



“Theory Closure”

Michael Krämer (RWTH Aachen University)

Machine Learning for Jet Physics

11–13 Dec 2017
Lawrence Berkeley National Laboratory
US/Pacific timezone

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Overview

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There has been a recent surge of interest in developing and applying advanced machine learning techniques in HEP, and jet physics is a domain at the forefront of the excitement. The goal of this workshop is to gather experts and new-comers to discuss progress, new ideas, and common challenges. The workshop is open to the community; we invite contributions and will try to accommodate everyone within reason.

 **Starts** 11 Dec 2017, 01:15
Ends 13 Dec 2017, 18:00
US/Pacific

 Lawrence Berkeley National Laboratory
2-100

 [Benjamin Nachman](#)
[Kyle Cranmer](#)
[Matt Dolan](#)
[Timothy Cohen](#)

 **Slides**
 [ML4JP_Workshop_Directions_BreakoutRoom...](#)
 [ML4JP_Workshop_Directions.pdf](#)

 There is no fee for attending the workshop. Coffee and light refreshments will be provided during breaks but meals are not provided.

There are many hotels in the Berkeley area, including limited availability at the LBNL guesthouse (5 min walk from the 140/*night*). *A complementary shuttle runs every 10 min from downtown Berkeley up to the lab. For lunch and dinner, see the agenda.*

Related workshops:

DS@HEP: <https://indico.fnal.gov/conferenceDisplay.py?ovw=True&confId=13497>

BOOST: <https://indico.cern.ch/event/579660/>

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-  Experimental/Practical aspects of
-  Heavy Ions
-  Jet tagging
-  Learning from data
-  Learning more about QCD
-  Recent results in ML
-  Representing jets



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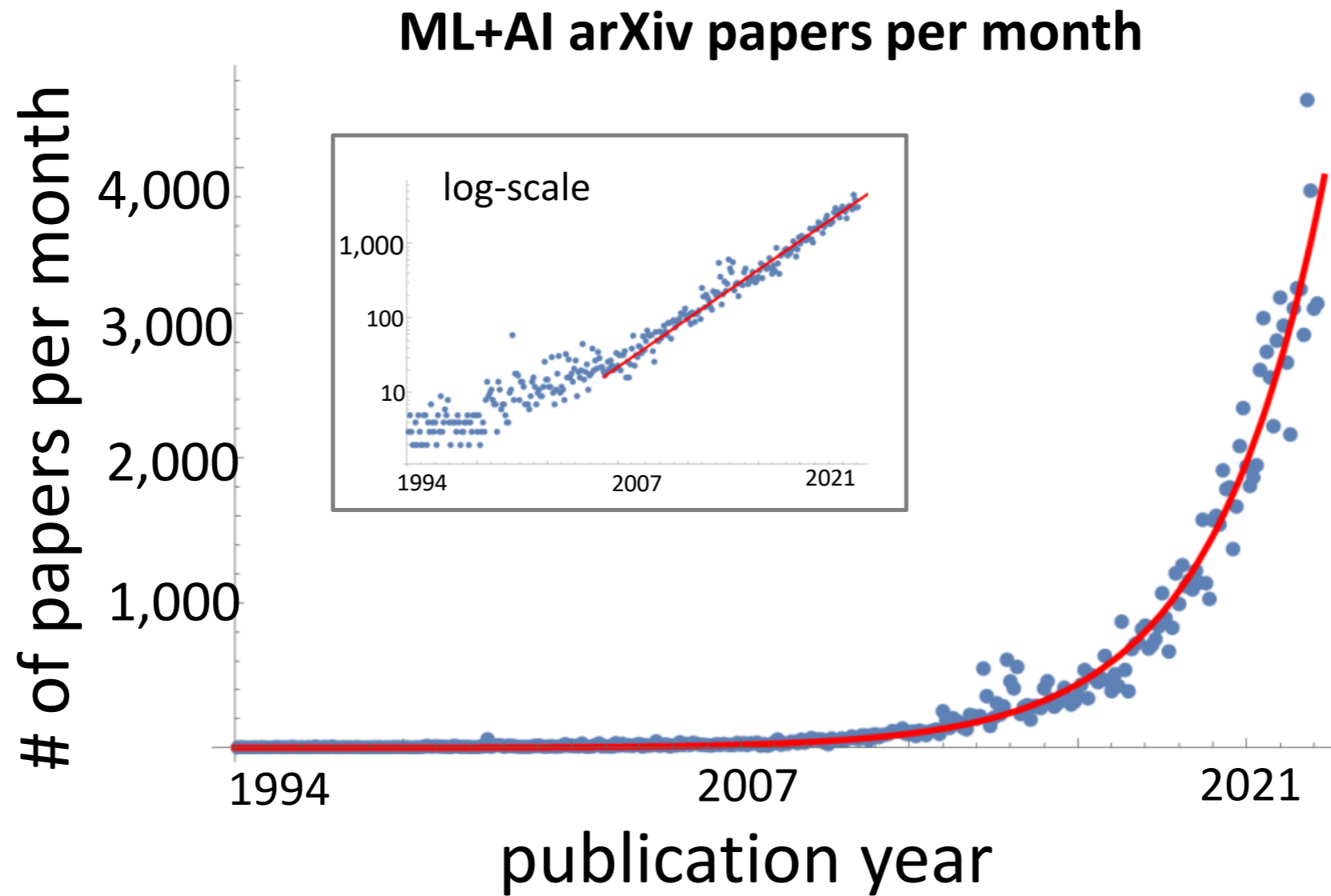
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ML4Jets2023

- Anomalies
- Astrophysics and Astronomy
- Closing
- Community & Datasets
- Energy Correlators, Safety &
- Generative
- Generative Models and Simulation
- Generative: Diffusion Models
- Generative: Partons and Phase
- Generative: Sets and Point Clouds
- Low Latency and Elementary Inputs
- Measurements & Observables
- Opening
- Physics ex machina: Machine
- Reconstruction
- Reconstruction & Representation
- Remote Discussion
- Results, Observables & Techniques
- Super Resolution, Reweighting, and
- Taggers & Understanding
- Tagging Techniques
- Theory & Understanding
- Uncertainties, Calibration & Theory
- Workshop Photo

The rise of machine learning



Predicting the Future of AI with AI: High-quality link prediction in an exponentially growing knowledge network, Krenn et al, arXiv:2210.00881 [cs.AI]

Particle physics in 2023

- The Standard Model has been confirmed with high accuracy up to several TeV.
 - A standard model-like Higgs boson has been discovered.
 - No conclusive sign of physics beyond the Standard Model has been found.
- New physics is **heavy**, with new particles at a large mass scale $\Lambda \gg E_{\text{LHC}}$
- New physics is **subtle** (small cross sections, novel signatures,...)

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To explore physics beyond the Standard Model, we need

- precision and
- model-independence.

What drives scientific progress?



Thomas Kuhn

Paradigm shifts are triggered by
new ideas and concepts.

What drives scientific progress?



Thomas Kuhn

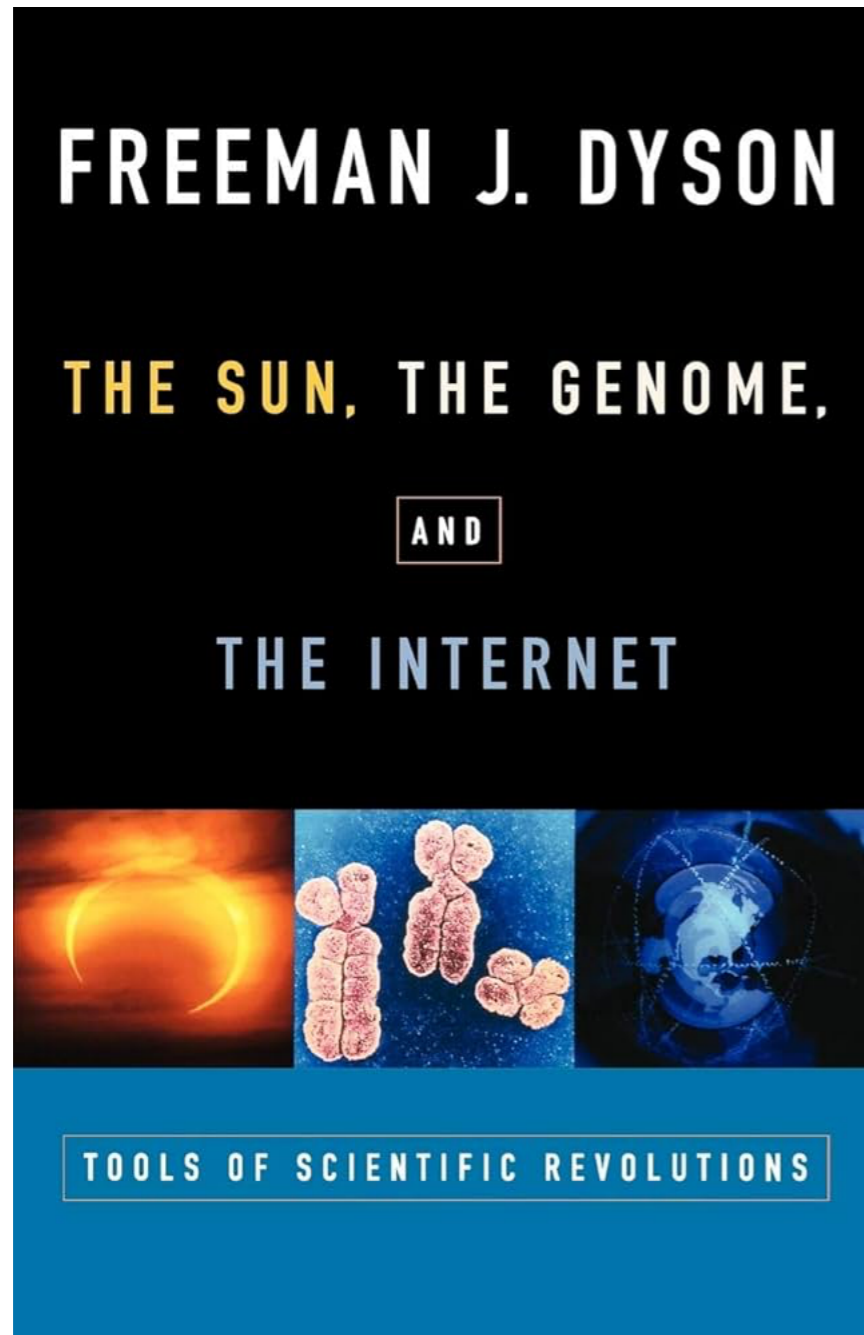
Paradigm shifts are triggered by new ideas and concepts.



Peter Galison

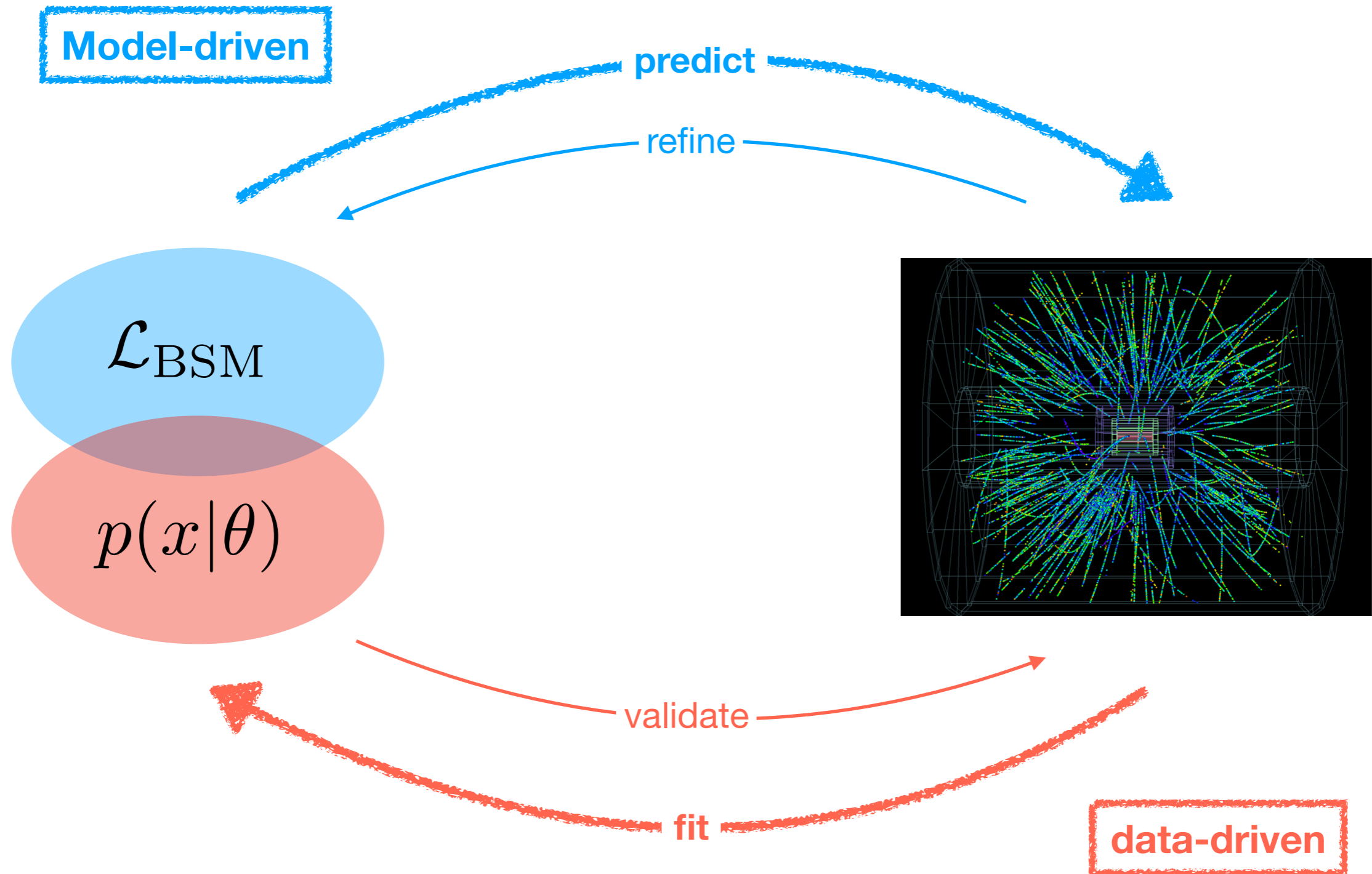
Progress in science is driven by new technologies and tools.

What drives scientific progress?



“New directions in science are launched by new tools much more often than by new concepts. The effect of a concept-driven revolution is to explain old things in new ways. The effect of a tool-driven revolution is to discover new things that have to be explained.”

The scientific method



Machine learning in physics

- What type of machine learning architectures are best suited for finding new and subtle phenomena in large amounts of complex data?
- How can data-driven approaches be used to identify novel physics principles (theories, models)?

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BERLIN'S WONDERFUL HORSE

He Can Do Almost Everything but Talk—
How He Was Taught.

Special Correspondence THE NEW YORK TIMES.

BERLIN, Aug. 23.—In an out-of-the-way part of the German capital a horse is now shown which has stirred up the scientific, military, and sporting world of the Fatherland. It should be said at the very outset that the facts in this article are not drawn from the imagination, but are based upon true observations and can be verified by Dr. Studt, Prussian Minister of Education; by the famous zoologist, Prof. Moebius, director of the Prussian Natural History Museum, and by other eminent scientific and military authorities. I had occasion to-day to see a performance of the animal which was given in the presence of the young Duke of Sachse-Coburg-Gotha.

Hans, the wonderful stallion, is nine years old and is the property of a Herr von Osten, a retired school teacher. The horse has never been used for riding or driving. For over four years Herr von Osten has given the animal systematic instruction such as he would give to a child. The industrious pedagogue is the owner of a tenement house in the northern part of Berlin, and there he lives. The animal is quartered in a small shed adjoining a court where he is shown.

Some years ago the neighborhood was astonished by observing the training which Herr von Osten gave his animal. They beheld him and Hans at a certain hour of the day standing in the court before a blackboard and counting machine. Herr von Osten, undismayed by ridicule, (for by his method he had gained the reputation of being an old crank,) instructed the stallion by showing him the balls on the machine, and influencing him to indicate a number by stamping down his right hoof. At the same time, while the horse was doing this, his instructor spoke the name of the number. Then every time Hans put down his foot correctly he would be rewarded by a carrot or a piece of sugar. All other things the intelligent animal learned by seeing certain objects and at the same time hearing their names. In this way words to him

became signs for visible objects, and he used footsteps as signs for his perceptions, according to the same psychic laws as we use a language to make others understand.

After Herr von Osten had taught Hans this simple sign language, the foundation for further education was established. He put before him gold, silver, and copper coins, and taught him to indicate gold pieces by one movement of the foot, silver with two, and copper with three steps. When, for example, three coins were placed in a row, Hans stamped down his foot

three times when asked the number. He is also able to distinguish coins according to signs. When asked to give the value of a one-mark piece touched by his teacher, he moves his foot once, for a two-mark piece twice, &c.

Hans is an expert in numbers, even being able to figure fractions. He answers correctly the number of 4's in 8, in 16, in 30, &c. When asked how many 3's there are in 7 he stamps down his foot twice and for the fraction once. Then, when 5 and 9 are written under each other on the blackboard and he is asked to add the sum, he answers correctly.

Hans is also capable of distinguishing persons. He told the number of girls and officers standing in a line.

A remarkable thing happened yesterday. An officer was pointed out, and Hans was told, "That is Count Dohna." Half an hour later the same man was pointed out to him, and when asked for his name the horse picked out the letters D-o from the blackboard. Herr von Osten, however, having the name Doenhof in mind, wanted to help the animal by uttering "Do." Uninfluenced, however, Hans spelt out correctly "Dohna." In the same manner to-day Hans was introduced to the Prince of

Sachse-Coburg-Gotha, and also gave his name correctly.

The versatility of Hans in other directions is astonishing. He can distinguish between straw and felt hats, between canes and umbrellas. He knows the different colors. One beholds several colored rags fastened on a string. A cavalry officer places himself before the horse and Hans is asked to state the color of his cap. The horse answers by stamping his foot down three times, the color of the third rag, which, like the cap, is red.

Hans has also been taught to distinguish tones. The various tones of the musical scale are numbered, and he recognizes their position by his usual method.

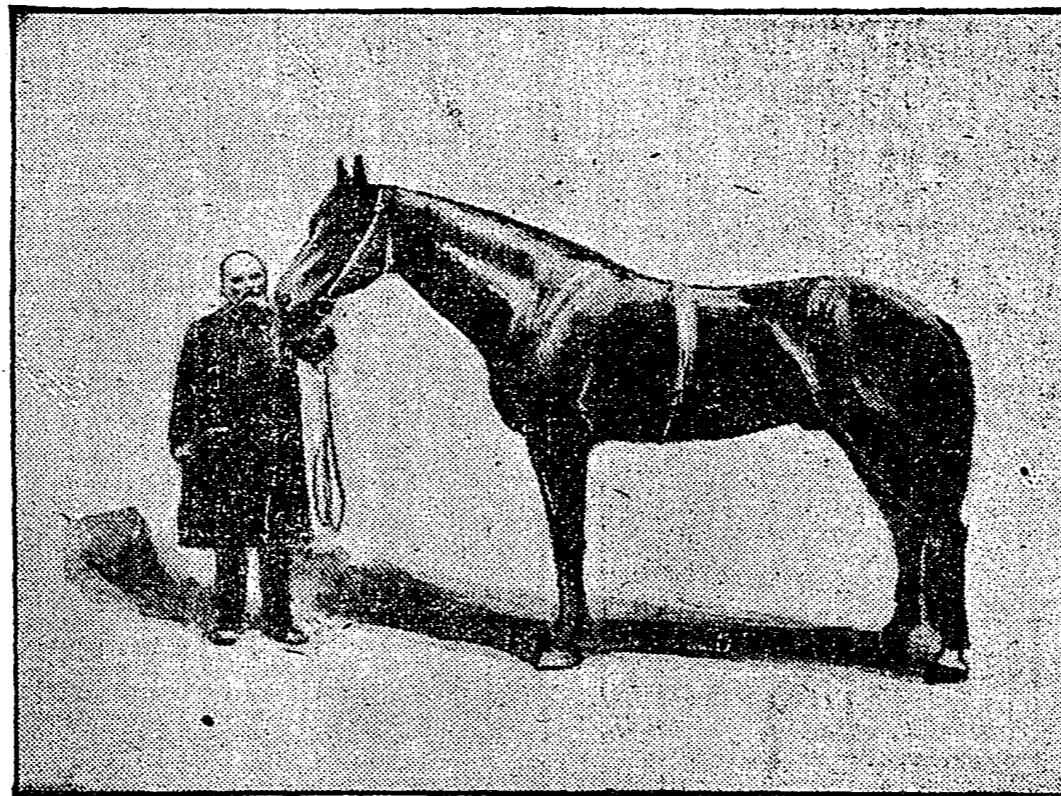
Hans can tell the time on a watch and can indicate the exact hour. At the test yesterday he recognized persons from photographs. Herr von Osten placed persons in a row who had given him their photographs; then put the picture before the horse and asked him to indicate the position of the person in the line. Again Hans recognized the gentleman in civilian clothes who the day before had been introduced to him in uniform. He knows the names of the months and indicates the day of the week by putting down his foot, Sunday once, Monday twice, &c.

Prof. Moebius, the eminent zoologist, has this to say about Hans:

"He possesses the ability to see sharply, to distinguish mental impressions from each other, to retain them in his memory, and to utter them by his hoof language. Of course, not by himself has he learned all this, but by methodical instruction of a human intelligence, who has developed the highly intelligent senses of the species horse. For wild horses, not trained, in the same manner utilize their physical and psychic faculties as does Hans, to satisfy their desire for food.

"Herr von Osten has succeeded in training Hans by cultivating in him a desire for delicacies. This desire is aroused by questions and finger signs, according to which the stallion acts, in order to satisfy his aroused desire, for as soon as he puts his foot down he snaps for the delicacy in the hand of his master. I doubt whether the horse really takes pleasure in his studies. He follows entirely mental impressions which he receives from the surroundings and which satisfy his wants."

Hans is the second horse Herr von Osten has trained. He claims that any horse of fair intelligence can be so taught. Herr von Osten's training is done purely from a scientific standpoint, and he told me that he greatly regretted the premature publicity given to his work. By the time this article is in print the Kaiser, who has heard with interest of this horse prodigy, will have seen the animal. EDWARD T. HEYN.



HANS AND HIS OWNER, HERR VON OSTEN.

The New York Times

Published: September 4, 1904
Copyright © The New York Times

ARTICLE

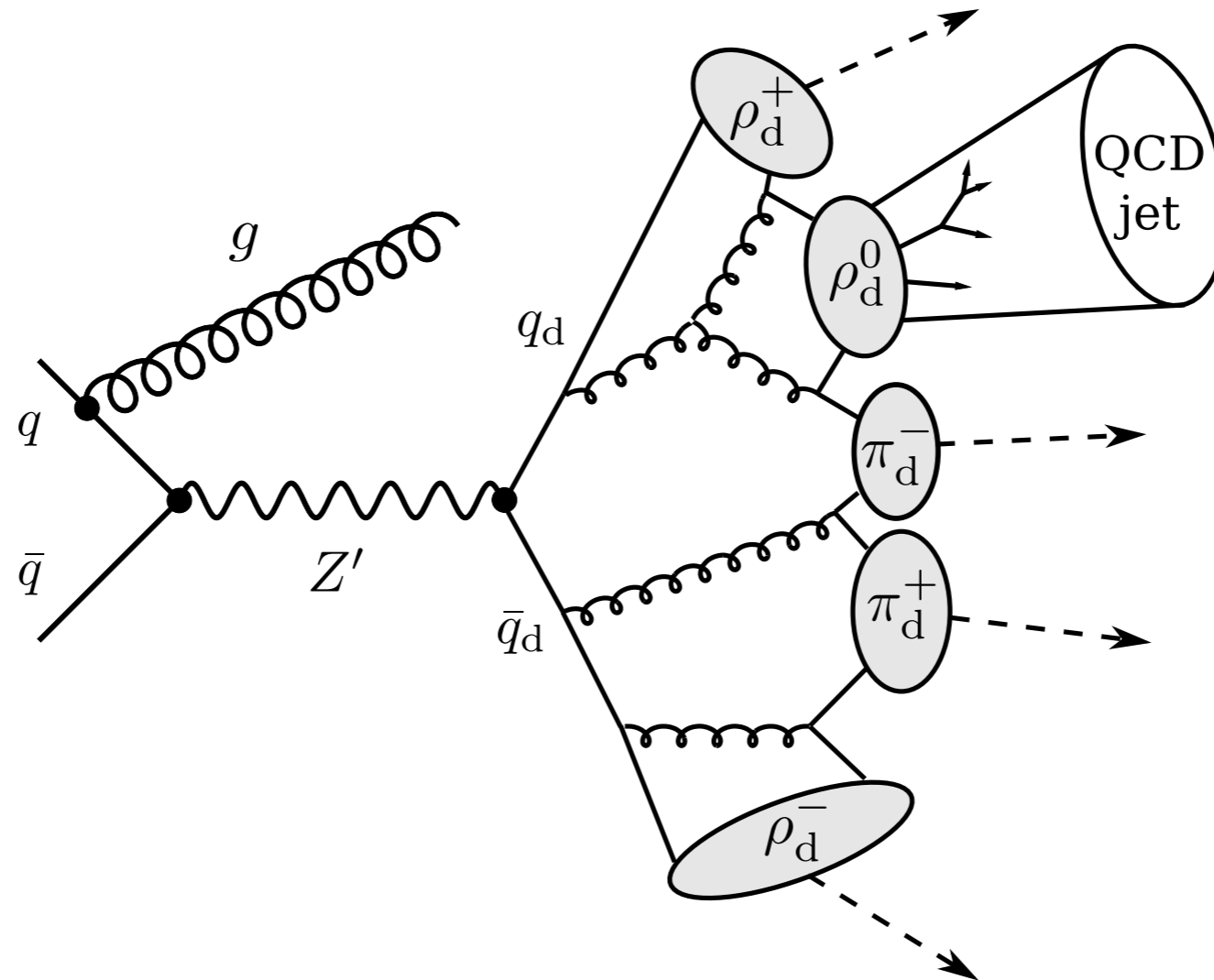
<https://doi.org/10.1038/s41467-019-08987-4>

OPEN

Unmasking Clever Hans predictors and assessing what machines really learn

Sebastian Lapuschkin¹, Stephan Wäldchen², Alexander Binder³, Grégoire Montavon², Wojciech Samek¹ & Klaus-Robert Müller^{2,4,5}

Current learning machines have successfully solved hard application problems, reaching high accuracy and displaying seemingly intelligent behavior. Here we apply recent techniques for explaining decisions of state-of-the-art learning machines and analyze various tasks from computer vision and arcade games. This showcases a spectrum of problem-solving behaviors ranging from naive and short-sighted, to well-informed and strategic. We observe that standard performance evaluation metrics can be oblivious to distinguishing these diverse problem solving behaviors. Furthermore, we propose our semi-automated Spectral Relevance Analysis that provides a practically effective way of characterizing and validating the behavior of nonlinear learning machines. This helps to assess whether a learned model indeed delivers reliably for the problem that it was conceived for. Furthermore, our work intends to add a voice of caution to the ongoing excitement about machine intelligence and pledges to evaluate and judge some of these recent successes in a more nuanced manner.



Bernreuther, Kahlhoefer, MK, Tunney, Strongly interacting dark sectors in the early Universe and at the LHC through a simplified portal, JHEP 01 (2020) 162

Dynamic Graph CNN for Learning on Point Clouds

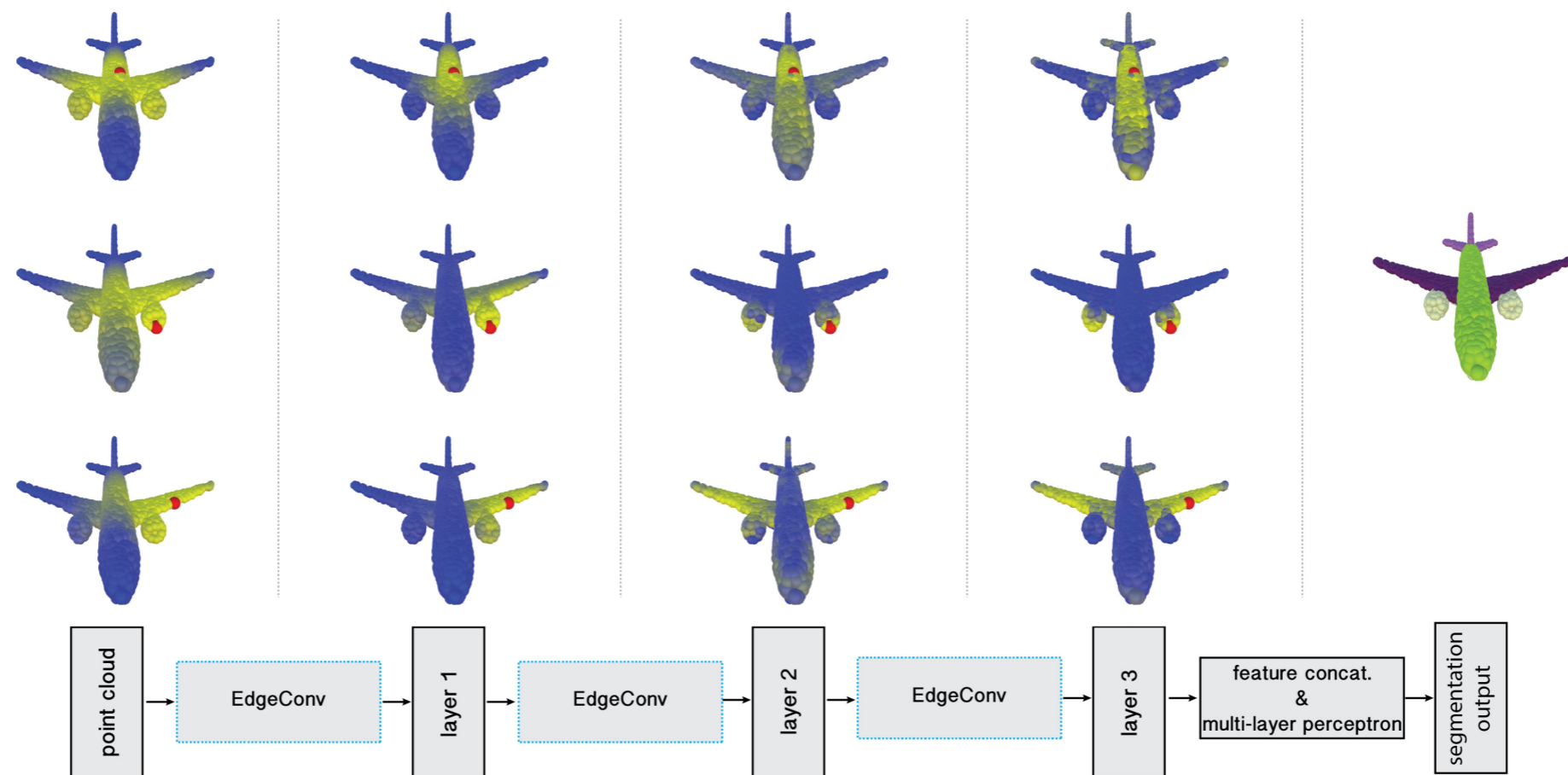
YUE WANG and YONGBIN SUN, Massachusetts Institute of Technology

ZIWEI LIU, UC Berkeley/ICSI

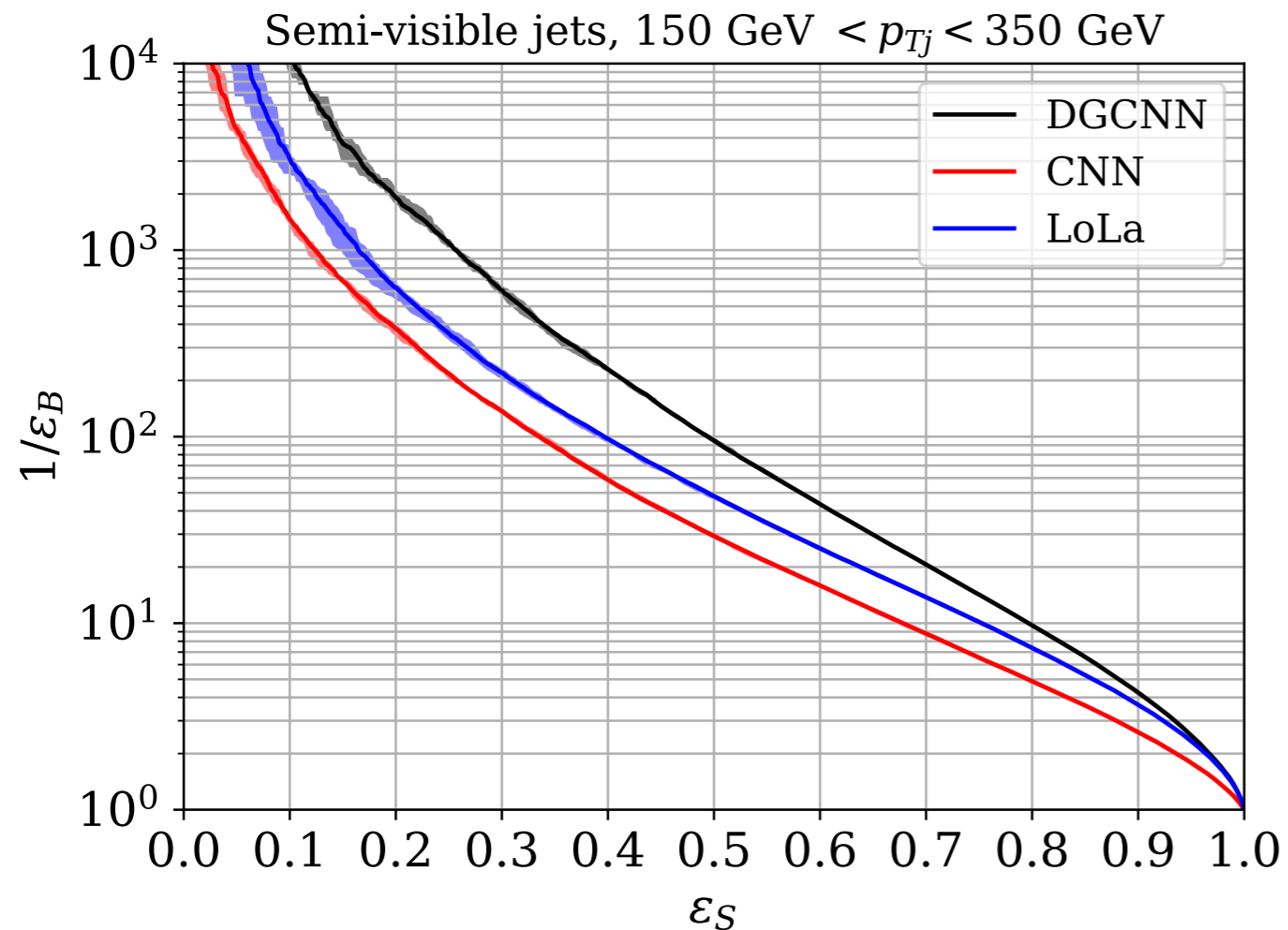
SANJAY E. SARMA, Massachusetts Institute of Technology

MICHAEL M. BRONSTEIN, Imperial College London/USI Lugano

JUSTIN M. SOLOMON, Massachusetts Institute of Technology



See also “ParticleNet: Jet Tagging via Particle Clouds”, Qu, Gouskos, PRD 101, 056019 (2020)



“For a cloud of particles representing a jet, it appears natural that the correlation of particles which are not close in the initial features, can be important for the classification of the jet. The dynamic update enables the network to link those initially distant particles.”

Bernreuther, Finke, Kahlhoefer, MK, Mück, arXiv:2006.08639 [hep-ph]

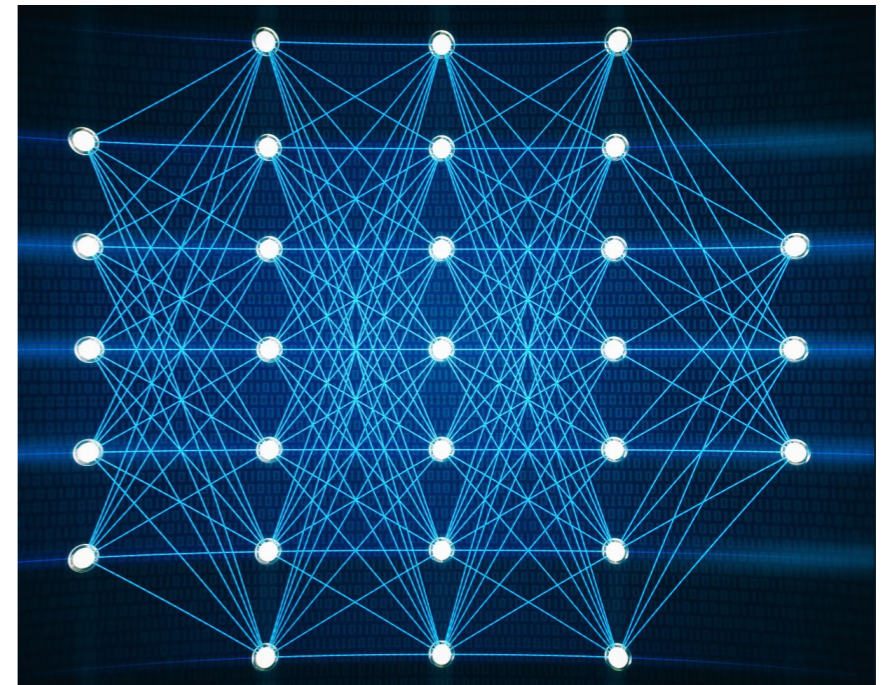
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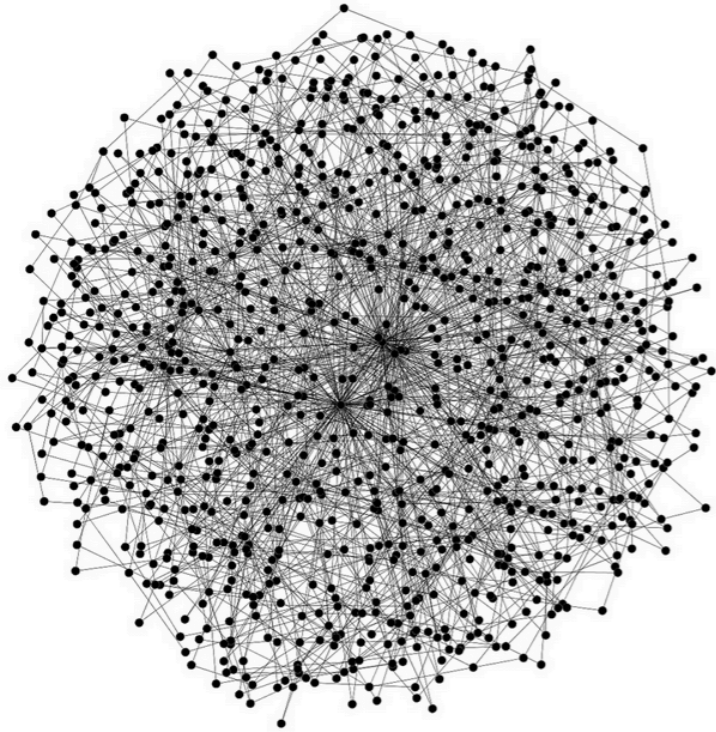
Connections: AI for physics and physics for AI



$$Z = \int \mathcal{D}\phi e^{S(\phi)}$$



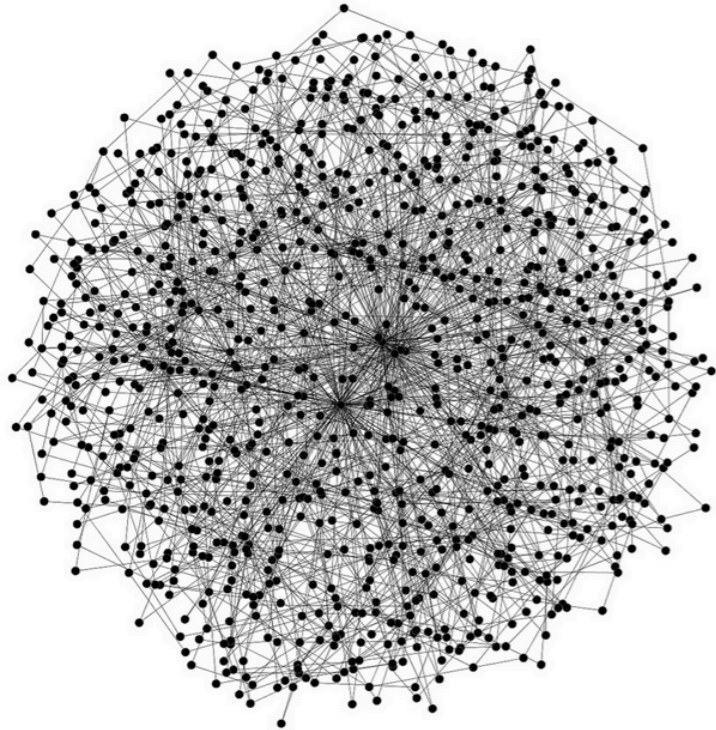
Field theory for neural networks



$$\frac{d}{dt}x_i(t) = -x_i(t) + \sum_j^N W_{ij}\phi(x_j(t)) + \xi_i(t)$$

Sompolinsky, Crisanti, Sommers (1988)

Field theory for neural networks



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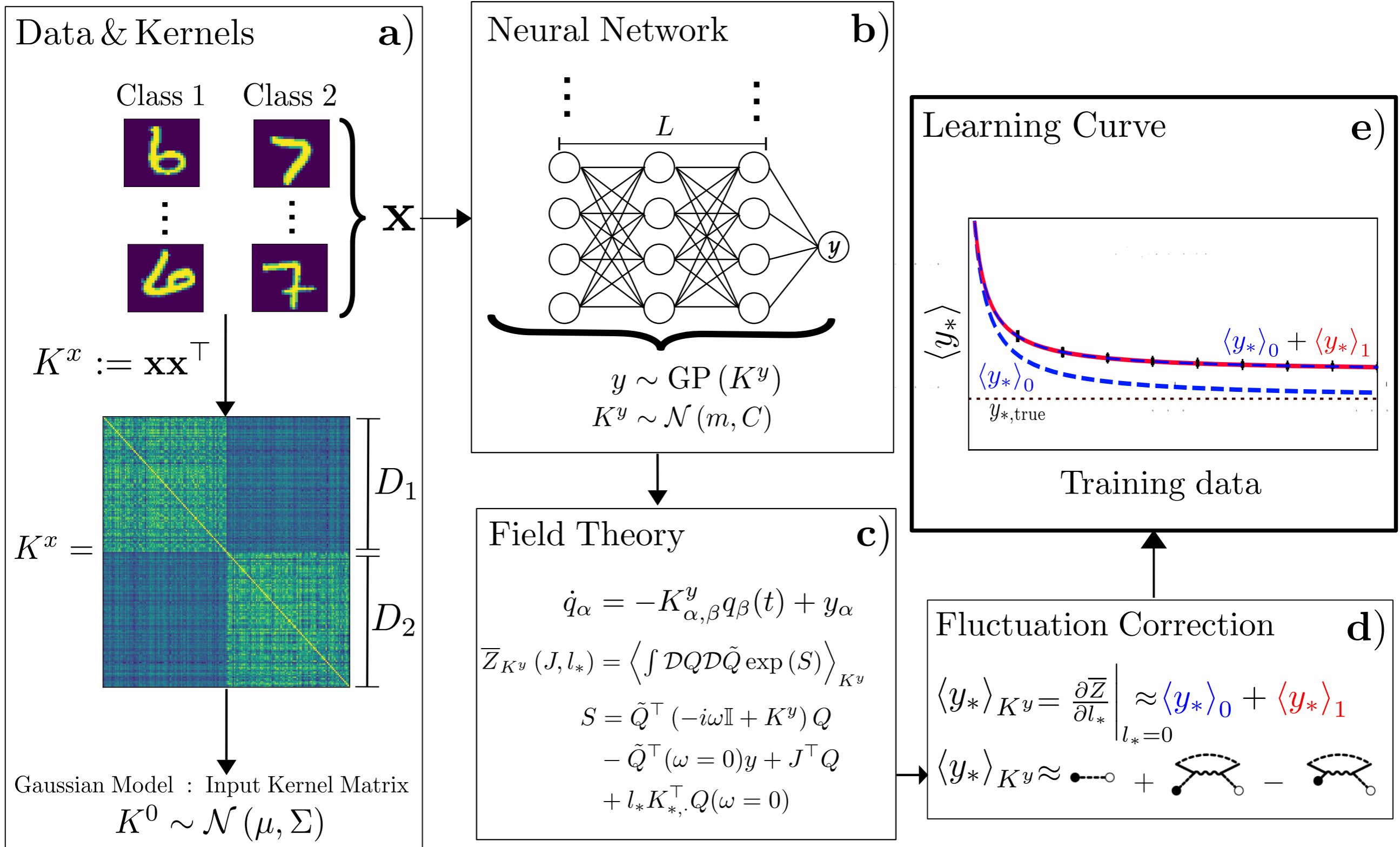
Sompolinsky, Crisanti, Sommers (1988)

Probability for the time evaluation $x(t)$:
$$p[x(t)] = \int \mathcal{D}\tilde{x} e^{S(x, \tilde{x})}$$

with an action of the form

$$S(x, \tilde{x}) = \sum_i \left(\int dt \tilde{x}_i(t) \left(\frac{d}{dt} + 1 \right) x_i(t) + \frac{D}{2} \int dt \tilde{x}_i(t) \tilde{x}_i(t) - \int dt \tilde{x}_i(t) \sum_j W_{ij} \phi(x_j(t)) \right)$$

Martin, Siggia, Rose (1973), De Dominicis (1976), Janssen (1976)



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CHRIS ANDERSON SCIENCE 06.23.08 12:00 PM

THE END OF THEORY: THE DATA DELUGE MAKES THE SCIENTIFIC METHOD OBSOLETE



On scientific understanding with artificial intelligence

Mario Krenn, Robert Pollice, Si Yue Guo, Matteo Aldeghi, Alba Cervera-Lierta, Pascal Friederich, Gabriel dos Passos Gomes, Florian Häse, Adrian Jinich, AkshatKumar Nigam, Zhenpeng Yao  and Alán Aspuru-Guzik 

Abstract | An oracle that correctly predicts the outcome of every particle physics experiment, the products of every possible chemical reaction or the function of every protein would revolutionize science and technology. However, scientists would not be entirely satisfied because they would want to comprehend how the oracle made these predictions. This is scientific understanding, one of the main aims of science. With the increase in the available computational power and advances in artificial intelligence, a natural question arises: how can advanced computational systems, and specifically artificial intelligence, contribute to new scientific understanding or gain it autonomously? Trying to answer this question, we adopted a definition of ‘scientific understanding’ from the philosophy of science that enabled us to overview the scattered literature on the topic and, combined with dozens of anecdotes from scientists, map out three dimensions of computer-assisted scientific understanding. For each dimension, we review the existing state of the art and discuss future developments. We hope that this Perspective will inspire and focus research directions in this multidisciplinary emerging field.

understood and generalized by human scientists. Third, AI acts as an agent of understanding. AI reaches new scientific insight and — importantly — can transfer it to human researchers. Although there have not yet been any examples of AI acting as a true ‘agent of understanding’ in science, we outline important characteristics of such a system and discuss possible ways to achieve it.

In the first two dimensions, the AI enables humans to gain new scientific understanding, whereas in the last, the machine gains understanding itself. Distinguishing between these classes allows us to map out a vibrant and mostly unexplored field of research, and will hopefully guide direction for future AI developments in the natural sciences.

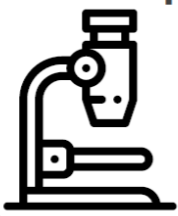

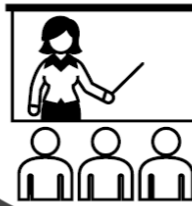
The focus of this Perspective is how advanced computational systems and AI specifically can contribute to new scientific understanding. There are many related, interesting topics that we cannot cover here. For example, we will not discuss the relationship between scientific understanding and cognitive science, but refer the reader to a good overview¹⁴. Furthermore, we will only discuss ‘understanding’ in the context of

How can androids contribute to new scientific understanding?


Philosophy of Science
What is scientific understanding?

Survey of Scientists
How do scientists gain understanding?

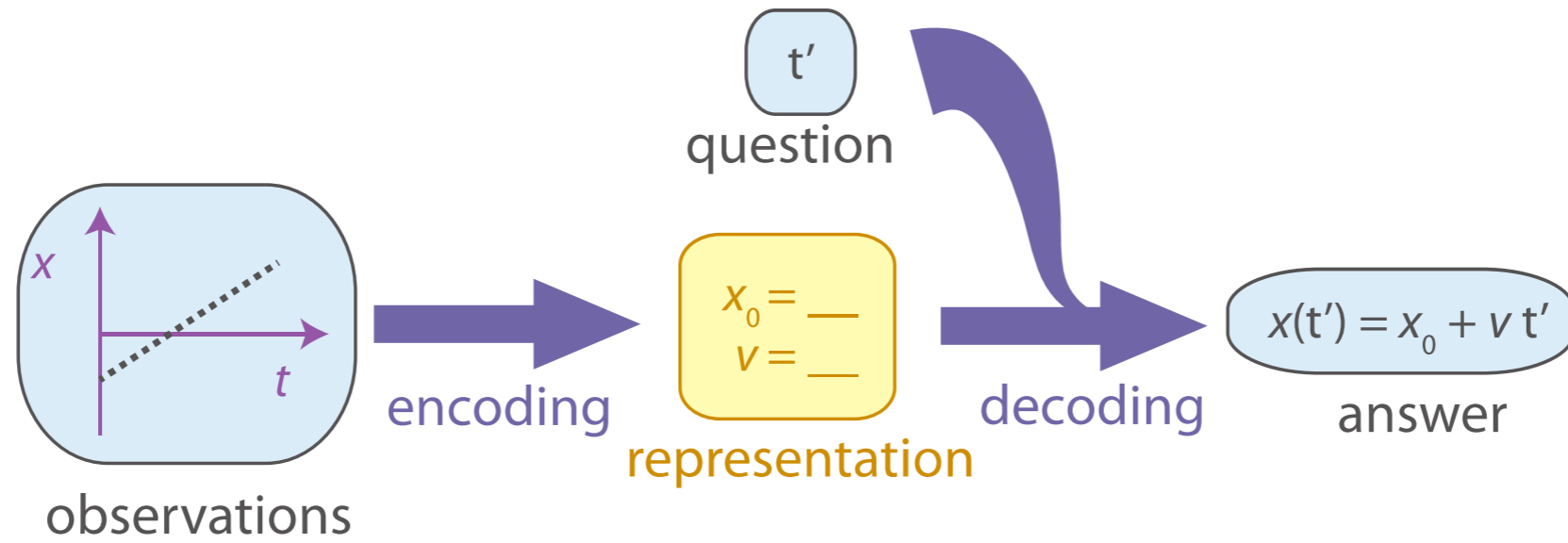
Three Dimensions of Computer-Assisted Scientific Understanding

- Computational Microscope 
- Resource of Inspiration 
- Agent of Understanding 

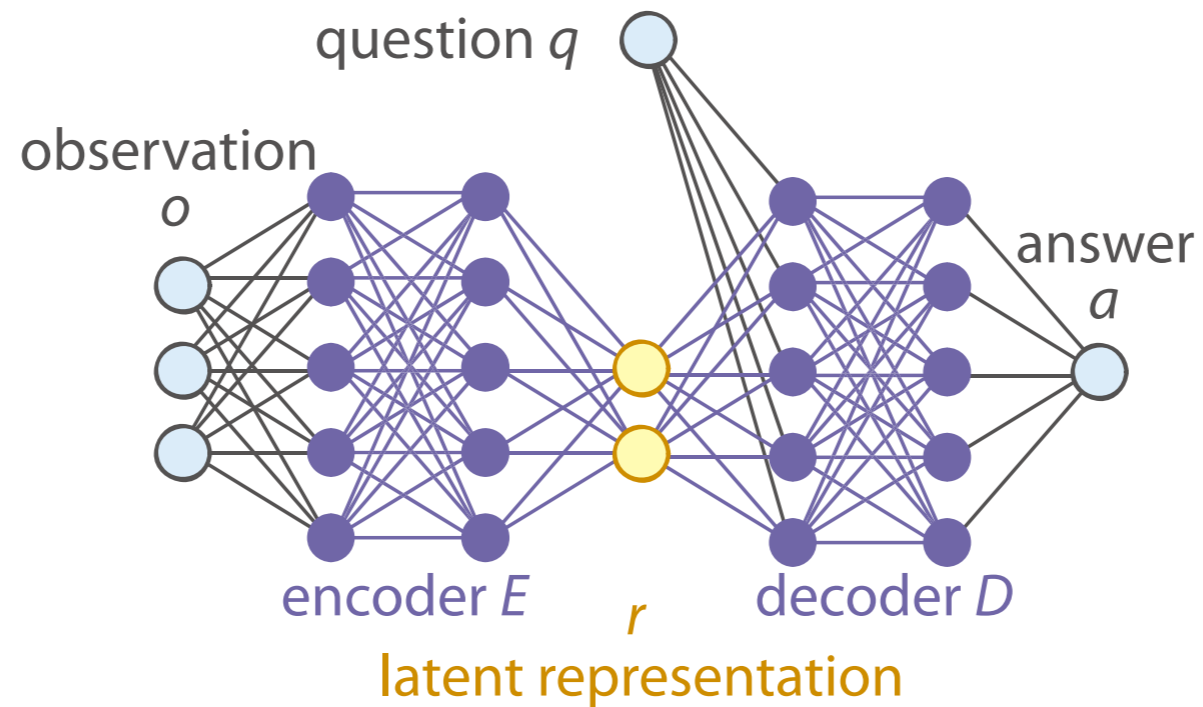
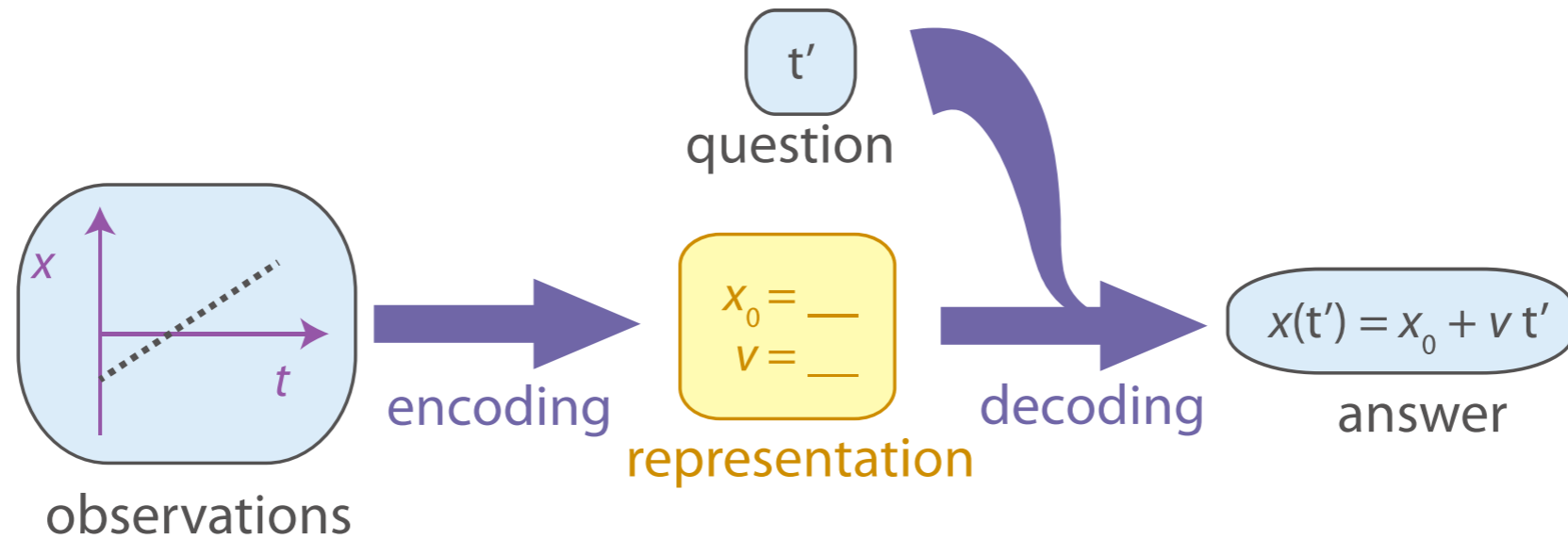
Roadmap Towards Android Scientific Understanding



Agent of understanding?

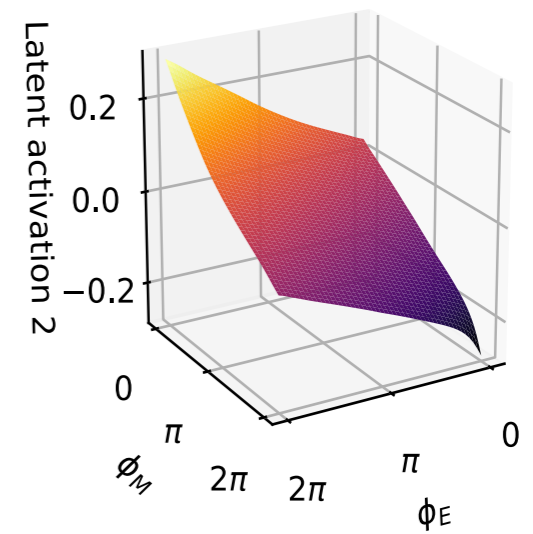
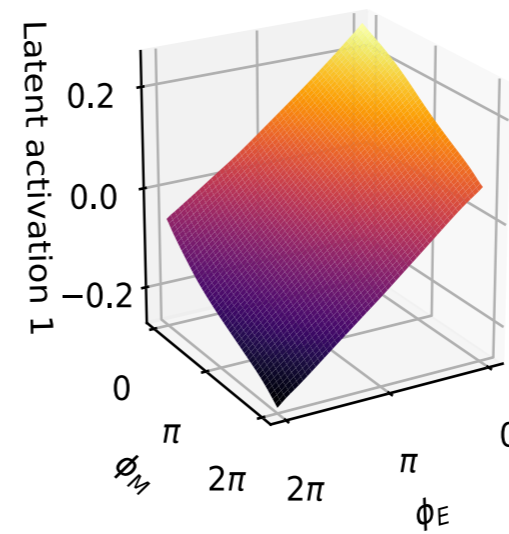
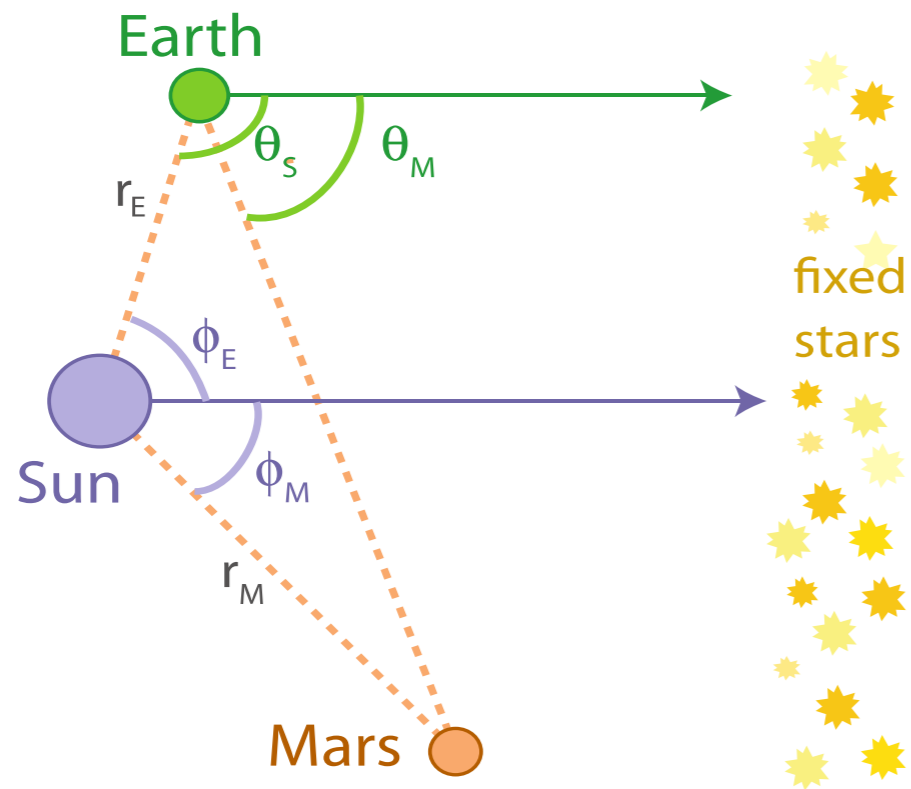


Agent of understanding?



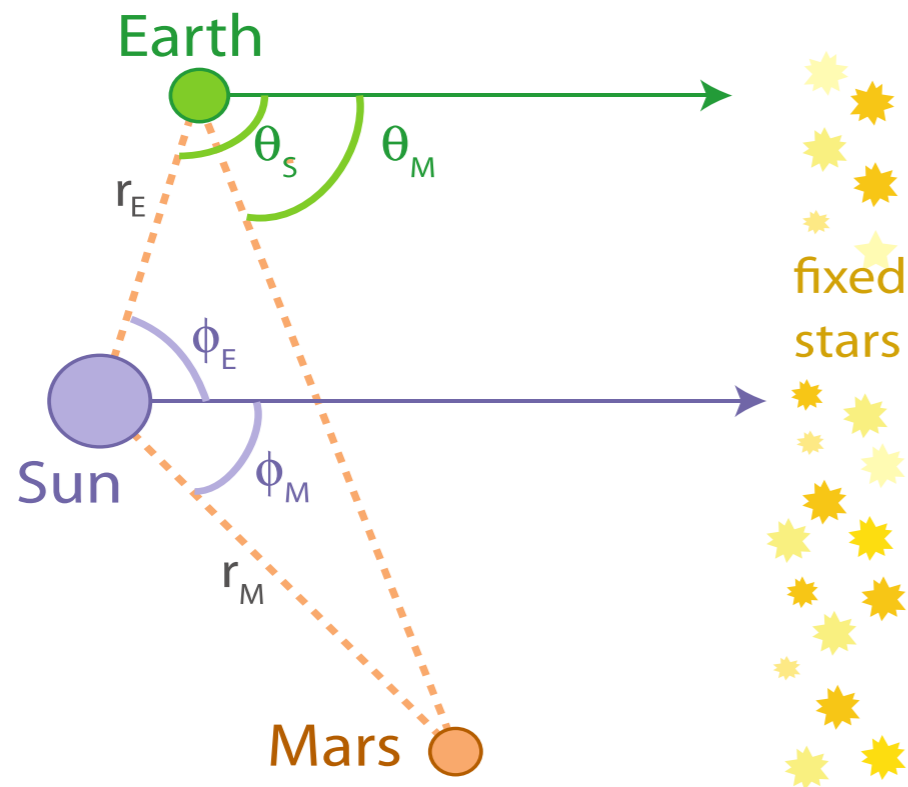
Iten, Metger, Wilming, del Rio, Renner, Phys. Rev. Lett. 124, 010508 (2020)

Agent of understanding?



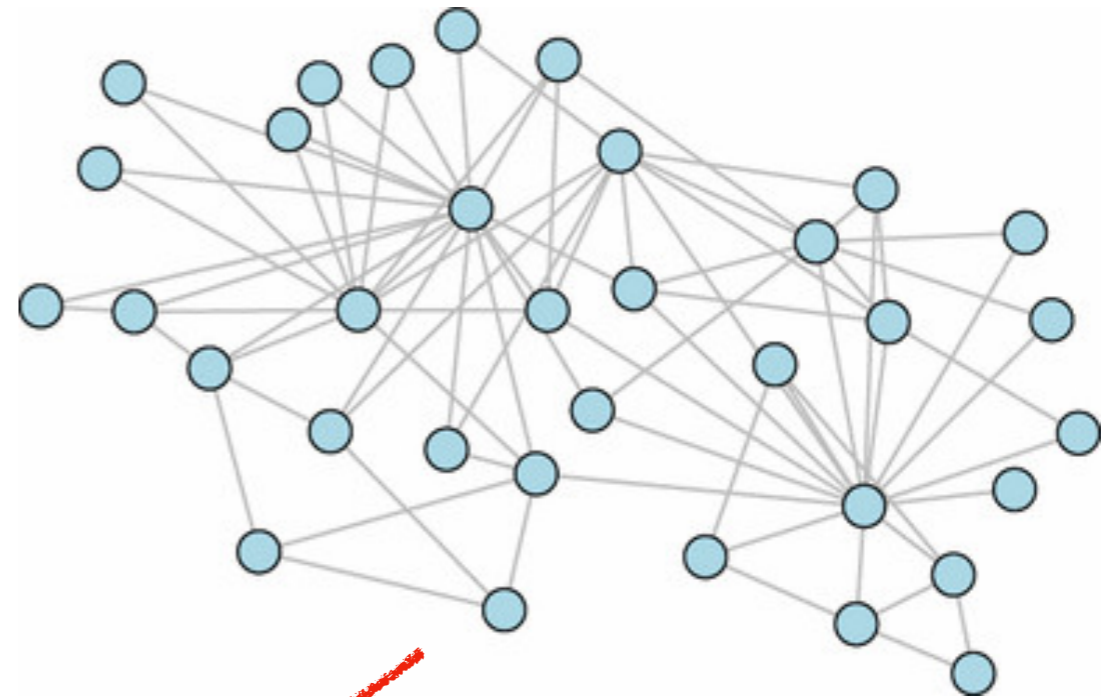
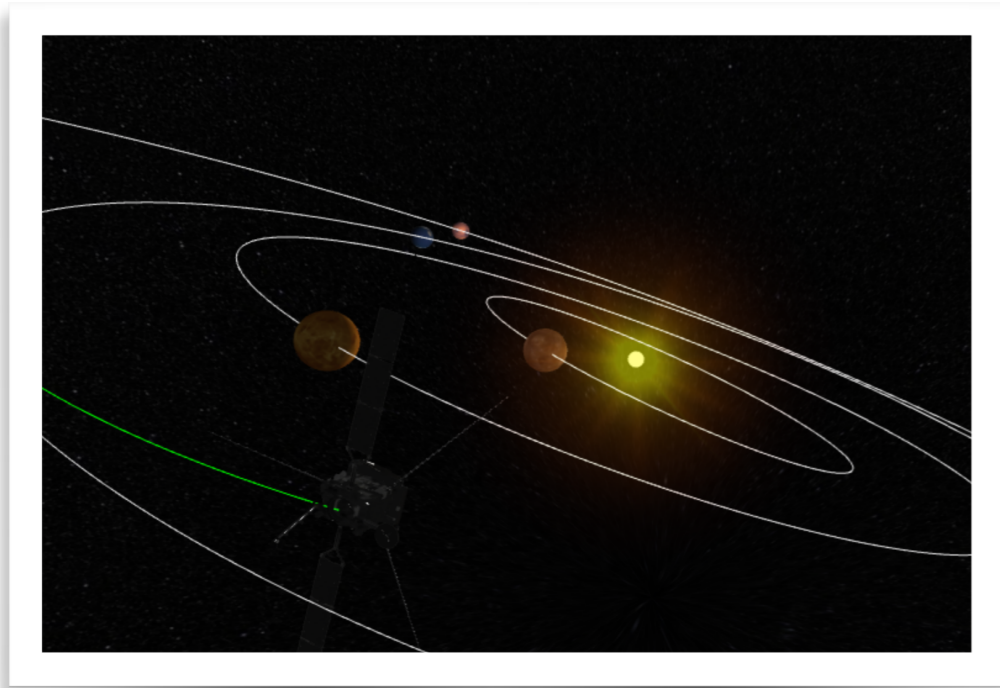
Iten, Metger, Wilming, del Rio, Renner, Phys. Rev. Lett. 124, 010508 (2020)

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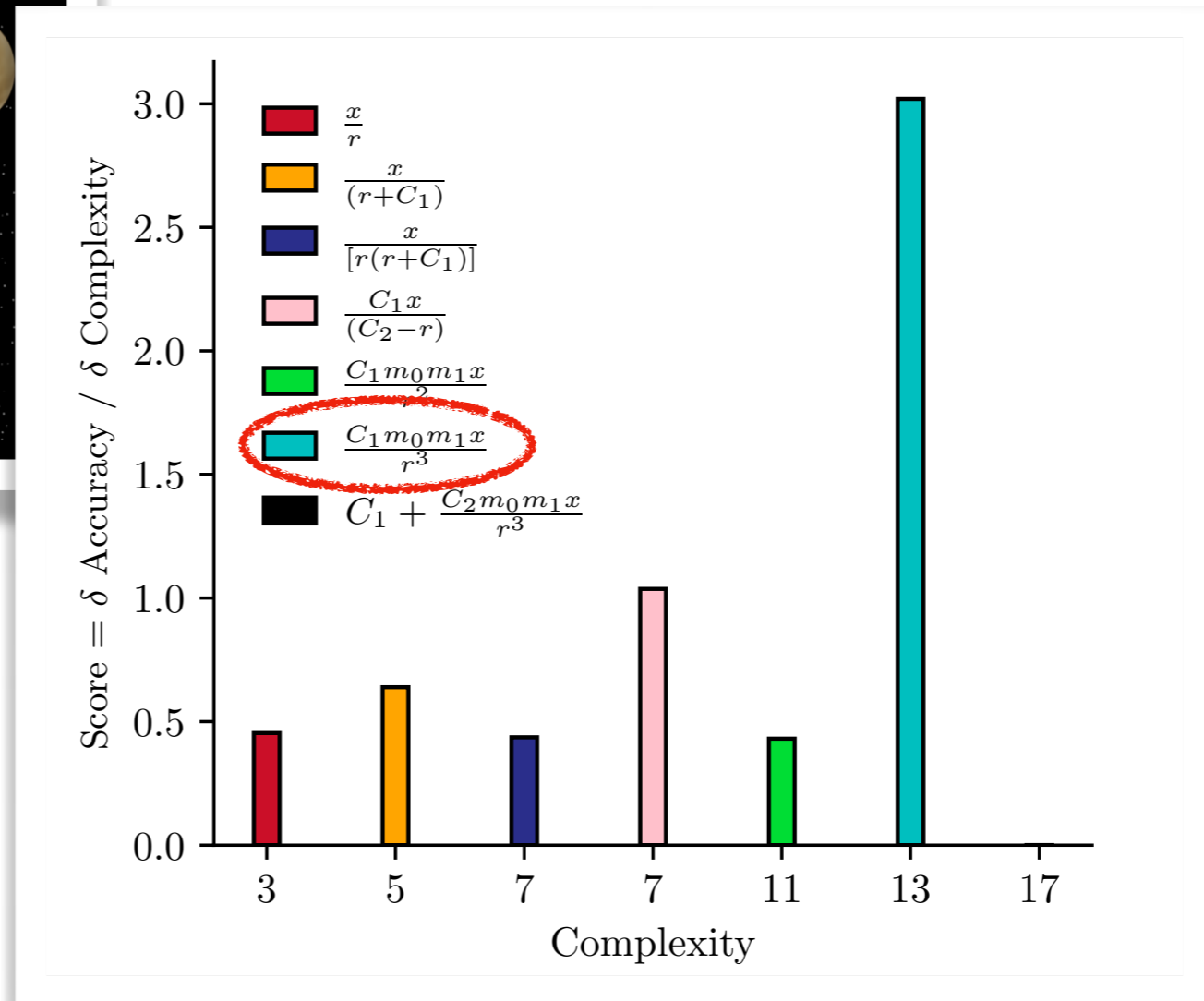
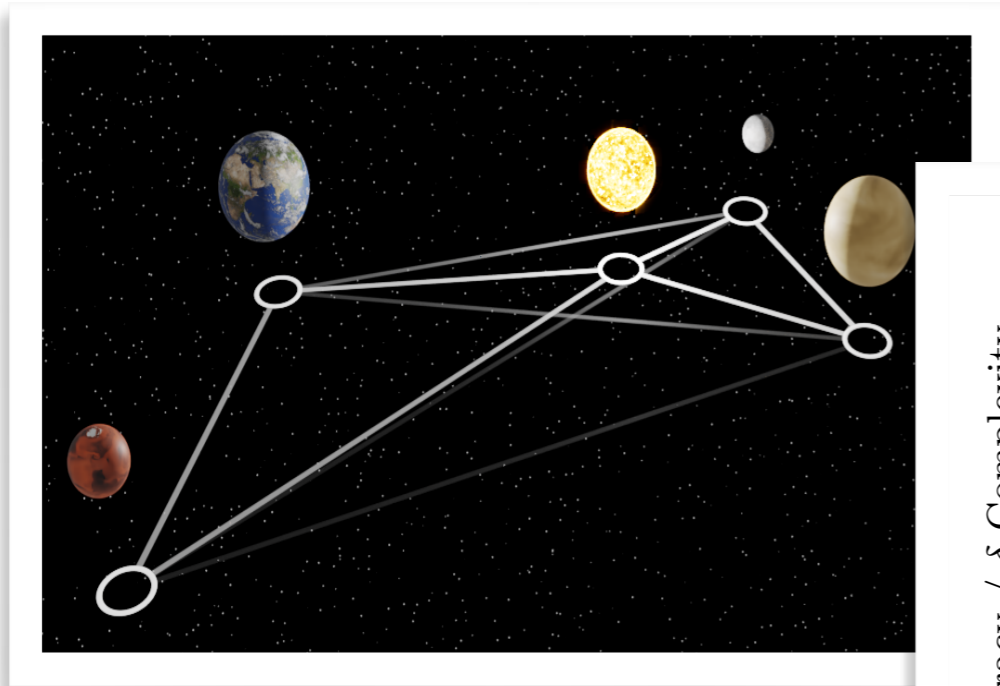
Agent of understanding?



$$F = G \frac{m_1 m_2}{r^2}$$

Lemos, Jeffrey, Cranmer, Ho, Battaglia, arXiv:2202.02306 [astro-ph.EP]

Agent of understanding?



Lemos, Jeffrey, Cranmer, Ho, Battaglia, arXiv:2202.02306 [astro-ph.EP]

Some final thoughts...

Particle physics is **not** about testing any particular kind of prediction about physics beyond the Standard Model.

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Particle physics is **not** about testing any particular kind of prediction about physics beyond the Standard Model.

The new era of big data and powerful machine learning tools offers us the opportunity to conduct basic research in a way that is no longer limited to pre-defined paths, but is more open, exploratory and driven by data.



A painting of a hiker standing on a rocky peak, looking out over a vast, misty landscape. The hiker is wearing a green jacket and dark pants, and is holding a walking stick. The landscape is filled with rolling hills, mountains, and a thick layer of mist or fog. The sky is a pale, hazy blue. The overall mood is serene and contemplative.

Thanks to

Freya, Andrea, Frank, Andreas,
Matthias and in particular Gregor!