

# Machine Learning in Particle Physics



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AI generated image by  
Việt Vun Vút





Hà Ly Phúc Toàn

Harry Potter

ART  
AIhug.ART  
[fb.com/AIhugART](https://fb.com/AIhugART)

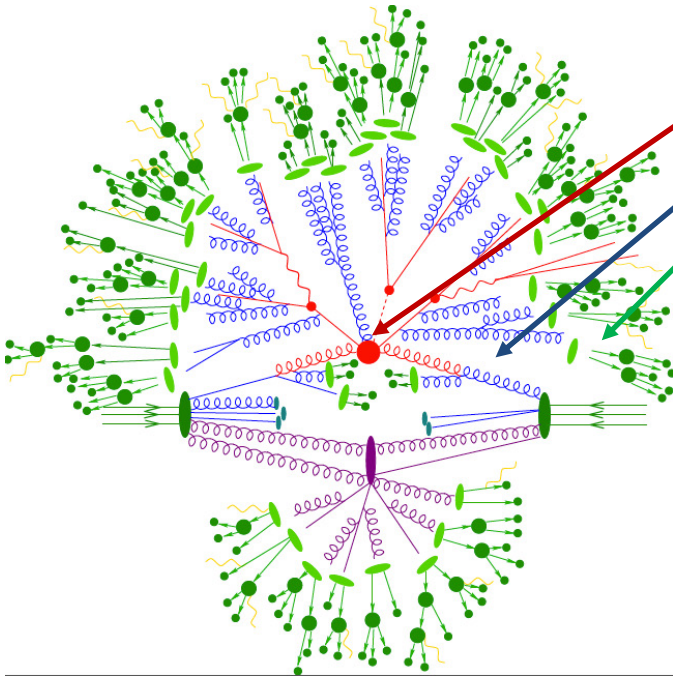
Ảnh bảo cho người xem. Sản phẩm này do AI Art Generator tạo ra mang tính chất tham khảo để lên ý tưởng, dùng để học hoặc truyền cảm hứng, không dùng cho mục đích thương mại. Đọc kỹ hướng dẫn trước khi xem/ sử dụng.



# How is ML used in particle physics?

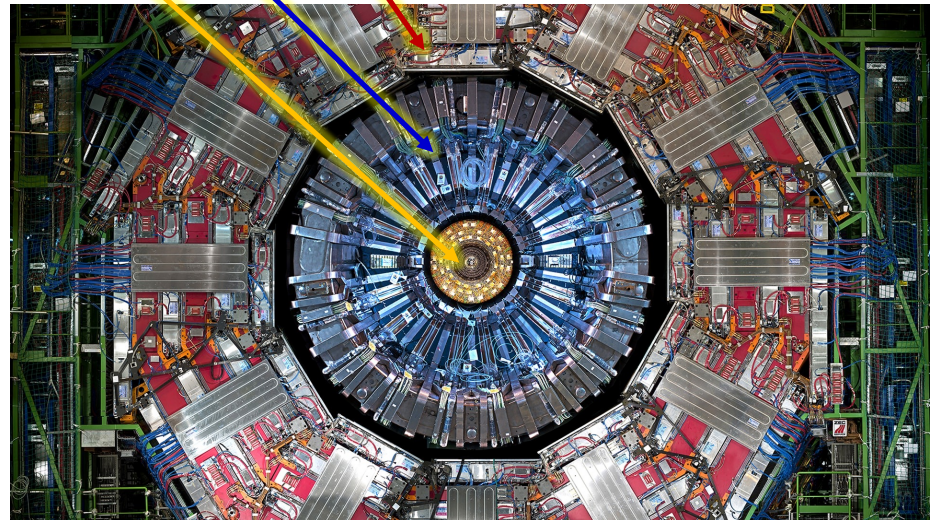
Main use so far is in **collider physics**

- Can generate billions of simulated events on a laptop
- Simulations accurate over **20 orders of magnitude!**
- Unheard of in any other area of science

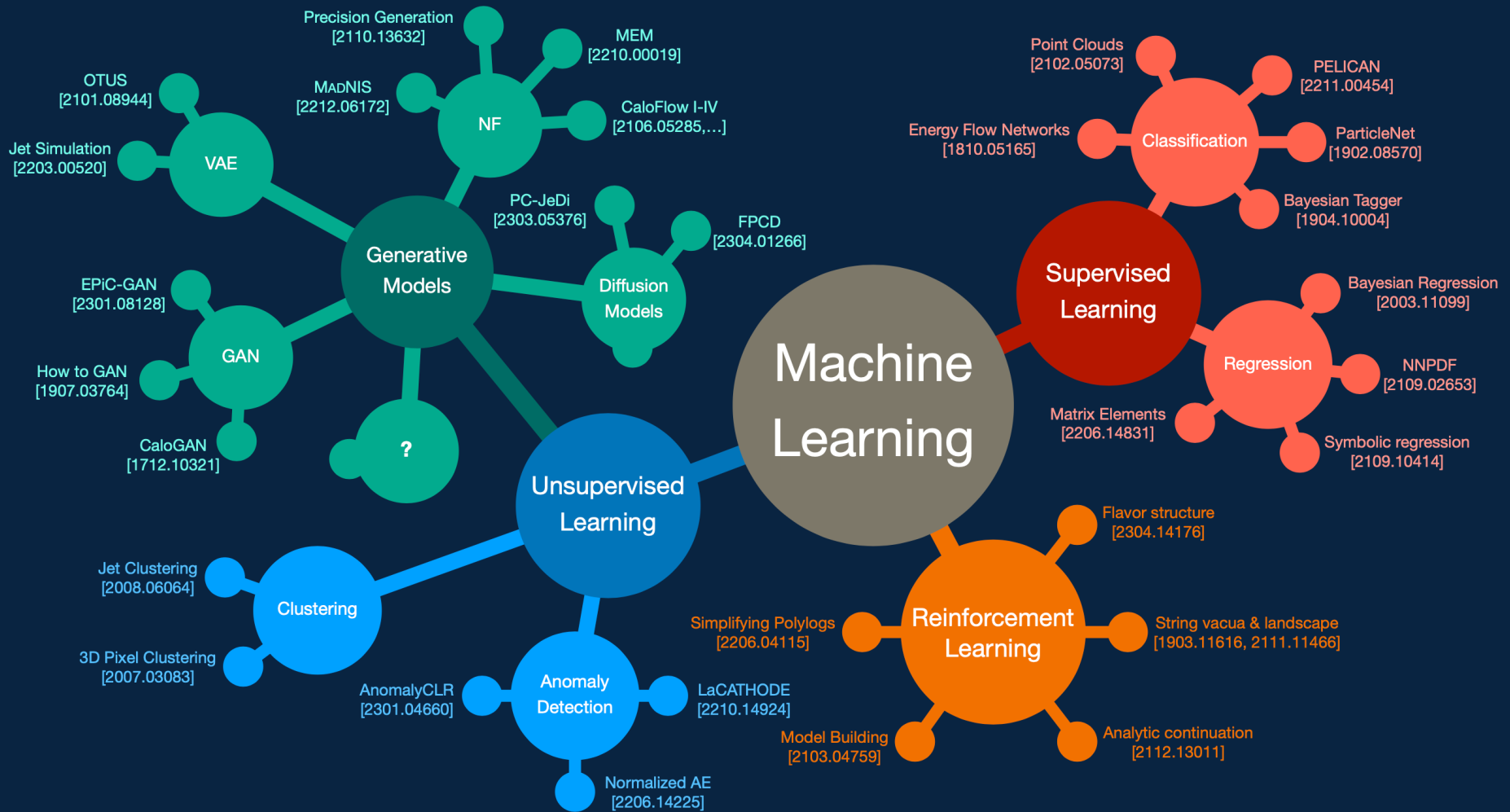


Simulation pipeline:

- **Perturbative QCD:  $10^{-19}\text{m} - 10^{-16}\text{ m}$**
- **Parton shower:  $10^{-16}\text{ m} - 10^{-14}\text{ m}$**
- **Hadronization/fragmentation  $10^{-14}\text{m} - 10^{-12}\text{ m}$**
- **tracker/ecal/hcal simulation  $10^{-12}\text{ m} - 10^2\text{ m}$**



# Most results heavily use these simulations



# Current areas of progress

## 1. Lattice QCD

- Normalizing flows, Monte Carlo sampling, Spectral reconstruction, ...

## 2. Simulation/unfolding

- Learn to reproduce simulations with a neural network
- Can speed up simulations by factors of  $10^3 - 10^5$
- Can be used for unfolding: remove effects of simulation on data

## 3. Anomaly detection

- Search for deviations from background
- No signal hypothesis necessary (?)

## 4. Data representation

- Can ML provide a better way to categorize and understand data?
- e.g. optimal transport, graph networks, etc.

## 5. Classification

- Top tagging, W tagging, Q v G discrimination, new physics searches

## 6. Symbolic regression

- Large language models (chatGPT) ?



# Anomaly detection



ART  
hug.ART  
om/AlhugART

Cho người xem: Sản phẩm này do AI Art Generator tạo ra, mang tính chất tham khảo để lấy ý tưởng, dùng để học  
liên cảm hứng, không dùng cho mục đích thương mại. Vui lòng hướng dẫn trước khi xem và dùng.  
Viewers: This product created by AI Art Generator is for reference purposes only, for learning or inspiration, not

# Anomaly detection

The Dream:

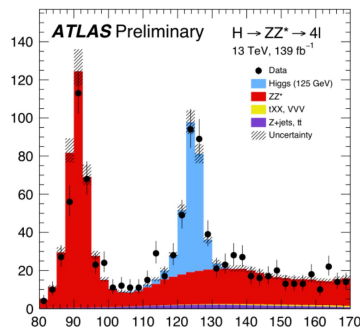
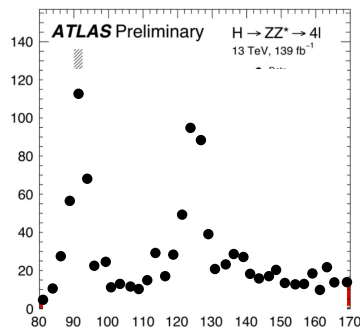
- ML sees something unusual in the data, new physics is found!
- dream is **an unsupervised method**: do not need a signal hypothesis
- Way to find “unknown unknowns”

The main idea:

- Background is understood well enough by ML that statistical outliers are seen

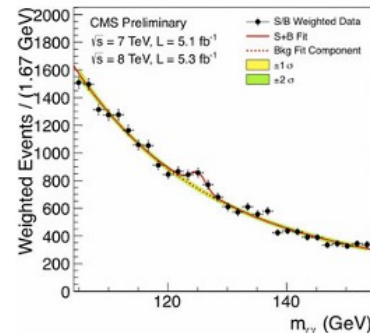
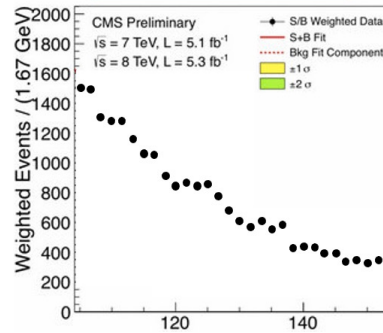
Easy: outliers

$$h \rightarrow e^- e^+ \mu^- \mu^+$$

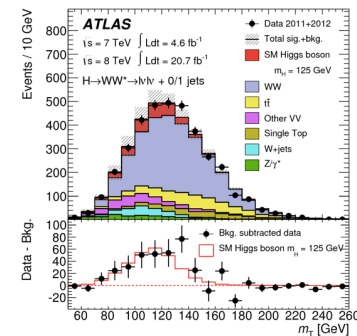
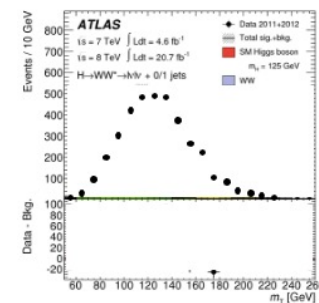


Hard: overdensities

$$h \rightarrow \gamma\gamma$$



$$h \rightarrow e^- \mu^+ \bar{\nu} \nu$$



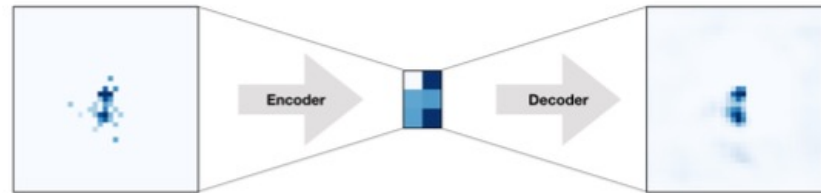
- Collins et al: 1805.02664
- D'Angelo and Wulzer: 1806.02350
- Collins et al: 1902.02634
- D'Angelo et al: 1912.12155
- Nachman & Shih: 2001.04990
- Stein et al: 2012.11638
- Carron et al: 2106.10164
- Hallin et al: 2109.00546

- Hajer et al: 1807.10261
- Heimel et al: 1808.08979
- Farina et al: 1808.08992
- Cerri et al: 1811.10276
- Roy + Vijay: 1903.02032,
- Atkinson et al: 2105.07988
- Carron et al: 2106.10164
- Ngairangbam et al: 2112.04958
- ...

# Autoencoders

Variational autoencoders: [Farina et al: 1808.08992]

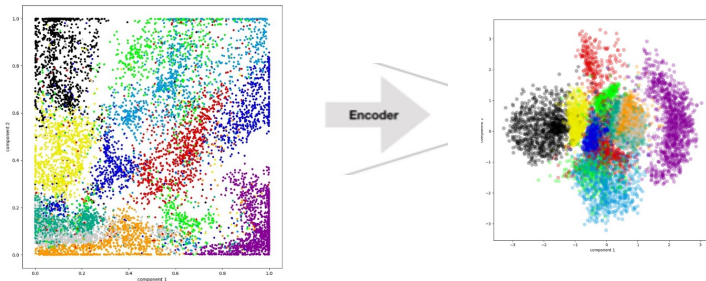
- Compress the background/data to a low-dimensional latent space



- Uncompress back to data space.
- Poorly reconstructed events are anomalies

Fraser, MDS, et al: 2110.06948

- Can look for anomalies directly in low-dimensional latent space



Metric	Number of medoids	Method	Top jet		W jet	
			AUC	$\epsilon_S(\epsilon_B = 0.1)$	AUC	$\epsilon_S(\epsilon_B = 0.1)$
Wass(1)	-	Avg	0.81	0.33	0.62	0.02
	1	Medoid	0.83	0.28	0.63	0.02
	3 (elbow)	Medoids (min)	0.85	0.43	0.67	0.04
	5	Medoids (min)	<b>0.87</b>	<b>0.54</b>	0.60	0.05
Wass(5)	7	Medoids (min)	0.87	0.54	0.61	0.05
	4 (elbow)	Medoids (min)	0.67	0.22	0.41	0.04
MAE	1	Medoid	0.82	0.40	<b>0.71</b>	0.07
	3 (elbow)	Medoids (min)	0.82	0.49	0.61	<b>0.08</b>

- Use k medoids or Wasserstein optimal transport metric
- Use event-to-ensemble distance for anomaly score
- Take home messages:
  - Performance depends on metric and sample
  - Cannot optimize in signal-independent manner

$$d_{Wass}^{(p)} = \left( \min_f \sum_{i,j} f_{ij} (c_{ij})^p \right)^{1/p}$$



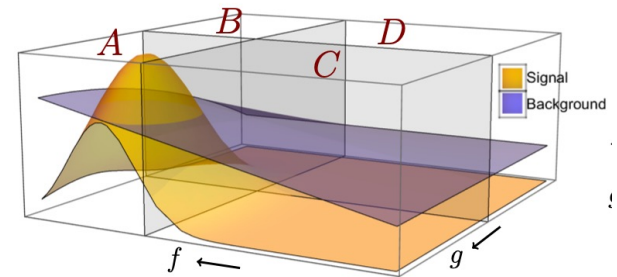
# ABCDDisCo: ML the ABCD method

ABCD method:

- Standard experimental sideband technique
- Estimate background in region A via  $N_A = \frac{N_B N_C}{N_D}$
- Requires two features  $f$  and  $g$  to be uncorrelated
  - E.g.  $f$  = mass and  $g$  = rapidity

Distance Correlation (DisCo): alternative to adversarial networks

- Decorrelates observables, easy to train



Kasieczka and Shih [arXiv: 2001.05310]

- Single DisCo



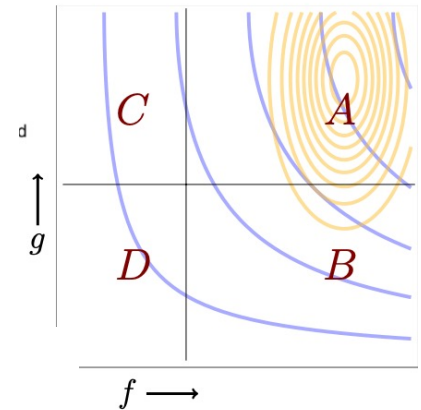
$f$  is fixed (e.g. mass)  $g$  is learned

Kasieczka, Nachman, MDS, Shih [arXiv: 2007.14400]

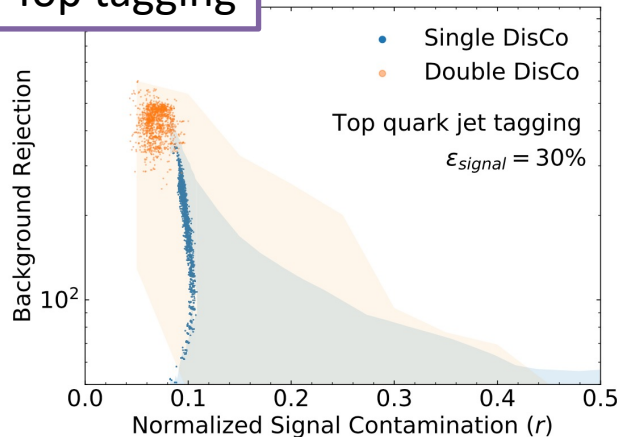
- Double DisCo



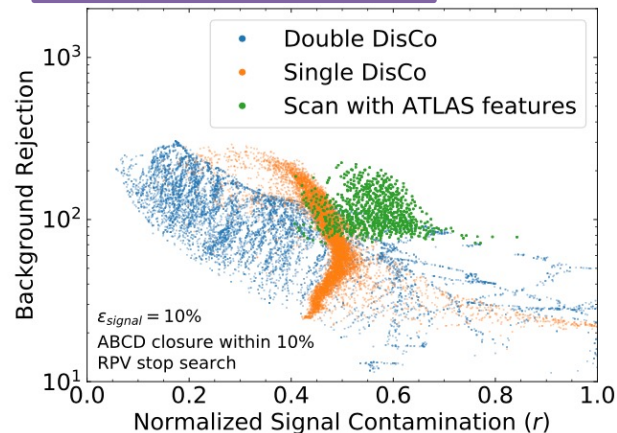
$f$  and  $g$  are learned



Top tagging

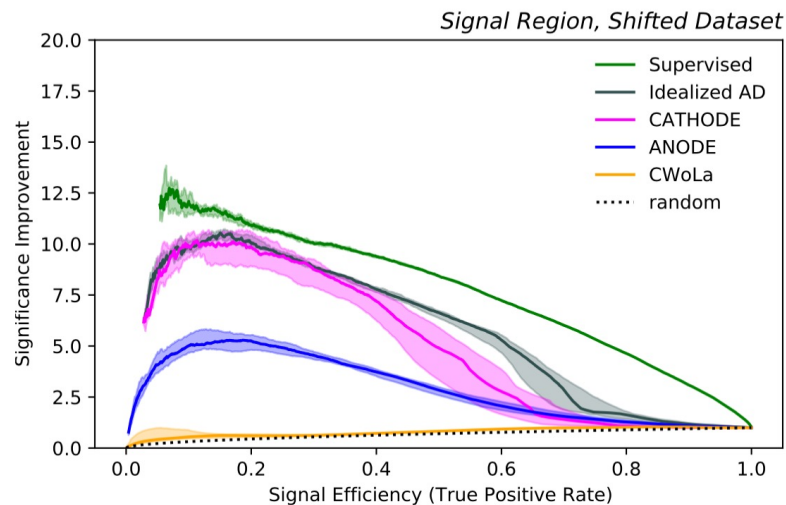


RPV squark search



# Challenges for Anomaly Detection

- Background regions are **signal dependent**
  - e.g. if looking for a dijet resonance, need a dijet background
  - No such thing as a signal-independent background
- **Looking under the lampost**
  - We only know how to look for resonances/new particles
  - Different signals are too varied to be pooled together
- Very **sensitive to metric** for what is anomalous
  - Tails of backgrounds are unique in their own way
- Supervised classifiers always do better



[Hallin et al. 2109.00546]

# Classification



Gia tinh

Đậu Biếc

Dobby



# Classification: top tagging

e.g. top tagging

## Jet substructure approach (2008-2017):

- Think about physics
- Deconstruct jet
- Look for W within top jet
- Look at helicity angle
- Hopkins Top Tagger (2008)

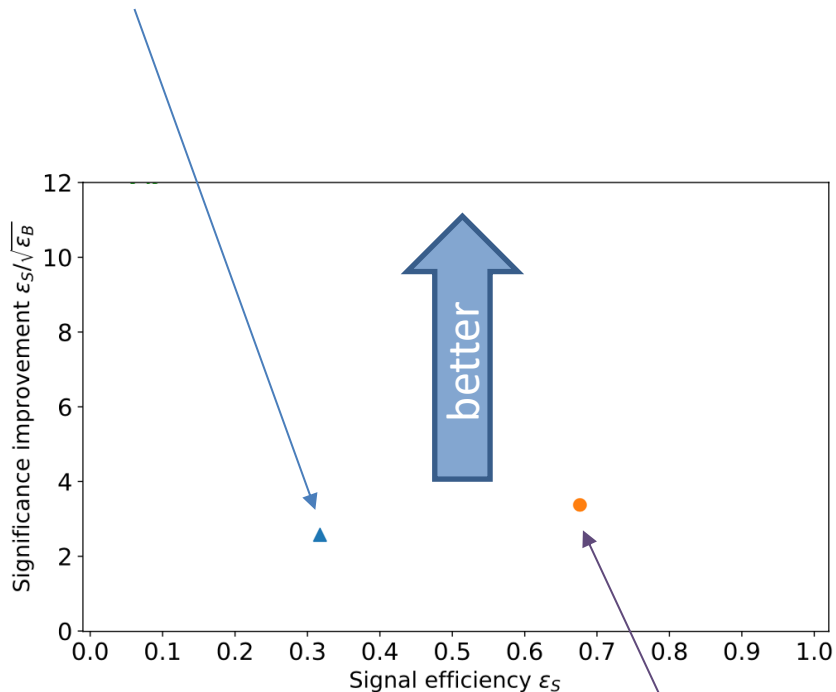
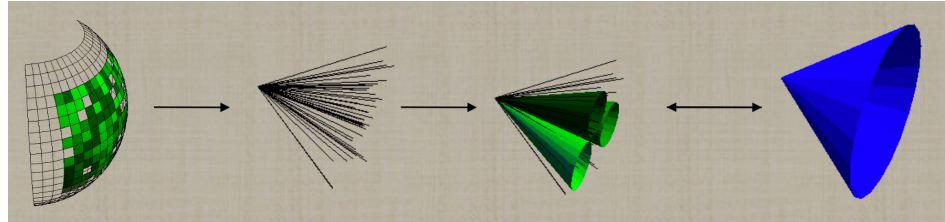


fig from 2103.12226

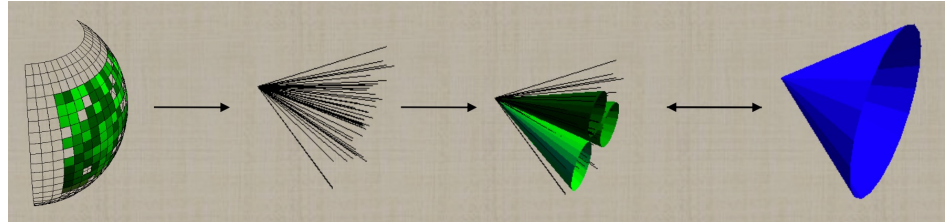
best jet substructure algorithm (2014)

# Classification: top tagging

e.g. top tagging

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- Think about physics
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## Machine learning methods are much better

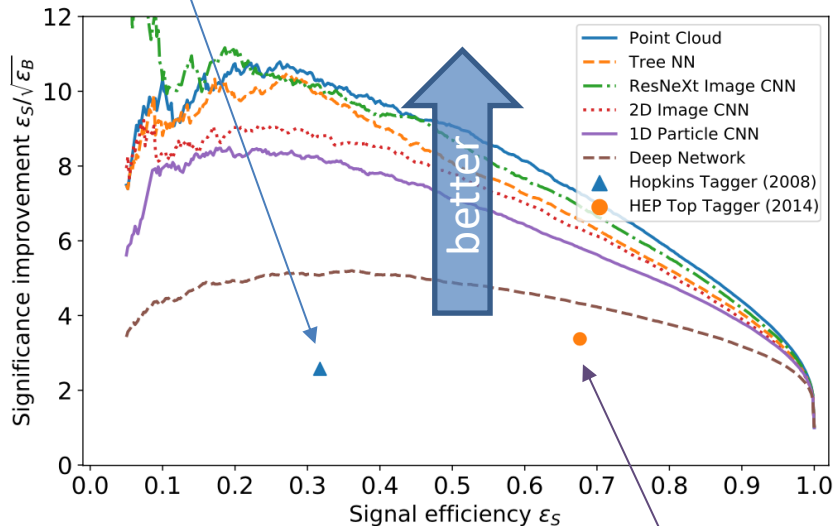
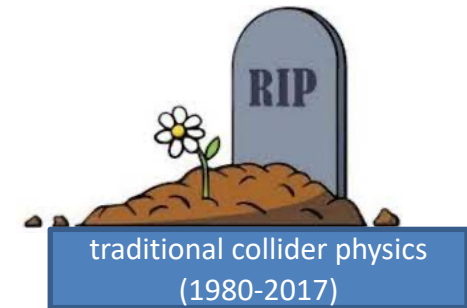


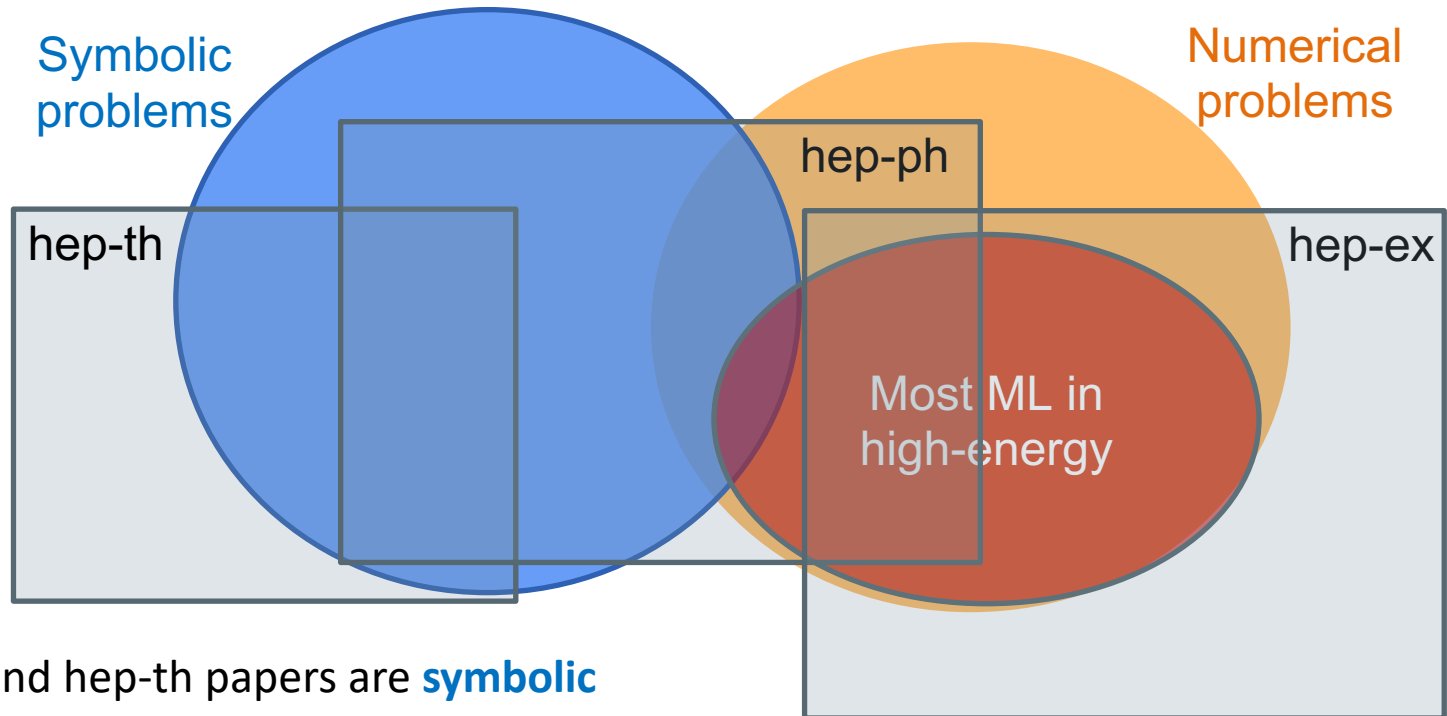
fig from 2103.12226

best jet substructure algorithm (2014)



- ML requires less “thinking”
- Provides less physical insight
- Better performance

# What subfield will ML make obsolete next?



Most hep-ph and hep-th papers are **symbolic**

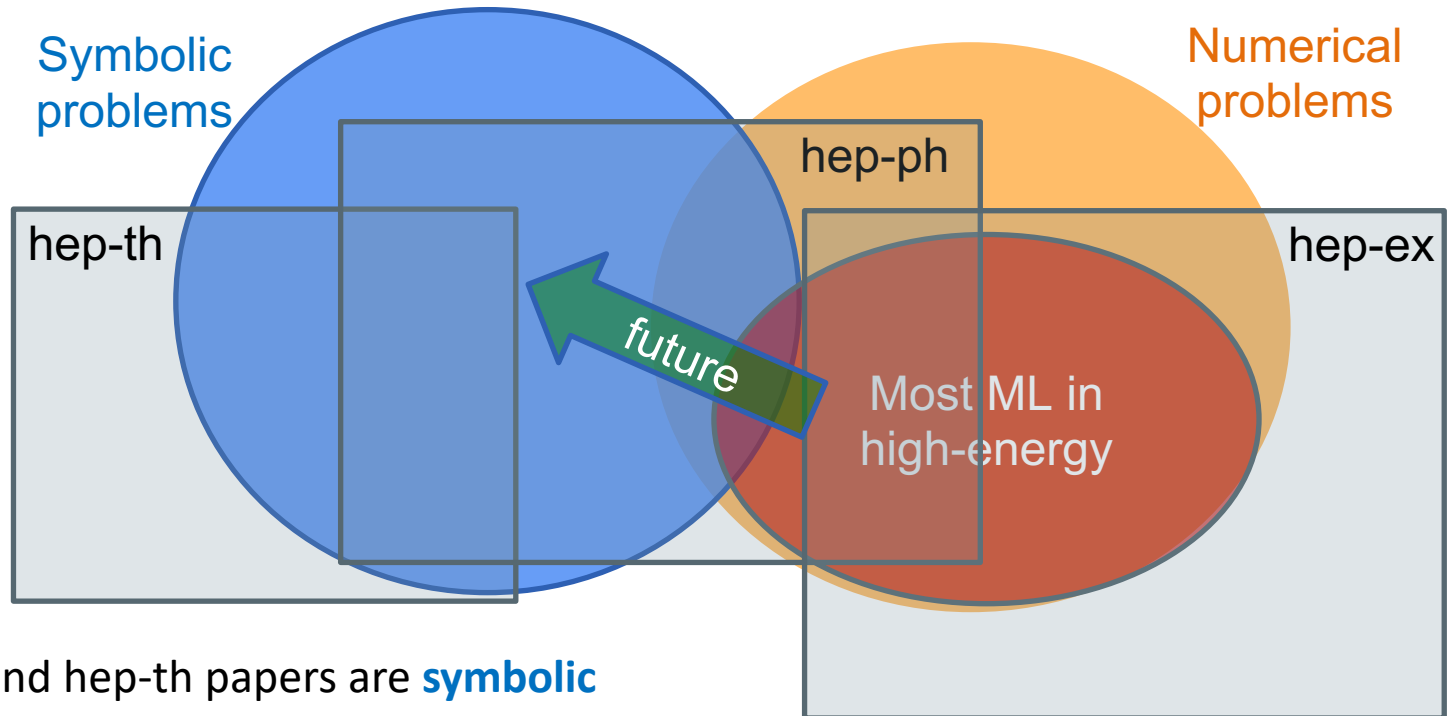
- Qualitative understanding of some simplified model
- Approximate but exact solutions to some equation
- Analytic computations in some system

So far, most ML in physics is highly **numerical**

- Collider physics data is millions of numbers
- Approximate answers are ok



# What subfield will ML make obsolete next?



Most hep-ph and hep-th papers are **symbolic**

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Symbolic ML methods will be **essential** for the future of High Energy Physics

- The world is changing because of **symbolic** large language models

# Symbolic regression



# 1. Simplifying polylogarithms

Given some polylogarithmic expression:

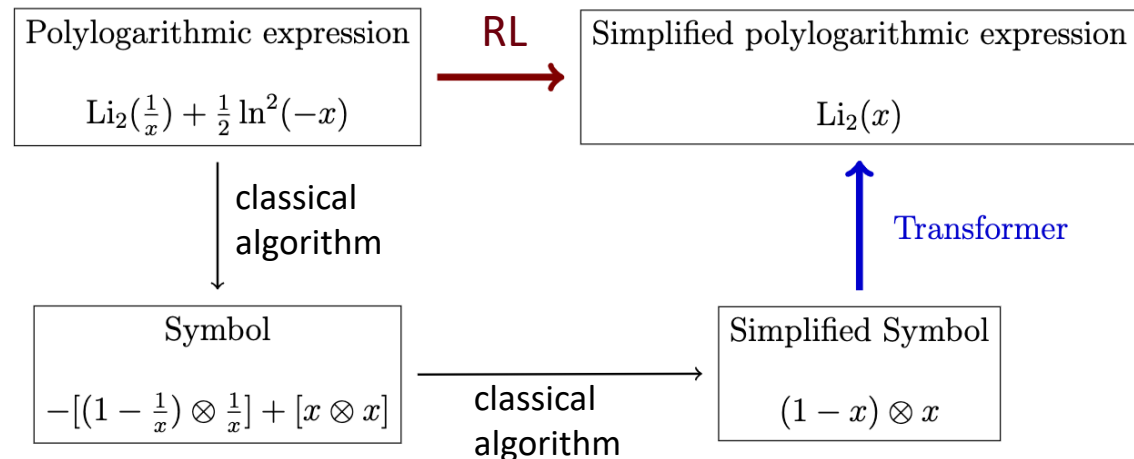
Dersy, Schwartz, Zhang arXiv:2206.04115)

$$f(x) = 9 \left( -\text{Li}_3(x) - \text{Li}_3 \left( \frac{2ix}{-i + \sqrt{3}} \right) - \text{Li}_3 \left( -\frac{2ix}{i + \sqrt{3}} \right) \right) \\ + 4 \left( -\text{Li}_3(x) + \text{Li}_3 \left( \frac{x}{x+1} \right) + \text{Li}_3(x+1) - \text{Li}_2(-x) \ln(x+1) \right) \\ - 4 \left( \text{Li}_2(x+1) \ln(x+1) + \frac{1}{6} \ln^3(x+1) + \frac{1}{2} \ln(-x) \ln^2(x+1) \right)$$

1. What is its simplest form?
2. Does it simplify to zero?
3. What identities do we apply in what order to simplify it?

Two approaches

1. Reinforcement learning
2. Transformer networks





# Example use case

1. Loop calculation gives some function of GPLs with complex arguments

$$f(x) = 4\zeta_3 + 9 \left[ G(0, 0, 1, x) + G\left(0, 0, \frac{-1 - \sqrt{3}i}{2}, x\right) + G\left(0, 0, \frac{-1 + \sqrt{3}i}{2}, x\right) \right] \\ + 4 \left[ -G(-1, -1, -1, x) + G(-1, 0, -1, x) + G(0, -1, -1, x) + G(0, 0, 1, x) - G\left(0, 0, 1, \frac{x}{x+1}\right) \right]$$

2. Express in terms of classical polylogs

$$f(x) = 9 \left( -\text{Li}_3(x) - \text{Li}_3\left(\frac{2ix}{-i + \sqrt{3}}\right) - \text{Li}_3\left(-\frac{2ix}{i + \sqrt{3}}\right) \right) \\ + 4 \left( -\text{Li}_3(x) + \text{Li}_3\left(\frac{x}{x+1}\right) + \text{Li}_3(x+1) - \text{Li}_2(-x) \ln(x+1) \right) \\ - 4 \left( \text{Li}_2(x+1) \ln(x+1) + \frac{1}{6} \ln^3(x+1) + \frac{1}{2} \ln(-x) \ln^2(x+1) \right)$$

3. Compute the symbol and simplify

$$\mathcal{S}[f(x)] = 9(x^2 + x + 1) \otimes x \otimes x + 13(1 - x) \otimes x \otimes x + 4(x + 1) \otimes x \otimes x$$

4. Integrate the symbol with a transformer network

$$f(x) = -\text{Li}_3(x^3) - \text{Li}_3(x^2) + 4\zeta_3 \quad \checkmark$$

highly non-trivial  
powerful dedicated  
neural network

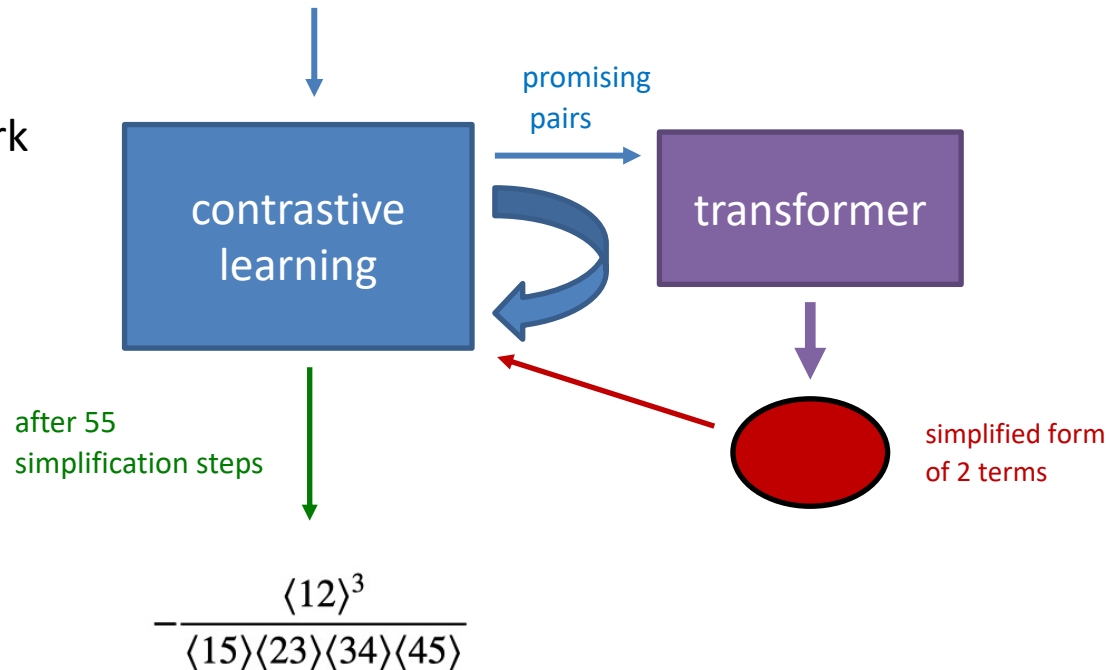
# 2. Simplifying Spinor-helicity amplitudes

[Cheung, Dersy, MDS, in preparation]

1. Compute 5-point MHV amplitude with Feynman diagrams: 390 terms
2. Choose some smart reference vector to reduce to 79 terms  
(smarter choice can reduce to 17)

$$\frac{\langle 12 \rangle^2 \langle 15 \rangle^2 \langle 24 \rangle \langle 34 \rangle [12] [14] [15] [23] [25] + \langle 12 \rangle^2 \langle 15 \rangle \langle 23 \rangle \langle 34 \rangle \langle 45 \rangle [12] [15] [23] [25] [34] + \dots 77 \text{ terms}}{\langle 15 \rangle^2 \langle 23 \rangle \langle 34 \rangle^2 \langle 45 \rangle^2 [12]^2 [15] [23] [45]}$$

3. Feed to network



4. Output when simplification completes

# 3. S-matrix bootstrap

What is the S-matrix bootstrap?

- Use analyticity, unitarity, crossing symmetries, etc. to completely fix S
- Stalled in 1960s: math too hard
- Recent revitalization: new insights from toy models, susy, numerical methods, etc.

Penedones et al 1708.06756

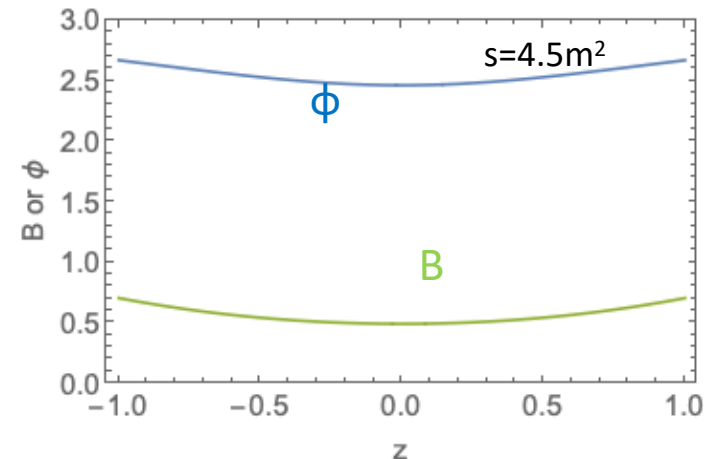
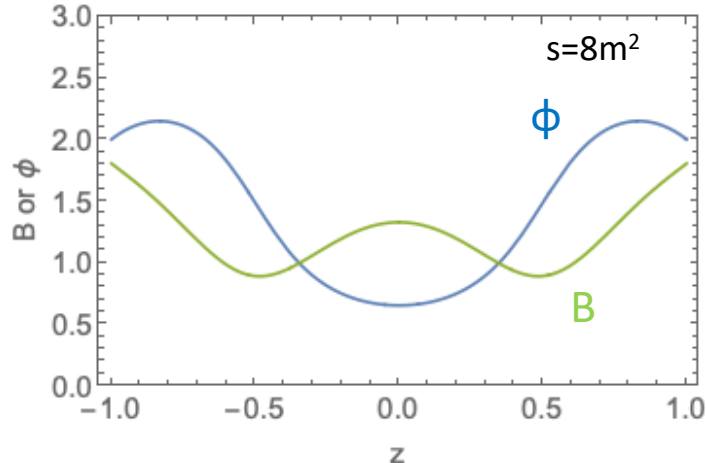
Fitzpatrick et al 2207.12448

Example ML application:

Dersy, MDS, Zhiboedov, to appear

For a given cross section  $\sigma \sim |F|^2$

- Does there always exist a phase  $\phi$  so that  $F = B e^{i\phi}$ ?

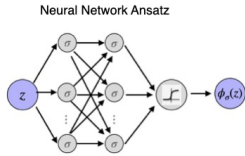


Open questions:

- A. How do we determine  $\phi$  from  $B$ ?
- B. Can there be many phases  $\phi_1, \phi_2, \dots$  for the same  $B$ ?

# A. Can we find $\phi(z)$ given $B(z)$ ? ... Yes!

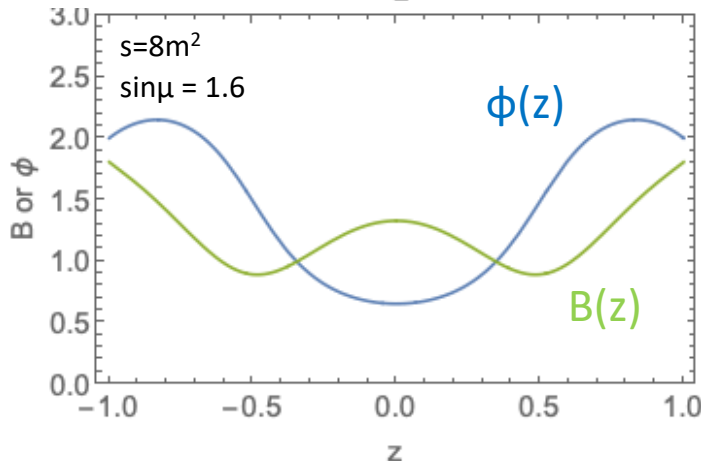
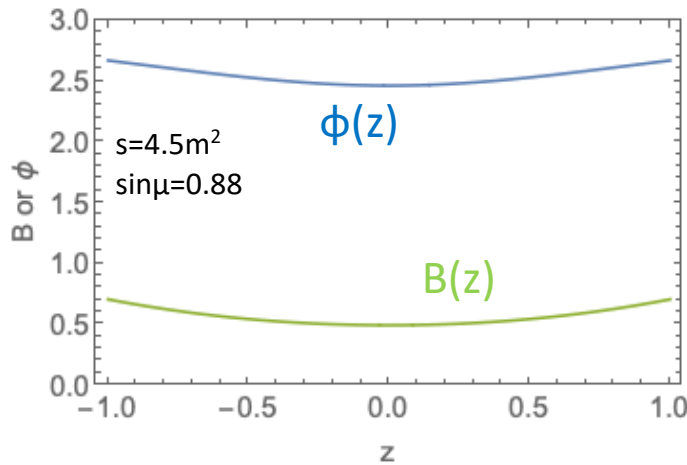
- Parametrize  $\phi(z)$  as a neural network



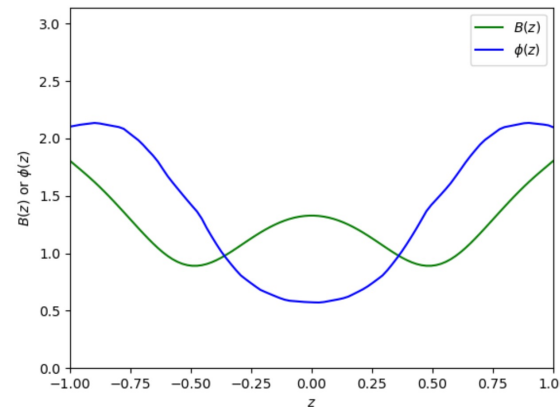
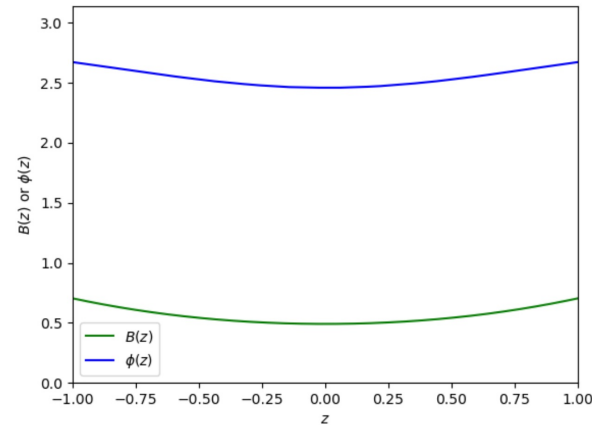
- Loss function is unitarity condition

$$\mathcal{L} = \mathbb{E} \left\| \left| B(z) \sin \phi(z) - \frac{1}{4\pi} \int_{-1}^1 dz_1 \int_0^{2\pi} d\phi_1 B(z_1) B(z_2) \cos(\phi(z_1) - \phi(z_2)) \right| \right\|^2$$

## S-matrix bootstrap results



## $\phi$ from $B$ using ML



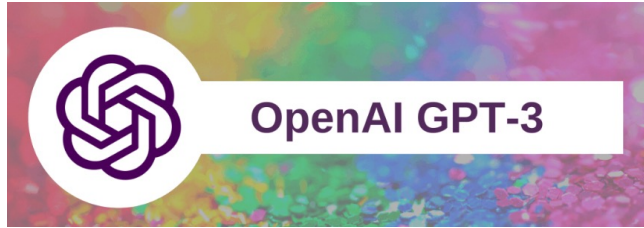
excellent agreement with known results



# The future

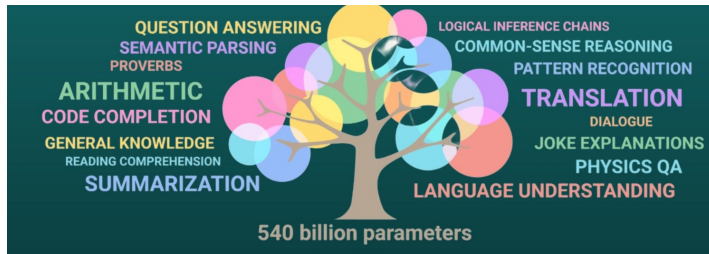


# Future of AI



- 3<sup>rd</sup> generation model (2020)
- 175 billion parameters

Google : PaLM (2022)  
540 billion parameters



Human brain

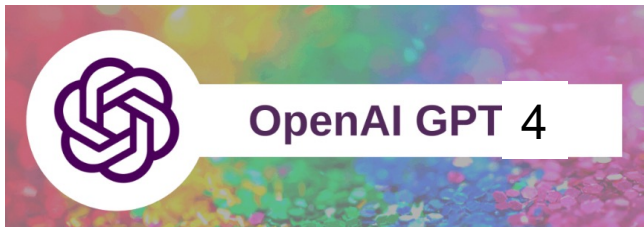


80 billion neurons  
150 trillion synapses

Cat brain



0.760 billion neurons  
10 trillion synapses

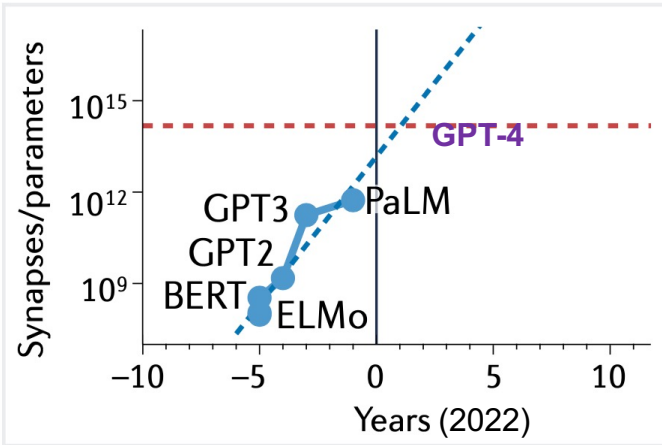


**170 trillion parameters!**

2023 ... 2040... 2100? ...3000...?

# Future of AI

**Should artificial intelligence be interpretable to humans?** MDS, Nature reviews physics (2022)



- ELMo (94 million parameters, 2018)
- GPT2 (1.5 billion parameters, 2019)
- GPT3 (175 billion parameters, 2020)
- PALM (540 billion parameters, 2022)
- GPT4 (110 trillion parameters, 2023)

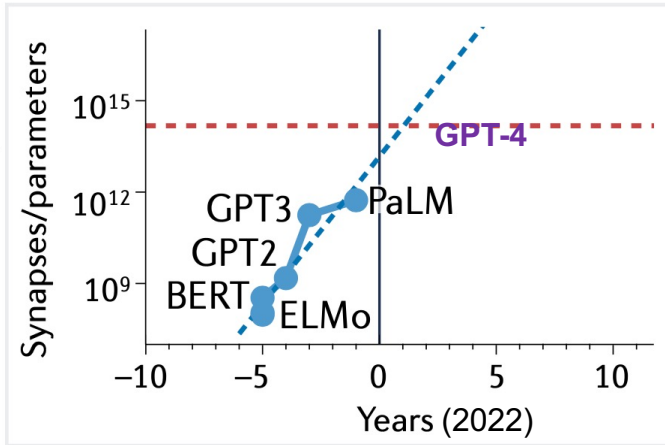
AI grows by factor of  $\sim 10$ /year

# Future of AI

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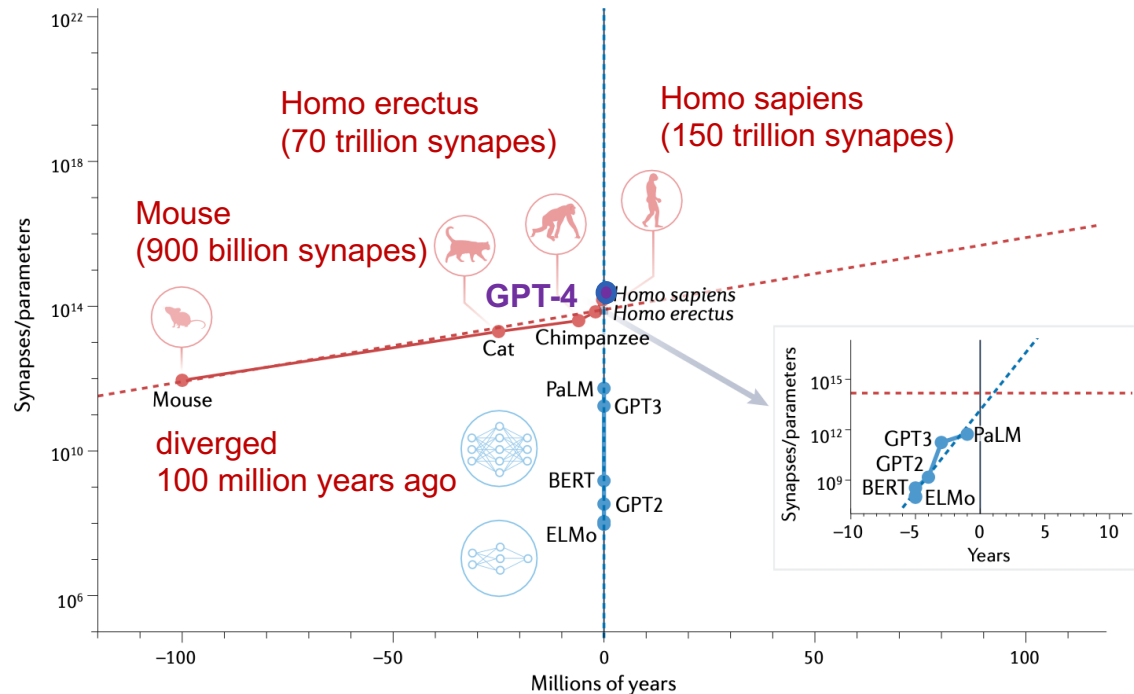
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AI grows by factor of ~10/year



Biological intelligence grows by a factor of 2 in  $10^6$  years

- Both AI and biological intelligence grow exponentially
- Factor of  $10^6$  difference in exponent (!!)





# Does AI look like biological intelligence?

Exam	GPT-4
SAT Math	700 / 800 (~89th)
Graduate Record Examination (GRE) Quantitative	163 / 170 (~80th)
Graduate Record Examination (GRE) Verbal	169 / 170 (~99th)
AP Environmental Science	5 (91st - 100th)
AP Macroeconomics	5 (84th - 100th)
AP Microeconomics	5 (82nd - 100th)
AP Physics 2	4 (66th - 84th)

- GPT4 can do freshman level college physics very well
- In ~ 1 year will do it perfectly
- In ~ 3 years it will have mastered college

MA

Write me a good sophomore level physics problem about vietnam



### Problem: Cable Car in Ba Na Hills

The Ba Na Hills cable car near Da Nang, Vietnam, holds the world record for the longest non-stop single track cable car at 5,801 meters in length. It also boasts a staggering height difference between its departure and arrival station, offering passengers an impressive view of the surrounding scenery.

Imagine a physics experiment conducted aboard this cable car. A student suspends a simple pendulum of length 0.5 meters from the ceiling of the cable car. The pendulum consists of a small weight at the end of a lightweight, inextensible string. As the cable car ascends the hill with a constant upward acceleration of  $a = 0.2 \text{ m/s}^2$ , the student notices the pendulum no longer hangs vertically but makes an angle  $\theta$  with the vertical line.

1. Determine the angle  $\theta$  that the pendulum makes with the vertical due to the acceleration of the cable car.

**Hint:** Consider the effective gravitational acceleration in the frame of reference of the accelerating cable car.

Solution...

Thus, due to the acceleration of the cable car, the pendulum makes an angle of approximately  $1.17^\circ$  with the vertical.

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## Can the improvements continue?

- Already use all available training data (the internet)

# Does AI look like biological intelligence?

Exam	GPT-4
SAT Math	700 / 800 (~89th)
Graduate Record Examination (GRE) Quantitative	163 / 170 (~80th)
Graduate Record Examination (GRE) Verbal	169 / 170 (~99th)
AP Environmental Science	5 (91st - 100th)
AP Macroeconomics	5 (84th - 100th)
AP Microeconomics	5 (82nd - 100th)
AP Physics 2	4 (66th - 84th)

- GPT4 can do freshman level college physics very well
- In ~ 1 year will do it perfectly
- In ~ 3 years it will have mastered college

## Can the improvements continue?

- Already use all available training data (the internet)

Yes!

- It would be foolish to say this is the endpoint
- ML can learn just like we do
  - Data augmentation
  - Create and solve toy problems
  - Fewer sociological pressures than human beings have



# Conclusions

Machine learning is having a huge impact on high energy physics

- QCD
- Anomaly detection
- Detector simulation/unfolding
- Jet substructure/classification

Future of ML in high energy will likely be more symbolic

- Begin with hybrid numerical/symbolic problems
  - (polylogarithms, spinor helicities, Feynman diagrams)
- Eventually exploit large language models to understand physical systems like we do



The future is bright!

ML provides hope at finally solving problems too difficult for human beings