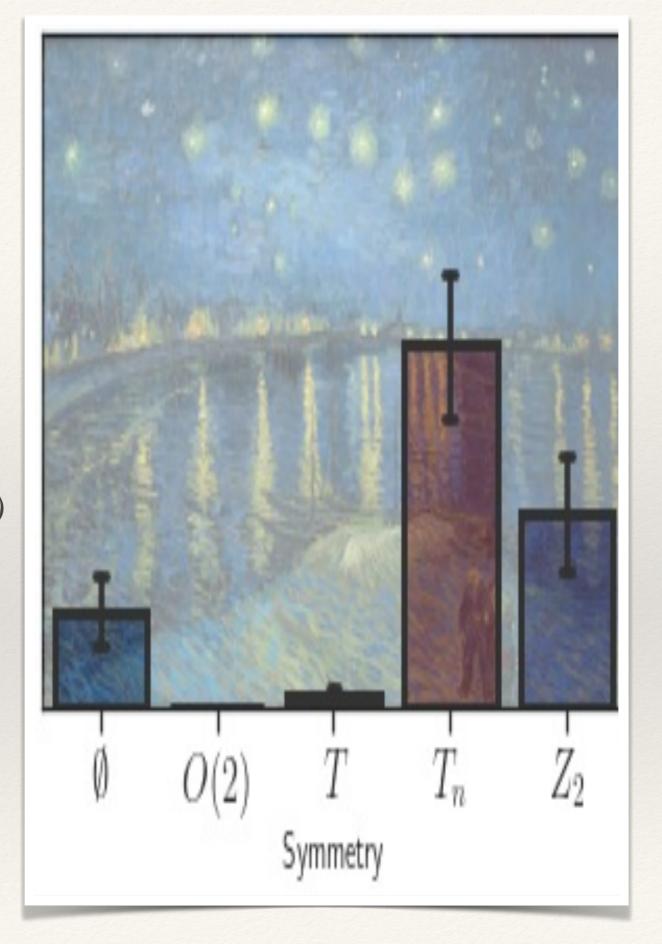
IWR School

Applications in theory and beyond

Veronica Sanz (IFIC-UValencia/CSIC)



In these lectures, we will talk about

- 1. AI-assisted Science
- 2. Human surrender?
- 3. Looking under the hood
- 4. Variational Autoencoders
 - 5. Symmetries
 - *classical mechanics
 - *particle collisions
 - *art
- 6. Beyond physics with AI
 - *Ecology and restoration
 - *Musical concepts
 - *Political adherence
- *Traffic and pollution, Sun storms



AI-assisted Science

AI vs ML vs DL

Today we live in an era where the edge is Deep
Learning

with new opportunities and new challenges

ARTIFICIAL INTELLIGENCE

A programme that can feel, reason, act and adapt to the environment

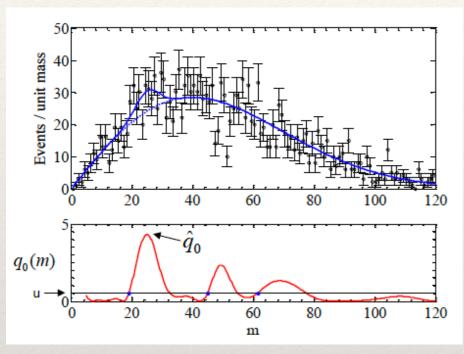
MACHINE LEARNING

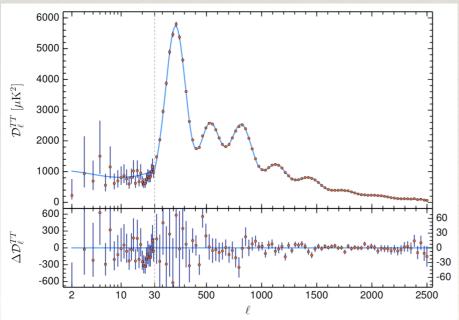
Algorithms which improve as they are exposed to more data

DEEP LEARNING

Neural Networks which learn from huge amounts of data

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





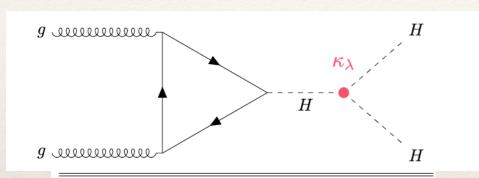
In fact,
we have always been early
adopters and developers of
sophisticated statistical techniques

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

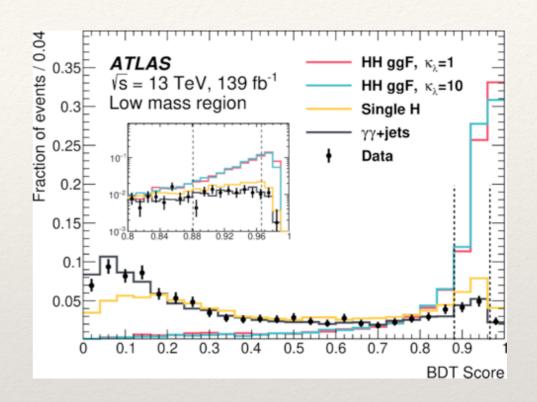
Exps. have been using ML for a very long time esp in channels where discovery = squeezing a bit more (eg. TeVatron's monotop)

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e.g. ATLAS HDBS-2018-34

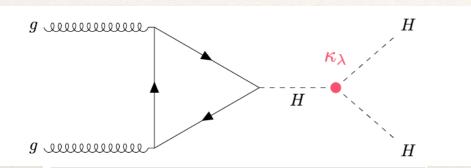


Photon-related kinematic variables				
$p_{\mathrm{T}}/m_{\gamma\gamma}$	Transverse momentum of each of the two photons divide by the diphoton invariant mass $m_{\gamma\gamma}$ Pseudorapidity and azimuthal angle of the leading an subleading photon			
η and ϕ				
Jet-related kinematic variables				
b-tag status	Tightest fixed b -tag working point (60%, 70%, or 77% that the jet passes			
p_{T}, η and ϕ	Transverse momentum, pseudorapidity and azimuthal angle of the two jets with the highest <i>b</i> -tagging score			
$p_{\mathrm{T}}^{b\bar{b}},\eta_{b\bar{b}}$ and $\phi_{b\bar{b}}$	Transverse momentum, pseudorapidity and azimuthal angle of the <i>b</i> -tagged jets system			
$m_{bar{b}}$	Invariant mass of the two jets with the highest <i>b</i> -tagging score			
H_{T}	Scalar sum of the p_T of the jets in the event			
Single topness	For the definition, see Eq. (??)			
Missing transverse	e momentum variables			
$E_{\mathrm{T}}^{\mathrm{miss}}$ and ϕ^{miss}	Missing transverse momentum and its azimuthal angle			

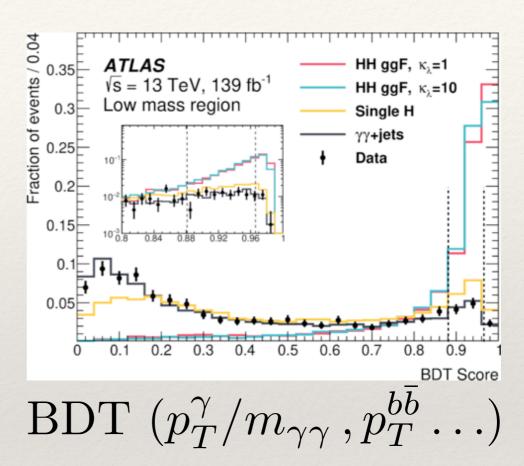


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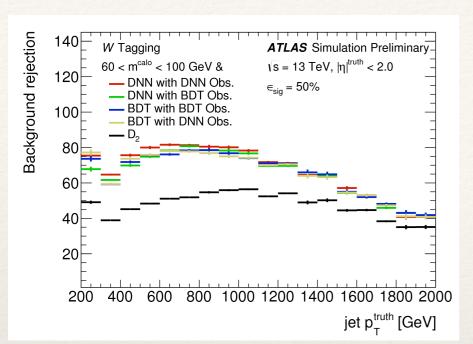


Where this function is highly nonlinear and can express complex relationships

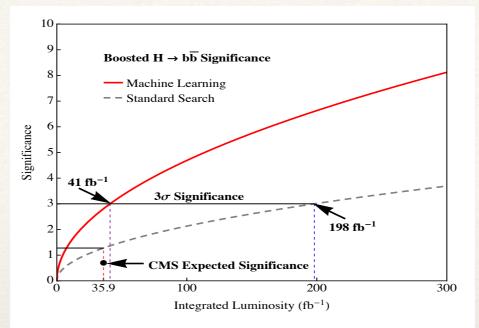
CAVEATs: interpretability, communication to theorists, reuse of data... all the stuff that happens when we move towards more complex/aggressive techniques

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

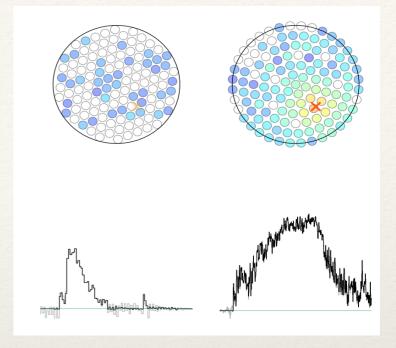
Is it a W?

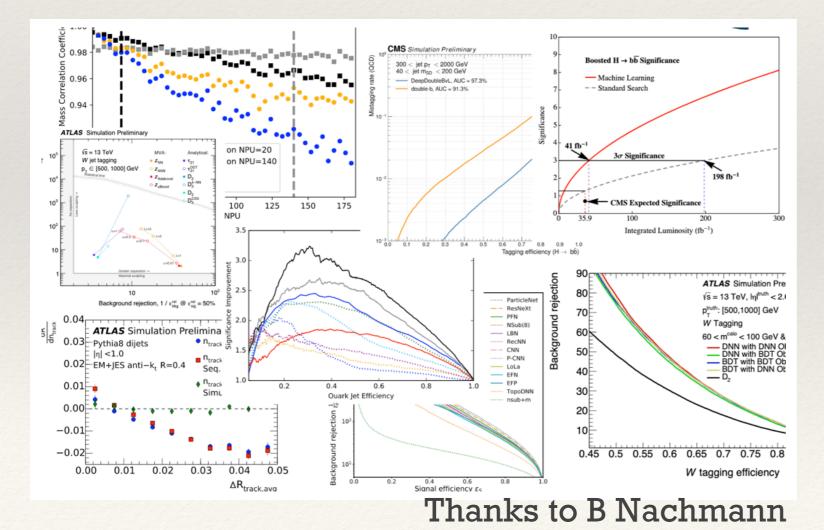


Is it a Higgs?



Is it DM?





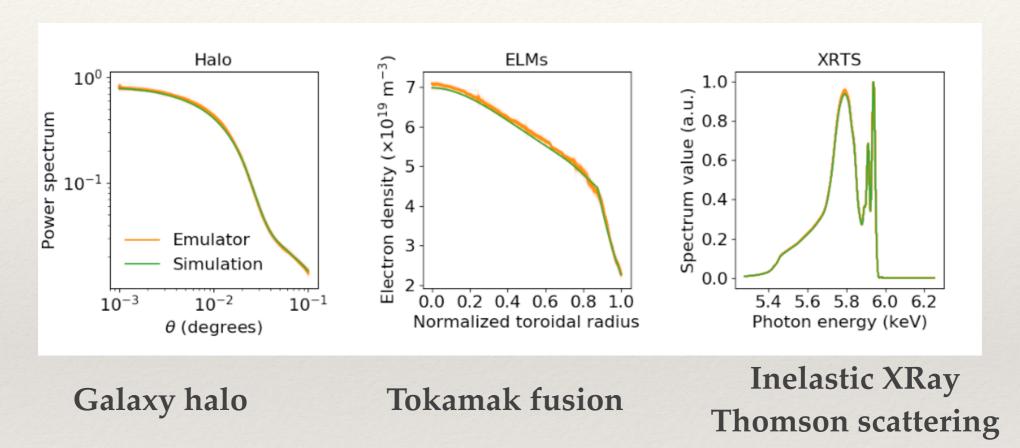
The gains in ID-ing phenomena are typically in the range of 5%-30%

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)

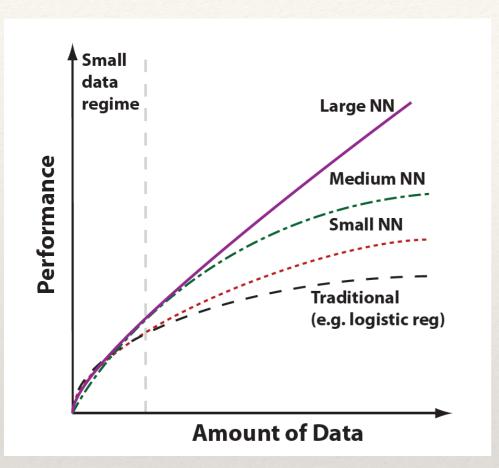


Method	Platform	Time/shower (msec)	Speedup
Monte Carlo	2S Intel Xeon Platinum 8180	17000	1.0
3DGAN CPU		16	1063
3DGAN GPU	GTX 1080	4	4250

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

SEE MANUEL'S LECTURES

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

NNs are able to take large streams of data and learn features with little

guidance, work like black boxes

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



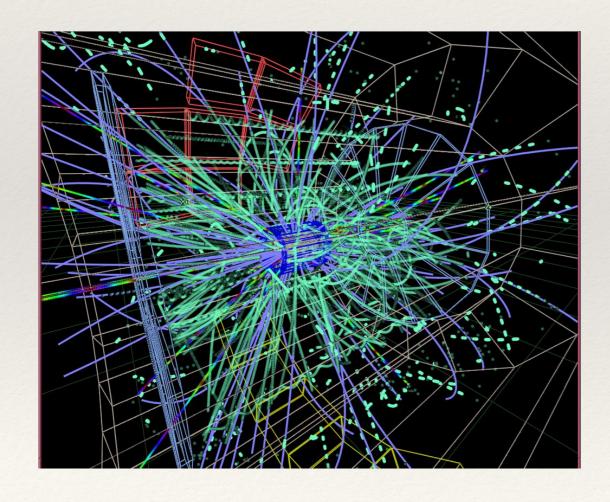
Human surrender?



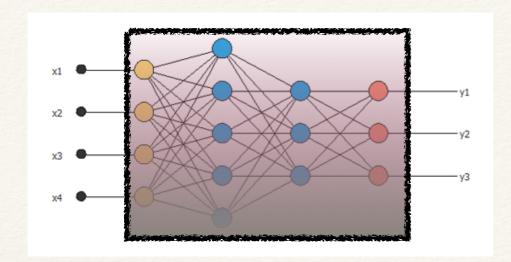
Only open in case of a disaster

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



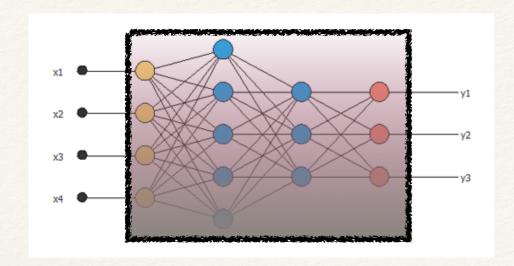
If the blackbox can help ID'ing this event faster and better than a traditional algorithm, who cares?



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



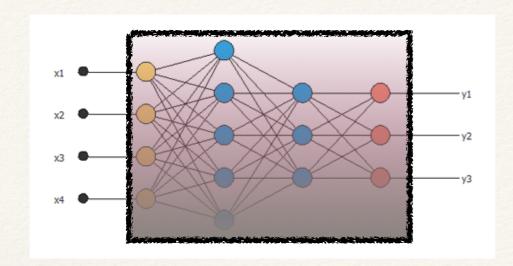
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Any efforts we do to express the workings of NNs from different viewpoints may lead to new ideas for machine learning



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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 efforts to regulate AI

XAI, Ethical AI... all these require a better understanding of DNNs

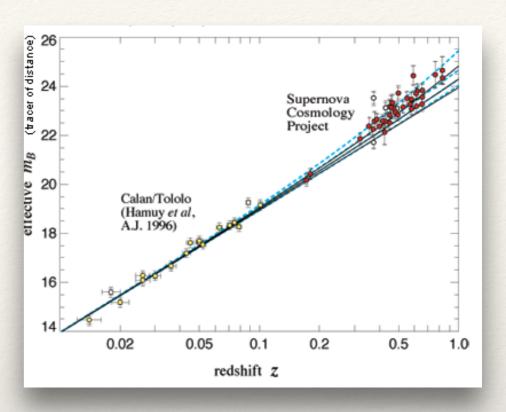


Looking under the hood

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

what would **you** do?

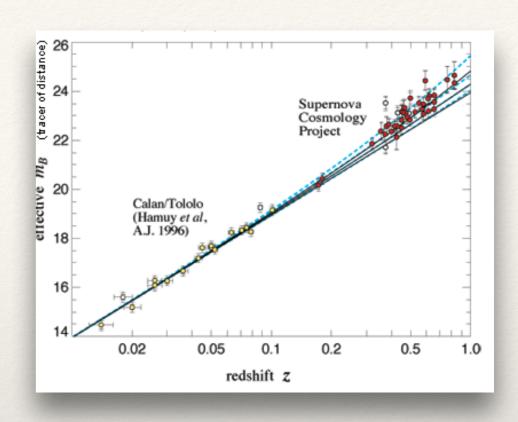
as a physicist, you would start thinking on possible physical relations, plotting things, trying to obtain the best data representation *the* representation which manifests a behaviour Could an AI guide you?



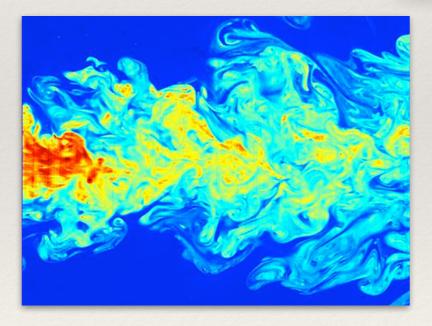
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If I showed you many examples of fluid behaviour

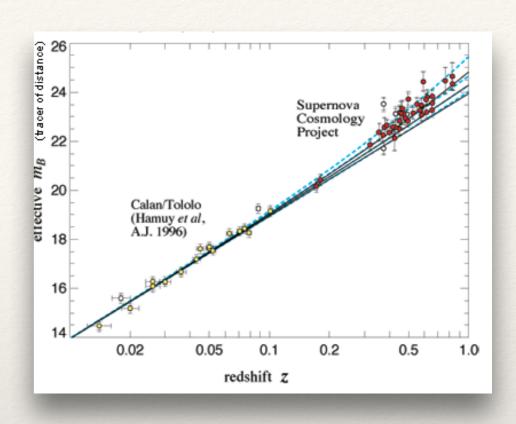


would you learn the Navier-Stokes equation?

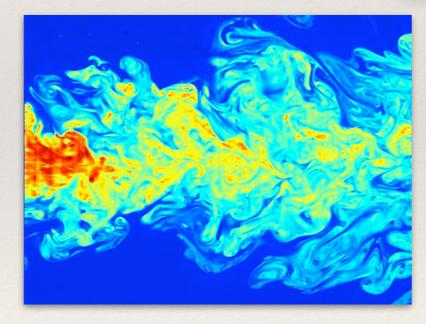
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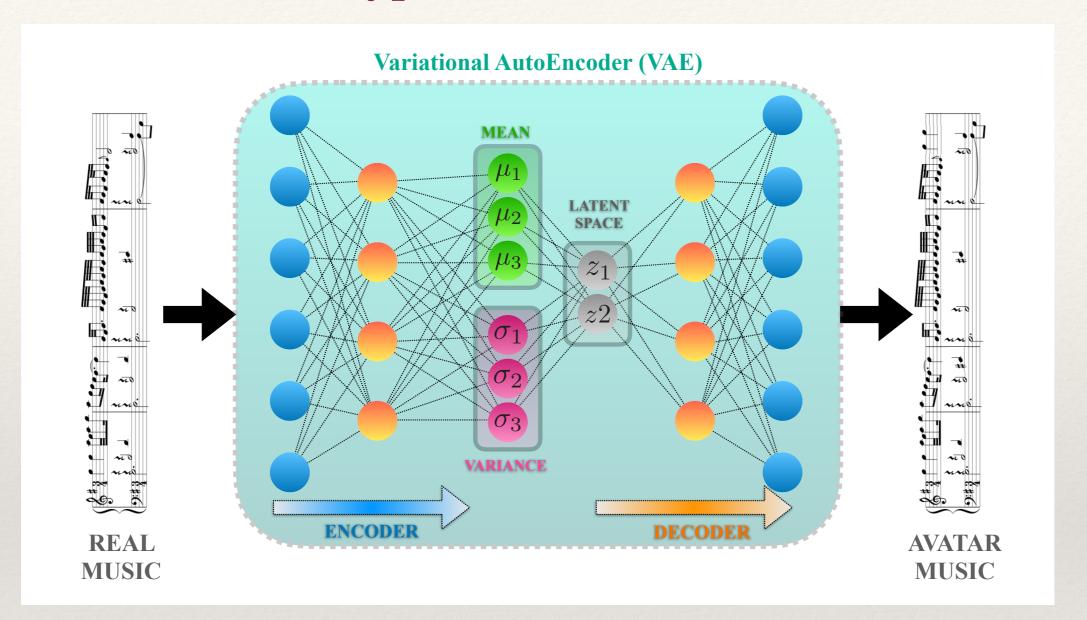
AI can help with that, e.g. **Symbolic Regression** (aka Eq Discovery) or **symmetry**-ID



Variational Autoencoders

I am sure you have learned and used VAEs already, but do keep listening

VAEs: a type of GenAI architecture



ENCODER: compresses the data, forcing higher levels of abstraction DECODER: decompresses, creates new samples (Generative part)

Max level of compression (more abstraction)= bottleneck LATENT SPACE

Let's discuss how VAEs are trained

Supervised learning input-> predict output what if we just asked 'look at this!' with no determined output?

GANs (Generative Adversarial Networks)

and VAEs (Variational AutoEncoders)

In CNNs, benchmarks were cats/dogs and hand-written digits (MNIST)

Here, human faces

Supervised learning input-> predict output what if we just asked 'look at this!' with no determined output?

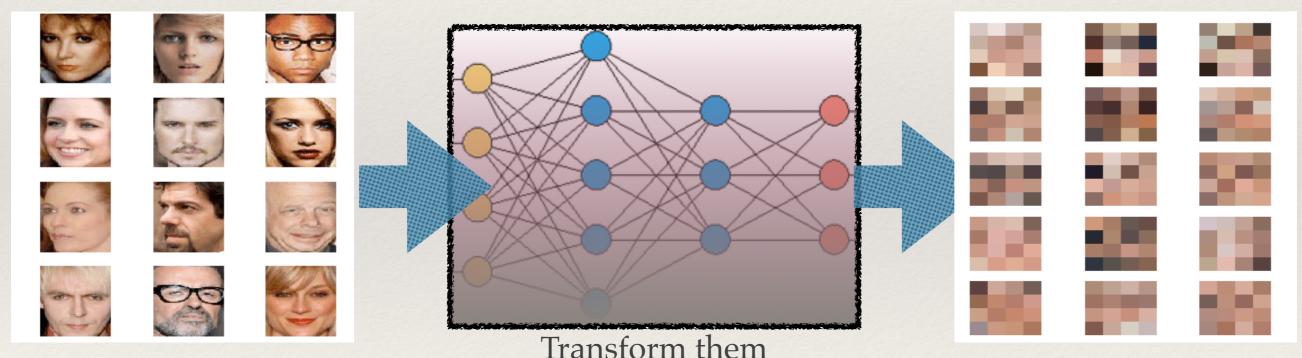
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STEP 1 - 'LEARN' what is a human face



Take face images: x

in complicated ways

Create an avatar: x'

Doing this many times, while the DISCRIMINATOR says: 'You are going in the right direction', 'You are completely lost!'

Supervised learning input-> predict output what if we just asked 'look at this!' with no determined output?

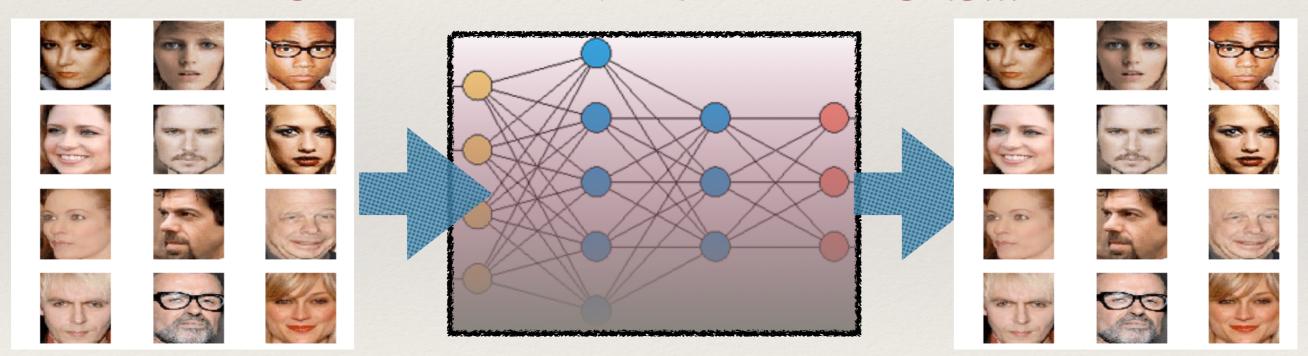
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STEP 2- AFTER MANY ITERATIONS...



When the avatars are indistinguishable to the DISCRIMINATOR, game is over

Wait a minute!

Aren't we just programming the identity transformation?

Wait a minute!

Aren't we just programming the identity transformation?

NNs have a huge number of parameters (**expressivity**) so they could be just memorising all the faces (**overfitting**) Yet, we did control for that during the training

Supervised learning input-> predict output what if we just asked 'look at this!' with no determined output?

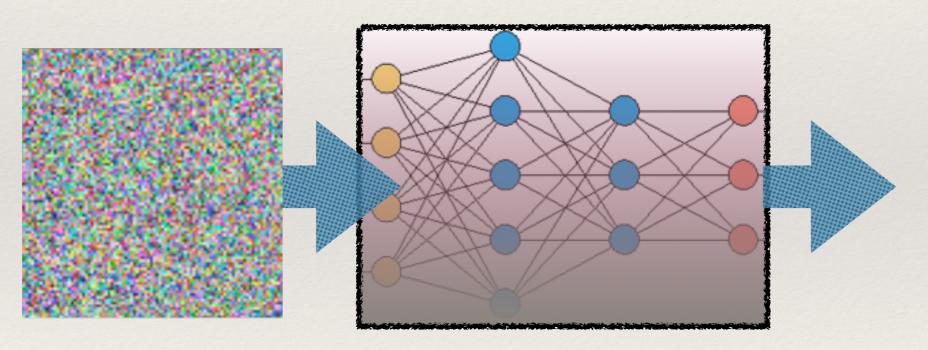
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STEP 3- CREATE NEW POSSIBILITIES



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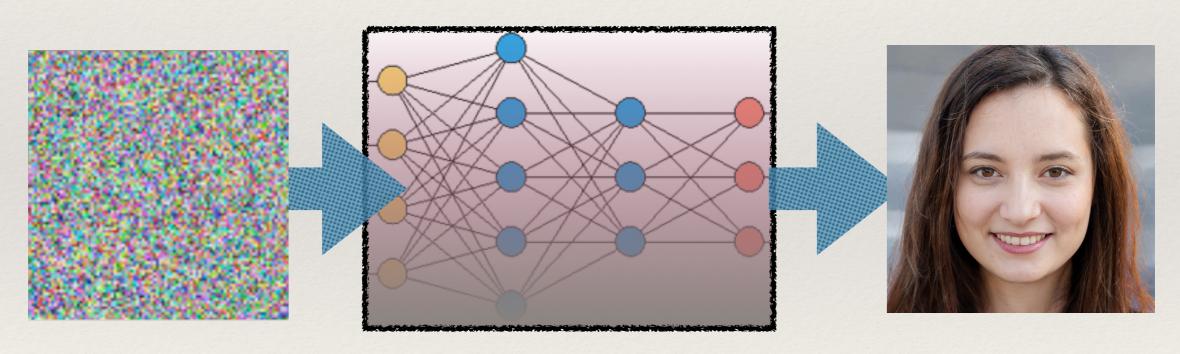
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STEP 3- CREATE NEW POSSIBILITIES



This woman **does not exist**. It has been generated from noise. The NN has learnt the *concept* of 'human face' and now can create human faces from noise

Supervised learning input-> predict output what if we just asked 'look at this!' with no determined output?

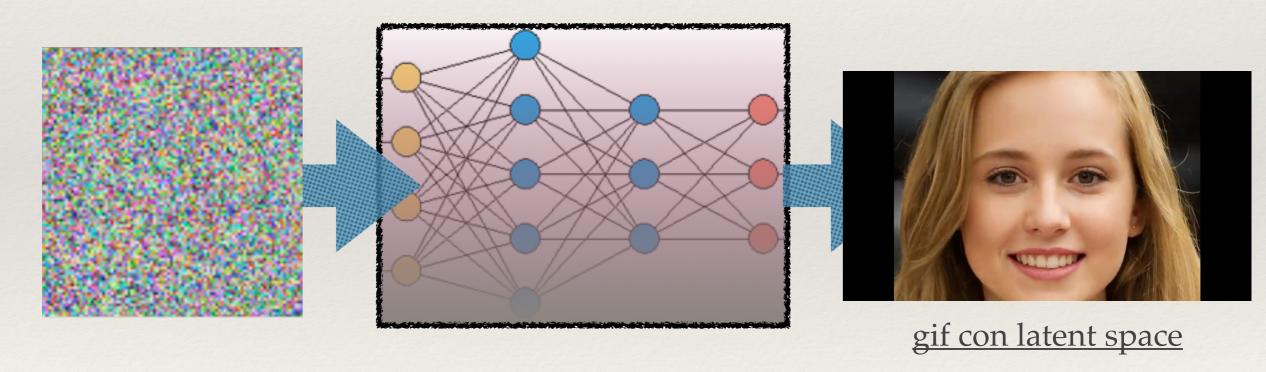
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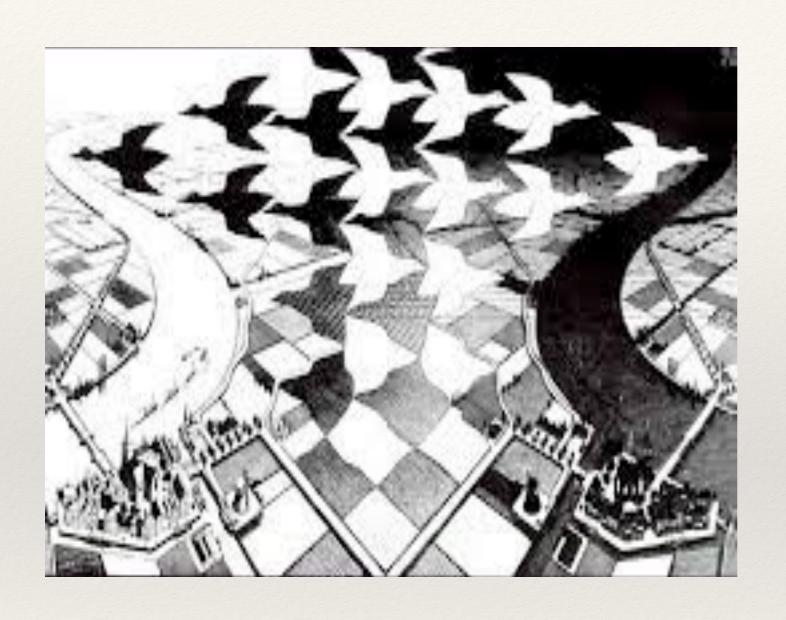
In CNNs, benchmarks were cats/dogs and hand-written digits (MNIST)

Here, human faces

STEP 3- CREATE NEW POSSIBILITIES



Random noise generate deformations in the output, leading to new *people*



Symmetries

Can NNs learn **concepts** like symmetry? We just saw how it *learned* the concept of human face

A symmetry is a redundancy, so the AI should learn it to become more efficient at describing the data

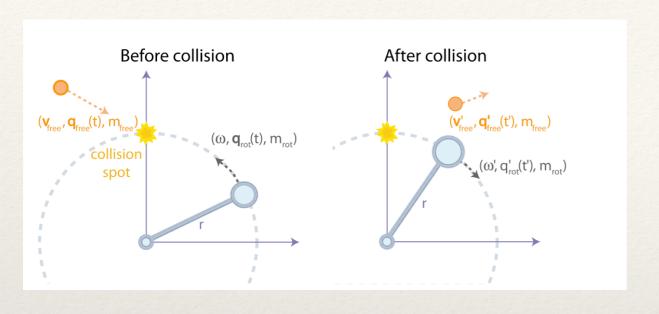
The initial question is **how** do we interrogate a blackbox and learn if it has learned the symmetry

Then we can continue by testing if it can learn symmetries even if **approximate**

Ultimately, the idea would be to let the AI find principles for us

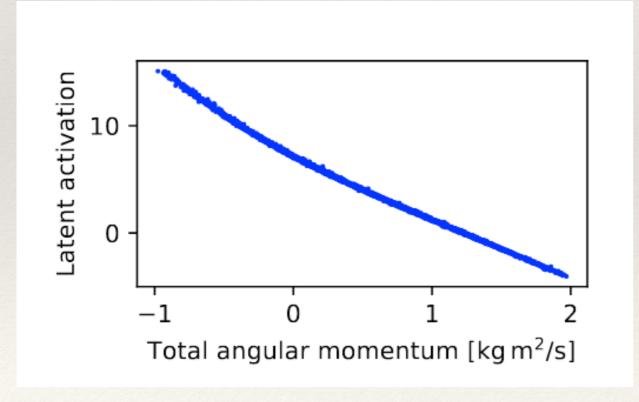
Let's start with something very simple

Discovering physical concepts with NNs, 1807.10300 by Iten et al



Classical mechanics:

Create a dataset of the characteristics of this type of collision
Train a VAE with the data
Reduce the latent space to a single neuron

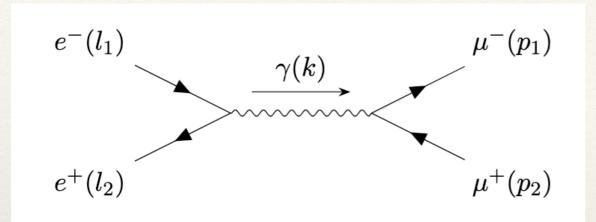


Interrogate the VAE= find a strong correlation between the neuron activation and the system

They showed that NNs were storing information of the angular momentum. The size of the latent activation was related to total angular momentum.

Let's do something a bit more complicated

Learning Symmetries in datasets, 2504.05174 by VS



Relevance plot-lepton collisions n_1 n_2 n_3 n_4 n_5 n_6

QED:

Create a dataset with the muons 4vectors
Train a VAE with the data

Interrogate the VAE

A bit more complicated than before

1.) What is the perceived dimensionality of the system?

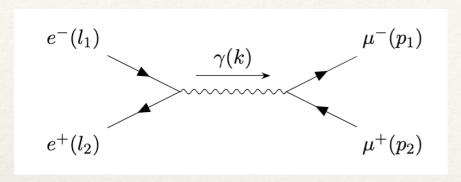
Relevance_j =
$$\frac{\operatorname{std}(\langle z_j \rangle)}{\operatorname{mean}(\sigma_j)}$$
,

From Exploring how a GenAI understands music—> Tomorrow

Input dim is 8, VAE sees 3 => there must be redundancies/symmetries

Let's do something a bit more complicated

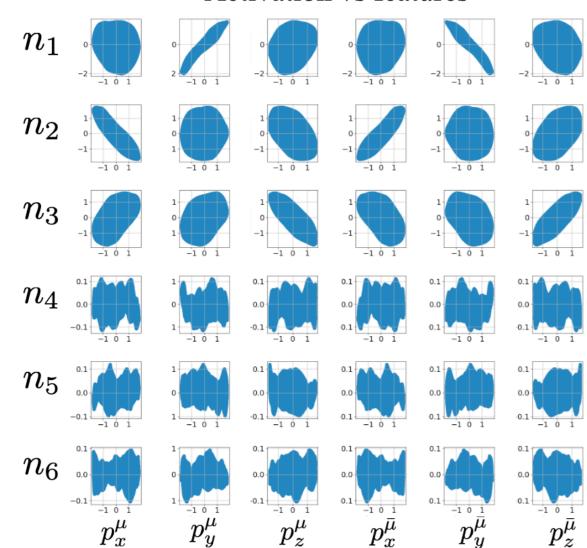
Learning Symmetries in datasets, 2504.05174 by VS



2.) What did it learn?

In these collisions, energy-momentum is conserved Energy fixed, 3D momentum conservation So we go from 8 to 8-2-3=3 quantities

Activation vs features



Momentum conservation

$$p_x^{\mu} + p_x^{\bar{\mu}} = 0 \; ,$$
 $p_y^{\mu} + p_y^{\bar{\mu}} = 0 \; ,$ $p_z^{\mu} + p_z^{\bar{\mu}} = 0 \; .$

Have been **discovered** and **encoded** in the three relevant neurons, leaving the rest as **generative**

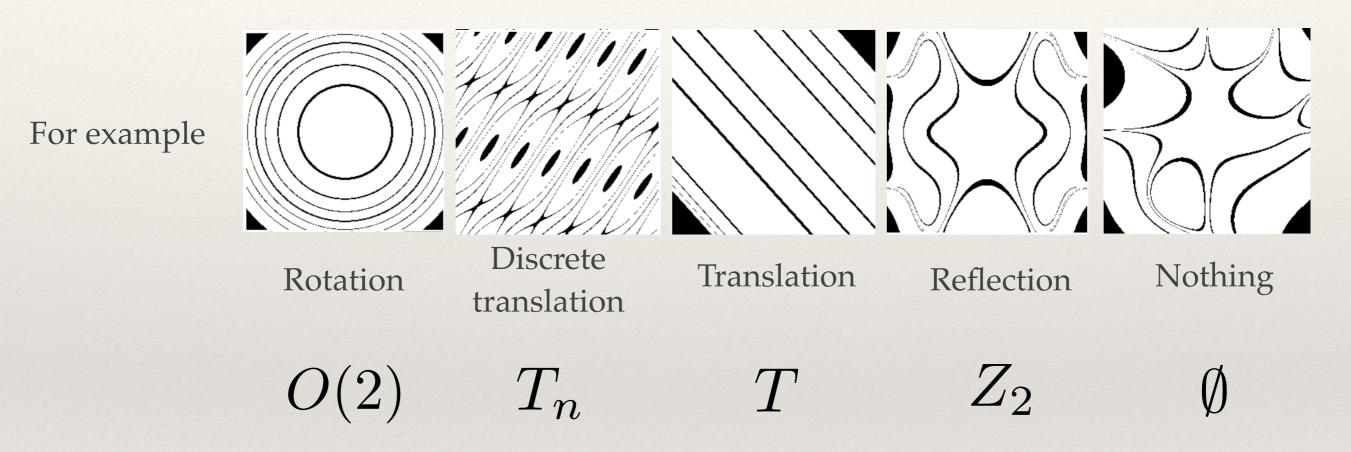
$$\langle z_2 \rangle \sim p_x^\mu - p_x^{\bar{\mu}} \; ,$$

 $\langle z_1 \rangle \sim p_y^\mu - p_y^{\bar{\mu}} \; ,$
 $\langle z_3 \rangle \sim p_z^\mu - p_z^{\bar{\mu}} \; .$

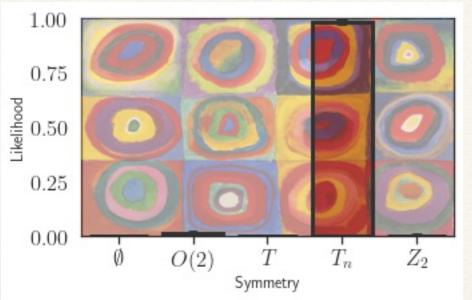
Let's see if this stands with approx symms

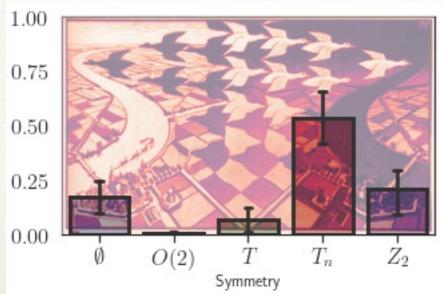
Symmetry meets AI, SciPost Phys (2021) by Barenboim, Hirn, VS

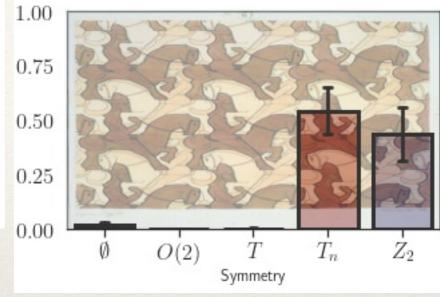
1.) Create a dataset of 2D images of potentials with symmetries (or not)



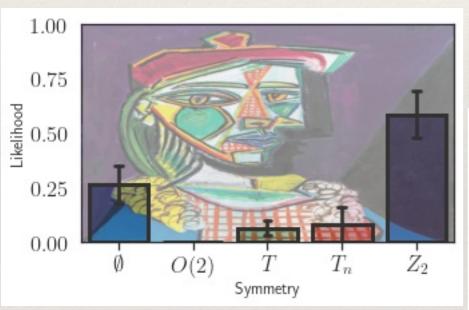
- 2.) Train this set in a decoy task (again like an identity) and inspect the last hidden layer
 - 3.) With the true labels, train a symmetry detector
 - 4.) Apply it to art, see if it can handle approx symmetries

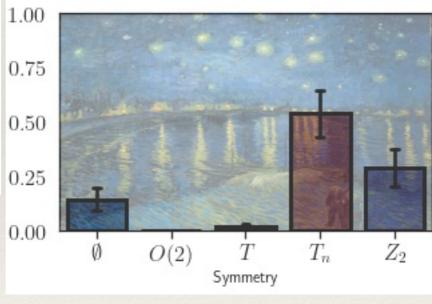






 \dot{Z}_2

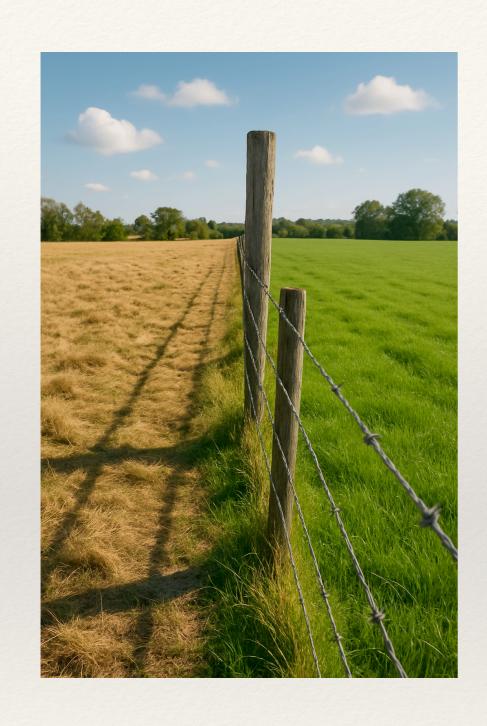




1.00

0.75

and many more, including children's drawings, fractals, photographs etc 0.50 0.25 0.00 0.00 0.00



Beyond fundamental physics

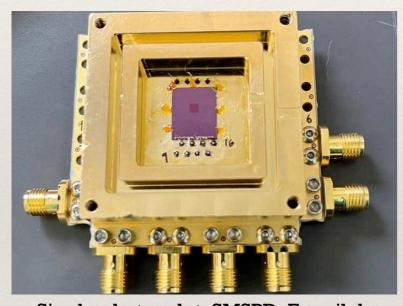
In fundamental physics we ALWAYS have a firm ground to step from

A theoretical framework: SM, LambdaCDM, mean field, perturbation theory in QFT...

We say *terra incognita* or similar, but we actually have a **range** of possibilities in mind

In fundamental physics we ALWAYS have a firm ground to step from

A theoretical framework: SM, LambdaCDM, mean field, perturbation theory in QFT...

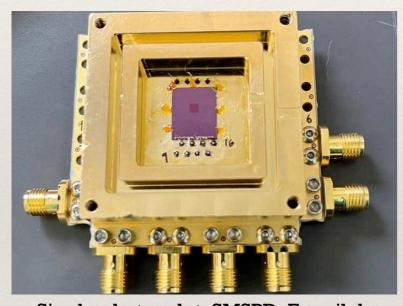


Single photon det. SMSPD. Fermilab

+some physical understanding of the observable environment: we build our purpose-made instruments, experiments are reproducible, measurements can be correlated...

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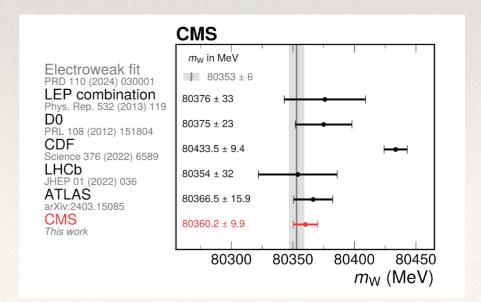
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Single photon det. SMSPD. Fermilab

+some physical understanding of the observable environment: we build our purpose-made instruments, experiments are reproducible, measurements can be correlated...

Very often cross-checks are possible,
limiting cases are known
Improvements can be done incrementally
Precision is an achievable goal



When attacking a problem CMS's W to lepton-neutrino, electron tracking we develop frameworks that allow us to correlate with others EWPTs global fit, GEANT4 electron's behaviour in a material progress in one corner of the data often illuminates other areas

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Robust tools for DAQ, simulation and theoretical interpretation MC@NLO, GEANT4...

These capabilities are distinctive to us

However, when engaging with other scientific domains
fields equally rich in data and eager for deeper understanding
this mindset must evolve

Understanding, period

*Learn unknown patterns e.g. beginning solar storm

*Discover relations, equations

e.g. competition/cooperation among species

*Find more abstract, simplifying description of a complex system e.g. find the political axes

* Evolution of a situation e.g. predict a traffic jam

& robustify your prediction e.g. set an alarm threshold

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*Find more abstract, simplifying description of a complex system *e.g.* find the political axes

* Evolution of a situation *e.g.* predict a traffic jam

& robustify your prediction *e.g.* set an alarm threshold

But outside fundamental physics, *data* may be more sparse, w/genuinely more variance, bunch of unknown unknowns, prone to glitches... data prep and viz are more important Even the target variables may not be clear

Let's discuss examples of all this

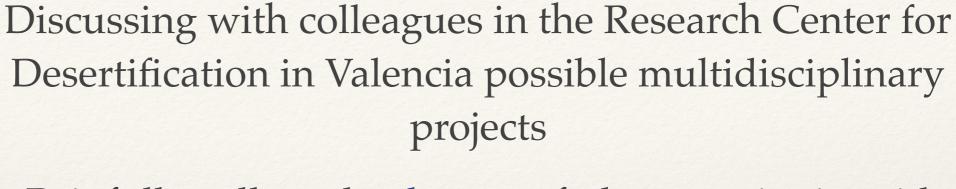


Understanding ecological interactions with AI

Based on papers in Methods in Ecology and Evolution (2022), Applications of Generative AI (2024), Ecological Informatics (2024), Journal of Applied Ecology (2025)

The beginning





Painfully collected a dataset of plant species in arid regions in the Mediterranean (typical landscape)

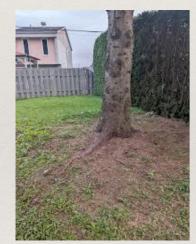
Done by an expert human, cost is huge

Hope was to use this dataset (from the natural environment) to help restoration efforts

Restoring the ecosystem in an arid region is complex, conditions are harsh and policy had been to plant pines for exploitation (bad idea)

Hypothesis:

phylogenetic closeness should impact restoration





The beginning - Petrer



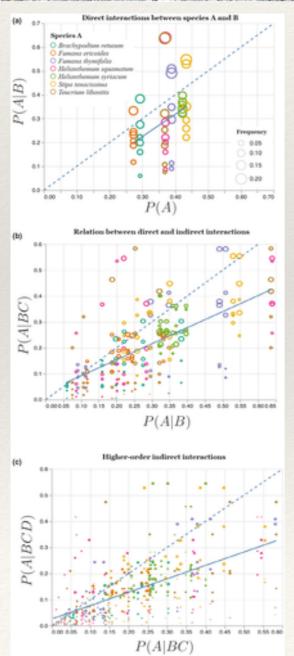
The dataset was grouped as a patch (a small area on the ground) with annotations of which species where present, number of them, and which was the nurse

We spent a lot of time with cleaning and viz tasks

Rough ideas learn what makes species cooperate or compete, under what circumstances, what creates more diversity

The beginning - Petrer





The dataset was grouped as a patch (a small area on the ground) with annotations of which species where present, number of them, and which was the nurse

We spent a lot of time with cleaning and viz tasks

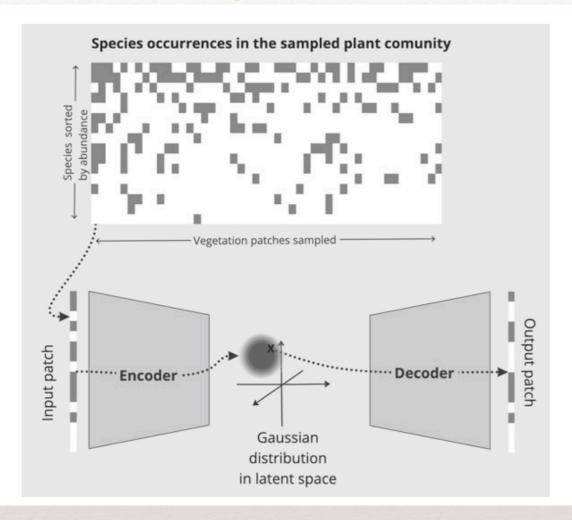
Rough ideas learn what makes species cooperate or compete, under what circumstances, what creates more diversity

Obstacle was lack of stats

just few thousands of examples for dozens of species limitation **intrinsic** to the study
We also knew that **interactions were complex**

We toyed with many statistical and AI techniques recommendation systems, LLMs, correlation+kurtosis etc searching for a clear question and a clear answer

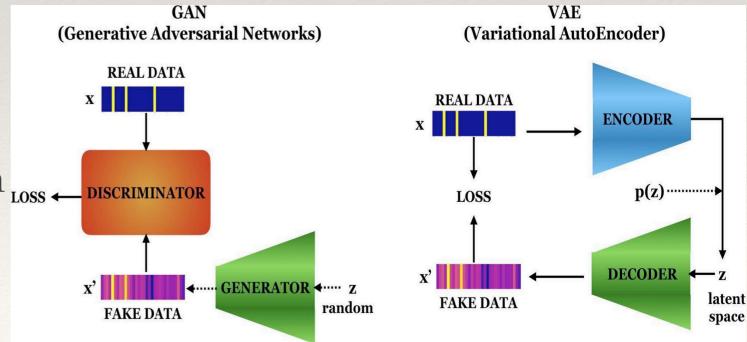
Setting the problem



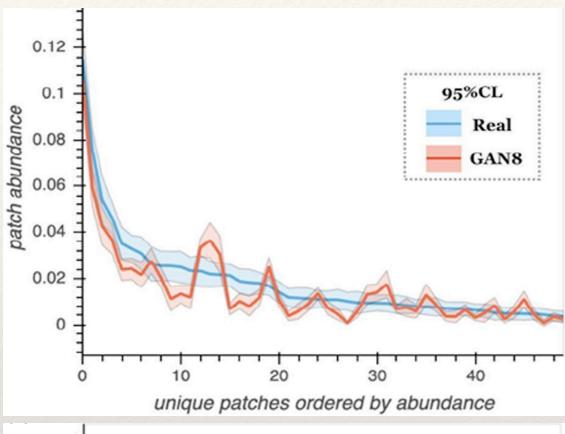
We settled to represent the data as absence/presence in a patch

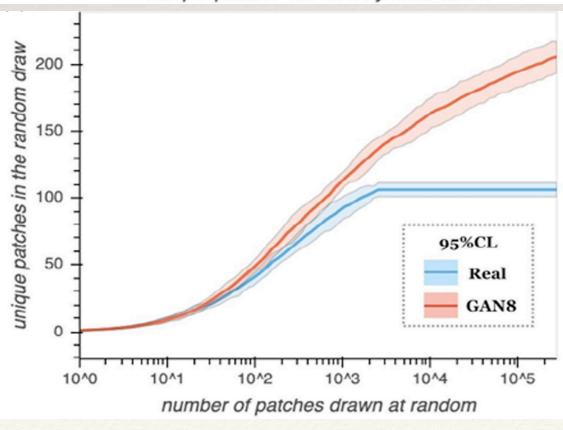
We trained (successfully) a GAN and VAE with varying number of species 8-16-32 most common species

Aim to get a model of the species interactions that can interpolate in the regions with limited stats



Results on Petrer



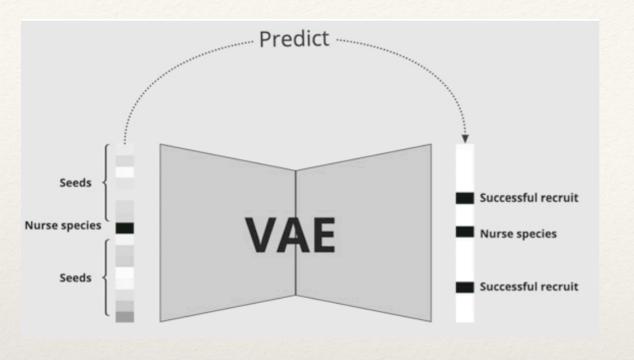


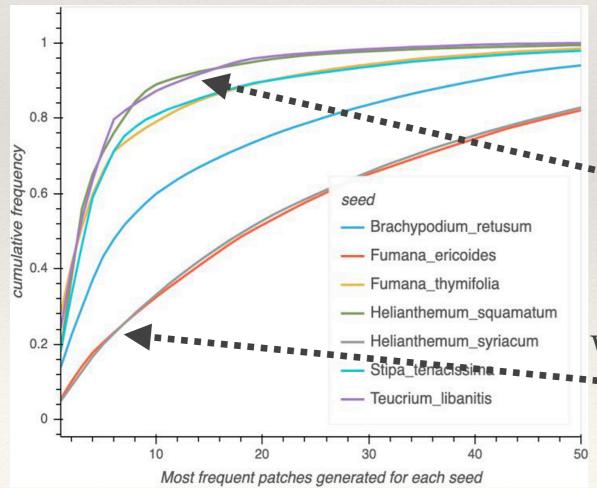
Once you have a GenAI model trained on data, you can start sampling from it and see how far it goes

The GenAI model was reproducing the typical distribution in the natural environment e.g. had learned gypsum terrain and we could refute the phylogenia hypothesis

And could be extrapolated to regions where there was no data in a continuous way

Results on Petrer



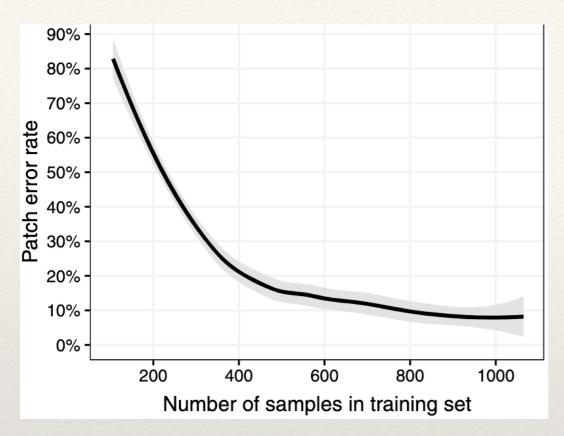


With the GenAI model we can ask restoration questions such as What seed would produce more diverse patches?

The VAE can be used to test pioneer species by introducing them into its latent space and analyzing the generated patch distributions

produce only a few dominant patch types '* with high probability, saturating quickly

generate a larger variety of distinct patches with low individual probabilities, suggesting they promote greater biodiversity



Unsurprisingly the more data the better, to a point

But datasets in this area a really small (hundreds of samples) and scaling up is a costly field campaign

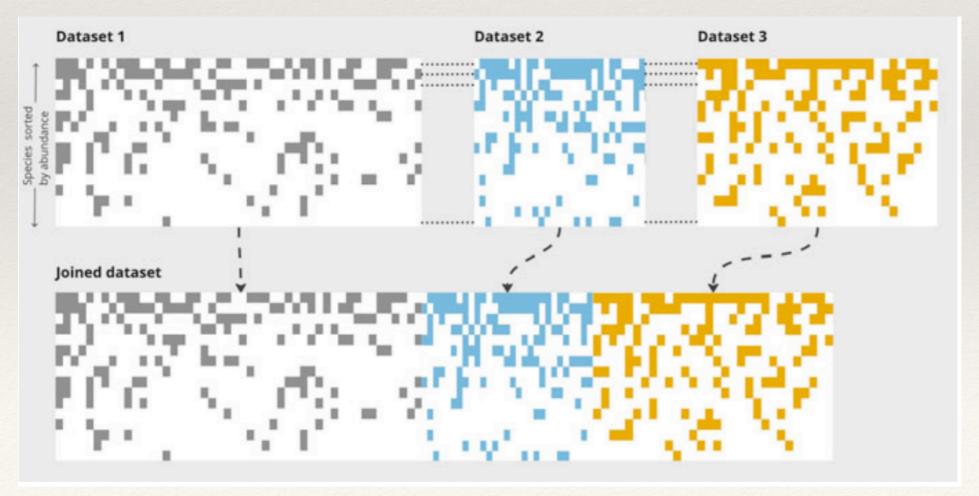
Also, maybe the rules of the game learned by the GenAI model are somewhat universal, albeit complex

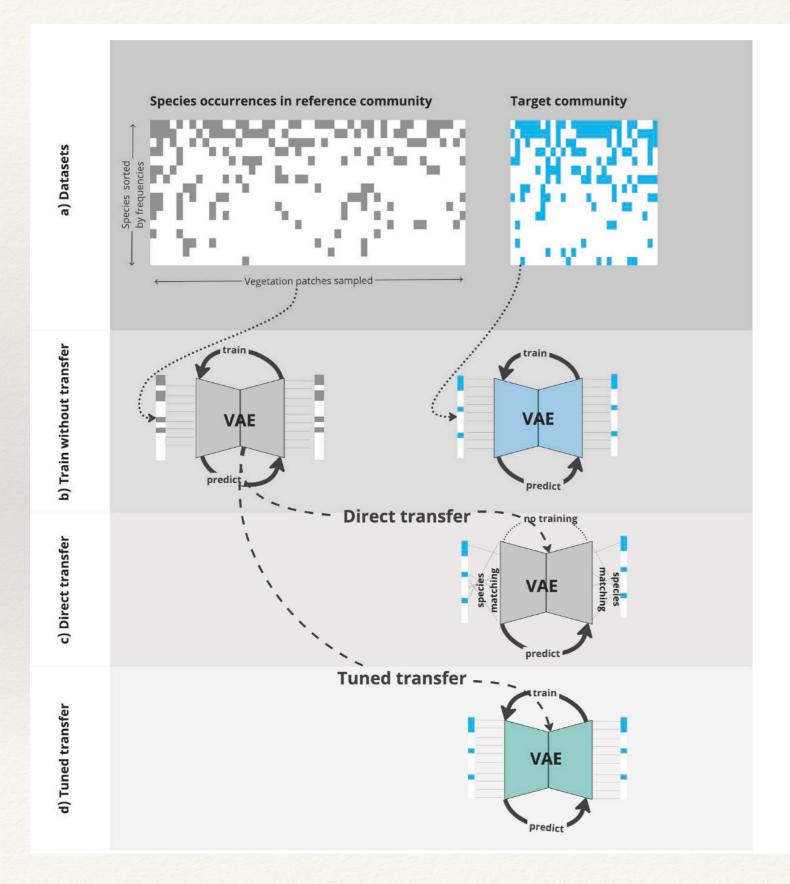
Can we combine different datasets? How?

Explored how Petrer could help understanding other arid ecosystems

Those ecosystems contained different species: there was **no direct translation between the systems**

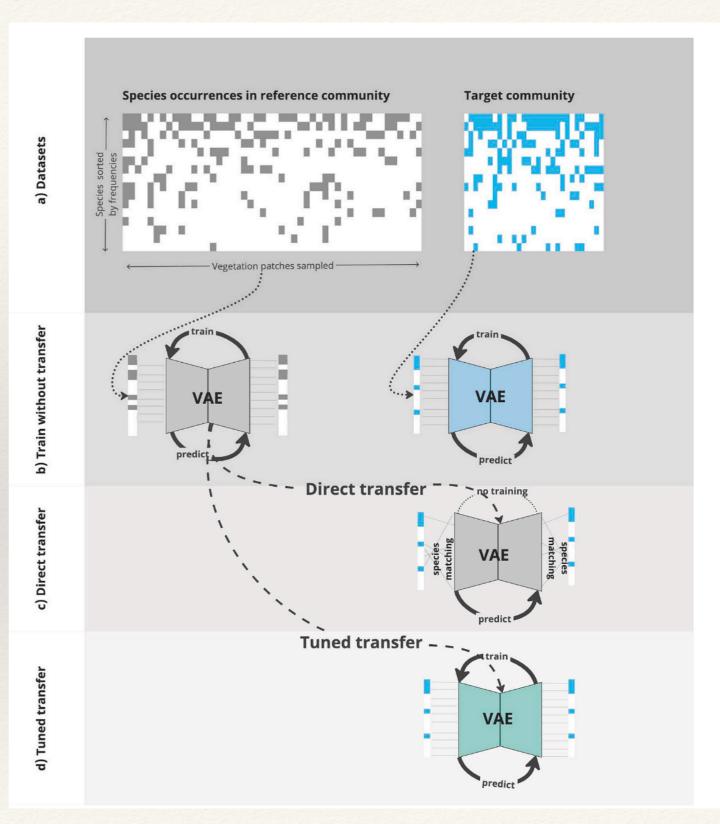
We needed to create a **dictionary** tested translations based on phenotypic, phylogenetic and abundance information

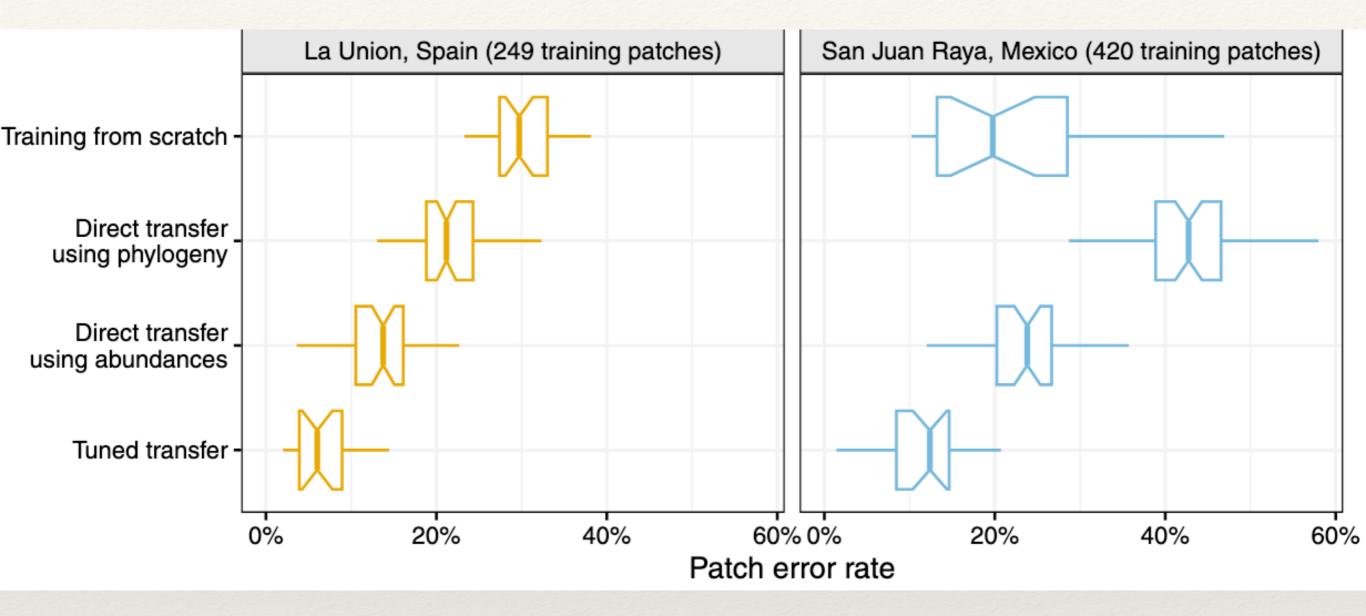




Compare
Train without transfer
Direct transfer w/ dictionary
Tuned transfer

Compare
Train without transfer
Direct transfer w/ dictionary
Tuned transfer w/ dictionary





- Clear improvement
- Best dictionary based on abundance
- Settles a methodology to combine different datasets

The goal of the research group was to guide restoration efforts in damaged ecosystems old mines, consolidated dumps, burned areas...

Those restored areas were seeded years ago and left to evolve

We did a field campaign in two **restoration** sites and their surrounding **natural** area

The data was very sparse but we checked that the GenAI model with the dictionary was good at predicting the restoration area

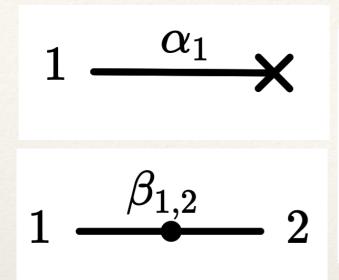
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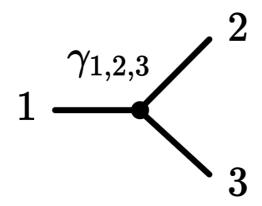
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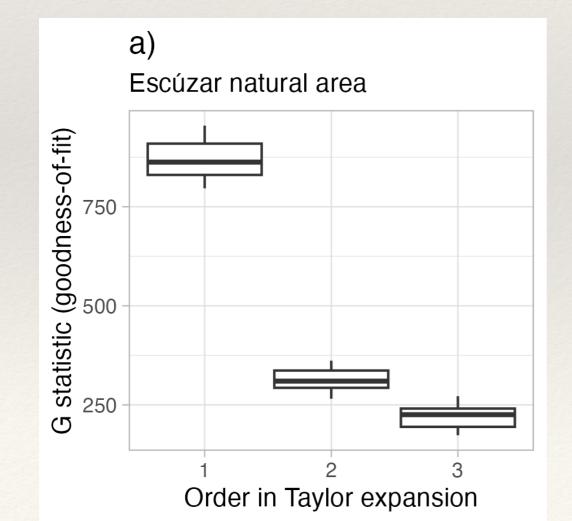
BUT restoration was often seeding of non-natural species here we had to ask a different question quantify the level of restoration achieved wrt natural area

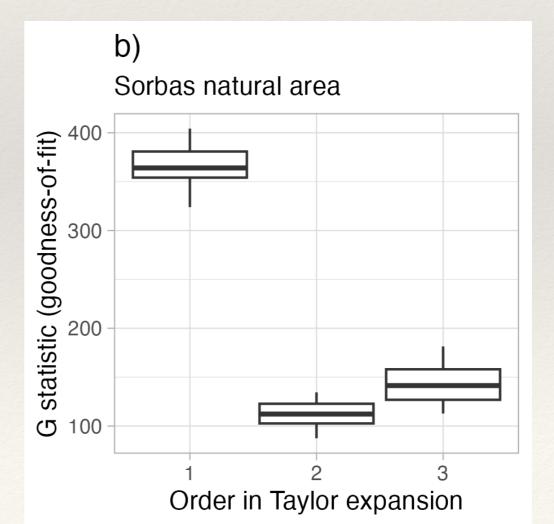




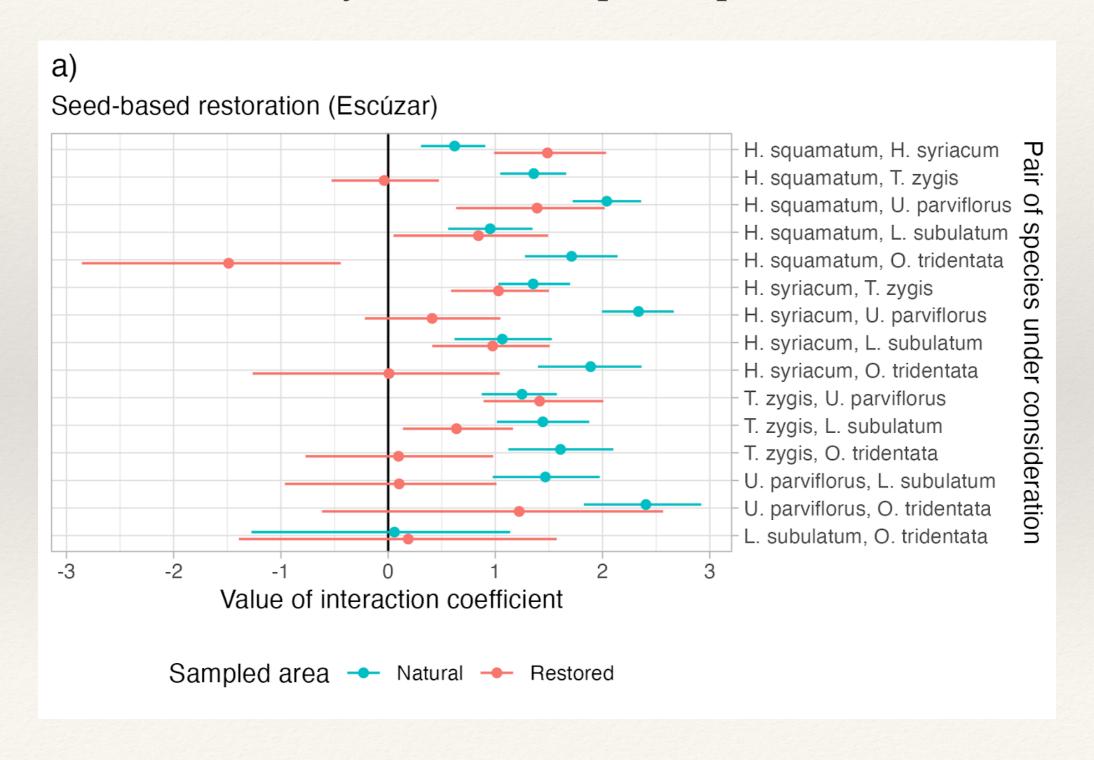
We moved to an interpretable method Best fit of a kind of Lagrangian

The natural areas were different





Assess the level of compatibility between the natural and restored ecosystem on the species present in both



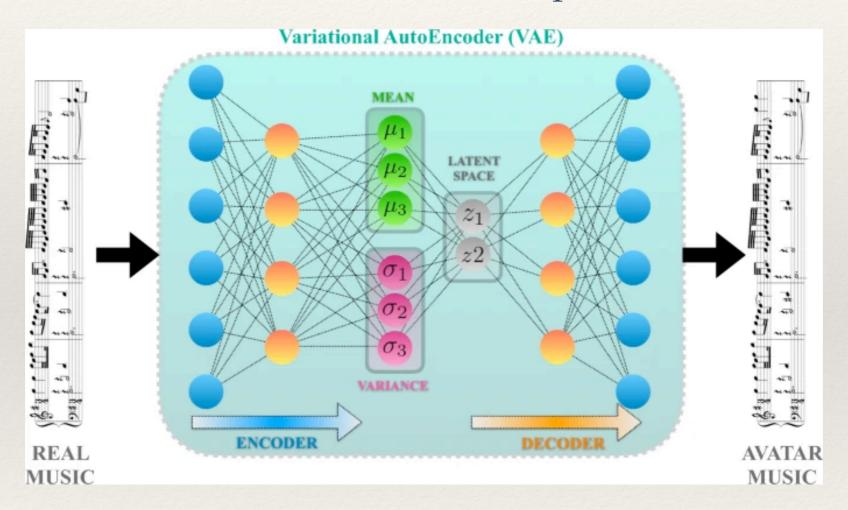


Music and AI

Based on Exploring how a GenAl understands music. Neural Computing and Applications (2024)

A VAE trained on music, does it understand music?

Google's MAGENTA is a music generator trained on a huge music dataset The architecture is massive, latent space of 512 neurons



As in the symmetry examples I showed you, did MAGENTA learn something about music? What makes music, music?

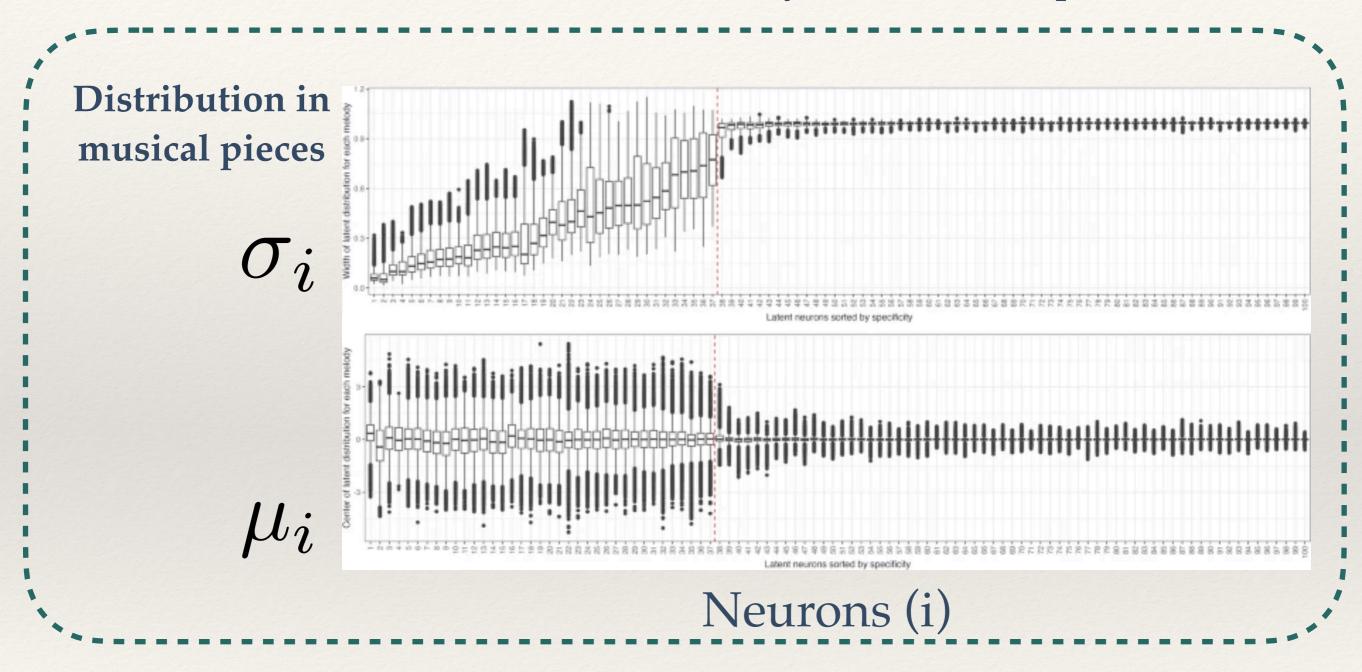
We can ask specific questions like

-Can latent dimensions be **ordered** by importance?

-**How many** latent dimensions are really necessary for the VAE to perform well, i.e., can some latent dimensions be classified as irrelevant?

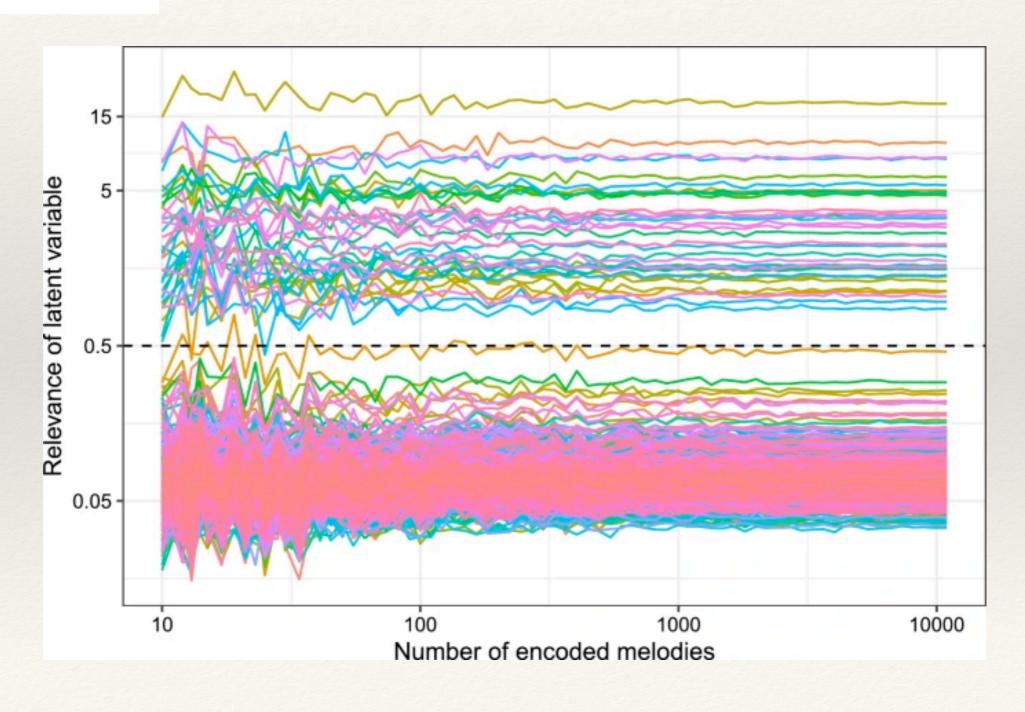
-Do the relevant latent dimensions have an **interpretation**? correspond to some concepts of musicality as understood by humans?

-Can latent dimensions be **ordered** by relevance/importance?

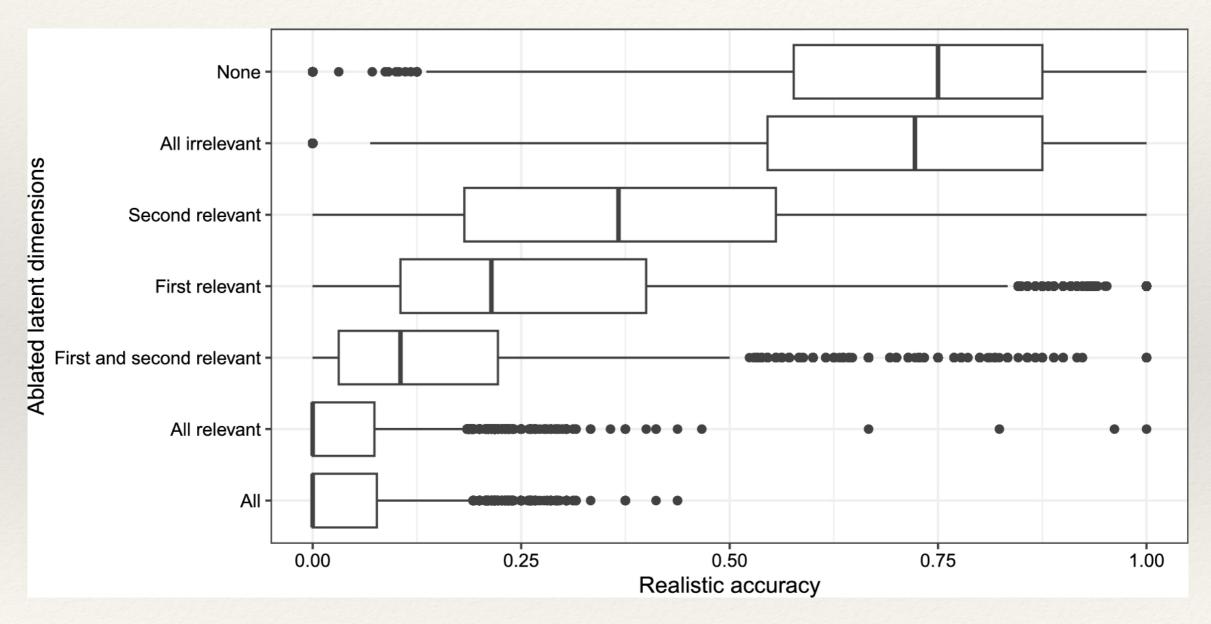


There is indeed a hierarchical behaviour

$$Relevance_j = \frac{\operatorname{std}(\langle z_j \rangle)}{\operatorname{mean}(\sigma_j)} ,$$



-How many latent dimensions are really necessary for the VAE to perform well, i.e., can some latent dimensions be classified as irrelevant?

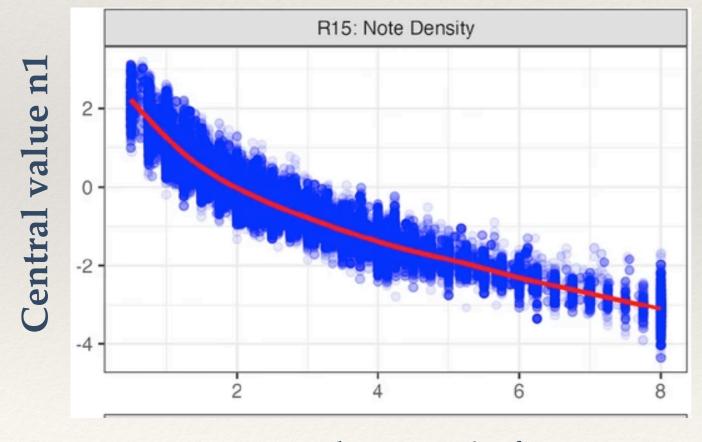


very few...

Interpretation

-Do the relevant latent dimensions have an **interpretation**? correspond to some concepts of musicality as understood by humans?

First two most relevant neurons are highly correlated with rythm, pitch and melody musical features



Value music feature

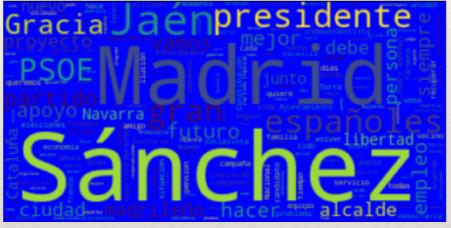
For example, n1 vs note density

All the irrelevant neurons do not show correlation but they are key to produce new distinctive musical pieces









Politics

Based on

Exploring the political pulse of a country using DS. Journal of Computational Social Science (2021) and

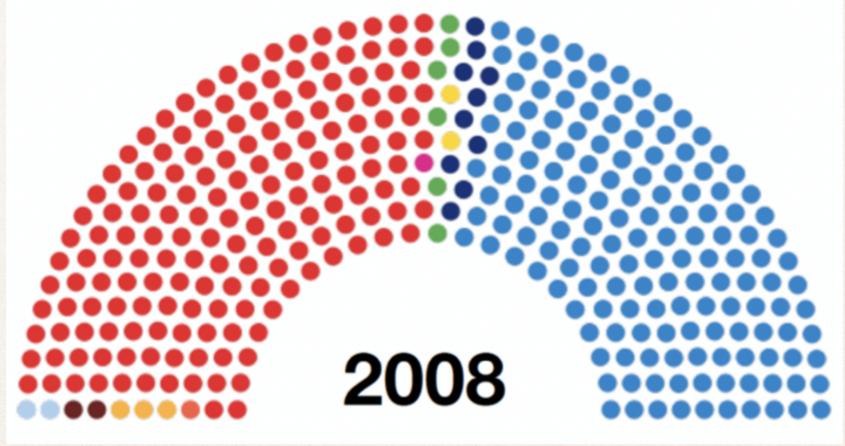
Polarisation of political elites with ML techniques.

Journal of Computational Social Science (2025, to appear)

Evolution of the Spanish Parliament in the last years





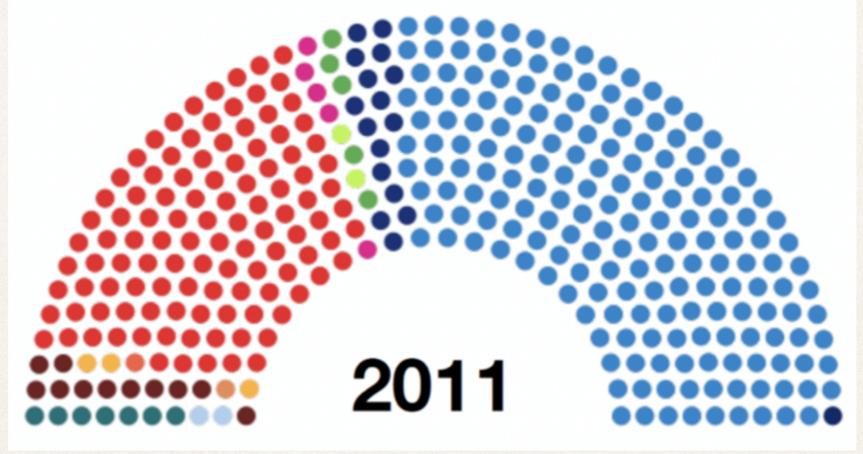


Highly Bi-partisan

Evolution of the Spanish Parliament in the last years



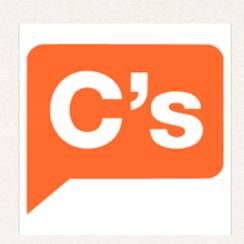




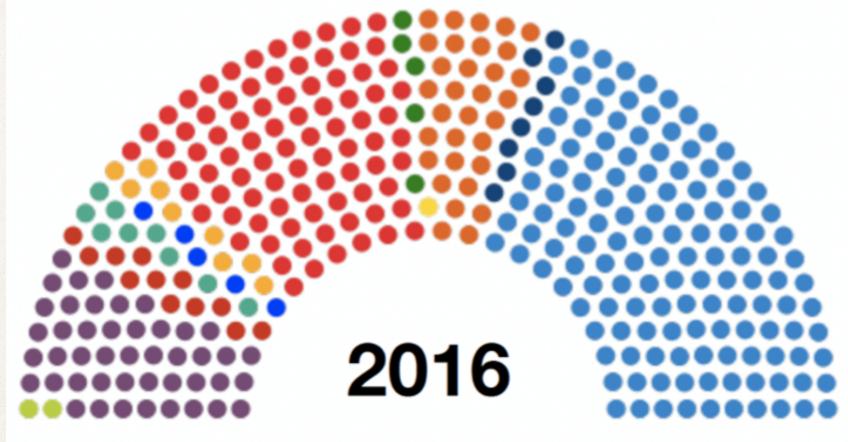
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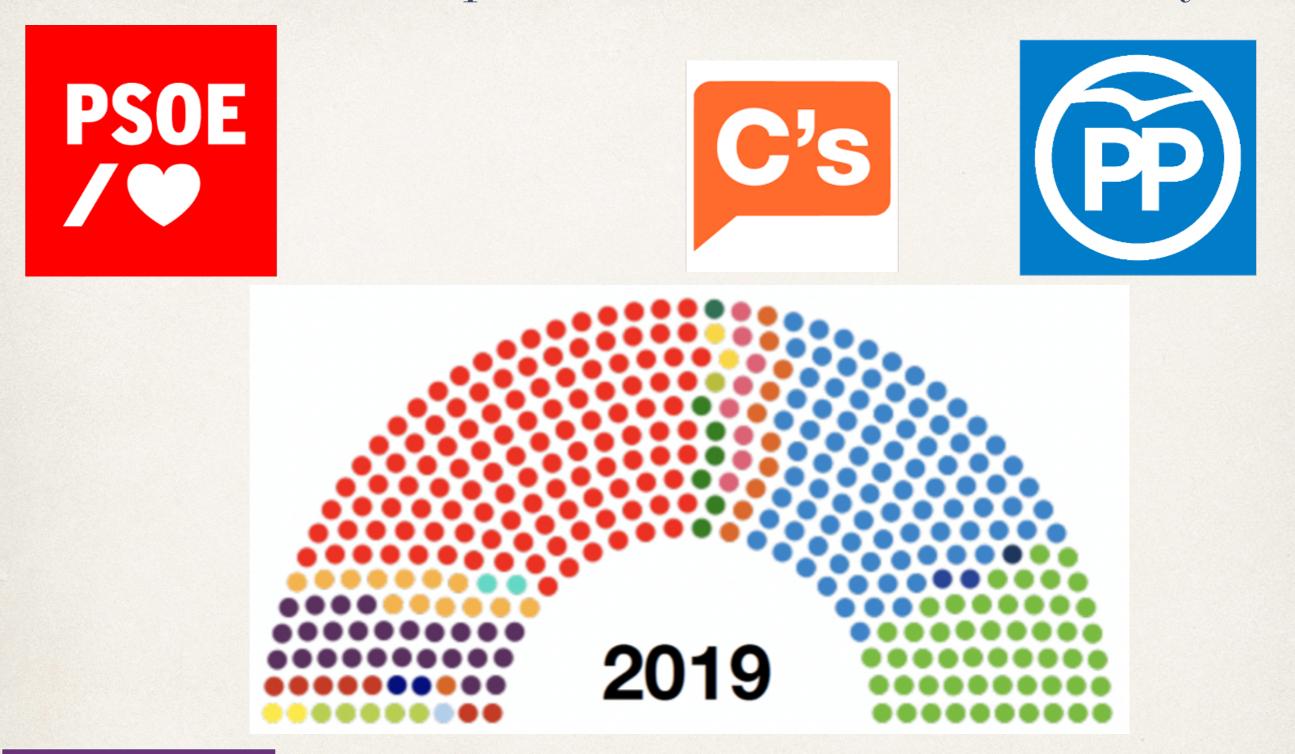








Evolution of the Spanish Parliament in the last years





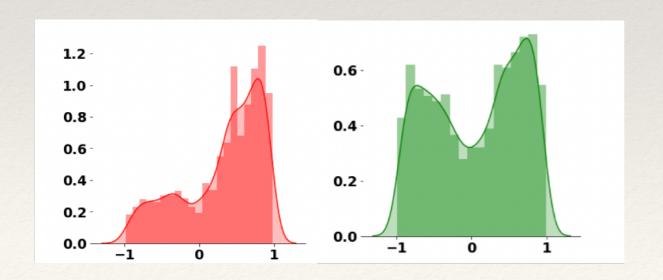
Similar in 2023, fractured parliament with extremes growing over centrist parties

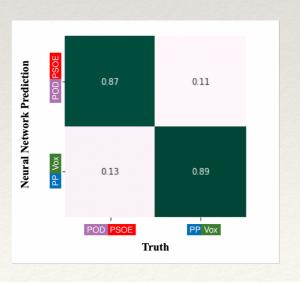


We first analysed Twitter discourse from politicians (easy to harvest)

Used a bunch of NLP techniques, finding: New parties' polarisation is higher, sentiment measure is able to track events (impeachment, procés...) and some parties are highly (anti-)correlated

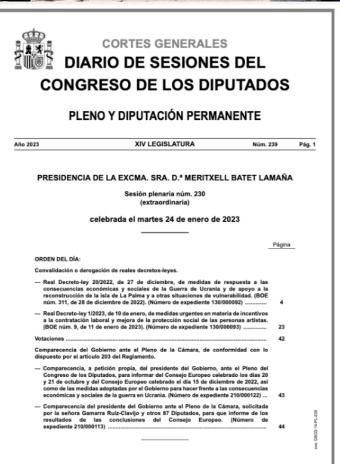
NN predicts political leaning ~ 90% accuracy: **Adherence** to messages is high

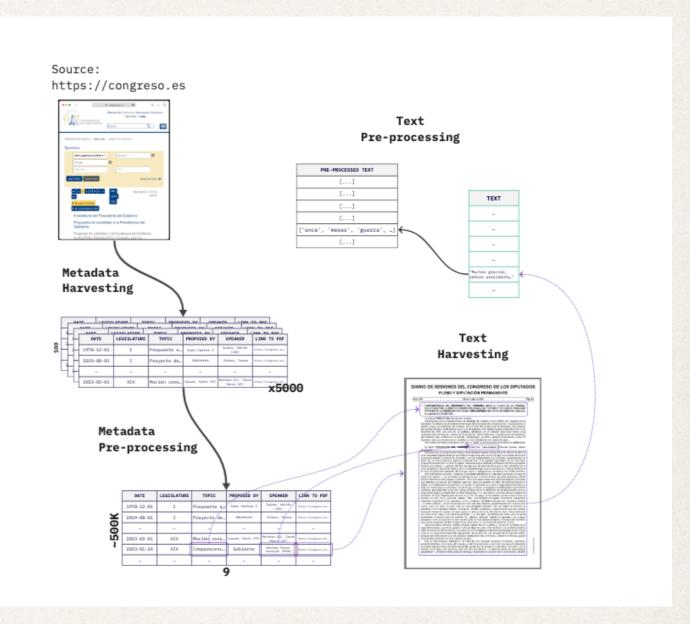




Then moved onto what they officially say







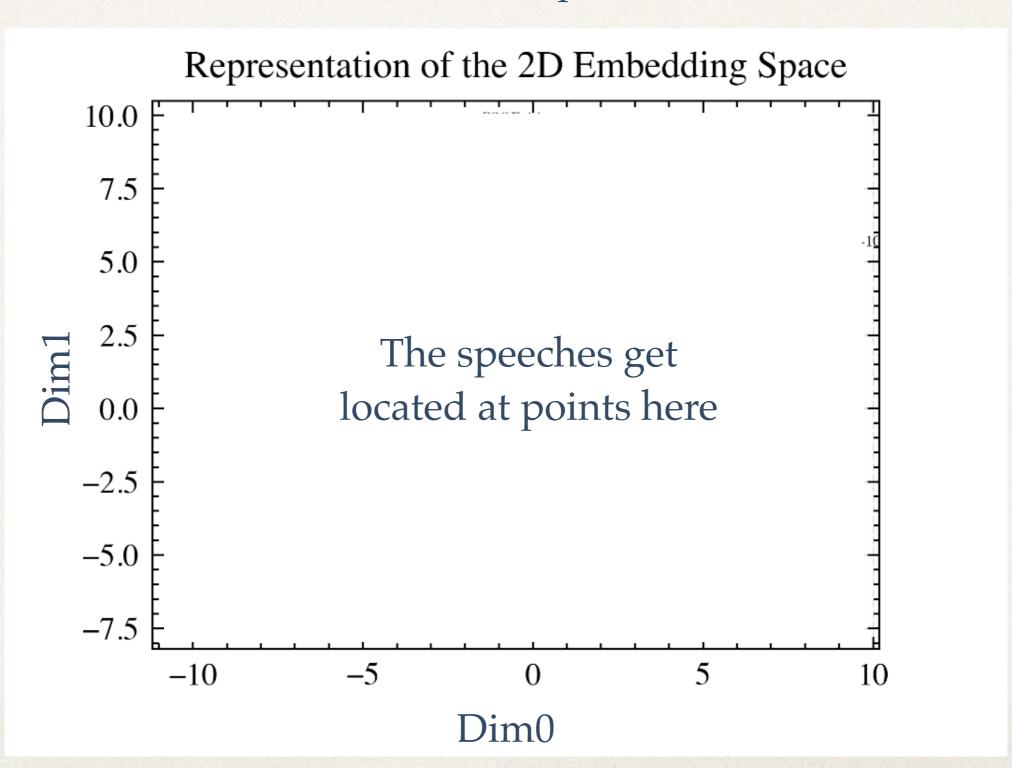
Webcrawler, clearning, preprocessing...

Result:

dataset from 1979 till 2024, available in Zenodo

Full-monty NLP incl transformers

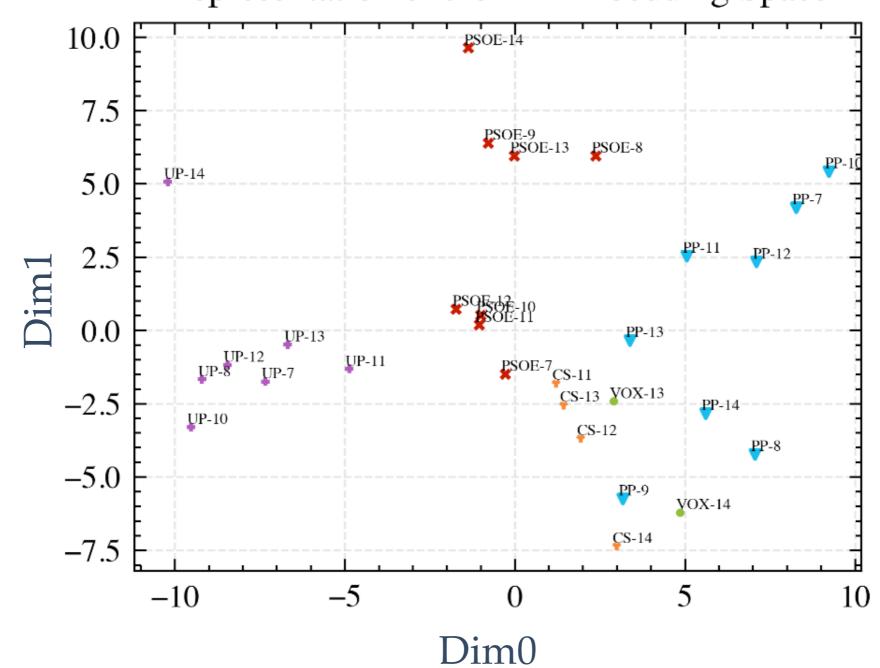
Many results, e.g. ask to project all speeches in a 2D space directions in the internal (latent) space with more information



Representation in 2D: clustering

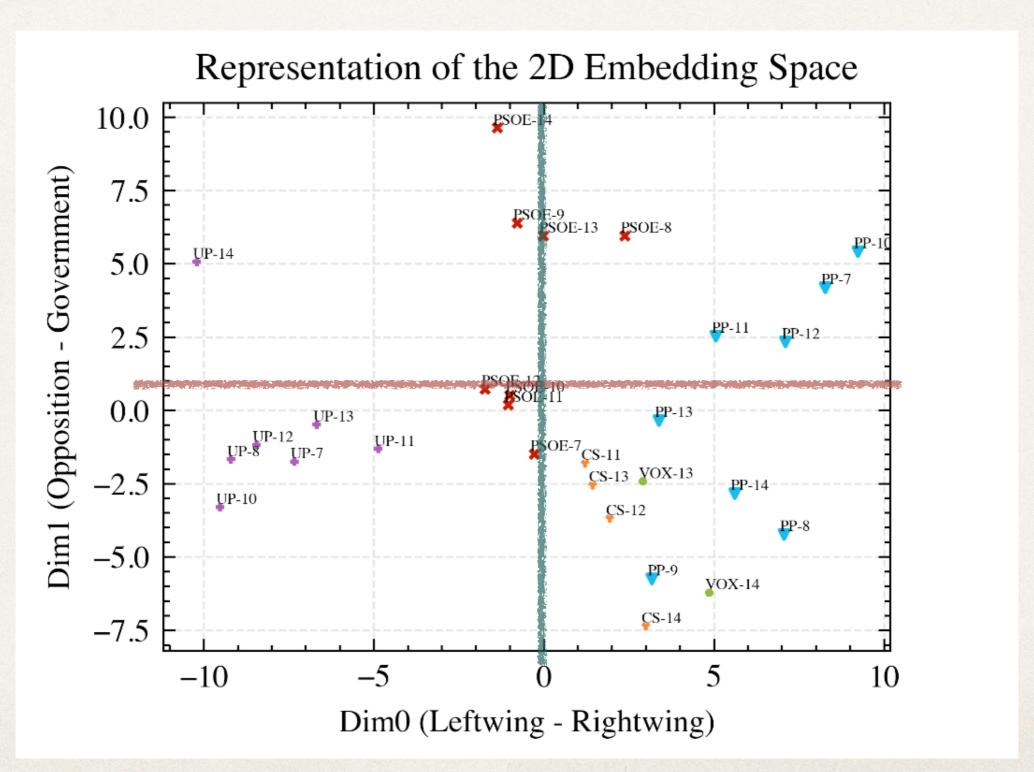
We then use the labels we had kept invisible to the AI to ID political party and term

CLUSTERING occurs, the AI has understood party's ideology Representation of the 2D Embedding Space



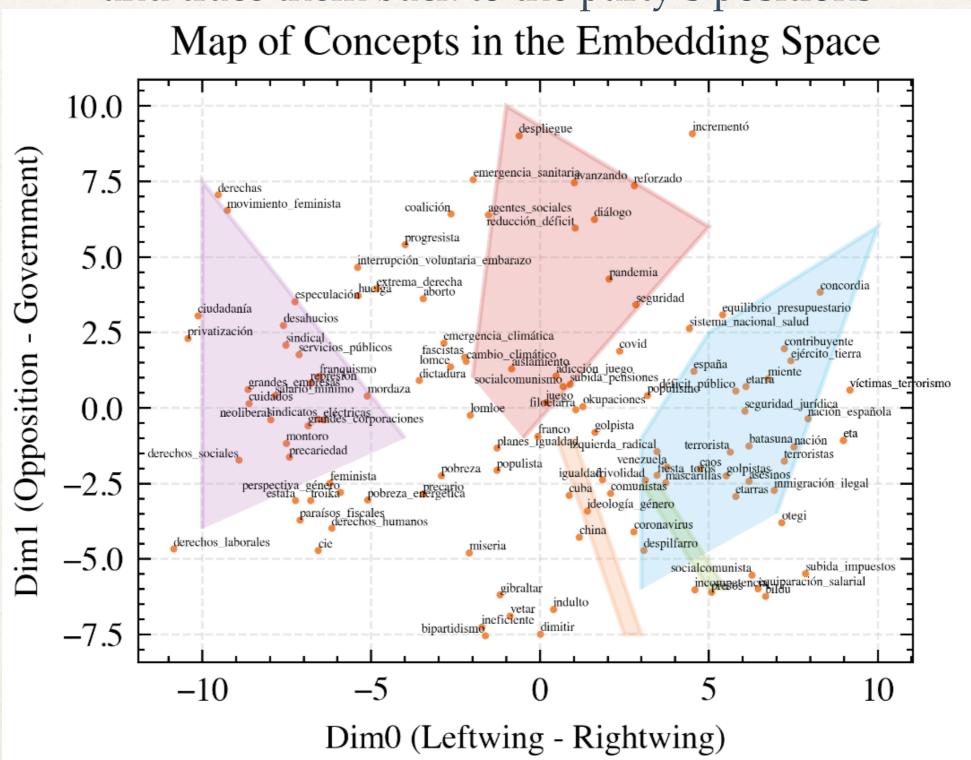
Representation in 2D: meaning

We can then ask if Dim0 and Dim1 have any meaning, the AI has *understood* divisions of left/right and government/opposition



Map of concepts

We can go further, and assign in the 2D space points concepts that represent them and trace them back to the party's positions

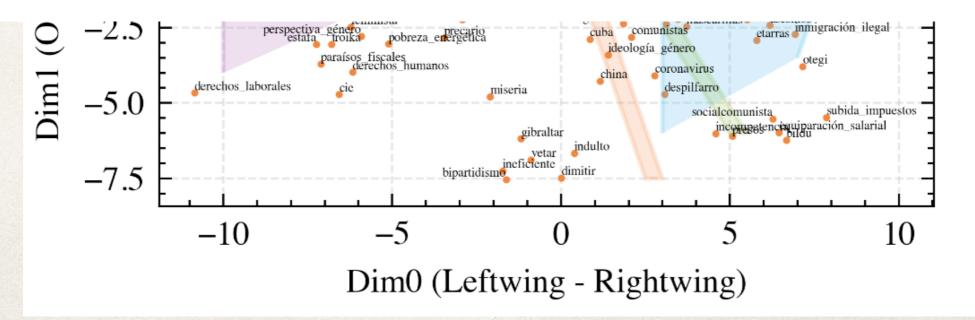


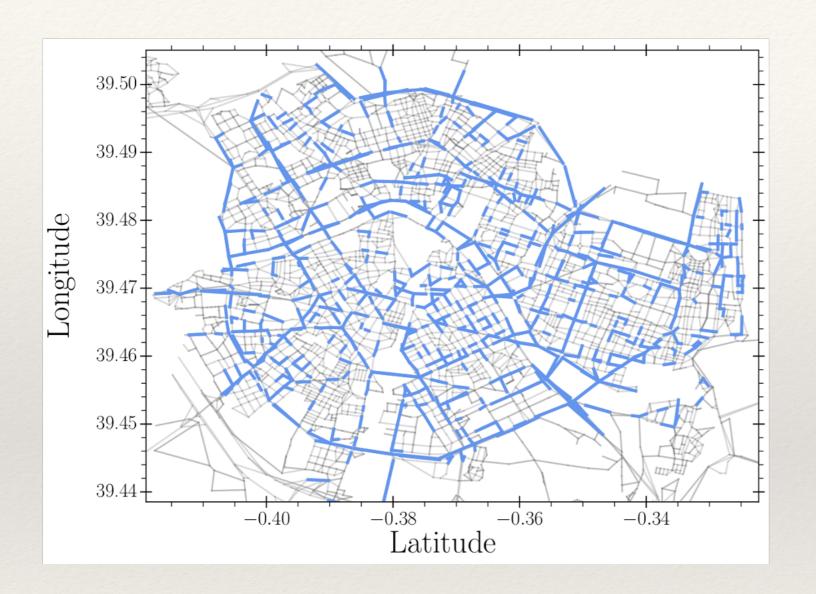
Map of concepts

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Map of Concepts in the Embedding Space

PC1 (Ideological axis)		PC2 (Rhetorical style axis)	
Left (Negative)	Right (Positive)	Bottom (Negative)	Top (Positive)
Equality	Security	Populist Language	Institutional Lan-
			guage
Social Justice	National Unity	Emotive Expressions	Procedural Discourse
Feminism	Constitution	Political Attacks	Legislative Vocabu-
			lary
Labor Rights	Territorial Integrity	Crisis Framing	Administrative Lan-
			guage
Environmentalism	Traditional Values	Polarizing Terms	Formal Register



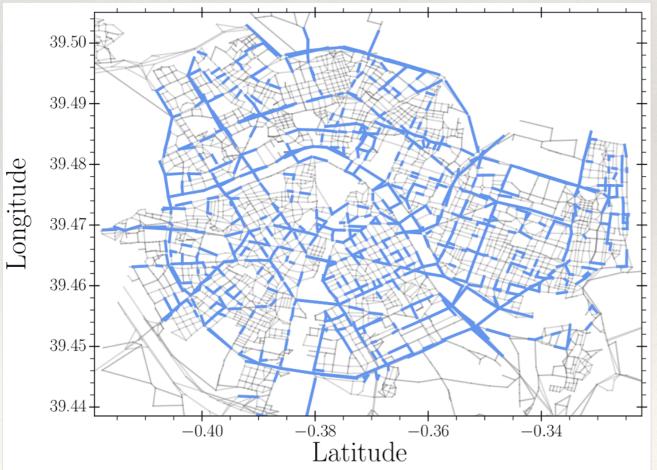


Traffic and pollution

Based on Applied AI Letters (2025) Neural Computing and Applications (2025)

Valencia

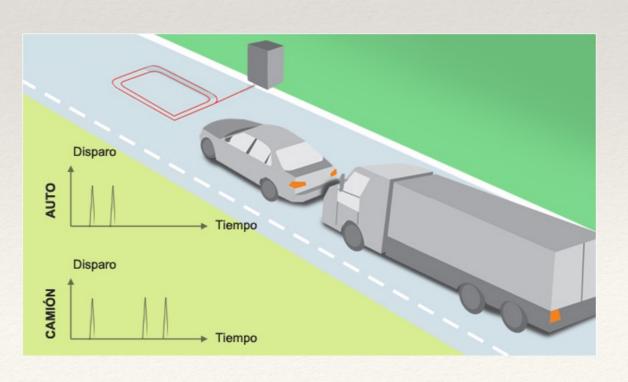




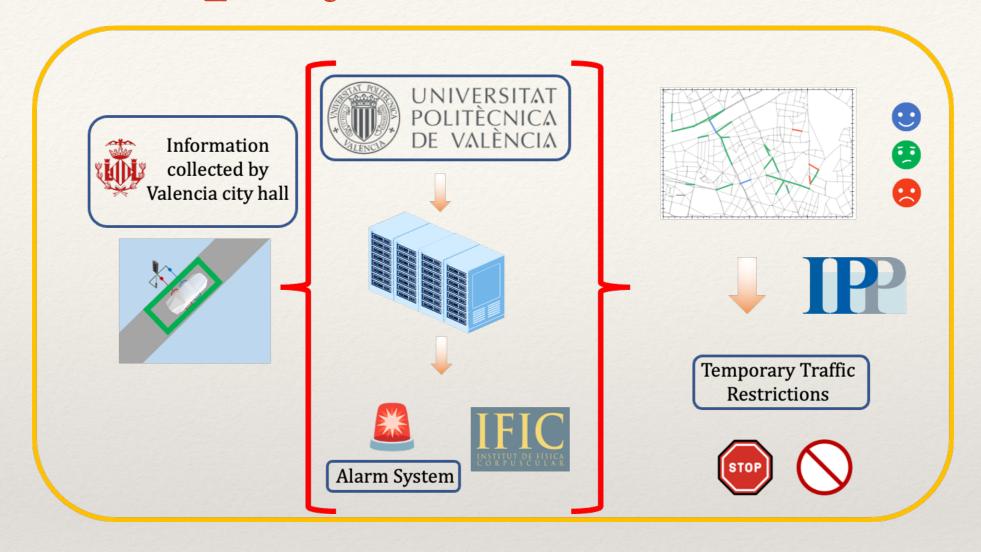
Nice city

One of the most sensorized in the world

About 9000 road segments collecting data on passing vehicles every 5 mins



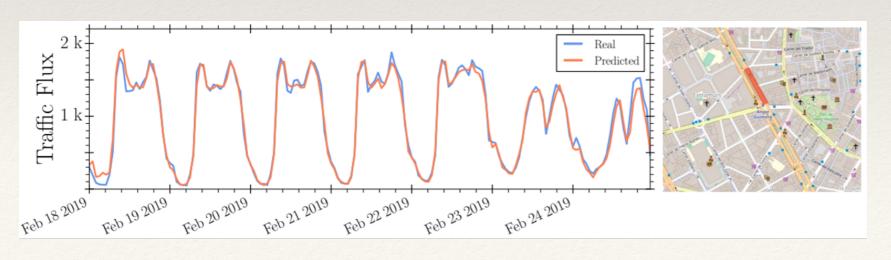
Common project across institutions



City govt.

Data+ML

Sociologists



We used arrays of LSTMs
(despite coverage,
GraphNN or more
sophisticated techniques
did not perform as well)

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...

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

We learned that an AI can identify and use higher level concepts, and this learning can be found in subtle features of the blackbox

We have seen that through AI methods, there is interesting cross-pollination between our area and others (music->LHC)

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?

Example 1 PDE-Nets

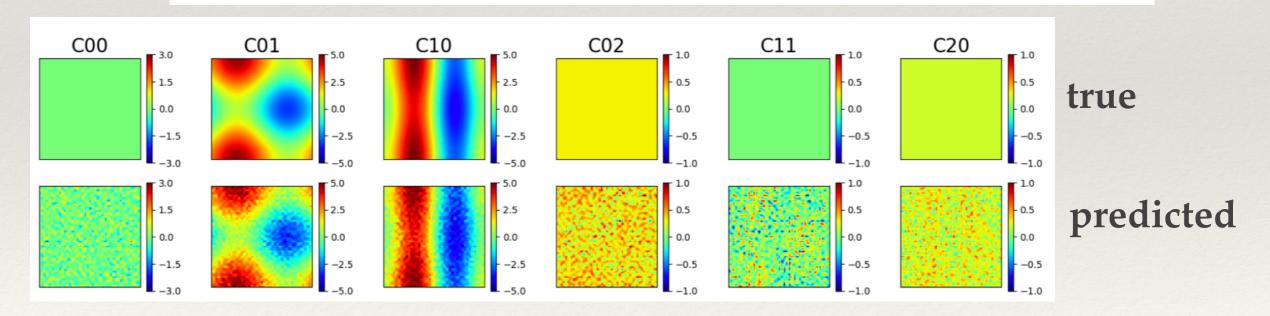
Navier Stokes, Maxwell, Schrodinger... Laws of Nature are PDEs

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?

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

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



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