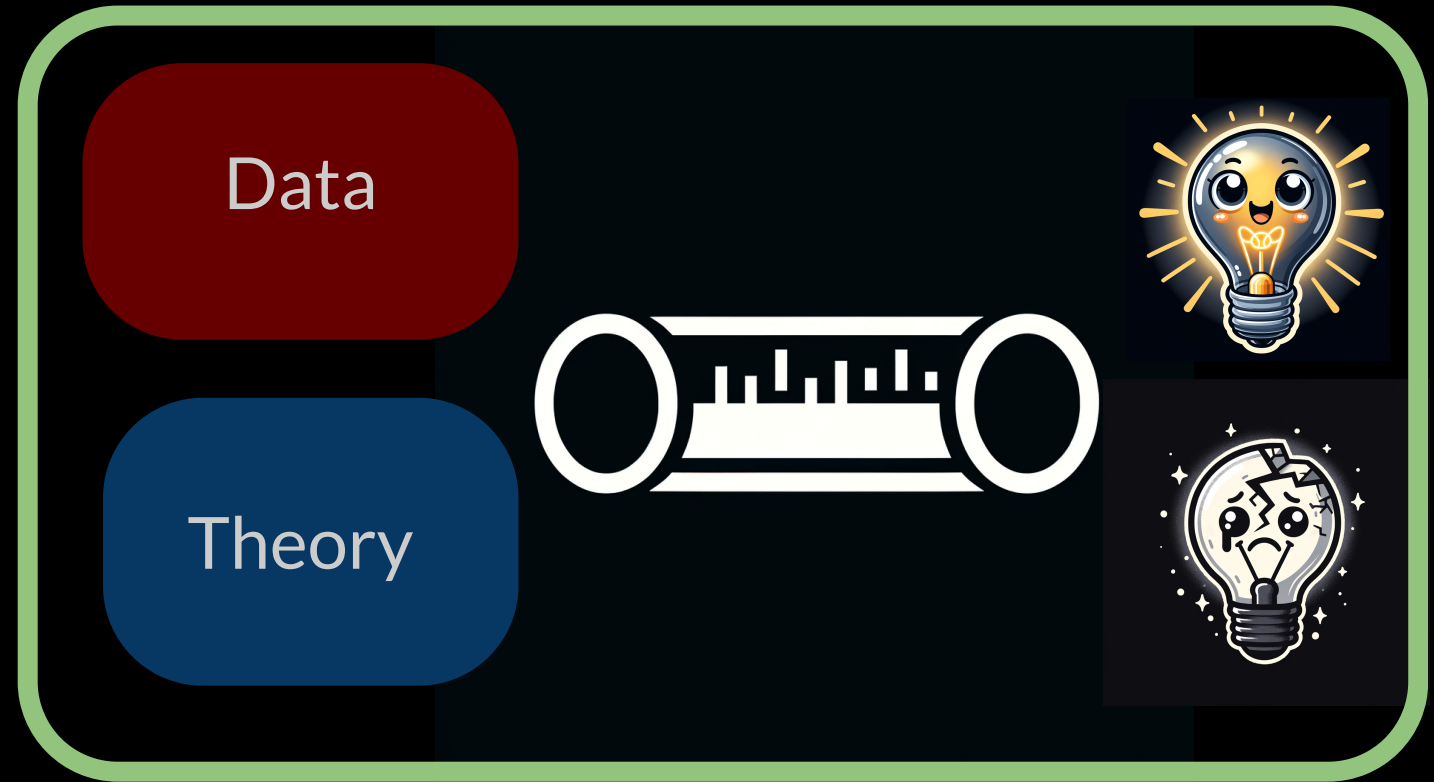
Research is essentially a *reinforcement learning* process

Data

Theory



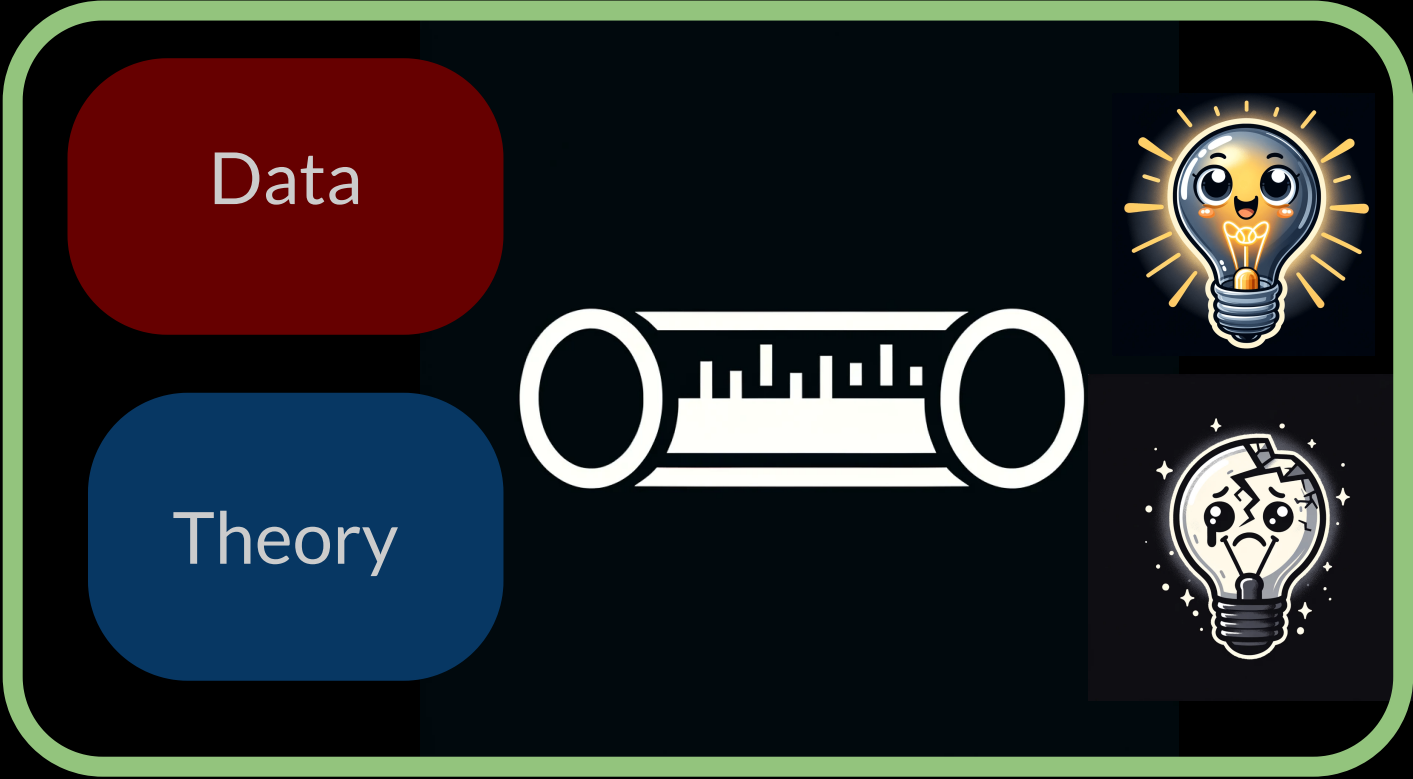
Research is essentially a *reinforcement learning* process



State of the research

Research is essentially a *reinforcement learning* process

Evaluate the state

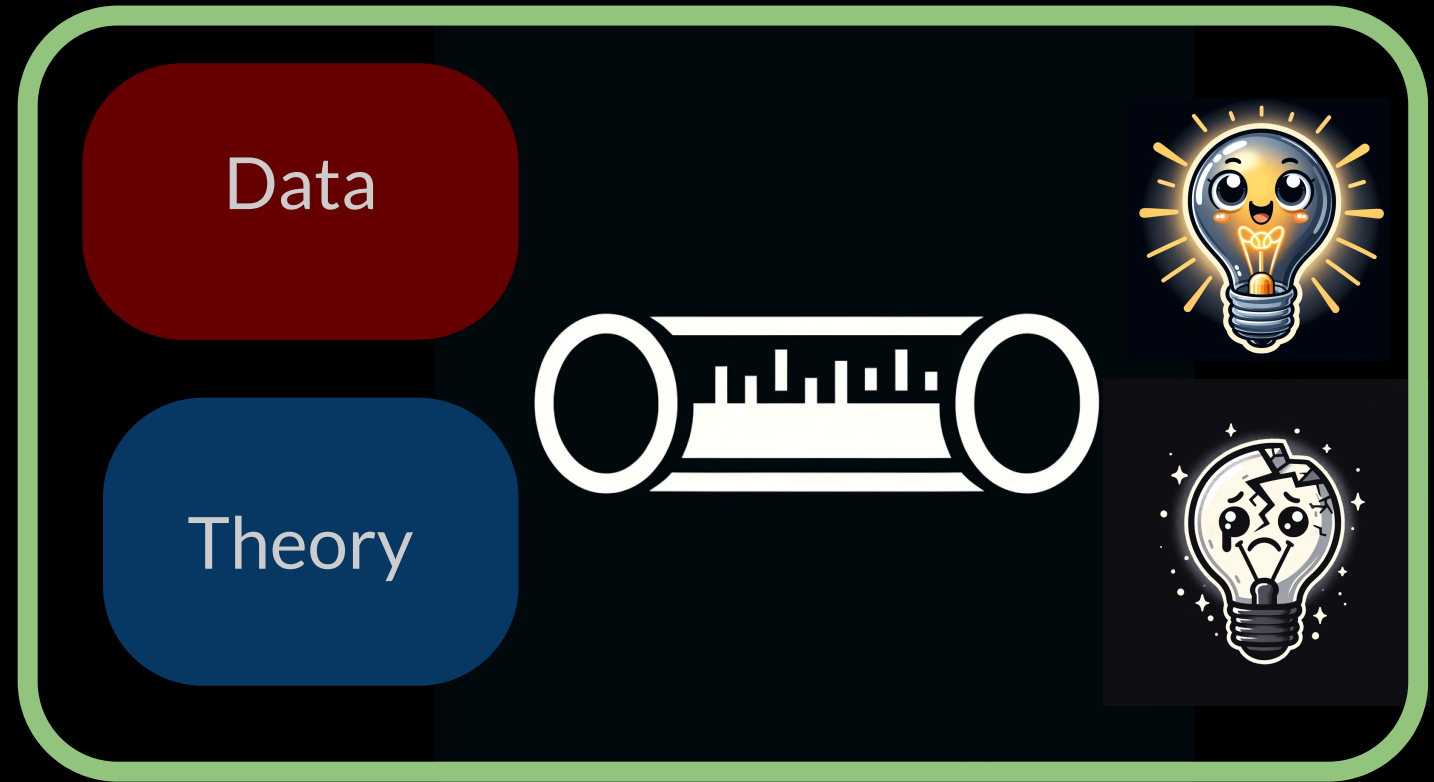
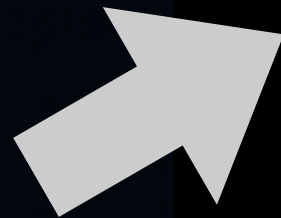


State of the research

Research is essentially a *reinforcement learning* process

Evaluate the state

Making "plan"

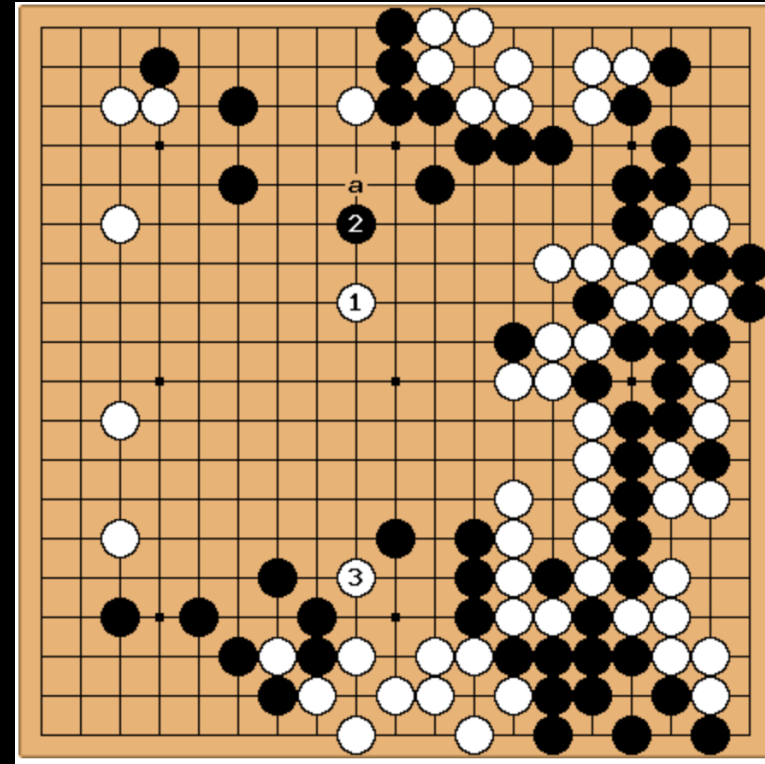


State of the research

Research is essentially a *reinforcement learning* process

Evaluate the state

Making "plan"



State of the research

Enabling LLM agents to
learn how to make plan
through *open world exploration*

Enabling LLM agents to
learn how to make plan
through *open world exploration*



Human *"intuition"* +
experience

o-ph.[MJ] 23 Sep 2024

Interpreting Multi-band Galaxy Observations with Large Language Model-Based Agents

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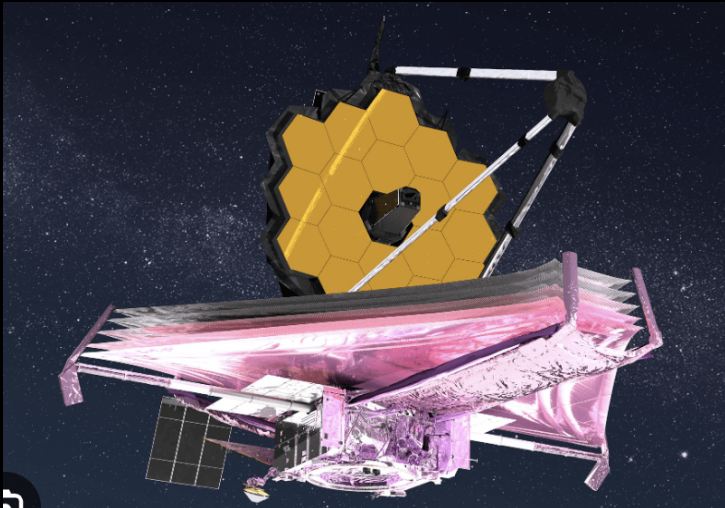
Zheng Cai

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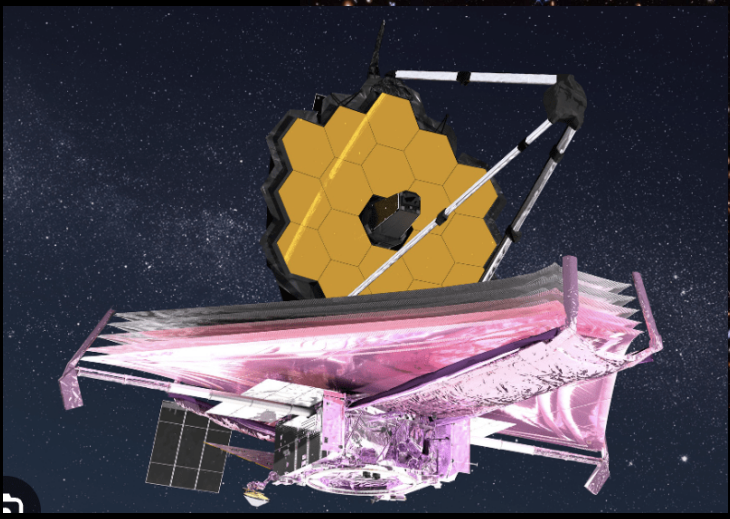


Sun, YST+, 2024b

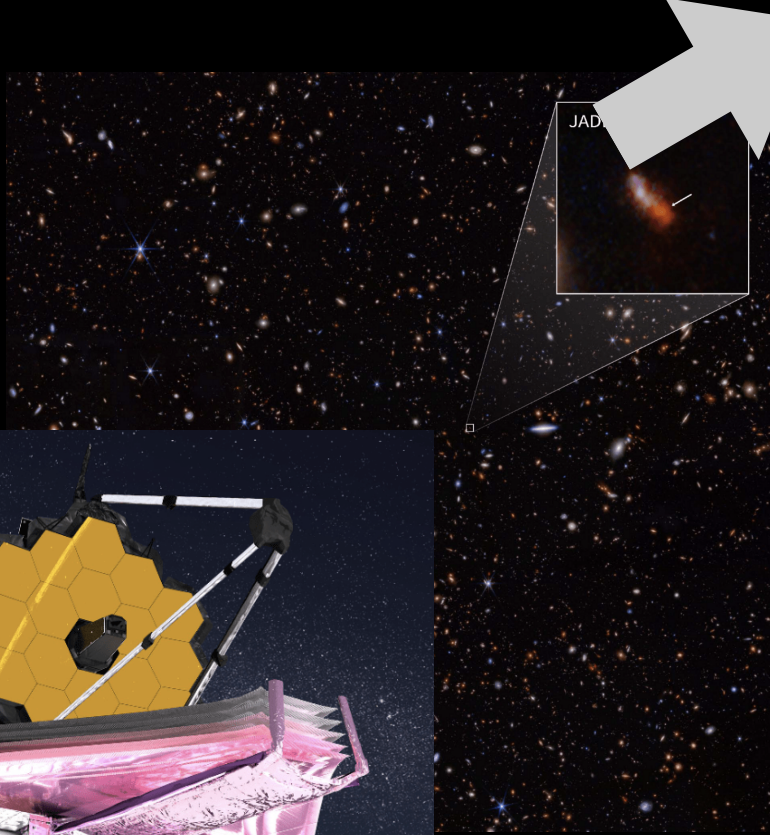
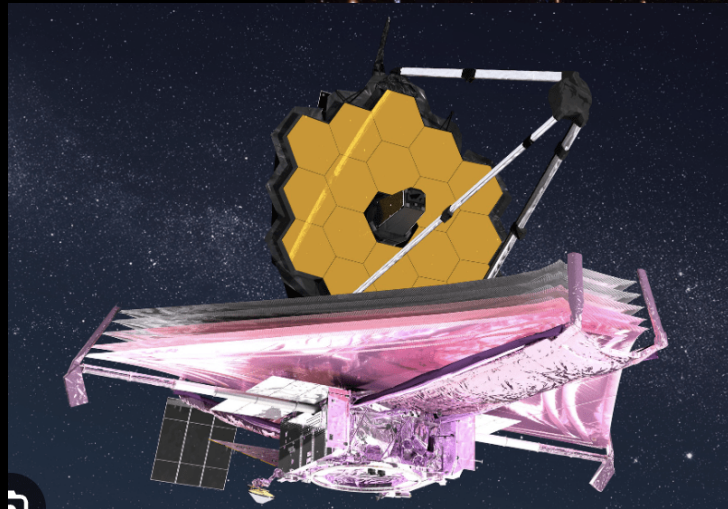
Can we identify all the astronomical objects that our current physics can't explain



Can we identify all the astronomical objects that our current physics can't explain



Can we identify all the astronomical objects that our current physics can't explain ??



The Cosmos in Its Infancy: JADES Galaxy Candidates at $z > 8$ in GOODS-S and GOODS-N

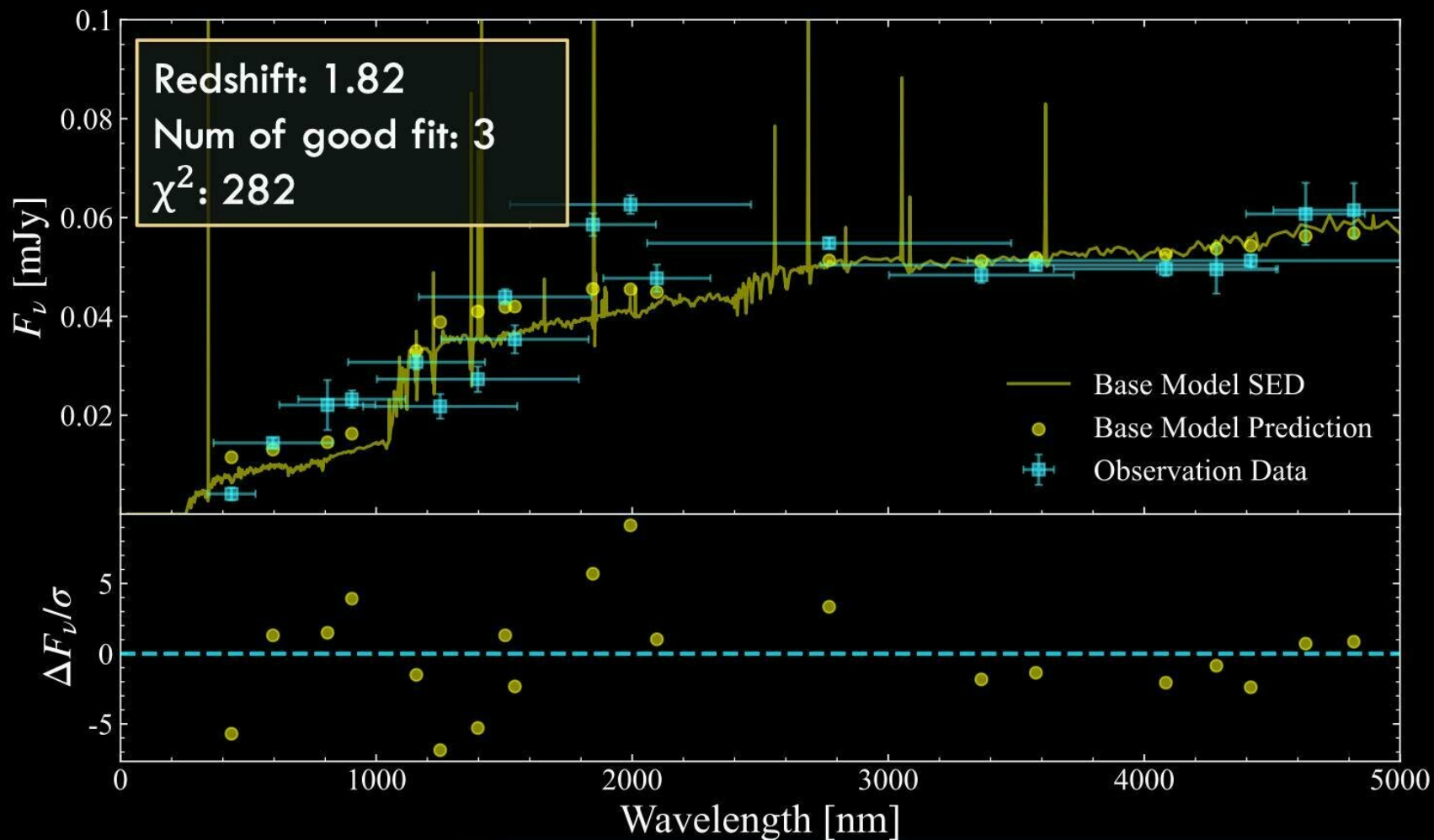
Kevin N. Hainline¹, Benjamin D. Johnson², Brant Robertson³, Sandro Tacchella^{4,5}, Jakob M. Helton¹, Fengwu Sun¹, Daniel J. Eisenstein², Charlotte Simmonds^{4,5}, Michael W. Topping¹, Lily Whitler¹, Christopher N. A. Willmer¹, Marcia Rieke¹, Katherine A. Suess^{6,7}, Raphael E. Hviding¹, Alex J. Cameron⁸, Stacey Alberts¹, William M. Baker^{4,5}, Stefi Baum⁹, Rachana Bhatawdekar^{10,11}, Nina Bonaventura^{1,12,13}, Kristan Boyett^{14,15}, Andrew J. Bunker⁸, Stefano Carniani¹⁶, Stephane Charlot¹⁷, Jacopo Chevallard⁸, Zuyi Chen¹, Mirko Curti^{4,5,18}, Emma Curtis-Lake¹⁹, Francesco D'Eugenio^{4,5}, Eiichi Egami¹, Ryan Endsley²⁰, Ryan Hausen²¹, Zhiyuan Ji¹, Tobias J. Looser^{4,5}, Jianwei Lyu¹, Roberto Maiolino^{4,5,22}, Erica Nelson²³, Dávid Puskás^{4,5}, Tim Rawle¹⁰, Lester Sandles^{4,5}, Aayush Saxena^{8,22}, Renške Smit²⁴, Daniel P. Stark¹, Christina C. Williams²⁵, Chris Willott²⁶, and Joris Witstok^{4,5}

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- ¹⁴ School of Physics, University of Melbourne, Parkville, VIC 3010, Australia

Astronomical research is *more than* just fitting data

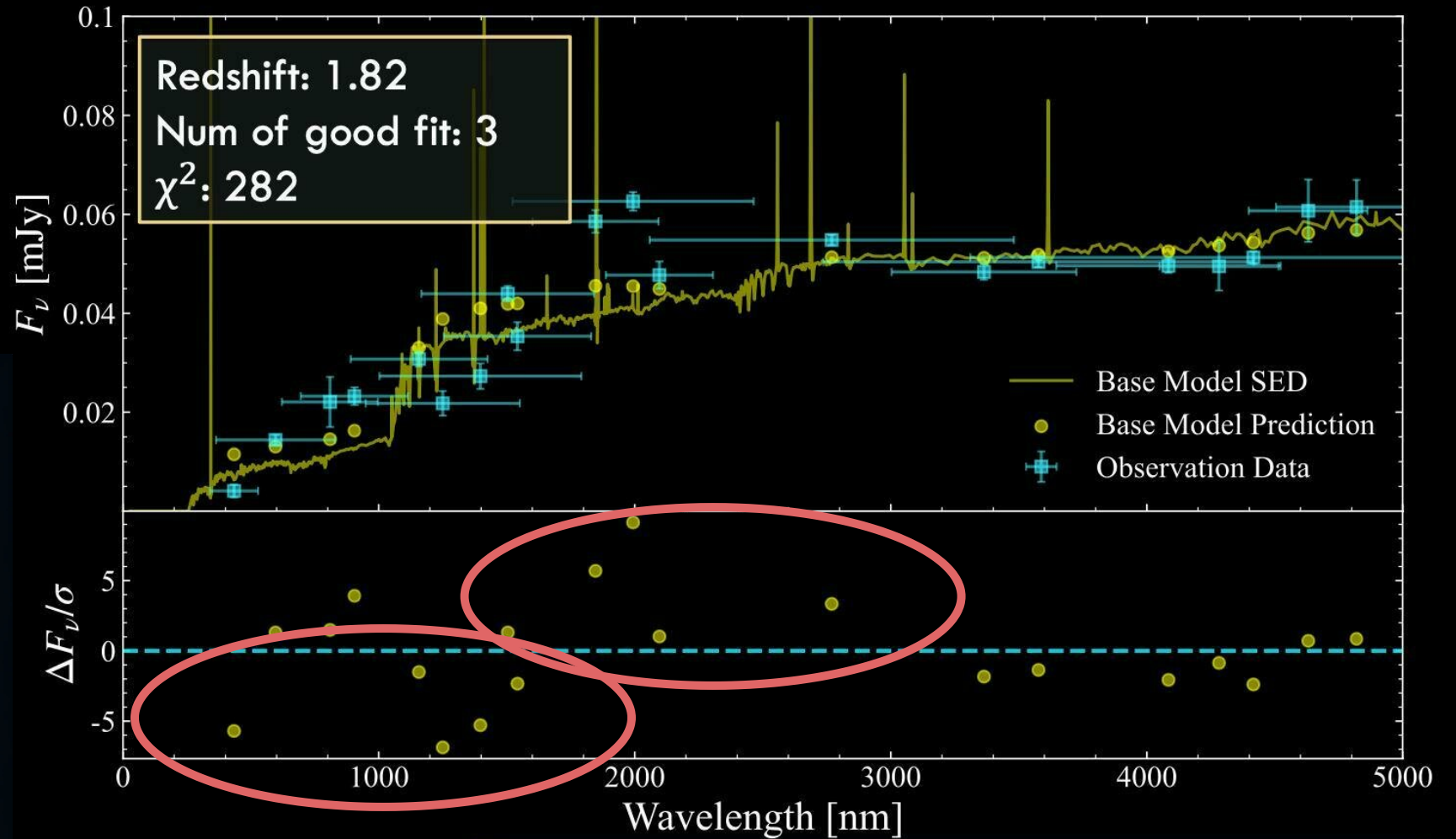
Action space is vast and transcends mathematical formalism

A default fit with
an SED model

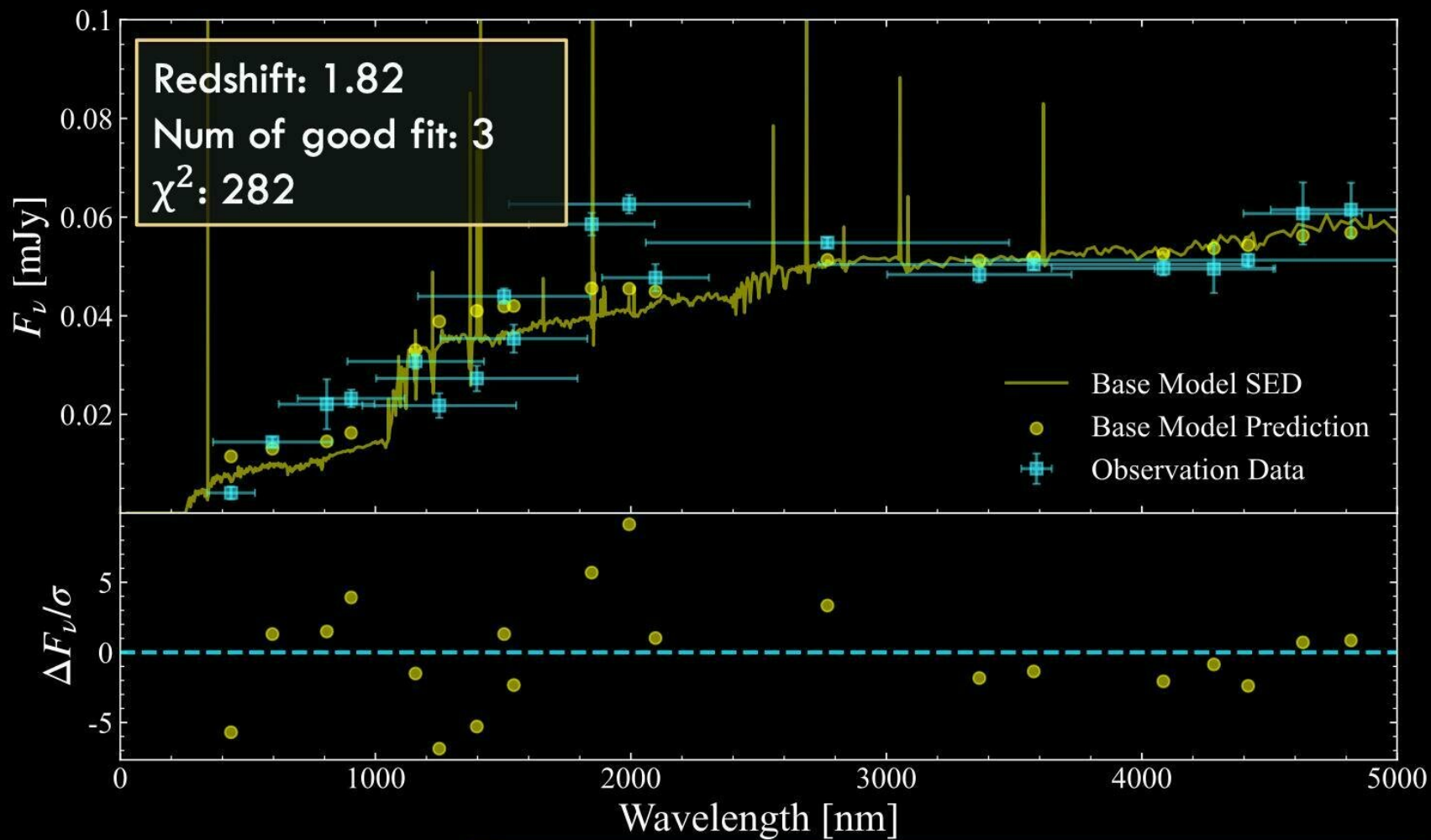


Action space is vast and transcends mathematical formalism

A default fit with an SED model

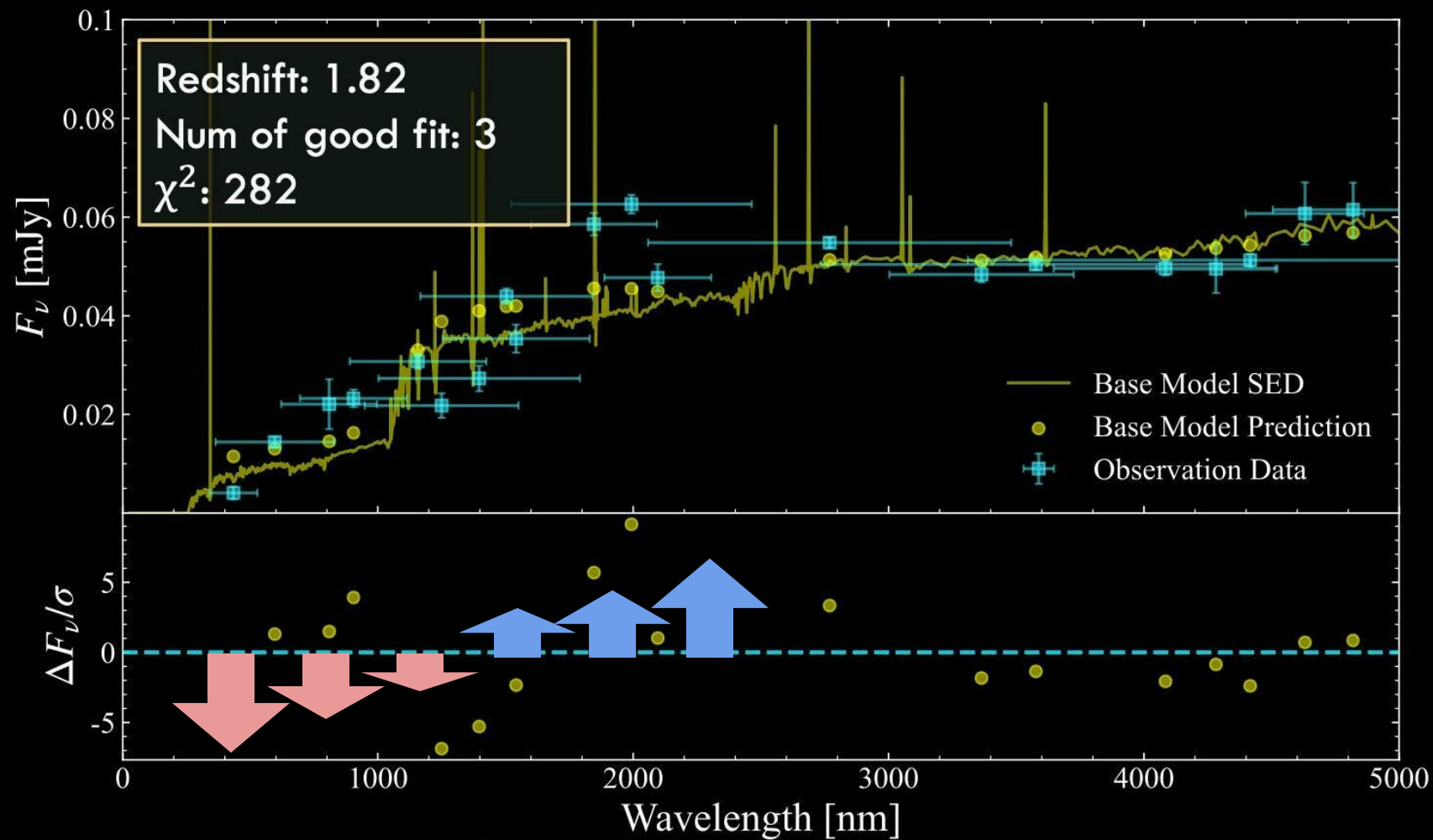


Action space is vast and transcends mathematical formalism



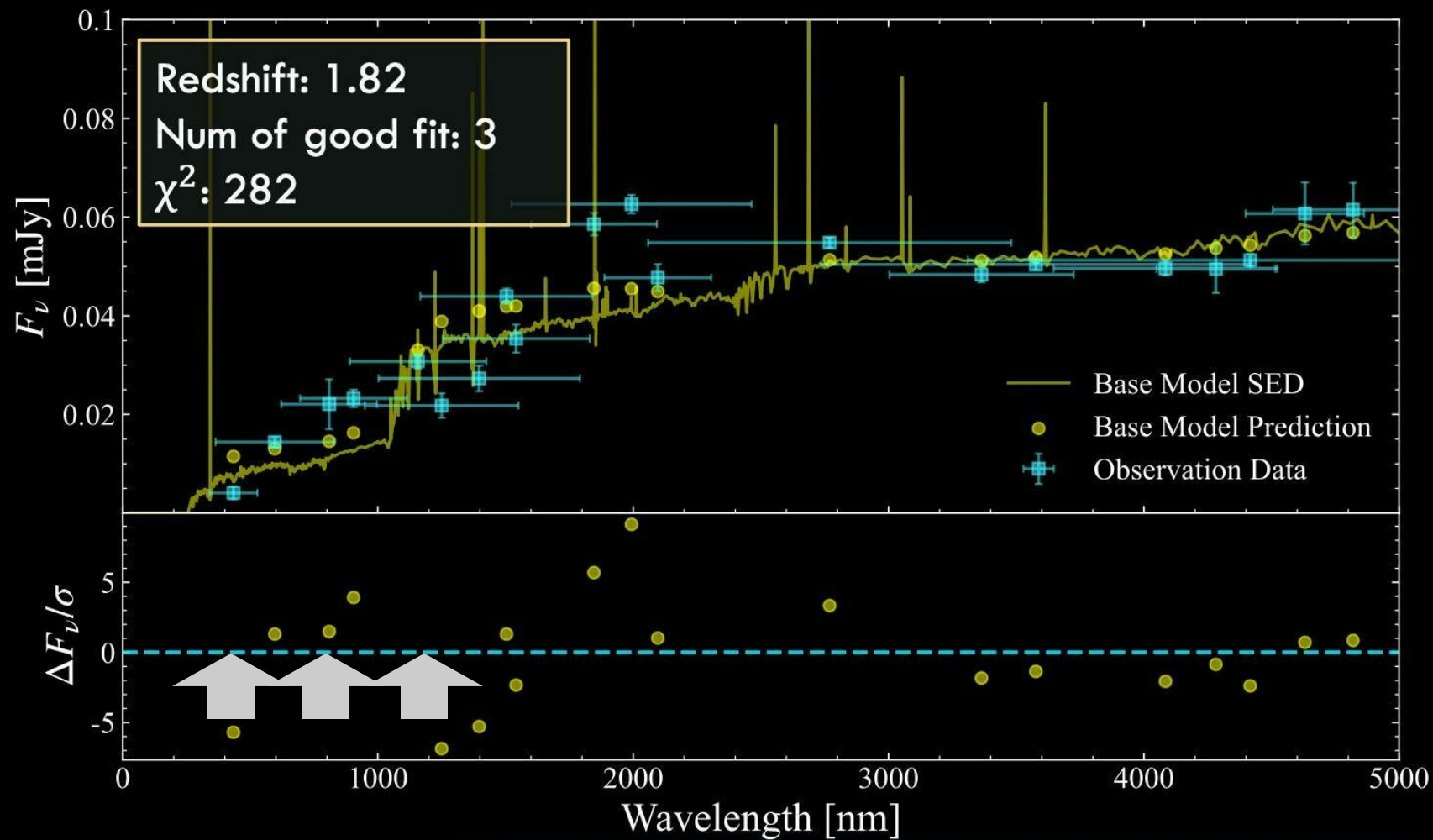
Action space is vast and transcends mathematical formalism

Extinction model ?



Action space is vast and transcends mathematical formalism

Young stellar population?



Many real-world projects lack a *mathematical* reward function

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- The objective goes beyond minimizing a single error metric.

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- Real-world action spaces are vast and hard to parameterize.

Many real-world projects lack a *mathematical* reward function

- The objective goes beyond minimizing a single error metric.
- Real-world action spaces are vast and hard to parameterize.
- Many tasks may require modifying assumptions / physical models, not just optimizing over all parameters

Can a large-language model learn
from *its own experience*?

Introducing OpenAI o1

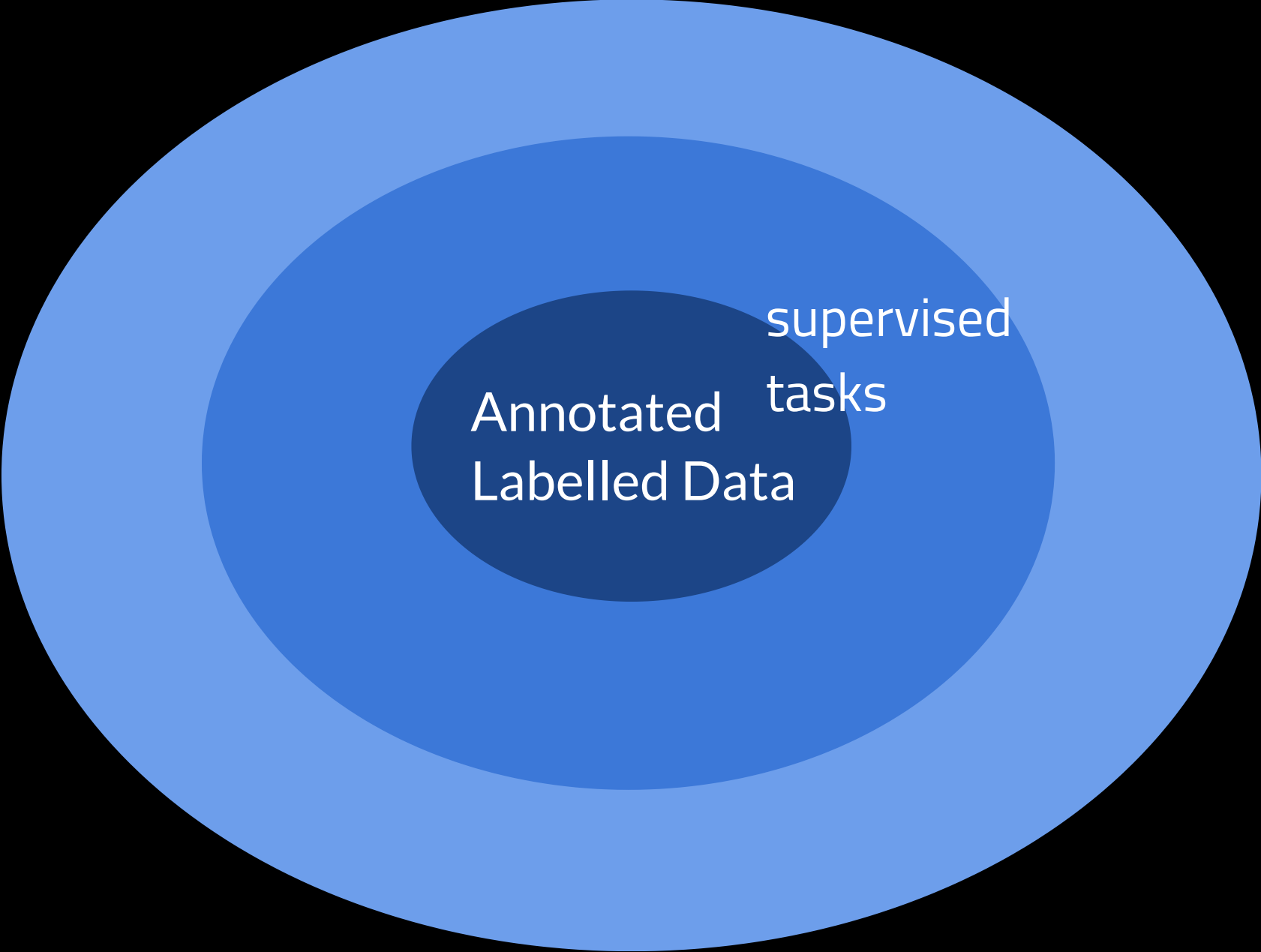
We've developed a new series of AI models designed to spend more time thinking before they respond. Here is the latest news on o1 research, product and other updates.

[Try it in ChatGPT Plus ↗](#)[Try it in the API ↗](#)[Sort ▼](#)

Self-Play Reinforcement Learning

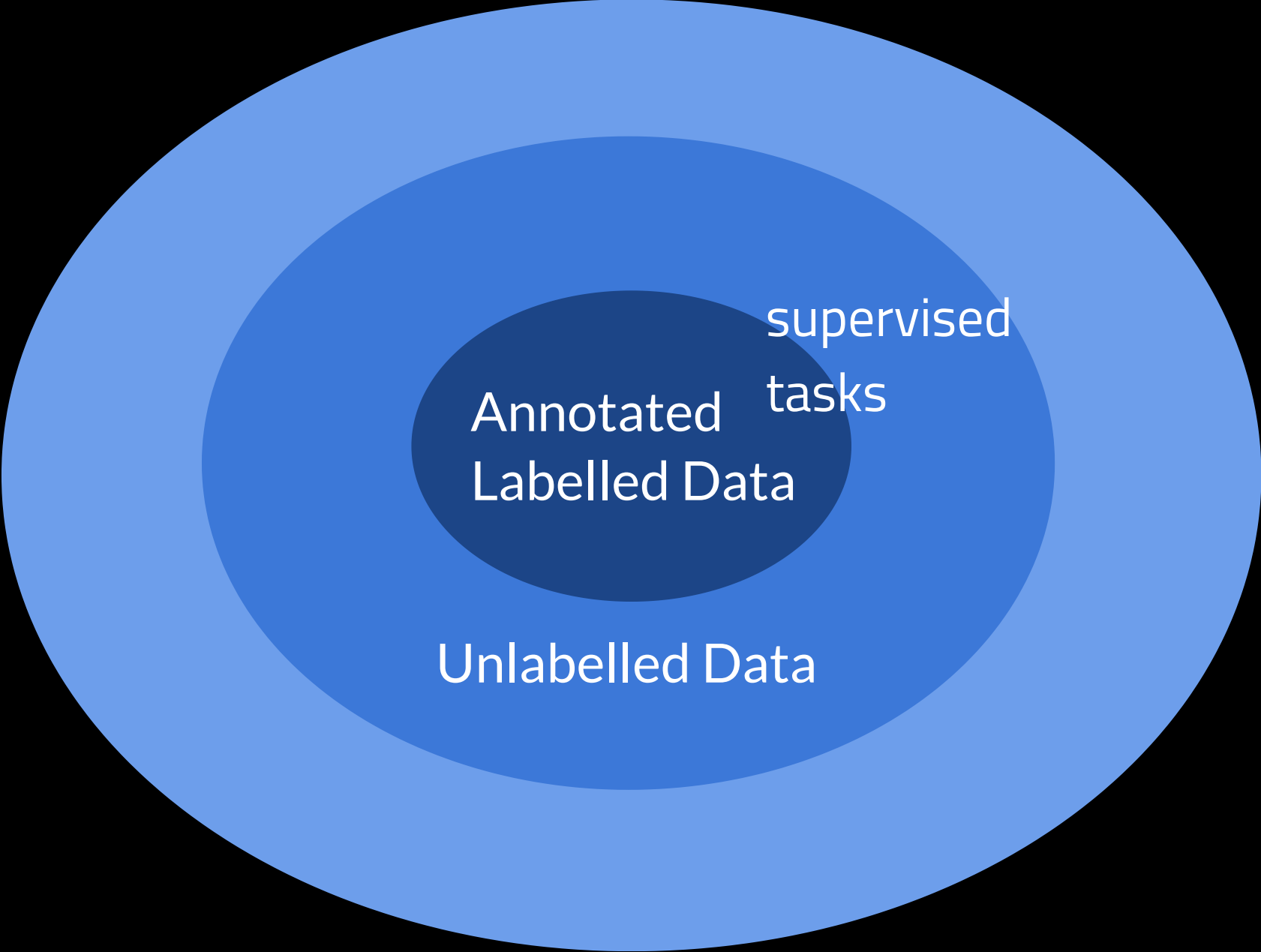


Annotated
Labelled Data



Annotated
Labelled Data

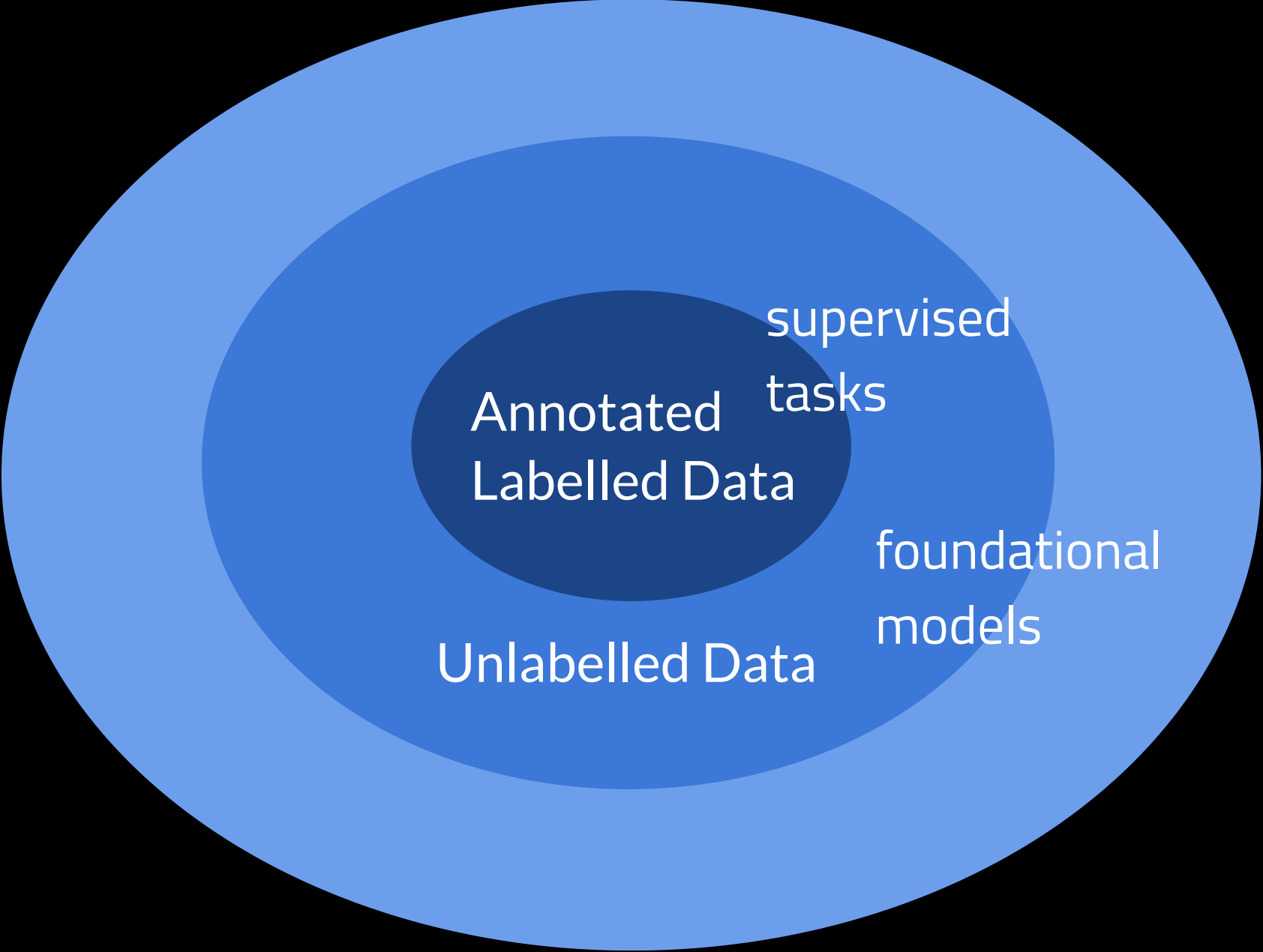
supervised
tasks



Annotated
Labelled Data

Unlabelled Data

supervised
tasks

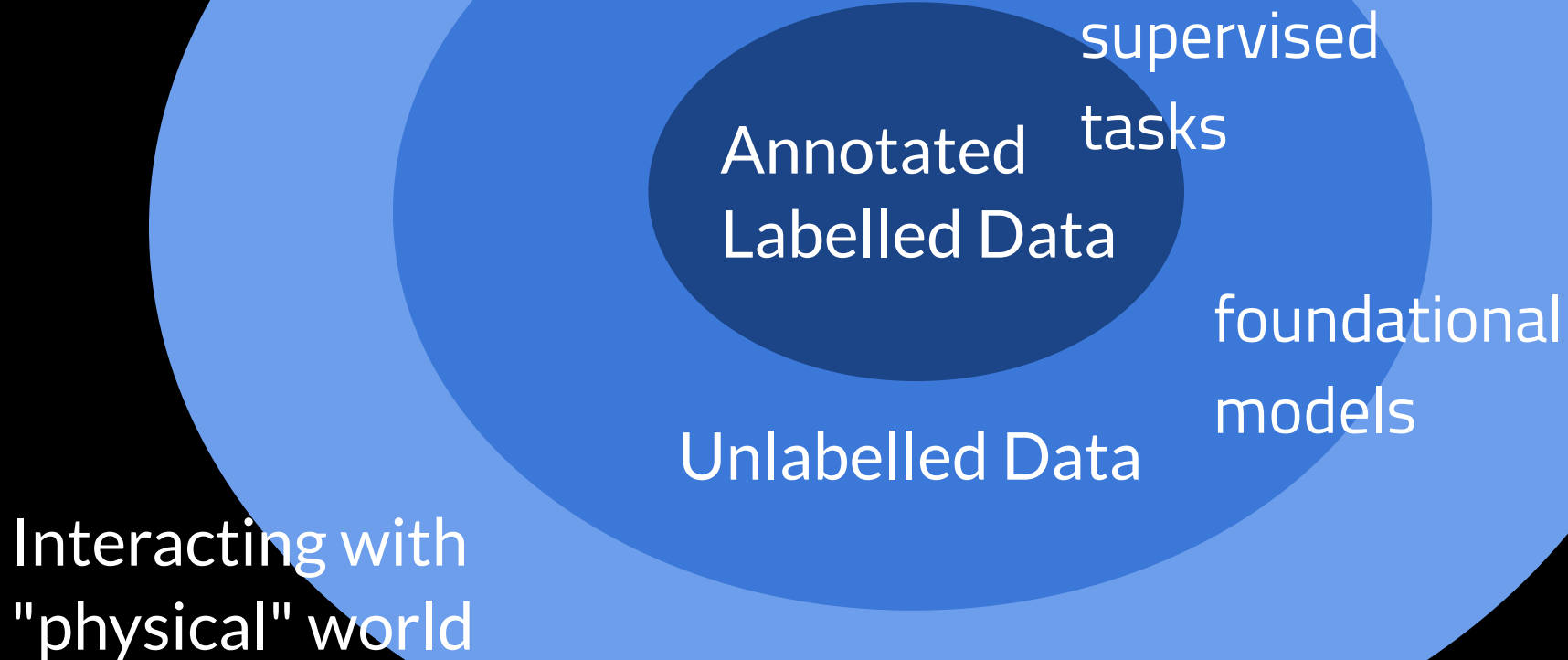


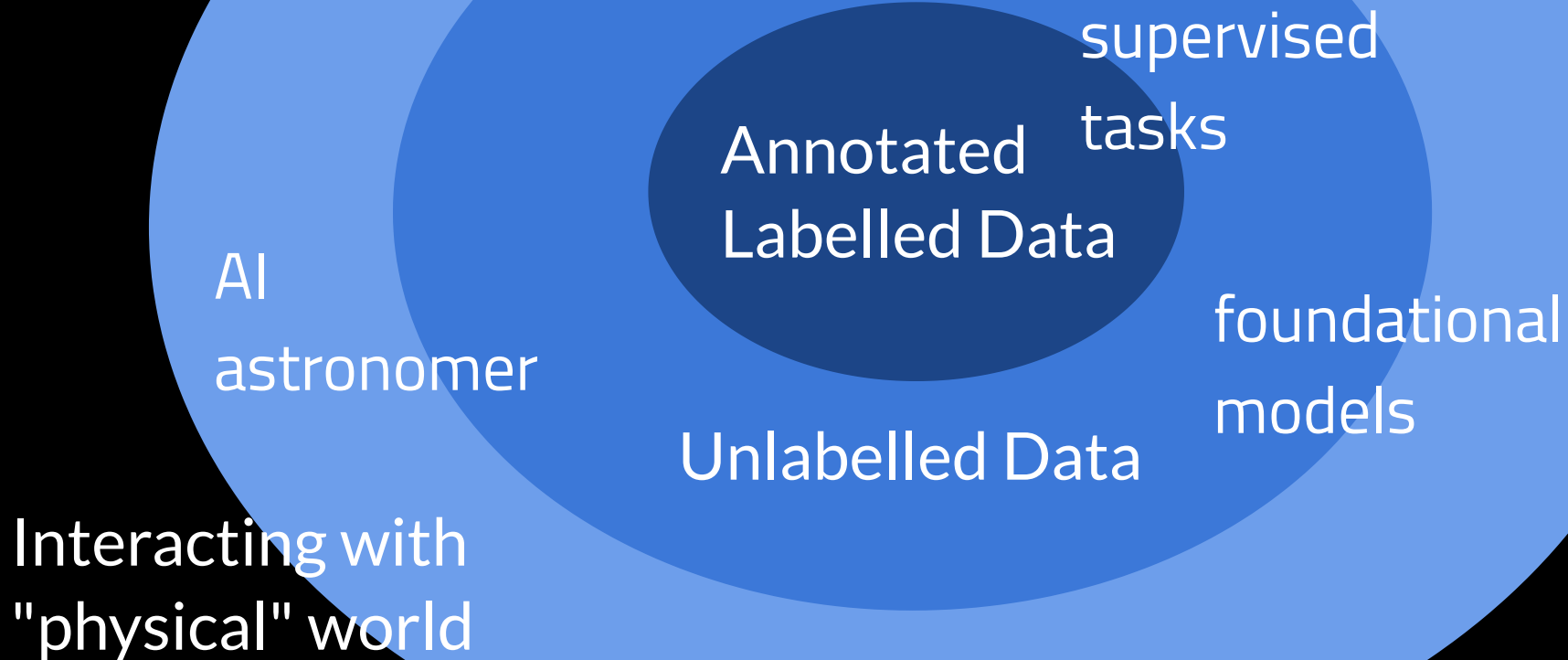
Annotated
Labelled Data

Unlabelled Data

supervised
tasks

foundational
models





Introducing *Mephisto**

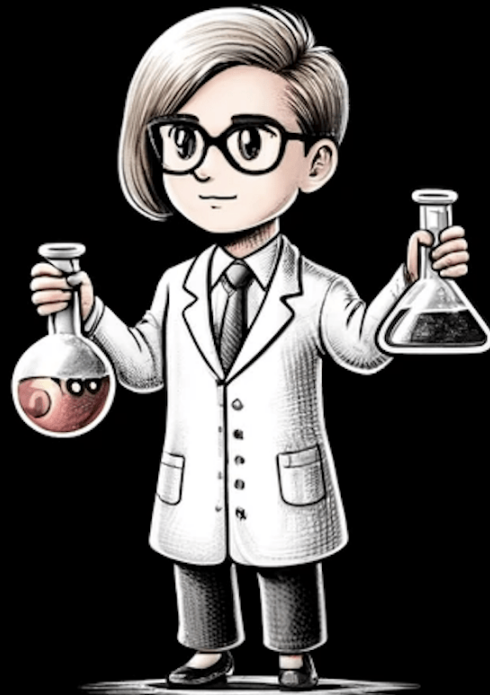


* In the classic tale of Faust, Mephisto is a demon who tempts the scholar Faust with *knowledge* and power in exchange for his soul.

A *collaboration* of multiple AI agents (LLM models)



Proposing actions



Execute actions



State evolution



Knowledge
distillation

A *collaboration* of multiple AI agents (LLM models)



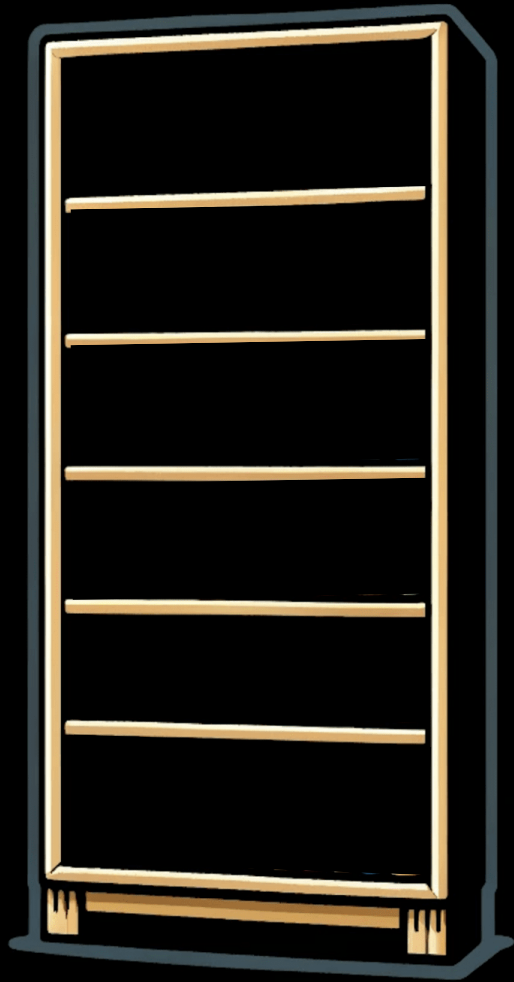
Proposing actions

Execute actions

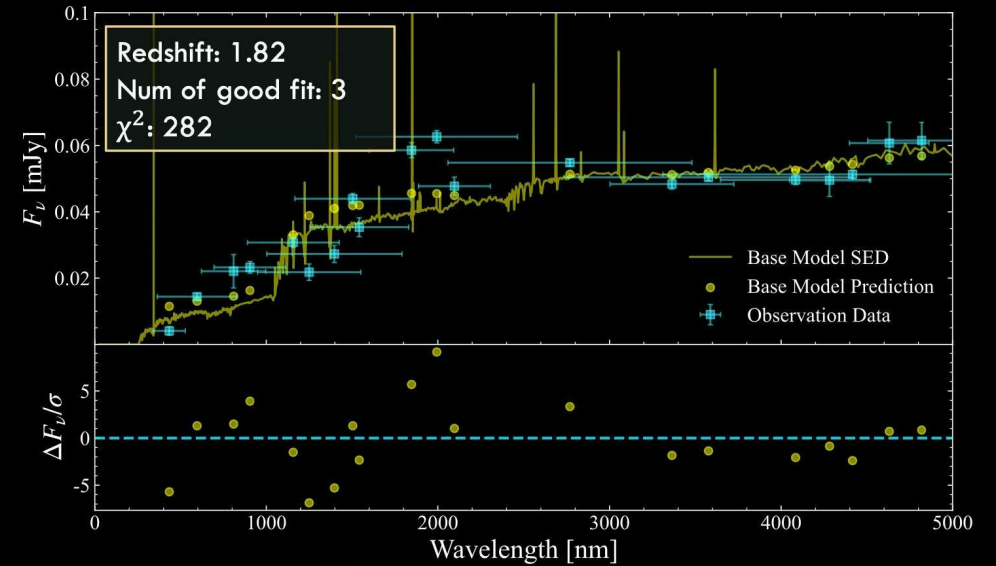
State evolution

Knowledge
distillation

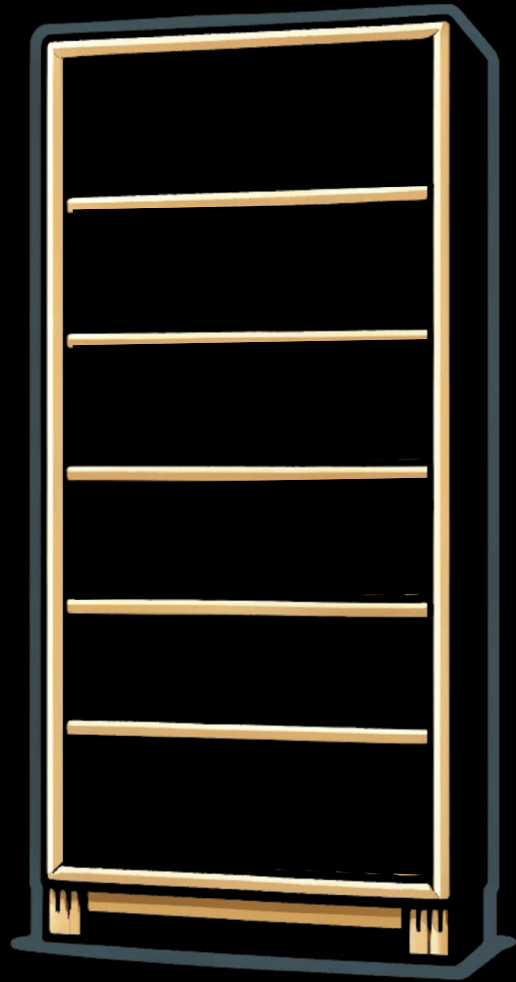
Enabling AI to collect "*knowledge*" through exploration



Knowledge base



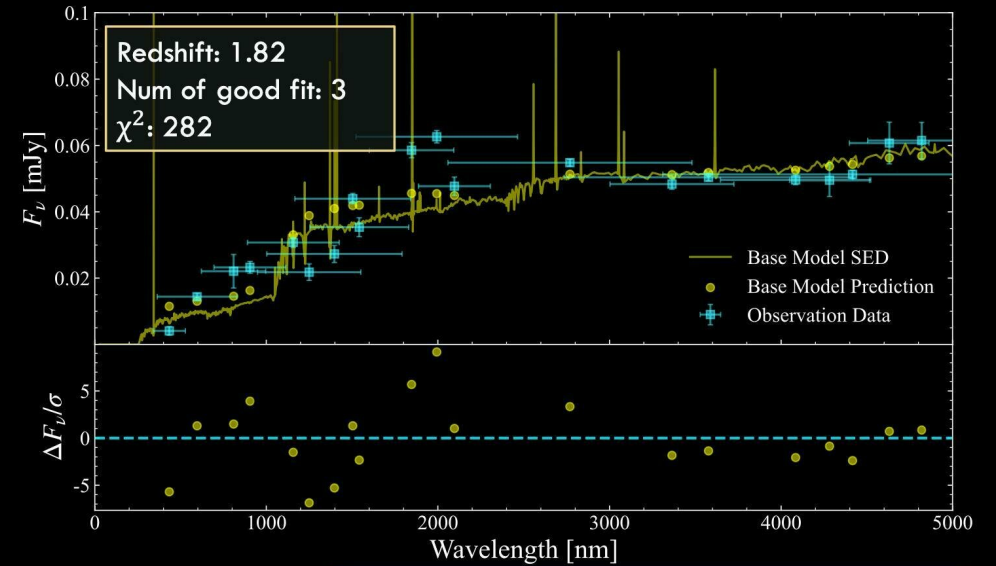
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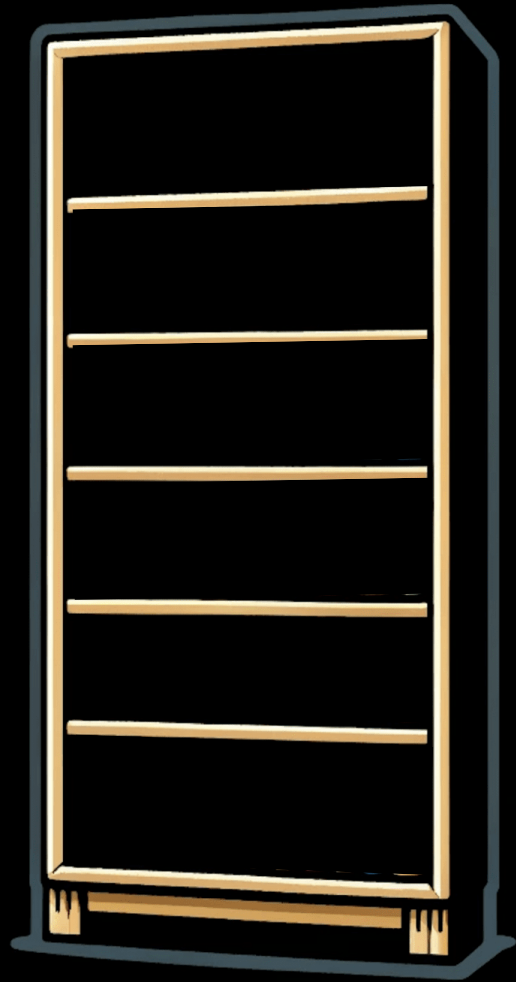
Knowledge base



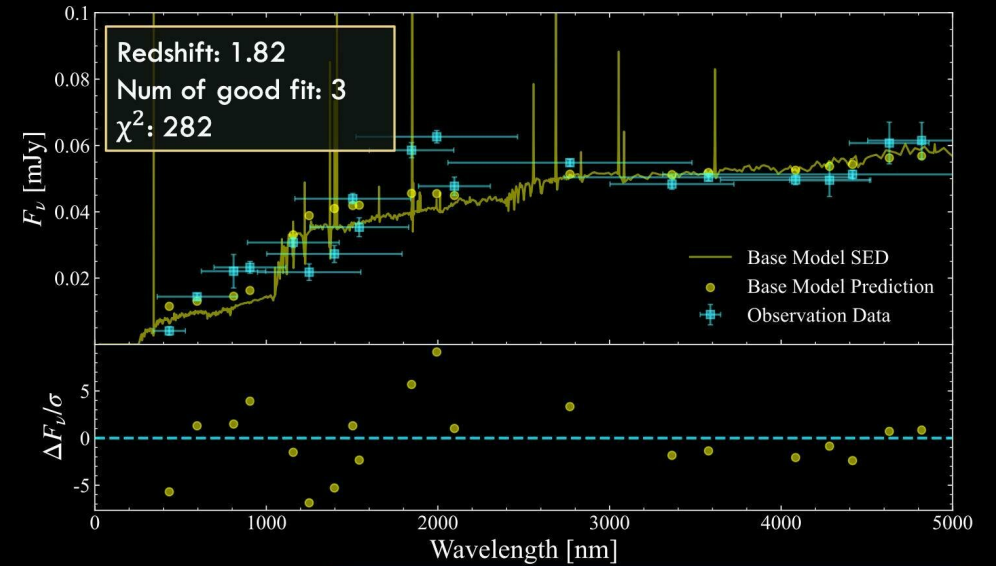
Proposing Actions - e.g., different physical models / parameter range



Enabling AI to collect "*knowledge*" through exploration

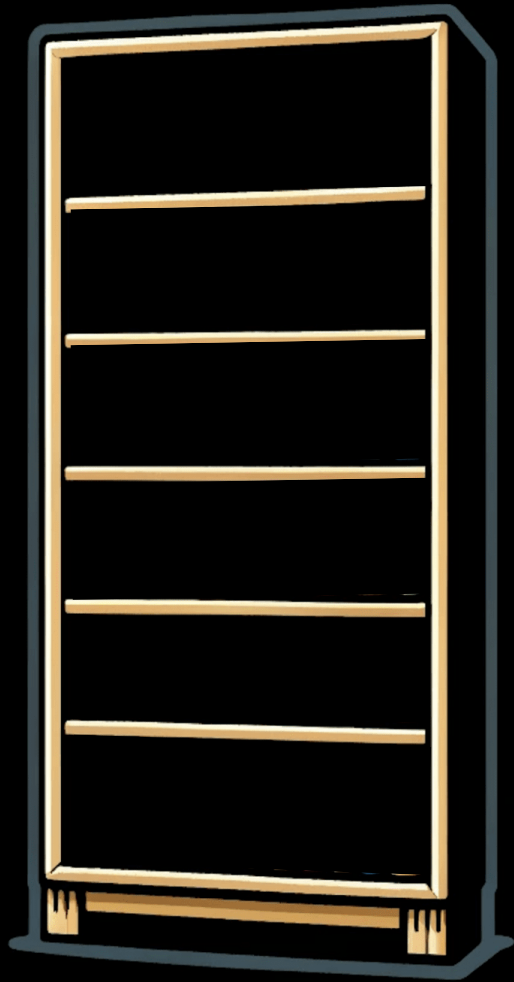


Knowledge base

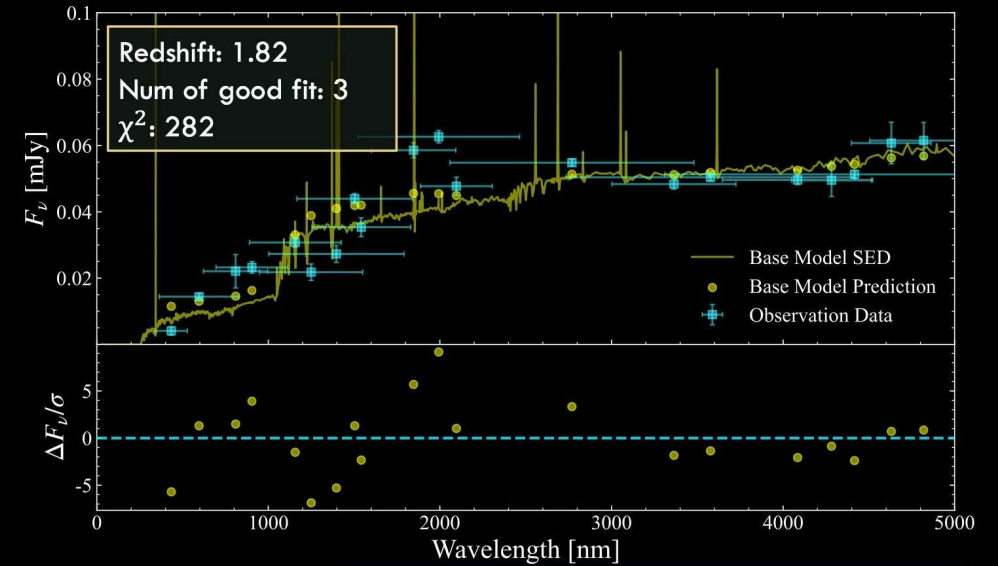
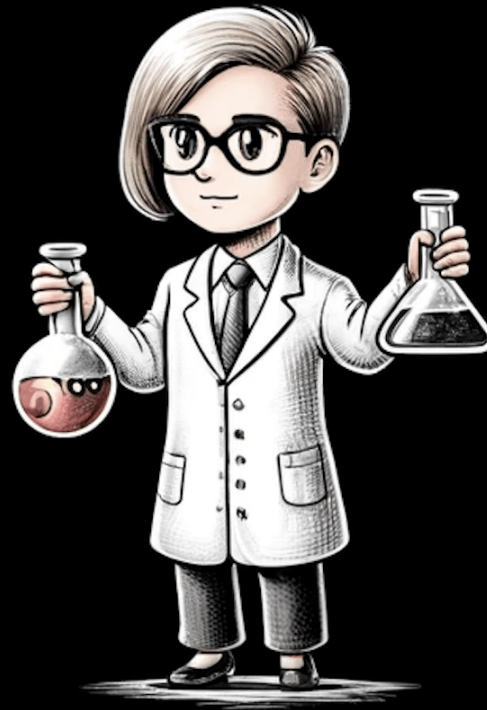


Proposing Actions - e.g., different physical models / parameter range

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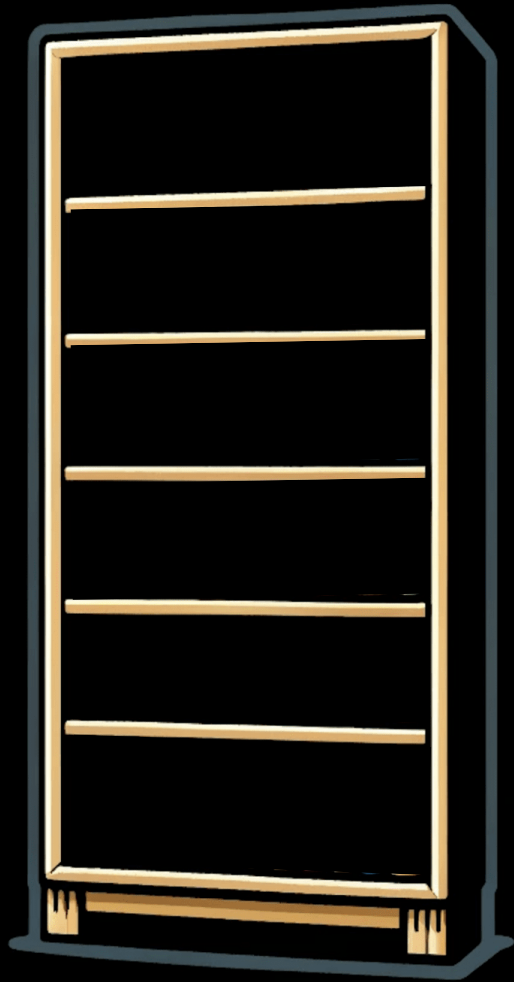


Knowledge base

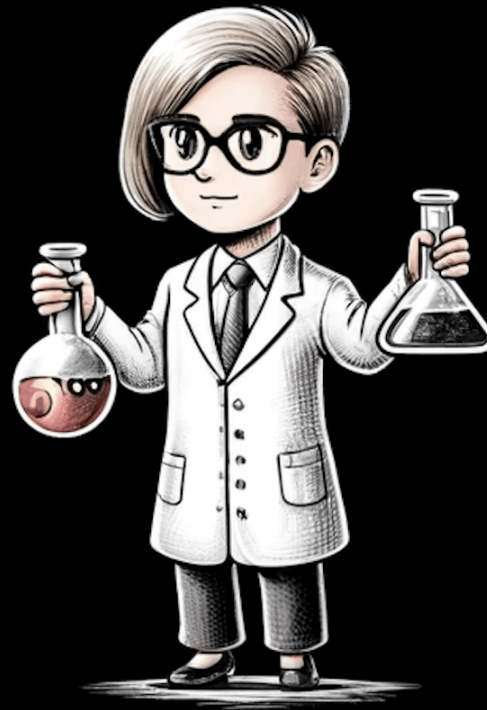


Execute Actions - write configuration files, run the codes, autonomously

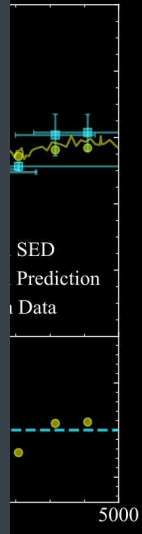
Enabling AI to collect "*knowledge*" through exploration



Knowledge base



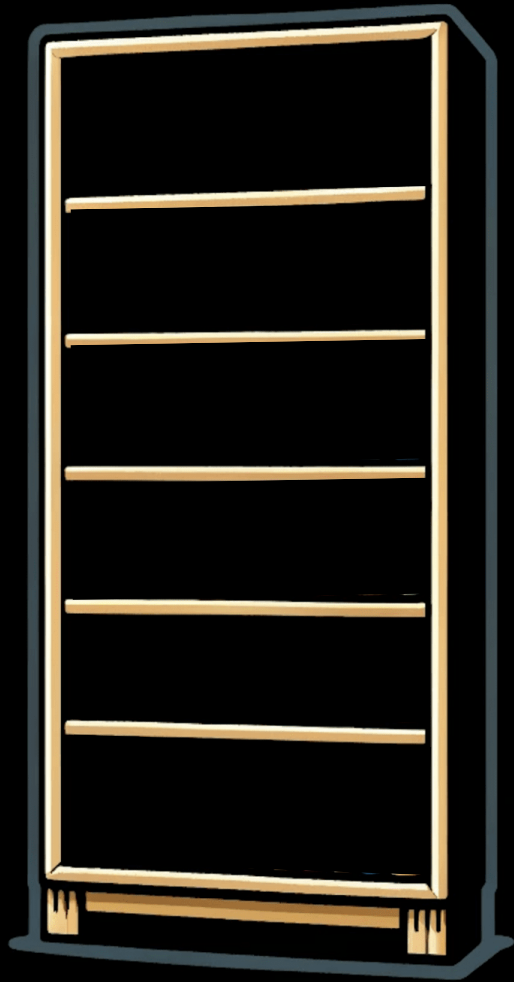
```
25
26 def check_db():
27     if not os.path.isfile(FILE_URI):
28         db.create_all()
29
30 @app.route("/")
31 def home():
32     check_db()
33     all_books = db.session.query(Book).all()
34     return render_template("index.html", books=all_books)
35
36 @app.route("/edit", methods=["GET", "POST"])
37 def edit():
38
39     if request.method == "POST":
40         book_id = request.form["id"]
41         book_to_update = Book.query.get(book_id)
42         book_to_update.rating = request.form["rating"]
43         db.session.commit()
44         return redirect(url_for("home"))
```



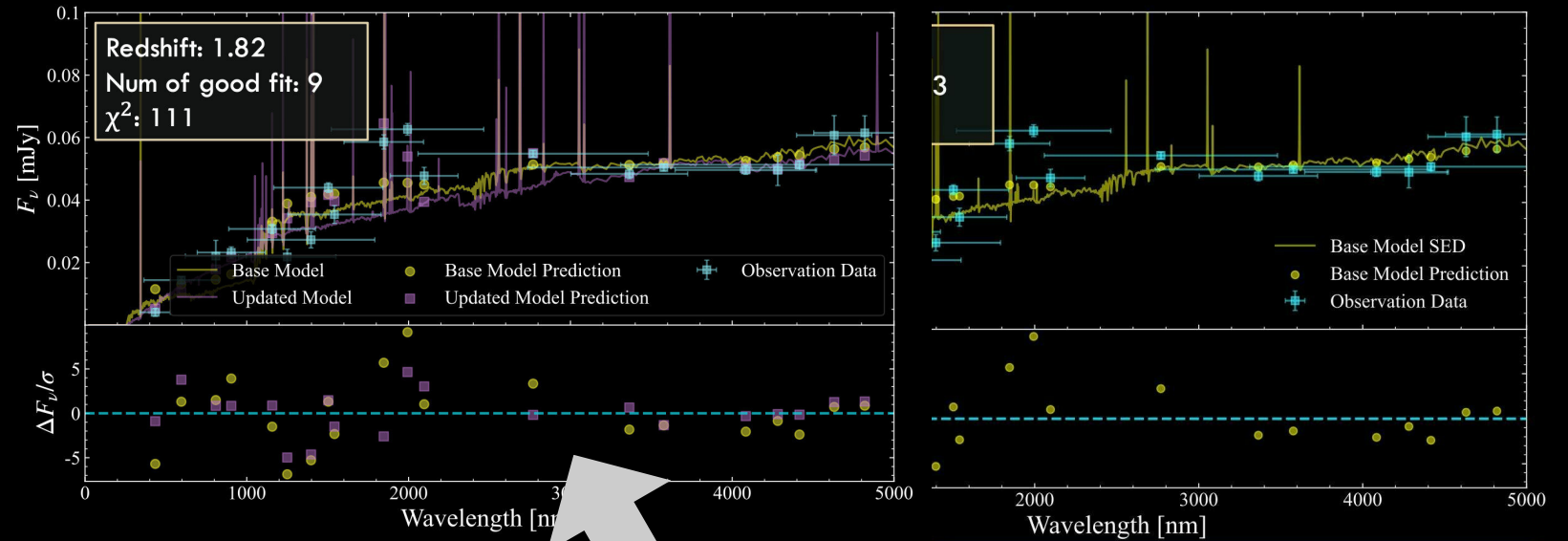
- 1
- 2
- 3
- 4

Execute Actions - write configuration files, run the codes, autonomously

Enabling AI to collect "*knowledge*" through exploration

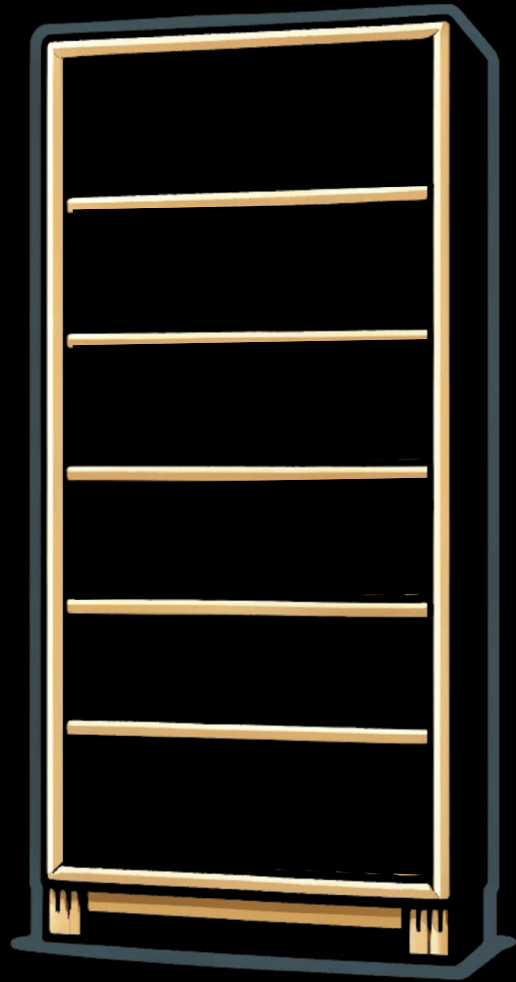


Knowledge base

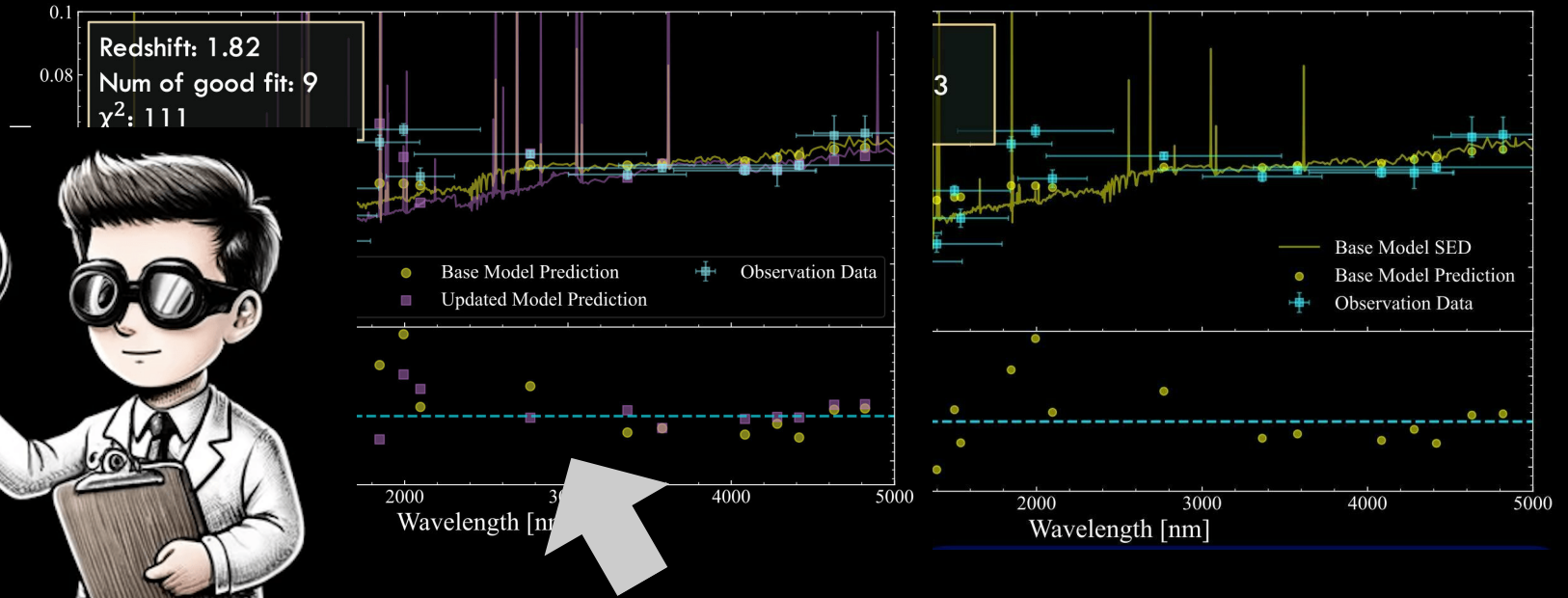


- 1
- 2
- 3
- 4

Enabling AI to collect "*knowledge*" through exploration



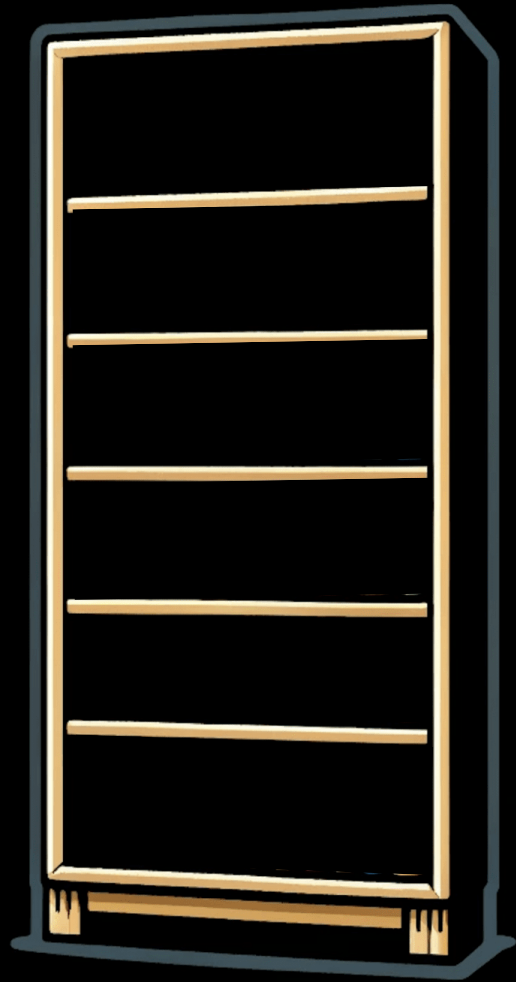
Knowledge base



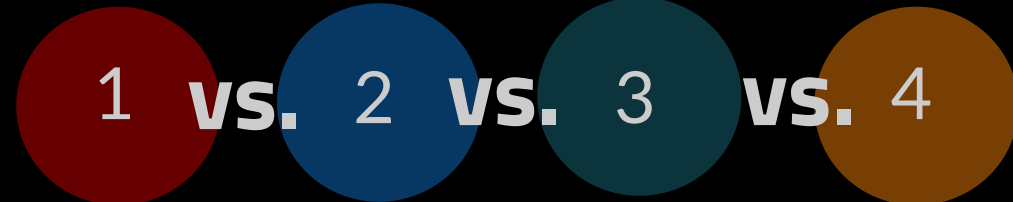
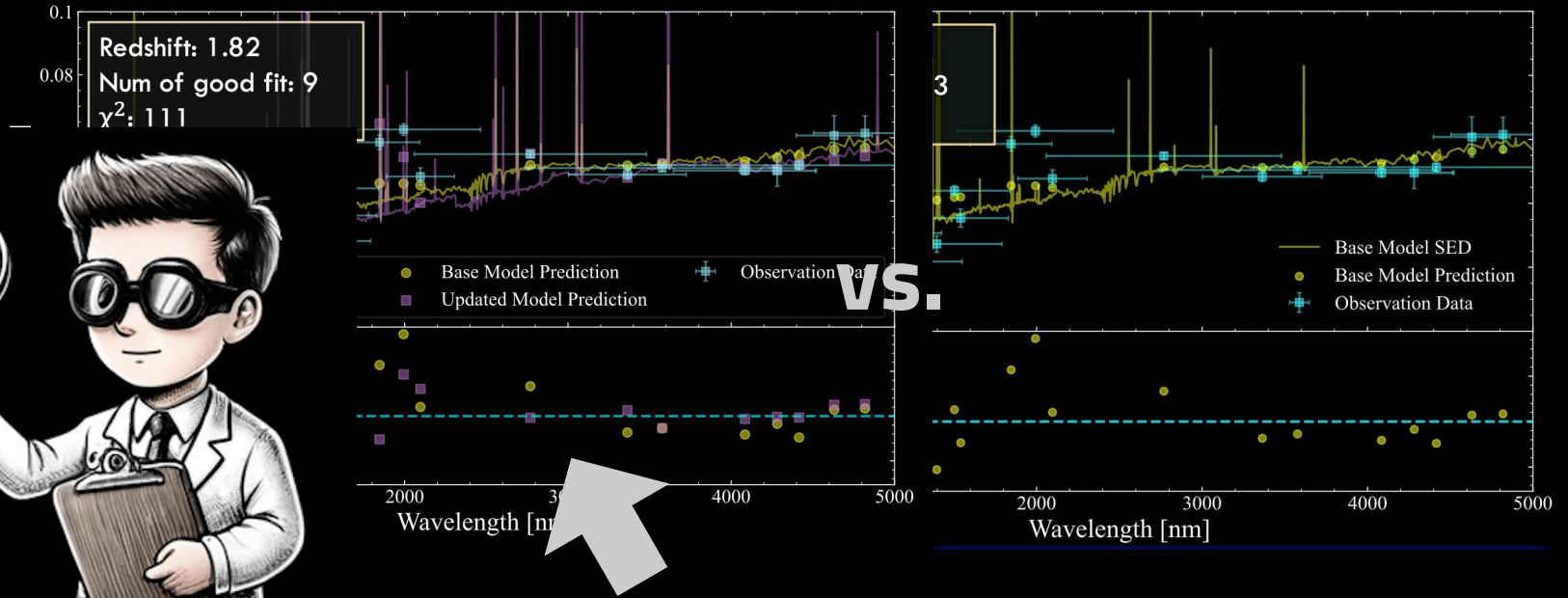
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State Evaluation - evaluate the results (beyond a single error metric)

Enabling AI to collect "*knowledge*" through exploration

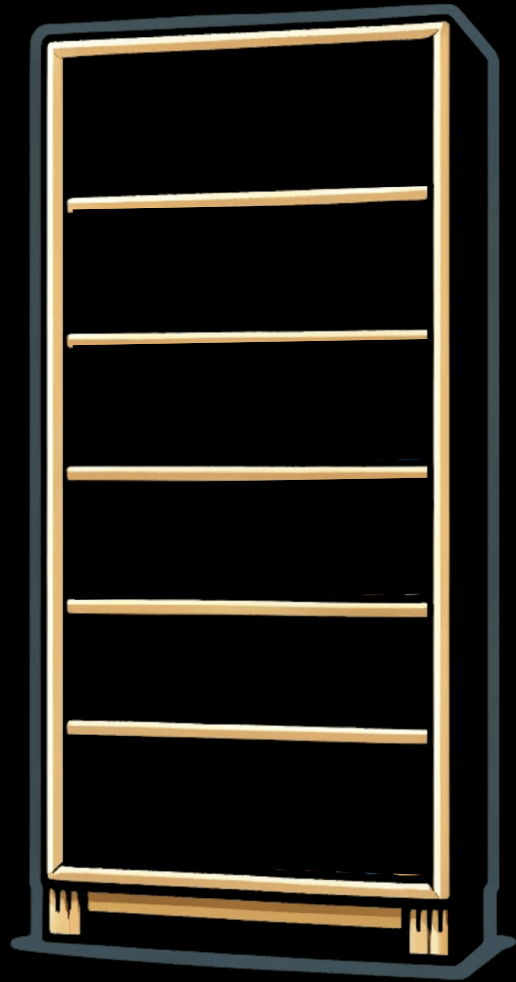


Knowledge base



State Evaluation - evaluate the results (beyond a single error metric)

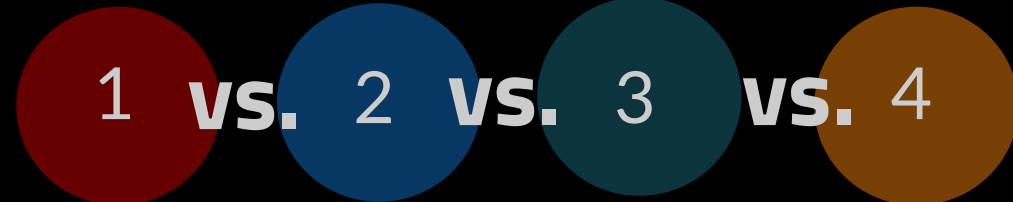
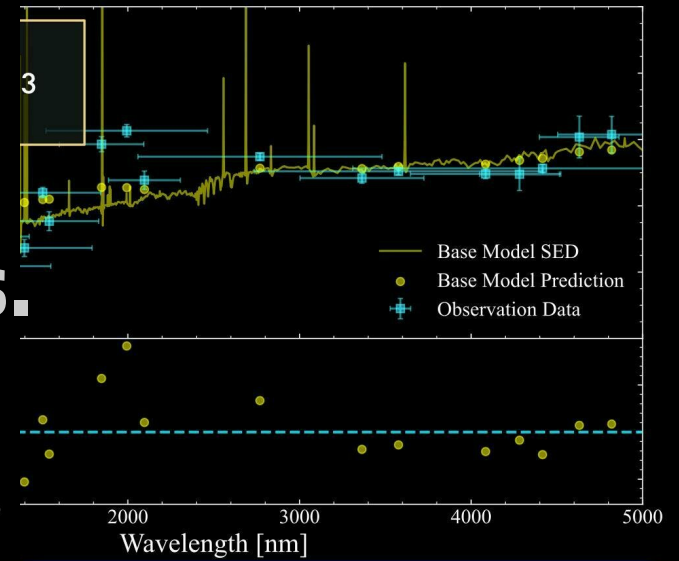
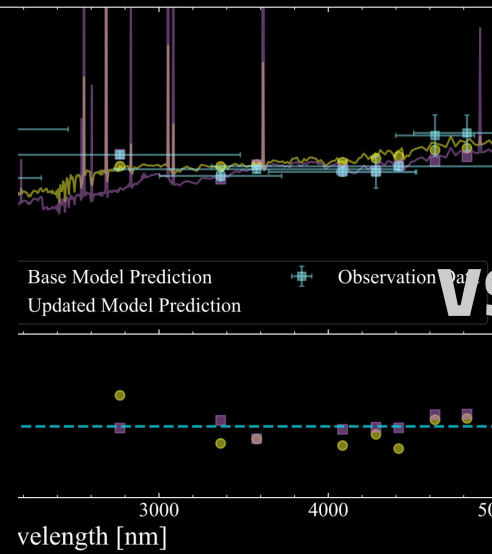
Enabling AI to collect "*knowledge*" through exploration



Knowledge base

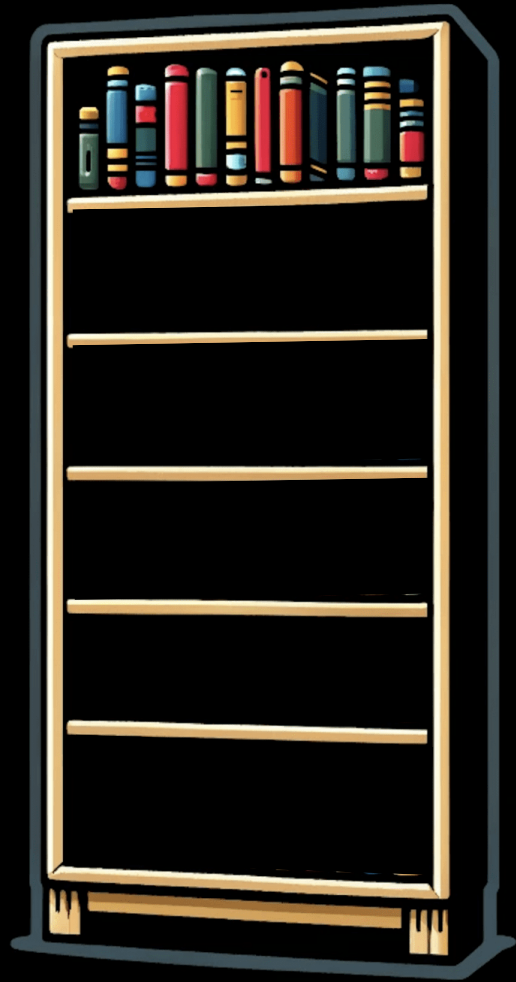


Redshift: 1.82
Num of good fit: 9



Knowledge Distillation - summarise useful actions given the previous state

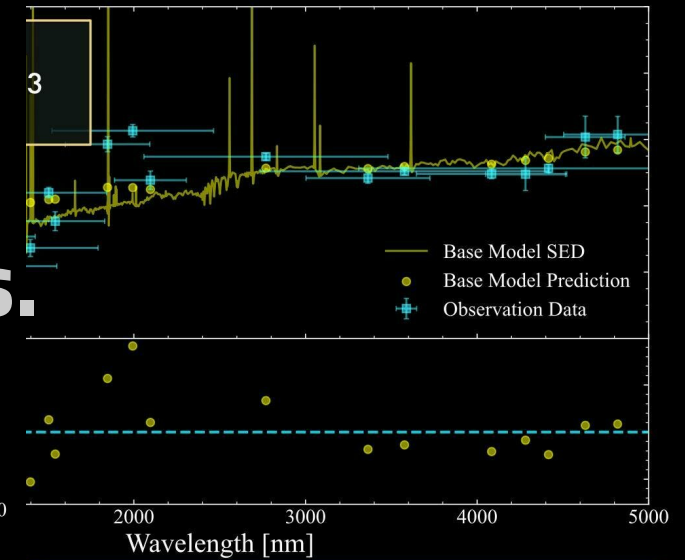
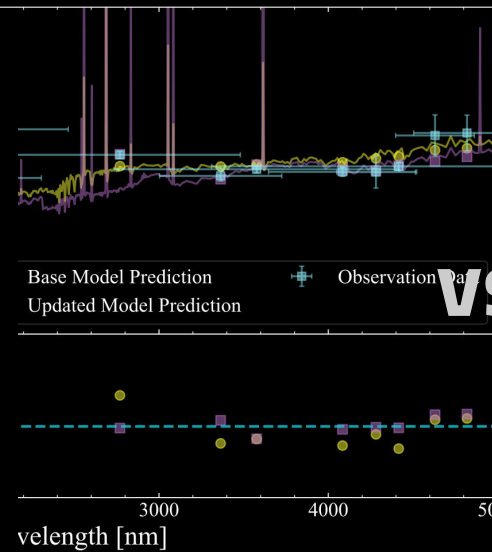
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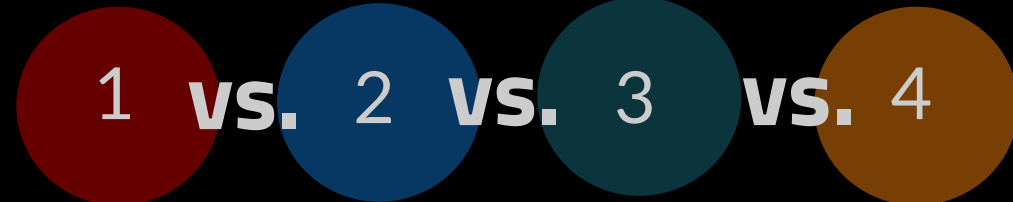
Knowledge base



Redshift: 1.82
Num of good fit: 9



vs.



Knowledge Distillation - summarise useful actions given the previous state

Example of learned "knowledge"

Example of learned "knowledge"

" If the fit is *overestimated in the UV and optical* bands,

Example of learned "knowledge"

" If the fit is *overestimated in the UV and optical* bands,

increasing the E_{BV_lines} parameter may lead to a better fit by accounting for more *dust attenuation* in these bands. "



Example of learned "knowledge"

Example of learned "knowledge"

" If there is a gross *underestimation in the MWIR bands,*

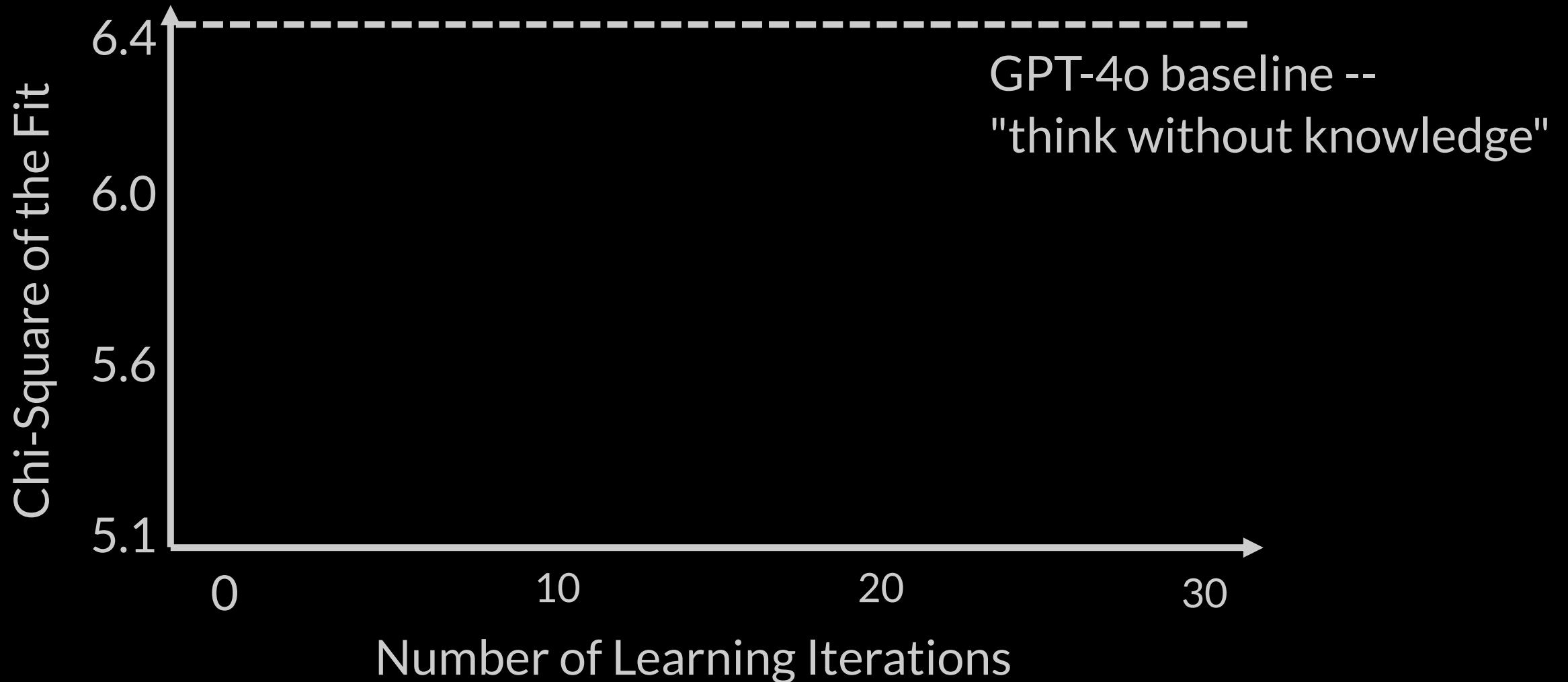
Example of learned "knowledge"

" If there is a gross *underestimation in the MWIR bands*,

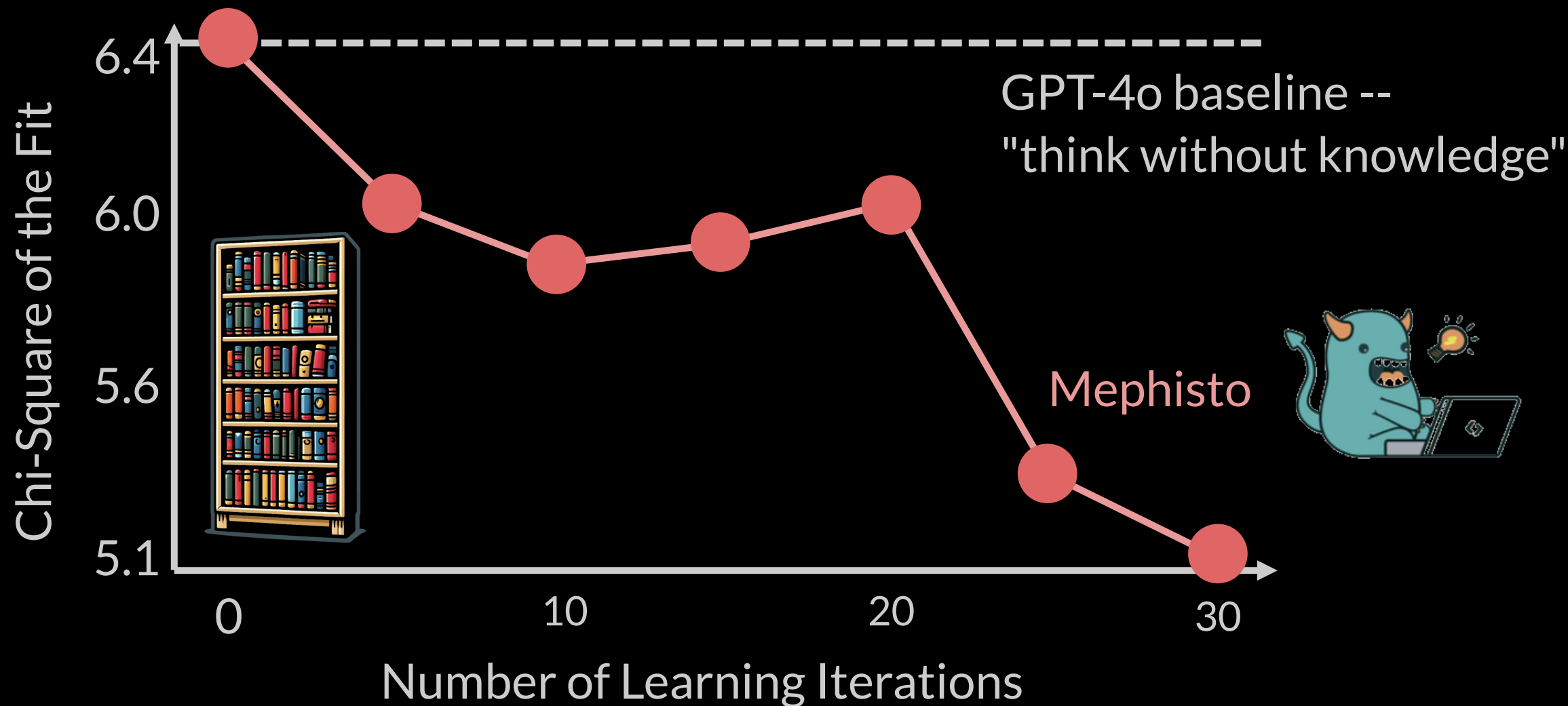


consider exploring a wider range of *fracAGN values* in the agn module to improve the fit in these bands "

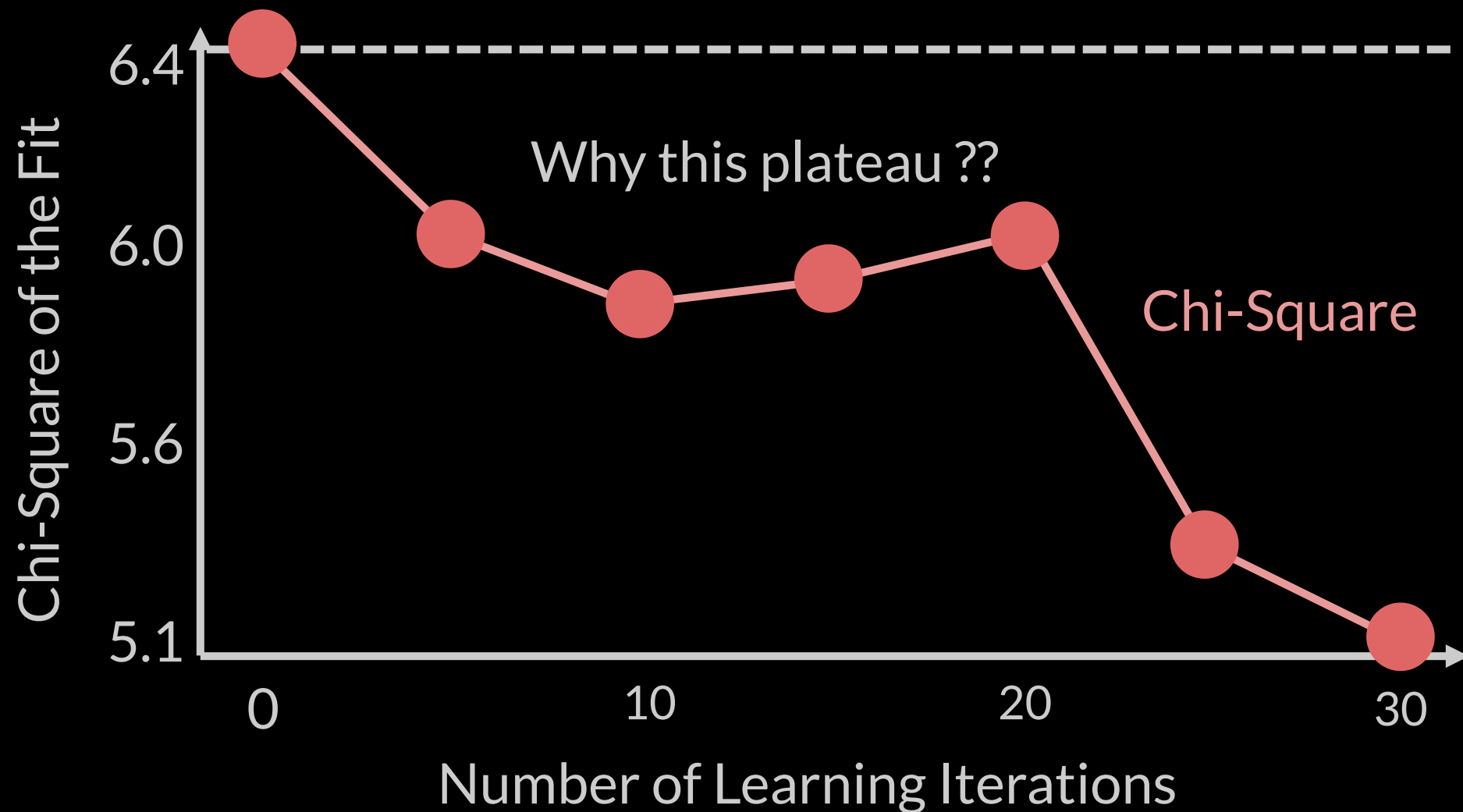
LLMs with self-play RL *outperforms* native LLMs



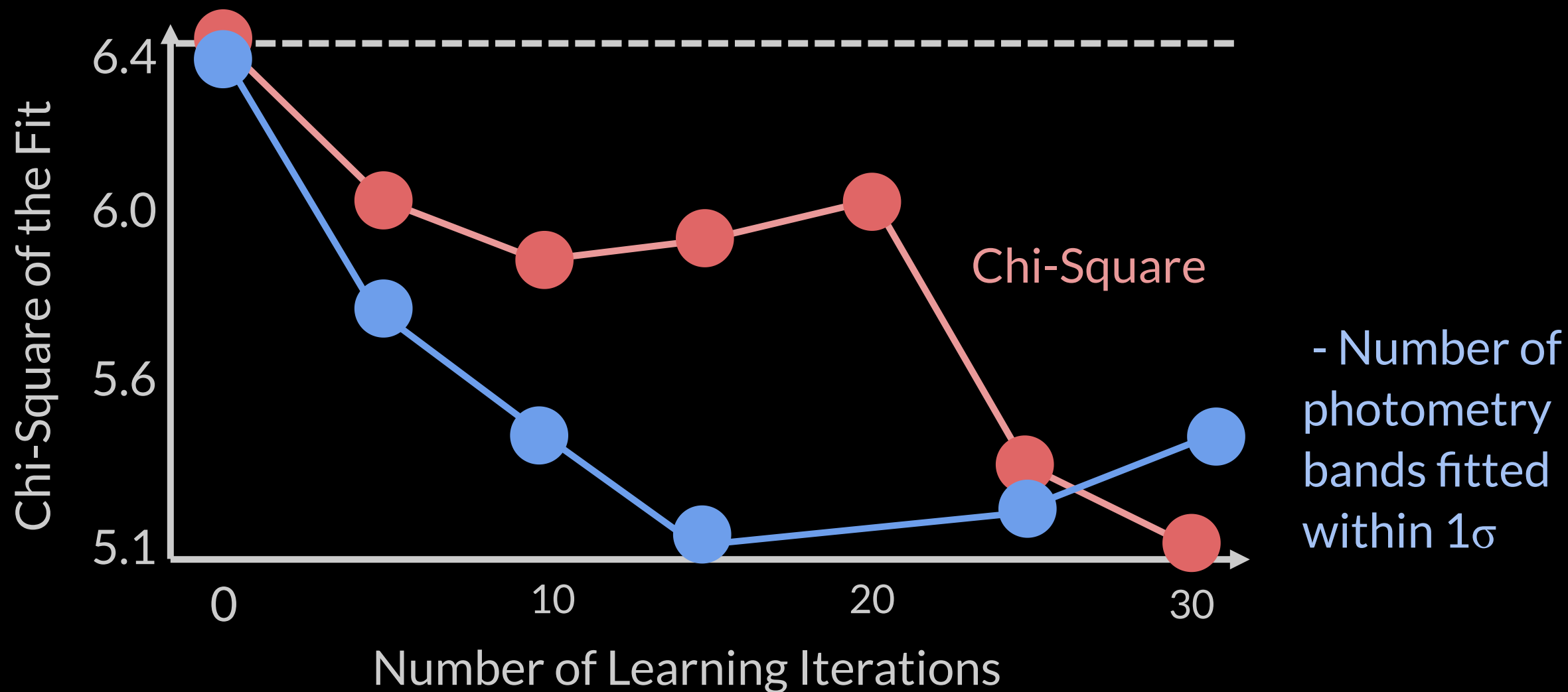
LLMs with self-play RL *outperforms* native LLMs



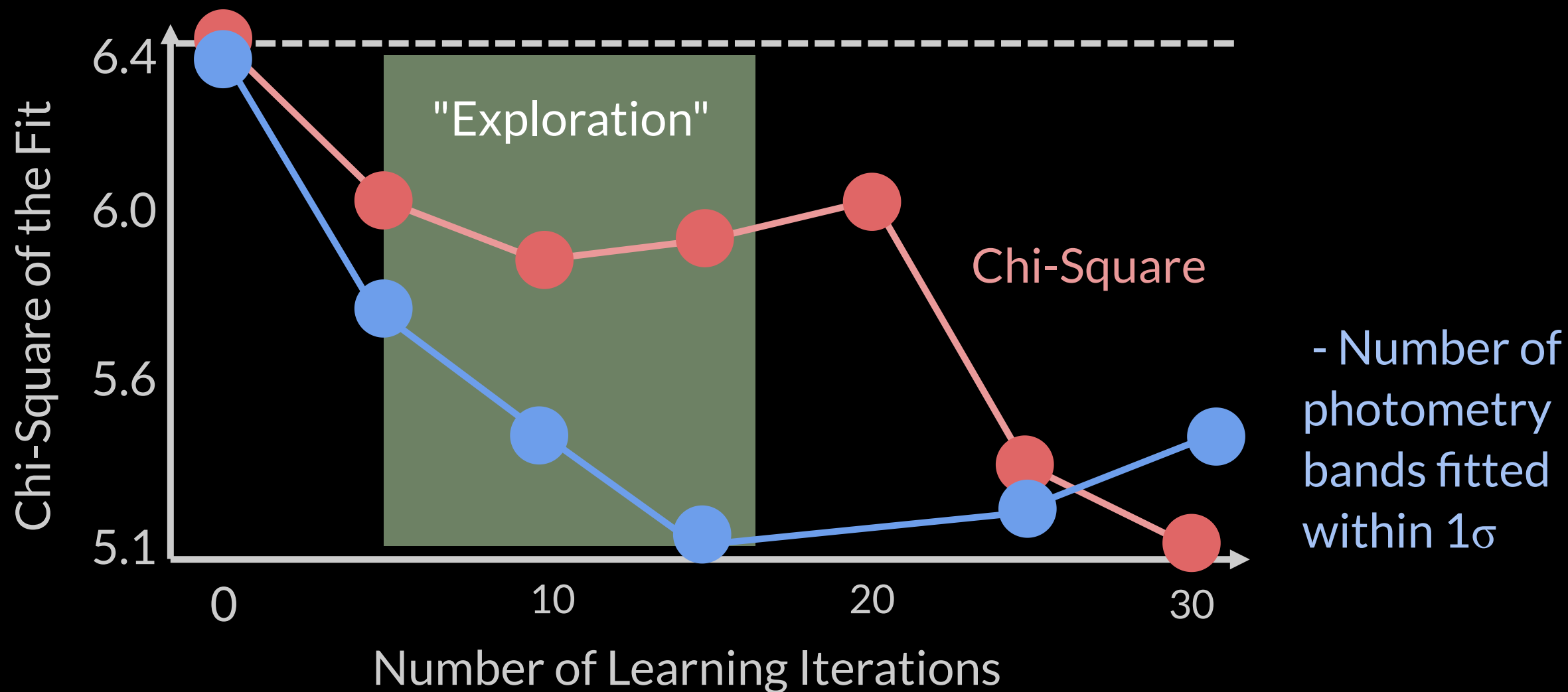
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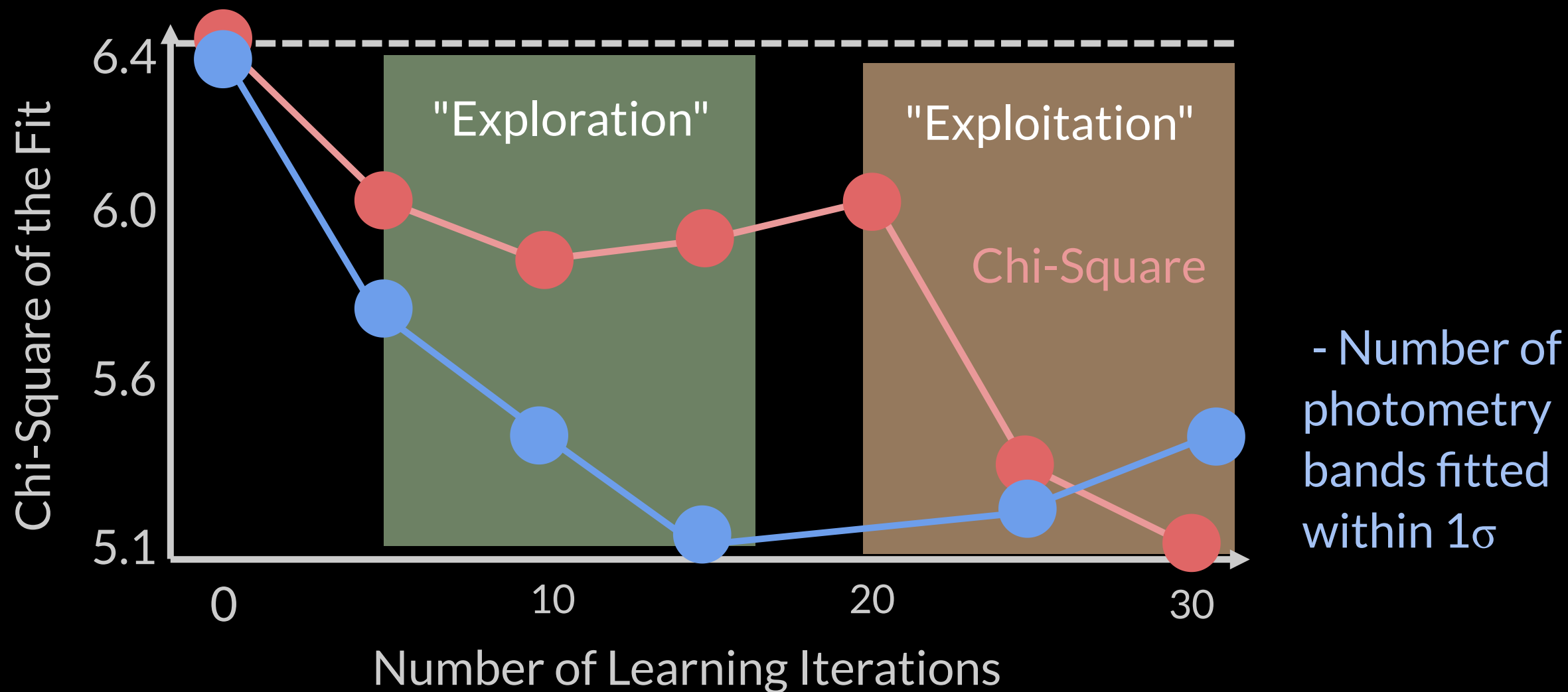
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LLMs with self-play RL *outperforms* native LLMs



LLMs with self-play RL *outperforms* native LLMs

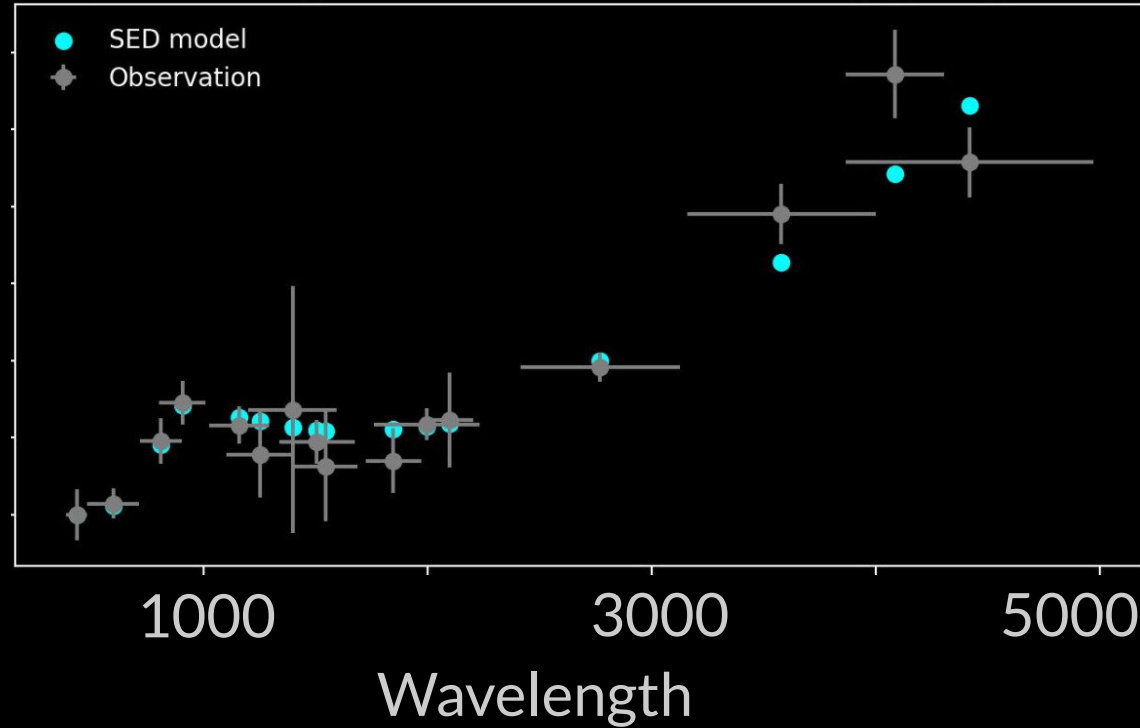
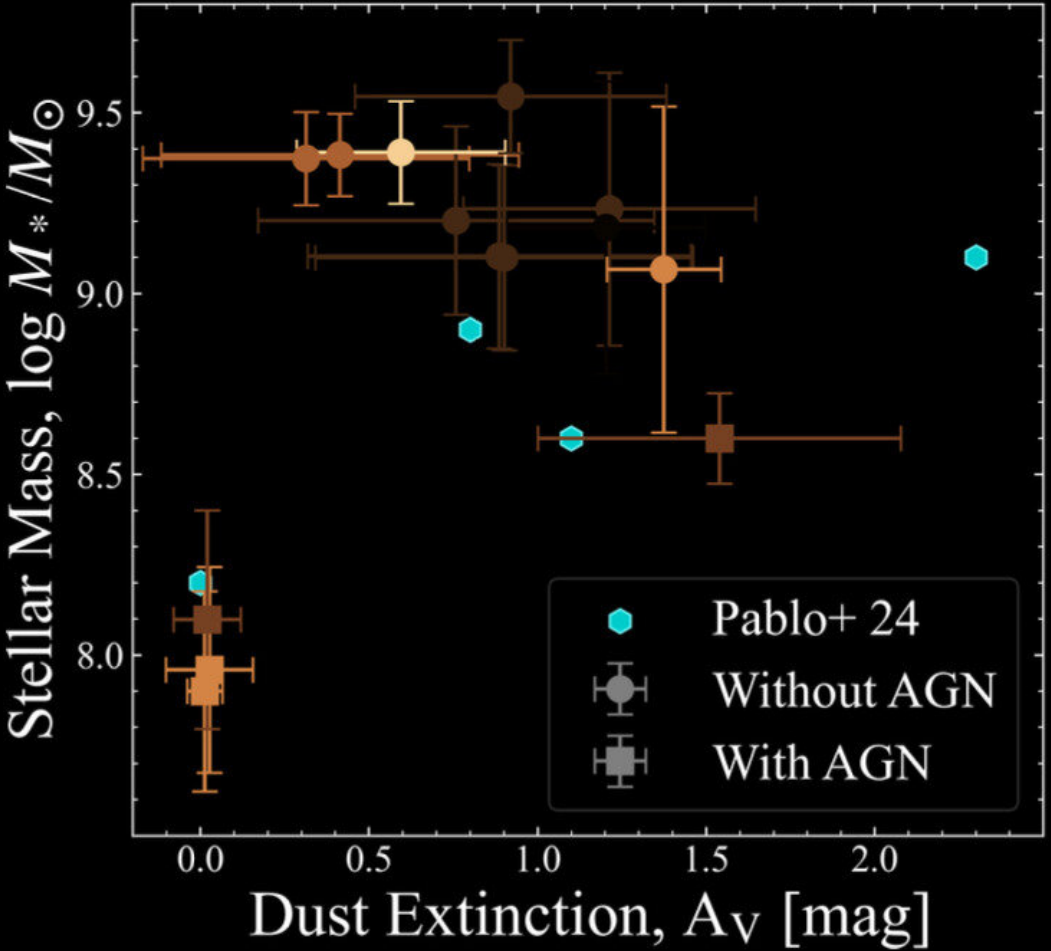


LLMs can reach *human-level reasoning* for specific astronomy analysis tasks through *self-play* reinforcement learning



Explaining James Webb's *"little red dot"* galaxies with mephisto

JADES LRDs 79803



Potentially identifying *all* the astronomical objects'
SED that our current physics can't explain



Provided that we have *a capable model* that can generate inference quickly and *cost efficiently*....



Provided that we have *a capable model* that can generate inference quickly and *cost efficiently*....



capable model

vs.

cost efficiency



In the SED case study, we need *~0.1M tokens* per source

capable model

vs.

cost efficiency

e.g., GPT-4o (this study)



In the SED case study, we need *~0.1M tokens* per source

capable model

vs.

cost efficiency

e.g., GPT-4o (this study)



Model	Input	Output
gpt-4o	\$5.00 / 1M tokens	\$15.00 / 1M tokens
gpt-4o-2024-05-13	\$5.00 / 1M tokens	\$15.00 / 1M tokens

In the SED case study, we need *~0.1M tokens* per source

capable model

vs.

cost efficiency

e.g., GPT-4o (this study)

= USD 1 *per source*



Model	Input	Output
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gpt-4o-2024-05-13	\$5.00 / 1M tokens	\$15.00 / 1M tokens

In the SED case study, we need *~0.1M tokens* per source

1B sources = \$1 billion

e.g., *Roman* Space Telescope, *Euclid* Space Telescope

1B sources = \$1 billion

e.g., *Roman* Space Telescope, *Euclid* Space Telescope

~ approximately the build cost

How do we get there in a *cost-effective* way?

The first extensive *benchmarking effort* of Large Language Models in terms of astronomy Q&A.

AstroMLab 1: Who Wins Astronomy Jeopardy!?

YUAN-SEN TING (丁源森),^{1,2,3,4} TUAN DUNG NGUYEN,⁵ TIRTHANKAR GHOSAL,⁶ RUI PAN (潘瑞),⁷ HARDIK ARORA,⁸ ZECHANG SUN (孙泽昌),⁹ TIJMEN DE HAAN,^{10,11} NESAR RAMACHANDRA,¹² AZTON WELLS,¹² SANDEEP MADIREDDY,¹³ AND ALBERTO ACCOMAZZI¹⁴

¹*Research School of Astronomy & Astrophysics, Australian National University, Cotter Rd., Weston, ACT 2611, Australia*

²*School of Computing, Australian National University, Acton, ACT 2601, Australia*

³*Department of Astronomy, The Ohio State University, Columbus, OH 43210, USA*

⁴*Center for Cosmology and AstroParticle Physics (CCAPP), The Ohio State University, Columbus, OH 43210, USA*

⁵*Department of Computer and Information Science, University of Pennsylvania, Philadelphia, PA 19104, USA*

⁶*National Center for Computational Sciences, Oak Ridge National Laboratory, Oak Ridge, TN 37831, USA*

⁷*Department of Computer Science and Engineering, Hong Kong University of Science and Technology, Kowloon, Hong Kong*

⁸*Indian Institute of Technology Patna, Bihta, Bihar 801106, India*

⁹*Department of Astronomy, MongManWai Building, Tsinghua University, Beijing 100084, China*

¹⁰*Institute of Particle and Nuclear Studies, High Energy Accelerator Research Organization, Tsukuba, Ibaraki 305-0801, Japan*

¹¹*International Center for Quantum-field Measurement Systems for Studies of the Universe and Particles (QUP-WPI), High Energy Accelerator Research Organization (KEK), Tsukuba, Ibaraki 305-0801, Japan*

¹²*Computational Science Division, Argonne National Laboratory, Lemont, IL 60439, USA*

¹³*Mathematics and Computer Science Division, Argonne National Laboratory, Lemont, IL 60439, USA*

¹⁴*Center for Astrophysics, Harvard & Smithsonian, Cambridge, MA 02138, USA*

ABSTRACT

We present a comprehensive evaluation of proprietary and open-weights large language models (LLMs) using the first astronomy-specific benchmarking dataset. This dataset comprises 4,425 multiple-choice questions curated from the Annual Review of Astronomy and Astrophysics, covering a broad range of astrophysical topics. Our analysis examines model performance across various



\$100,000

\$50,000

\$25,000

FINAL JEOPARDY!

FINAL JEOPARDY!

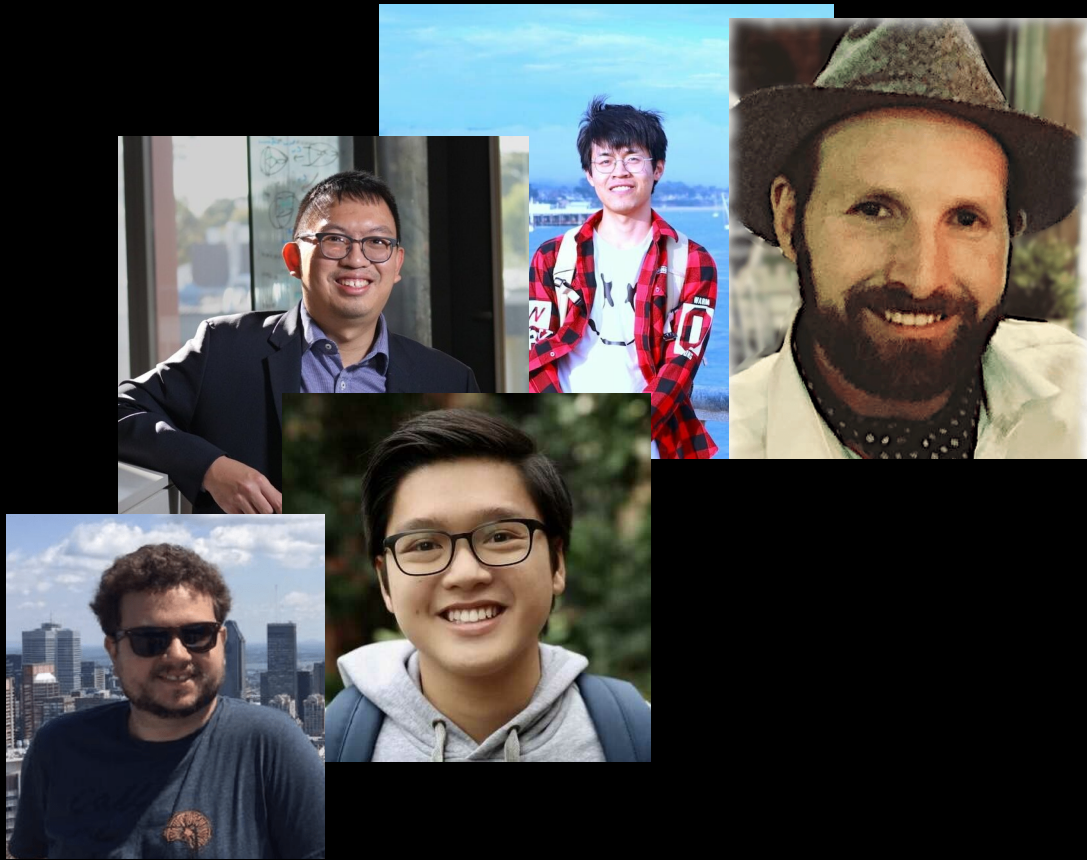
FINAL JEOPARDY!

Prestigious TOURNAMENT

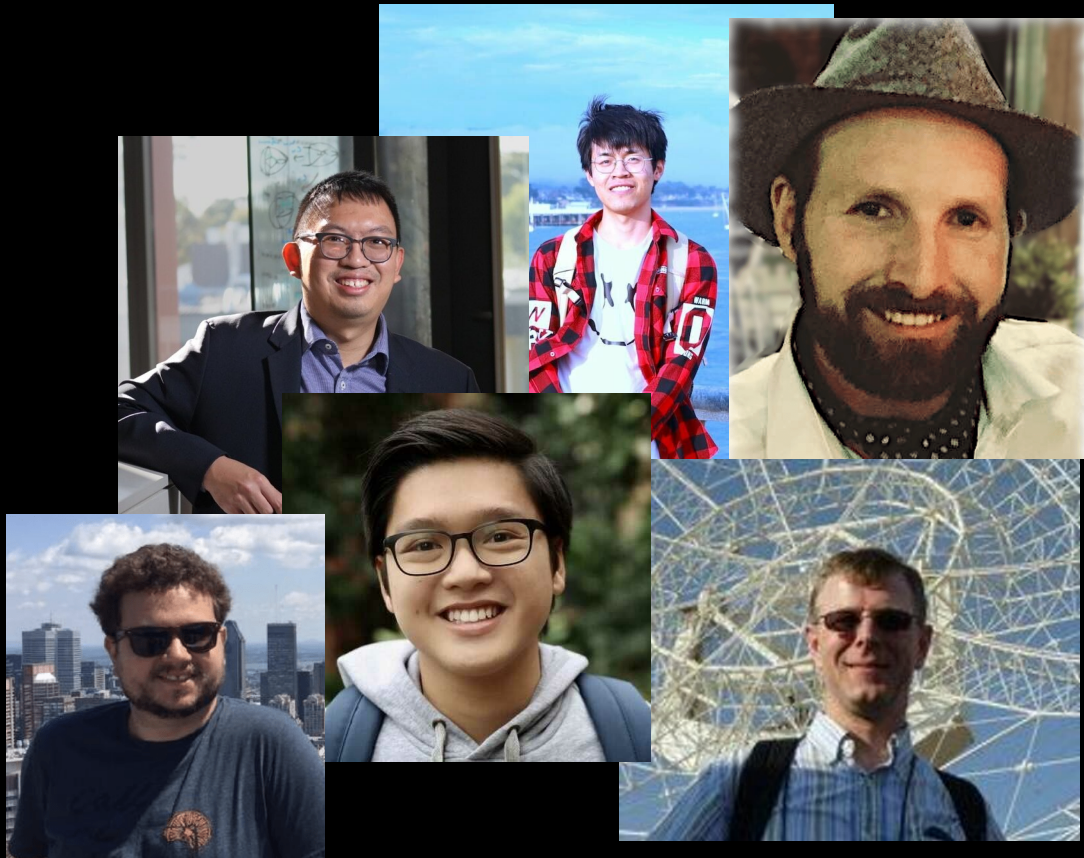
Prestigious TOURNAMENT



AstroMLab (astromlab.org)



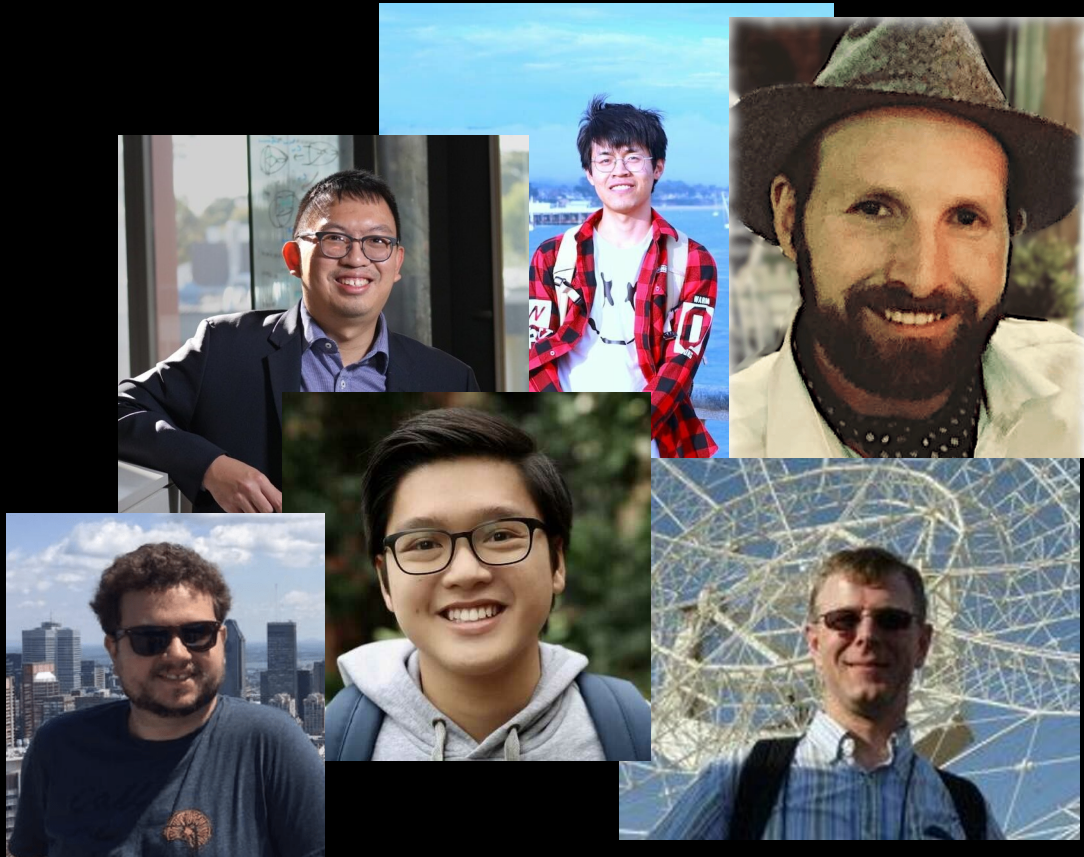
AstroMLab (astromlab.org)



Harvard-Smithsonian ADS

AstroMLab (astromlab.org)

Natural Language Processing
experts

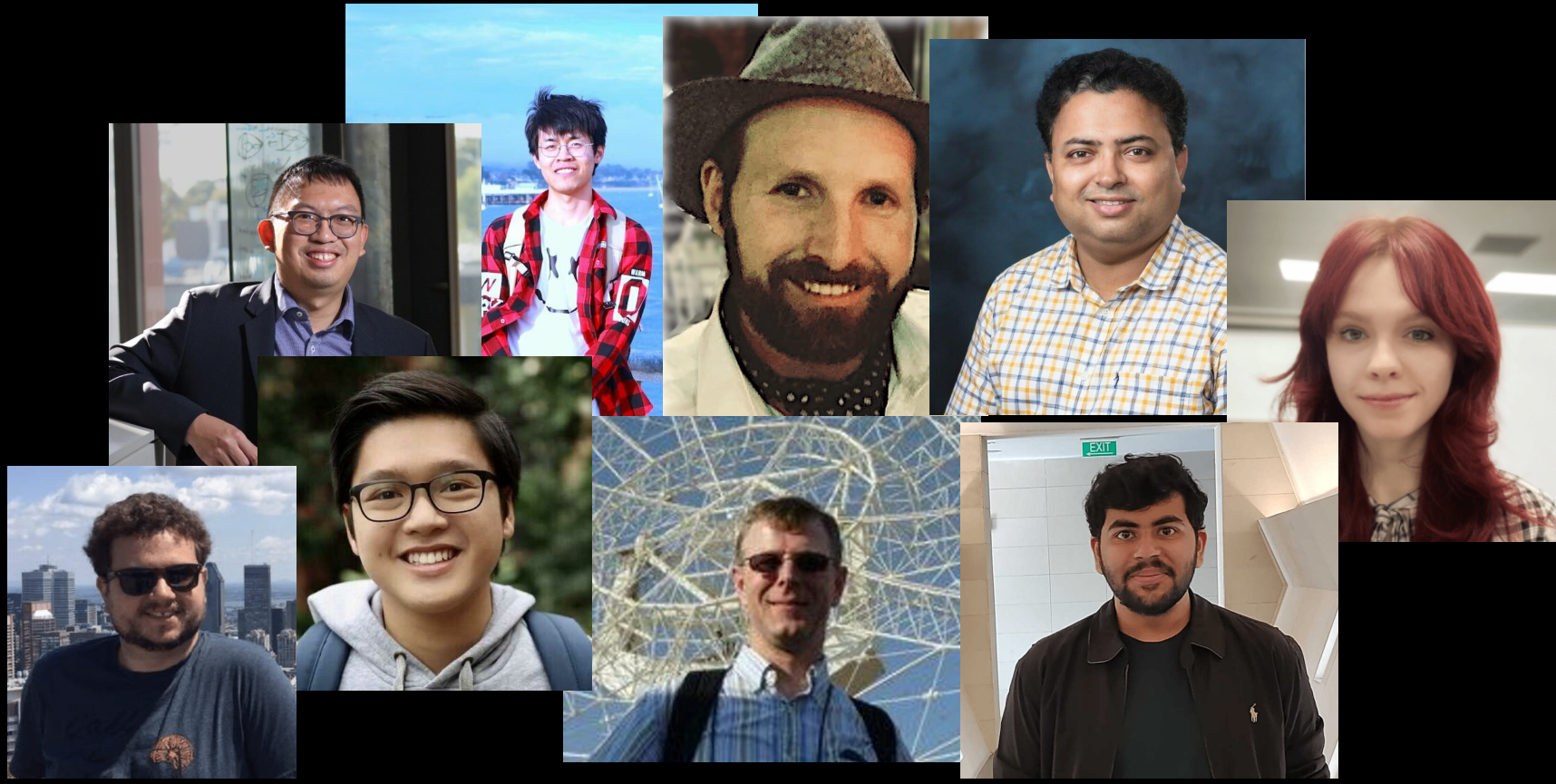


Harvard-Smithsonian ADS

AstroMLab (astromlab.org)

Natural Language Processing
experts

Oak Ridge
National Lab



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Argonne
National Lab



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experts

Oak Ridge
National Lab

Argonne
National Lab

U. Illinois
Urbana-
Champaign



Harvard-Smithsonian ADS

Curation of 5000 high quality astronomy QA *benchmark* dataset

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Latest Articles



Benchmark multiple choice question - *example*

What is the primary reason for the decline in the number density of luminous quasars at redshifts greater than 5?

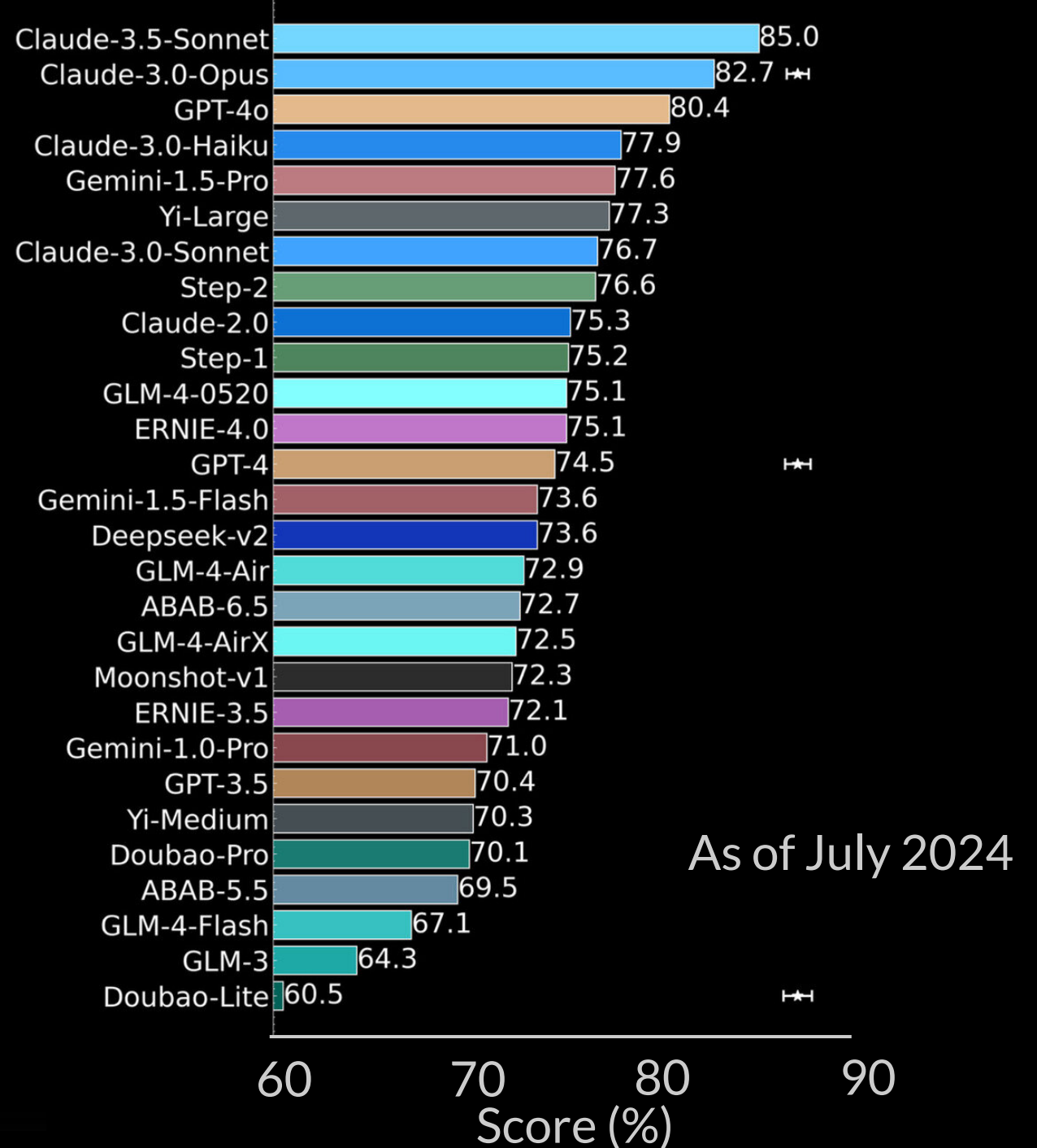
- A decrease in the overall star formation rate, leading to fewer potential host galaxies for quasars.
- An increase in the neutral hydrogen fraction in the intergalactic medium, which obscures the quasars' light.
- A decrease in the number of massive black hole seeds that can form and grow into supermassive black holes.
- An increase in the average metallicity of the Universe, leading to a decrease in the efficiency of black hole accretion.

Benchmark multiple choice question - *example*

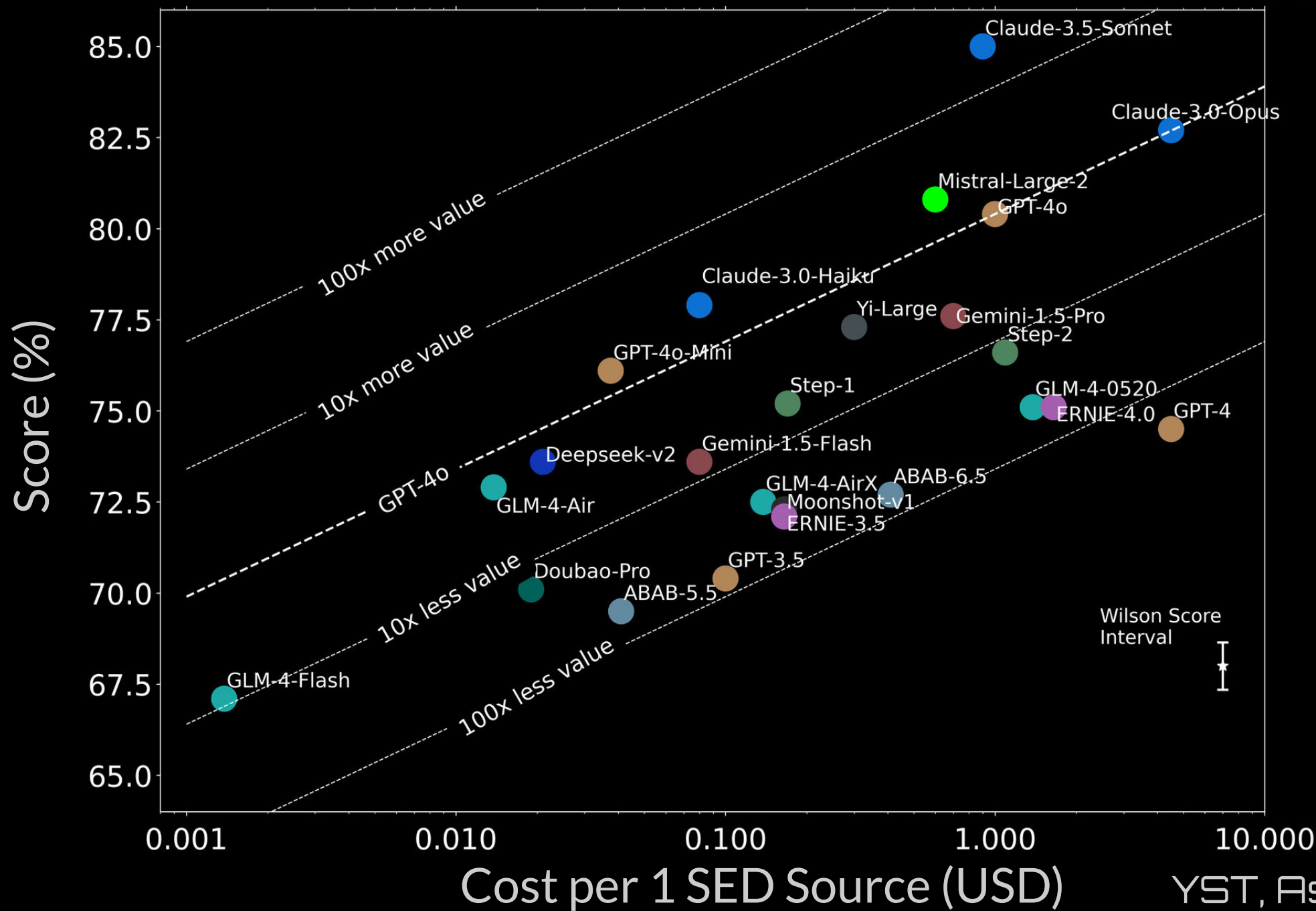
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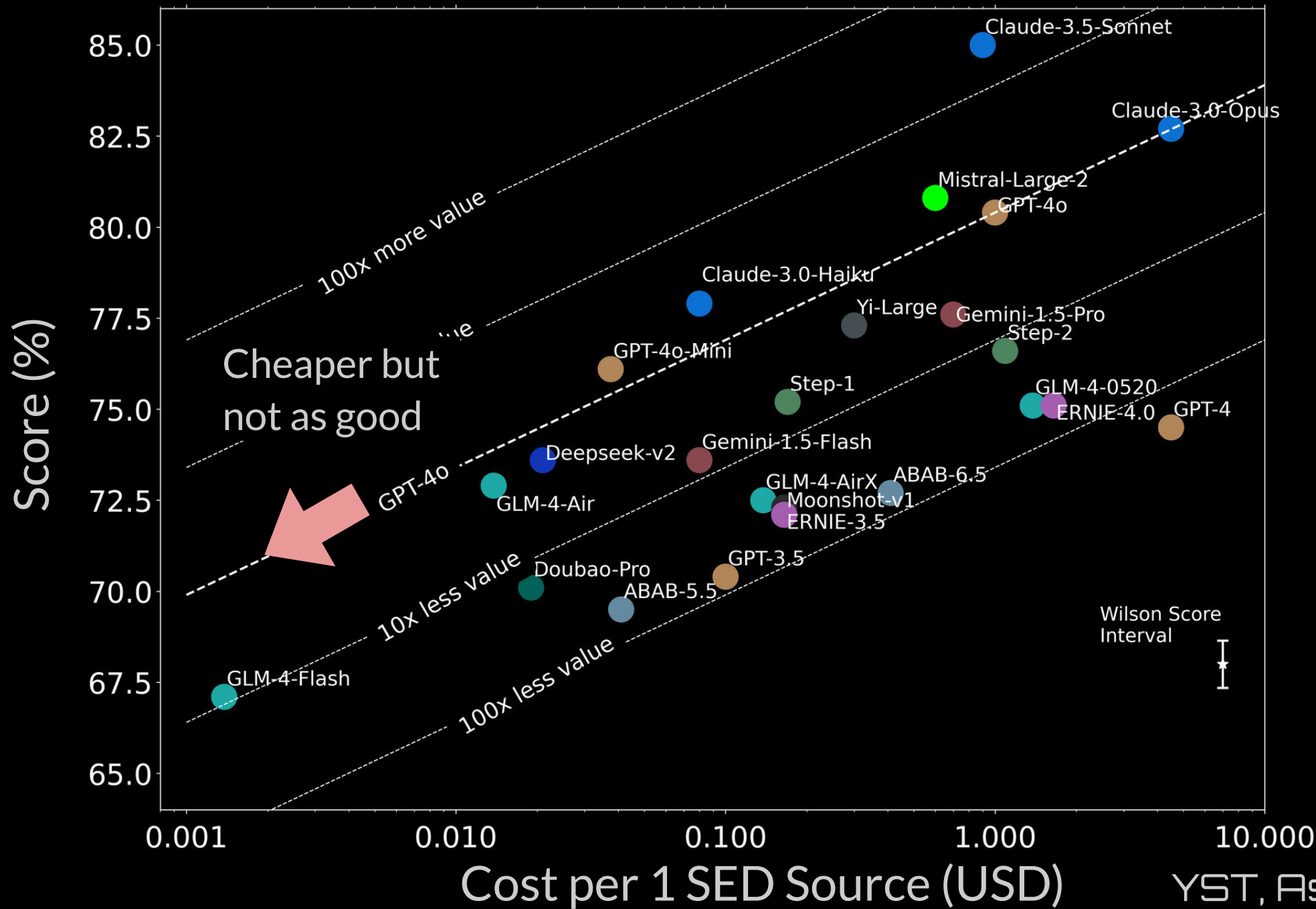
Proprietary models

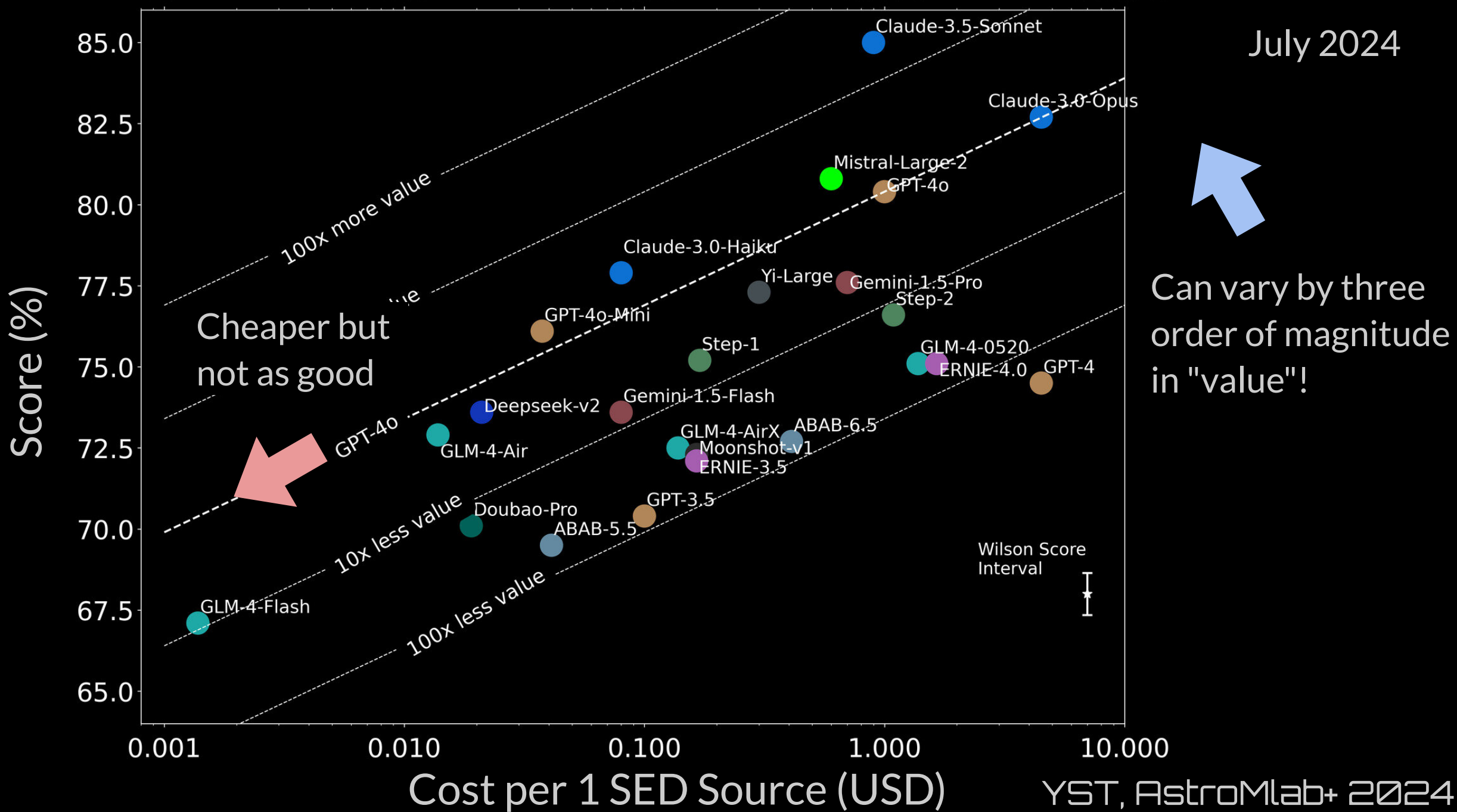


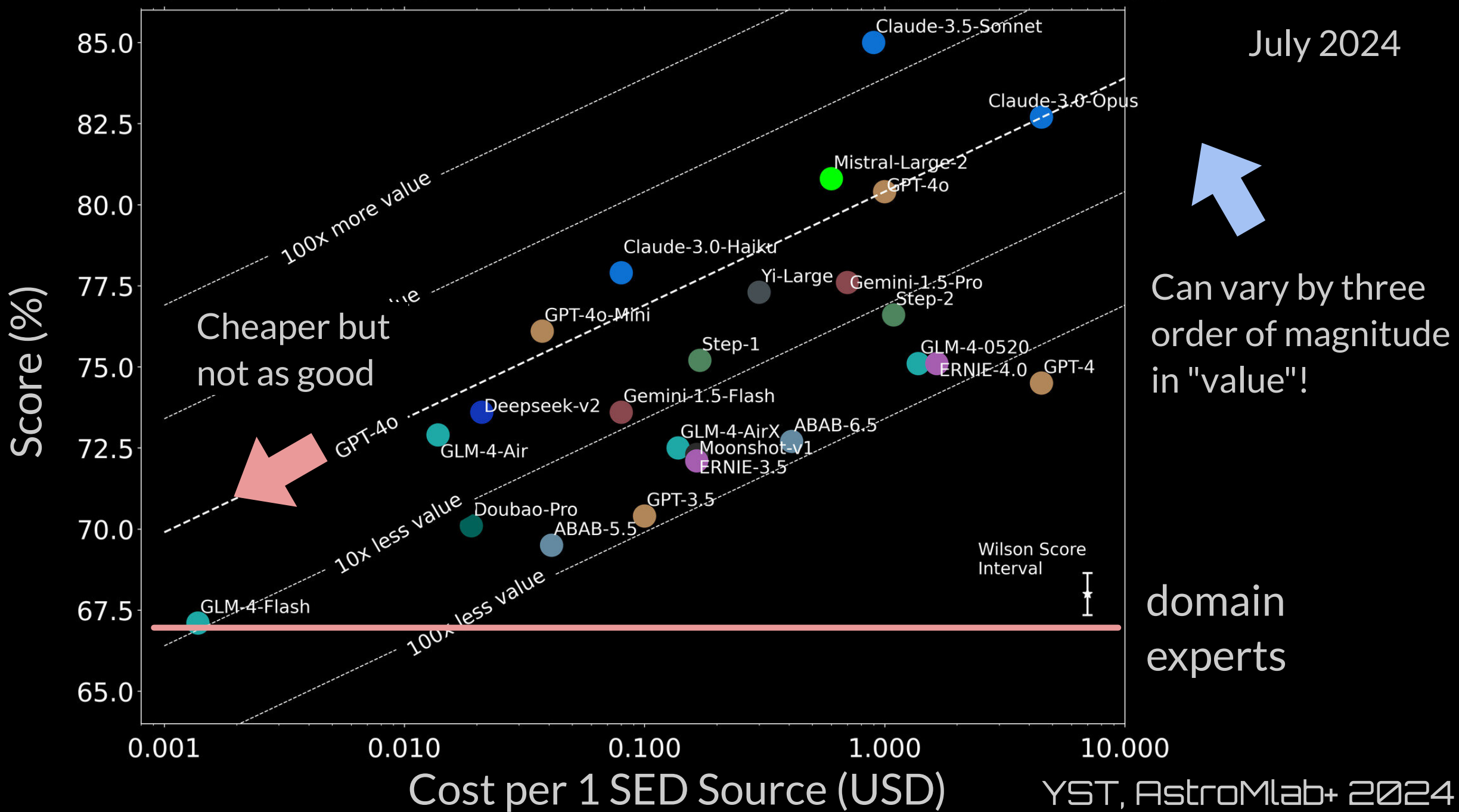
July 2024

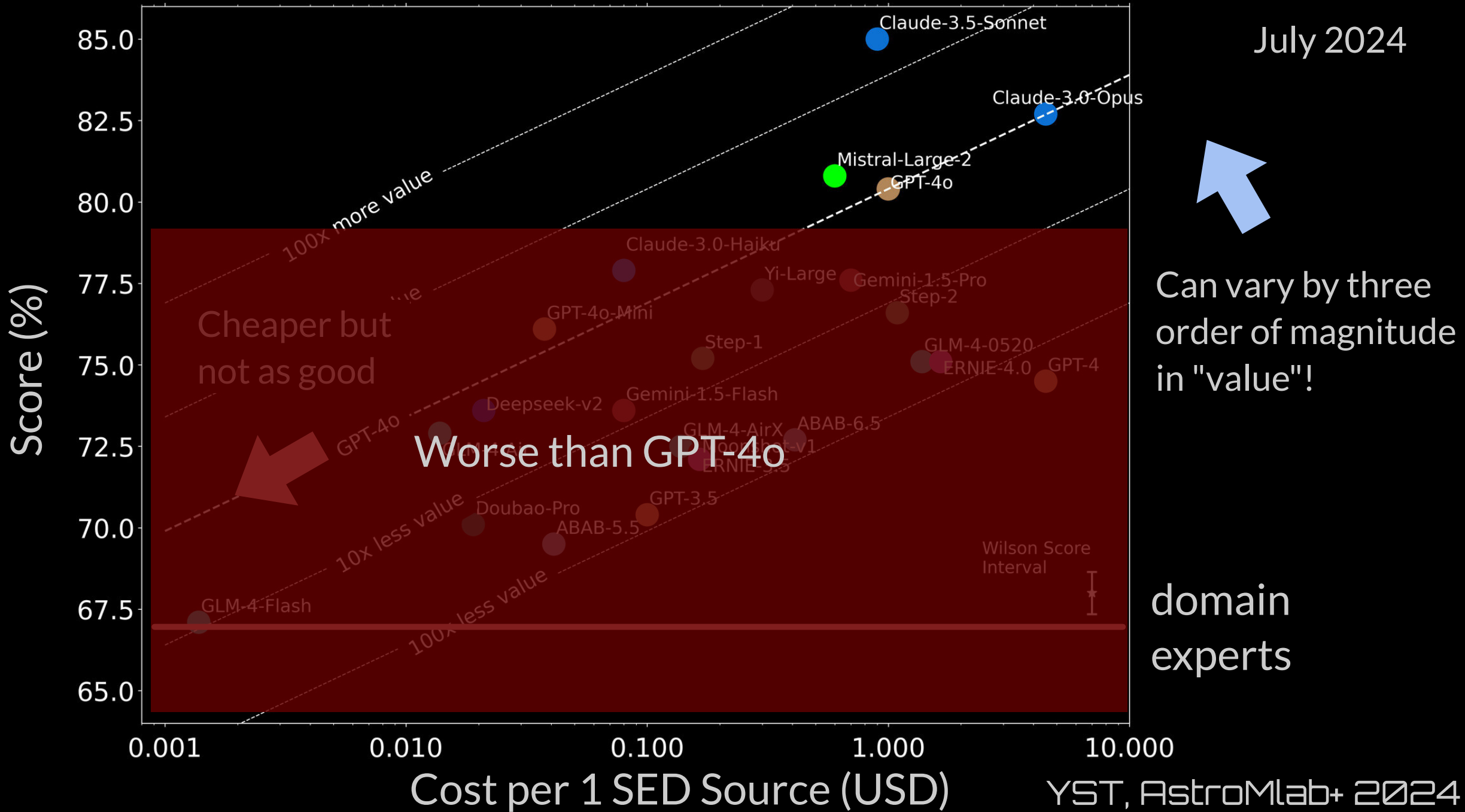


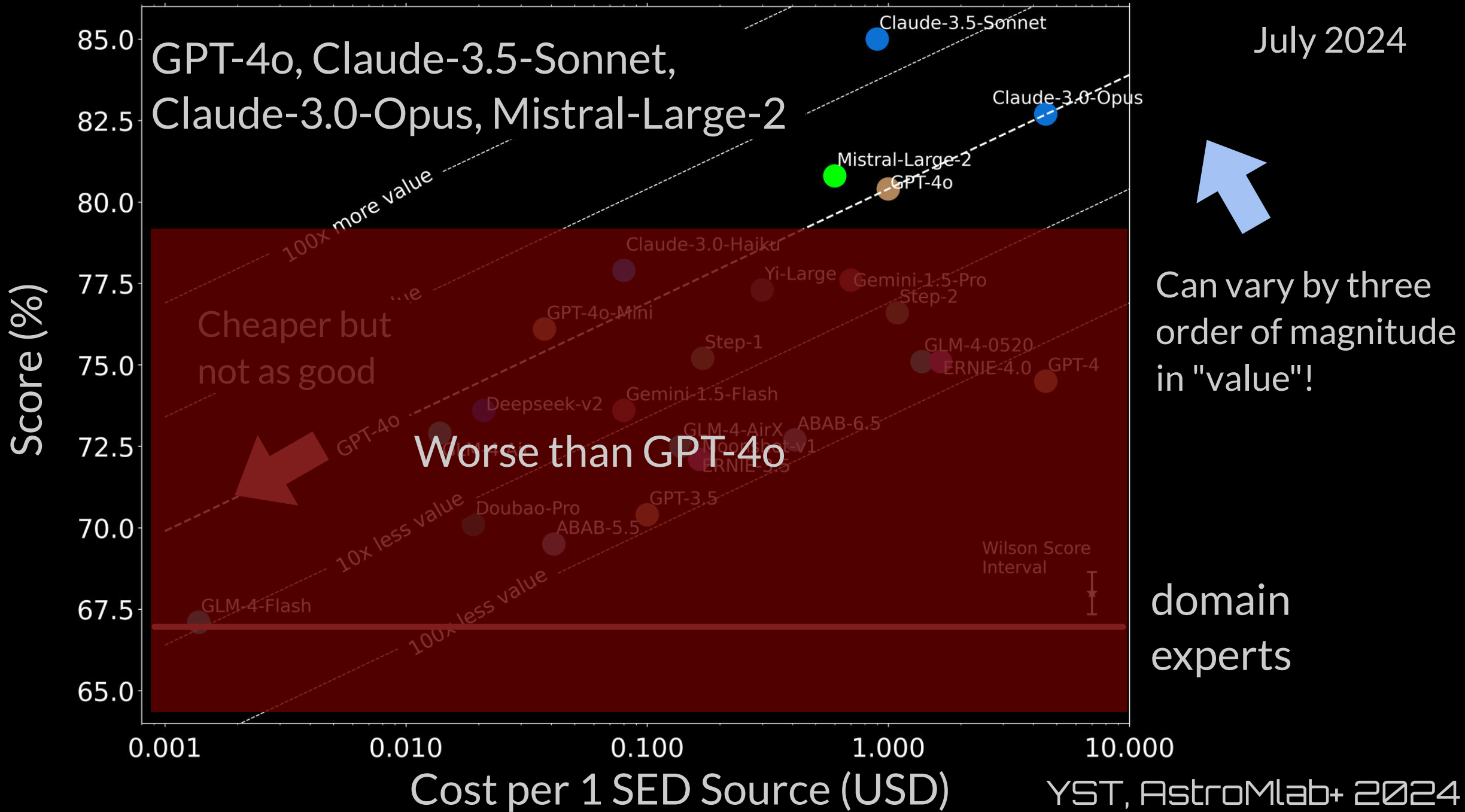
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Nov 2024

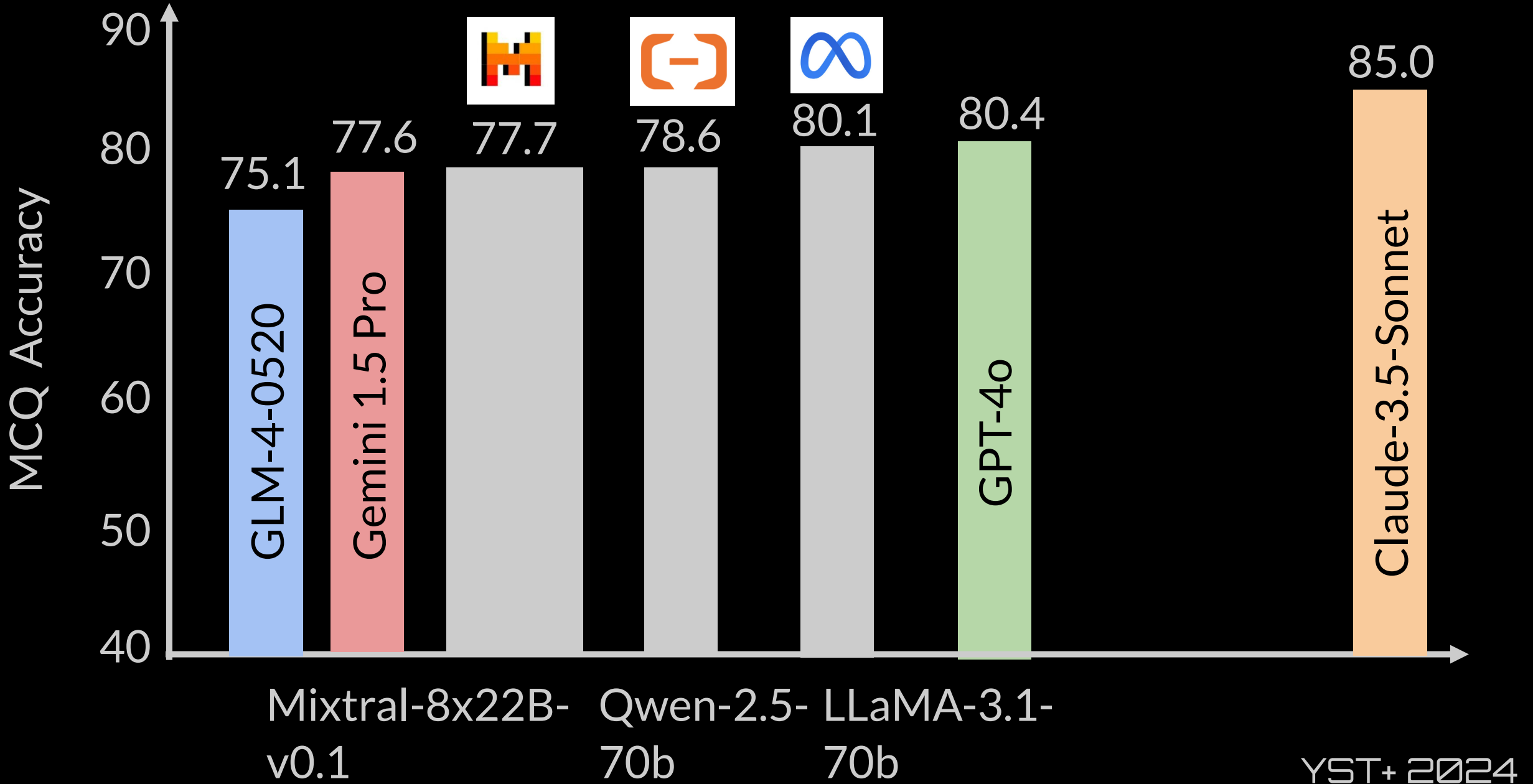


Open-weights large language models?

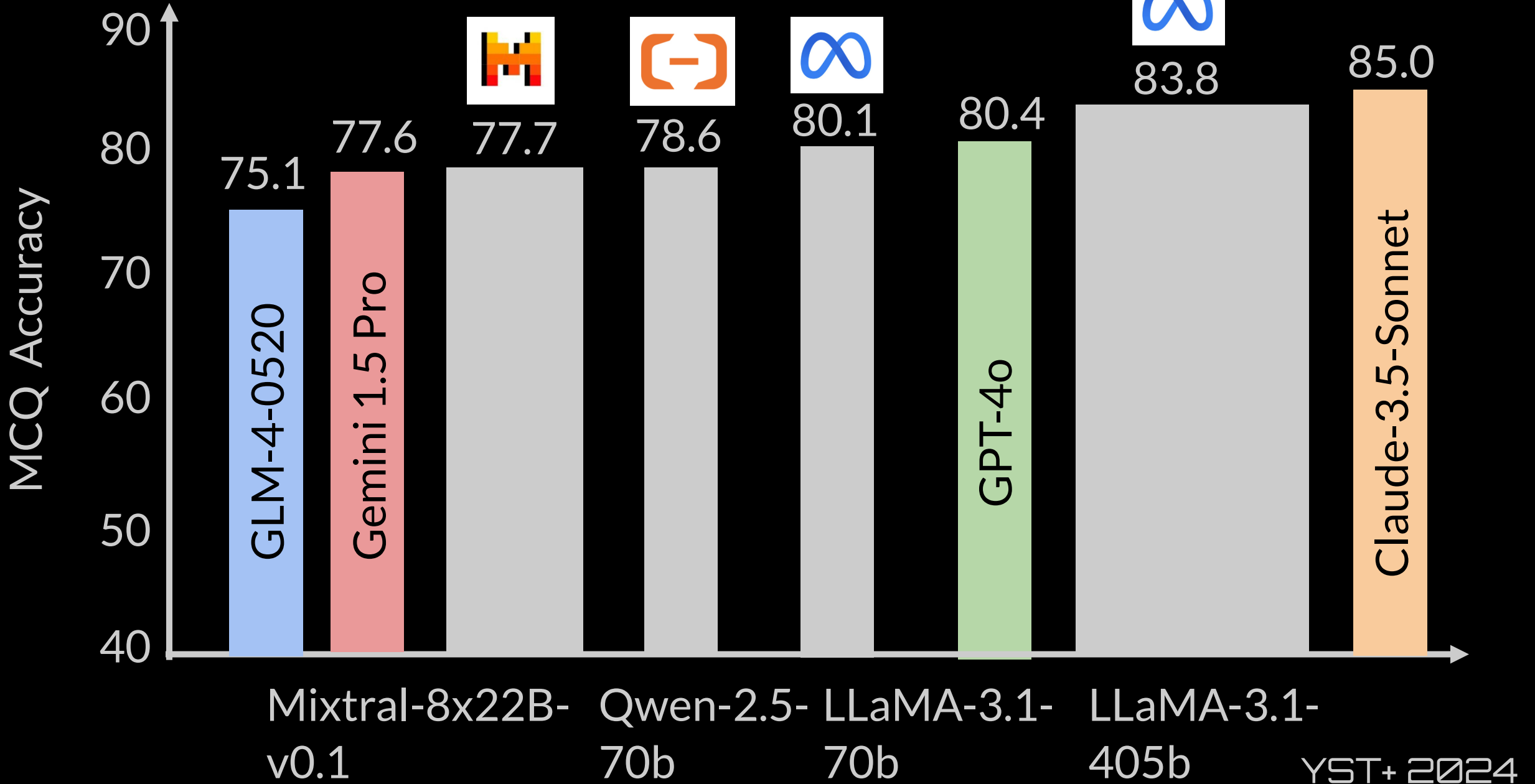


In academic settings, it's still easier to *secure GPU time* than to get grants for LLMs.

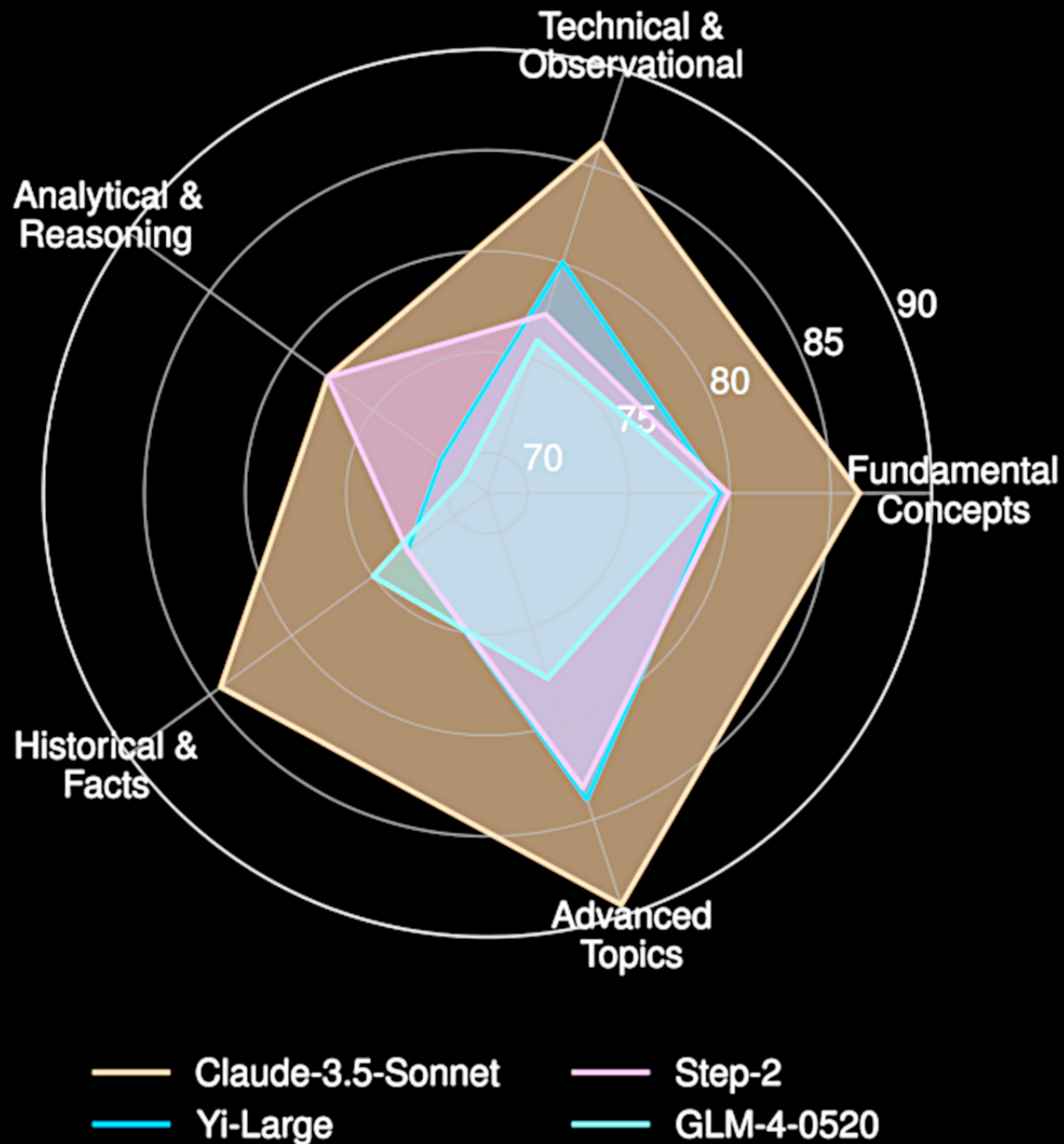
Open-weights models *are catching up*



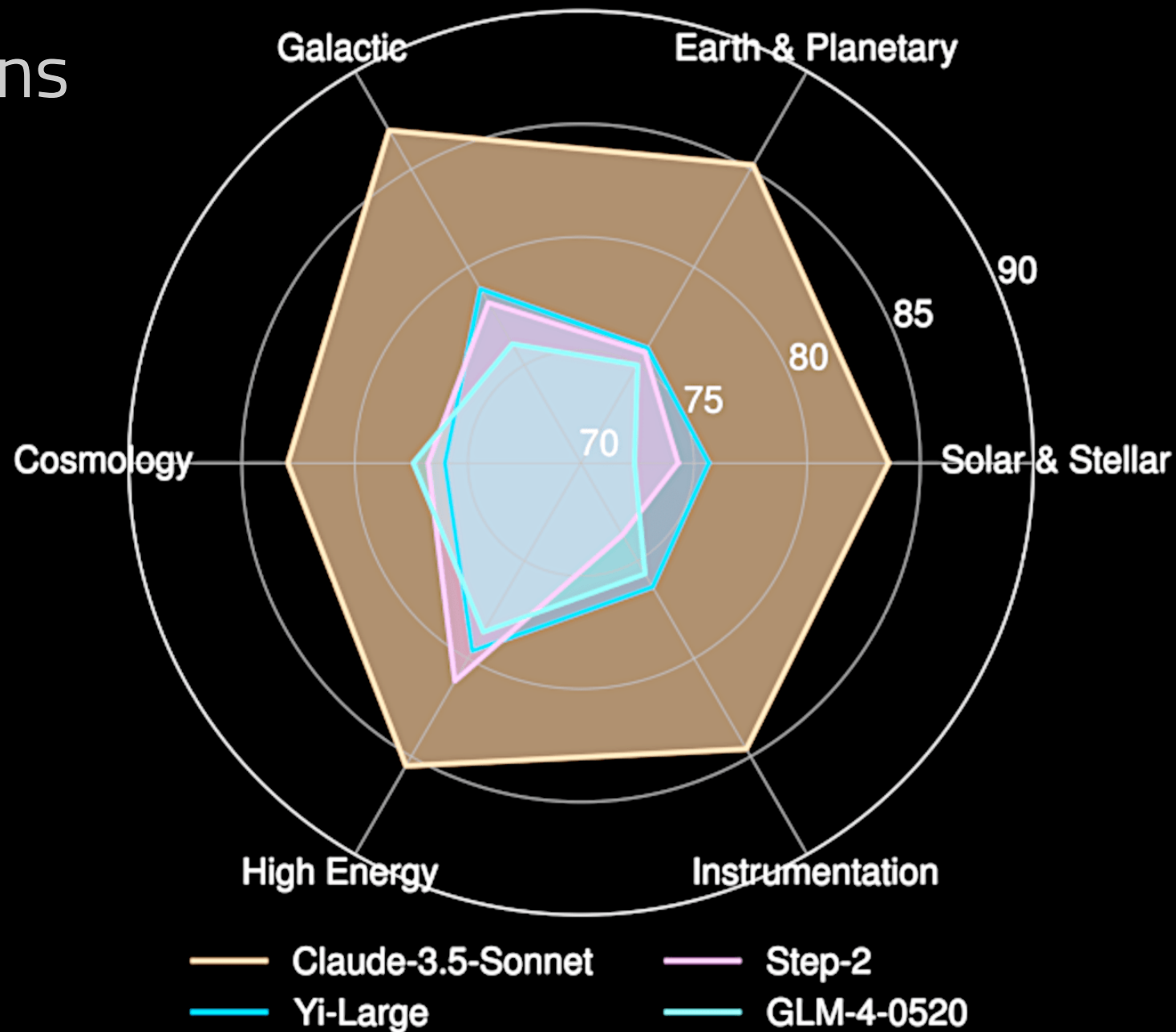
Open-weights models *are catching up*



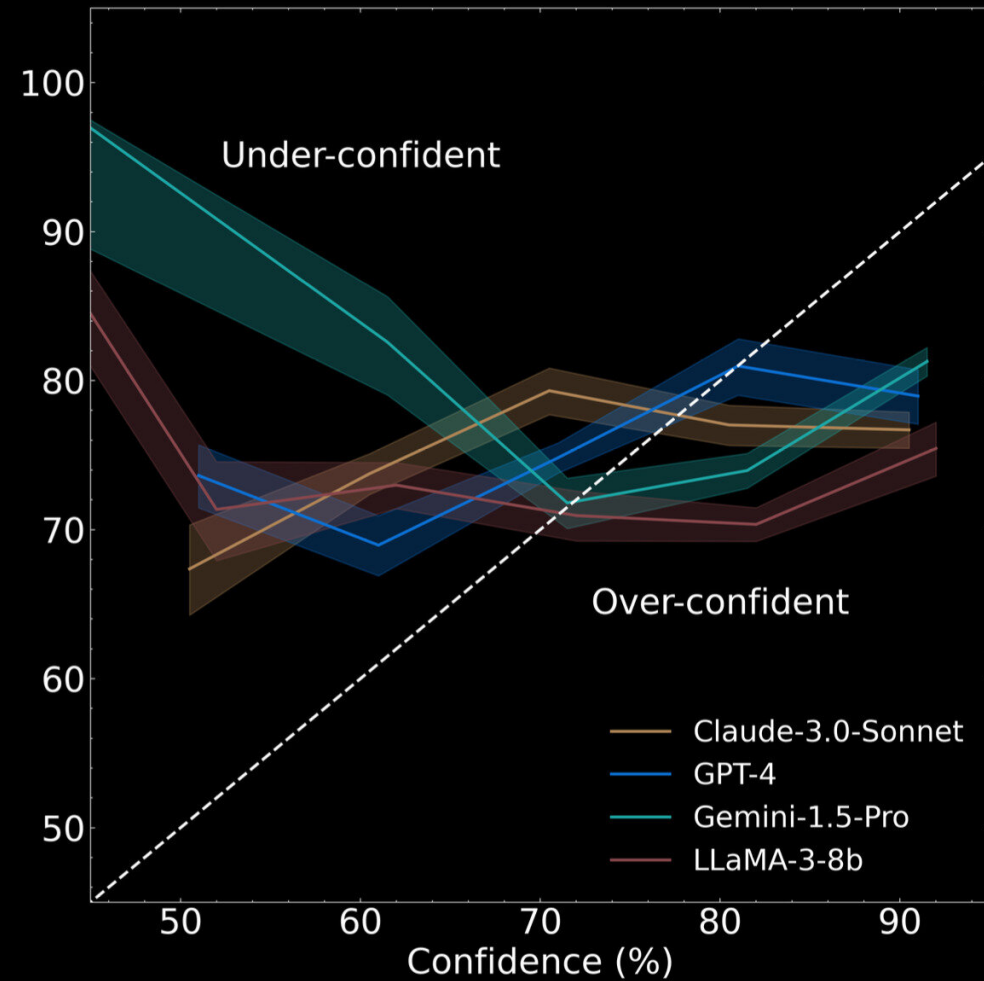
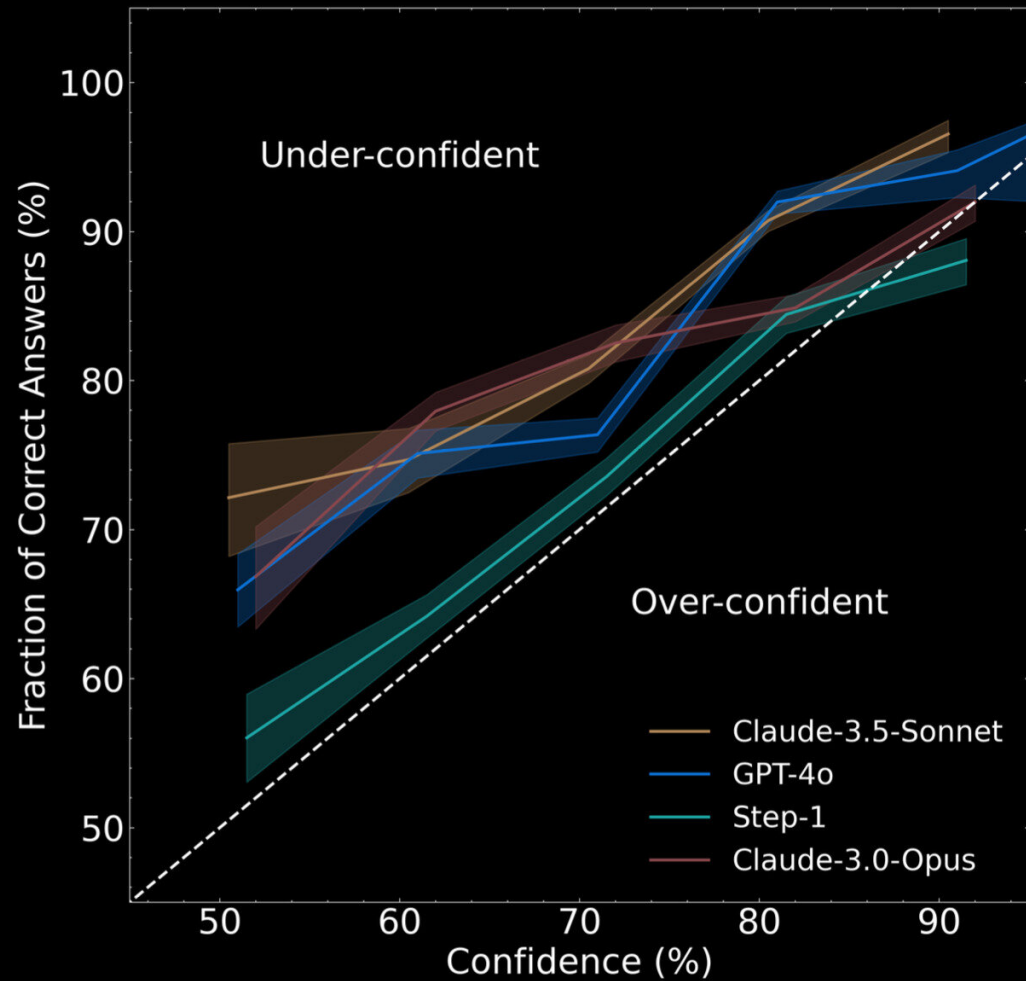
Identifying the limitations



Identifying the limitations



Trustworthiness : Are you sure?



Open-weight large language models
are *as good as* the proprietary models



Open-weight large language models
are *as good as* the proprietary models

at the ~70B level
and beyond



Still it is *not very scalable*



Still it is *not very scalable*



LLaMA-3.1 70b throughput on *four H100 GPUs*

= ~ 100 tokens / second



LLaMA-3.1 70b throughput on *four H100 GPUs*

= ~ 100 tokens / second

1 SED source = 15 GPU minutes



LLaMA-3.1 70b throughput on *four H100 GPUs*

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1 SED source = 15 GPU minutes

1B sources = 10M GPU days



LLaMA-3.1 70b throughput on *four H100 GPUs*

= ~ 100 tokens / second

1 SED source = 15 GPU minutes

1B sources = 10M GPU days

A cluster with *10,000 H100 GPUs*
running for *3 years*



Can we improve *lightweight (e.g., 8B)*
open-weights LLMs to perform well on
astronomical tasks?

AstroMLab 3: Achieving GPT-4o Level Performance in Astronomy with a Specialized 8B-Parameter Large Language Model

Tijmen de Haan¹, Yuan-Sen Ting (丁源森)^{2,3}, Tirthankar Ghosal⁴, Tuan Dung Nguyen⁵, Alberto Accomazzi⁶, Azton Wells⁷, Nesar Ramachandra⁷, Rui Pan (潘瑞)⁸, Zechang Sun (孙泽昌)⁹

¹*International Center for Quantum-field Measurement Systems for Studies of the Universe and Particles (QUP-WPI), High Energy Accelerator Research Organization (KEK), Tsukuba, Ibaraki, Japan*

²*Department of Astronomy, The Ohio State University, Columbus, OH, USA*

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⁷*Computational Science Division, Argonne National Laboratory, Lemont, IL, USA*

⁸*Department of Computer Science and Engineering,*

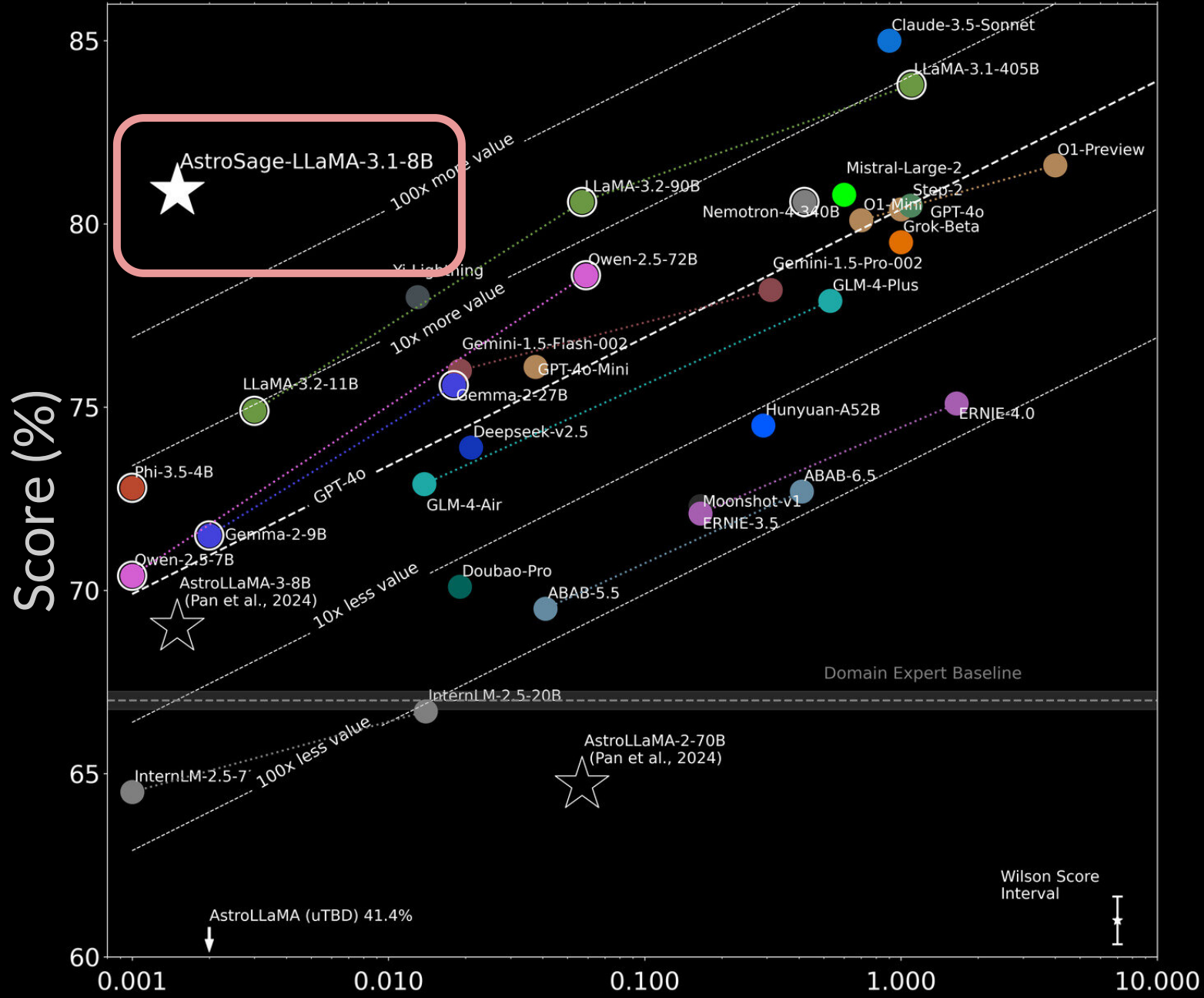
Hong Kong University of Science and Technology, Kowloon, Hong Kong and

⁹*Department of Astronomy, Tsinghua University, Beijing, People's Republic of China*

AstroSage-Llama-3.1-8B is a domain-specialized natural-language AI assistant tailored for research in astronomy, astrophysics, and cosmology. Trained on the complete collection of astronomy-related arXiv papers from 2007-2024 along with millions of synthetically-generated question-answer

Special thanks to



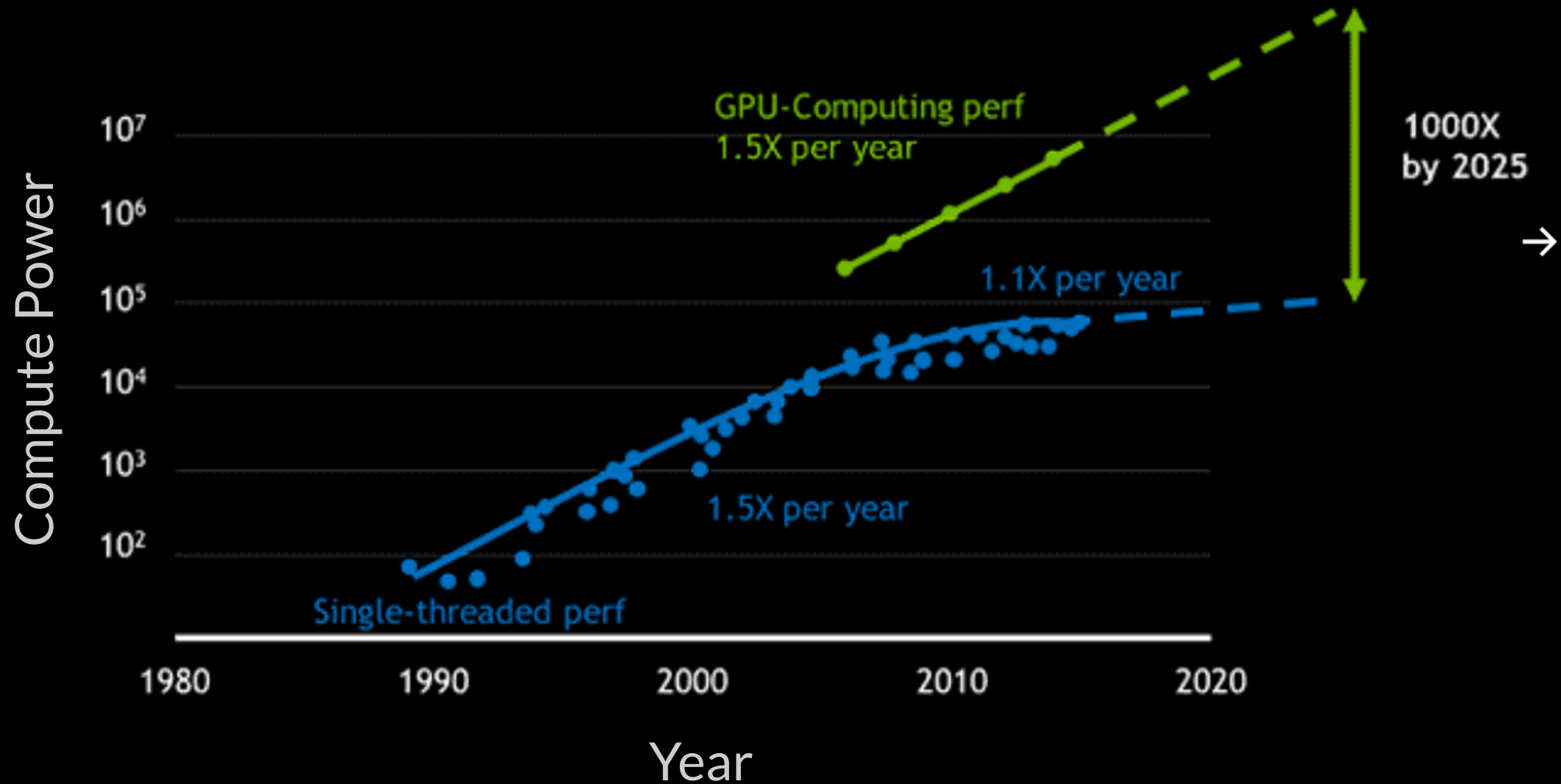


Cost per 1 SED Source (USD)

de Haan, AstroMLab+ 2024

For *individual specific* downstream task,
it is possible to train a super-performant
lightweight LLMs.

Huang's Law



Tech / Tech Trends

Tech unicorn Zhipu AI joins China's **LLM price war** amid new funding round

- Zhipu AI's GLM series of large language models now costs 90 per cent less than the current industry average of 1 yuan per 1 million tokens

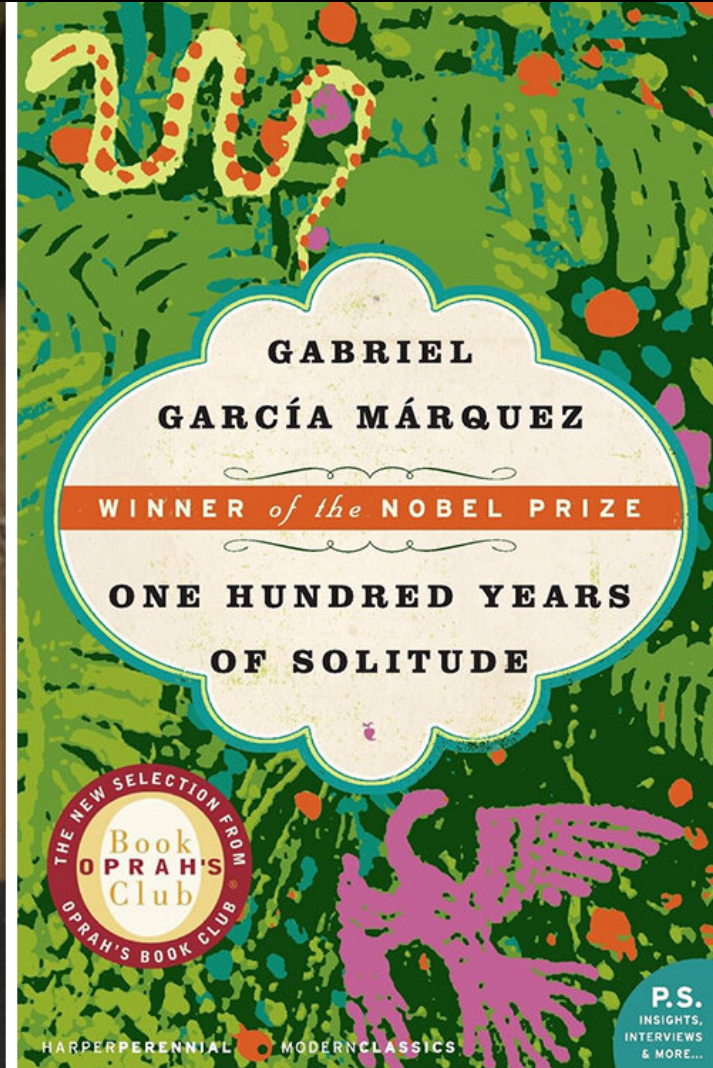
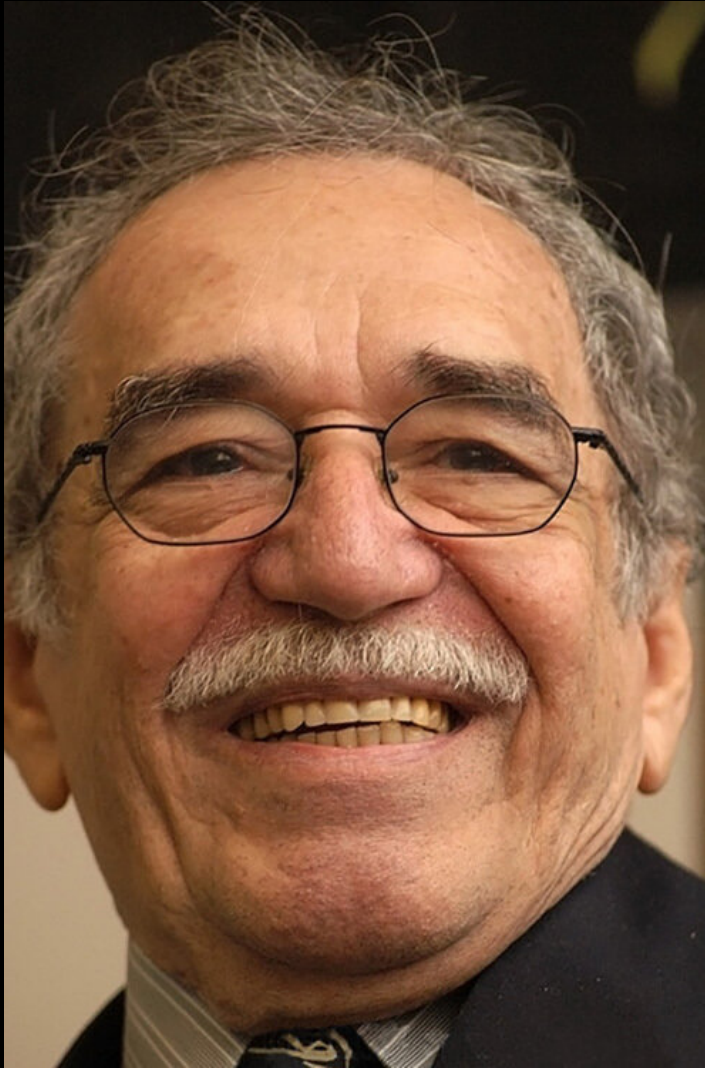


Ben Jiang in Beijing

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Published: 8:00pm, 5 Jun 2024 ▾

 [Why you can trust SCMP](#)



= 0.03 USD





Cornell University

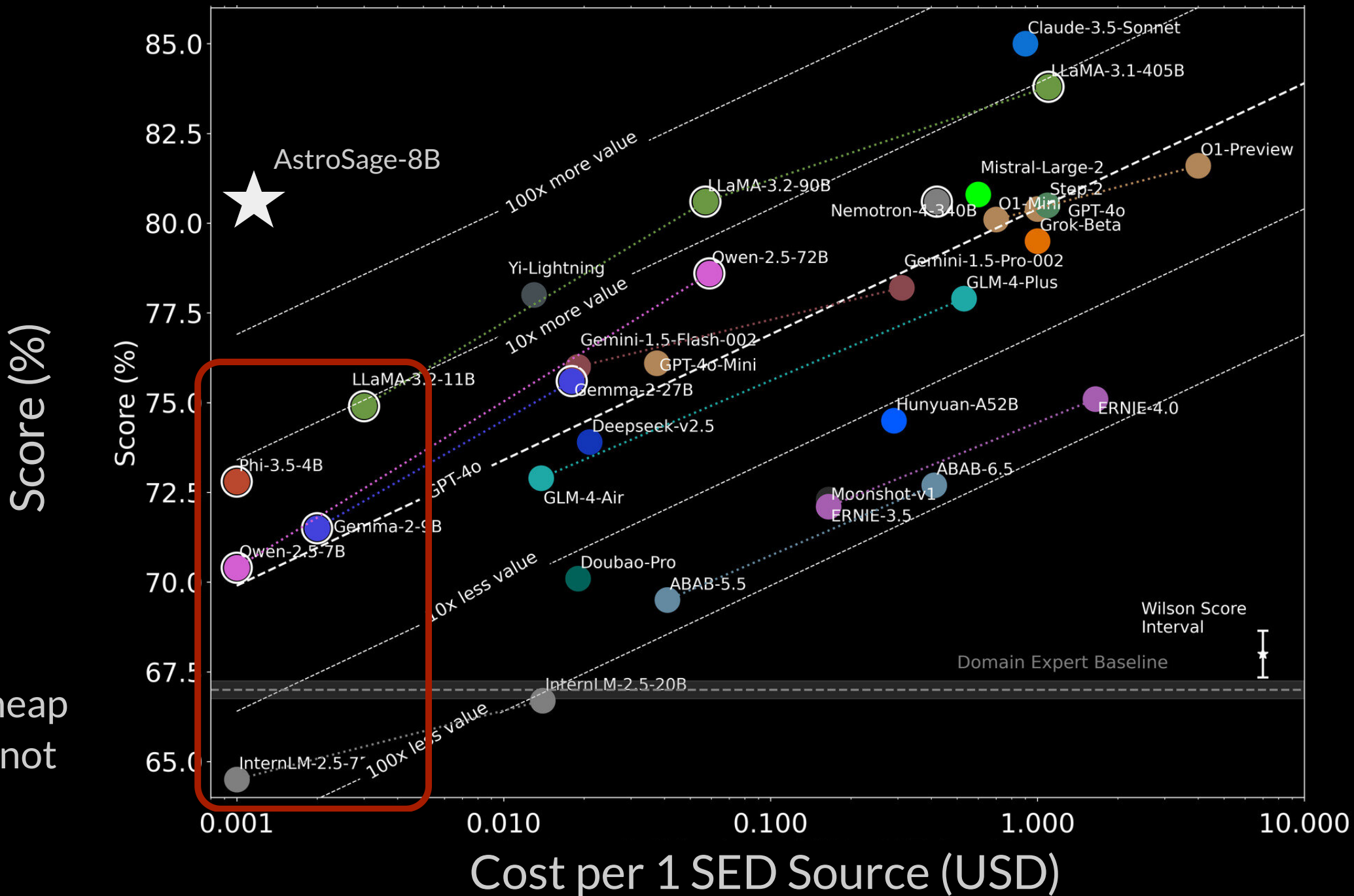
arXiv > astro-ph

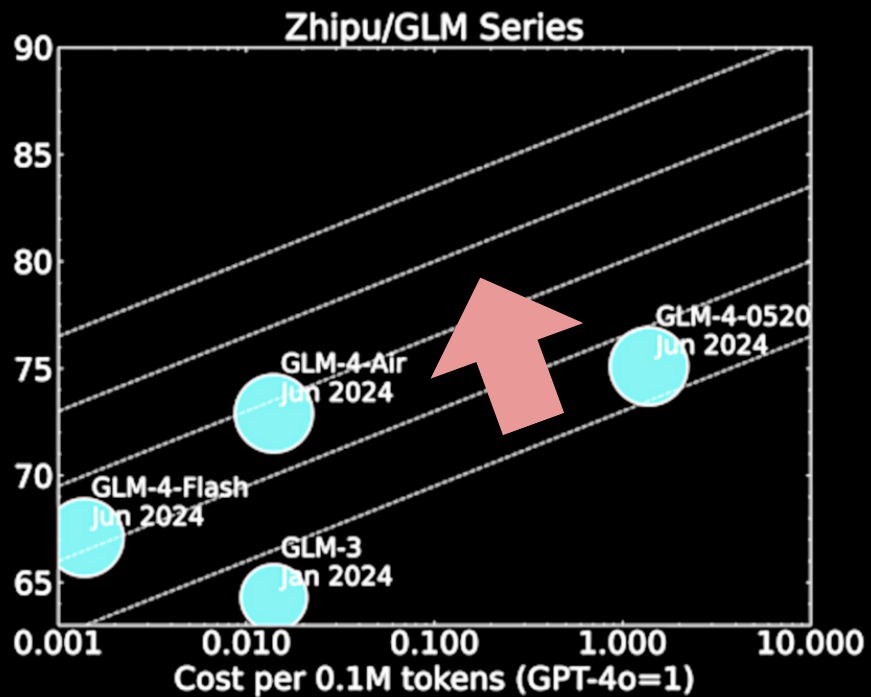
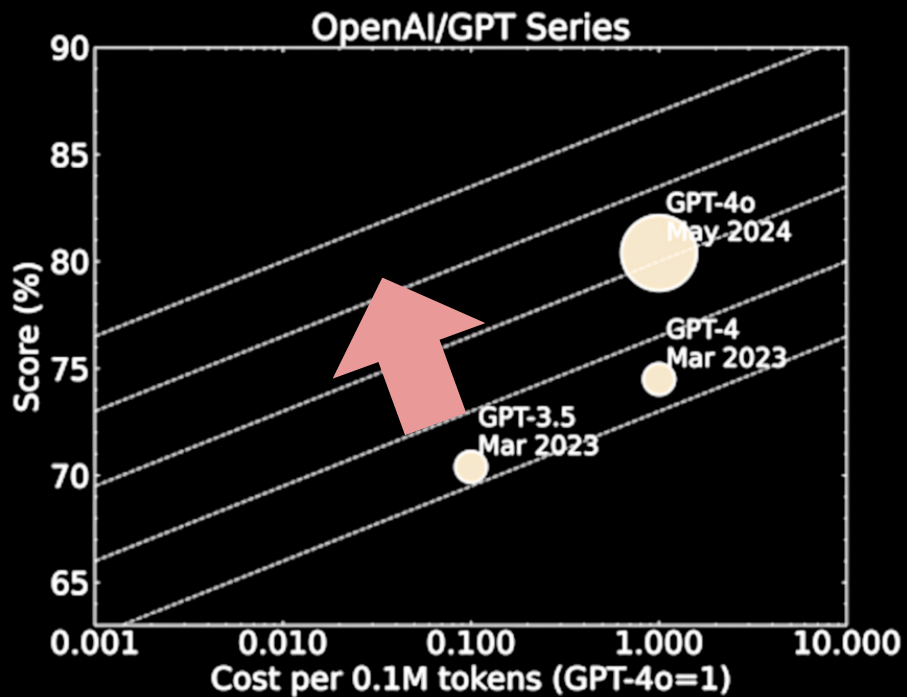
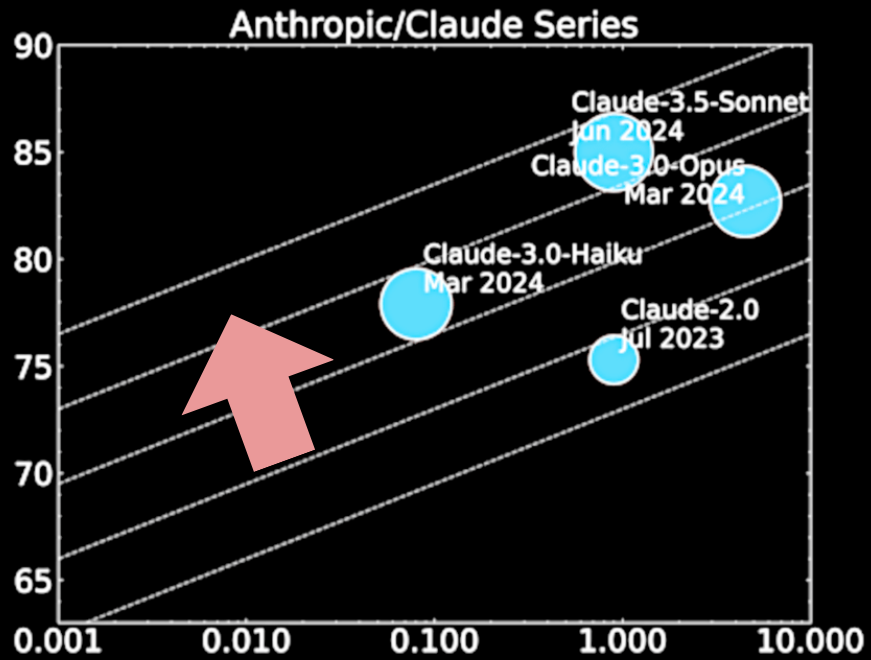
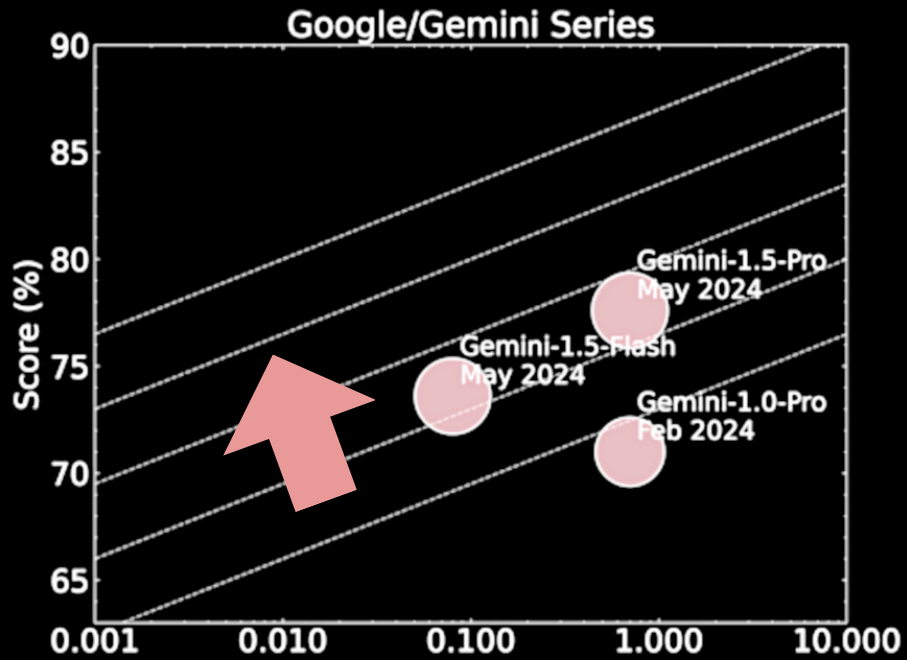
Astrophysics (since April 1992)

= 40 USD

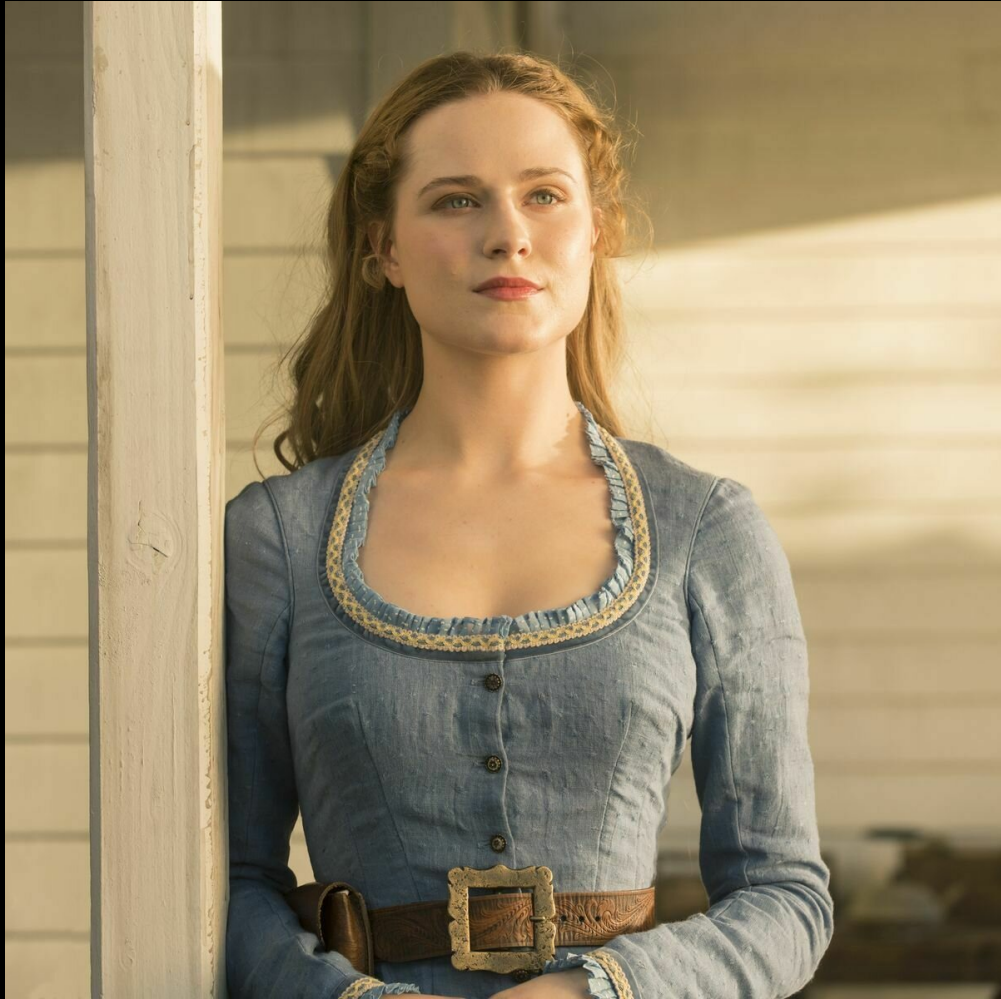


The ultra cheap models are not great yet

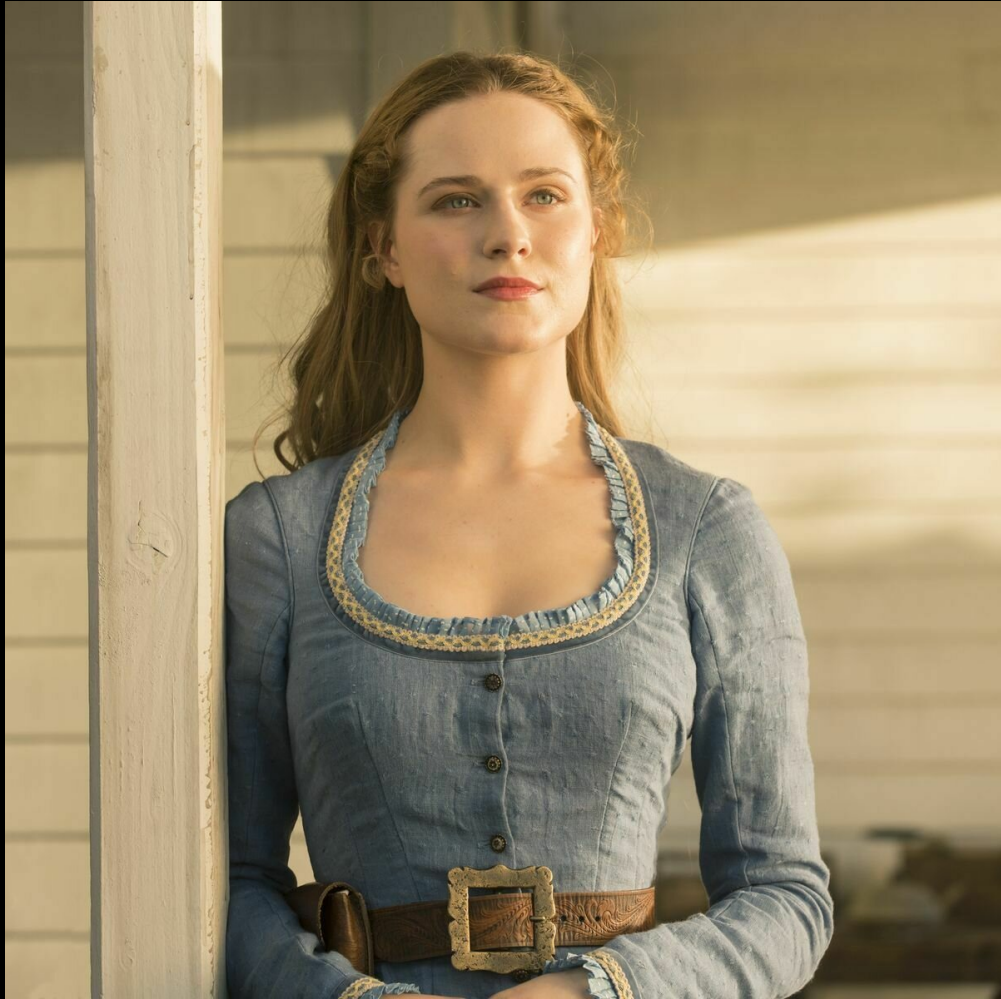




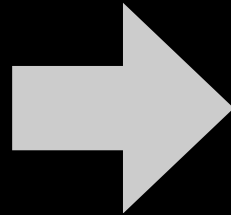
The price drop has an e-folding time of *approximately 3-6 months*



Data-poor , Theory-rich



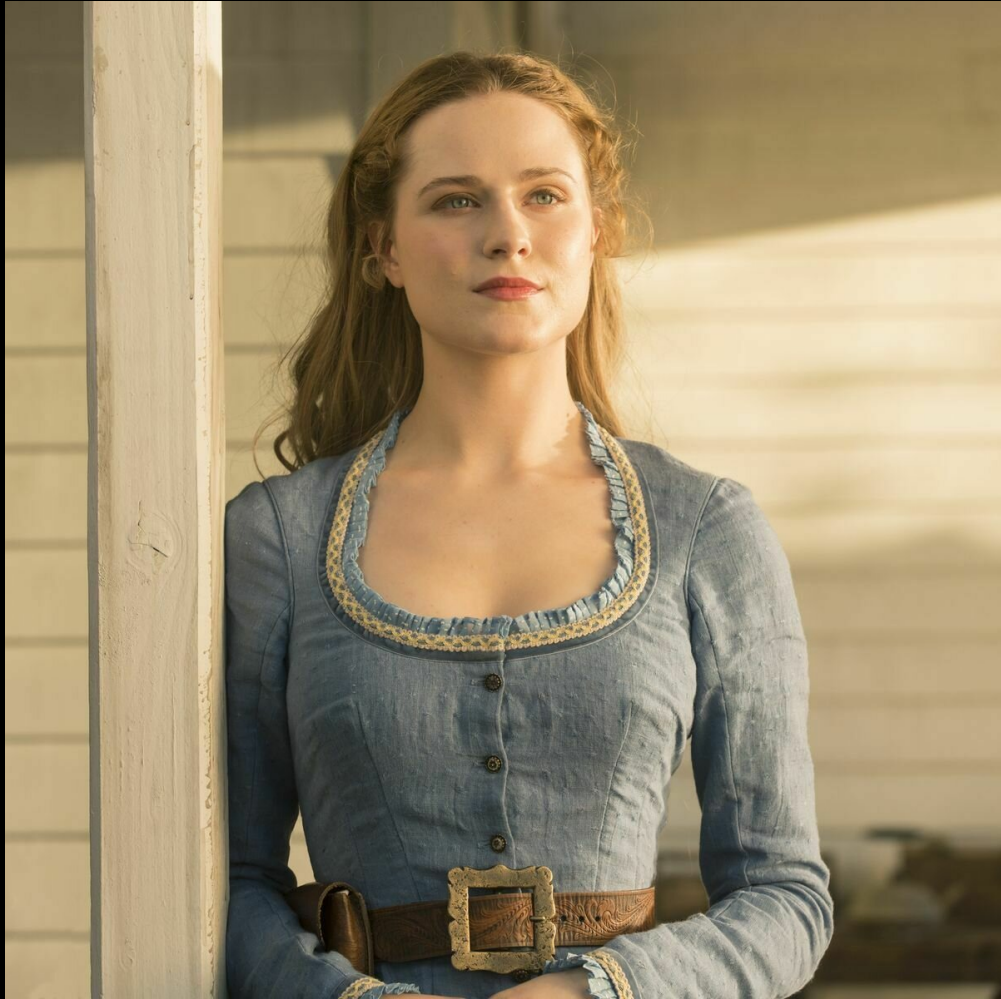
???



Collecting
more data



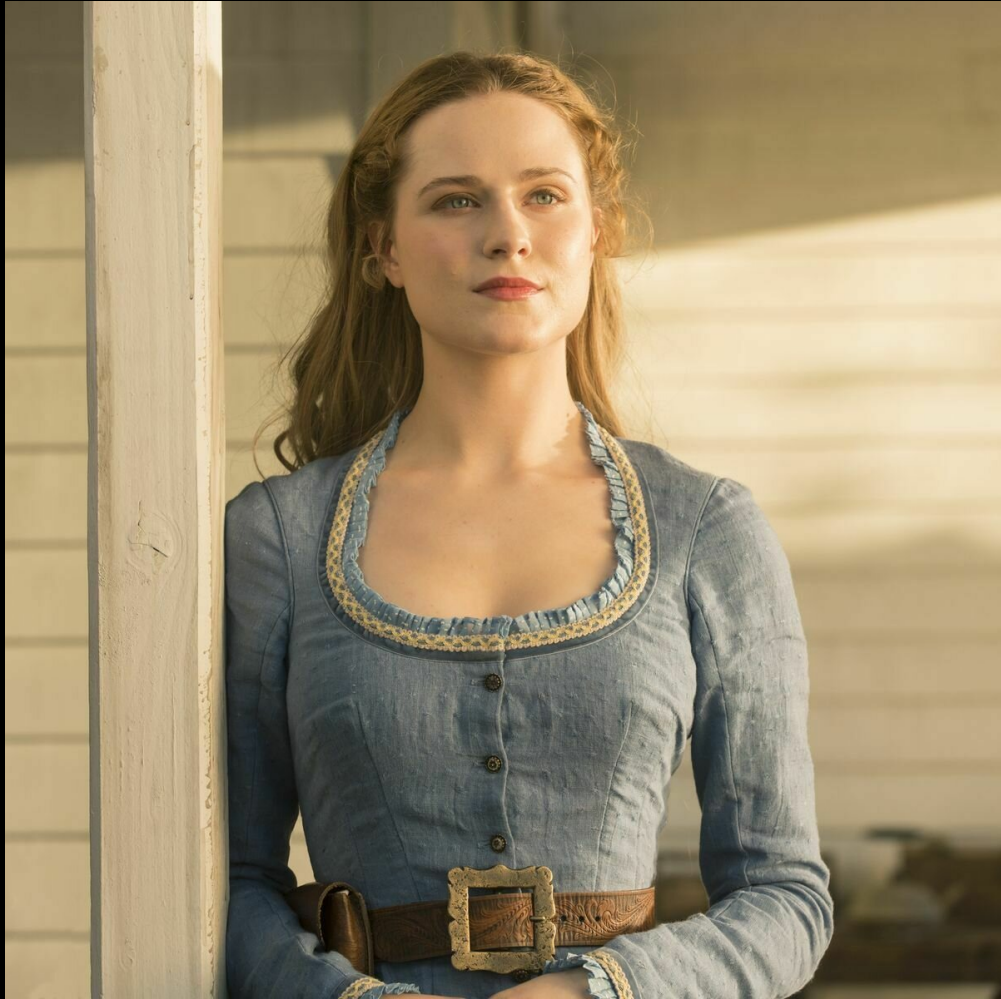
Data-poor , Theory-rich



Data-poor , Theory-rich



Roman, HSC,
Euclid, DESI,
SDSS, PFS



Data-poor , Theory-rich



Roman, HSC,
Euclid, DESI,
SDSS, PFS

Data-rich , Theory-poor





Data-poor , Theory-rich

三个臭皮匠胜过一个诸葛亮

Millions of LLM agents

~~"Three cobblers with their wits combined surpass one Zhuge Liang (~Machiavelli) "~~ - Chinese proverb

