# Machine Learning in HEP : trends and successes

**David Rousseau**

**LAL-Orsay**

**rousseau@lal.in2p3.fr**

**CHEP 2018, Sofia**

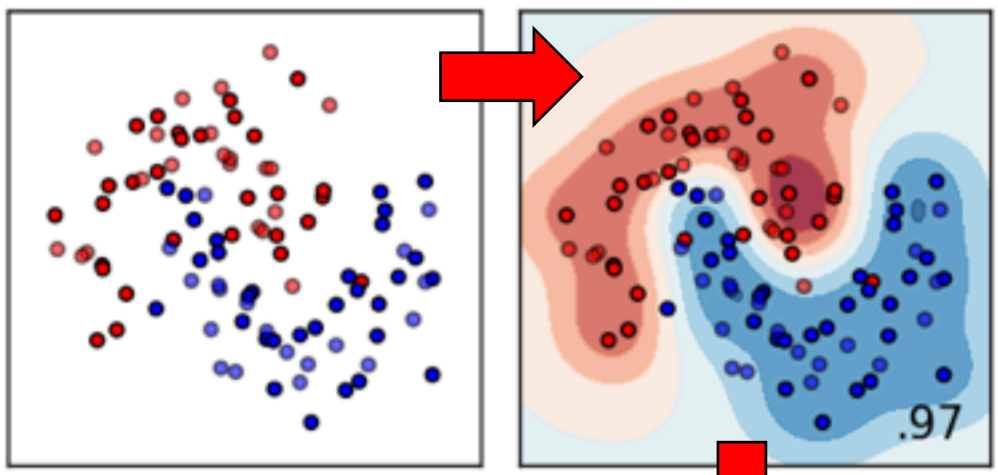
# Outline

- ML basics
- ML in analysis
- ML in reconstruction
- ML in simulation
- Wrapping up

- Focus on applications rather than details of the techniques
- Sometimes blunt statements that I'd love to see challenged
- Deliberately incomplete (sorry…)
- No parameterised learning, no jet images, no likelihood free inference, no classification without labels, no recurrent NN, no review on ML software, no application to distributed analysis, no GAN to uniformity, no Bayes optimisation, no reinforcement learning, no adversarial example, no probablistic programming, no learning with quantum computing….

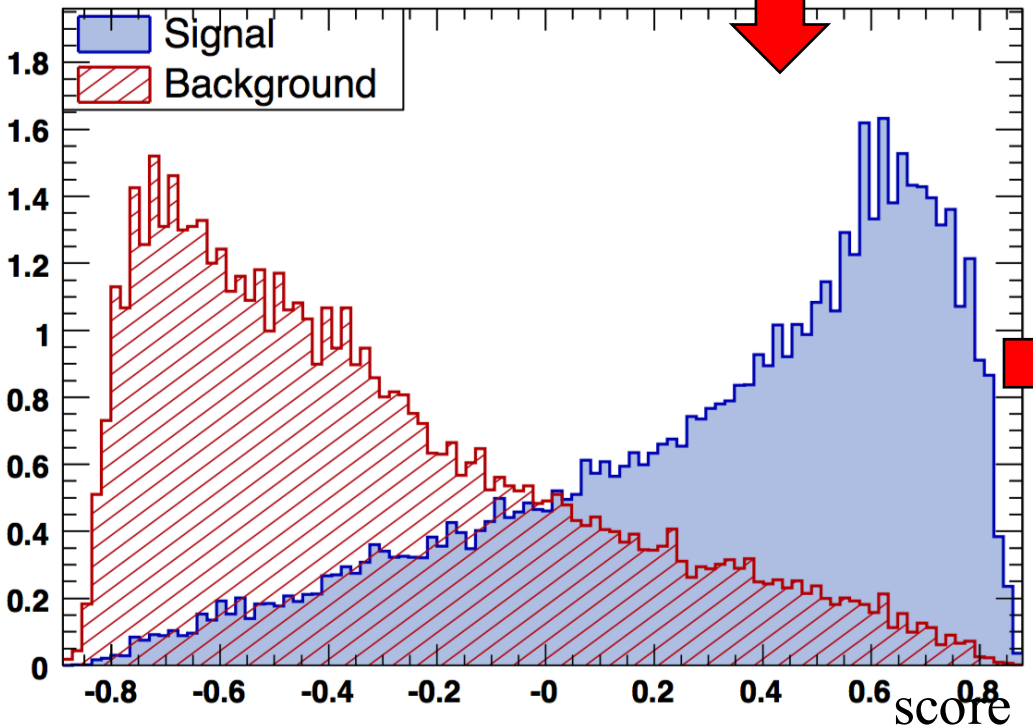
See also "Machine Learning in High Energy Physics Community White Paper" on arXiv 1807.02876 today but no pretension to mirror it here

# Classifier basics

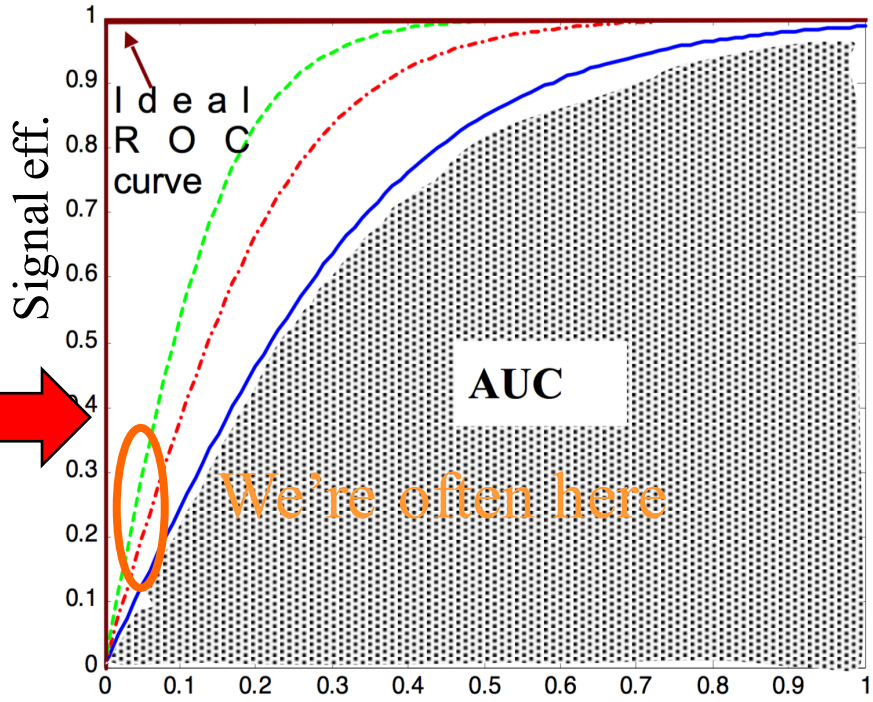



Train on Signal and Background Monte-Carlo
➔learn the separation between S and B distribution
Apply on test sample
Apply on data

Note: instead of *classifiying* 0 or 1, can *regress* !



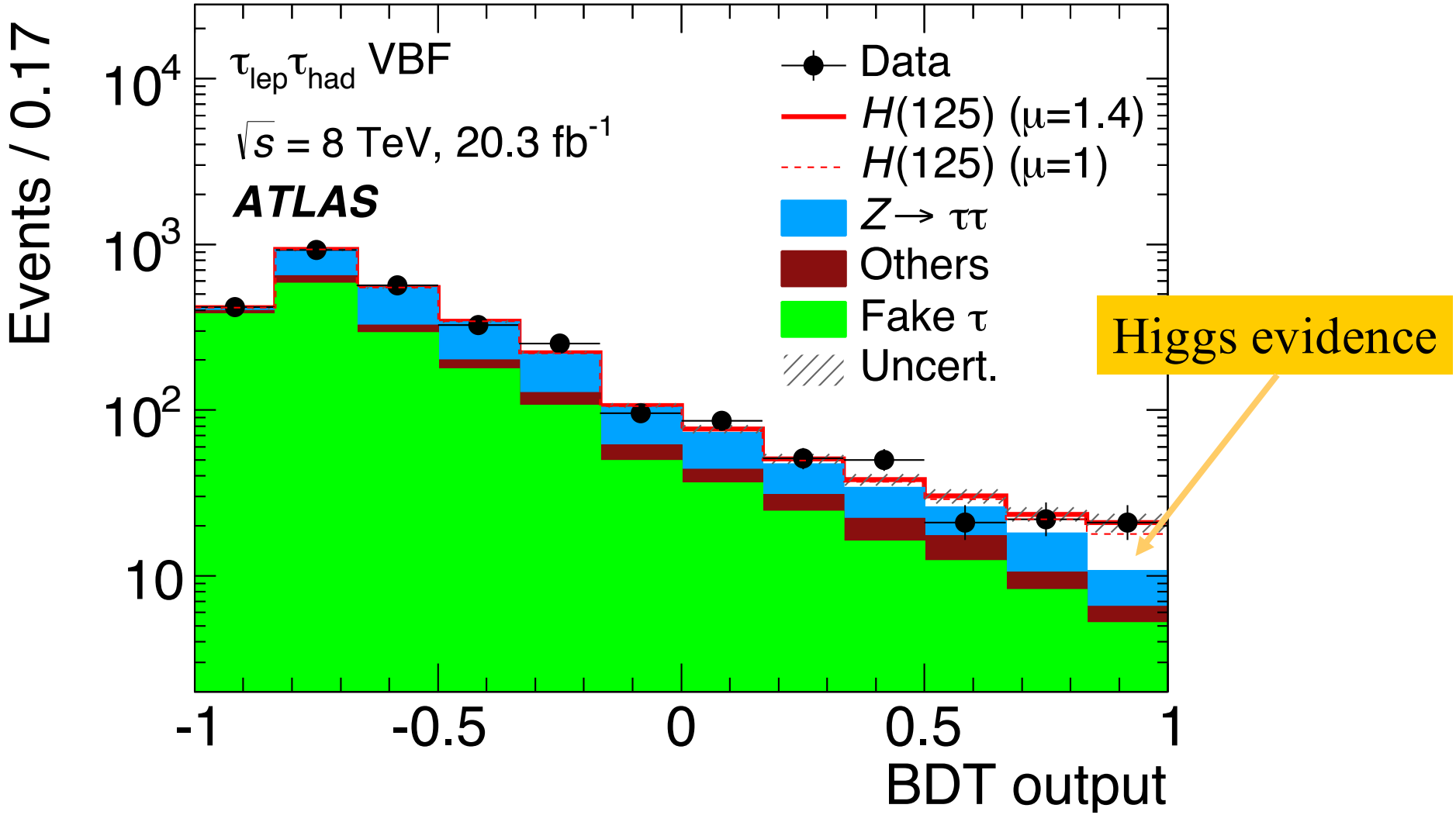

AUC : Area Under the (ROC) Curve



# Classifier (2)

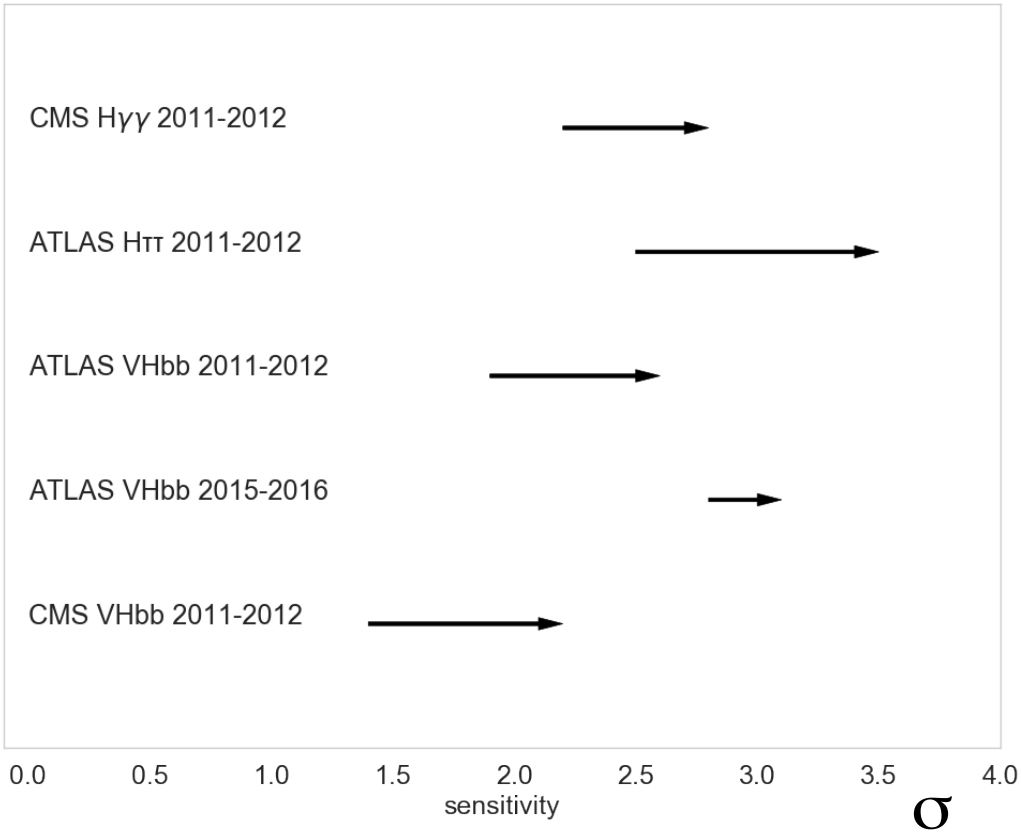
JHEP 04, 117 (2015) 1501.04943

Boosted Decision Tree (BDT) using ~dozen of high level variables



# ML on Higgs Physics

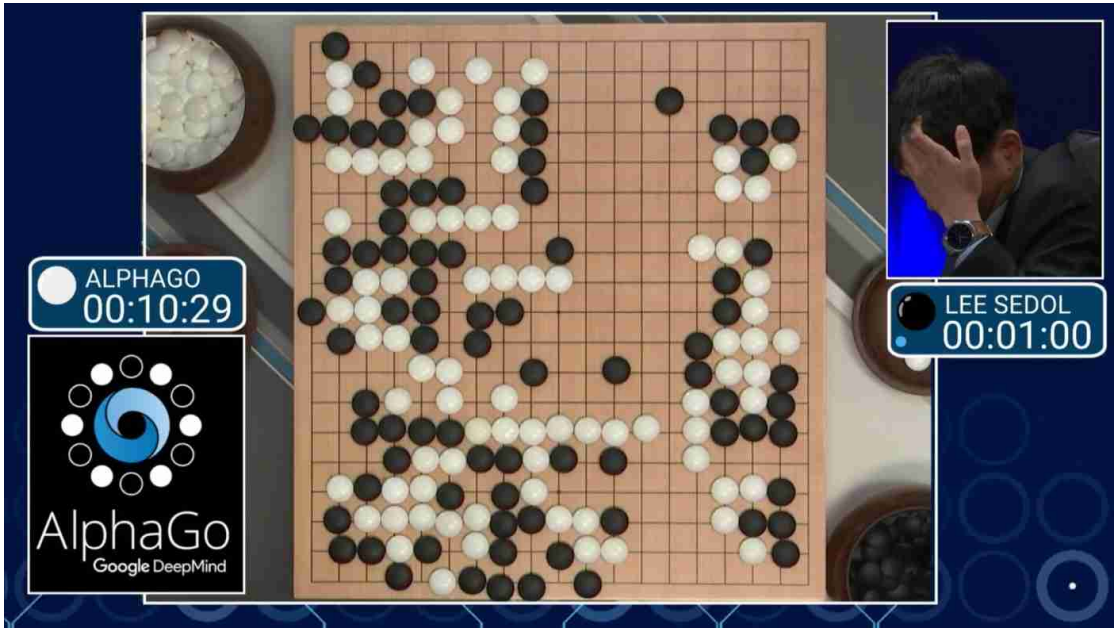
- At LHC, Machine Learning used almost since first data taking (2010) for reconstruction and analysis
- In most cases, Boosted Decision Tree with Root-TMVA, on ~10 variables
- For example, impact on Higgs boson expected sensitivity at LHC:




➔~50% gain on LHC running

# ML in HEP

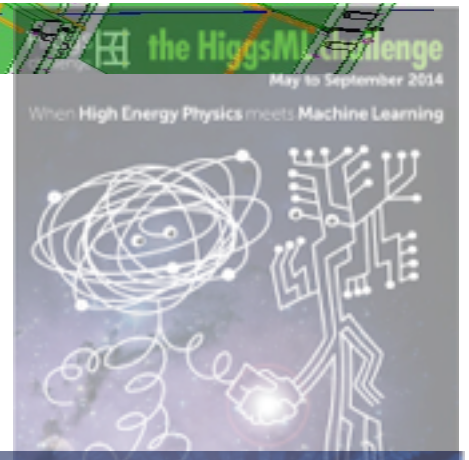
- Meanwhile, in the outside world :



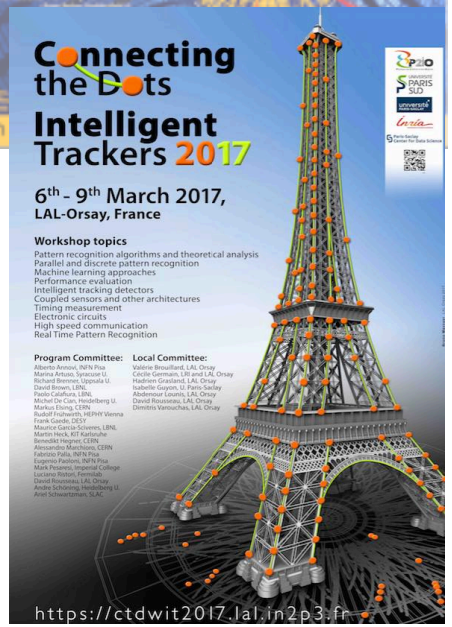

- "Artificial Intelligence" not a dirty word anymore!
- We (in HEP) have realised we're been left behind! Trying to catch up now…

# Multitude of HEP-ML events

- HiggsML Challenge, summer 2014
  - ➔HEP ML NIPS satellite workshop, December 2014
- Connecting The Dots, Berkeley, January 2015
- Flavour of Physics Challenge, summer 2015
  - ➔HEP ML NIPS satellite workshop, December 2015
- DS@LHC workshop, 9-13 November 2015
- Moscou/Dubna ML workshop 7-9th Dec 2015
- Heavy Flavour Data Mining workshop, 18-21 Feb 2016
- Connecting The Dots, Vienna, 22-24 February 2016
- Hep Software Foundation workshop 2-4 May 2016 at Orsay, ML session
- Connecting The Dots, LAL-Orsay, 6-9 March 2017
- LHC Interexperiment Machine Learning group
  - IML workshop @CERN 20-22 March 2017, 9-12 April 2018
- DS@HEP workshop @FNAL 8-12 May 2017
- Hammers and Nails, Weizmann, Jul 2017
- ACAT conference Seattle, Sep 2017
- Connecting The Dots, 20-22 March 2018
- CHEP, July 2018 (ML now acknowledged in Track name)
- Tracking ML challenge, summer 2018
- ACAT conference, Saas Fe, March 2019

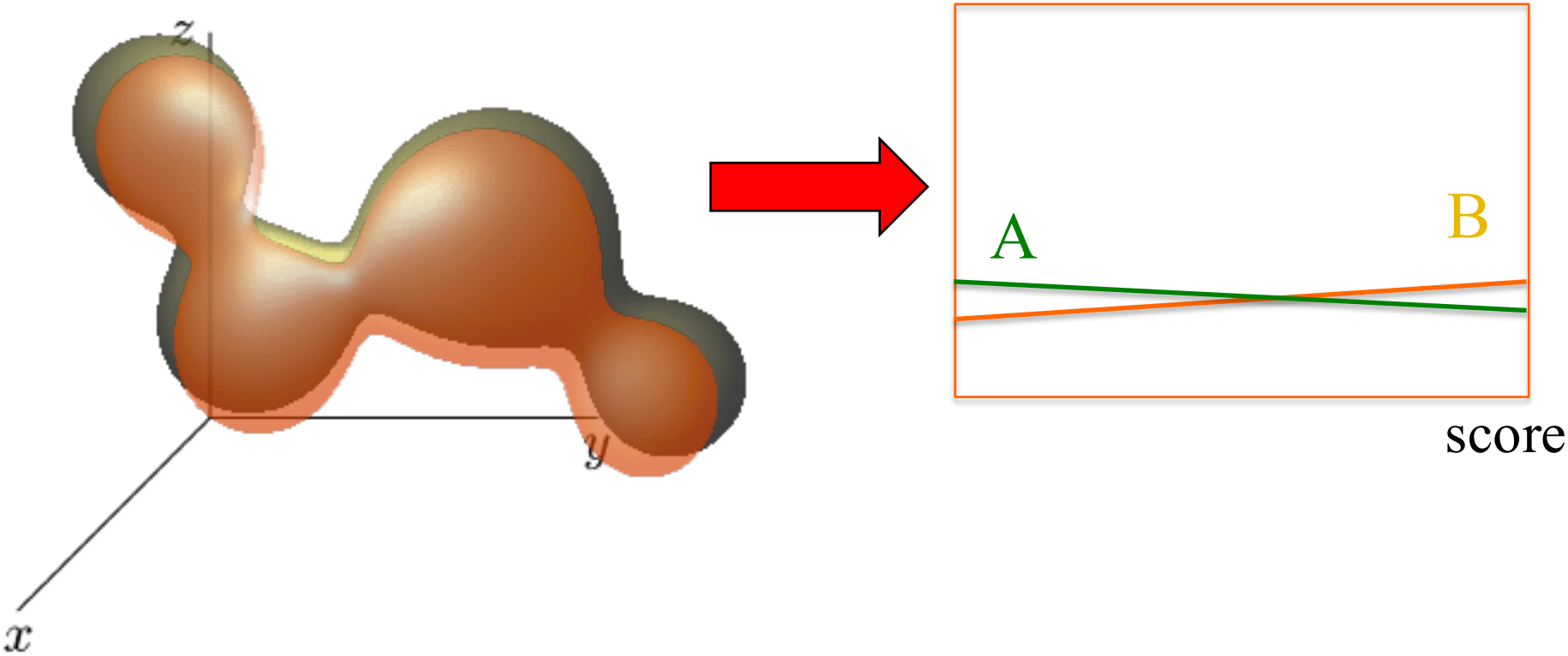






# ML Basics

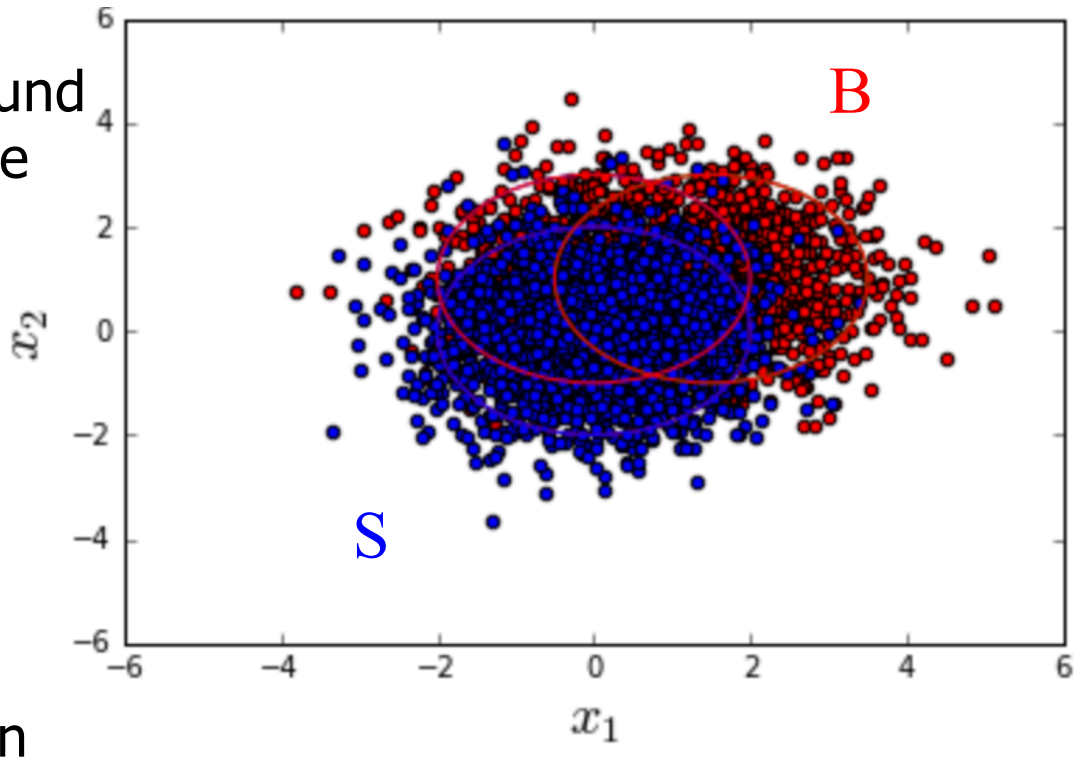
# What does a classifier do?




- The classifier "compresses" the two multidimensional "blobs" maximising the difference, without (ideally) any loss of information

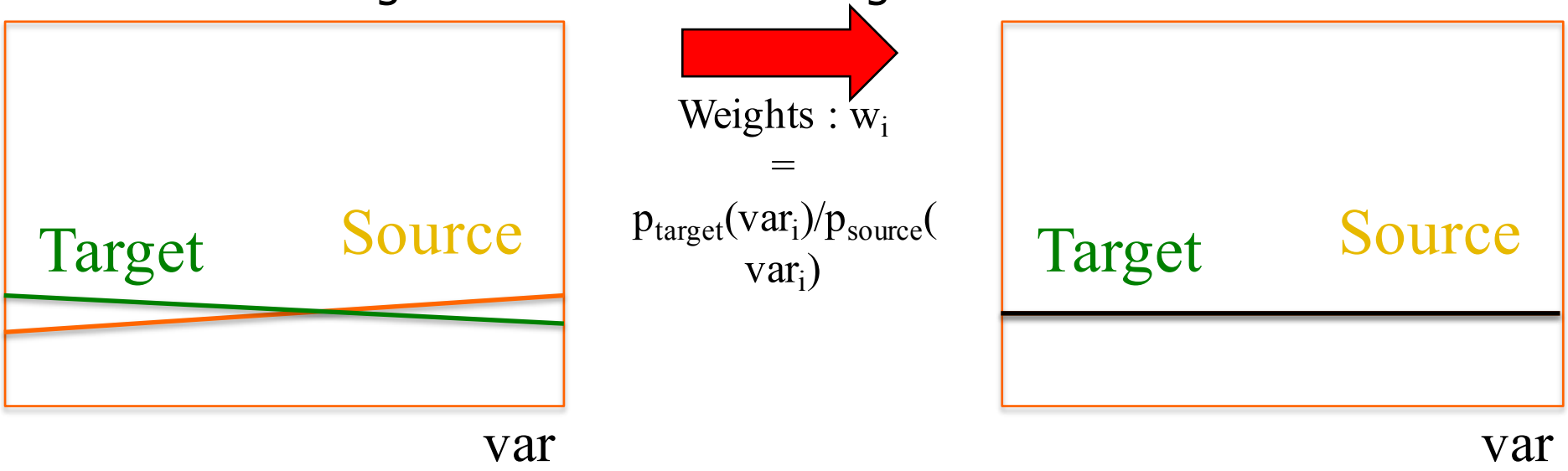
# No miracle

- ML (nor Artificial Intelligence) does not do any miracles
- For selecting Signal vs Background and underlying distributions are known, nothing beats ihihood ratio! (often called "Bayesian limit"):
  - $L_S(x)/L_B(x)$
- OK but quite often $L_S$ $L_B$ are unknown
  - + x is n-dimensional
- ML starts to be interesting when there is no proper formalism of the pdf
- ➔mixed approach, if you know something, tell your classifier instead of letting it guess



# Re-weighting

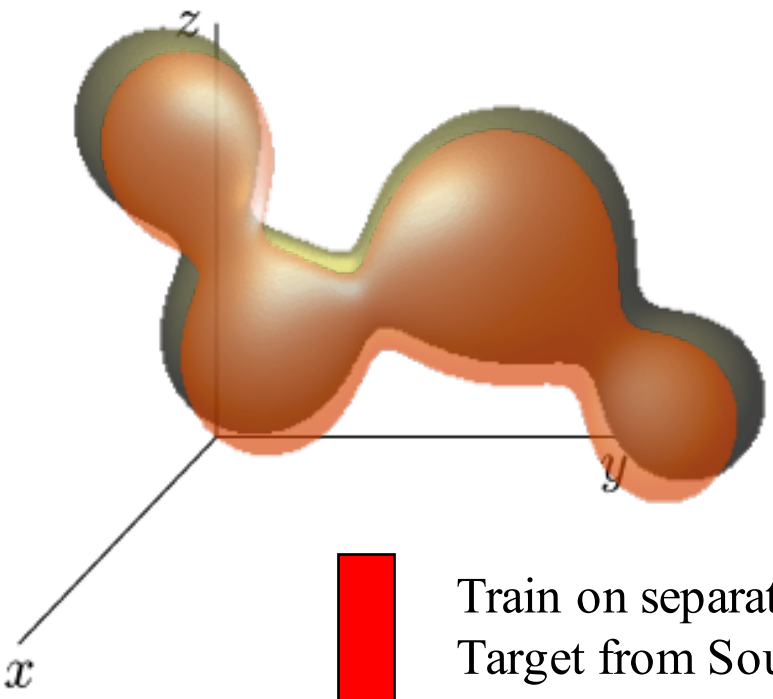
- Suppose a variable distribution is slightly different between a Source (e.g. Monte Carlo) and a Target (e.g. real data)
  - ➔reweight!  …then use reweighted events



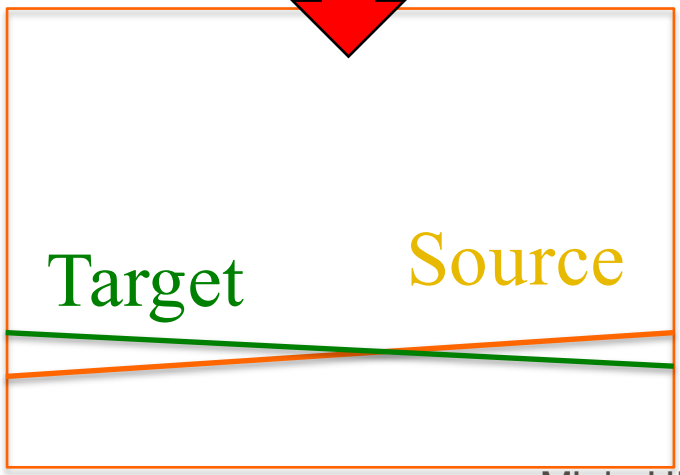

- What if multi-dimension ?
- Usually : reweight separately on 1D projections, at best 2D, because of quick lack of statistics
- Can we do better ?

# Multidimension reweighting

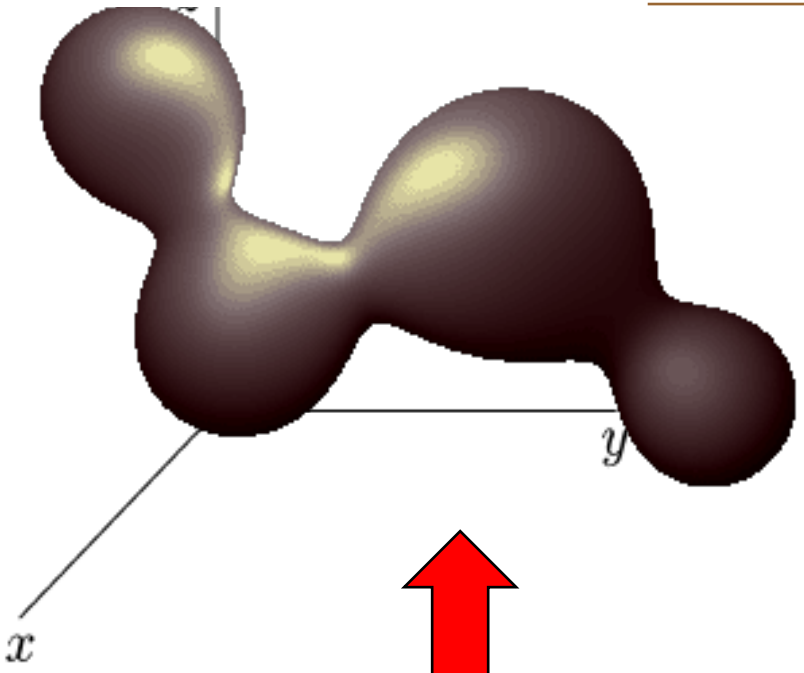
See demo on Andrei Rogozhnikov github and also Kyle Cranmer's github Related : uBoost

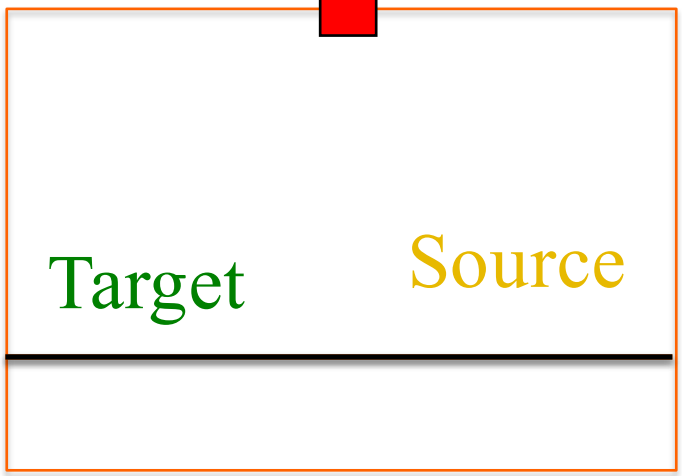



Train on separating
Target from Source




Weights : $w_i$
=
$P_{target}(score_i)/p_{source}(score_i)$



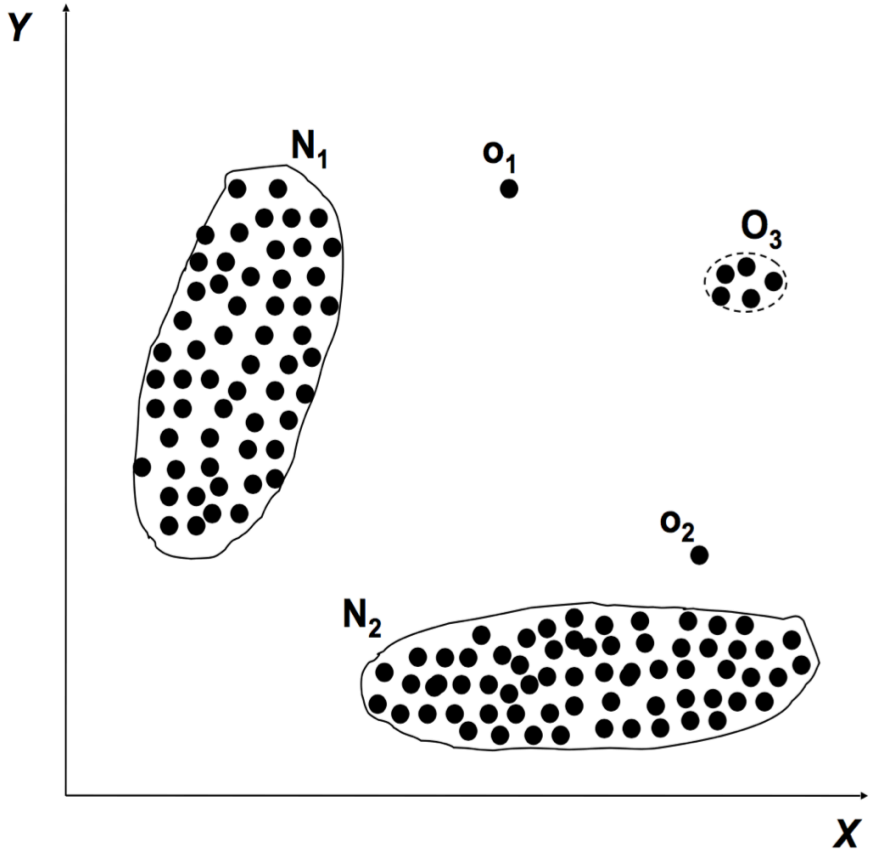



# Multi dimensional reweighting (2)

- Reweighting the Source distribution on the score allows multidimensional reweighting without statistics problem
- Usual caveat still hold : Target support should be included in Source support, distributions should not be too different otherwise unmanageable very large or very small weights
- (Note : "reweighting" in HEP language <==> "importance sampling" in ML language)
- Only use (that I know off) in published analyses in LHCb
- Why ?

# Anomaly detection

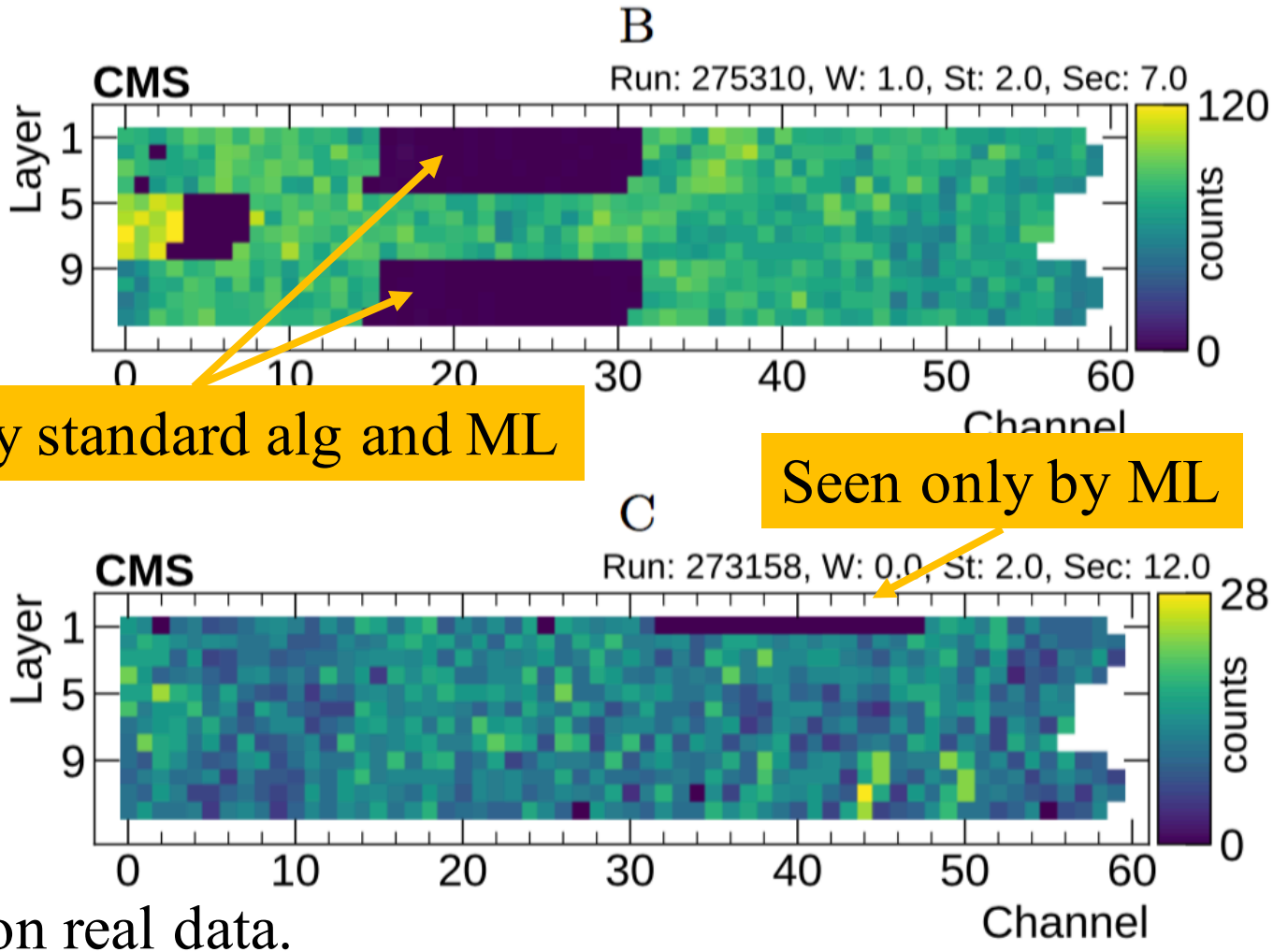
- Also called outlier detection
- Three approaches:
  - Unsupervised : give the full data, ask the algorithm to cluster the bulk N1 N2 and find the lone entries : o1, o2, O3
  - Semi-supervised : train the algorithm on the bulk N1 N2, and find the lone entries o1 O2 O3
  - Supervised : train algorithm on the bulk and possible model of outliers



# Anomaly : DQM application

Adrian Alan Pol, this conference

- Example application CMS muon chamber monitoring (with Convolutional Neural Net)

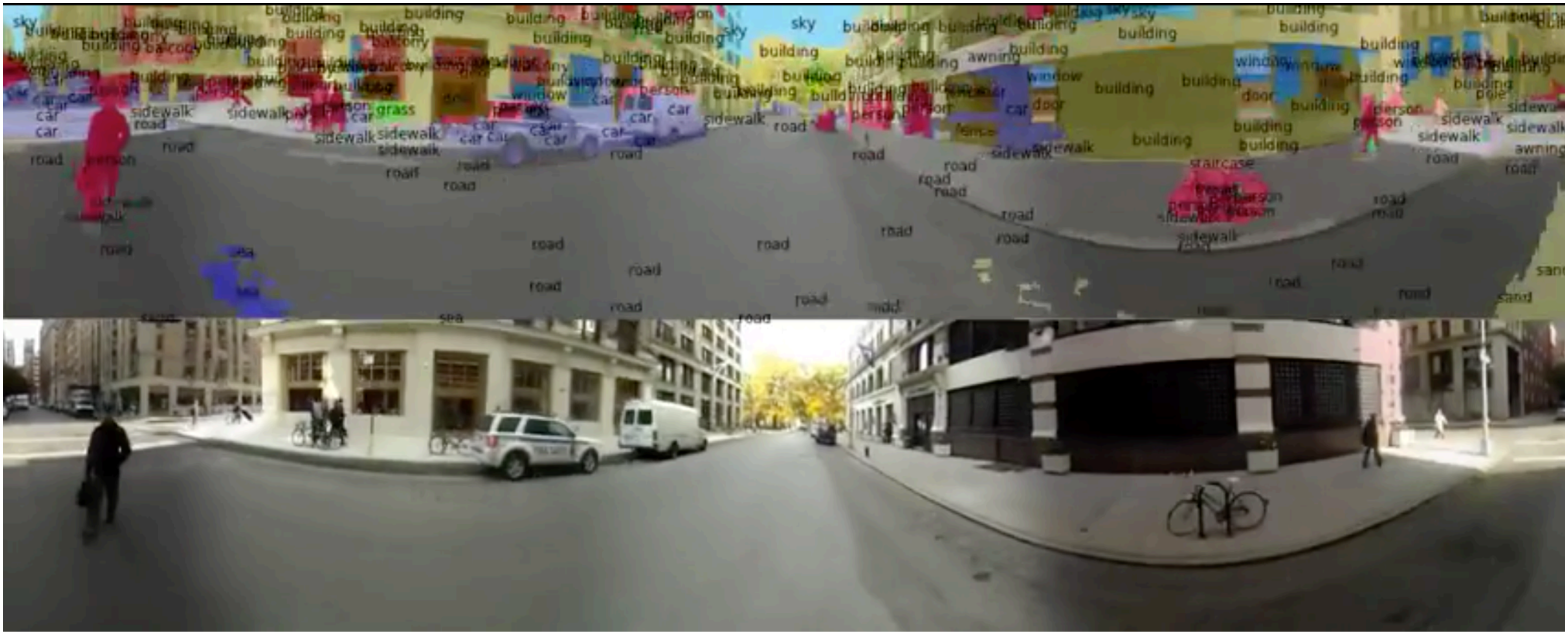



Demo on real data.

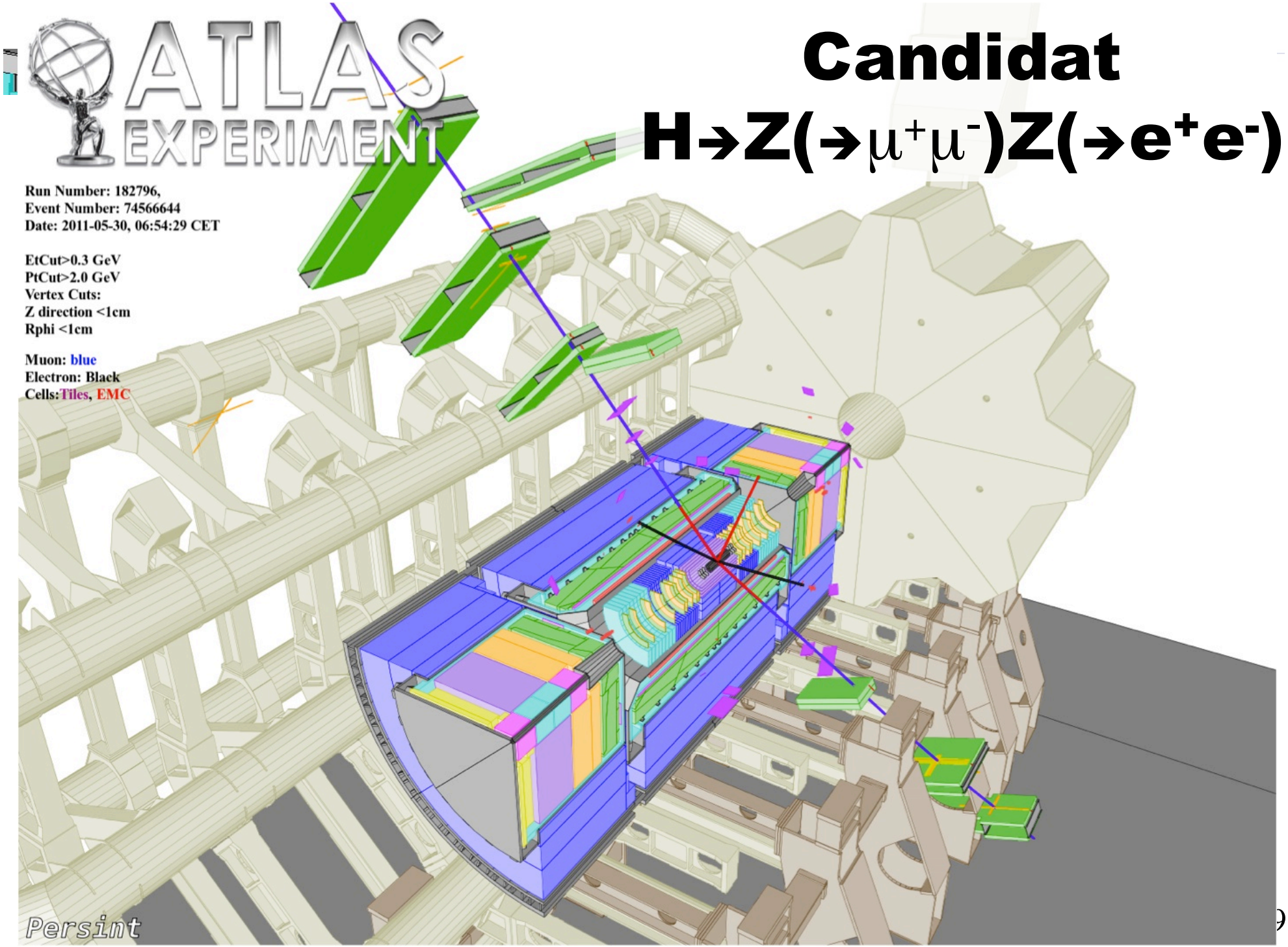
# Anomaly detection for physics

# ML in analysis

# Typical Deep Learning application

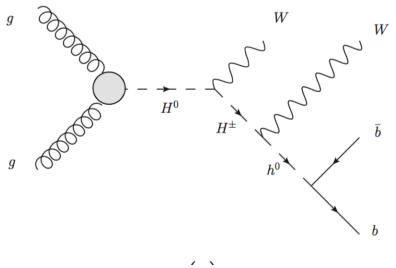


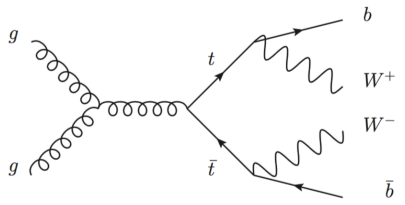
# Candidat
# $H \to Z(\to \mu^+\mu^-)Z(\to e^+e^-)$

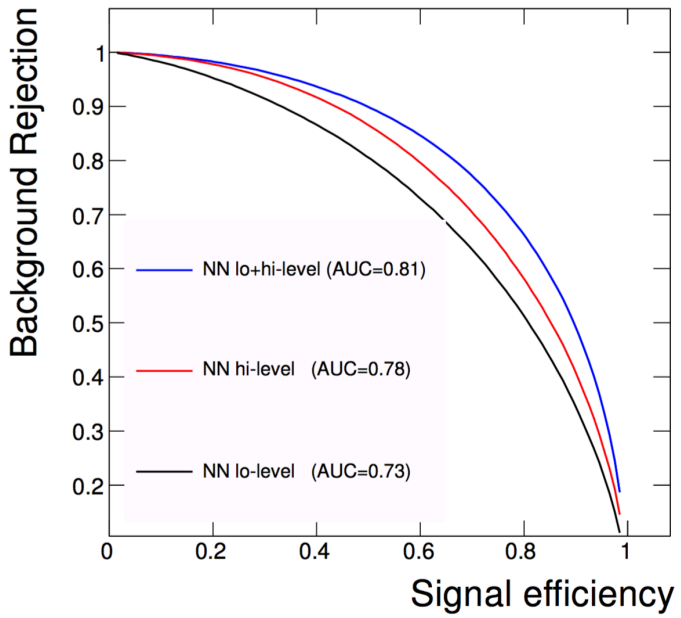


# Deep learning for analysis

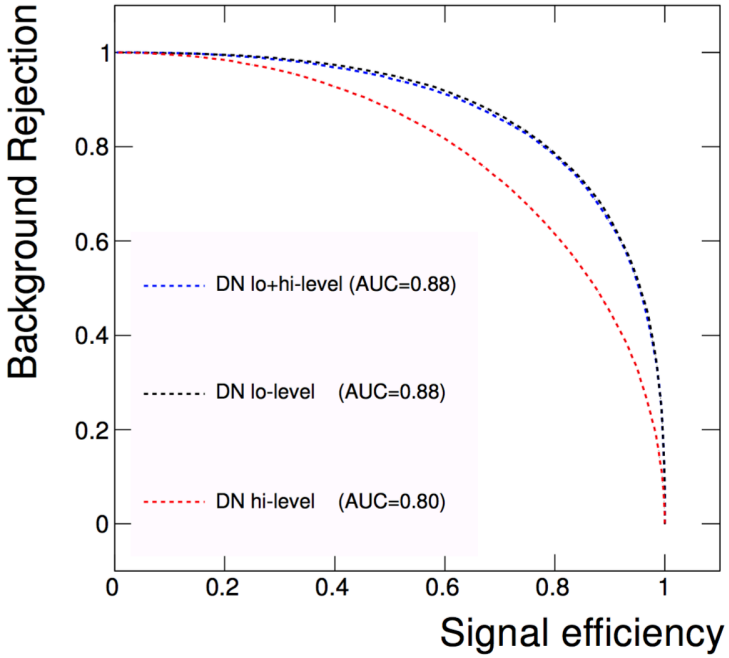
1402.4735 Baldi, Sadowski, Whiteson



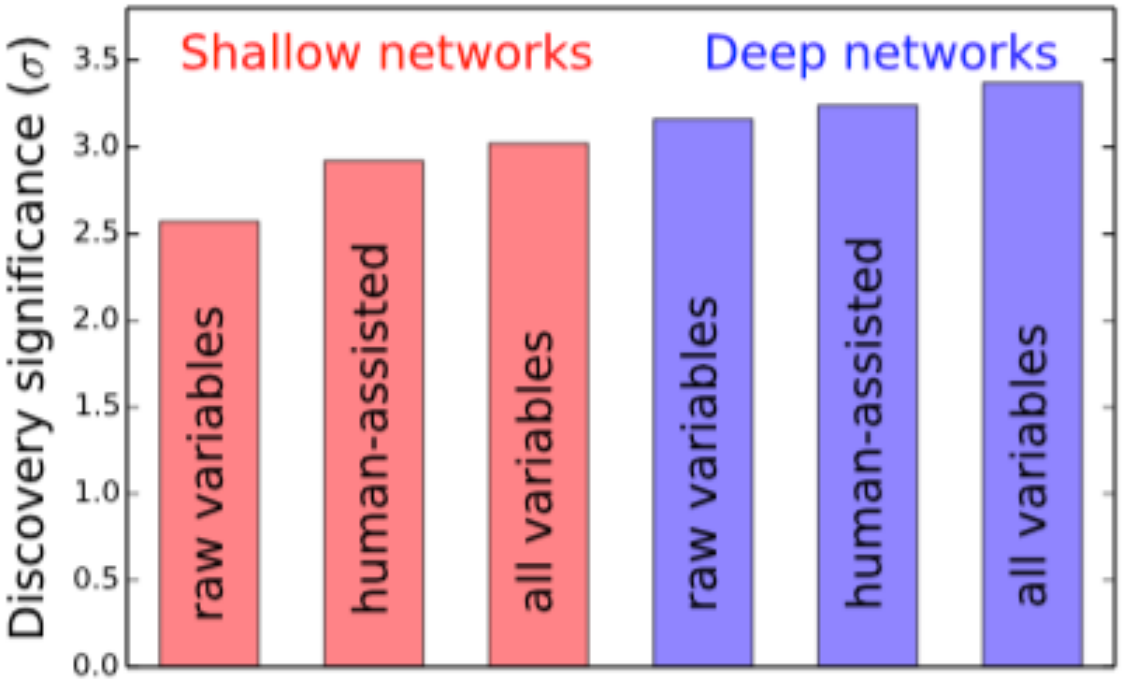

- MSSM at LHC : $H^0$➔WWbb vs tt➔WWbb
- Low level variables:
  - 4-momentum vector
- High level variables:
  - Pair-wise invariant masses
- Deep NN outperforms NN, and does not need high level variables
- DNN learns the physics ?



# 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 improved on NN but still needed high level features
- Both analyses with Delphes fast simulation
- ~100M events used for training (>>100* full G4 simulation in ATLAS)

# DL for analysis (3)

- No published LHC analyses using DL (CMS 2018 ttH « DNN » just two layers)
- Recent trend is to feed more (up to 20) variables to classifiers, even low level ones (2/3-vectors of particles) (see recent ATLAS/CMS ttH papers)
- A few NN in top and Higgs physics paper but no clear advantage wrt BDT
  - XGBoost (de facto BDT standard in ML) starts to be used
- Not completely clear why no DL

# Systematics-aware training

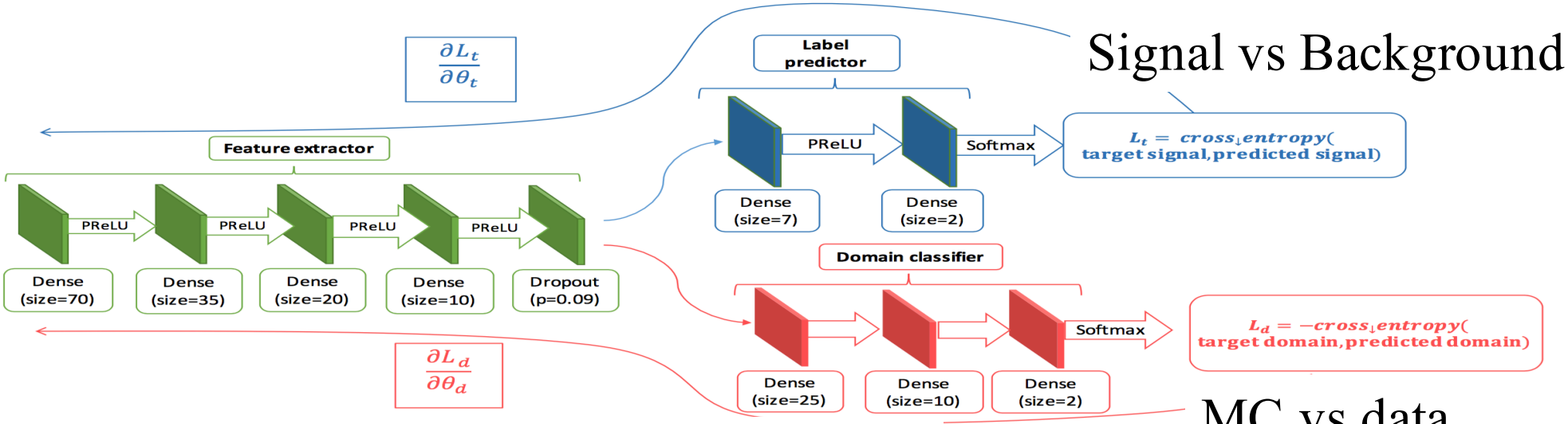
See Victor Estrade's, this conference

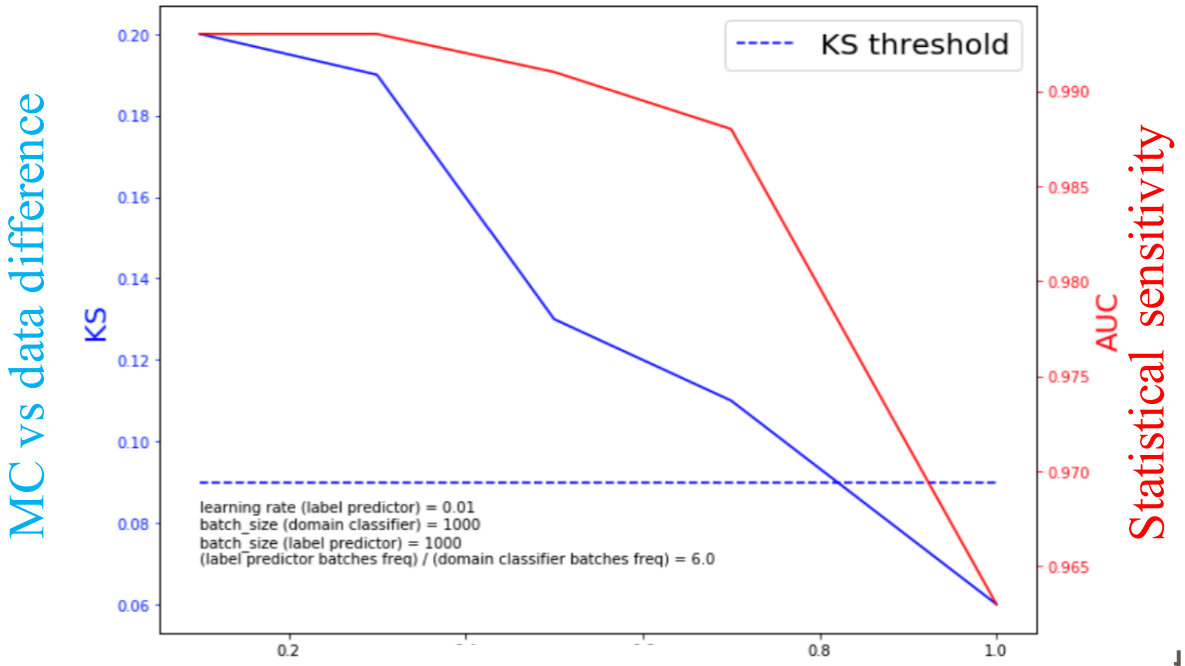
- Our experimental measurement papers typically ends with
  - measurement = m ± σ(stat) ± σ(syst)
  - σ(syst) systematic uncertainty : known unknowns, unknown unknowns…
- Name of the game is to minimize quadratic sum of :

  σ(stat) ±σ(syst)
- ML techniques used so far to minimise σ(stat)
- Impact of ML on σ(syst) or even better global optimisation of σ(stat) ± σ(syst) is an open problem
- Worrying about σ(syst) untypical of ML in industry
- 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

# Syst Aware Training: adversarial

- Inspired from 1505.07818 Ganin et al : ACAT 2017 Ryzhikov and Ustyuzhanin




Tuning parameter

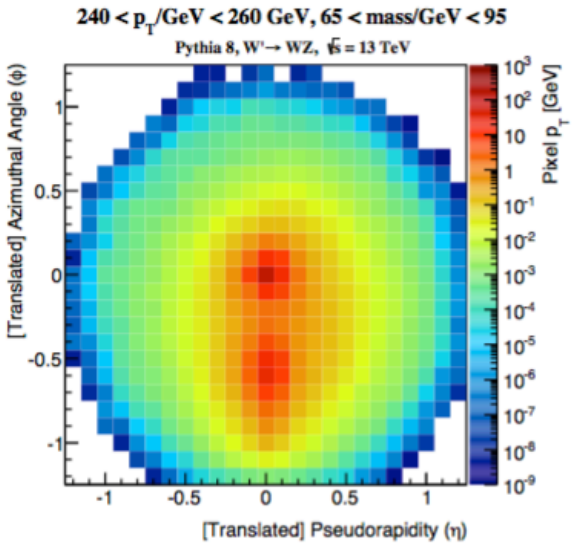
# ML in reconstruction

# Jet Images

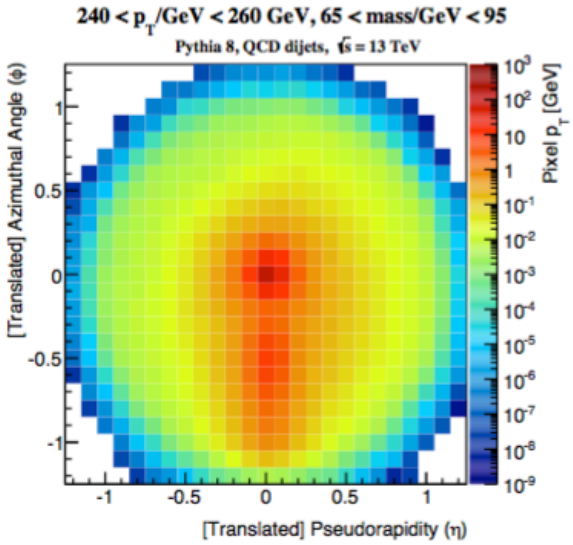
arXiv 1511.05190 de Oliveira, Kagan, Mackey, Nachman, Schwartzman

- Distinguish boosted W jets from QCD
- Particle level simulation
- Average images:

Boosted W➔qq jet

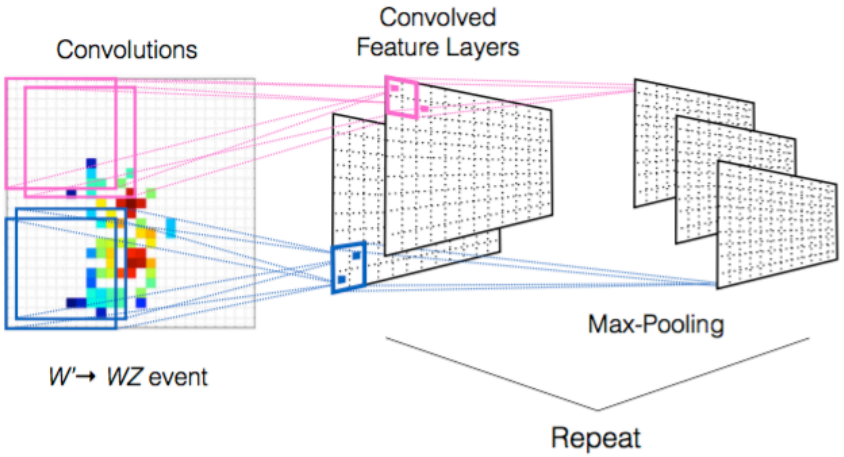


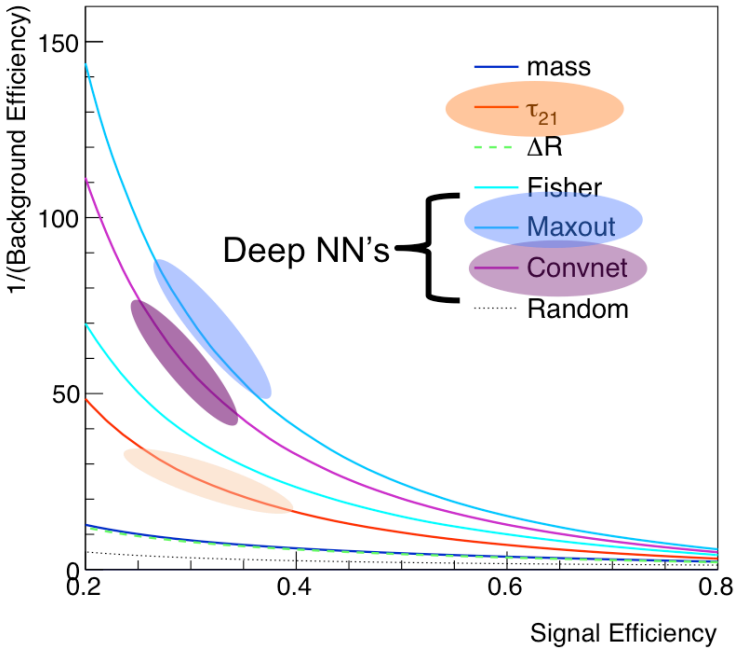

QCD



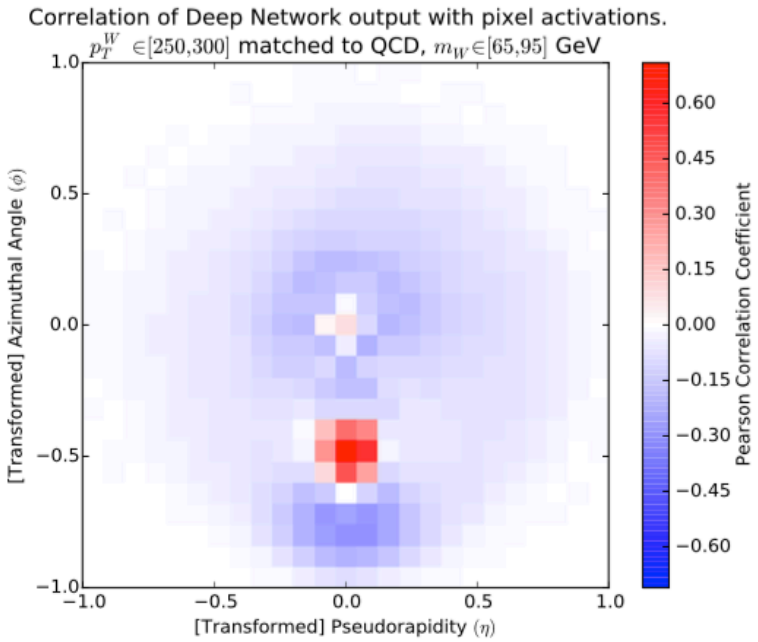
# Jet Images : Convolution NN

arXiv:1511.05190

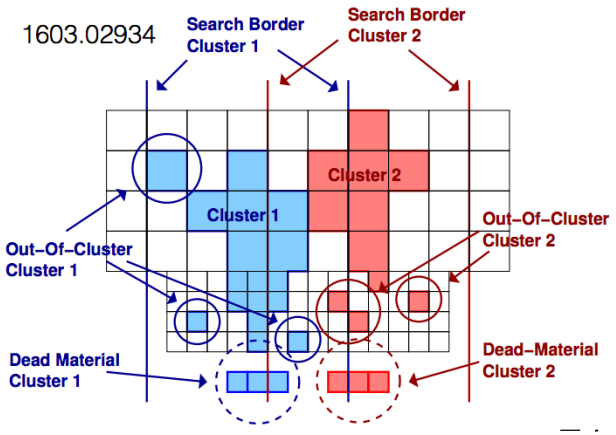



- Variables build from CNN outperform the more usual ones



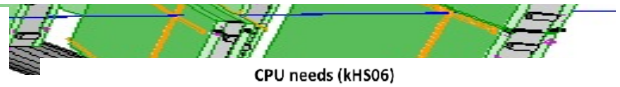

- What the CNN sees (the "cat" neurone")
- Now need proper detector and pileup simulation ATL-PHYS-PUB-2017-017
- ➔3Dimension ?



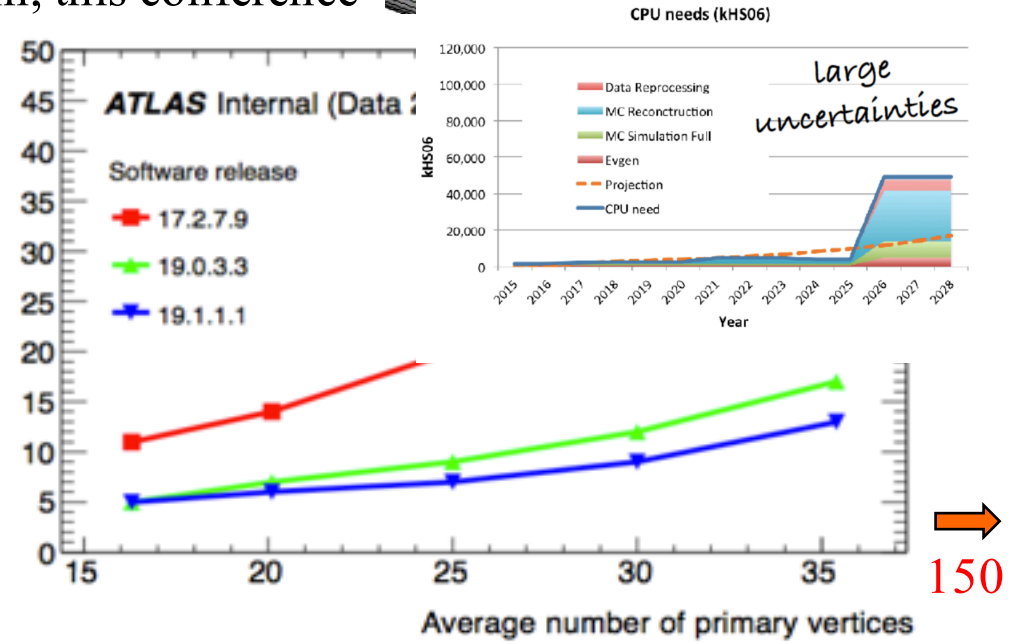

, David Rousseau, CHEP 2018,

# Tracking competition

See Moritz Kiehn, this conference



- Tracking (in particular pattern recognition) dominates reconstruction CPU time at LHC
- HL-LHC (phase 2) perspective : increased pileup :Run 1 (2012): <>~20, Run 2 (2015): <>~30,Phase 2 (2025): <>~150
- CPU time quadratic/exponential extrapolation (difficult to quote any number)
- Large effort within HEP to optimise software and tackle micro and macro parallelism. Sufficient gains for Run 2 but still a long way for HL-LHC.
- >20 years of LHC tracking development. Everything has been tried?
  - Maybe yes, but maybe algorithm slower at low lumi but with a better scaling have been dismissed ?
  - Maybe no, brand new ideas from ML (i.e. Convolutional NN)
- ➔Tracking challenge launched 1st May 2018
- 125 events x ( 10'000 tracks / 100'000 points)
- Follow us on twitter @trackmllhc !

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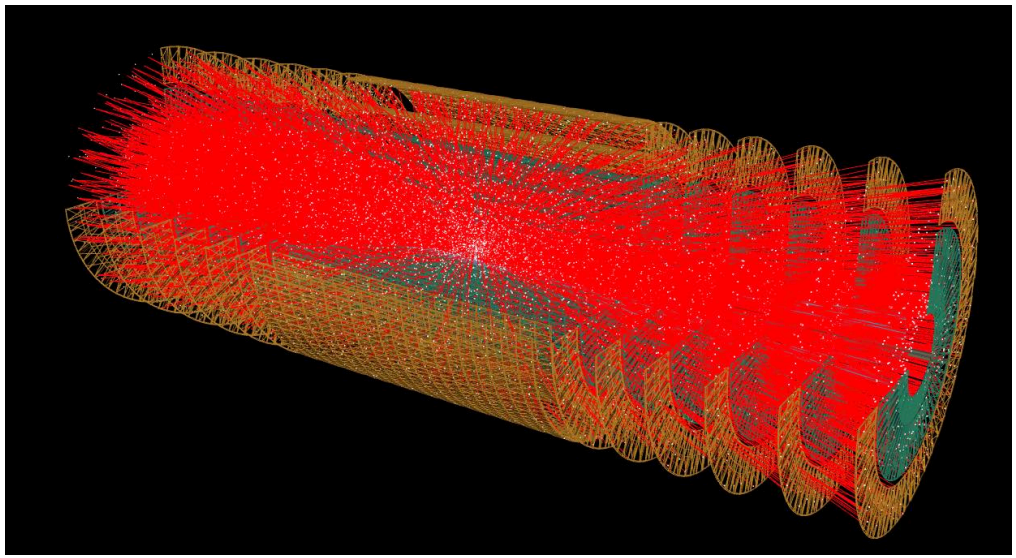
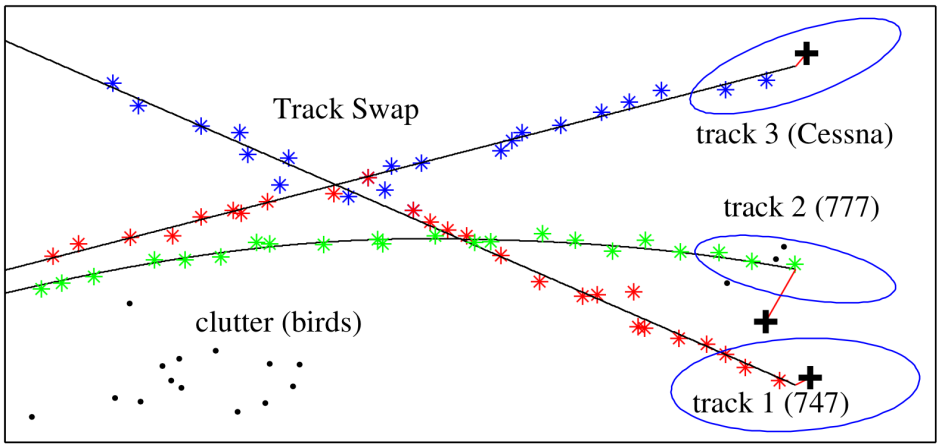
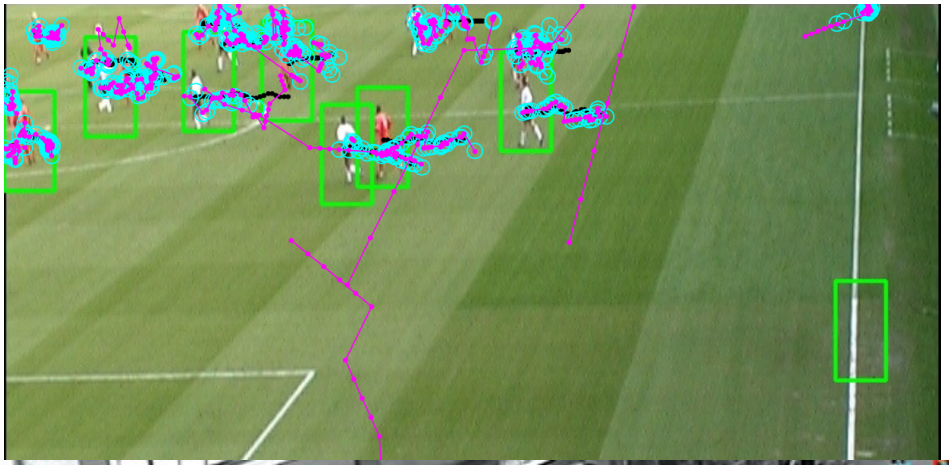
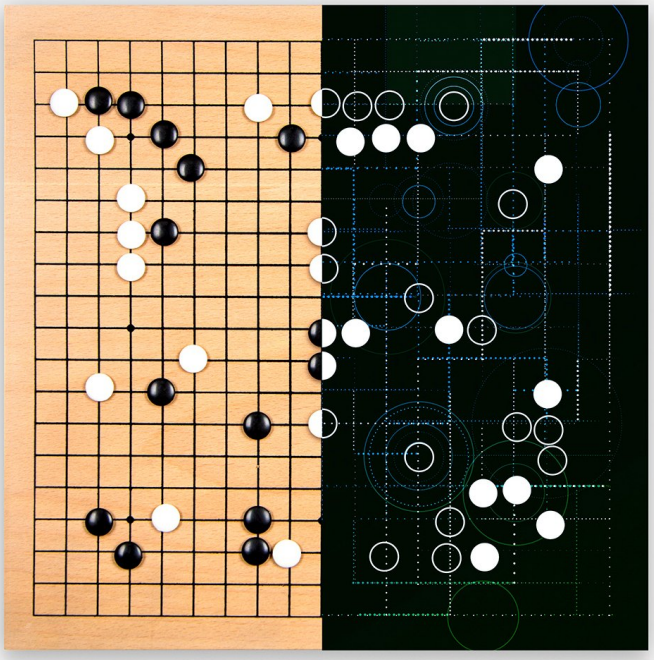


# Pattern Recognition/Tracking

- Pattern recognition/tracking is a very old, very hot topic in Artificial Intelligence, but very varied
- Note that these are real-time applications, with CPU constraints





# Aparté on ML in HEP history

Computer Physics Communications 49 (1988) 429–448
North-Holland, Amsterdam

## NEURAL NETWORKS AND CELLULAR AUTOMATA IN EXPERIMENTAL HIGH ENERGY PHYSICS

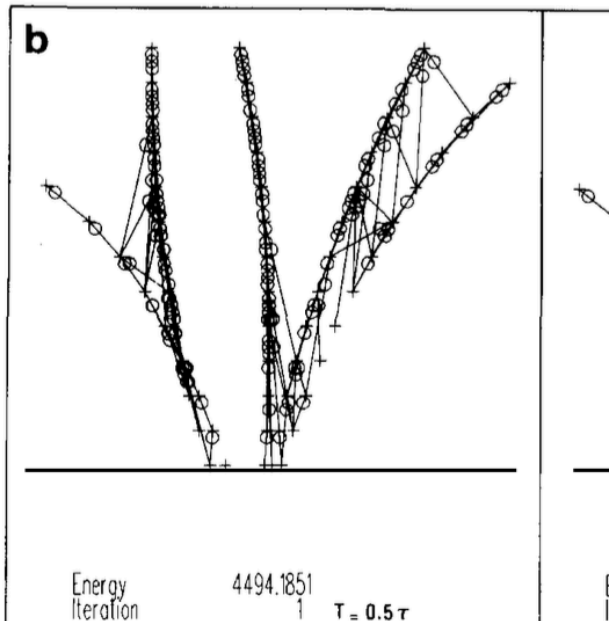
B. DENBY

*Laboratoire de l'Accélérateur Linéaire, Orsay, France*

Received 20 September 1987; in revised form 28 December 1987

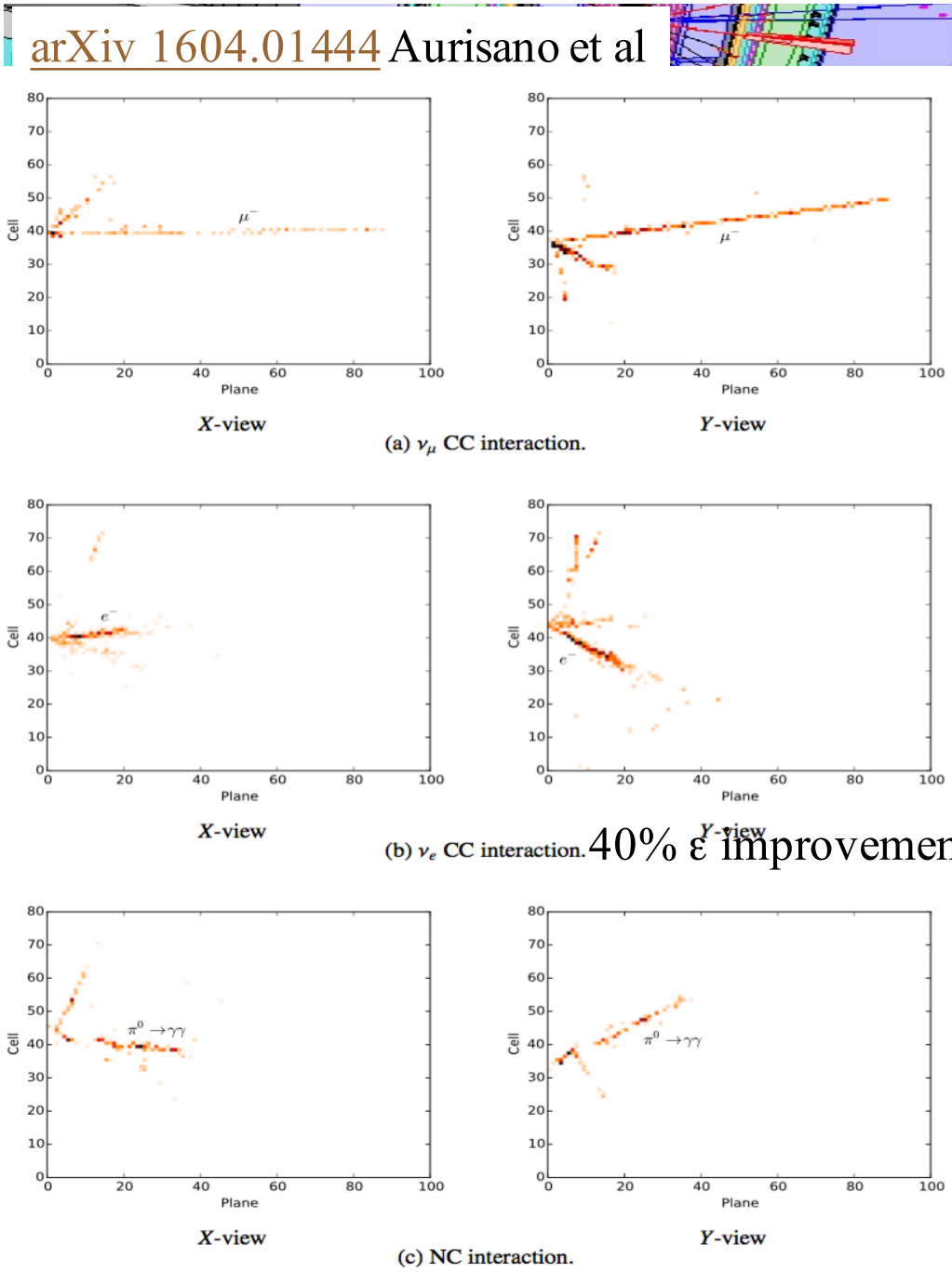
Bruce Denby

- 1987 Very first Neural Net in HEP paper known
- NN for tracking and calo clustering
- B. Denby then moved from Delphi at LEP to CDF at Tevatron. He still active outside HEP: 2017 analysis of ultrasonic image of the tongue
- 1992 JetNet Carsten Peterson, Thorsteinn Rognvaldsson (Lund U.) , Leif Lonnblad (CERN) (~500 citations) really started NN use in HEP



# A recent success with ν : NOVA

arXiv 1604.01444 Aurisano et al




40% ε improvement

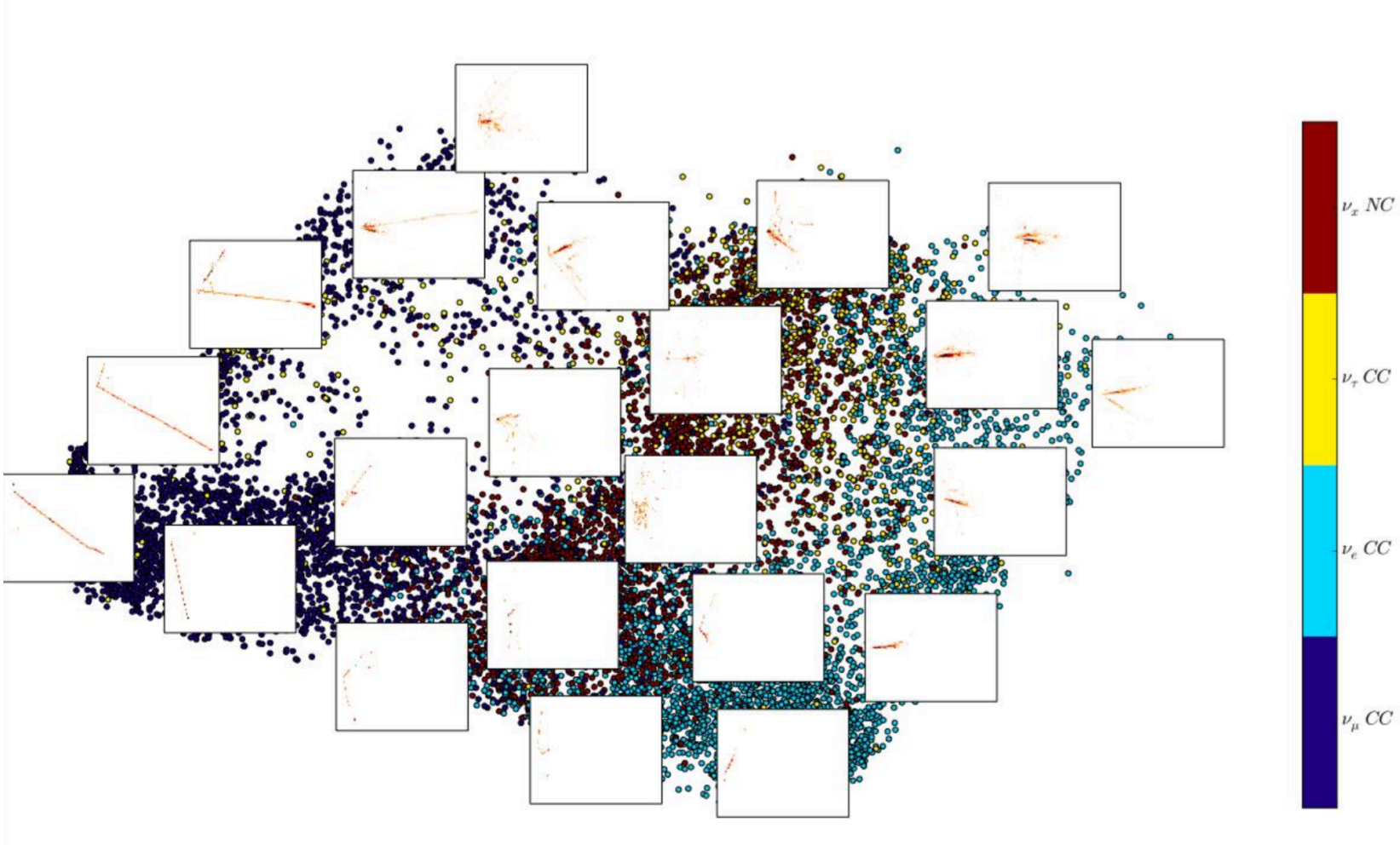
Neutrino interaction classification
Using Convolutionnal Neural Network (GoogleNet)

**Actually used in physics results 1703.03328 and 1706.04592**

# Aparté on t-SNE

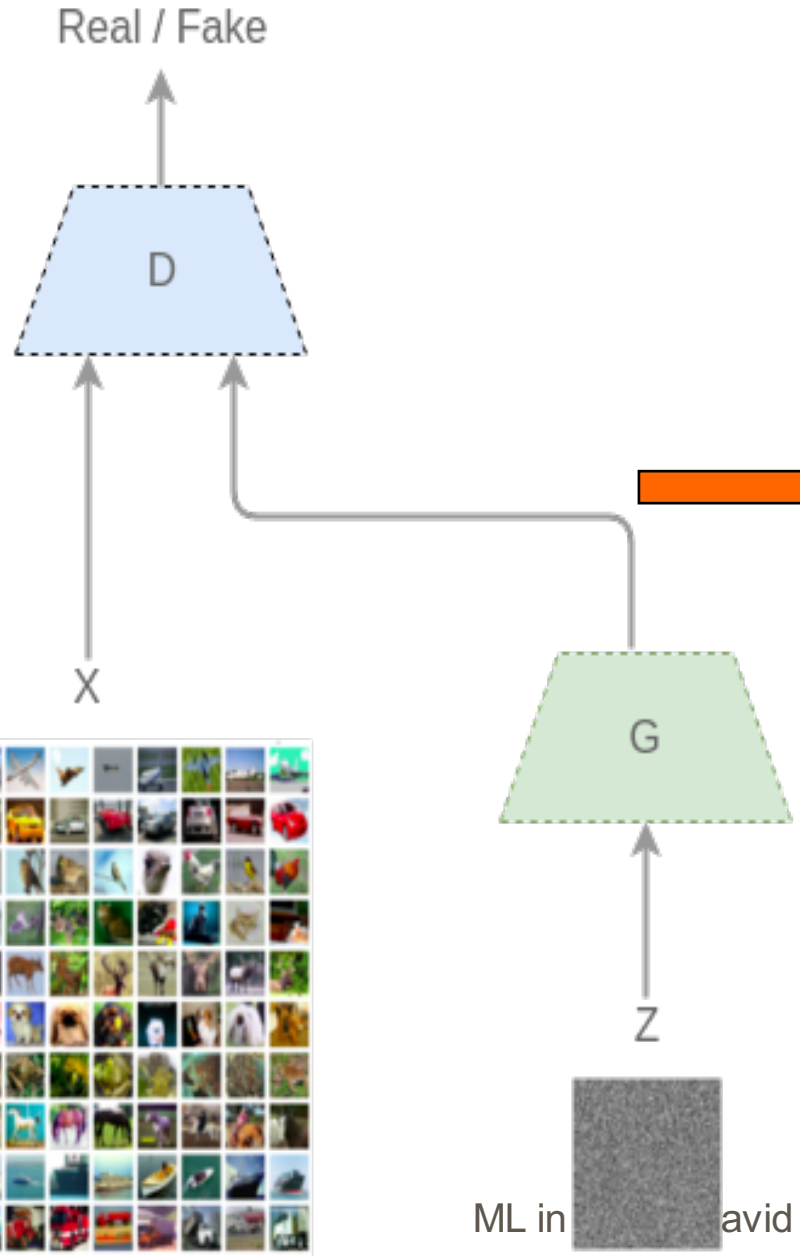
van der Maaten and Hinton. JMLR 9 2008

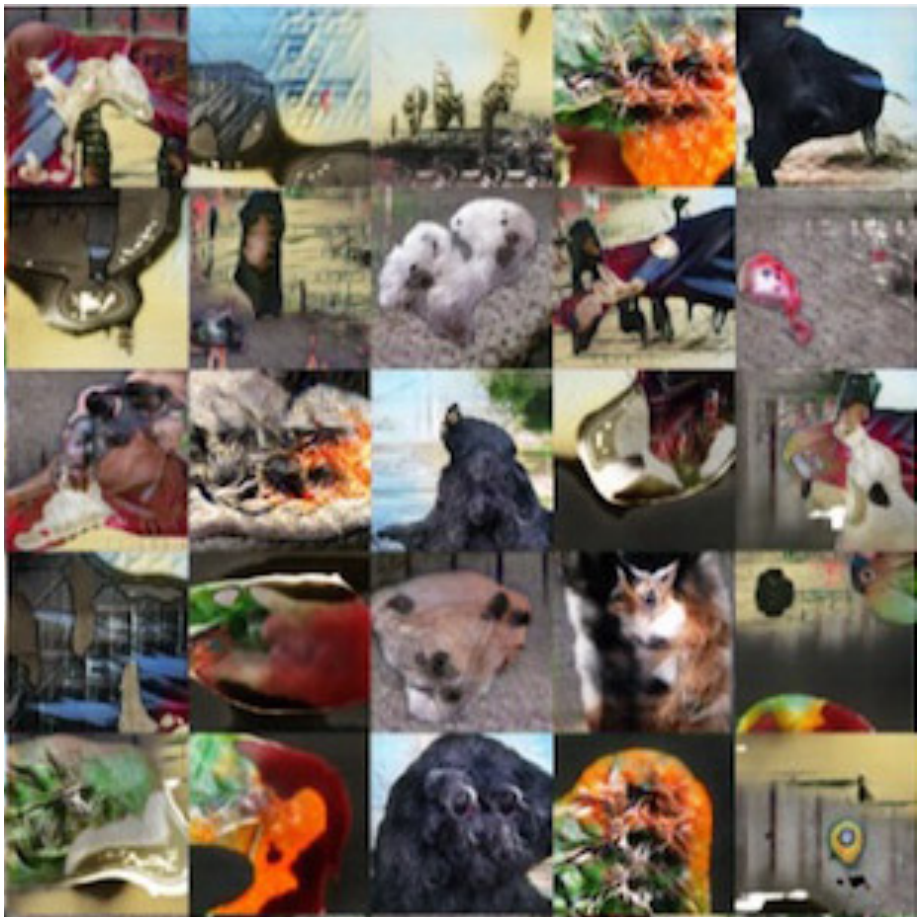
- Non-linear dimensionality compression, very popular in ML, unknown (almost) in HEP, except NOVA:



# ML in simulation

# Generative Adversarial Network



# Condition GAN

Text to image

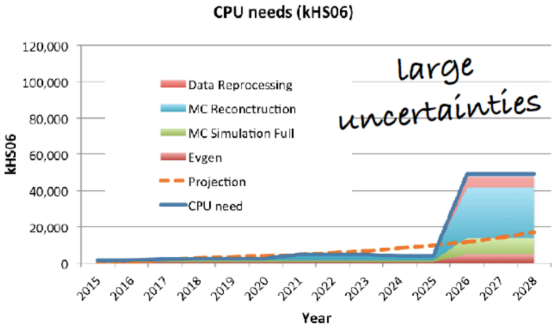
this small bird has a pink breast and crown, and black primaries and secondaries.

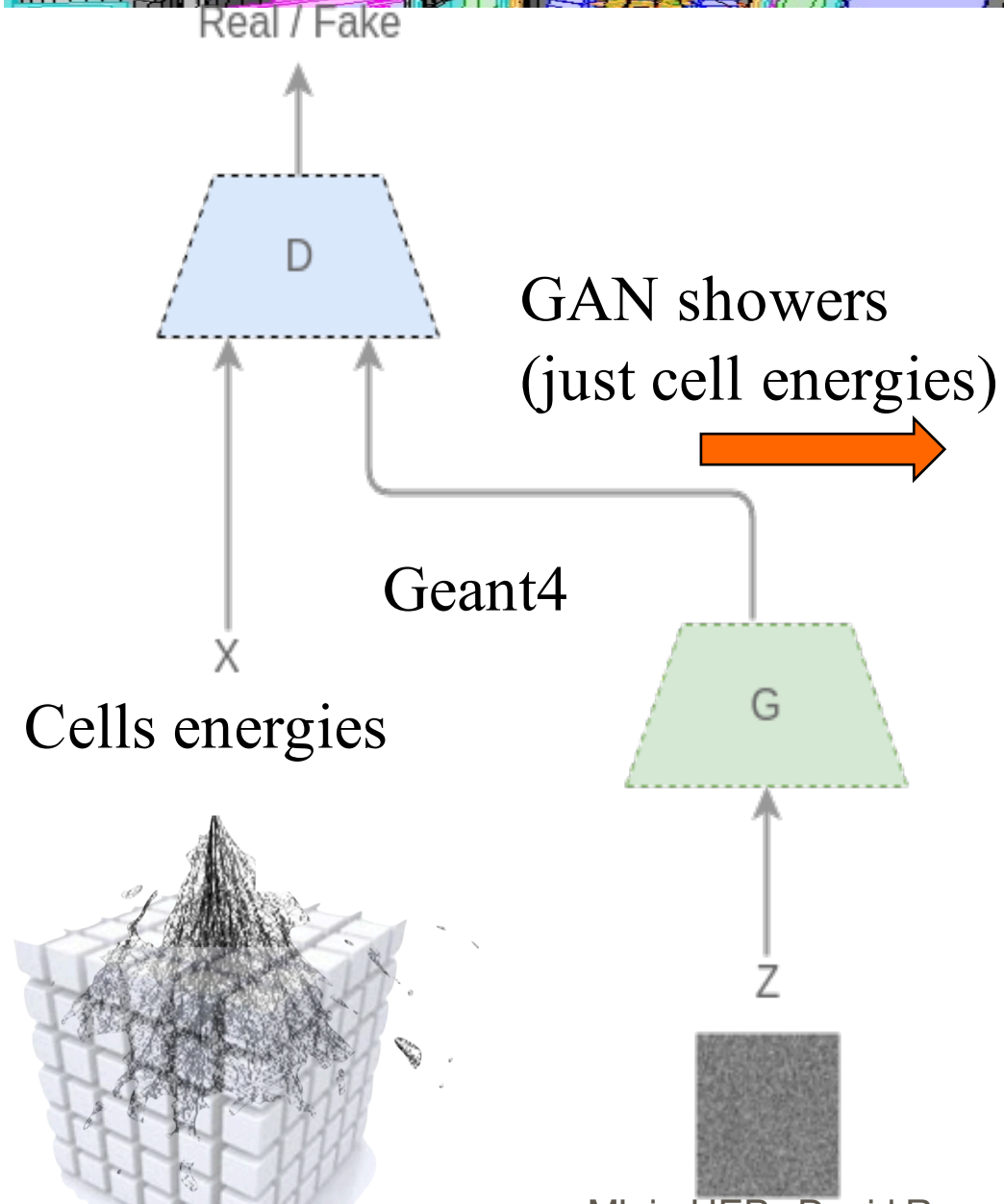
this magnificent fellow is almost all black with a red crest, and white cheek patch.

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

# GAN for simulation (1)

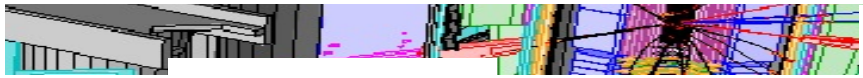


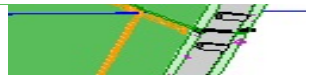

- Half of LHC grid computers (~300.000 cores) are crunching Geant4 simulation 24/24 365/365
- …while LHC experiments are collecting more and more events
- ➔reducing CPU consumption of simulation is very important

- Imagine training a GAN on single particle showers of all types and energies
- Then when an event is simulated it would ask for GAN showers on request (superfast by 3-4 order of magnitude)
- Would replace current fast simulation, frozen shower libraries….
- If/when it works, would require large GPU clusters

# GAN for simulation (2)

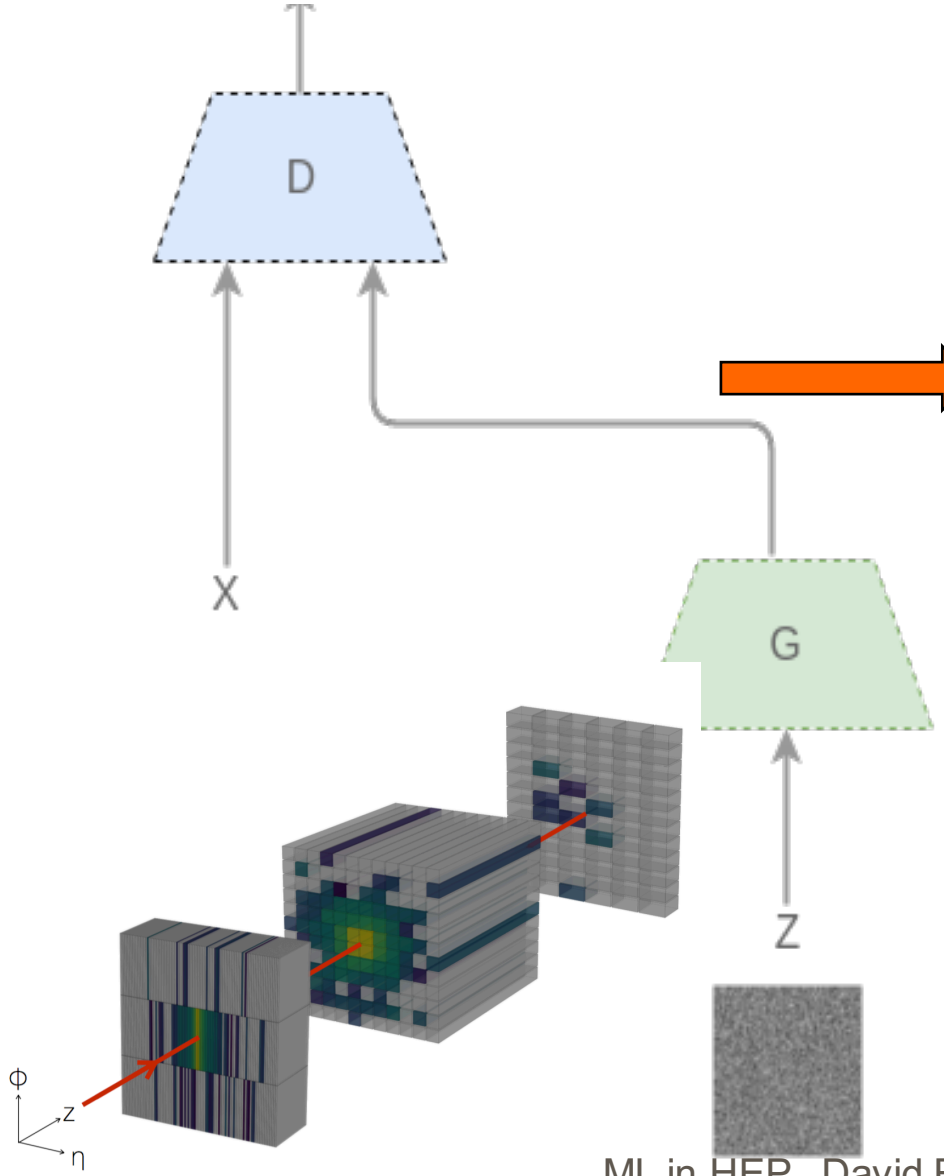


Chekalina, Vallecorsa, this conference

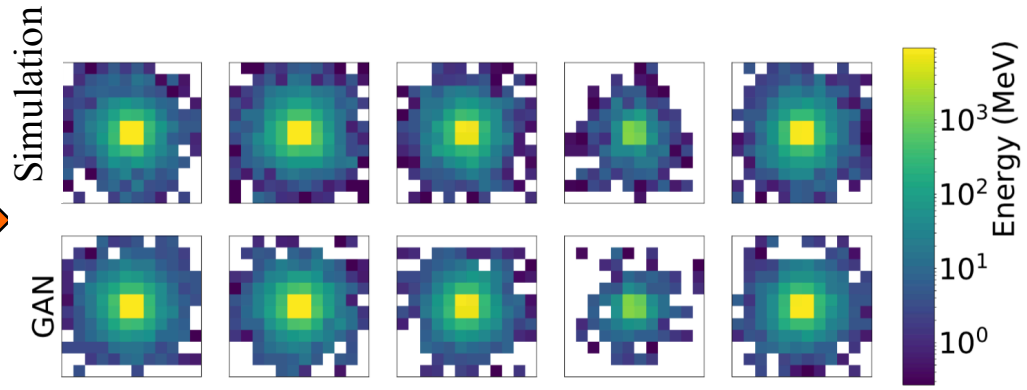


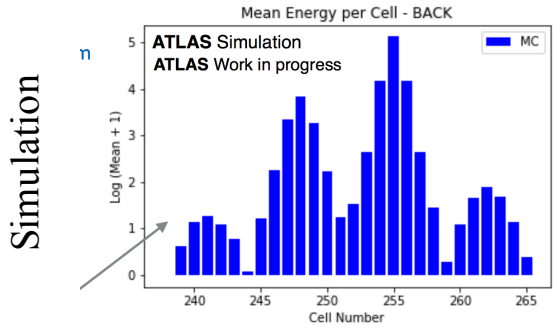
True/False

Paganini et al 1705.02355.

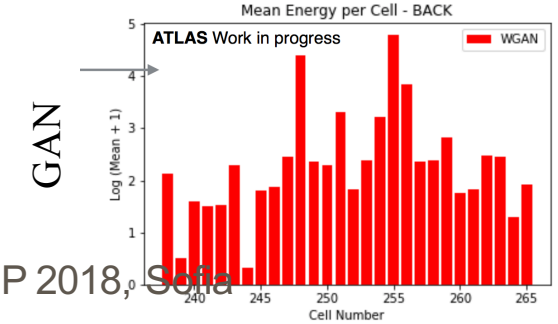



Computing speed-up single shower x1000




Simulation

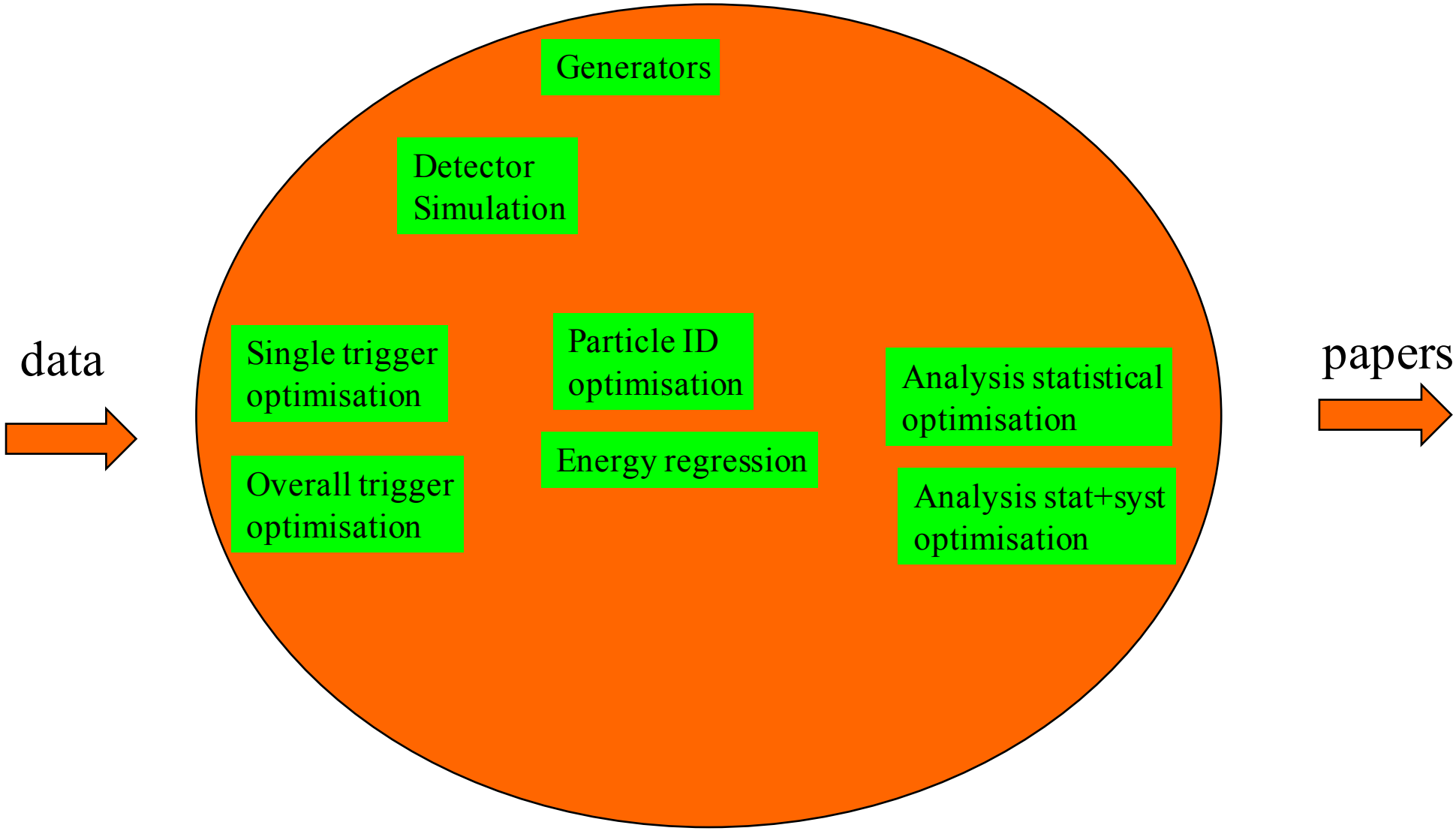



GAN

Still lot of work to have this work in production

# Wrapping-up

# ML playground



# ML Collaborations

- Many of the new ML techniques are complex➔difficult for HEP physicists alone
- ML scientists (often) eager to collaborate with HEP physicists
  - prestige
  - new and interesting problems (which they can publish in ML proceedings)
- Takes time to learn common language
- Access to experiment internal data an issue, but there are ways out➔more and more Open Dataset
- Very useful/essential to build HEP - ML collaborations : study on shared dataset, thesis (Computer Science or HEP)
- There is always a friendly Machine Learner on a campus!

# Open Data

Simko this conference

- Public dataset are essential to collaborate (beyond talking over beer/coffee) on new ML techniques with ML experts (or even physicists in other experiments)
  - can share without experiments Non Disclosure policies
- Some collaborations built on just generator data (e.g. Pythia) or with simple detector simulation e.g. Delphes
  - good for a start, but inaccurate
- Effort to have better open simulation engine (e.g. Delphes 4-vector detector simulation, ACTS for tracking)
- UCI dataset repository has some HEP datasets
- Role of CERN Open Data portal, need be more and more pupulated

# Conclusion (1)

- We (in HEP) are analysing data from multi-billion € projects➔should make the most out of it!
- Recent explosion of novel (for HEP) ML techniques, novel applications for Analysis, Reconstruction, Simulation, Trigger, and Computing
- Some of these are ~easy, most are complex: open source software tools are ~easy to get, but still need (people) training, know-how
- Sometimes contradictory results
- Never underestimate the time for :
  - (1) Great ML idea➔
  - (2) …demonstrated on toy dataset➔
  - (3) …demonstrated on semi-realistic simulation ➔
  - (4) …demonstrated on real experiment analysis/dataset ➔
  - (5) …experiment publication using the great idea

# (2) Faster ML to production

- Training of HEP students post-docs
  - ... and senior scientists
- Campus-level sustained HEP ML collaborations
  - … not just workshops or challenges
- Public datasets
  - …not just toys but also real experimental ones
- Release software with papers
  - …matching "reproducibility" movement in ML
- Computing resources
  - …although (not yet) the limiting factor