Symmetry

meets AI

Veronica Sanz Universitat de Valencia - IFIC (Spain) & Sussex University (UK)

Colloquium@Torino'23



Today, we will talk about

*Human vs Machine Learning *Supervised Learning *Going further: unsupervised *Human surrender *Looking under the hood *From Physics to Art: Paintings and music

My aim is

if you know about ML, make you think a bit differently if you don't, motivate you to have a closer look

Human vs Machine Learning



repeat and improve on a task



repeat and improve on a task

predict the evolution of a situation



repeat and improve on a task

predict the evolution of a situation

discover unknown relations



repeat and improve on a task

predict the evolution of a situation

Previous experience discover unknown relations

choose the option that maximises return



repeat and improve on a task

predict the evolution of a situation

Previous experience discover unknown relations

choose the option that maximises return

imagine new possibilities

VERY IMPRESSIVE, YET human learning is limited by our personal viewpoint, our collective intelligence (*newspeak?*) & our inherent capacity to process information (amount , speed, level of detail)

ON THE OTHER HAND

the ultimate limitations of machine learning are unknown (if they do exist) CPU-> GPU, TPU, FPGA, IPU -> ... Quantum Computing, Neurophotonics...





Machine learning

repeat and improve on a task **SUPERVISED MACHINE LEARNING** predict the evolution of a situation **TIME-SERIES LEARNING**

discover unknown relations CLUSTERING/UNSUPERVISED

choose the option that maximises return **REINFORCEMENT LEARNING**

> imagine new possibilities GENERATIVE AI

Nowadays, Machine Learning is in the middle of a revolution: processing speed and storing capacity have increased enormously but **more importantly** the *way* machines learn has changed

TRADITIONALLY

learning was limited to lines of code we (humans) were writing

we can write *extremely complex* codes and the machine can improve in performing tasks but the structure of *thought* behind decision making is human if something_is_in_the_way is True:
 stop_moving()
else:

continue_moving()



The Machine can't describe relations we haven't coded in *like a born-blind person who is asked to think of blue*

A new way of thinking: Neural Networks

Structures made of units called *neurons* and organised by *layers*



The network learns from data with no structured instructions

Neural networks are able to explore relations between inputs and outputs which cannot be contained in lines of codes their degree of expressivity is immense *and* it is extremely fast built from simple units and in a layered architecture

A new way of thinking: Neural Networks

Structures made of units called *neurons* and organised by *layers*



This technology is truly disruptive

we are unable to predict how fast is going to evolve and the extent of its applications

new algorithms and applications appear every day, and this tendency does not seem to slow down **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



Learning by example: Supervised ML repeat and improve on a task

A basic task: good or bad?



Is it a crocodile? Yes/No answer



A basic task: good or bad?



Is it a crocodile? Yes/No answer



To learn, dataset $\mathcal{D}(x_i, y_i) \ y \in \{0, 1\}$ with labels



Cat or dog?

Is this New Physics?

Training a binary network



init network \longrightarrow transform all images in numbers *y* the prediction (cat/dog)



The network applies many non-linear check the statistical transformations on the input \longrightarrow accuracy of your the result y(x) is highly non-linear result

we adjust the direction depending on learning slope we start over, checking the prediction accuracy again

change the init parameters a bit

A lot of ML in Particle Physics is answering YES/NO questions Is it a W? Is it a Higgs? Is it DM?



mostly using Neural Networks to deal with images (CNNs)



A lot of ML in Particle Physics is answering YES/NO questions Is it a W? Is it a Higgs? Is it DM?



mostly 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

intellectually, not super-exciting



Going further

imagine new possibilities

Here be dragons!

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? **GANs (Generative Adversarial Networks)** and **VAEs (Variational AutoEncoders)** In CNNs, benchmarks were cats/dogs and hand-written digits (MNIST) Here, human faces

STEP 1 - 'LEARN' what is a human face



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? **GANs (Generative Adversarial Networks)** and **VAEs (Variational AutoEncoders)** In CNNs, benchmarks were cats/dogs and hand-written digits (MNIST) Here, human faces

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?

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

Example in Particle Physics with Mike Soughton and Charanjit Khosa SciPost



Ask to look only to Standard Model ('normal') events

Learns to ID outliers ('New Physics')

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

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? **GANs (Generative Adversarial Networks)** and **VAEs (Variational AutoEncoders)** In CNNs, benchmarks were cats/dogs and hand-written digits (MNIST) Here, human faces

STEP 3- CREATE NEW POSSIBILITIES





gif con latent space

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



Human surrender?



Institut de Ciències

icm

What's wrong with blackboxes?

Only open if a disaster happened

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

Example: collaboration with Seismicity experts

VNIVERSITAT



Tomography



Garcia et al, Seismological Research Letters



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*





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



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



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



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

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 with symmetries



Symmetry is a key concept in Physics

not just as a simplification method or connection with other problems deeper level: Laws of Physics, understanding of forces, stability...

Symmetries can help with **Machine Learning** problems e.g., CNNs and data augmentation





The **concept** of symmetry is part of our shared **human appreciation**

We asked ourselves: Can Machines Deep-Learn symmetries? in which ways? and what could we use this for?

Do Al's understand concepts?

EXAMPLE- CONSERVATION LAWS

Before collision (V_{free}, q_{free}(t), m_{free}) (w, q_{rot}(t), m_{rot}) (w, q_{rot}(t), m_{rot}) (w, q_{rot}(t), m_{rot}) (w, q_{rot}(t), m_{rot}) (w, q'rot(t'), m_{rot}) Iten et al Phys Rev Lett



They trained a VAE with many collision examples with input of just kinematic variables



The trained algorithm had somehow *learned* that the concept of angular momentum is important and was storing it in one single neuron We know the NN is realising higher level features of the data it seems to *somehow* realise of the presence of a conserved quantities

what about symmetries? and even more, what if the potential had no symmetry, or was only approximate? what if we wanted to learn about symmetries in datasets that have no straightforward interpretation?



We asked ourselves: Are there ways to learn about symmetries which detect no symmetry or approximate levels of symmetry? and that can be applied to a wide range of situations? We needed a very general procedure We had to start with something else, a simpler representation

an image with only two colours



and a universal task: try to learn as much as possible from this image

dataset = (x, y, 0/1)

and train a FCNN to learn to reproduce the image

then we can ask whether, while learning every detail of the image, it did realise there was some level of symmetry

To train the FCNN, we build a dataset made of **Physics templates**

where we know the symmetry properties, but this information is **not** known to the NN

We pay attention to not **overspecialise** in the physics potentials FCNN is not allowed to **overfit**, so that it may be more prone to identify the symmetry

we then get the PCA image from the last hidden layer

at first sight all the PCAs look different, changing from run to run and from image to image...

Putting it all together



If the FCNN, while paying attention to reproduce the image, has learnt that there was some symmetry, *the PCAs may encode this learning*



We train a CNN, using the PCAs and the physics labels, to identify symmetries

We find that the PCA- >symm classification does work, the PCA does contain *some encoding of the symmetry*

From Physics to Art

So far have developed an algorithm which takes simple images and produces a **symmetry score** It can be used in any type of 2D images: a children's sketch, a painting, a photograph...

Some examples from Art:

first images-> sketches, then run the algorithm as if they were physics potentials





SYMM SCORE?











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



MAGENTA VAE trained on millions of music pieces



latent space of 500 neurons!

Q: did it learn anything non-trivial, or did it just memorize things?

One mor example: the AI discovers human concepts in music

coming out soon!

Reordering in the latent space by specificity, distribution *Example of short (two-bar) music* **MEAN ACTIVATION**



SIGMA



If we then look at how this AI representation relates to human quantities...



If we then look at how this AI representation relates to human quantities...



e.g. EXCITATION NEURON 2





We are just starting to understand the applications of ML in Physics They go beyond a mere iteration of our traditional statistical methods: unsupervised methods, generative AI, reinforcement learning...



We are just starting to understand the applications of ML in 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

Summing up...

We are just starting to understand the applications of ML in 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

Yet 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

Summing up...

We are just starting to understand the applications of ML in 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

Yet 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 does identify and use symmetries, even if only approximate, when *inspecting* an image (decoy task) and this learning can be found in subtle features of the hidden layers

Summing up...

We are just starting to understand the applications of ML in 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

Yet 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 does identify and use symmetries, even if only approximate, when *inspecting* an image (decoy task) and this learning can be found in subtle features of the hidden layers

We applied this method to Art, finding that it matches human intuition

Without being explicitly told, just by performing a *decoy* task the AI can discover that there is a concept (symmetry, rythm...) which helps better characterising physics potentials, music, collisions

Big Q: Can the AI discover something we haven't thought about?

