#### Machine Learning Course 4 Advanced ML for HEP

(more on unsupervised learning, anomaly detection, clustering specific HEP challenges in Ana Peixoto's courses next week)



#### **Feature Selection**



BB.

#### **Feature Selection**

Example of an ATLAS experiment analysis, see transp

100



# **Feature selection techniques**



- Iterative addition: start with n=1, take best training of all n options. Then take best option of adding one more from remaining n-1 variables, etc. Ranking complexity scales as O(n<sup>3</sup>).
- Key role permutation importance
   <u>Iterative removal</u>: start with training on all variables and remove iteratively remove the one that degrades the performance the least, scales as O(n<sup>3</sup>).
  - > Hypothesis: better consideration of variables that only add to performance in combination with others.
- Correlation based: rank the variables based on their correlation to the BDT score computed with all variables. Computationally cheap, scales as O(n).
- <u>BDT selection frequency 'TMVA ranking'</u>: train once on all variables, rank by how often a variables provided the optimal decision in the BDT, scales as O(n).
- Separation based: rank by overlap of signal vs background shapes. Only method that establishes ranking without performing any training.
- Random choice: serves as reference, use a random subset of the variables. Repeat and average over 1000 trials.

Here performance is measured as integral of the ROC curve.



### **Results**



### **Deep Learning for Analysis**



# **Deep Learning for Analysis**



- □ MSSM at LHC :  $H^0 \rightarrow WWbb$  vs tt → WWbb
- Low level variables:
  - o 3-momentum vectors
- □ High level variables:
  - Pair-wise invariant masses
- Compare shallow NN (1 hidden layer) with (not so) deep NN (3 hidden layers)

### **Results**



Deep NN outperforms NN, and does not need high level variables
 DNN learns the physics ???

# **Deep learning for analysis (2)**

1410.3469 Baldi Sadowski Whiteson

#### □ H tautau analysis at LHC: H→tautau vs Z→tautau

- Low level variables (4-momenta)
- High level variables (transverse mass, delta R, centrality, jet variables, etc...)



- Here, the DNN improves on NN but ...
- DNN still needs high level features
- Both analyses with Delphes fast simulation ~100M events used for training (very unusual>>100\* full G4 simulation in ATLAS)
- No convincing proof so far deep dense NN better than shallow NN or BDT, in realistic consitions

11-11 IVIE COURSE 0, BUVIE ROUSSEUR, UNI 2024, CHACAL

#### **Deep Learning success : NOVA**

TTTTT





HEP ML Course 3, David Rousseau, Jan 2024, CHACAL



#### **End to end Learning**



## **End to end learning**

- Train directly for signal on « raw » event ?
   Start from RPV Susy search
- ATLAS-CONF-2016-057
- □ Fast Simulated events with Delphes
- Project energies on 64x64 ηxφ grid

Compare with usual jet Reconstruction and physics Analysis variables such as:





Bhimji et al, 1711.03573

(b) gluino cascade decay



## End to end learning (2)



HEP ML Course 3, David Rousseau, Jan 2024, CHACAL

## End to end learning (3)



- >x2 gain over BDT/shallow network using physics variable and 5 leading jet 4momenta
- $\Box$   $\rightarrow$  CNN extract information from energy grid which is lost in the jets ?
- □ Not sure, they should compare to applying DL on the jets HEP ML Course 3 , David Rousseau, Jan 2024, CHACAL

#### **Systematics Aware Training**



# **Systematics-aware training**

				///// See	· Victor Estrade	CHEP 2018
🖵 Our	experimenta	al measurem	ent papers	typically	y ends with	

• measurement = m  $\pm \sigma$ (stat)  $\pm \sigma$ (syst)

IIII

- o  $\sigma$ (syst) systematic uncertainty : known unknowns, unknown unknowns...
- □ Name of the game is to minimize quadratic sum of :

 $\sigma$ (stat)  $\pm \sigma$ (syst)

- $\Box$  ML techniques used so far to minimise  $\sigma$ (stat)
- Impact of ML on  $\sigma$ (syst) or even better global optimisation of  $\sigma$ (stat)  $\pm \sigma$ (syst) is an open problem
- □ Worrying about  $\sigma$ (syst) untypical of ML in industry (... until recently *fake news*)
- □ However, a hot topic in ML in industry: *transfer learning*
- E.g. : train image labelling on a image dataset, apply on new images (different luminosity, focus, angle etc...)
- □ For HEP : we train with Signal and Background which are not the real one (MC, control regions, etc...)→source of systematics

## **Experimental bias**

TTTT





Example of impact of the angle on handwritten digits





#### **Example mHiggs measurement**



FIG. 3 (color online). The impacts  $\delta m_H$  (see text) of the nuisance parameter groups in Table I on the ATLAS (left), CMS (center), and combined (right) mass measurement uncertainty. The observed (expected) results are shown by the solid (empty) bars.

## **Syst Aware Training: adversarial**



## Not conclusive yet



#### Fair Universe: HiggsML Uncertainty Challenge

 Extension of previous HiggsML challenge from 2014 (which was a classification problem for Higgs decaying to Tau leptons in an ATLAS simulation based on momenta of decay particles and derived quantities)

- Larger dataset, and include systematic variations
  - Tau Energy Scale, Jet Energy Scale, MET, backgrounds or simulators - TBD)
  - Systematics implemented both using in <u>Delphes</u> <u>detector simulation</u> and post-hoc scripts to compare
- Participants submit methods that go beyond classification: predict signal strength (μ) and an uncertainty interval
- Metric/score on precision and accuracy
- To run on Codabench summer 2024 as a NeurIPS competition
  HEP ML Course 3, David Rousseau, Jan

#### Higgs **the Higgs ML challenge**

May to September 2014

When High Energy Physics meets Machine Learning





#### **Generative Models**



#### **Generative Adversarial Network**



## **Condition GAN**

#### Text to image

#### 2016

this small bird has a pink breast and crown, and black almost all black with a red primaries and secondaries.



the flower has petals that are bright pinkish purple with white stigma







this white and yellow flower have thin white petals and a round yellow stamen





Here is the image of the small bird with a pink breast and crown, and black primaries and secondaries.

#### <sup>°</sup>Actually using diffusion model rather than GAN

HEP ML Course 3, David Rousseau, Jan 2024, CHACAL

2024

### Jan 2024





### **ATLAS calo simulation**



#### **Results**



#### **Simulation of energy resolution**



# **Another GAN application**

TTTTT



photo  $\rightarrow$  Monet



HEP ML Coule on Petric Roys son oto 2024, CHACAL





## **Application**



### Recurrent Neural Networks



## **Recurrent Neural Network**



HEP ML Course 3, David Rousseau, Jan 2024, CHACAL

# **RNN for jet tagging**

IIII TRASS



ATL-PHYS-**PUB**-2017-003

- Used in physics for identification of jets from b-quarks from the list of particles associated to the jet
  - Basic track information like d0, z0, pt-Fraction of jet, ...
  - Physics inspired ordering by d0-significance
- RNN outperforms other IP algorithms

- No explicit vertexing, still excellent performance
- First combinations with other algorithms in progress



#### **Transformers**



### **Reinforcement learning**



#### **Apprentissage par renforcement**



Alpha Zero : a appris tout seul contre lui-même en quelques jours à jouer (séparément) au Go, aux échecs ou aux échecs japonais, et bat tout le monde, homme ou machine HEP ML Course 3, David Rousseau, Jan 2024, CHACAL

# RL (1)

# **States & Actions**

Curent state of the system

IIII



Actions of the player



# **RL (2)**

# **Rewards & value**

Immediate reward

TT

total Value (including the future)

Reward  $r^t$  = score at time t as a result of the action



# **RL (3)**

# **Rewards & value**

Immediate reward

total Value (including the future)

Reward  $r^t$  = score at time t as a result of the action

the "Value" of the position includes future rewards

$$\mathcal{V}(\{a_t, s_t\}) = \sum_{\tau=t}^{\infty} \gamma^{\tau} r(\tau)$$



# **Application of jet grooming**



HER IVIL COULSE J, DAVIU NOUSSEAU, JAH ZUZ4, CHACAL

### **Results**

Train a « policy » (keep a branch or not) according to « reward » : best jet mass

Impact : more precise jet reconstruction

 $\Box$  (no follow up to the best of my knowledge)



#### **Possible RL application : experiment design**

Experiment design
 Data collection
 Success/failure ?

→could be used to optimise trigger menu, which can be easily virtualised

MODE collaboration

## Example of a bad ML idea: SuperTML



## **SuperTML : principle**



# ...then analyse image with fine tuned a pre-trained CNN (on cats and dogs)

### Super TML on HiggsML dataset

0. 937
225
. 200
014
78
5
2
16
8
6
2 A
0

(a)	Sup	perTML.	_EF	back-
gro	und	event ex	kamj	ole.

TTTTT

(b) SuperTML\_VF signal event example.

68.768

3. 473 44. 704 2. 039 164. 546 1. 414 0. 501

igure 4. Examples of SuperTML images for Higgs Boson .

## **SuperTML results**

TRACE

TTTT

*Table 3.* Comparison of AMS score on Higgs Boson. The first two rows are winners in the Higgs Boson Challenge.

Methods	AMS	
DNN by Gabor Meli	3.806	
XGBoost	3.761	
SuperTML_EF(224x224)	3.979	No Way!
SuperTML_VF (224x224)	3.838	Overtraining ?

...unreproducible....

#### ChatGPT, a brilliant but messy intern



Caveat : Most experiments from June 2023

## **GPT** in one slide

- provided by (not at all Open) OpenAI, funded mainly by Microsoft (hence connection to Bing and github Copilot)
- Generative Pre-Trained Transformer : trained to guess the next word

- □ learned from a well curated dataset (details unknown). Certainly not "the whole web", but wikipedia, arXiv, books etc. Multilingual. Frozen in Sep 2021. → now (Jan 2024) April 2023
- □ Fine Tuned to specific task (now GPTs)
- RLHF : Reinforcement Learning from Human Feedback to provide structured answers
- □ safeguards against hate speech etc... Kids can use it
- □ GPT3.5 ~10<sup>11</sup> parameters. Memory 10.000 "tokens" (entity a bit smaller than a word)
- □ GPT4~10<sup>12</sup> parameters. Memory 25.000 tokens

# **ChatGPT and Bing in one slide**

#### ChatGPT : https://chat.openai.com/chat register

- GPT3.5 free, GPT4 for 24\$/month.
- Does not look up the web, knowledge frozen in Sep 21 (but evidence earlier arXiv are missing)
- No sources. Reference and citation often wrong
- On the prompt one can reference a paper giving its title/authors (NOT the http! Wrong paper)
- o Tends to be very verbose
- History of all different chats are kept and can be continued
- o https://platform.openai.com/ai-text-classifier supposed to detect code written with GPT
- Bing : simply tag @bing in skype or within MS Edge
  - o uses GPT4
  - o my feeling: looks up on the web and interpret the first few hits
    - →sources are often quoted and correct
    - Inot as thorough as ChatGPT
  - newtopic ⇒starts new conversation and forgets the current one (which is still visible skype mode, however Bing answers are deleted after ~10 days)
  - o only text input but it is possible to indicate a web page with a pdf (arXiv or on google drive)
  - o for more details this set of rules seems to be followed still, and help understands Bing's behavior



□ Call for contributions within ATLAS collaboration (1992 created, international, ~3000 physicists including ~200 with AI experience)

 $\square$   $\rightarrow$  ~20 stories from experienced users of ChatGPT/Bing

Beyond anecdotes, can ChatGPT/Bing be useful to physicist' daily work ?

- $\bullet \rightarrow$  a clear yes !
- However one always has to stay on top of it
- However would benefit a specialised fine-tune

## **Public knowledge database**

ChatGPT more thorough than Bing, but sources missing are a real problem (plus ChatGPT's training DN frozen in Sep 2021) → now (Jan 2024) essentially fixed

Very good for textbook knowledge on A or B

Not so good to treat A and B, especially if cutting-edge (i.e. science and AI)

## **Private Knowledge database**

	U1			-	11 12	and the		#/F	地が北下		1
$\leftarrow \  \  \rightarrow$	C		$\bigcirc$	A ht	tps://ind	ico. <b>cer</b>	n.ch/eve	ent(1306	120/		!
<b>#</b> K	<	<b>^</b>	>	X	-		<b>•</b>	େ	Q		
CHACAL 2024											
	15–27 j Fuseau ho	anv. 2 oraire Af	024 rica/Joh	annesbu	rg						
	Accue	il									
	Ordre	du iou	ır								

Liste des contributions

Inscription

List of students

→ big potential if « fine tuning » to internal knowledge (public papers and corresponding internal discussions, internal documents, mailing lists, meeting slides... since ~2000)

(many startups are proposing companies to build a ChatGPT for their internal documentation)

□ Indico : >1 million CERN meetings with slides attached since 2000□ → incredible, unique, dataset about science as it is built

**CHACAL 2024:** 

and Applications CNRS

15-27 Jan 2024, University of Witwater

#### « Can Normalizing Flows be used at the LHC? »

3.

#### ChatGPT

Yes, normalizing flows can be used at the Large Hadron Collider (LHC) for various tasks, such as data analysis and simulation. Normalizing flows are a type of generative model that can be used to learn the probability distribution of high-dimensional data. In the context of particle physics, normalizing flows can be used to model the probability distribution of particle collision events.

One application of normalizing flows in particle physics is in the simulation of particle collisions. Simulating particle collisions is essential for predicting the outcomes of experiments at the LHC. However, simulating particle collisions is a computationally expensive task that can require significant computing resources. Normalizing flows can be used to speed up the simulation of particle collisions by learning the probability distribution of the particles produced in a collision and generating new samples from that distribution. This can reduce the computational resources required to simulate particle collisions, which can be especially useful for rare events.

Normalizing flows can also be used for data analysis at the LHC. For example, they can be used to learn the probability distribution of signal events and background events in a particle physics experiment. This can be useful for identifying signal events, which are events that are of particular interest to researchers, and distinguishing them from background events, which are events that are produced by other processes and can obscure the signal events.

In summary, normalizing flows can be a useful tool for various tasks in particle physics, including simulation and data analysis at the LHC.

HEP ML Course 3, David

Normalizing Flows are generative models which produce tractable distributions where both sampling and density evaluation can be efficient and exact 1. They are used for distribution learning 2.

Bing

I found a research paper titled "Normalizing Flows for LHC Theory" which discusses the use of normalizing flows in LHC theory 3. However, I couldn't find any other information about the use of normalizing flows at LHC.

Is there anything else I can help you with?

- 1. https://arxiv.org/abs/1908.09257
- 2. https://arxiv.org/abs/1505.05770

← best primary reference

https://www.researchgate.net/publication/368556193\_Normalizing\_Flow s for LHC Theory

- Bing has tried to make sense from the first few hits
- ChatGPT more thorough but absence of source a clear handicap
- …however one should ask followup questions ( A then B):

How can normalizing flows be used to learn probability distribution exactly ?

(...)

thanks, please provide as a full latex document Rousseau, Jan 2024, CHACAL Let's suppose we have a dataset  $\mathcal{D}$  of N samples, each of which is a highdimensional vector  $\mathbf{x} \in \mathbb{R}^D$ . The goal of a normalizing flow model is to learn a transformation  $f_{\theta}: \mathbb{Z} \to \mathcal{X}$ , parameterized by  $\theta$ , that maps a simple base distribution, such as a Gaussian distribution, to the target distribution. Specifically, we want to learn the transformation such that the probability density of the transformed samples  $p_X(f_{\theta}(z))$  matches the true probability density of the dataset  $p_D(\mathbf{x})$ .

The transformation  $f_{\theta}$  is constructed by composing a sequence of invertible mappings  $f_i$ :

 $f_{\theta} = f_K \circ f_{K-1} \circ \cdots \circ f_2 \circ f_1$ 

Each  $f_i$  is an invertible function that takes as input a vector  $\boldsymbol{u}_i$  and outputs a vector  $\boldsymbol{v}_i {:}$ 

 $\boldsymbol{v}_i = f_i(\boldsymbol{u}_i)$ 

The inverse function of  $f_i$  is denoted by  $g_i$ , such that  $g_i(v_i) = u_i$ . The log-likelihood of a sample x can be computed using the change of variables formula:

$$p_{\mathcal{X}}(oldsymbol{x}) = \log p_{\mathcal{Z}}(oldsymbol{u}) - \sum_{i=1}^K \log \left|\det rac{\partial f_i}{\partial oldsymbol{u}_i}
ight|$$

```
\theta^* = \arg \max_{\theta} \sum_{\boldsymbol{x} \in D} \log p_{\mathcal{X}}(\boldsymbol{x}; \theta)
```

This optimization can be performed using gradient-based methods, such as stochastic gradient descent.

# Jan 2024: chatGPT much better

#### Vous

Can Normalizing Flows be used at the LHC? Please provide references

#### ChatGPT

Normalizing Flows can indeed be used in the context of the Large Had (LHC) for various tasks such as data analysis, simulation, anomaly deter Here are some references that detail their application:

- 1. Data Analysis and Event Reconstruction: Normalizing Fl precision simulations and evaluating uncertainties in hig includes applications like event reconstruction [\*\*].
- Fast Simulation: There is research on using generative m Normalizing Flows, for detector response modeling at the and efficient simulations [17].
- Anomaly Detection: Studies discuss the improvement of strategies at the LHC using variational autoencoders anc anomaly detection [\*\*] [\*\*].
- Noise Reduction and Data Compression: Normalizing Fluid dimensional detector simulations, which include tasks like noise reduction in complex datasets [1].
- 5. Uncertainty Quantification: The application of Normalizi

quantification in high-energy physics simulations is also discussed in the literature [\*]

Article Full-text available

#### **Normalizing Flows for LHC Theory**

February 2023 · <u>Journal of Physics Conference Series</u> 2438(1):012004 DOI: <u>10.1088/1742-6596/2438/1/012004</u> License · <u>CC BY 3.0</u>

Anja Butter

#### **Normalizing Flows for High-Dimensional Detector Simulations**

Florian Ernst<sup>1,2</sup>, Luigi Favaro<sup>1</sup>, Claudius Krause<sup>1,3</sup>, Tilman Plehn<sup>1</sup>, and David Shih<sup>4</sup>

Improving Variational Autoencoders for New Physics Detection at the LHC With Normalizing Flows 2022 | Jawahar, Pratik; Aarrestad, Thea; Chernyavskaya, Nadezda; Pierini, Maurizio; Wozniak, Kinga A; Ngadiuba, Jennifer; Duarte, Javier; Tsan, Steven Published Web Location https://doi.org/10.3389/fdata.2022.803685

#### Generative Machine Learning for Detector Response Modeling with a Conditional Normalizing Flow

Allison Xu

Shuo Han

Xiangyang Ju

Haichen Wang

au, Jan 2024, CHACAL

# **Scientific reading**

☐ mediocre: « What are the important points of this paper? »→all points correct, but

- Some do not come from the paper (but from general knowledge)
- « important » is too vague

However specific questions can be correctly answered: « why is technique A used » ?

• →in general 80/20 correct vs BS

# **Scientific writing**

Very good at suggesting a paper structure/substructure

- Useless for the actual writing (we're writing about cutting edge science not available elsewhere...)
- □ Not bad at summarising (80/20)
- Good at outreach: I am in high school, please explain the Higgs boson to me

- what would be a good analogy for the Higgs boson if I am 18 ?
- The Higgs boson is a particle that helps give other particles mass, so here's an analogy that might help you understand it better:

Imagine a school hallway where students are moving around, but some of them are able to move faster than others. The faster students are like particles that have less mass, while the slower students are like particles with more mass. Now imagine that there's a teacher in the hallway, and every time a student passes by the teacher, the student gets slowed down a bit. This teacher is like the Higgs field, which particles interact with to acquire mass. The more a particle interacts with the Higgs field, the more massive it becomes.

And just like how some students might have more trouble getting past the teacher and thus end up moving slower, some particles have more trouble interacting with the Higgs field and thus end up being more massive.

## Code

- Very good at writing simple code snippets
  - o → 80% correct
- □ Can also explain/debug code in unfamiliar language →
- Good at using well known libraries
- Not as good for specific code (3 M lines of C++/Python in ATLAS) → would need a dedicated « fine tuning »

I get an error when I try:

\$ conda env create -f cpu\_environment.yml python=3.9 -n exatrk-cpu Solving environment: failed

CondaValueError: Malformed version string '~': invalid character(s).

It looks like there might be an error in the `cpu\_environment.yml` file that you are trying to use to create your conda environment. The error message you are seeing suggests that there might be an issue with the version number specified in the environment file.

To resolve this issue, you could try removing the `python=3.9` argument from your command and see if that works. Here is an updated version of the command:



ß