ASFAE 2024 workshop

AI in fundamental physics

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Today, we will talk about

AI-assisted Science

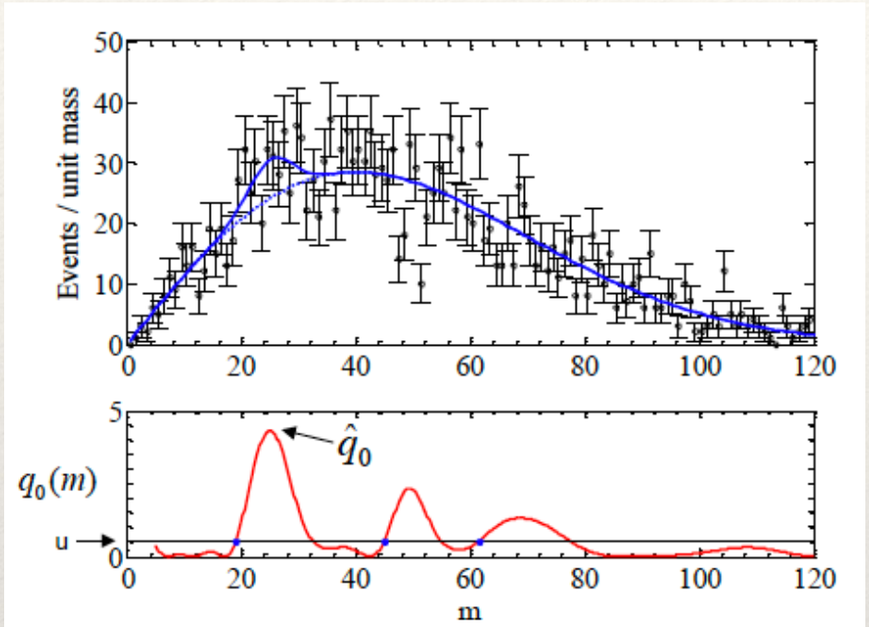
Human surrender?

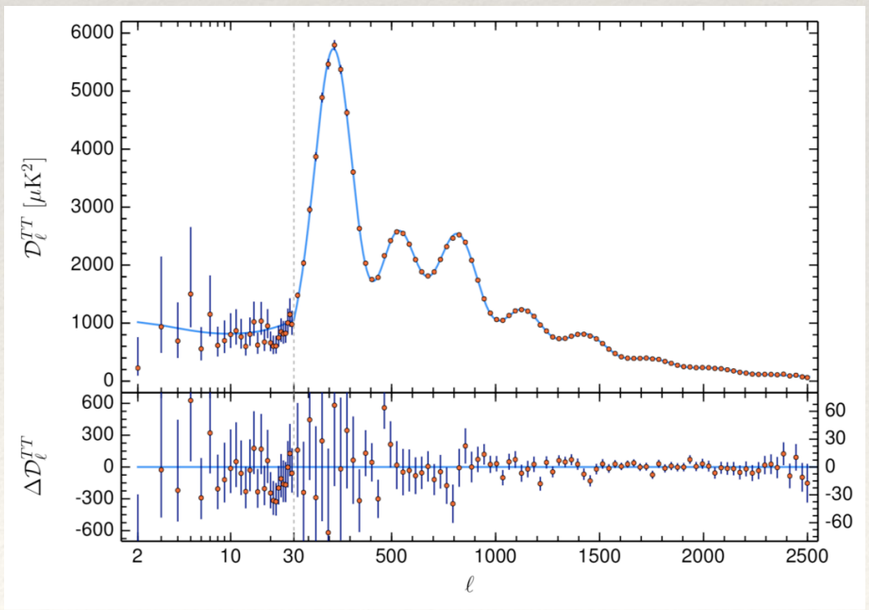
Looking under the hood

Explainable AI

AI-assisted Science

In particle, astro, cosmo & nuclear physics,
Artificial Intelligence techniques
are nowadays commonplace



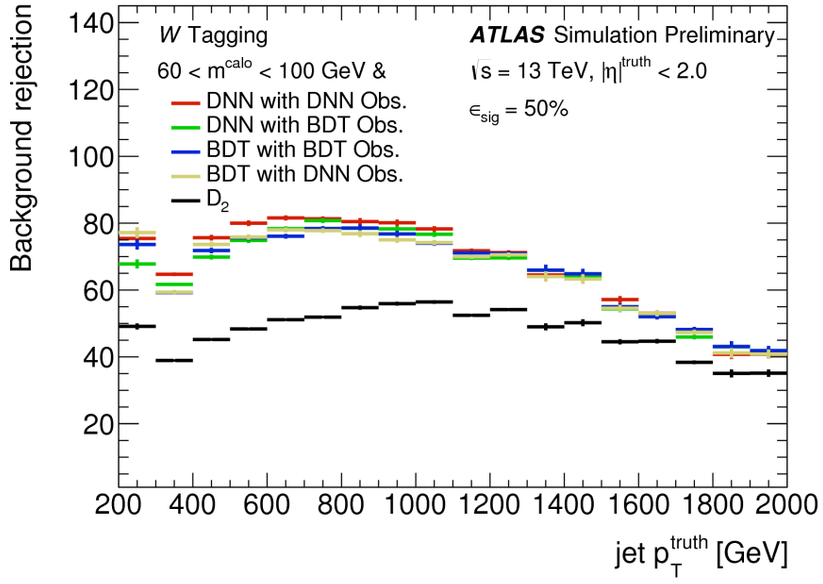


In fact,
we have always been early adopters and developers of sophisticated statistical techniques

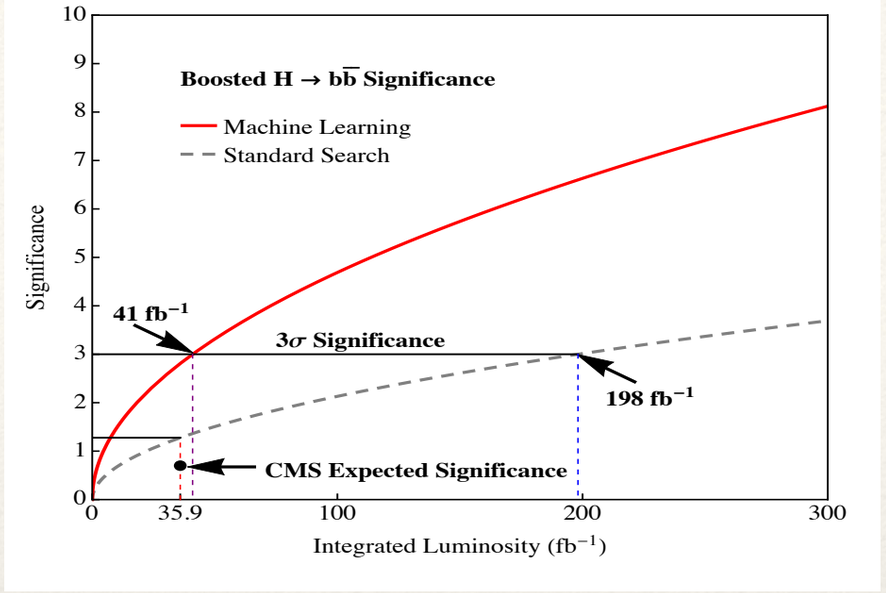
why? the stakes are high, the community is large and connected, we usually have a good physical understanding and can face increasingly complex questions

A lot of ML in Particle Physics is answering YES/NO questions

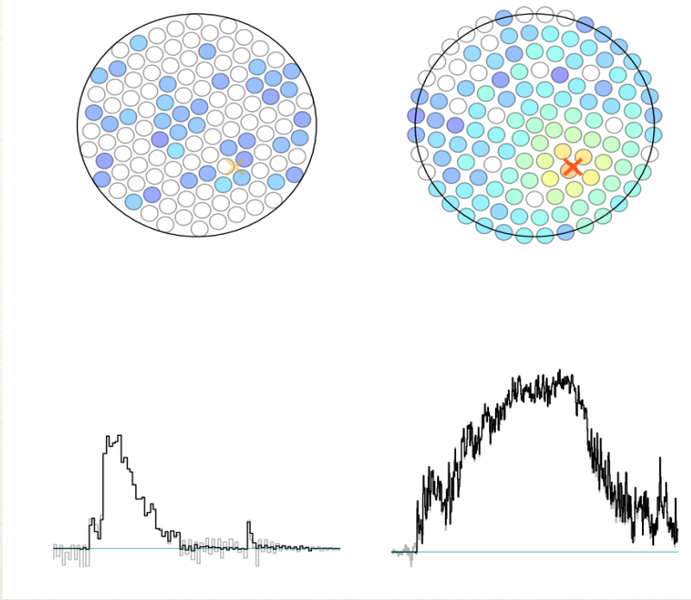
Is it a W?



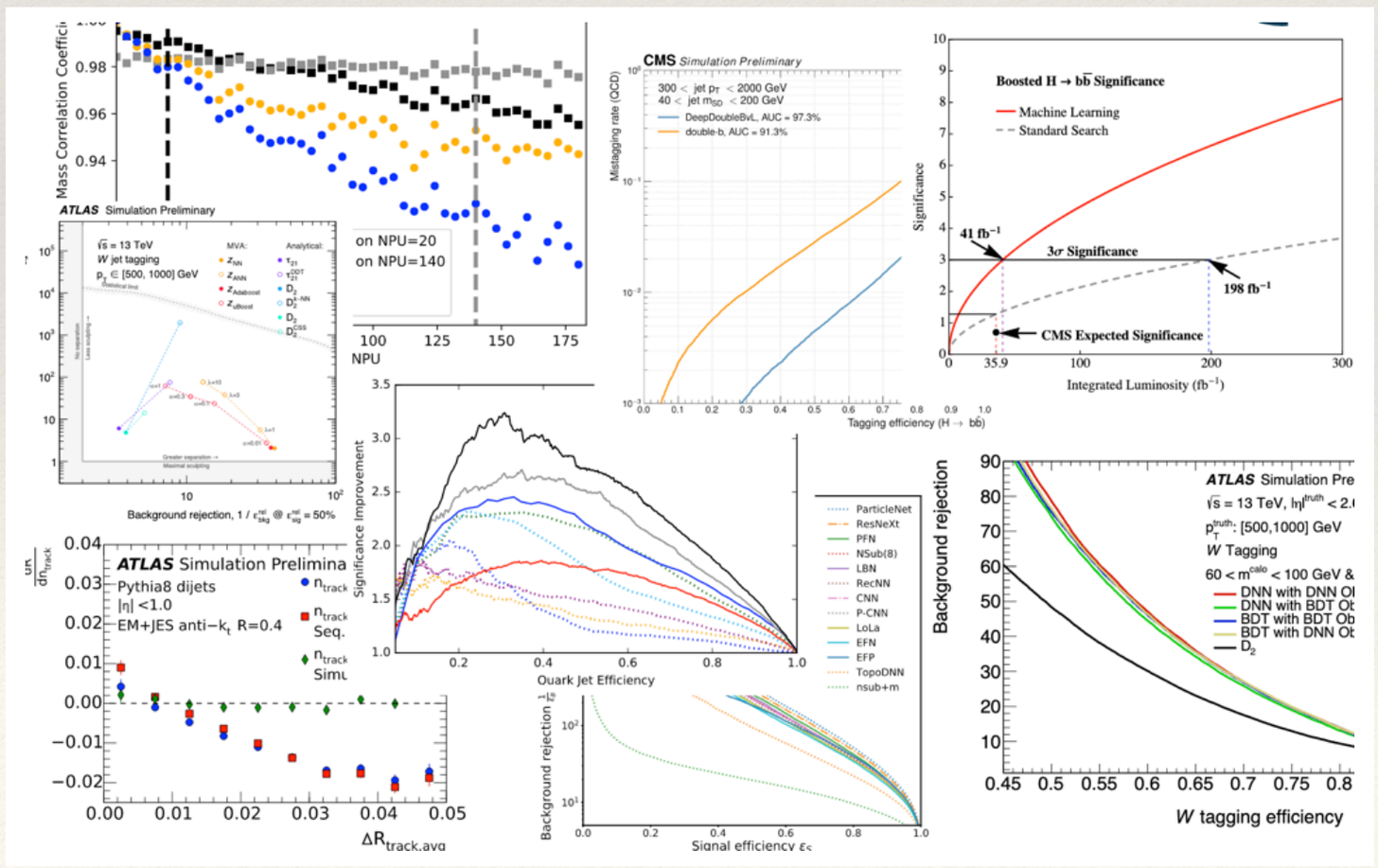
Is it a Higgs?



Is it DM?



often using Neural Networks to deal with images (CNNs)



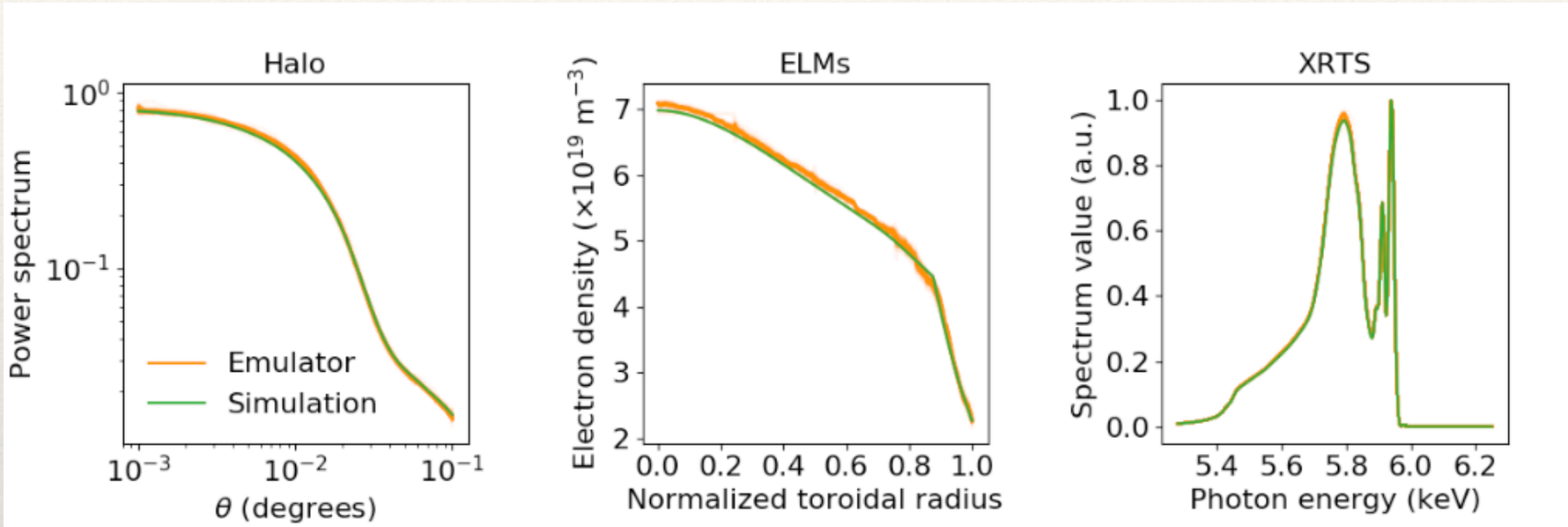
The gains in ID-ing phenomena are typically in the range of 5%-30%

for tricky environments: difference between **discovery or not**

Apart from better ID'ing, AI helps speeding up simulations

Here the gains respect to traditional techniques can be **huge**

Example: "*Up to two billion times acceleration of scientific simulations with deep neural architecture search*" (2001.08055)



Galaxy halo | **Tokamak fusion** | **Inelastic XRay Thomson scattering**

Method	Platform	Time/shower (msec)	Speedup
Monte Carlo	2S Intel Xeon Platinum 8180	17000	1.0
3DGAN CPU		16	1063
3DGAN GPU	GTX 1080	4	4250

And we are getting **even better** thanks to Generative AI
e.g. 2109.07388

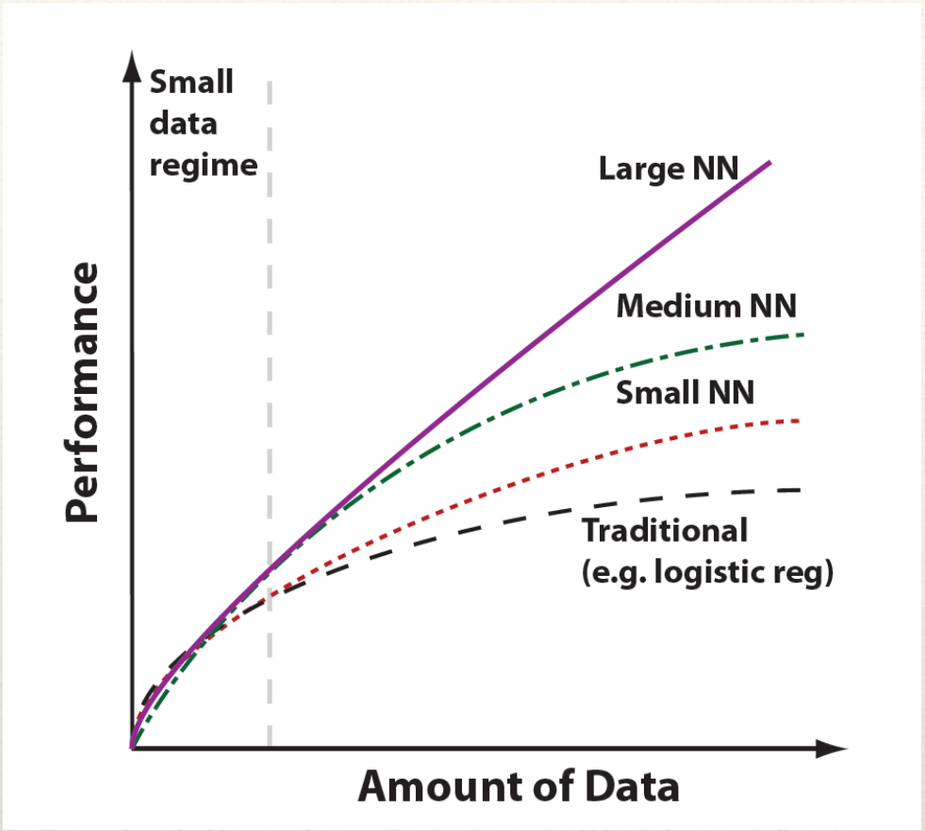
In both situations, ID and simulation,
AI comes to help in doing **better** what we
already know how to do

AI is *assisting*, enhancing the task
is not doing something radically new

Characteristic of fundamental physics:
we often have a way to tackle problems,
in our approximation to complex phenomena
we are strong followers of *reductionism*

Yet, Deep Learning seems to learn
beyond our naive expectations

Why are NNs so good at learning?



High-bias low-variance, 1803.08823

Good at handling large amounts of data: needle in a haystack

The NN structure (layers, 0/1 gates) allows a high representation power with moderate computational demands, e.g. allows parallelisation, use of GPUs…

It scales better than other learning methods (like SVMs)

Good at learning: ability to learn with little *domain knowledge*

That's something physicists (as humans) are good at

(Physics -> other things)

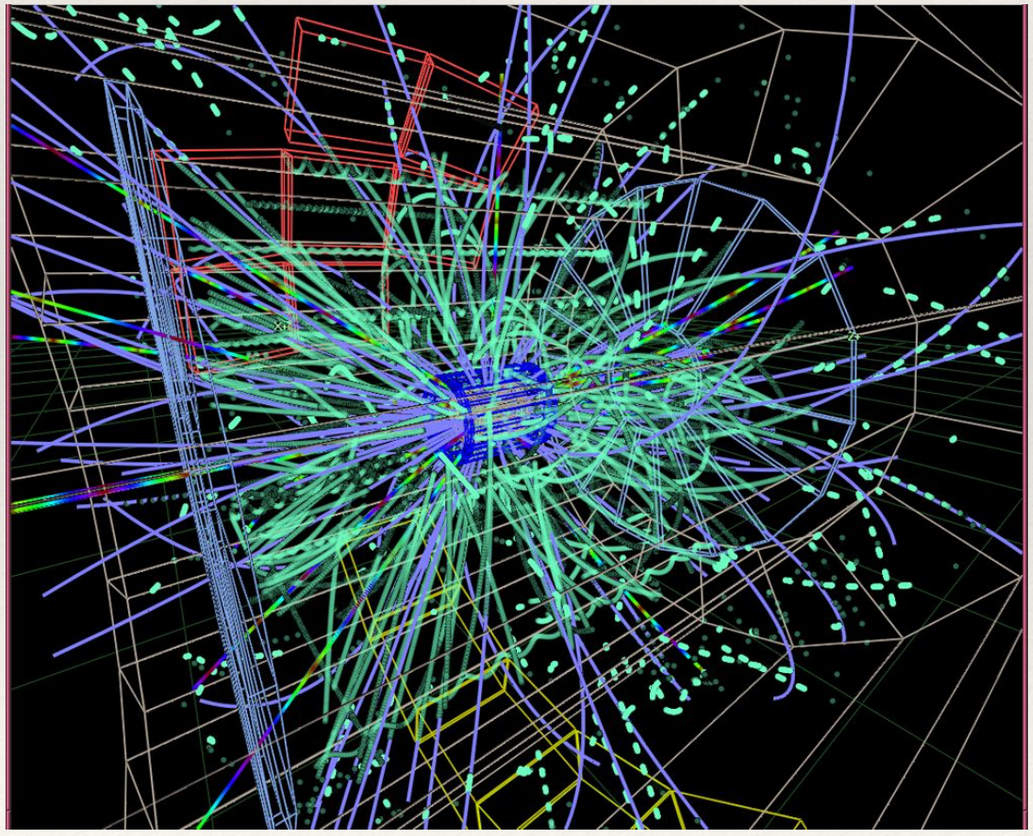
DNNs are good at this too, they are able to take large streams of data and learn features with little guidance, work like *black boxes*

Human surrender?

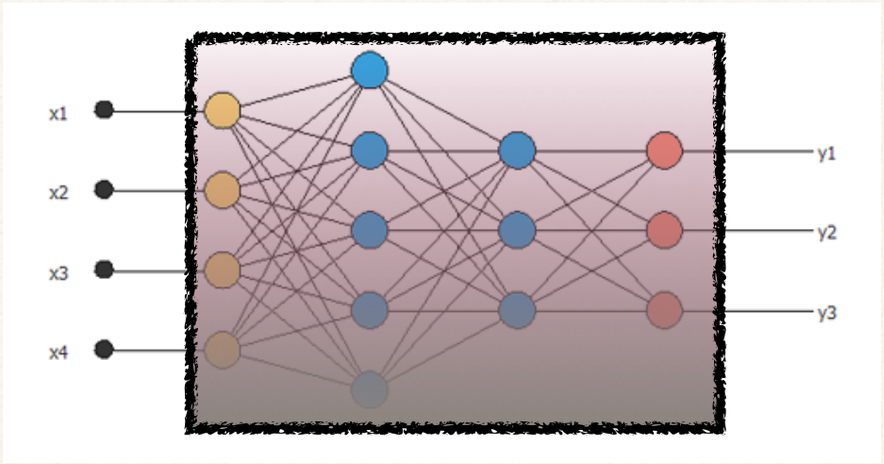
What's wrong with blackboxes?

Only open in case of a disaster

If it works, why fix it?
DL is very powerful, in a way that can be quantified and tensioned against human performance or other techniques



If the blackbox can help ID'ing this event faster and better than a traditional algorithm, who cares?



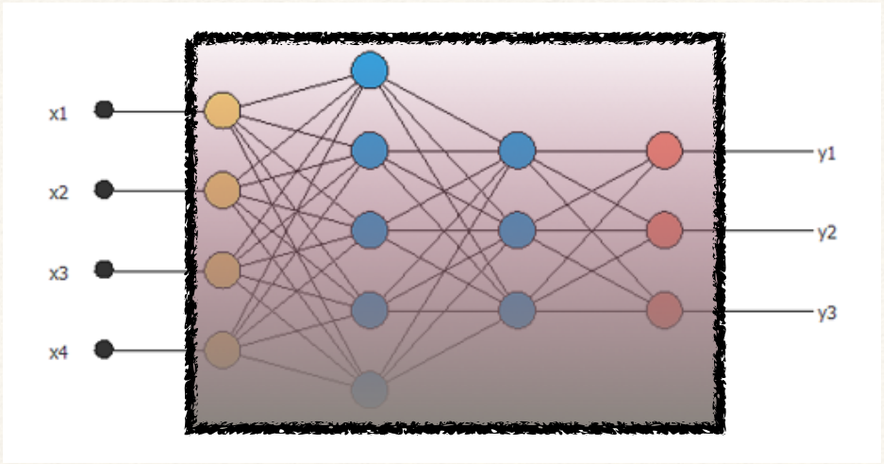
What's wrong with blackboxes?

If they do work, and help solve problems?

The lack of understanding hurts our pride as scientists

our job is to understand as much as we humanly can

"If you think you understand quantum mechanics, you don't understand quantum mechanics" R. Feynman, *The Character of Physical Law*



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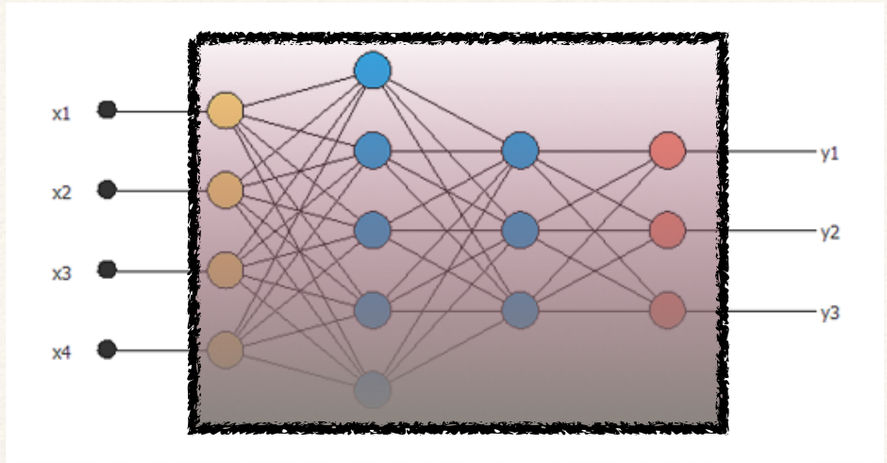
Any efforts we do to express the workings of NNs from different viewpoints may lead to *new ideas for machine learning*



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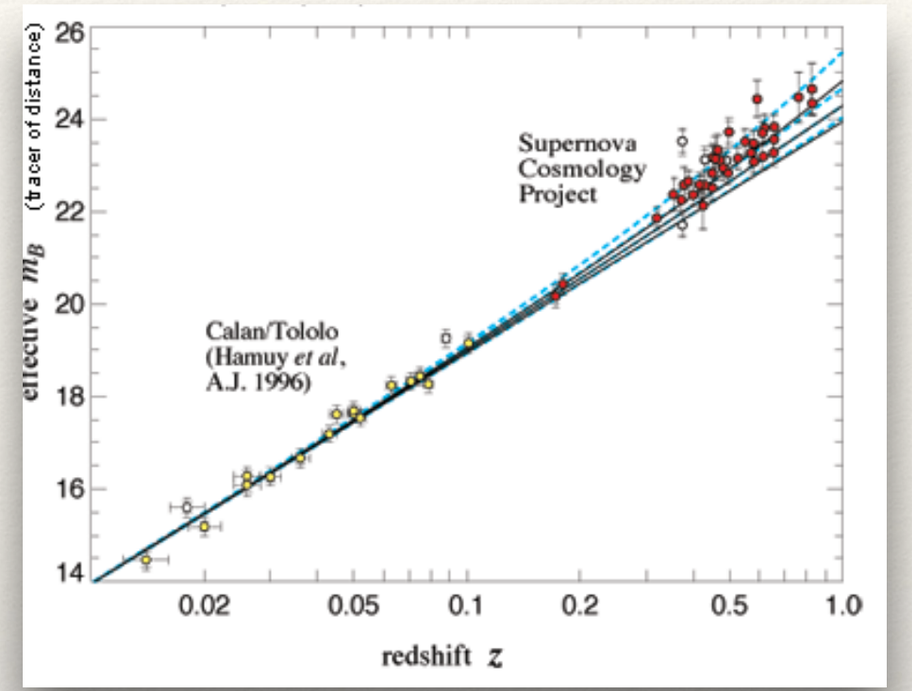
The depth and reach of AI in *decision making* is growing very fast
we should be concerned about our lack of control over this
e.g. see EU's draft on regulating AI, April 21st
XAI, Ethical AI… all these require a better understanding of DNNs

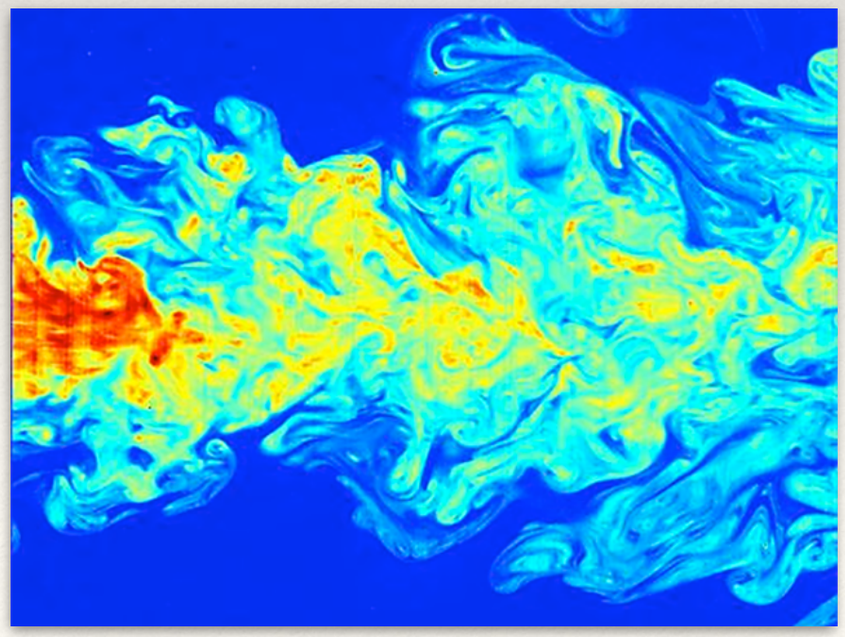
Looking under the hood

What if we didn't know what we were looking for?

what would **you** do?
as a physicist, you would start thinking on
possible physical relations, plotting things,
trying to obtain the best data representation
the representation which manifests a behaviour
Could an AI guide you?



If I showed you many examples of fluid behaviour



would you learn the
Navier-Stokes equation?

Example 1 PDE-Nets

Navier Stokes, Maxwell, Schrodinger…

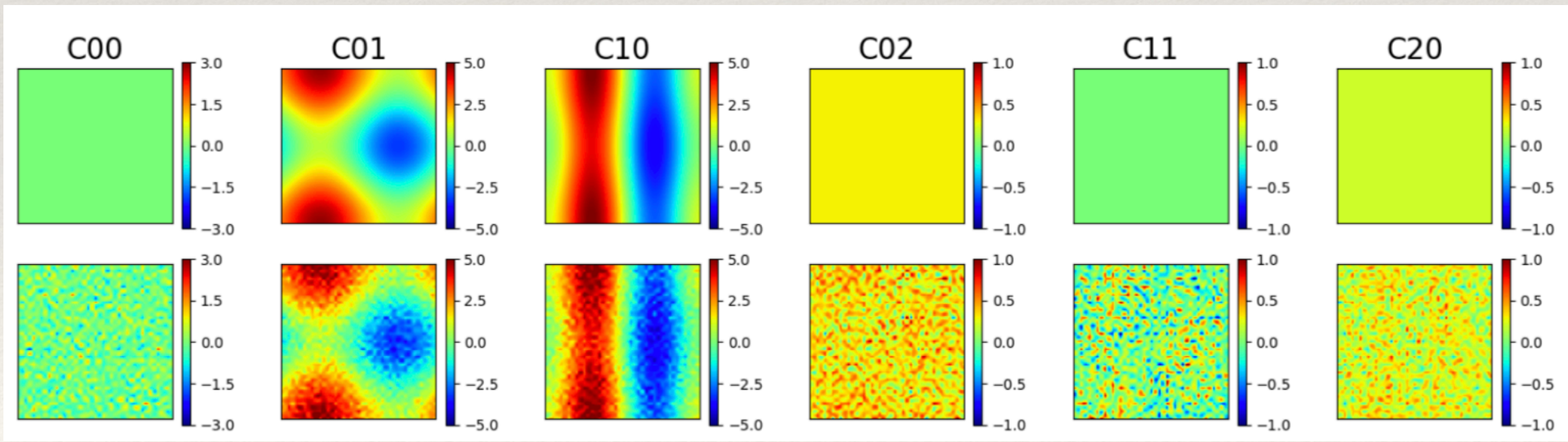
Laws of Nature are PDEs

But there are other areas in physics where equations are not known and even when we know them, they include assumptions

Pose an inverse problem: given an observed temporal distribution, can a NN learn the non-linear response?

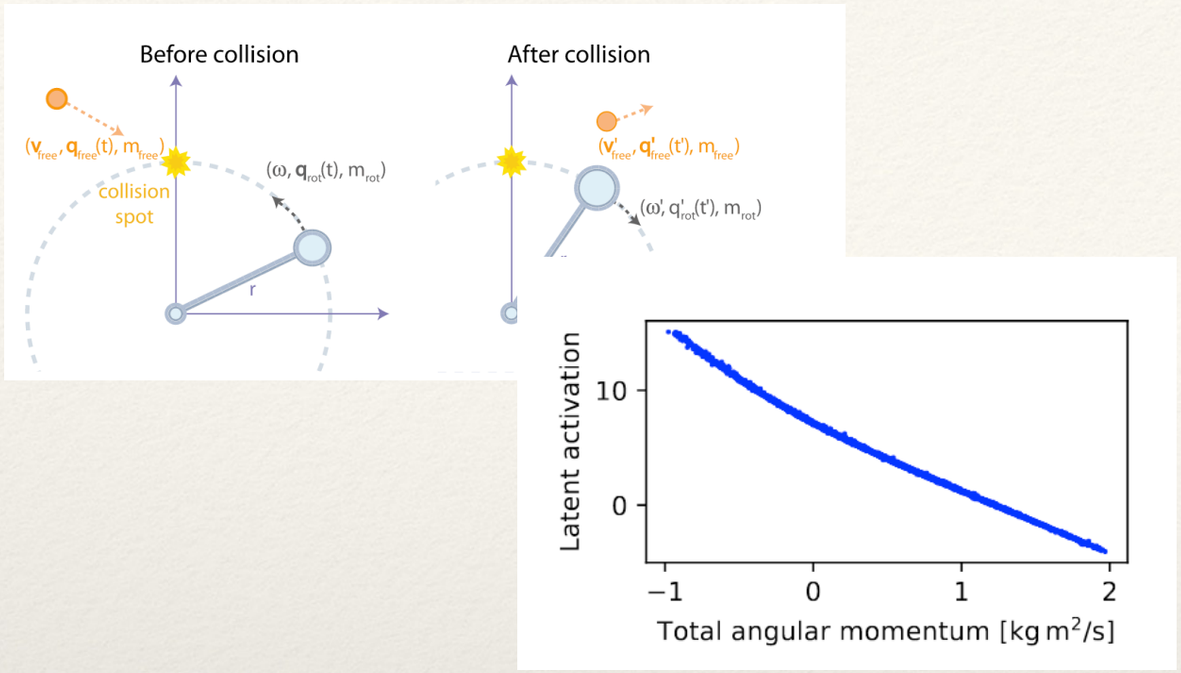
$$u_t = F(x, u, \nabla u, \nabla^2 u, \ldots), \quad x \in \Omega \subset \mathbb{R}^2, \quad t \in [0, T].$$

$$u_t(t, x, y) = F(x, y, u, u_x, u_y, u_{xx}, u_{xy}, u_{yy}, \ldots), \quad (x, y) \in \Omega \subset \mathbb{R}^2, t \in [0, T].$$



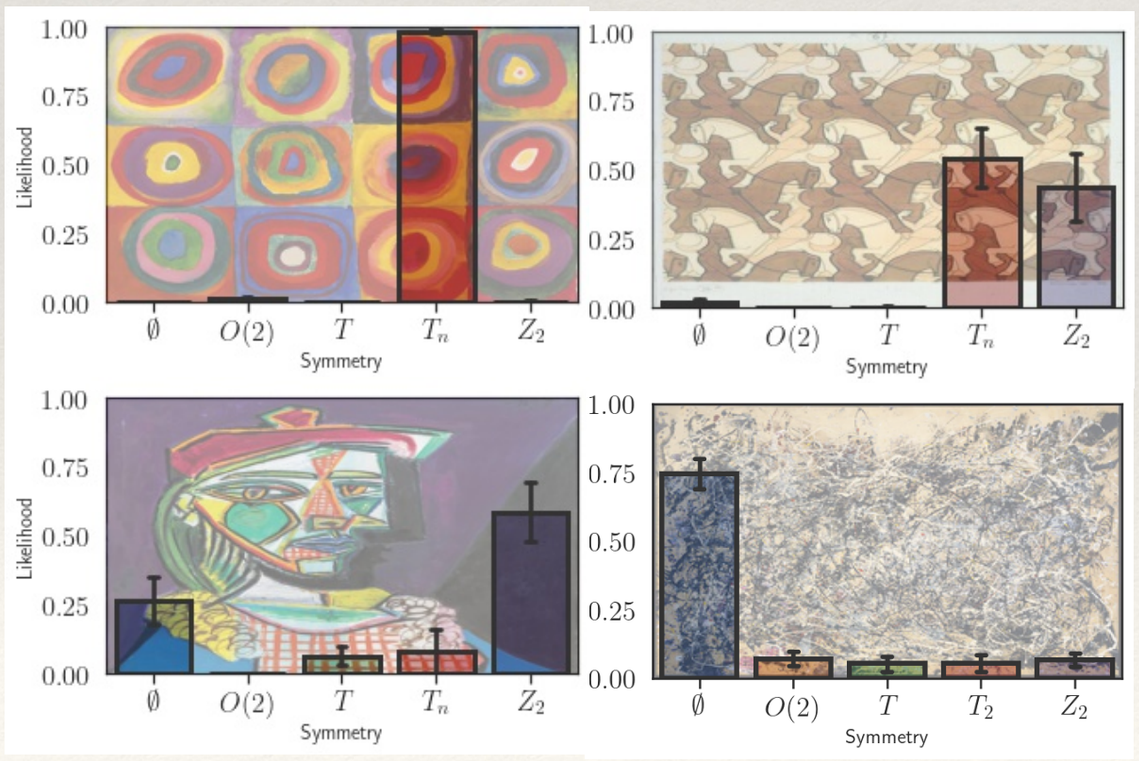
e.g PDE-Net, Long&Dong, 1812.04426

Example 2: Symmetries/conservation laws



Discovering physical concepts with NNs,
1807.10300 by Iten et al

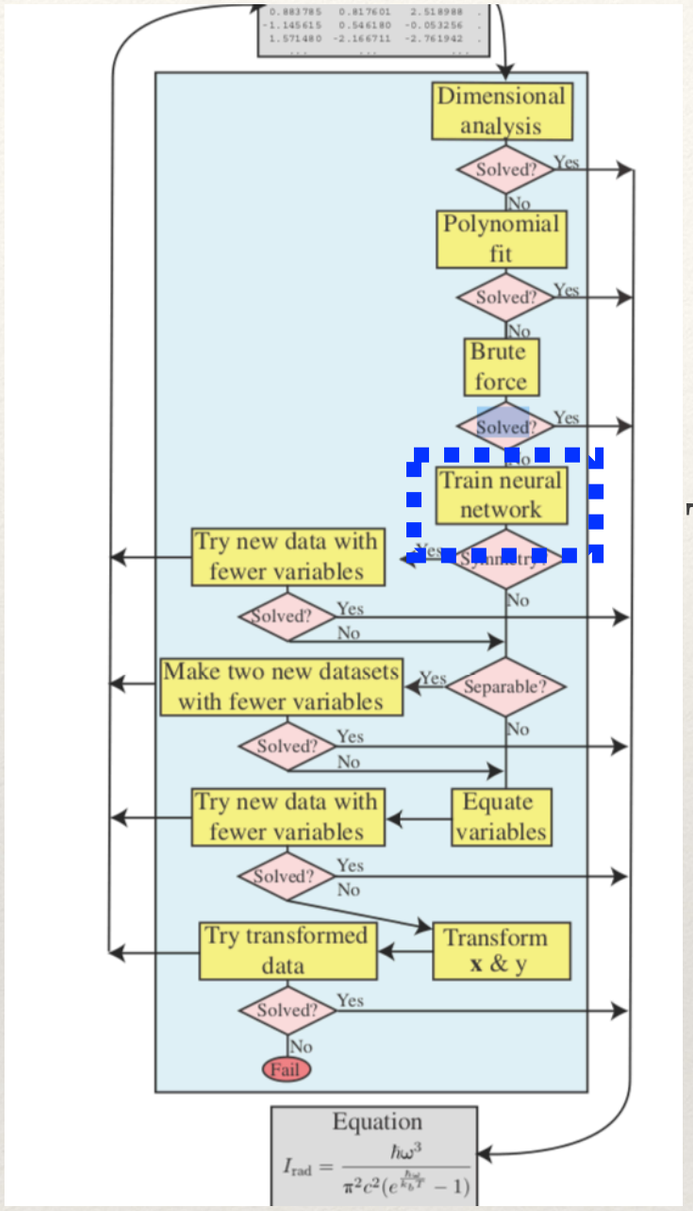
Showed that NNs were storing somehow information of the angular momentum
The size of the latent activation was related to total angular momentum



Symmetry meets AI,
2103.06115 by Barenboim, Hirn, VS

We give a task to an AI and then
interrogate it to understand if it *discovered*
the concept of symmetry—>
build a symmetry detector, apply it to art

Example 3: AI Feynman



Given a dataset (X, y) find the function y=f(X)

Clearly a task for a NN

The authors (physicists) use a set of

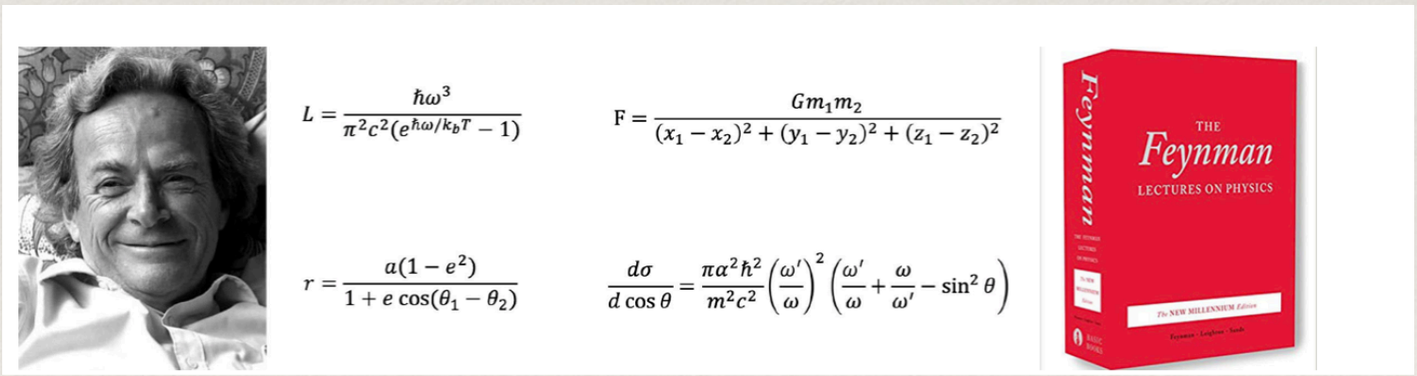
tricks to speed up things

(symmetries / dimensional analysis etc)

Then they test this procedure against hundreds of physics

equations in Feynman lectures

and compare with a commercial tool



AI Feynman, Udrescu & Tegmark, 1905.11481

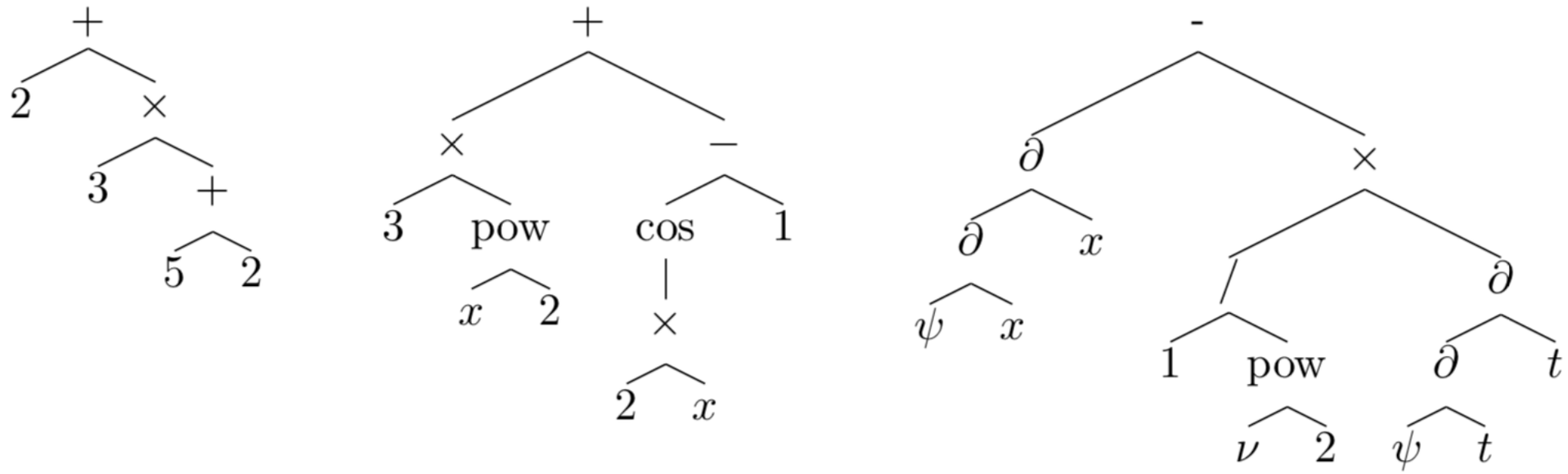
It's AI-assisted BRUTE FORCE

a more promising avenue:

using Transformers from Charton's group @ Meta

Example 4: Symbolic mathematics

expressions $2 + 3 \times (5 + 2)$, $3x^2 + \cos(2x) - 1$, and $\frac{\partial^2 \psi}{\partial x^2} - \frac{1}{\nu^2} \frac{\partial^2 \psi}{\partial t^2}$:



$x^2 \left(\tan^2(x) + 1\right) + 2x \tan(x) + 1$	$x^2 \tan(x) + x$
$1 + \frac{2\cos(2x)}{\sqrt{\sin^2(2x) + 1}}$	$x + \operatorname{asinh}(\sin(2x))$
$\frac{x \tan(x) + \log(x \cos(x)) - 1}{\log(x \cos(x))^2}$	$\frac{x}{\log(x \cos(x))}$
$-\frac{2x \cos\left(\operatorname{asin}^2(x)\right) \operatorname{asin}(x)}{\sqrt{1 - x^2} \sin^2\left(\operatorname{asin}^2(x)\right)} + \frac{1}{\sin\left(\operatorname{asin}^2(x)\right)}$	$\frac{x}{\sin\left(\operatorname{asin}^2(x)\right)}$
$\sqrt{x} + x\left(\frac{2x}{\sqrt{x^4 + 1}} + 1 + \frac{1}{2\sqrt{x}}\right) + x + \operatorname{asinh}\left(x^2\right)$	$x\left(\sqrt{x} + x + \operatorname{asinh}\left(x^2\right)\right)$
$\frac{-3 - \frac{3\left(-3x^2 \sin\left(x^3\right) + \frac{1}{2\sqrt{x}}\right)}{\sqrt{x} + \cos\left(x^3\right)}}{\left(x + \log\left(\sqrt{x} + \cos\left(x^3\right)\right)\right)^2}$	$\frac{3}{x + \log\left(\sqrt{x} + \cos\left(x^3\right)\right)}$
$\frac{-2 \tan^2(\log(\log(x))) - 2}{\log(x) \tan^2(\log(\log(x)))} + \frac{2}{\tan(\log(\log(x)))}$	$\frac{2x}{\tan(\log(\log(x)))}$

transform mathematical expressions into trees of relations

LANGUAGE TRANSLATION

Run a NLP algorithm to learn to symbolically solve integrals / differential equations etc

Benchmark against Mathematica / Matlab etc and obtain similar or better results

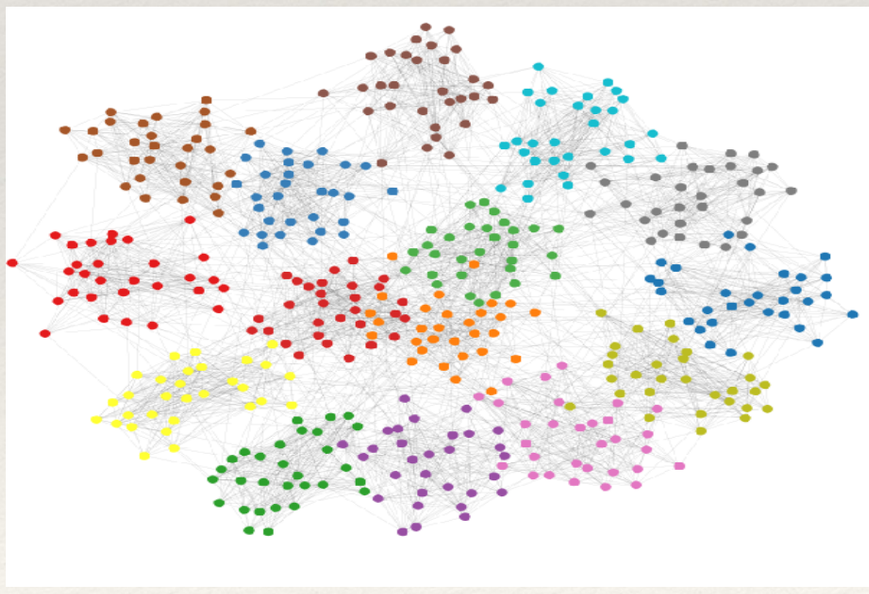
Explainable AI

Explainable AI?

We are talking about powerful stuff
with direct societal impact

With a simple hardware setup we can track and ID hundreds
of people in real time

we can scout online posts to gauge sentiment, cluster
individuals based on electricity use, predict sexual/political
orientation from a few clicks…



Explainable AI?

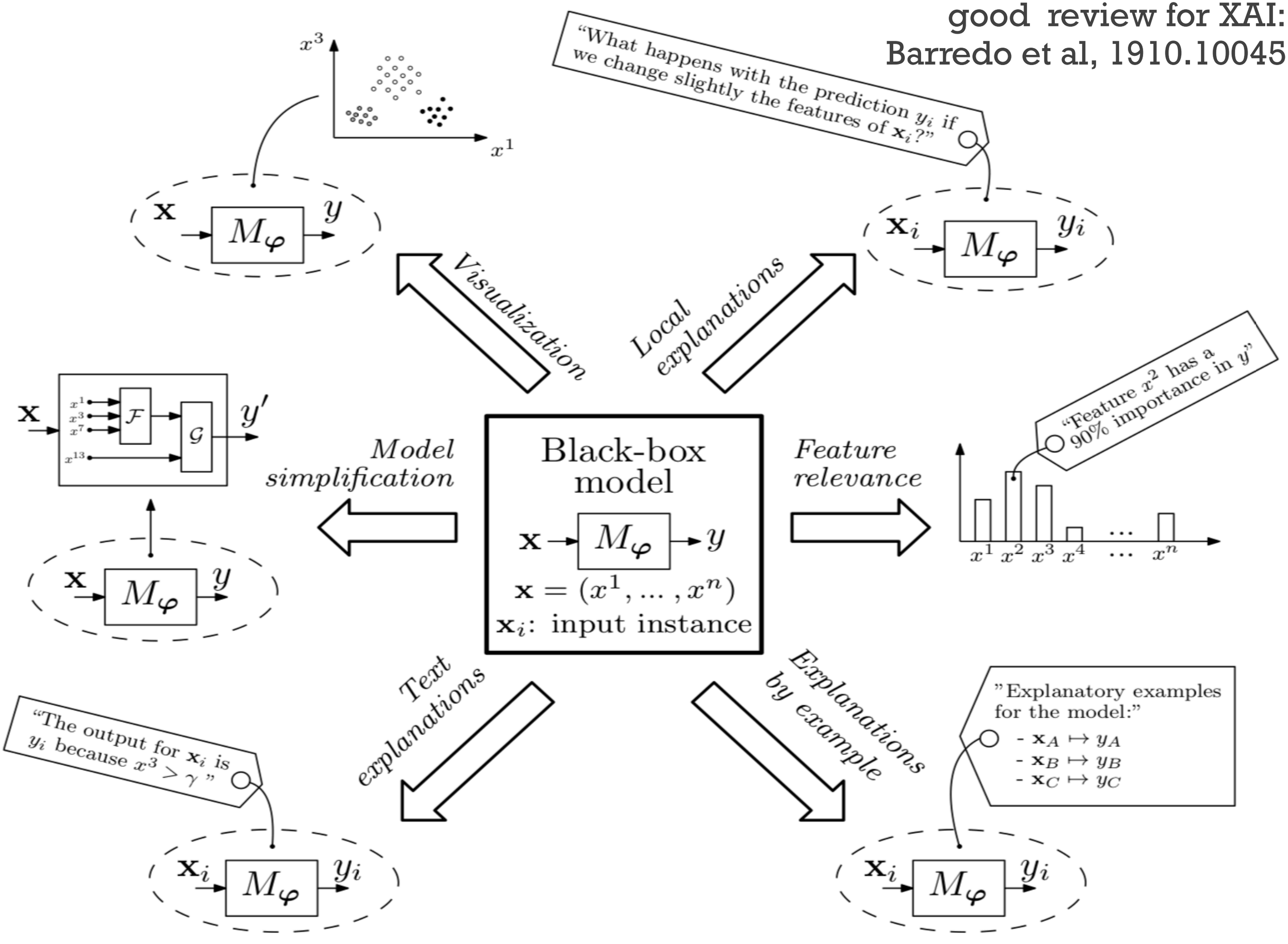
So, yes, we cannot just hold AI's hand,
close our eyes and jump with it

From an ethical perspective: we need to make sure decisions
based on AI comply with human policies
AI is a tool, not an aim

From a practical perspective: breakthroughs come from poking
around big solid castles like AI
Finding what AI *does* can help us discover new techniques

To trust AI's decisions and help on improving them
we need AI to become more 'human-readable'

good review for XAI:
Barredo et al, 1910.10045



Wrapping up…

We are just starting to explore the applications of ML in Fundamental Physics

They go beyond a mere iteration of our traditional statistical methods:
unsupervised methods, generative AI, reinforcement learning…

Through AI methods, there is interesting cross-pollination
between our area and others

A very efficient blackbox is not good enough for us,
we try to *communicate* with the AI,
to find ways to understand its inner workings

Today we learned that an AI can identify and use higher level concepts,
and this learning can be found in subtle features of the hidden layers

I believe that moving forward,
more thought needs to be placed on XAI methods
to make the AI inner workings closer to human intuition

Thanks for listening!

Questions?