

Machine Learning applications at IN2P3



ANF Machine Learning - 21-25 Septembre 2020, Orsay

Introduction

ML has been present since a long time in many research fields of the **IN2P3**

Since a few years **small revolution** with **modern** ML librairies and infrastructure

Access to ML more 'democratic' and widespread than before

A **lot of work** in this field: here just a **few** hand-picked results

To have a more **complete overview** of ML activities in the past year

- [Prospectives](#) Machine Learning de l'IN2P3 (oct. 2019)
- [Journées](#) Machine Learning et Physique Nucléaire (oct. 2019)
- IN2P3/IRFU Machine Learning [workshop](#) (jan. 2020)

Outline

Overview of ML activities @ IN2P3

- Detector / accelerator
- ML for HEP analyses
- Nuclear physics
- Astrophysics

Training and schools

Conclusion

Detectors / accelerators

Detector / accelerator

Detector design

ML for Accelerator developments

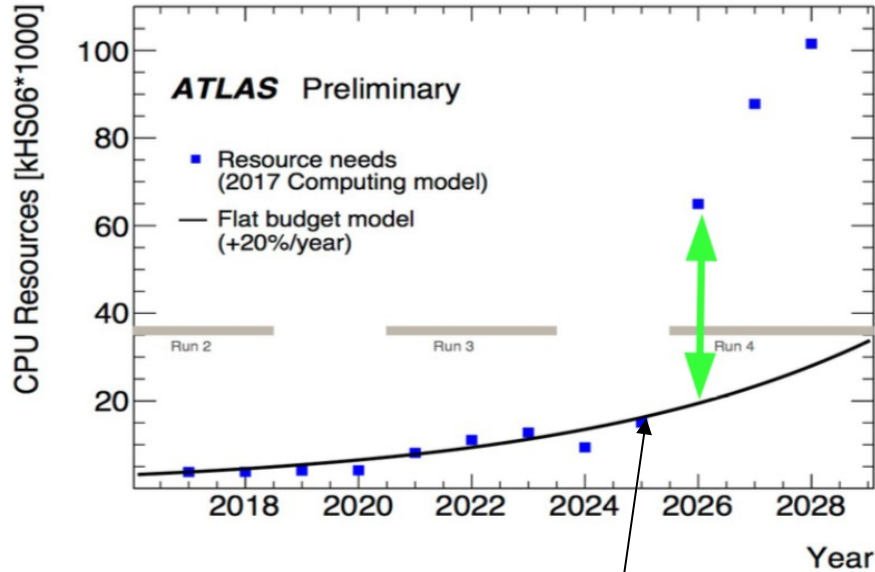
- ML for ThomX **experiment**

Simulation

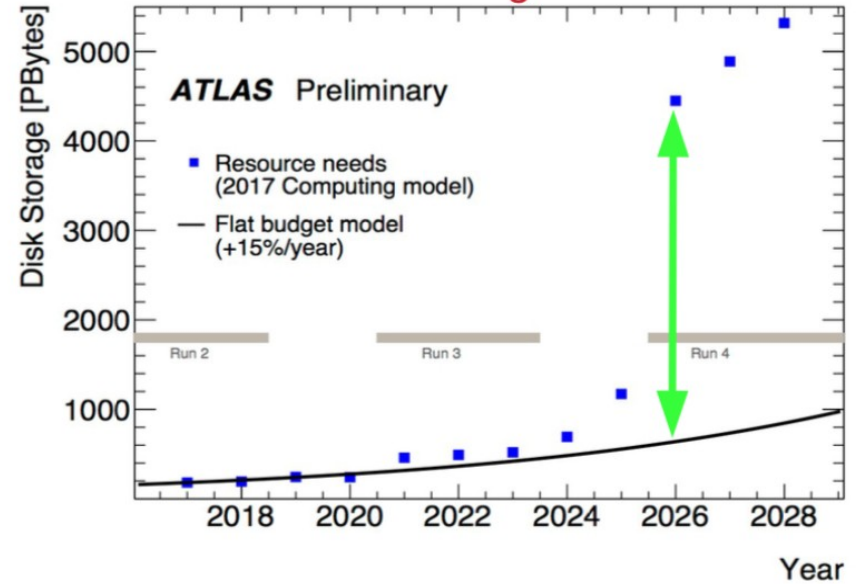
- Simulation of ATLAS **calorimeter** with GAN's

Fast simulation for High-Lumi LHC

CPU



Disk storage

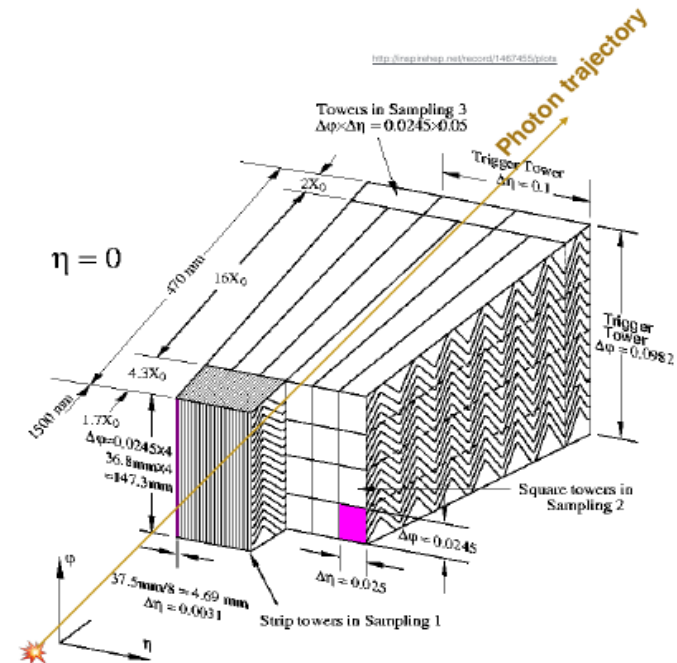
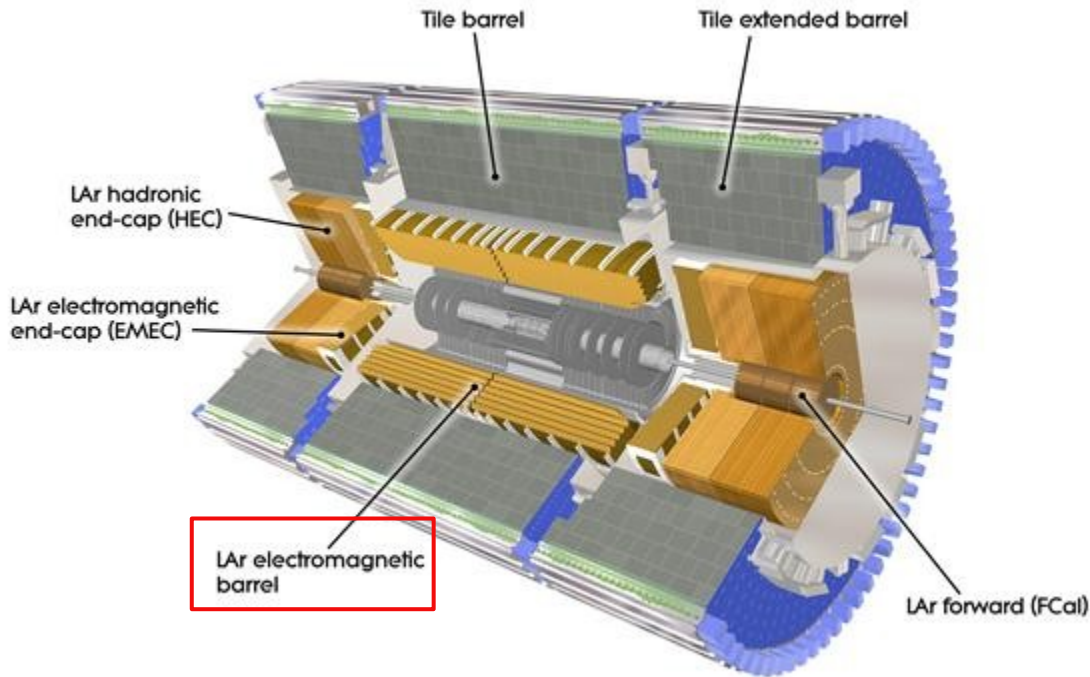


Dominated by : calorimeter simulation and tracking

ML used to design fast simulation algorithms

GAN for simulation for ATLAS

Simulation of liquid-argon electromagnetic calorimeter response with GAN's



Particle goes through 4 layers :

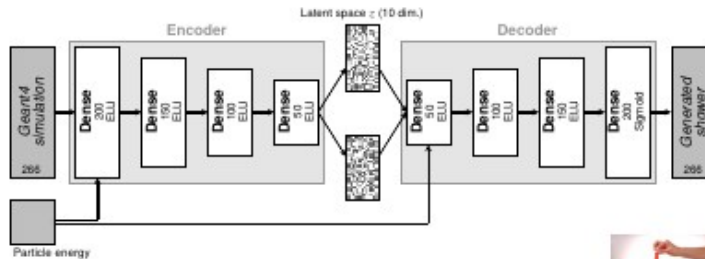
0. Pre-Sampler : (7x3) Some energy deposit
1. Strips: (56x3) Very granular in η ; more energy deposit
2. Middle: (7x7) Thickest layer, maximum energy deposit
3. Back: (4x7) Little Energy deposits

First results (2018)

D. Rousseau, A. Ghosh (LAL), G. Louppe (U Liège) et al.

[ATL-SOFT-PUB-2018-001](#) and update [ATLAS-SIM-2019-004](#)

VAE:



100 epochs, 2 mins, CPU



Flat vector of 266 cells are the output of both generators

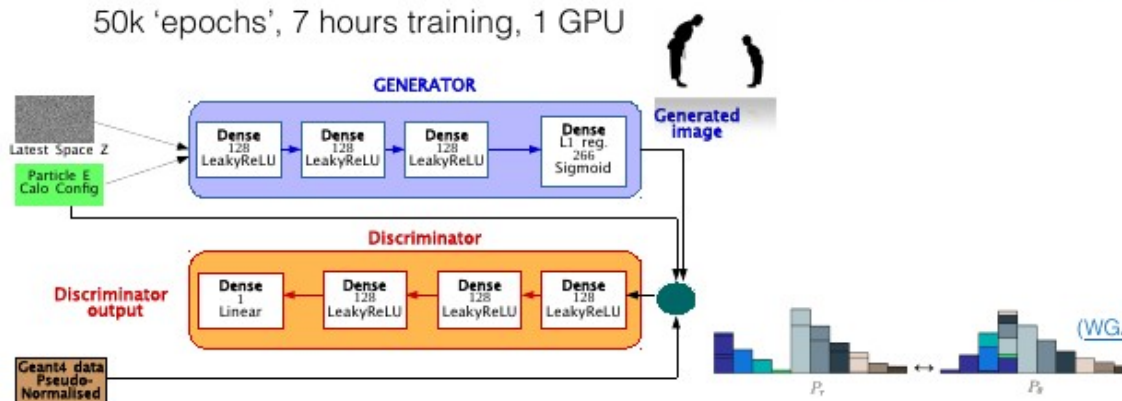
Not an ideal training dataset



Training dataset:

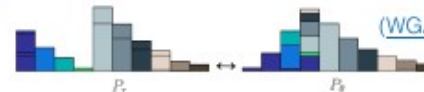
- Single **photon** samples from Geant4
- 88000 events
- 9 **discrete energy points** : {1, 2, 4, 8, 16, 32, 65, 131, 262} GeV
- $0.20 < |n| < 0.25$
- 4 electromagnetic calorimeter layers

50k 'epochs', 7 hours training, 1 GPU



GAN:

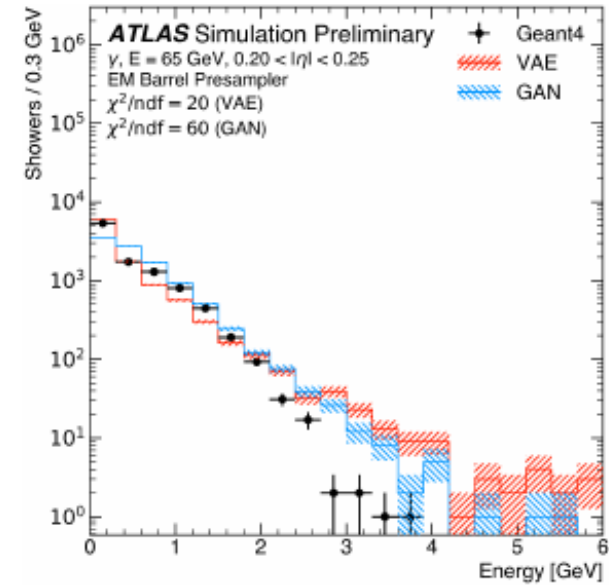
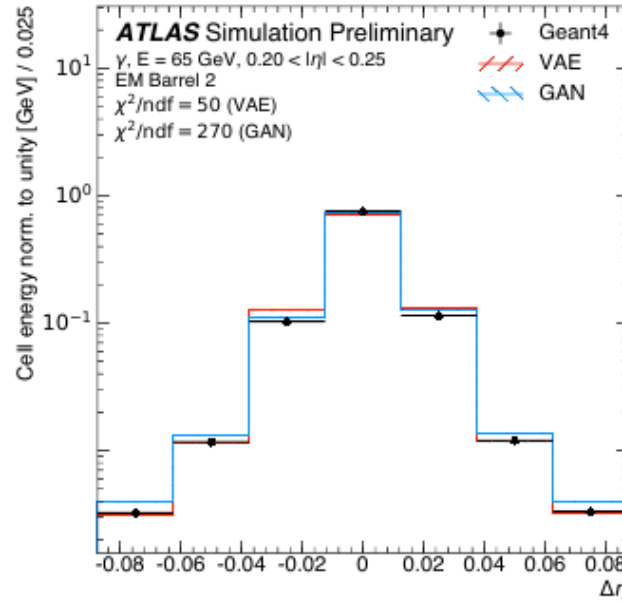
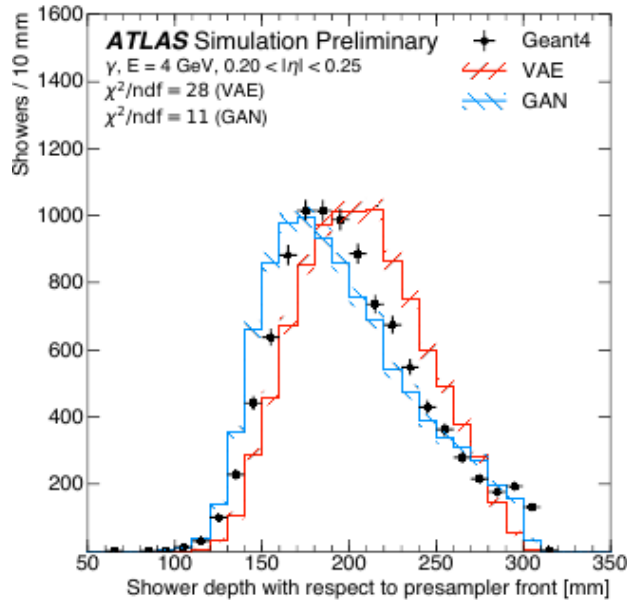
([WGAN-GP](#), Improved WGAN-GP nightmare on Ke...



Slide taken from Aishik Ghosh [talk 01/20](#)

First results (2018)

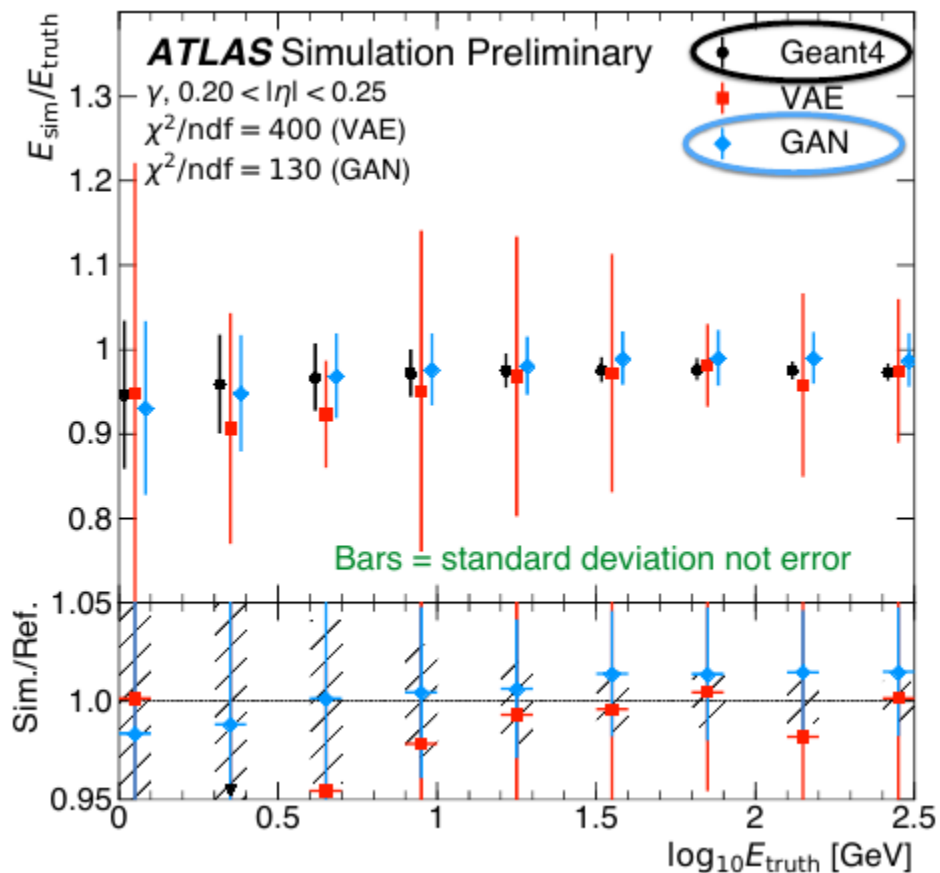
[ATL-SOFT-PUB-2018-001](#) and update [ATLAS-SIM-2019-004](#)



- < 1 ms instead of ~ 10 s to reconstruct an object
- x100 gain for a full event
- But some limitations: energy resolution, etc

First results (2018)

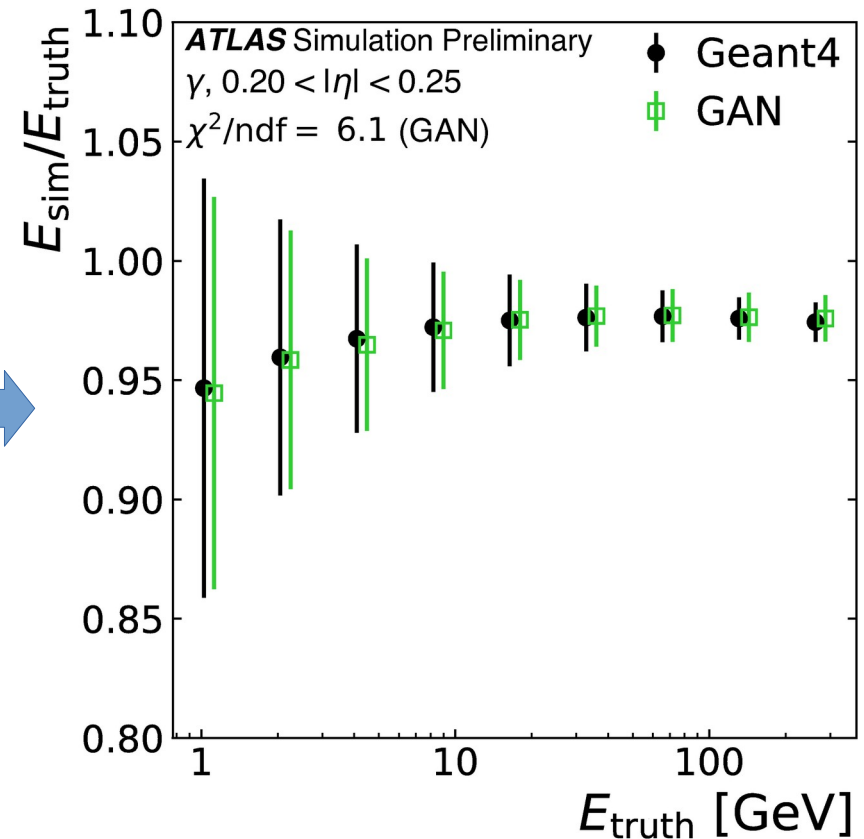
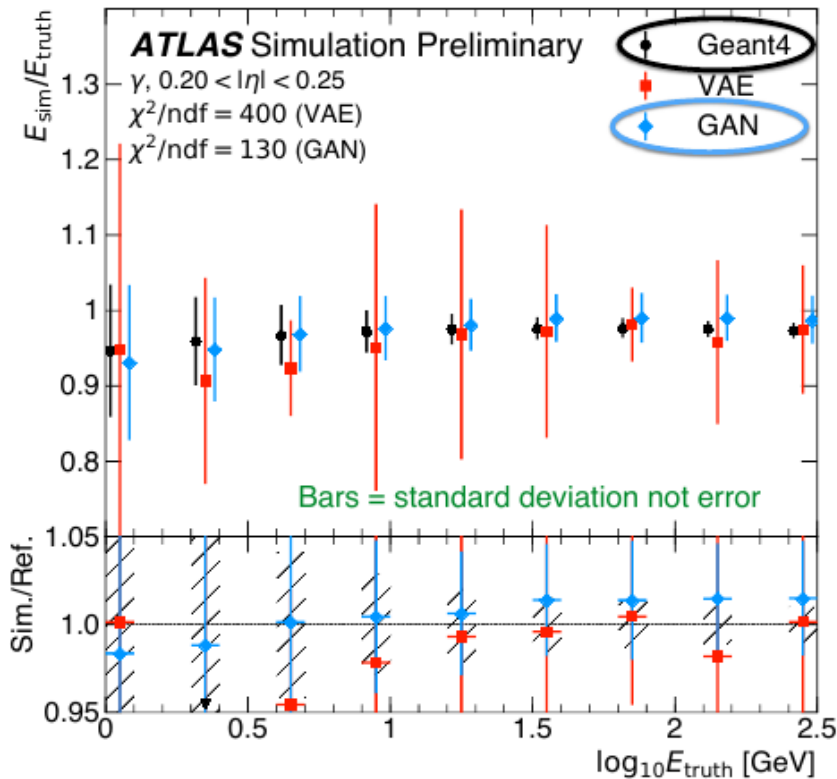
Problem: cannot model well detector resolution



GAN gets the means but not the widths of the energies

Improvements

New GAN architecture + conditioning (energy, position, geometry)
→ improved energy resolution, particle position



Impressive progresses but probably still a long road to go

(More details [here](#))

Machine learning for accelerators

General trend in ML for accelerators

Recently people from **PSI** (SLAC, DESY, CERN, MIT) started series of online seminars for physics of accelerators, and in particular **ML for accelerators**.

The **OWLE-Colloquium** is aimed at giving researchers a platform to share research and development results of very broad interest.

The **OWLE-ML seminar series** has a topical focus on machine learning and **experimental demonstration of AI-ML**.

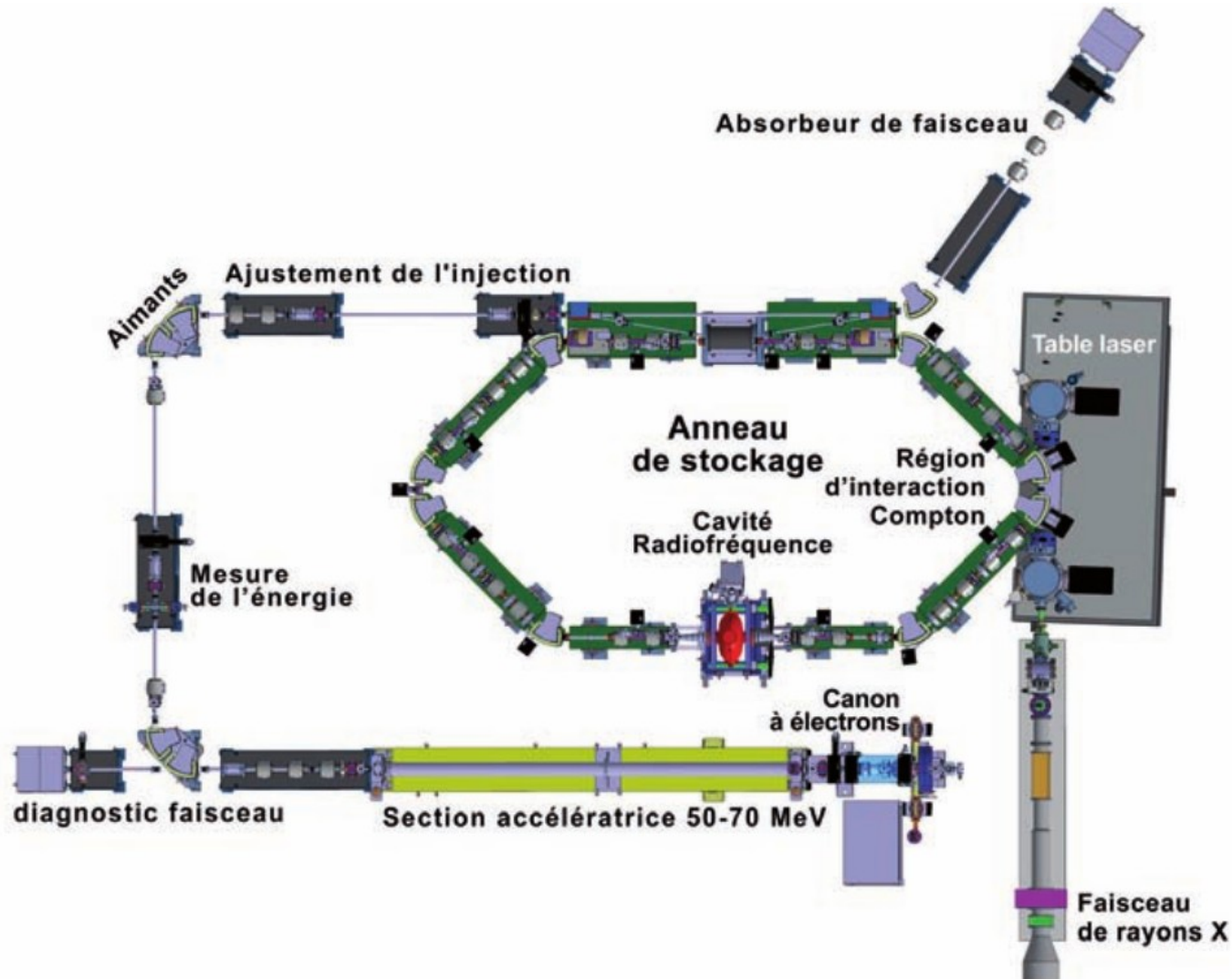
<https://sites.google.com/view/owle/home>



OWLE: The **O**ne **W**orld
partic**L**e acc**E**lerator
colloquium and seminars

Machine learning for accelerators

The ThomX project: high intensity and energy X-ray source produced by Compton interaction of photons (laser) and electron (accelerator ring)

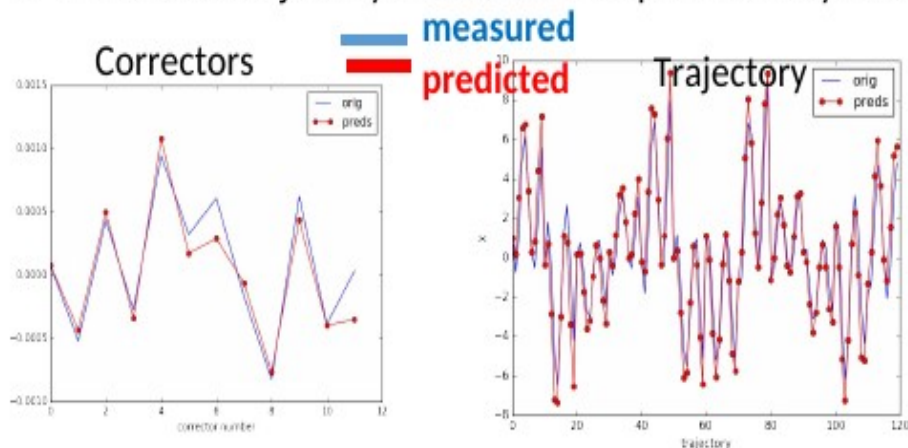


Supervised learning for accelerators

H. Guler, V. Kubyski et al. (IJCLAB)

ThomX RING : Single particle Trajectory (several turns)

1. Control parameter: Corrector magnets. 12 independent variables in transverse horizontal/vertical planes.
2. Measured: trajectory/n-turns/orbit represented by 120 variables (12 BMPs x 10 Turns).

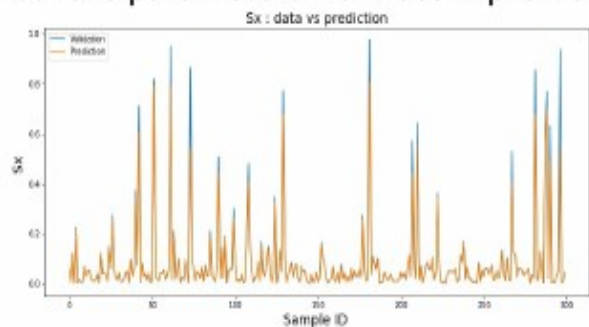


Model trained on simulation to predict correctors based on the trajectory input.

XGBRegressor + MultiOutputRegressor, or NN

ThomX LINAC : Reproduce beam longitudinal dynamics from simulation

1. Control parameter: Solenoid, RF phases, laser parameters (10 parameters)
2. Measured beam parameters (size, emittance, ...) : 6 observables
3. Retrieve parameters from beam profile (CNN)



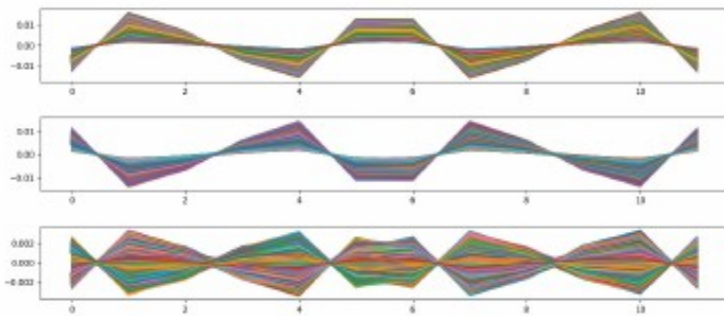
- Model trained on simulation (slow simulation 10 min per configuration)
- Neuronal network model for scalar data
- CNN for images data

Unsupervised and reinforcement learning

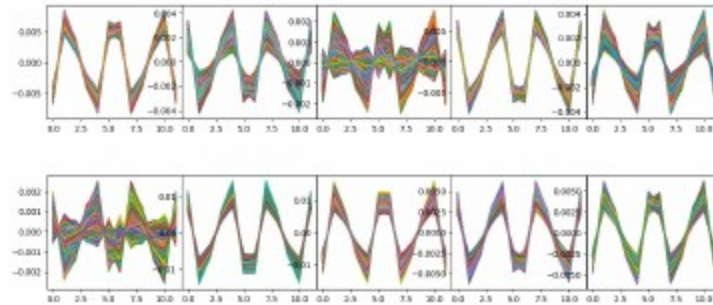
Classification of trajectories with K-Means.

Same dataset is easily regrouped to few categories/classes.

3 categories

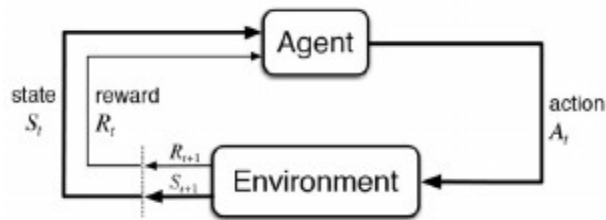


10 categories



Reinforcement Learning using model based on NN

Find special beam characteristics (example : minimum size, emittance etc)



OpenAI Gym environment used together with **Stable Baseline** and Tensorflow.

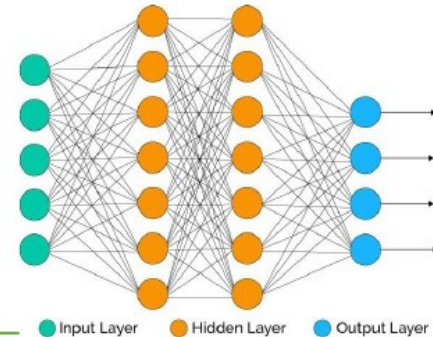
Different models benchmarked (DQN, DDQN, **TD3**, ...) with proper policy.

Could find beam minimum size after less than 20 epocs

Machine learning for accelerators

Typical workflow

1. Formulation of the problem
2. Preparing dataset and “understanding of the data”
3. ML model: development, training, improvement



Methods:

NN, CNN, XGBoost
RL

Tools:

Jupyter notebook, Keras,
Tensorflow, PyTorch, OpenAI

Hardware:

CPU (x48), GPU(GV100, Laptop)

Ongoing studies:

- prediction of correctors magnets currents
- Trajectory minimization
- Noise “filtering” in the data
- Model robustness
- Beta function reconstruction from TBT data
- Optimization of injection
- Orbit classification
- Failure/anomaly detection
- Inverse problems

When NN is not learning, search why :

- Dataset, more datapoints in trajectory
- NN architecture: layers, depth, activation
- learning rate
- Normalisation
- Optimizer
- Add noise

ML for HEP analyses

ML for HEP analyses

Historically a vast playground for ML approaches – many IN2P3 contributions

Object reconstruction, particle identification, calibration

Event classification, regression

Phenomenology and theory

Real time analysis and triggering

Treatment of uncertainties

Data reduction

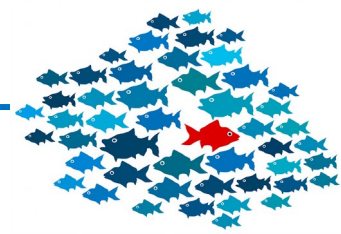
Search for anomalies

- **Searches for new physics at LHC**

Fundamental parameter inference

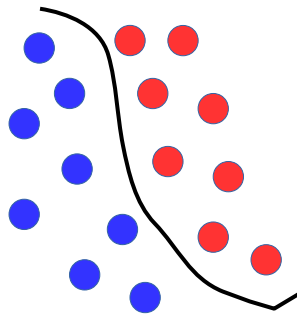
- **Likelihood free inference**

Anomaly detection



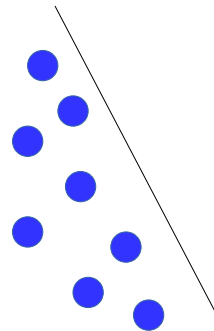
Supervised (labels)

DNN, BDT, SVM



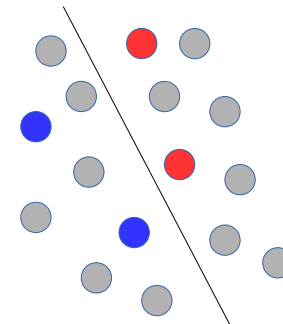
Unsupervised (no labels)

SVM-1class, **AE**, VAE,
WAE, **GAN-AE**,...

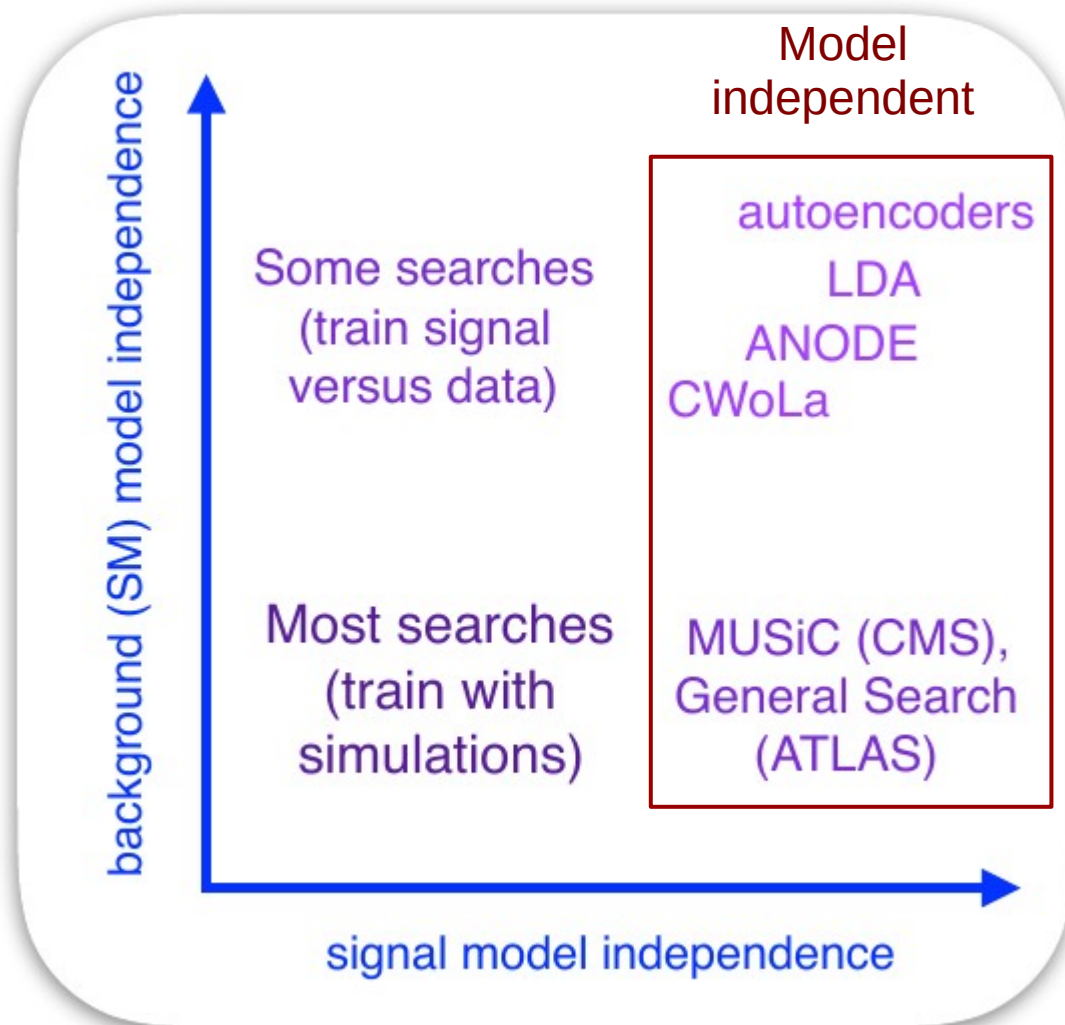


Semi-supervised (some labels)

triplet NN,...



Searches for New Physics at LHC



B. Nachman, D. Shih, [arxiv:2001.04990](https://arxiv.org/abs/2001.04990)

LHC Olympics challenge



Anomaly detection challenge using simulated data

Despite an impressive and extensive effort by the LHC collaborations, there is currently no convincing evidence for new particles produced in high-energy collisions. Goal is to ensure that the LHC search program is sufficiently well-rounded to capture “all” rare and complex signals.

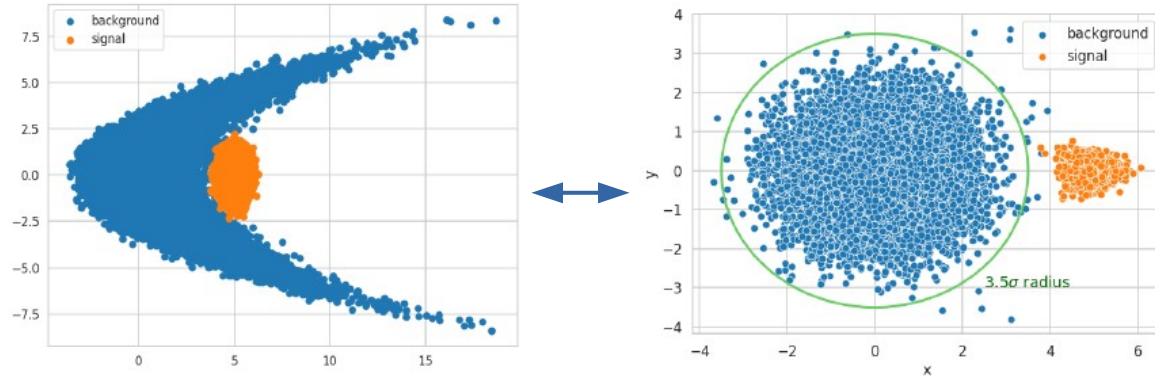
Two editions in 2020 (Winter and Summer): <https://lhco2020.github.io/homepage/>

Event-level anomaly detection methods

L. Vaslin, I. Dinu, J. Donini (LPC Clermont)

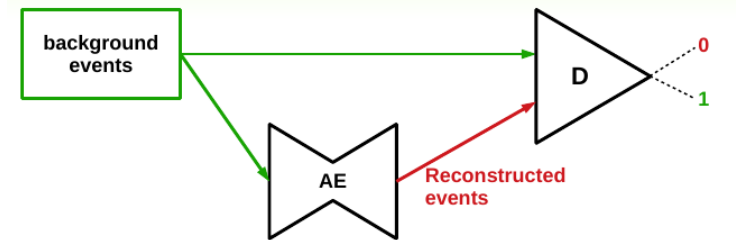
1. Normalizing flow for anomaly detection

Determine bijective transformations between background data and multivariate Gaussian



2. Autoencoders and generative models

Increase performances of AE using a GAN-like architecture

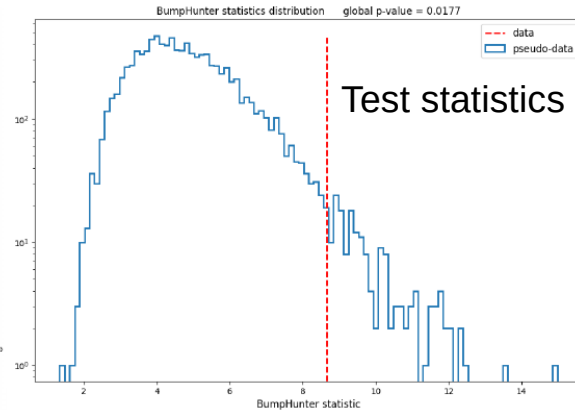
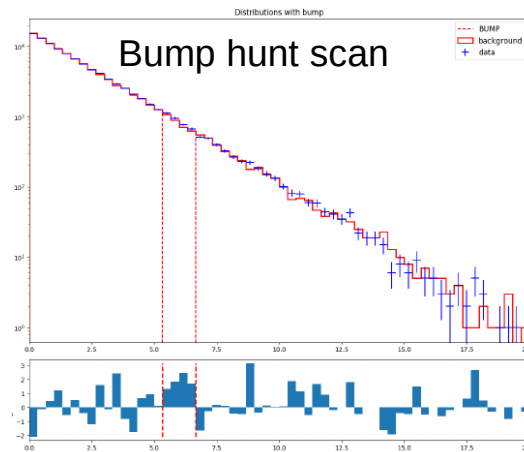


3. pyBumpHunter project

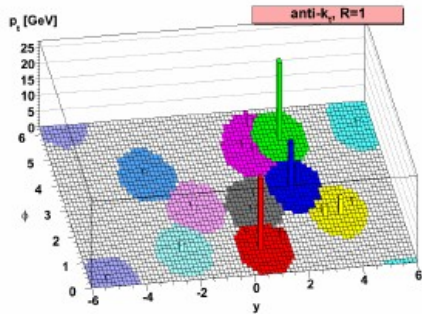
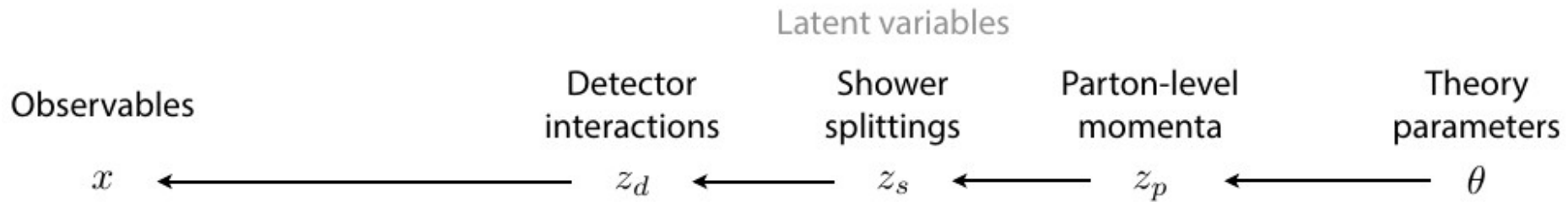
Python implementation of the popular [BumpHunter](#) algorithm

Code here: [pyBumpHunter](#)

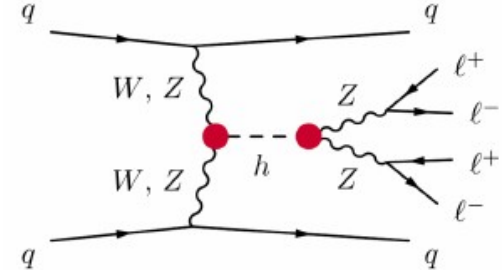
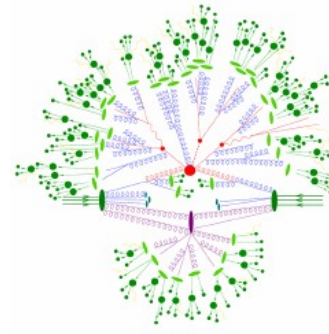
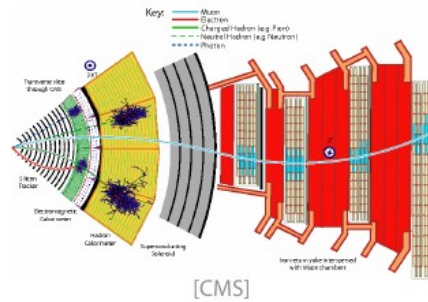
Implementation in scikit-hep



Likelihood free inference

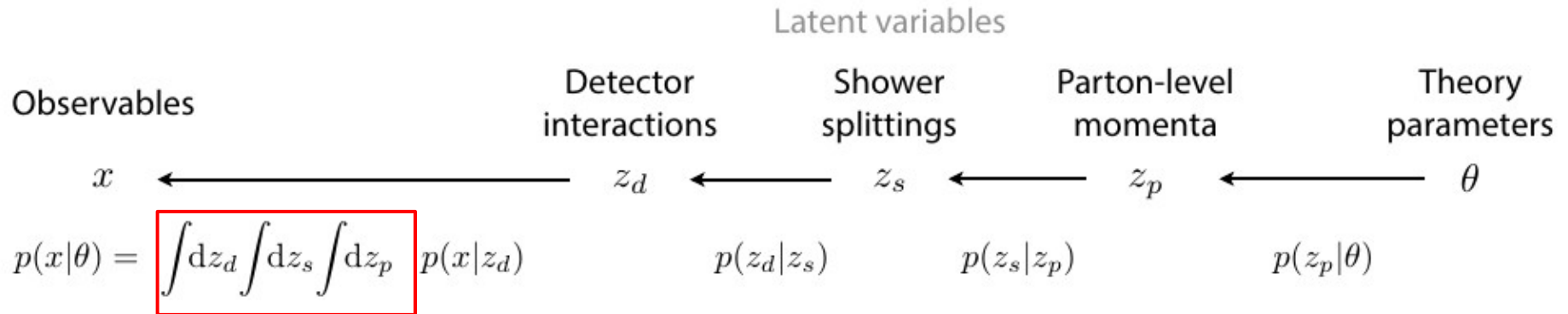


[M. Cacciari, G. Salam, G. Soyez 0802.1189]



For details see J. Brehmer [slides](#)

Likelihood free inference



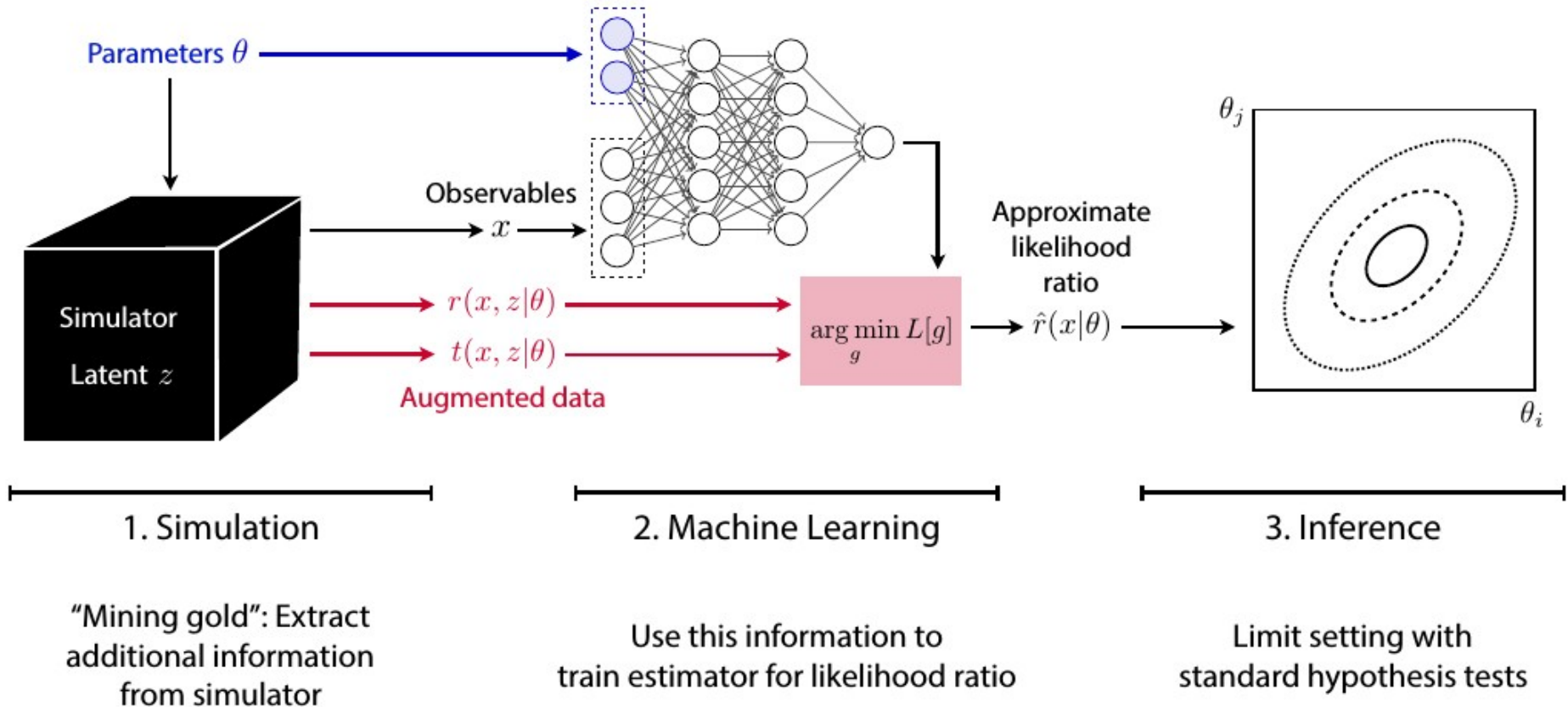
Impossible to calculate integral over enormous space

→ analysis at LHC generally rely on other approaches (collect data in form of histograms, etc)

Inference

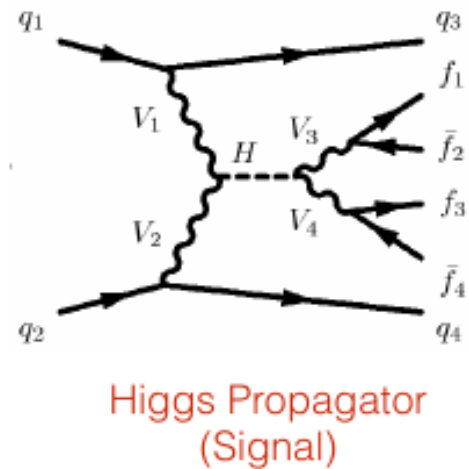
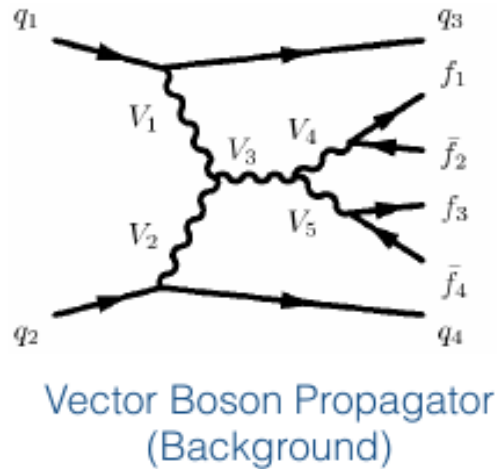
Likelihood free inference

Approach: use more informative targets to regress for a neural network



Likelihood free inference

Full example using this approach : **Measuring Quantum Interference in the Off-shell Higgs to 4 Leptons** (see A. Ghosh [presentation](#))



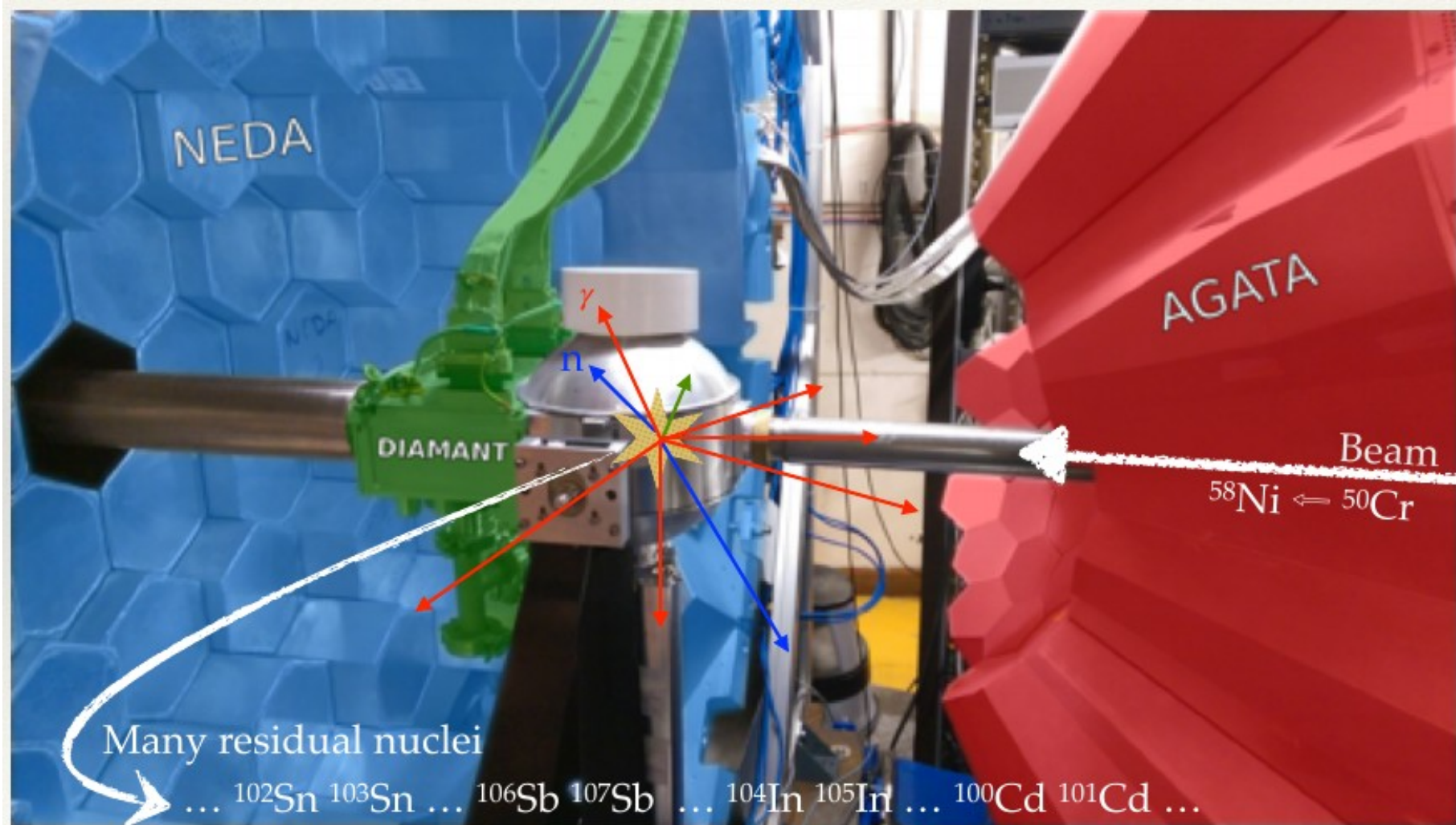
Aim: directly learn the likelihood using ML – results seem promizing

Nuclear physics

Pulse shape discrimination with NEDA

O. Stezowski et al. (IP2I)

Data from an experiment AGATA + NEDA + DIAMANT in coincidence [GANIL 2018]




(Slides O. Stezowski)

Pulse shape discrimination with NEDA

Data from an experiment AGATA + NEDA + DIAMANT in coincidence [GANIL 2018]

Modules fired in NEDA



PSD

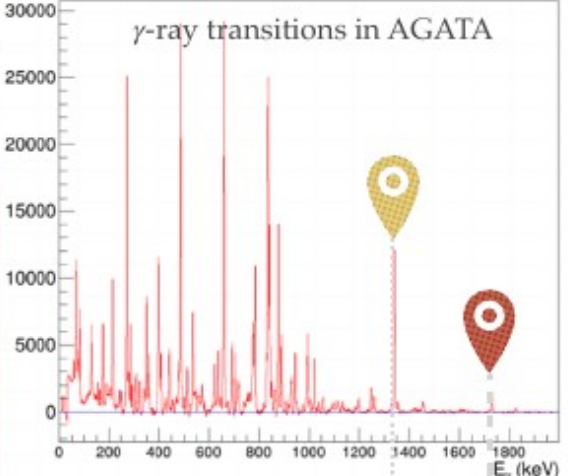
Artificial Neural Networks

We know the # x of neutrons detected

We can get the probability to be wrong

$$P(x_{\text{detected}} | y_{\text{emitted}})$$

Mislabel Probability $\equiv P(1n | 0n)$

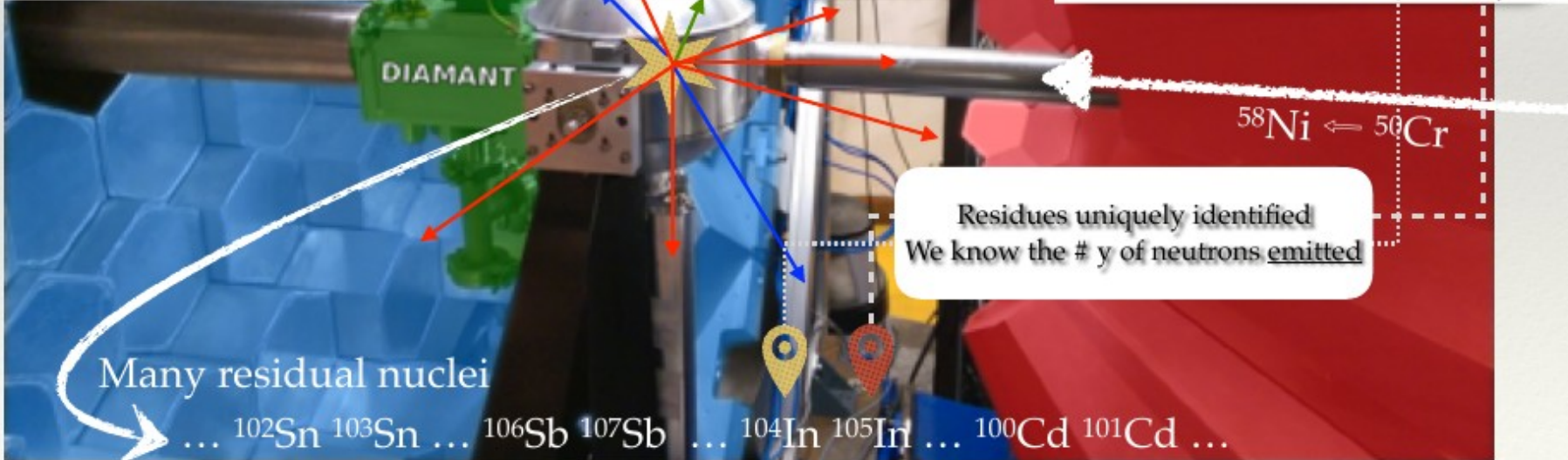


γ -ray transitions in AGATA

30000
25000
20000
15000
10000
5000
0

0 200 400 600 800 1000 1200 1400 1600 1800

E_γ (keV)



DIAMANT

γ

n

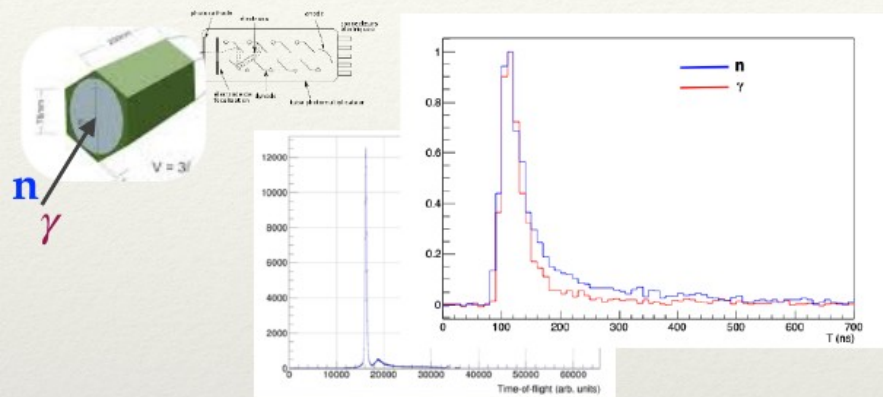
Residues uniquely identified
We know the # y of neutrons emitted

Many residual nuclei

... ^{102}Sn ^{103}Sn ... ^{106}Sb ^{107}Sb ... ^{104}In ^{105}In ... ^{100}Cd ^{101}Cd ...

$^{58}\text{Ni} \leftarrow ^{58}\text{Cr}$

Pulse shape discrimination with NEDA



Inputs used for the **Discrimination** :
the waveform - the amplitude - the time of flight

Common parametrisation of the signal

$$s(t) = A [\exp(-t/td1) - \exp(-t/tr)] + R^*(\exp(-t/td2) - \exp(-t/tr)) \text{ if } t > T0$$

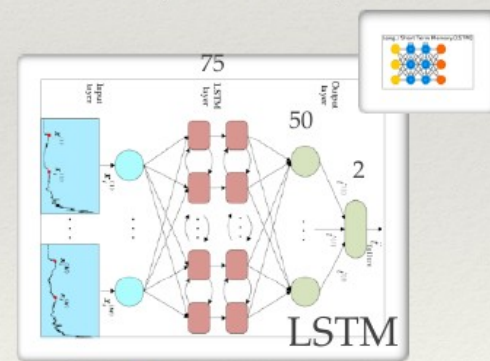
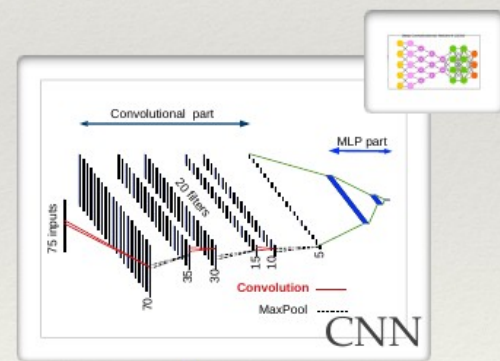
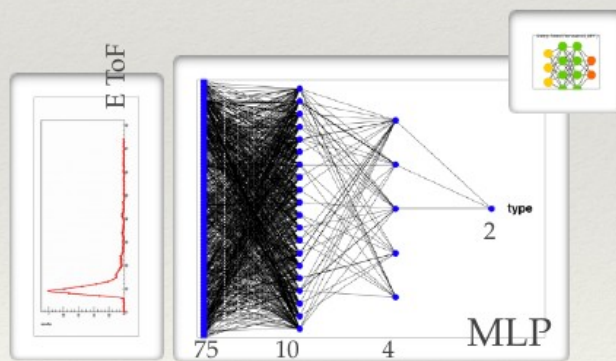
A amplitude = energy

T0 relies on how the signal is captured

td1, td2, tr independent of γ and n

R depends of the type of the particle

Three different Artificial Neural Network architectures tested : MLP / LSTM / CNN



👍 pattern

👍 time series

R&D NEDA

discrimination for low energy better than classical methods *

Implementation with ROOT - mono thread / CPU

➡ **Tensorflow / multi CPU / GPU**



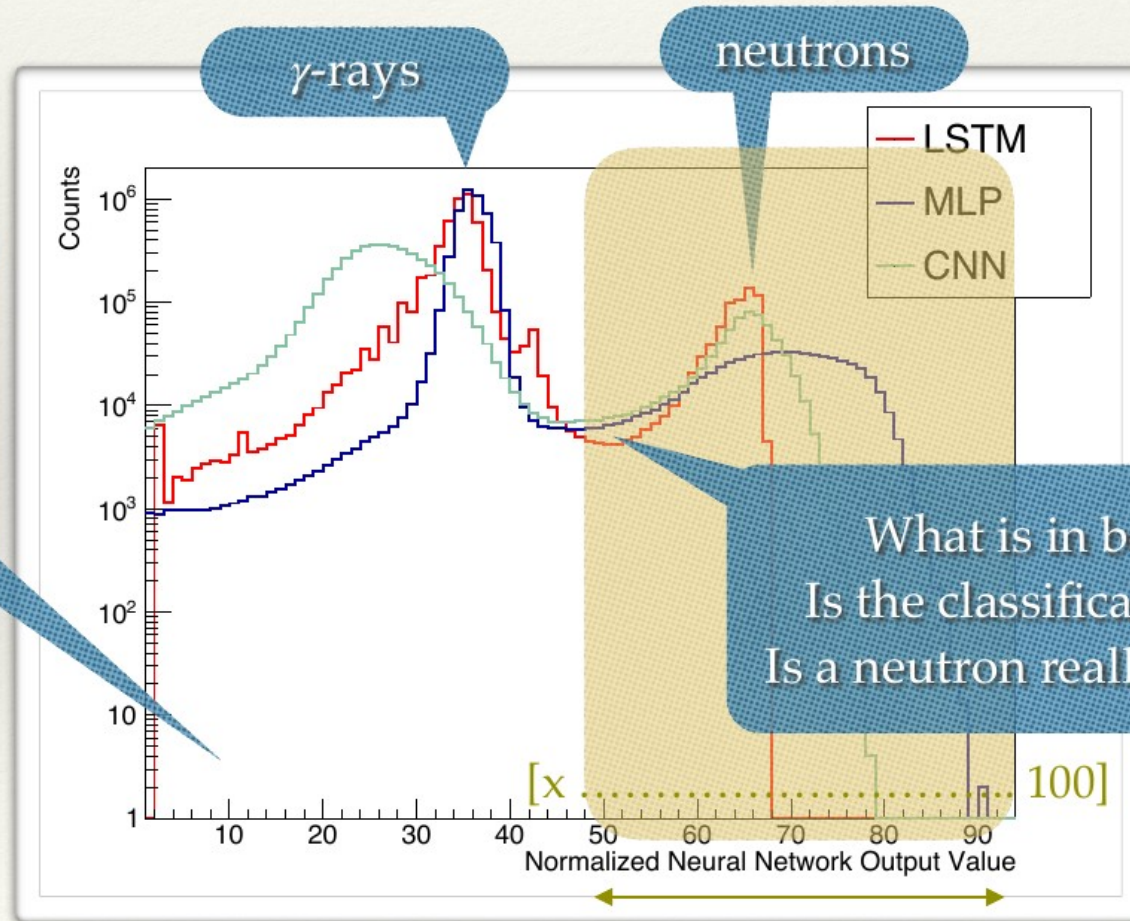
Number of parameters

MLP: 814, LSTM: 10502, CNN: 7042

* Ronchi et al., NIMA 610 (2009) 534–539

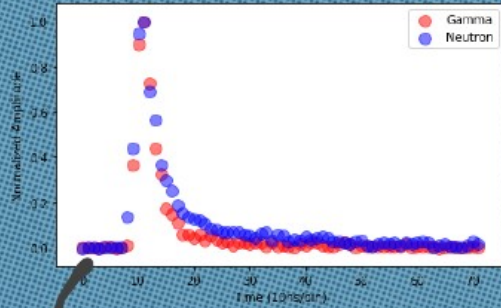
Pulse shape discrimination with NEDA

Distribution of the output value of the three different networks

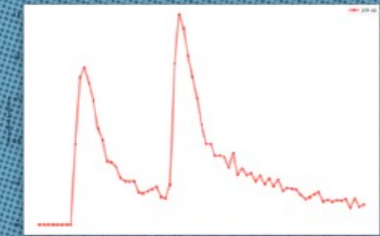
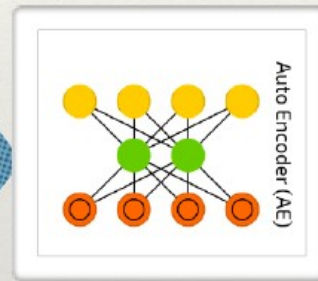
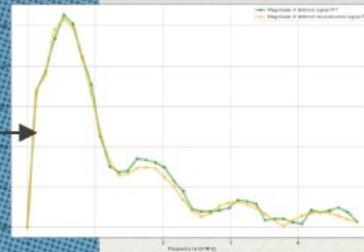
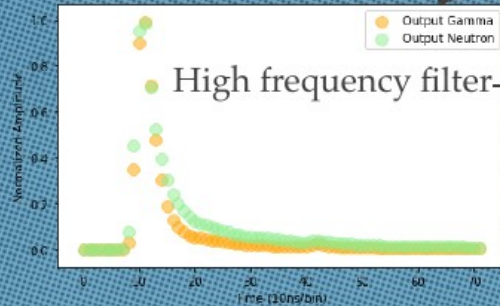


First steps in using Machine Learning for data processing, 3 ANN architectures studied

Signal and autoencoders

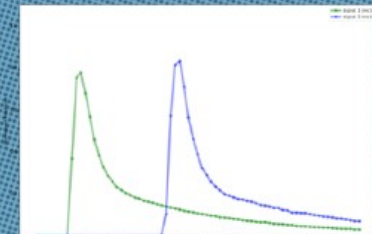
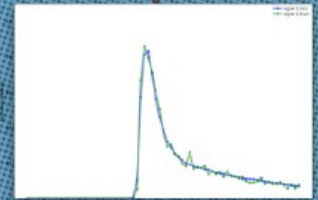
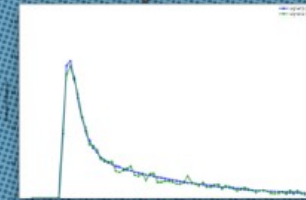


4
neurons
in bottleneck



Auto-encoder 1

Auto-encoder 2



Data compression !

Denosing : Pile-up deconvolution

Auto encoders into the game for compression / de-noising

Astrophysics

Astrophysics

Deep Learning

- Image analysis:
 - Characterization of gamma-ray events in CTA - LAPP
 - Photometry of blended galaxies with deep learning - APC
 - Photometric redshift estimation - CPPM
 - *Identification of tumors through real time imaging - IMNC*

- Events analysis:
 - Single detector glitches and signal identification in VIRGO - APC
 - Waveform reconstruction and characterization in LISA- APC
 - Classification of time-series from astronomical transients - LPC, CPPM

- Signal separation:
 - Generate pure EE/BB power spectra from CMB - APC
 - Deblending of galaxies with VAEs - APC
 - Galaxy signal / noise separation - CPPM

For a complete review see talk E. Ishida (journées prospectives IN2P3): [here](#)

Training and schools

Collaborations with CS/math

ML collaborations @ IN2P3

- Common project, co-supervision of PhD, post-doc
- Example of **(past) local** collaborations :
 - **LPC** and LIMOS/ISIMA (CS), LMBP (maths)
 - LSST (astronomical time series), ATLAS (anomaly detection), LHCb (bayesian learning)
 - **LPNHE** and Sorbonne (maths): ATLAS (fuzzy number systems)
 - **LAL** and LRI (CS): ATLAS (TrackML, Syst. Aware Training)
 - **CPPM** and LIS (CS): ATLAS (ttH), Cosmology (deep learning)
 - **LAPP** and LISTIC (CS): CTA (deep learning)
 - ...
- **International** collaborations: EU-projects with non-academics partners, ...

Obvious advantage in collaborating with ML experts but some caveats:

- Speaking same **language** & getting familiar with vast stat **litterature**
- Question of access to **confidential** experimental data and **authorship**
- **Publication** in journal of CS/math field
- Produce outcome **relevant** to collaborator

Training and schools

Being able to apply ML to practical problems requires understanding underlying statistical concepts and ML algorithms.

- **Target:** students (Master, PhD), staff IN2P3

Training courses exist in several universities / labs

- In general Master degree level some also open to staff for continuous training
 - Ex: [Diplome Universitaire Data Scientist](#)
- Training CNRS formation entreprise
 - Ex: [Introduction to ML and Deep learning](#)

Schools / workshops

- [IN2P3 School of Statistics](#) (organized every 2 years since 2008)
- Workshop CCIN2P3: [GPU and deep learning](#)

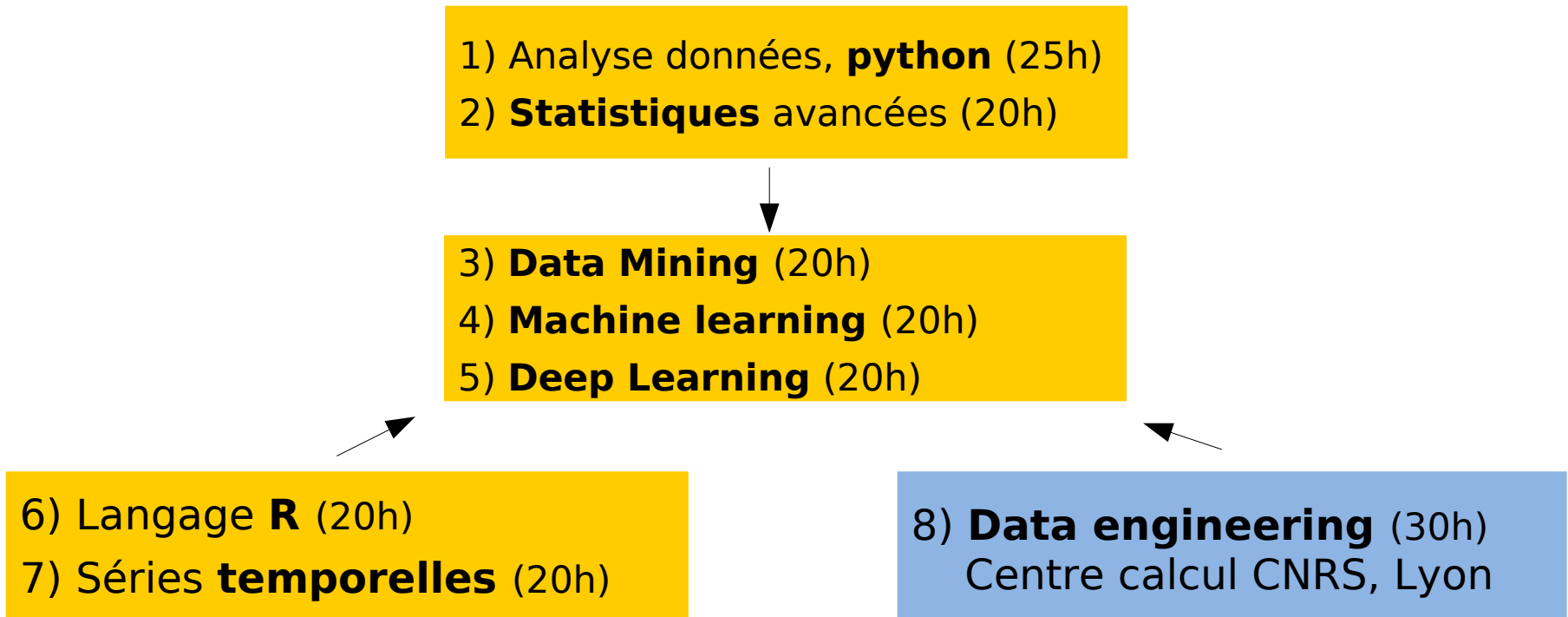
Uncovered needs should trigger specific training actions

Diplôme Universitaire Data Scientist (UCA)

Formation de l'Université Clermont Auvergne – partenariat CCIN2P3

8 semaines de cours réparties sur l'année

Ouvert à la formation continue



Toutes les informations disponibles [sur le site de la formation](#)

Conclusions

Usage of “traditional” **ML** since many years within IN2P3

Many research field at IN2P3 moved to **modern** ML approaches

Fast growing **expertise** on ML at IN2P3 but **training** is important

Huge research potential and many **opportunities**

Continuity and **support** is essential to maintain activities

Challenge: scalability, optimization, integration to experimental software

BACKUP

1. Detectors & accelerators

2. Simulation

Detector design

- Use ML to optimize detector design (LPNHE)

ML for Accelerator developments

- **Accelerator** tuning, lasers, virtual detectors (LAL)
- NN for particle **accelerator** operations and optimization (LPSC)

Simulation

- **Simulation of ATLAS calorimeter with GAN's** (LAL)
- MC sample **reweighting** in ATLAS (LPNHE)
- NN to simulate **fuel evolution** in nuclear reactors (IPNO)
- BDT's for multidim **reweighting** between MC (LAL)
- Gaussian Processes to **smooth MC** stat fluctuations (LAL)

Color code

Advanced
Studies
Interest

3. Object Reconstruction, Identification, and Calibration

Several contributions:

- **Tracking** ML challenge for LHC (LAL)
- **b-tagging** algorithms with BDT's for ATLAS (CPPM)
- **Particle identification** for LHCb (LPNHE)
- **Position reconstruction** of particles for med app (IMNC)
- Reconstruction **calorimeter** objects with CNN, RNN for LHCb (LAL)
- DNN to optimize **jet reconstruction** using RNN for ATLAS (LPSC)
- RNN for **tau ID** and QCD rejection for CMS (IP2I)
- Reco position, tracking **gamma** for nuclear app. (IP2I)
- Full **Event interpretation** algorithm with DNN, Belle 2 (IPHC)
- DNN for **calo reco** and transfert to FPGA for L1 ATLAS trigger (CPPM)

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5. Uncertainty Assignment

Contributions:

- **Systematic** aware training (LAL)
- ML tools for handling **uncertainties** ATLAS (LPNHE)

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6. Learning the Standard Model – searches for anomalies

Contributions:

- Search for **anomalies** (LPC)

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7. Matrix Element Method with ML —▶ **Uncovered ?**

8. Theory Applications

- LPSC: ML activities for HEP **phenomenology** (LPSC)

7. Computing Resource Optimization

- **CCIN2P3**

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