Advances in Machine Learning in High Energy Physics Deep Learning, GAN and more

David Rousseau

LAL-Orsay

rousseau@lal.in2p3.fr

CEA/DRF seminar

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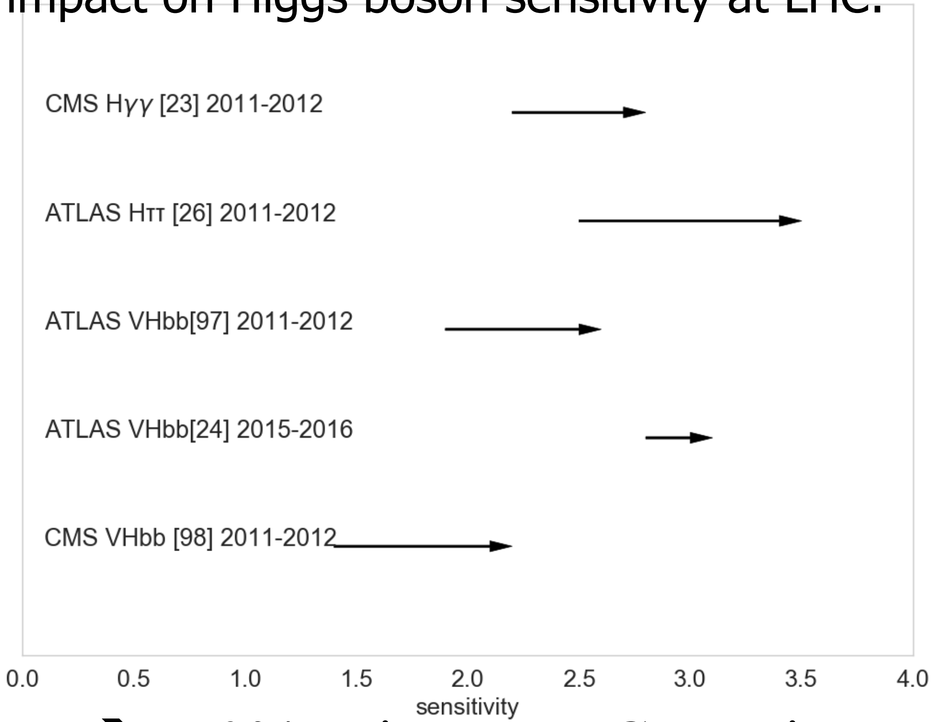
Outline

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

Focus on applications rather than details of the techniques

ML in HEP

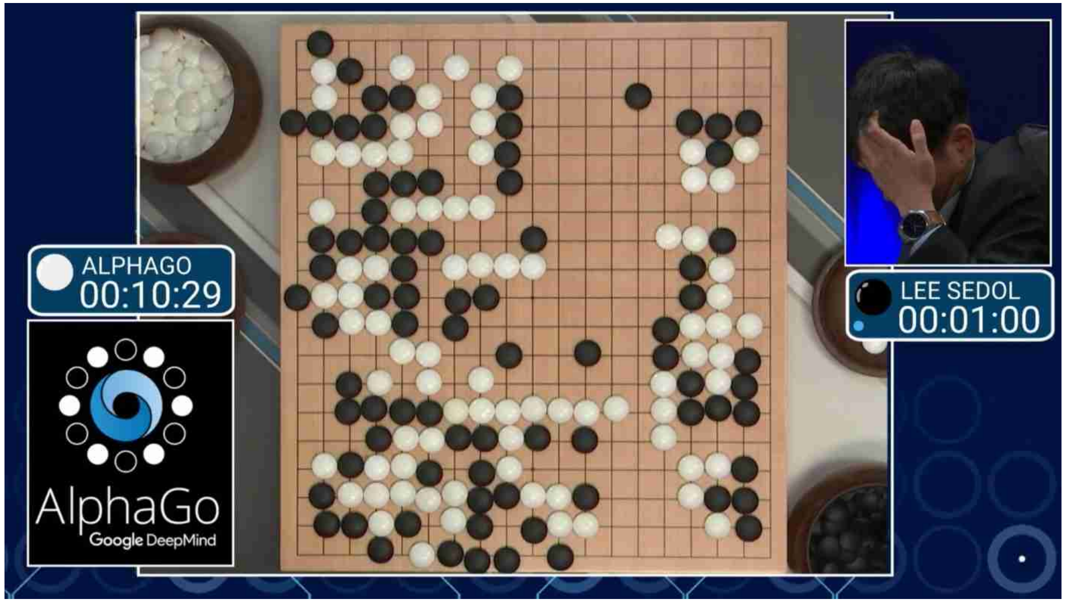
- Use of Machine Learning (a.k.a Multi Variate Analysis as we call it) already at LEP somewhat, much more at Tevatron (Trees)
- At LHC, Machine Learning used almost since first data taking (2010) for reconstruction and analysis
- In most cases, Boosted Decision Tree with Root-TMVA, on ~10 variables
- For example, impact on Higgs boson sensitivity at LHC:



➔~50% gain on LHC running

ML in HEP

- Meanwhile, in the outside world :



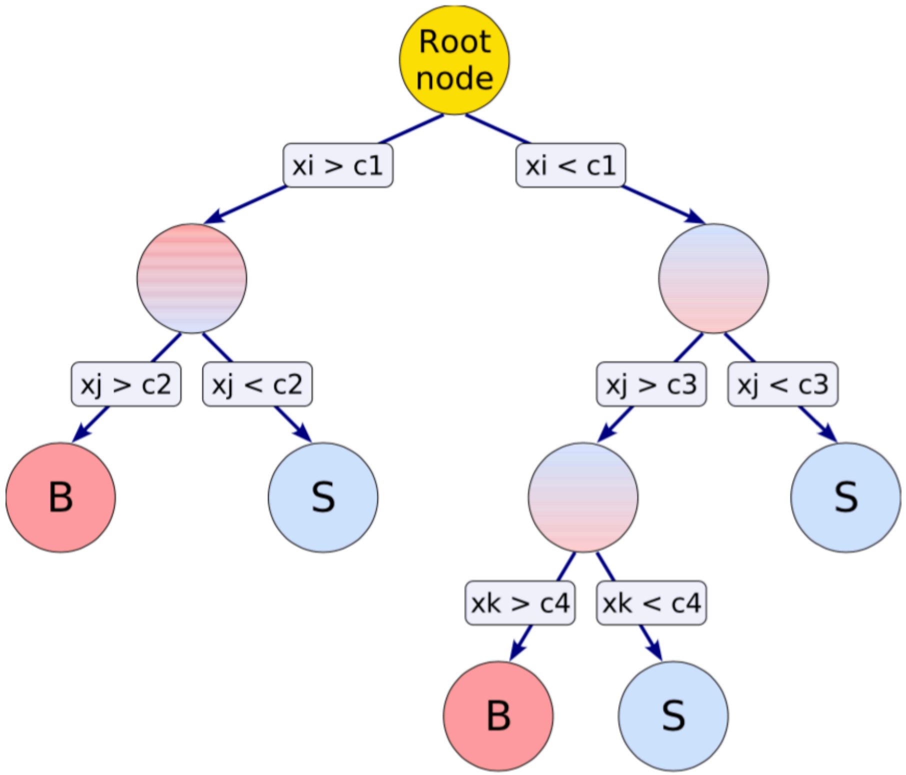
- “Artificial Intelligence” not a dirty word anymore!
- We (in HEP) have realised we’re been left behind! Trying to catch up now…
- This talk on very selected promising use of advanced ML in HEP

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
  - Started informally September 2015, gaining speed
  - IML workshop @CERN 20-22 March 2017, 9-12 April 2018
- DS@HEP workshop @FNAL 8-12 May 2017
- ACAT conference Seattle, Sep 2017
- Connecting The Dots, 20-22 March 2018

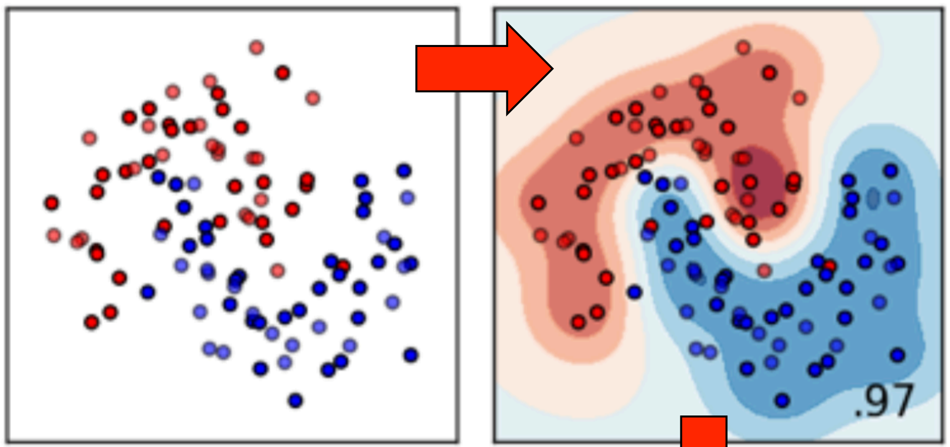
ML Basics

BDT in a nutshell



- Single tree (CART) <1980
- AdaBoost 1997 : rerun increasing the weight of misclassified entries ➔Boosted Decision Trees (Gradient BDT, random forest…)

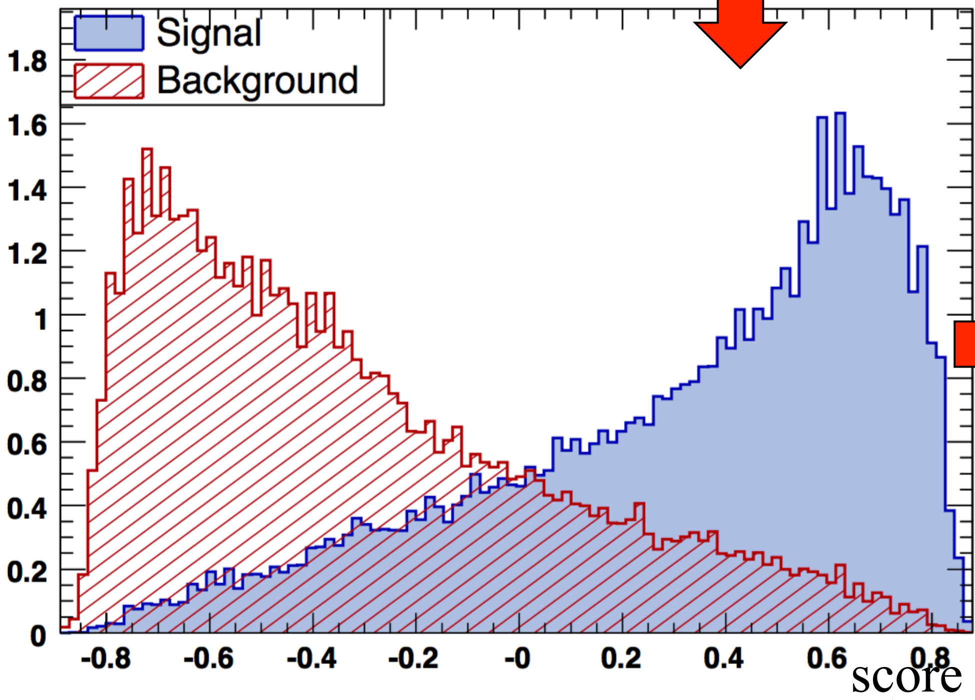
Classifier basics

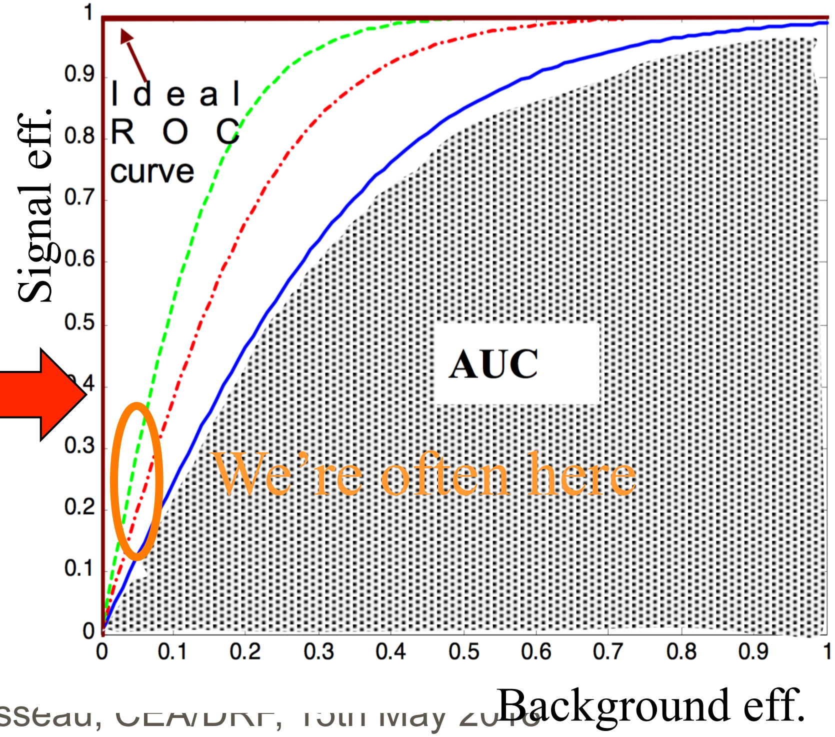


Train on Signal and Background Monte-Carlo
➔learn the separation between S and B distribution
Apply on test sample
Apply on data

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

AUC : Area Under the (ROC) Curve





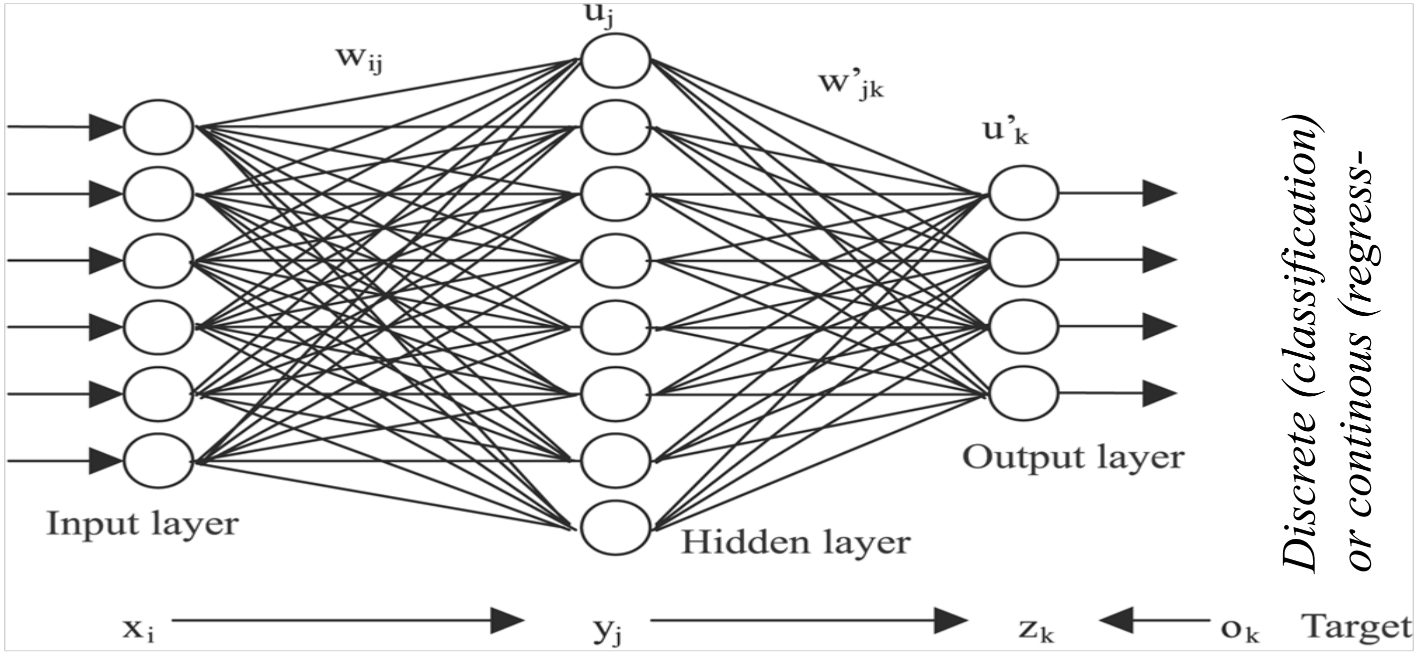
under/over training

Gilles Louppe, github

Some overtraining is good

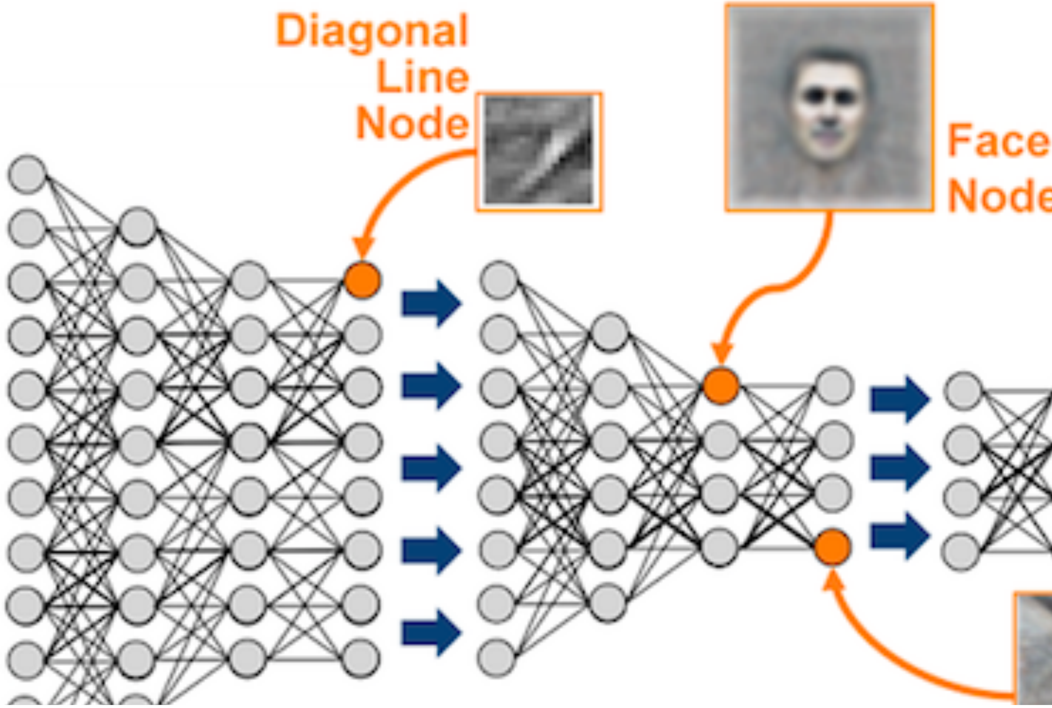
…provided CrossValidation done correctly!

Neural Net in a nutshell

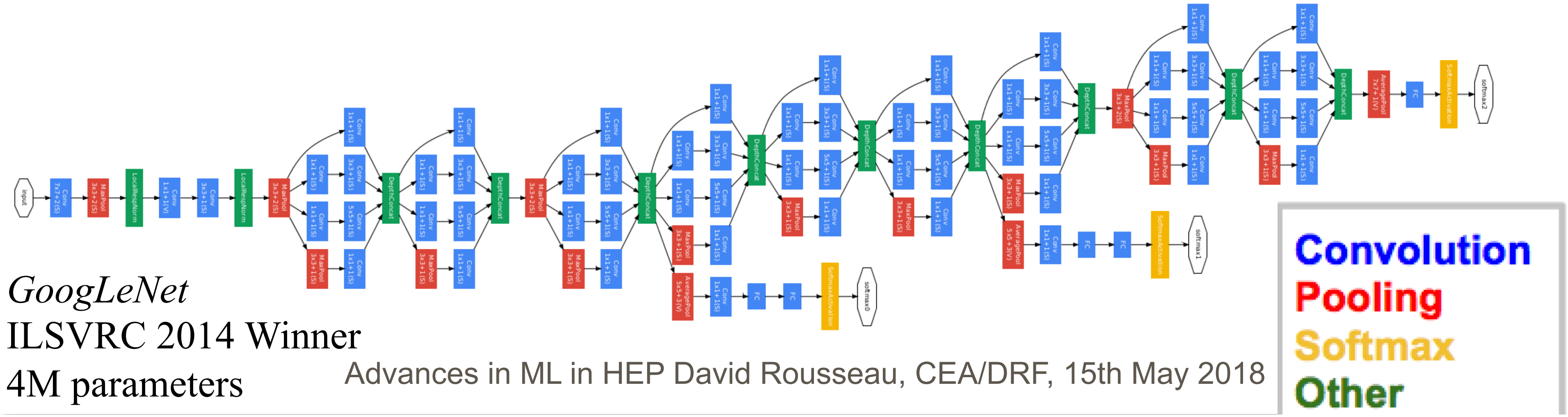


- Neural Net ~1950!
- But many many new tricks for learning, in particular if many layers (also ReLU instead of sigmoïd activation)
- “Deep Neural Net” up to 100 layers
- Computing power (DNN training can take days even on GPU)

Deep learning



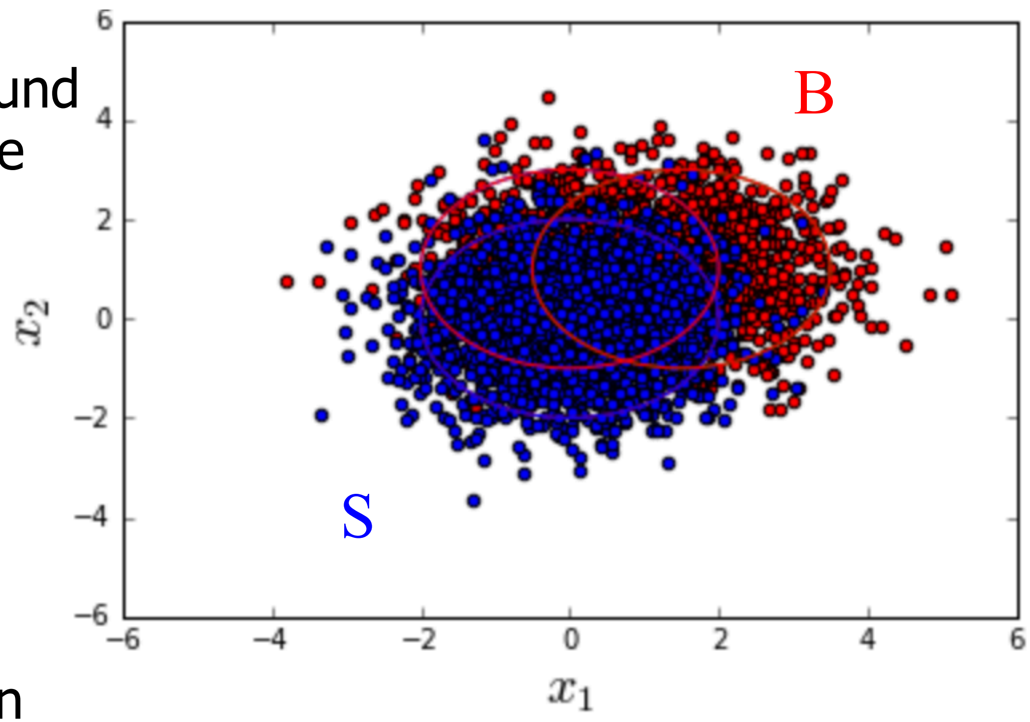
Optimal stimulus of a given neuron
Google 2012
http://arxiv.org/abs/1112.6209



GoogLeNet
ILSVRC 2014 Winner
4M parameters

No miracle

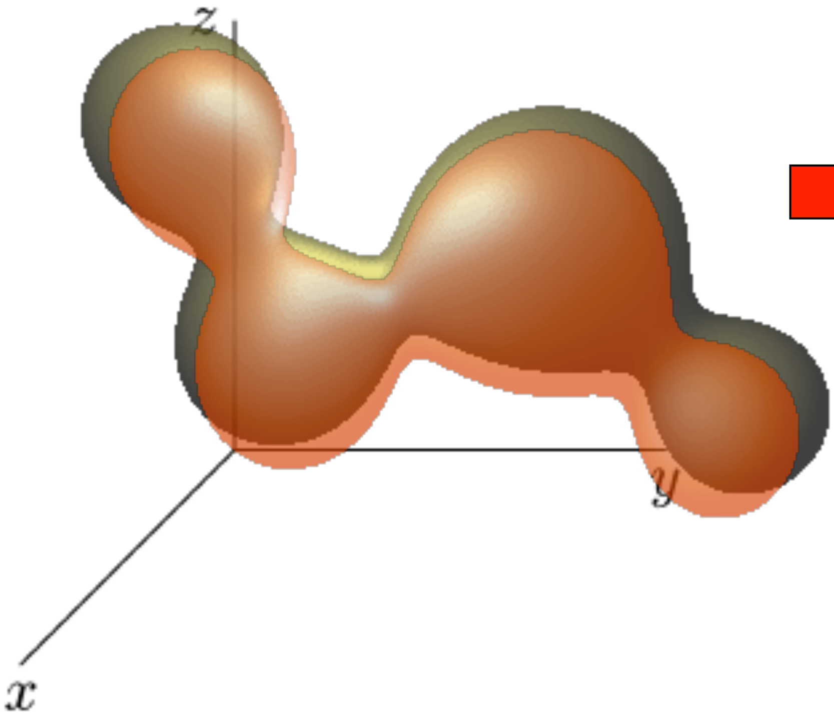
- ML (nor Artificial Intelligence) does not do any miracles
- For selecting Signal vs Background and underlying distributions are known, nothing beats ihihood ratio! (often called "bayesian limit"):
  - $L_S(x)/L_B(x)$
- OK but quite often L_S L_B are unknown
  - + x is n-dimensional
- ML starts to be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

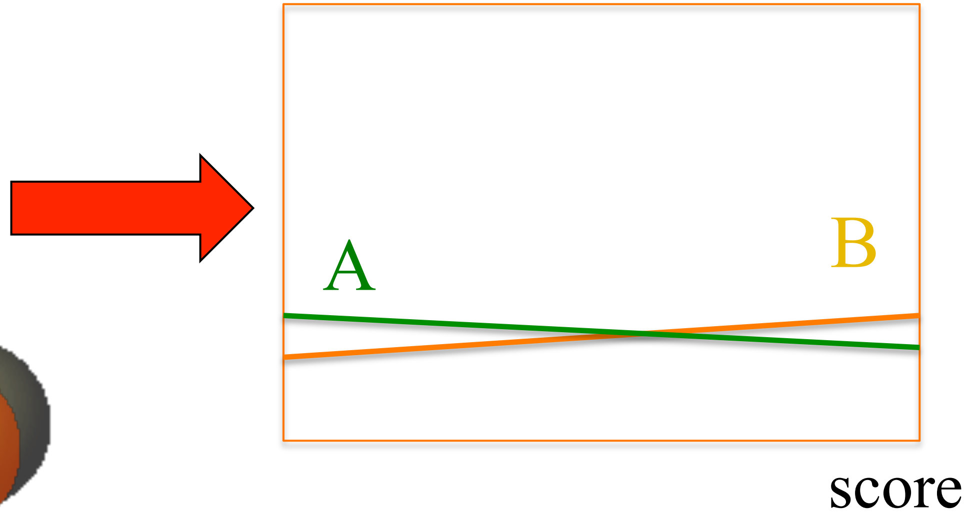


Modern Software and Tools

- New version of TMVA (root 6.0.8 on beyond) (see talk Lorenzo Moneta, Sergei Gleyzer IML workshop CERN March 2018)
  - Jupyter interface
  - Hyper-parameter optimisation / Cross-validation
  - Interface to R, sk-learn etc…
  - However : better convert ntuples to numpy array and use the software below
- Non HEP software
  - Sci-kit learn : de facto standard toolbox ML (except Deep Learning) (python, but fast)
  - Keras+Theano/TensorFlow : NN toolbox (build a NN in a few lines of python)➔ but pyTorch lately gaining speed
  - XGBoost best BDT, both speed and performance (c++ with python interface) (check T. Keck Comput Softw Big Sci (2017) 1: 2 for a comparison with TMVA and others). First use in physics paper :ATLAS Higgs ttH arxiv 1712.08891
- Note : for ~10 variable classification/regression task gradient BDT is still the tool of choice!
- Platforms
  - Your laptop is sufficient in many cases : install e.g. Anaconda https://docs.continuum.io/anaconda/install (demo)
  - If not, more and more platforms looking for users, maybe on your campus (with GPU DNN ==millions of parameter to optimise=>heavy duty linear algebra)
  - GridCL @ LLR (not for production but useful)
  - 50 GPU platform at Lyon CC-IN2P3, little used so far
- For CERN users:
  - SWAN interactive data analysis on the web see https://swan.web.cern.ch/content/machine-learning
  - CVMFS ML setup for any CVMFS enabled platform

What does a classifier do?

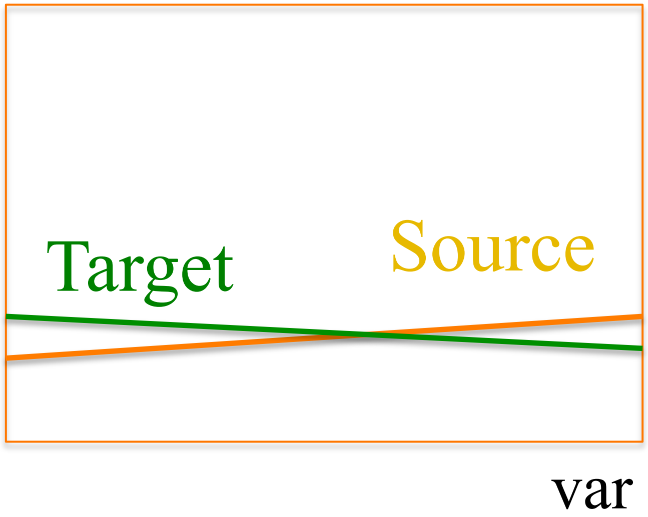




- The classifier "projects" the two multidimensional "blobs" maximising the difference, without (ideally) any loss of information

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

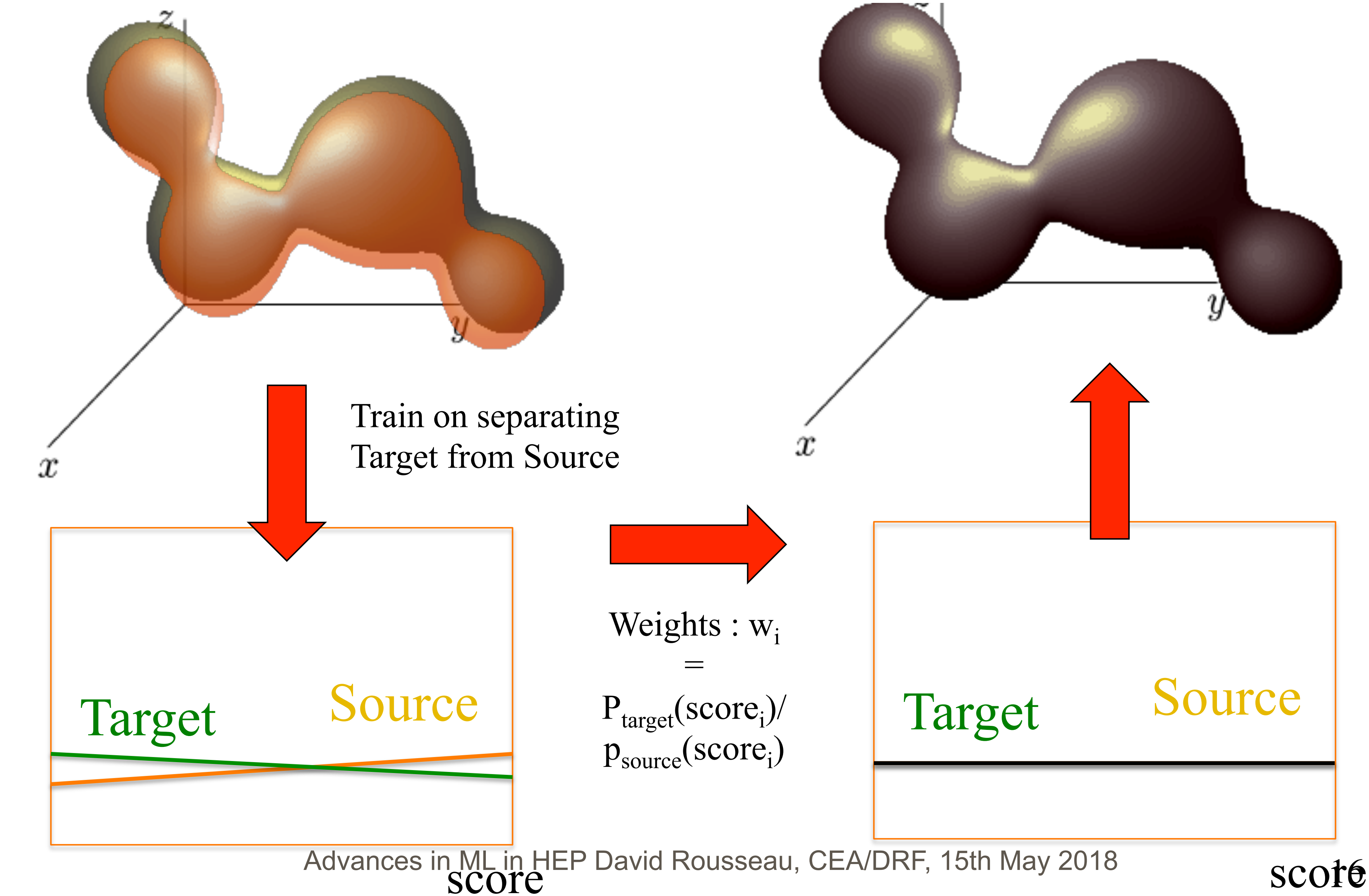


Weights : w_i = $p_{target}(var_i)/p_{source}(var_i)$

- 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



Multi dimensional reweighting (2)

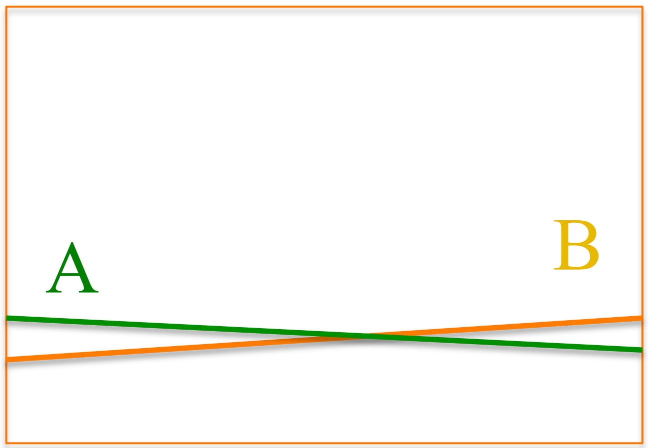
- Reweighting the Source distribution on the score allows multidimensional reweighting without statistics problem
- Usual caveat still hold : Target support should be included in Source support, distributions should not be too different otherwise unmanageable very large or very small weights
- (Note : “reweighting” in HEP language <==> “importance sampling” in ML language)

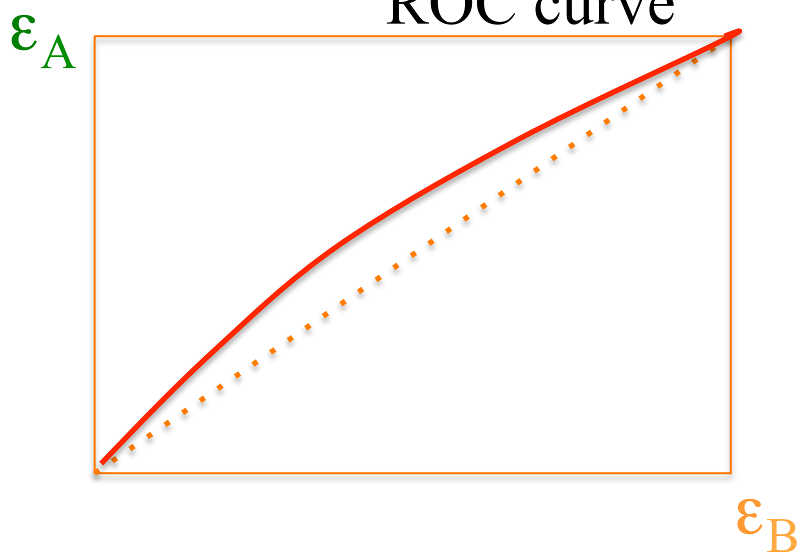
Anomaly detection

- Suppose you have two independent samples A and B, *supposedly* statistically identical. E.g. A and B could be:
  - MC prod 1, MC prod 2
  - MC generator 1, MC generator 2
  - Geant4 Release 20.X.Y, release 20.X.Z
  - Production at CERN, production at Lyon
  - Data of yesterday, Data of today
- How to verify that A and B are indeed identical ?
- Standard approach : overlay histograms of many carefully chosen variables, check for differences (e.g. KS test)
- One ML approach (not the only one): ~~ask an artificial scientist~~, train your favorite classifier to distinguish A from B, histogram the score, check the difference (e.g. AUC or KS test)
  - ➔only one distribution to check
- Being developped for accelerator monitoring, experiment Data Quality monitoring

Small non-local difference

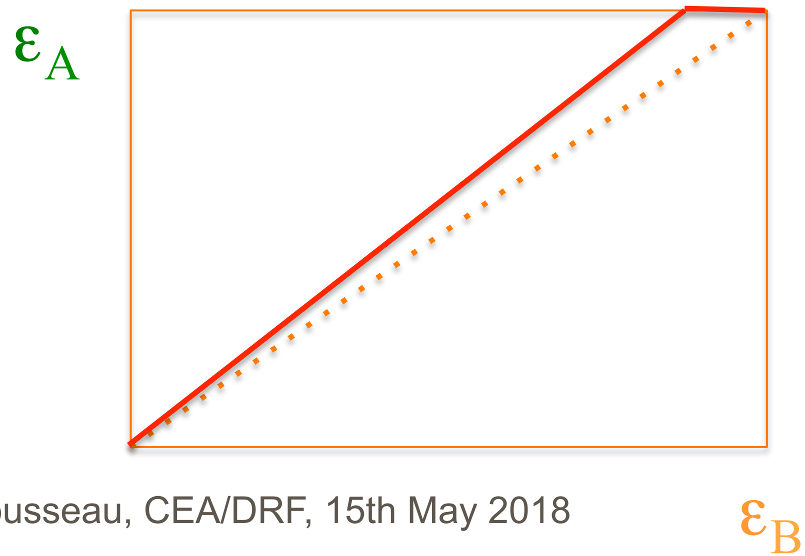
ROC curve





score

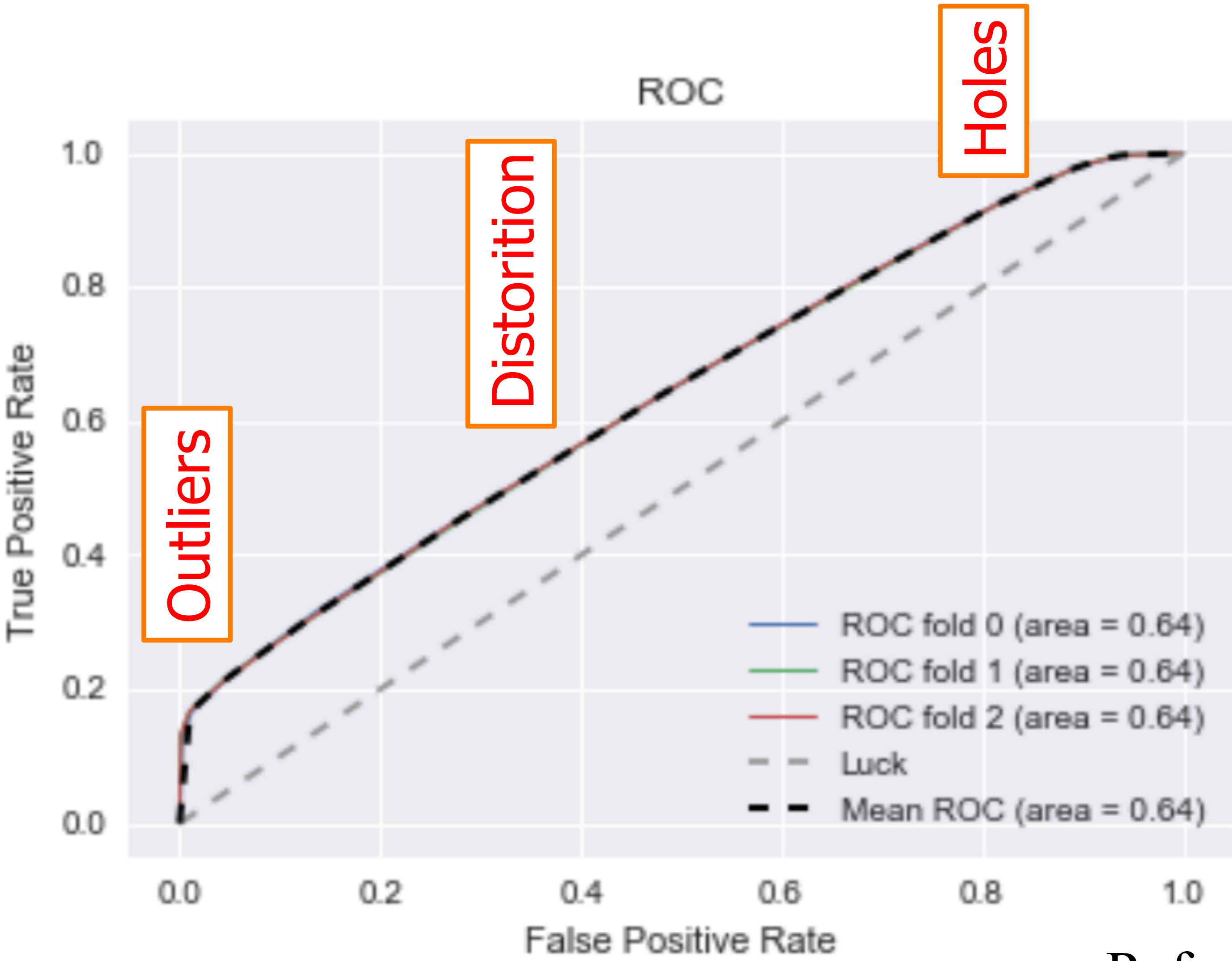
Local big difference (e.g. non overlapping distribution, hole)



score

HSF ML RAMP on anomaly (2)

Skewed

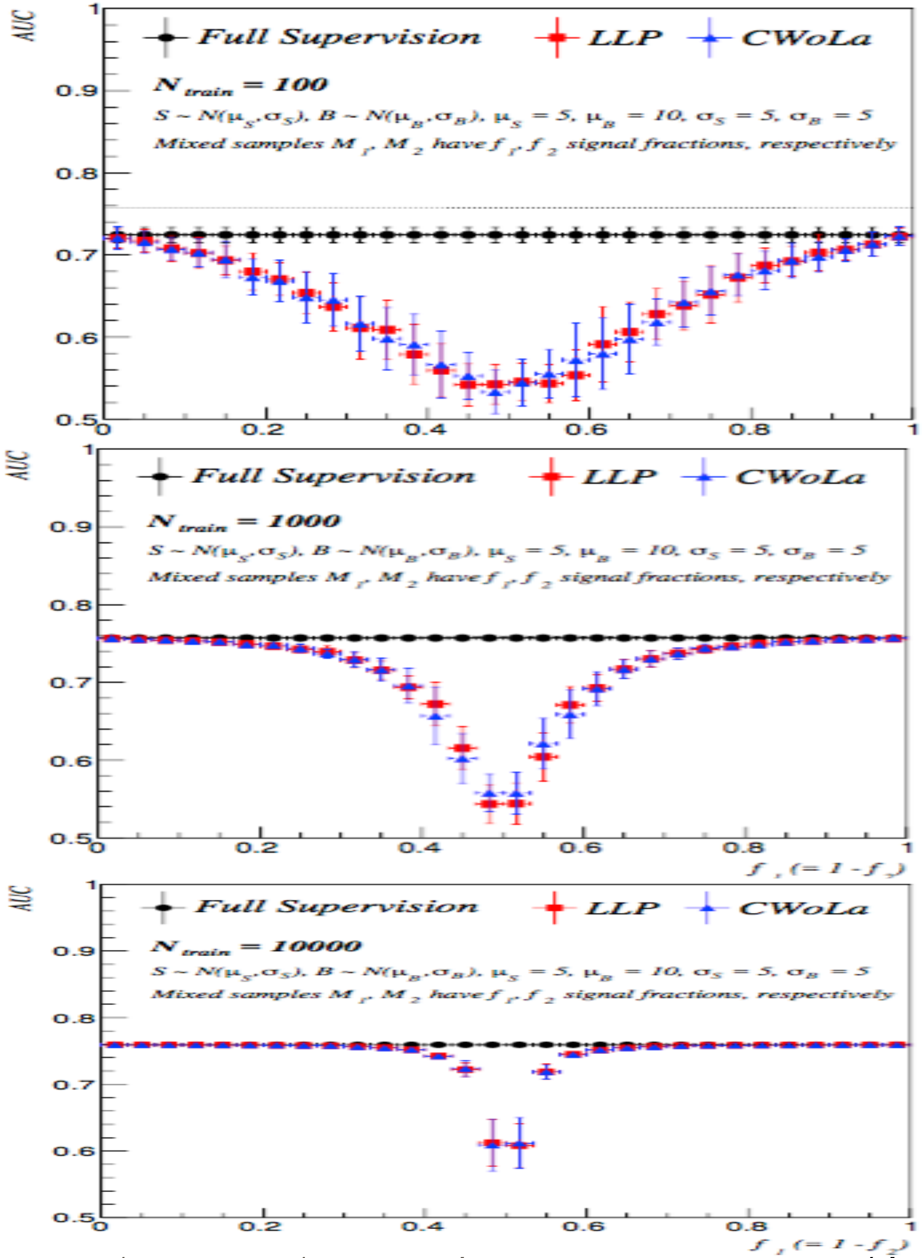


Reference

Classification without labels

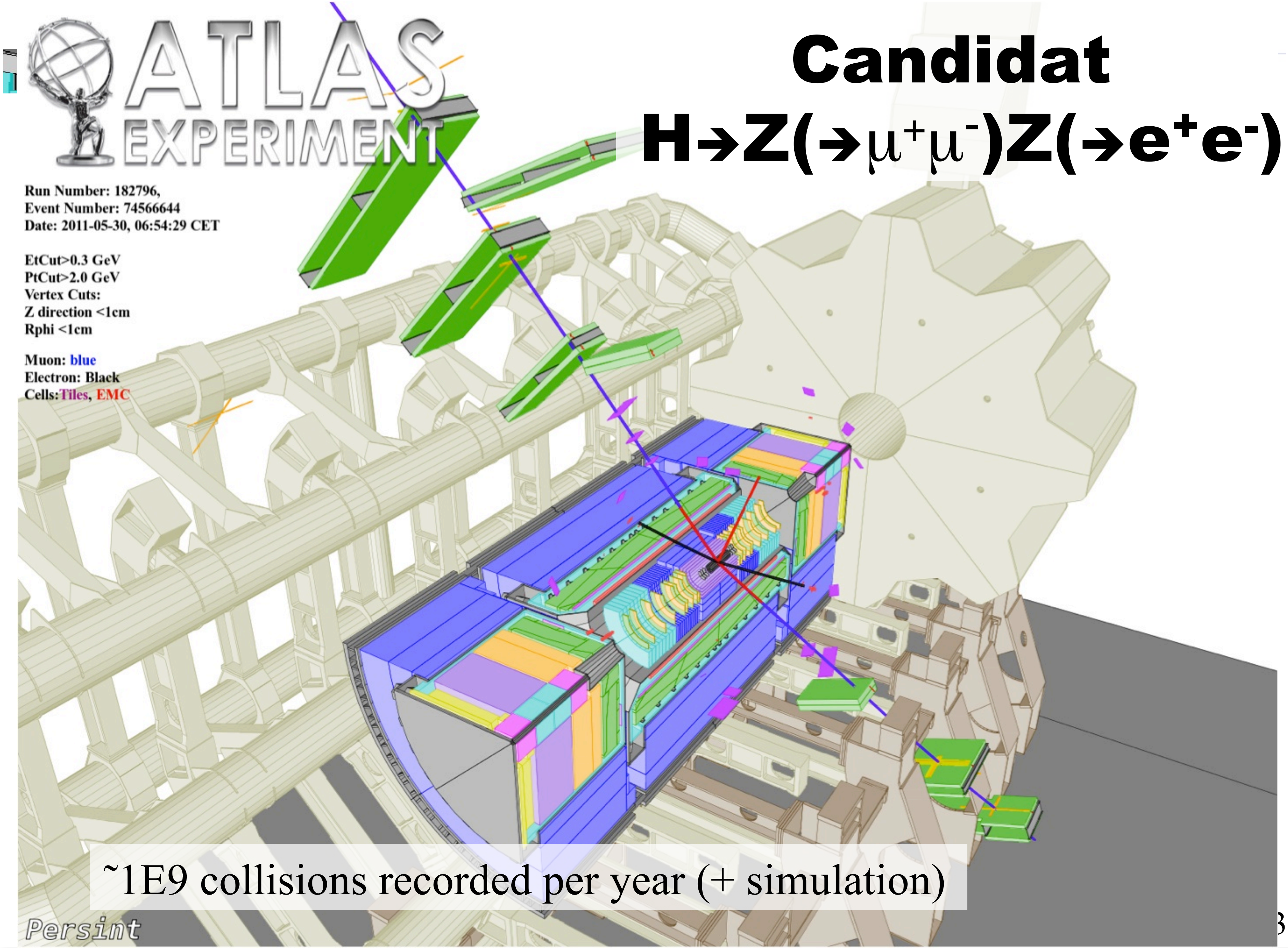
Metodiev et al, [1708.02949]

- Suppose one wants to separate S and B
- But one only has one signal rich sample Ms and one background rich sample Mb
- A classifier optimally trained with Ms and Mb (without information on fraction of S and B) is actually also optimal to separate S and B!
- ➔...allows training on data where it is hard to have very pure control sample
- ...one still need to evaluate classification perfomance
- Big caveat : works only if S and B pdf are indentical in Ms and Mb



ML in analysis

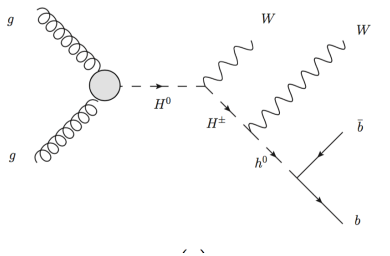
Candidat $H \rightarrow Z(\rightarrow \mu^+\mu^-)Z(\rightarrow e^+e^-)$

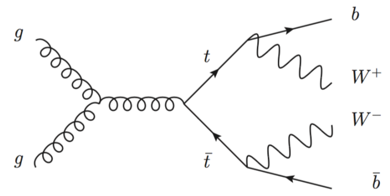


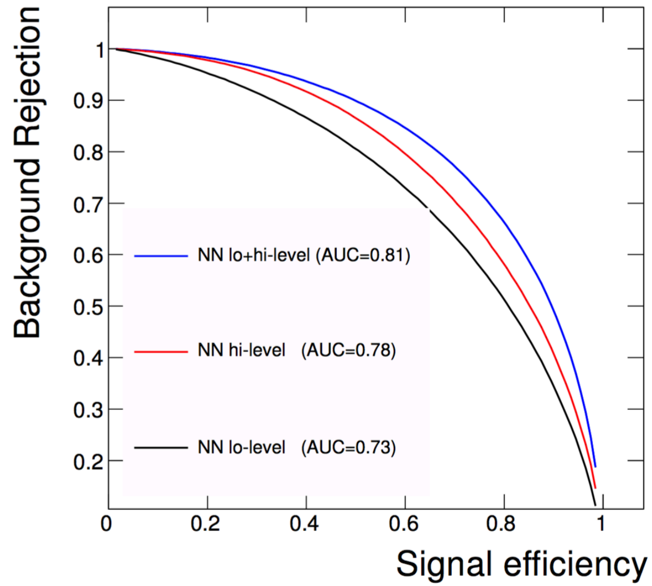
~1E9 collisions recorded per year (+ simulation)

Deep learning for analysis

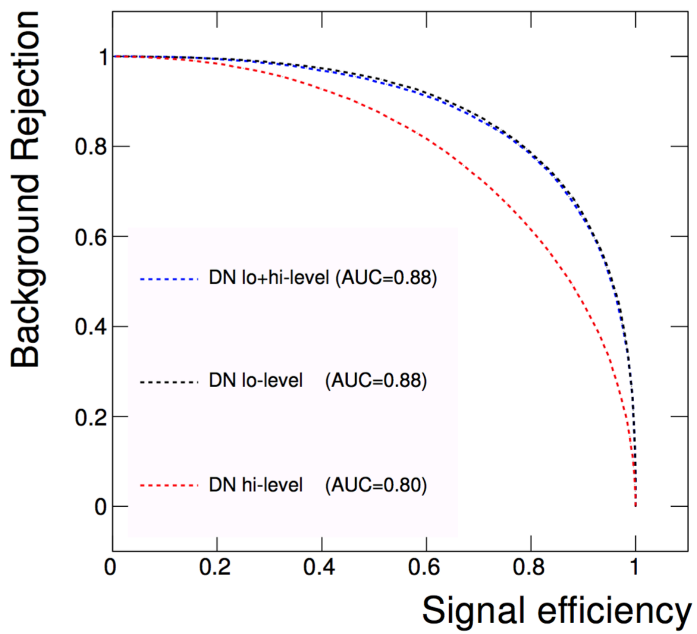
1402.4735 Baldi, Sadowski, Whiteson







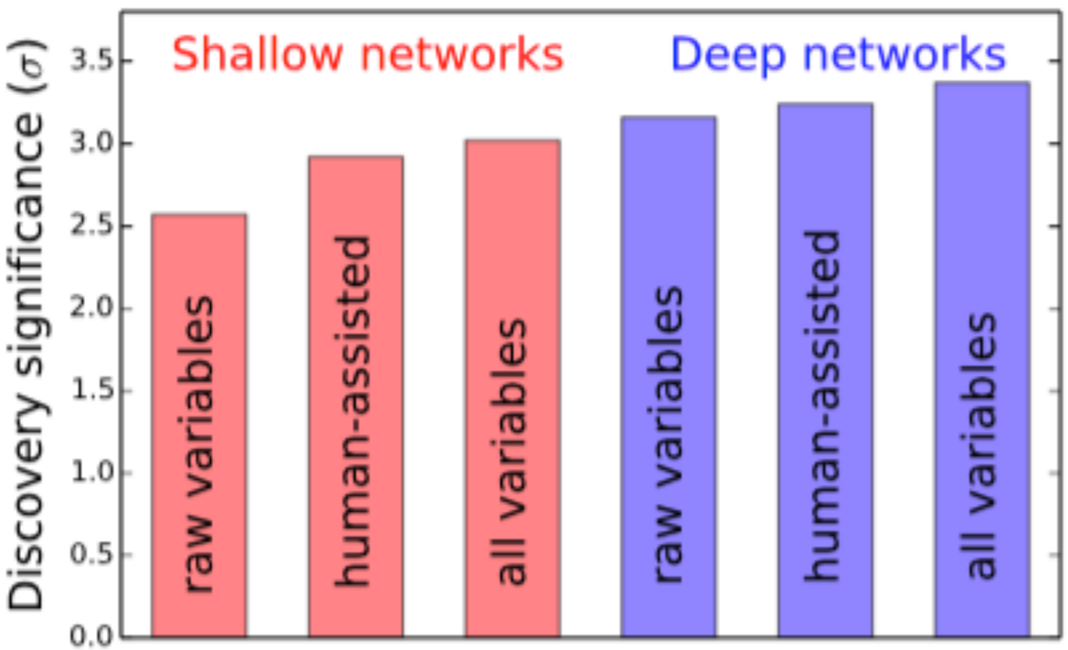
- MSSM at LHC : H^0➔WWbb vs tt➔WWbb
- Low level variables:
  - 4-momentum vector
- High level variables:
  - Pair-wise invariant masses
- Deep NN outperforms NN, and does not need high level variables
- DNN learns the physics ?



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)

Systematics-aware training

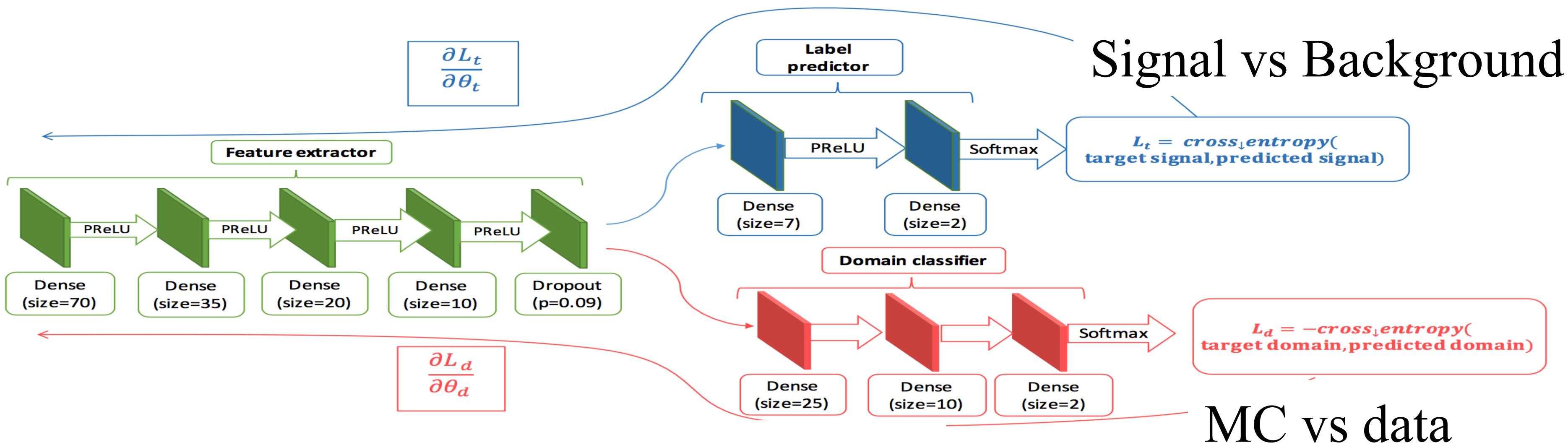
- Our experimental measurement papers typically ends with
  - measurement = m ± σ(stat) ± σ(syst)
  - σ(syst) systematic uncertainty : known unknowns, unknown unknowns…
- Name of the game is to minimize quadratic sum of :

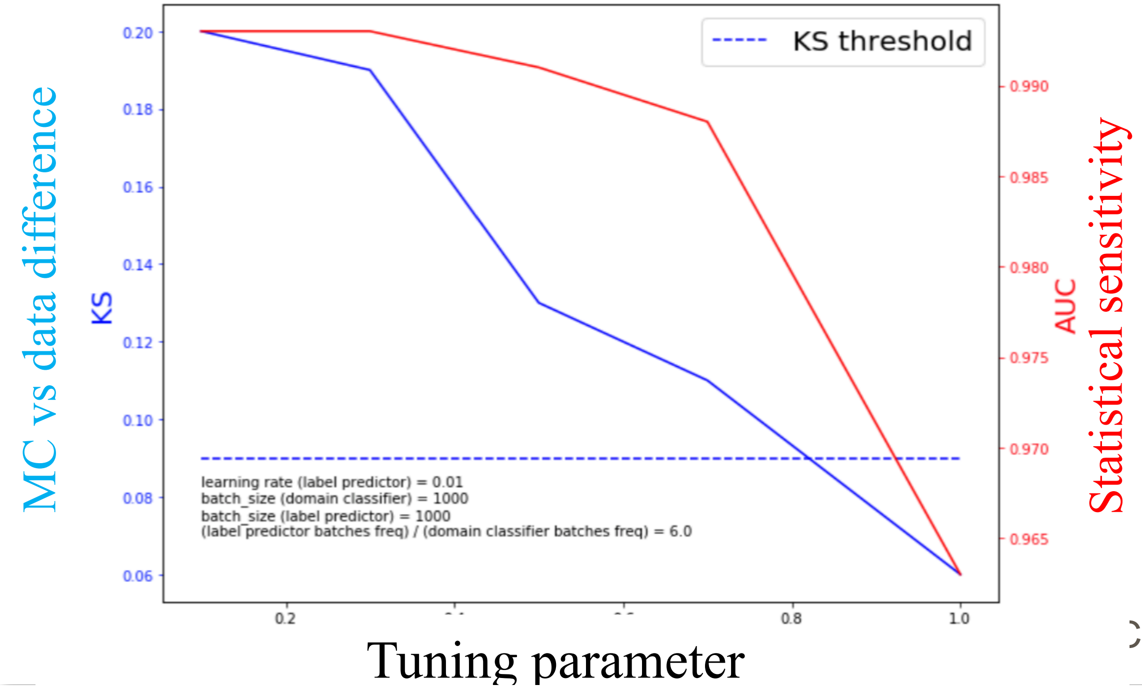
$$\sigma(\text{stat}) \pm \sigma(\text{syst})$$

- 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



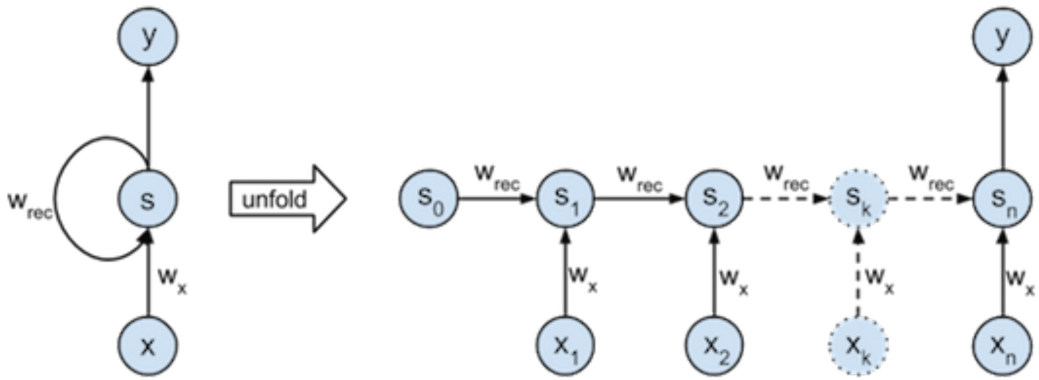


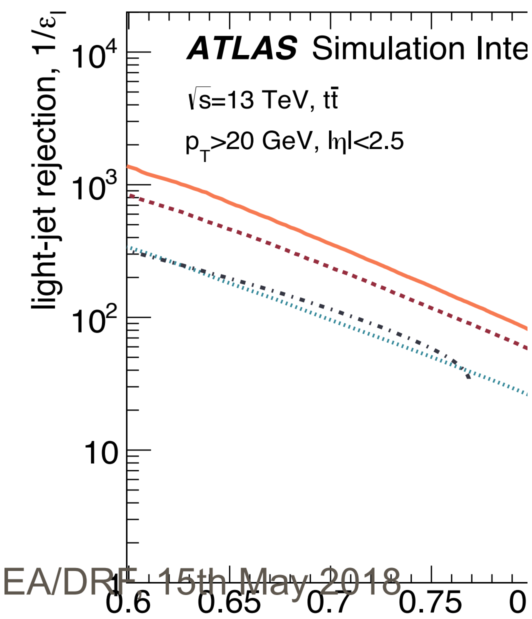
ML in reconstruction

RNN for b tagging

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

- BDT and usual NN expect a fix number of input. What to do when the number of inputs is not fixed like the tracks for b-quark jet tagging ?
- Recurrent Neural Networks have seen outstanding performance for processing sequence data
  - Take data at several “time-steps”, and use previous time-step information in processing next time-steps data
- For b-tagging, take list of tracks in jet and feed into RNN
  - 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
- Learning on sequence data may be important in other places!
  - Combining tracks with clusters? Track to vertex matching?



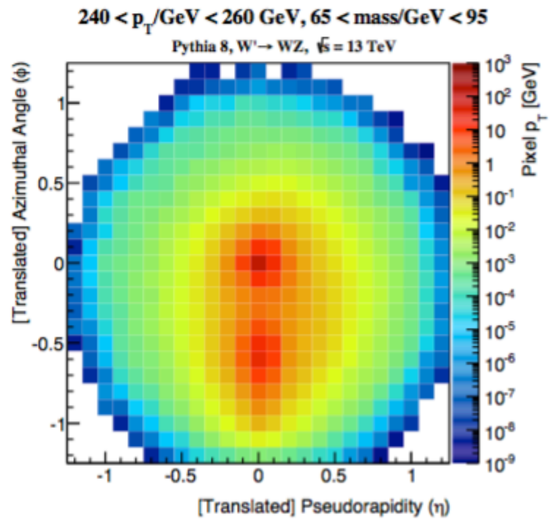


Jet Images

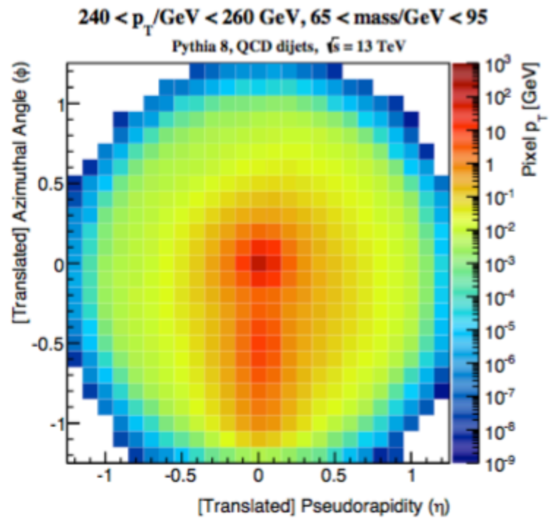
arXiv 1511.05190 de Oliveira, Kagan, Mackey, Nachman, Schwartzman 

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

Boosted W→qq jet

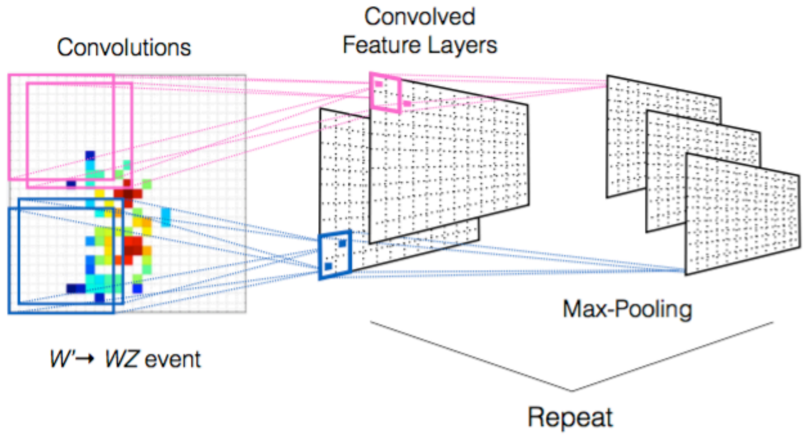


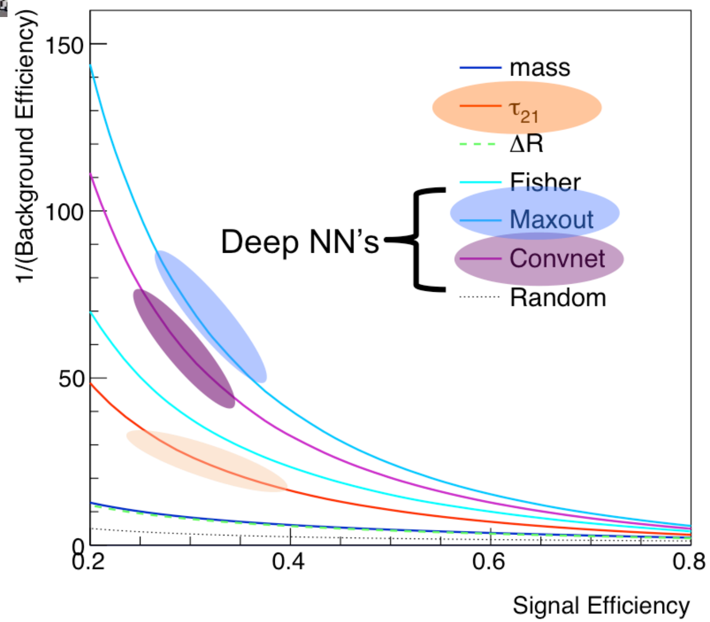
QCD



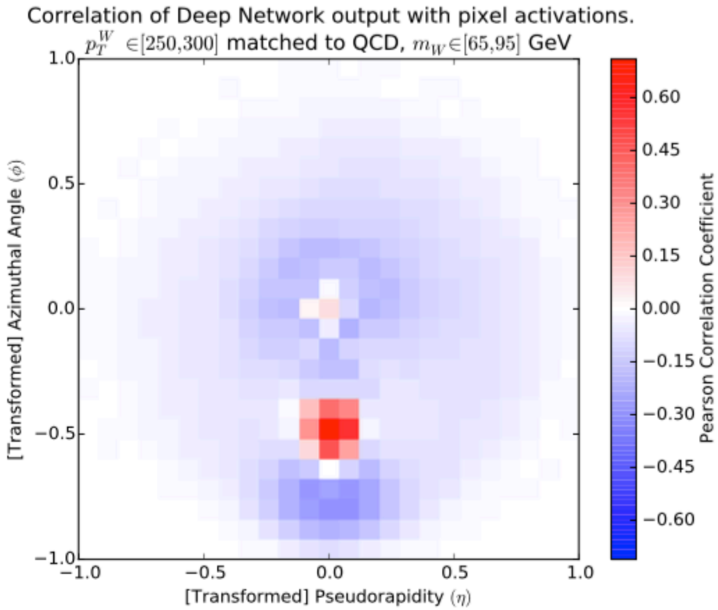
Jet Images : Convolution NN

arXiv:1511.05190



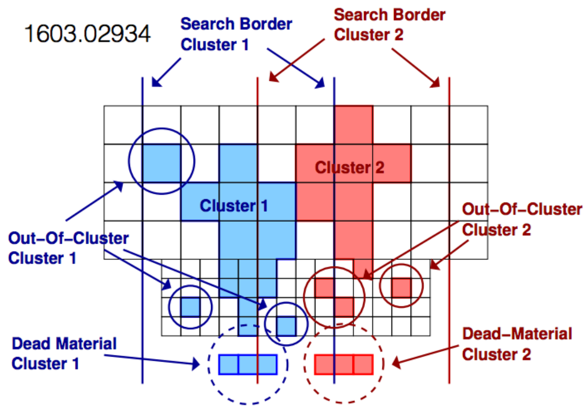


- Variables build from CNN outperform the more usual ones



- What the CNN sees (the "cat" neurone")
- Now need proper detector and pileup simulation
- ➔3Dimension

1603.02934



End to end Learning

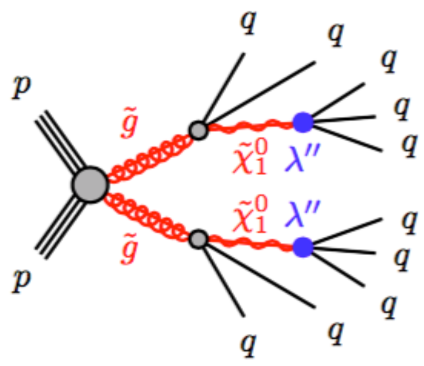
End to end learning

Bhimji et al, 1711.03573

- Train directly for signal on « raw » event ?
- Start from RPV Susy search

ATLAS-CONF-2016-057

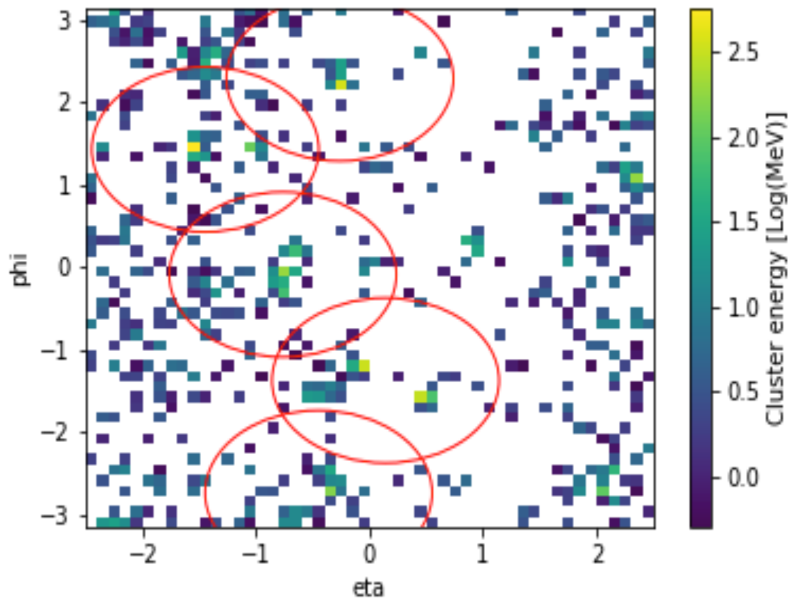
- Fast Simulated events with Delphes



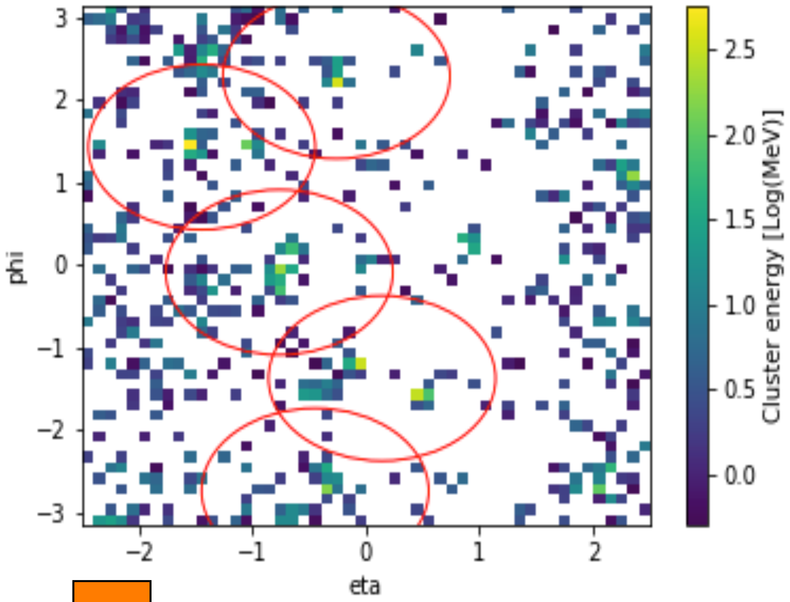
(b) gluino cascade decay

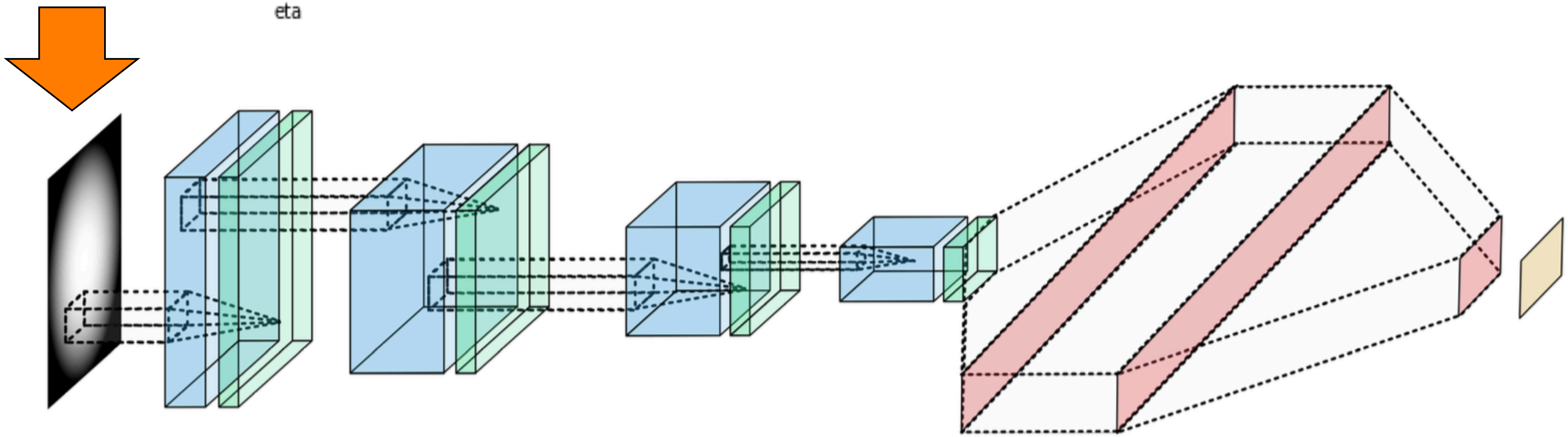
- Project energies on 64x64 ηxϕ grid
- Compare with usual jet Reconstruction and physics Analysis variables such as:

$$M_J^{\Sigma} = \sum_{\substack{p_T > 200\,\mathrm{GeV} \\ |\eta| \leq 2.0}}^{4} m^{\mathrm{jet}}$$

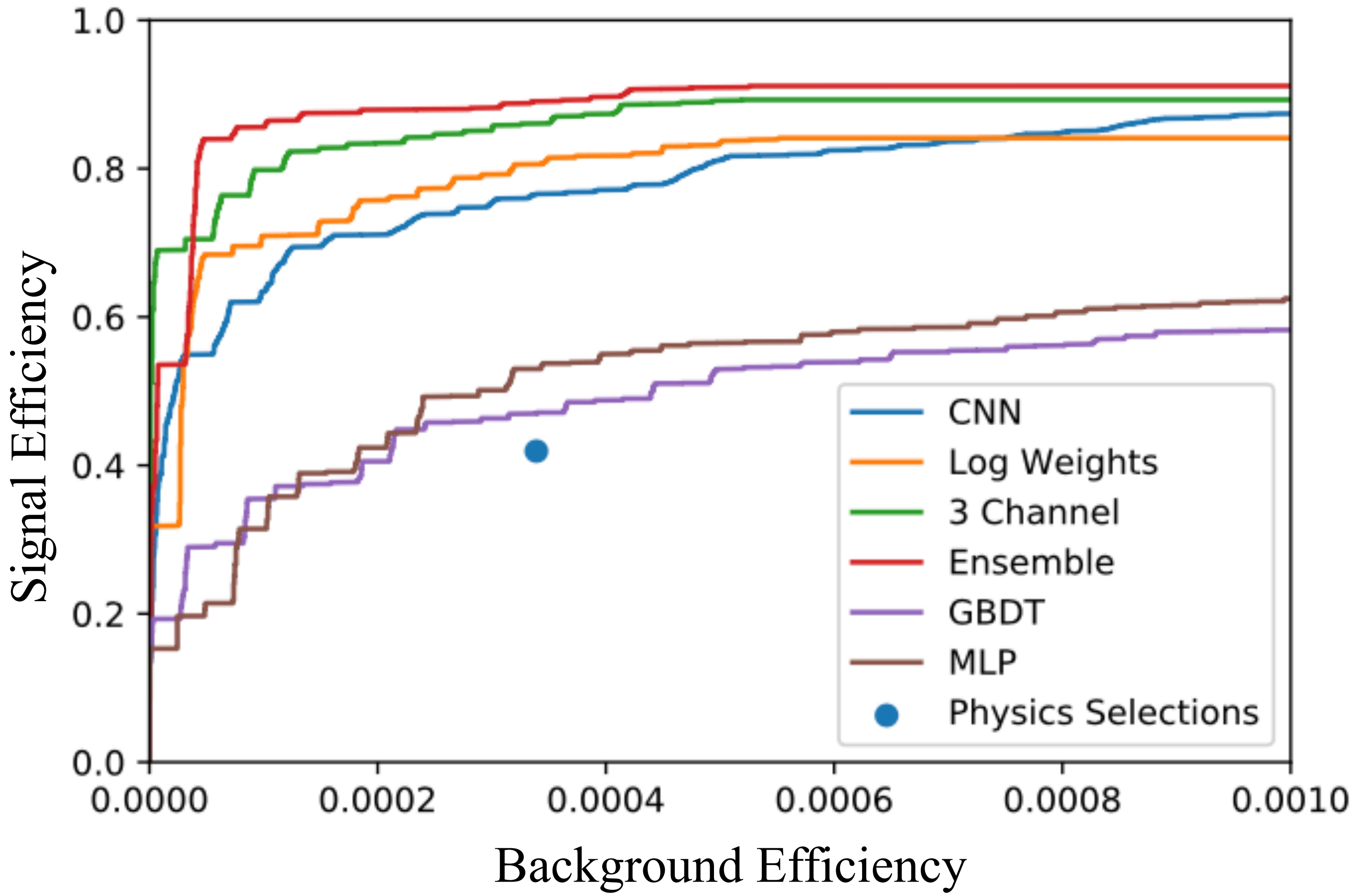


End to end learning (2)





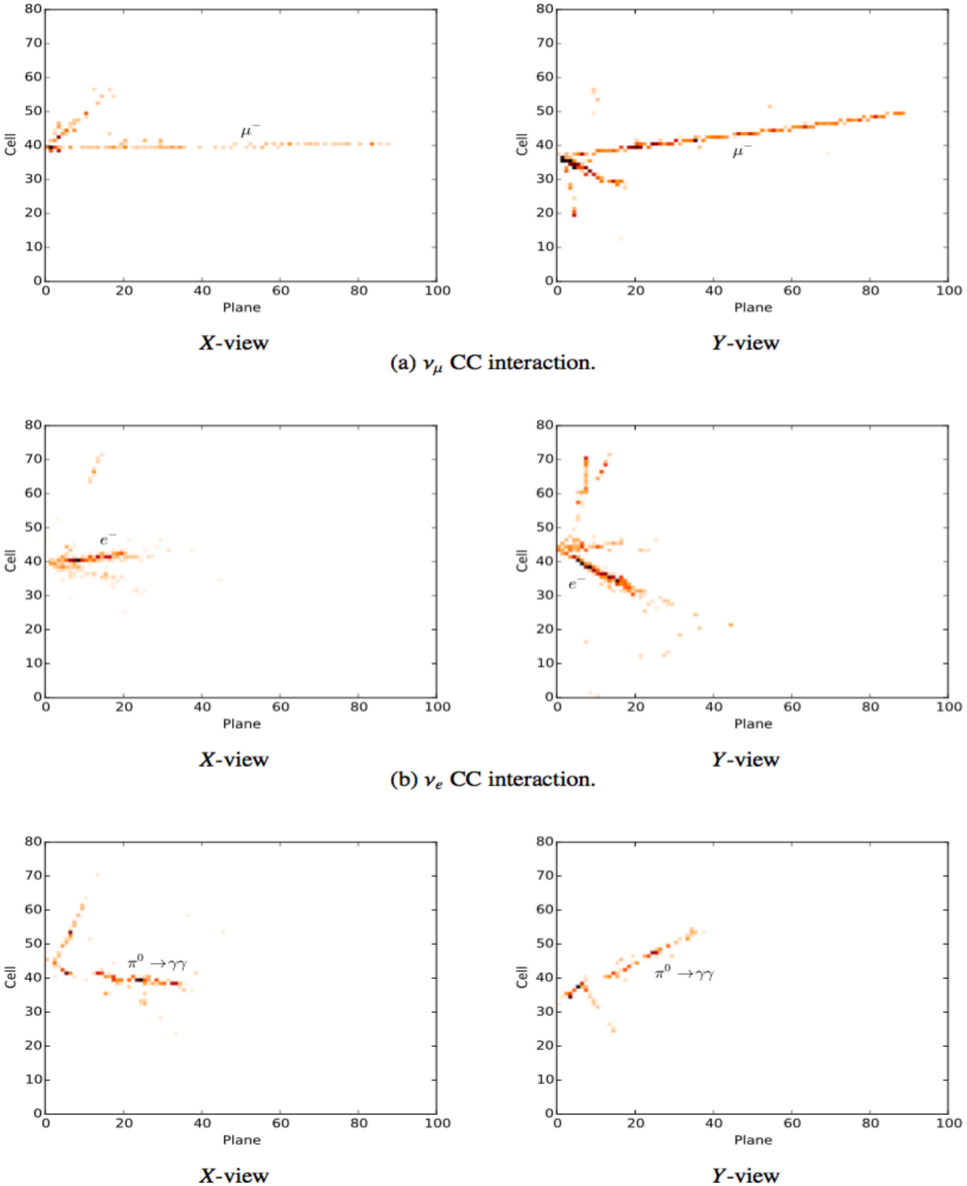
End to end learning (3)



- >x2 gain over BDT/shallow network using physics variable and 5 leading jet 4-momenta
- ➔CNN extract information from energy grid which is lost in the jets ?
- Not sure they should compare to applying DL on the jets

A recent success with ν : NOVA

arXiv 1604.01444 Aurisano et al



(a) ν_μ CC interaction.

(b) ν_e CC interaction.

(c) NC interaction.

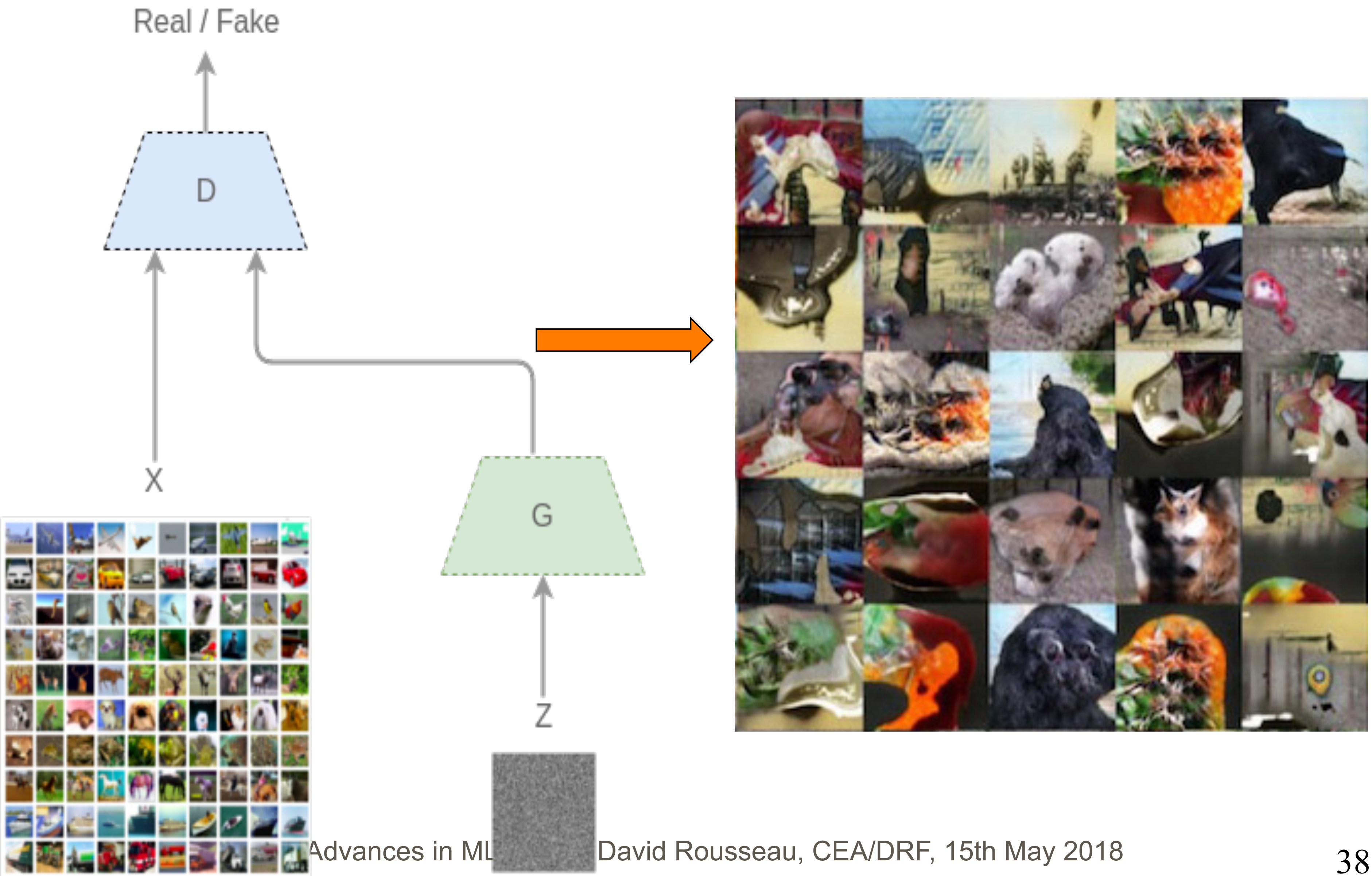
Neutrino interaction classification

Using Convolutional Neural Network (GoogleNet)

Actually used for analysis

ML in simulation

Generative Adversarial Network



Condition GAN

Text to image

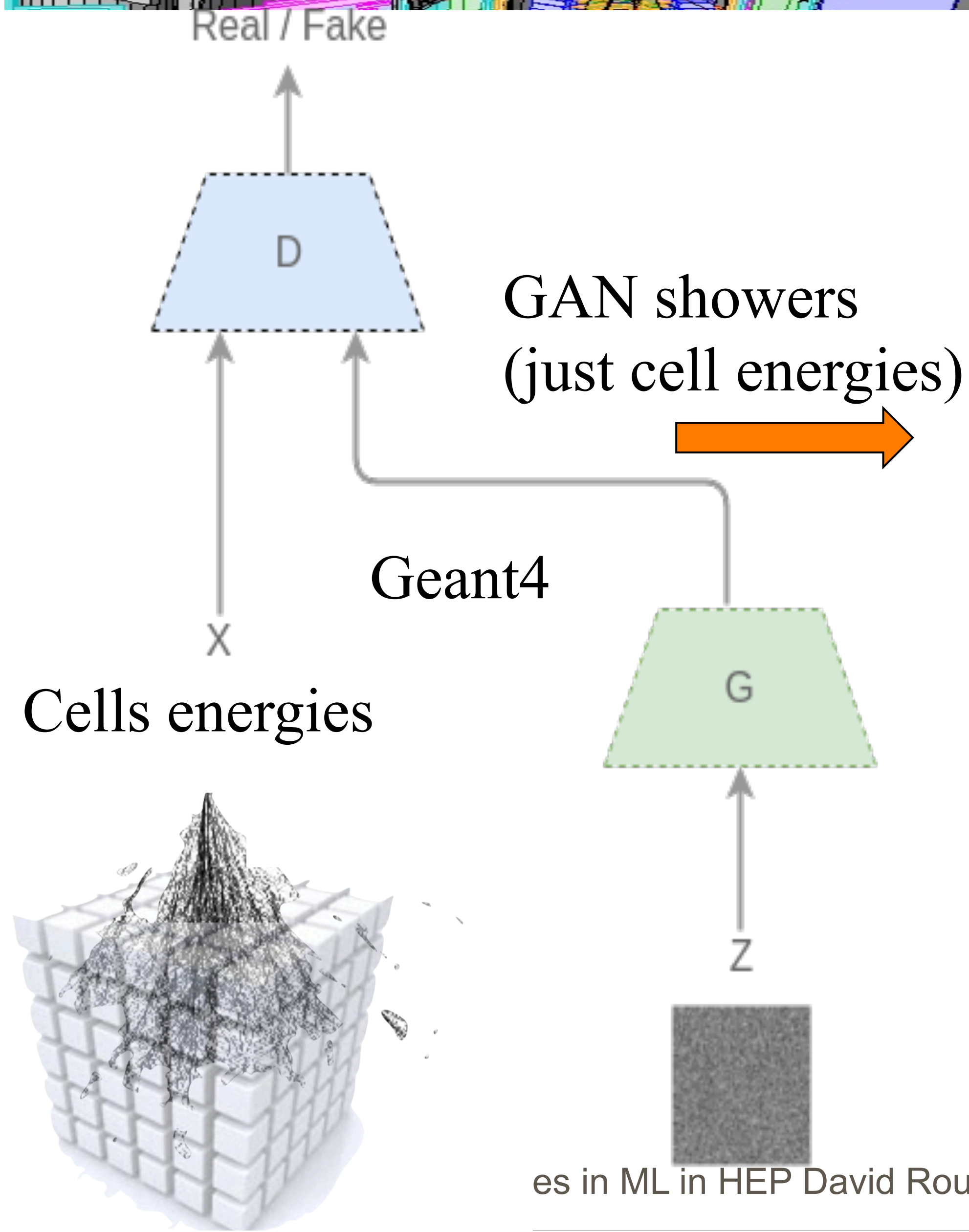
this small bird has a pink breast and crown, and black primaries and secondaries.

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)



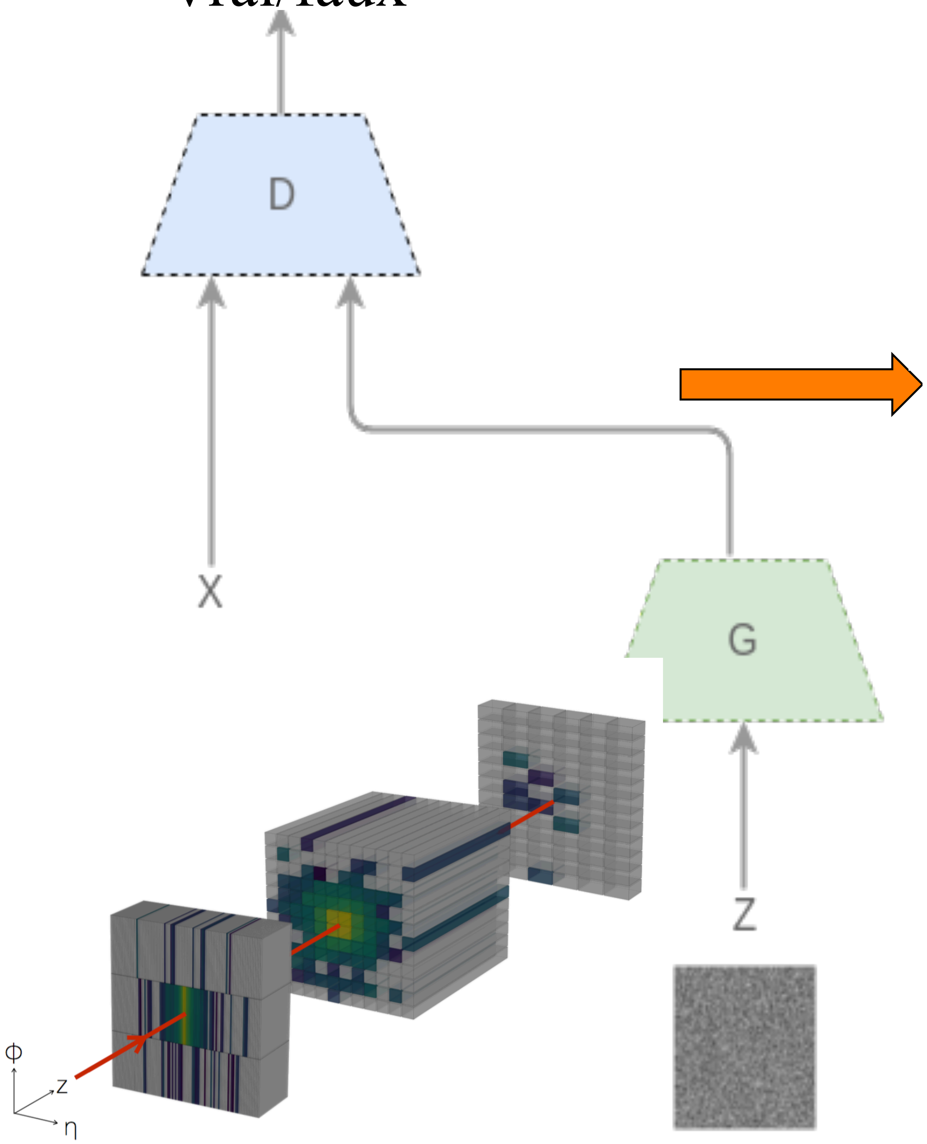
- Half of LHC grid computers (~300.000 cores) are crunching Geant4 simulation 24/24 365/365
- …while LHC experiments are collecting more and more events
- ➔reducing CPU consumption of simulation is very important

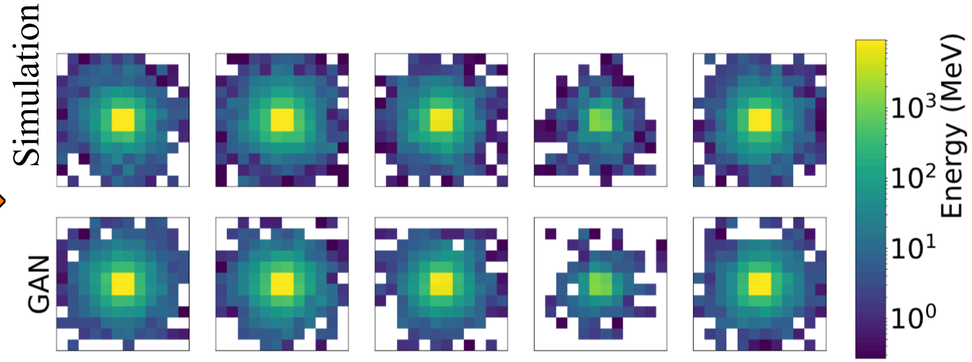
- Imagine training a GAN on single particle showers of all types and energies
- Then when an event is simulated it would ask for GAN showers on request (superfast by 3-4 order of magnitude)
- Would replace current fast simulation, frozen shower libraries….
- If/when it works, would require large GPU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

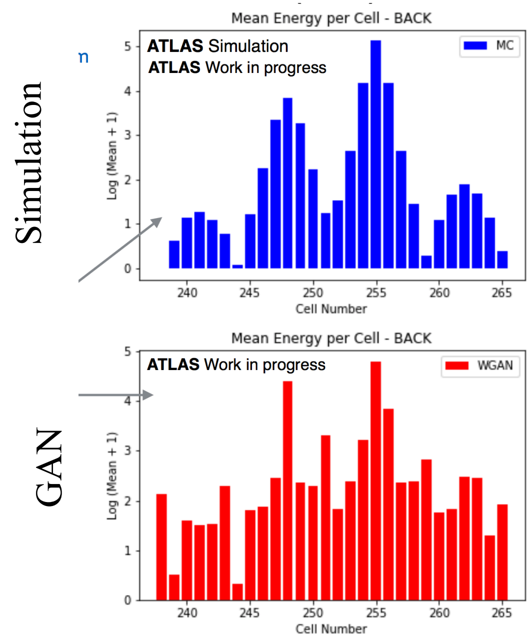
GAN for simulation (2)

Paganini et al 1705.02355.

Gain en temps de calcul x1000

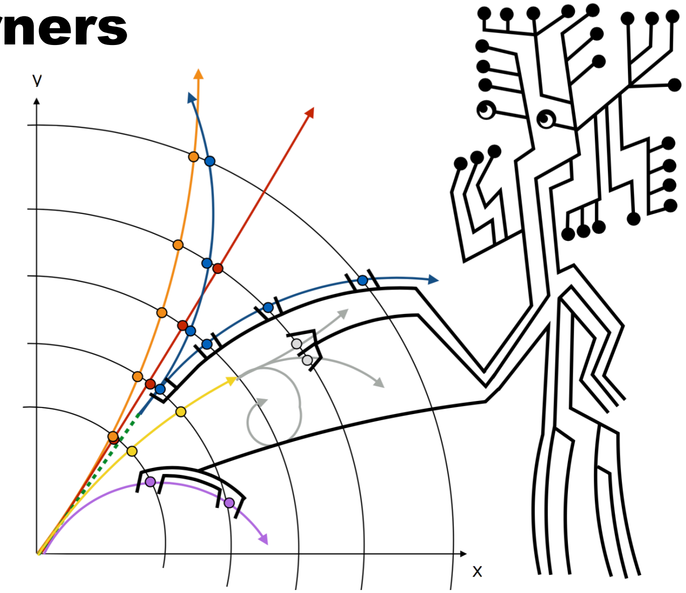






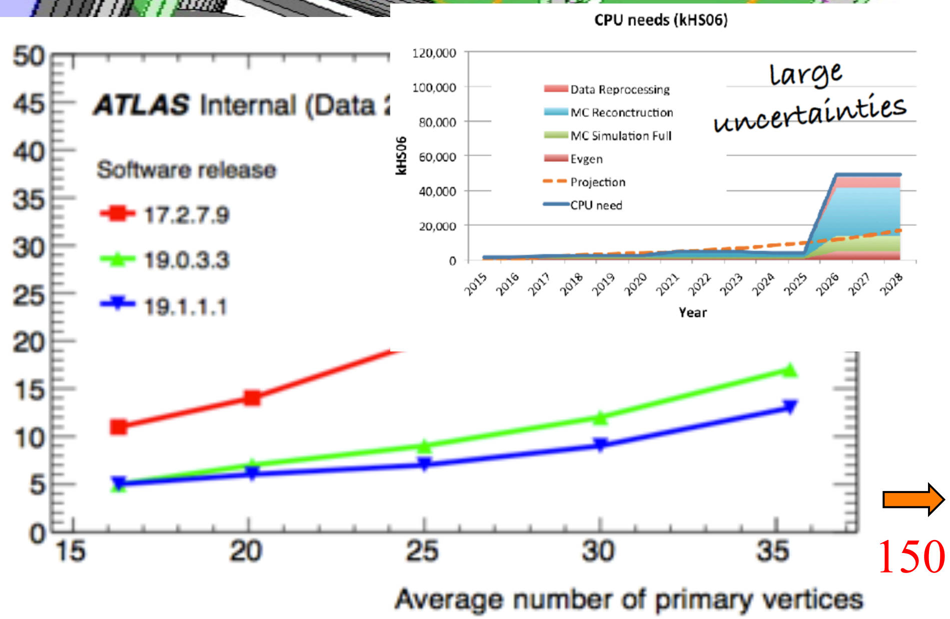
Tracking Machine Learning challenge 2018

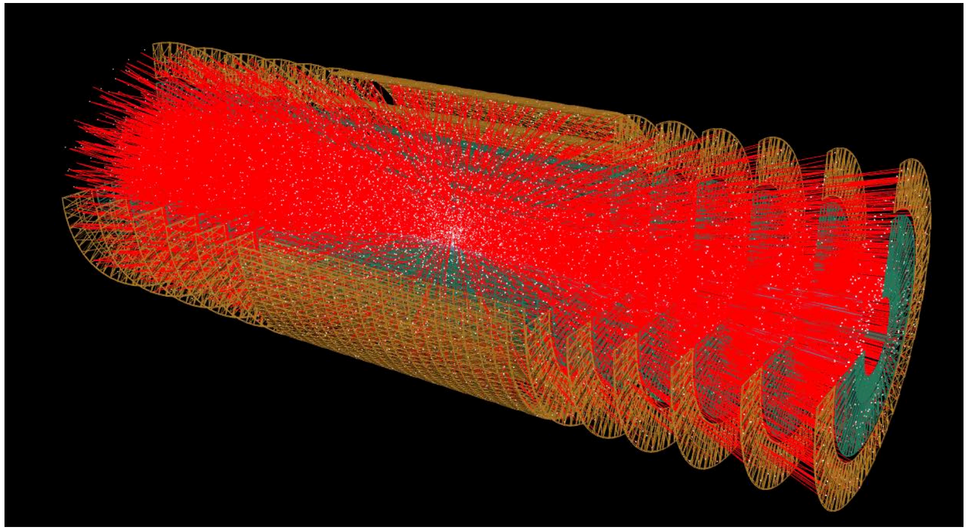
A collaboration between ATLAS and CMS physicists, and Machine Learners



TrackML : Motivation

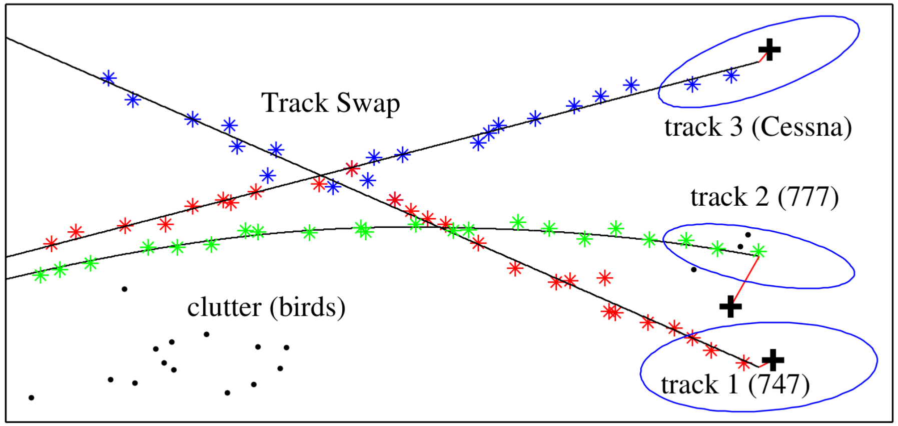
- Tracking (in particular pattern recognition) dominates reconstruction CPU time at LHC
- HL-LHC (phase 2) perspective : increased pileup :Run 1 (2012): <>~20, Run 2 (2015): <>~30,Phase 2 (2025): <>~150
- CPU time quadratic/exponential extrapolation (difficult to quote any number)
- Large effort within 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
- Follow us on twitter @trackmllhc !

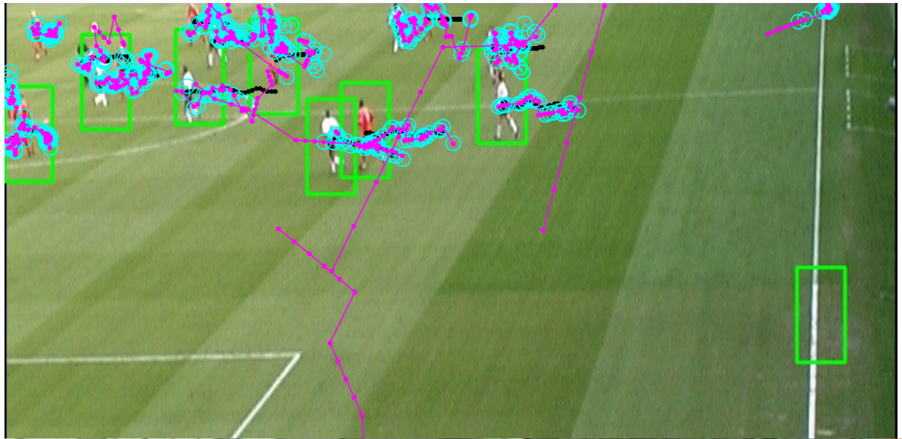


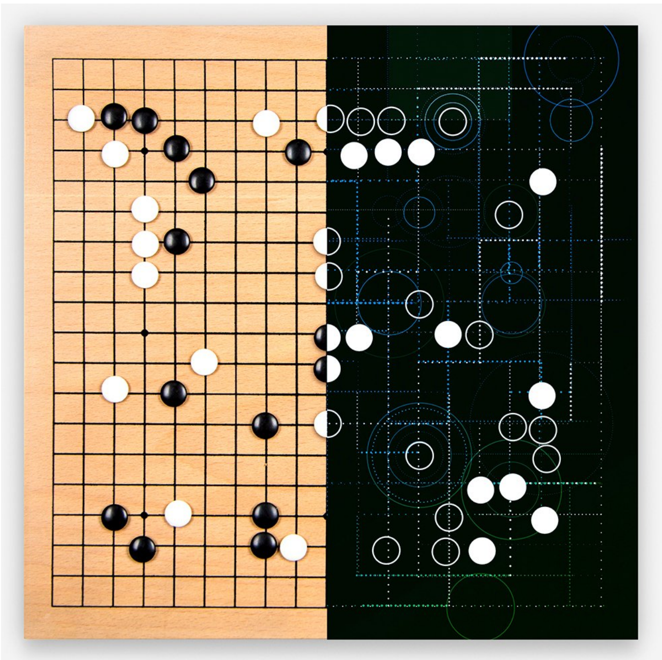


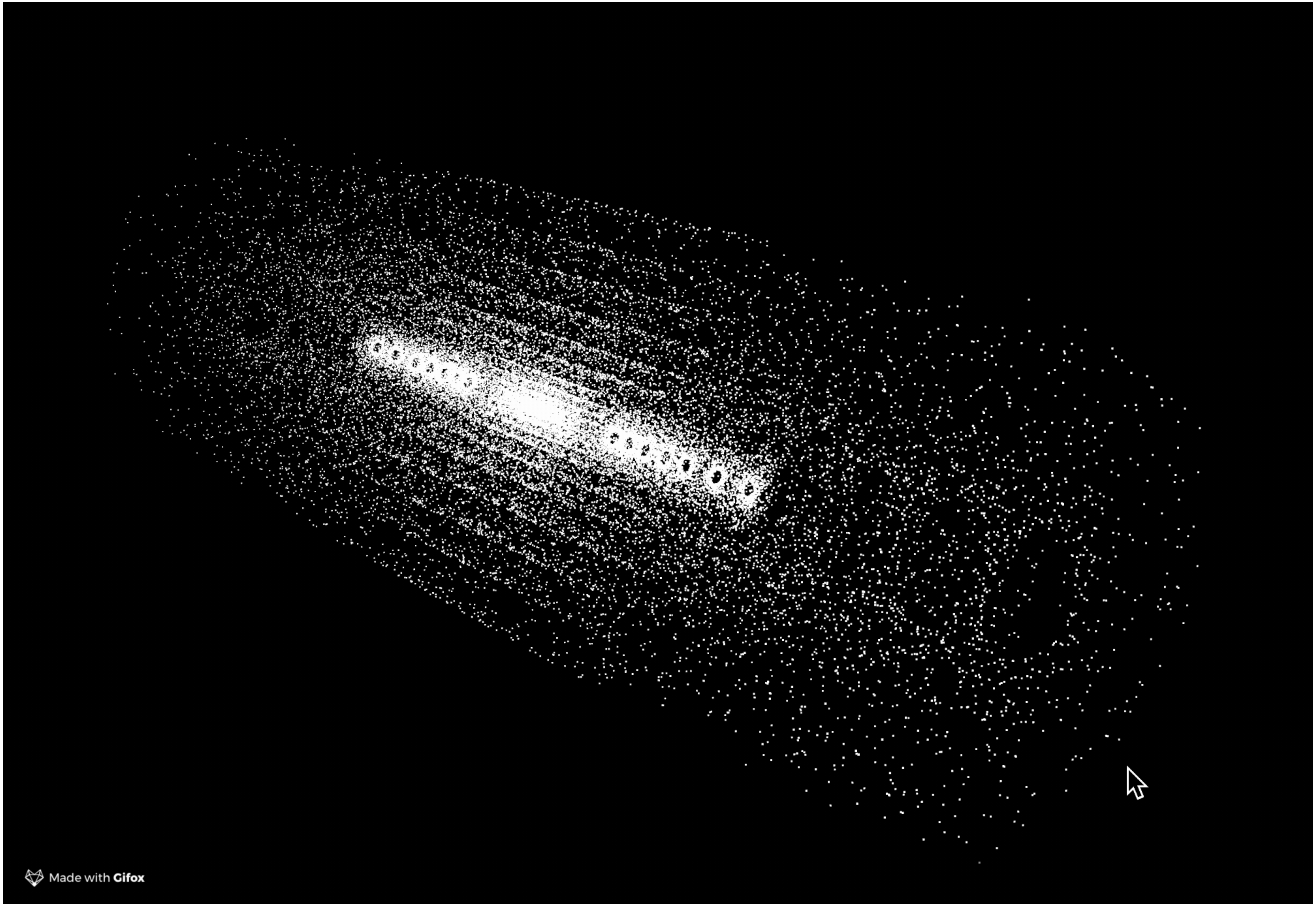
Pattern Recognition/Tracking

- 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








Made with Gifox

TrackML Leaderboard 15/05/08

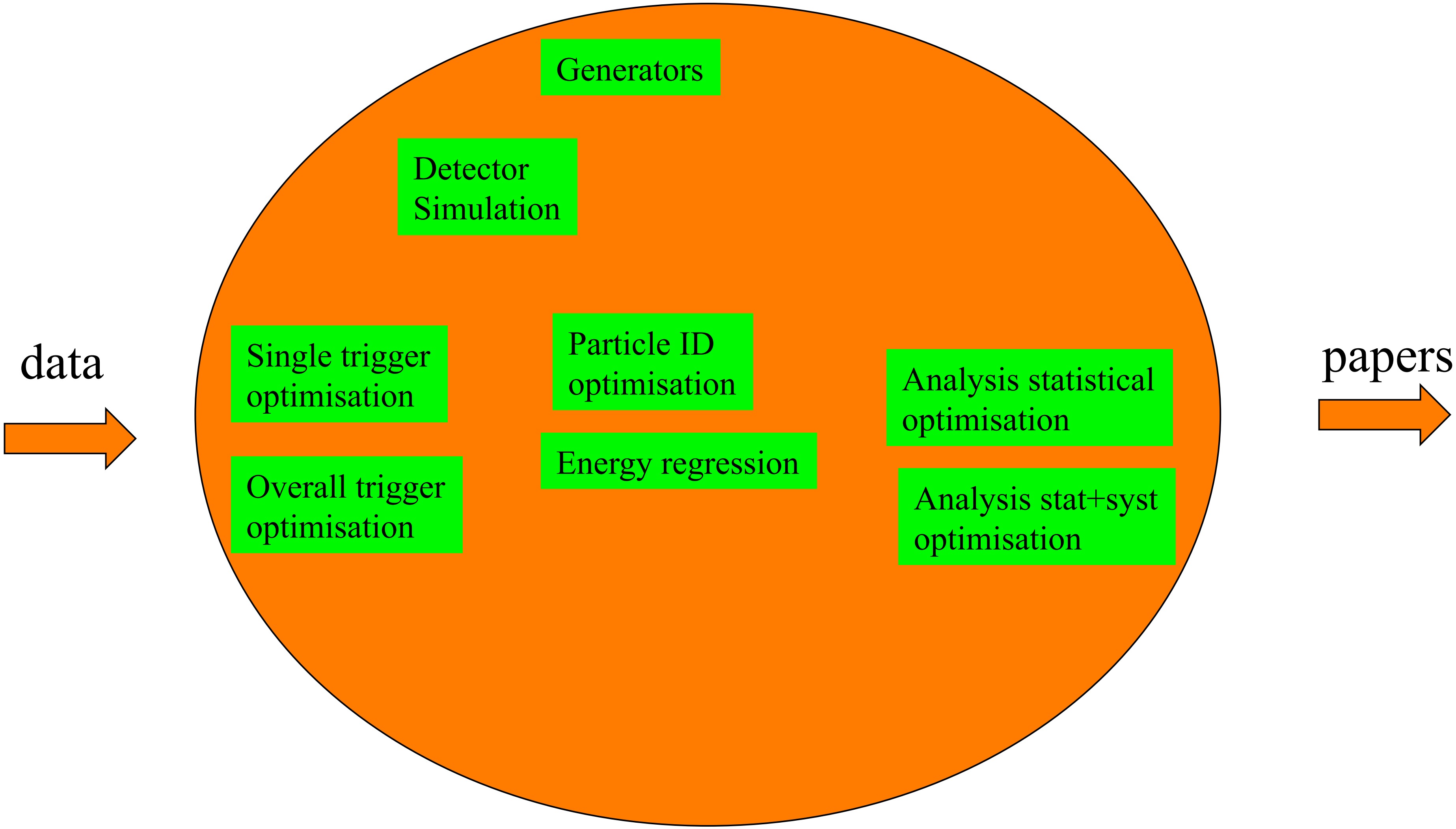
https://www.kaggle.com/c/trackml-particle-identification/leaderboard

~fraction of points correctly assigned

#	△1w	Team Name	Kernel	Team Membe...	Score	Entr...	Last
1	▲1	**Mickey**			0.4610	5	8h
2	▼1	**Grzegorz Sionkowski**			0.4225	6	3d
3	new	**Konstantin Lopuhin**			0.3254	3	1d
4	new	**Lin12345**			0.2969	7	1d
5	▲3	**Heng CherKeng**			0.2886	20	2d
6	▼3	**TeraFlops**			0.2819	14	6d
7	▲56	**Austin&Yair**			0.2697	10	2d
8	new	**Kimura**			0.2673	8	14h
9	▲3	**PEQNP . TECH**			0.2661	33	2h
10	—	**Bhaskar Lachman Khub...**			0.2630	43	14h
11	new	**FlaDM**			0.2610	2	15h

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
- Note : Yandex Data School of Analysis (with ~10 ML scientists) now a bona fide institute of LHCb
- 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

- 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:
  - We (ATLAS) initially saw its use for outreach purposes (CMS has been more open on releasing raw data)
  - But after all, ML collaboration is a kind of scientific outreach
  - ➔ATLAS uploaded there in 2015 the data from Higgs Machine Learning challenge (essentially 4-vectors from full G4 ATLAS simulation Higgs->tautau analysis)
  - ATLAS consider releasing more datasets dedicated to ML studies

Collection of links

- In addition to workshops mentioned in the first transparencies, and references mentioned in the talks
- Interexperiment Machine Learning group (IML) is gathering speed (documentation, tutorials, etc…). Topical monthly meeting. Workshop 20-22 March :
- An internal ATLAS ML group has started in June 2016. In CMS in June 2017
- https://higgsml.lal.in2p3.fr
- http://opendata.cern.ch/collection/ATLAS-Higgs-Challenge-2014: permanent home of the challenge dataset
- NIPS 2014 workshop agenda and proceedings http://jmlr.org/proceedings/papers/v42/
- Mailing list opened to any one with an interest in both Data Science and High Energy Physics : HEP-data-science@googlegroups.com and lhc-machinelearning-wg@cern.ch
- IN2P3 project starting – http://listserv.in2p3.fr/cgi-bin/wa?A0=MACHINE-LEARNING-L open to anyone with some interest to ML (planning on 2 x 1day workshop per year)
- NIPS 2017 DL in HEP workshop
- IN2P3 School of Statistics 28 May 1 June 2018 To be Confirmed (see SoS 2016)

Conclusion

- 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
- More and more open datasets/simulators
- More and more HEP and ML workshops, forums, schools, challenges
- More and more direct collaboration between HEP researchers and ML researchers
- HEP will need more and more access to (GPU) training resources
- Never underestimate the time for :
  - (1) Great ML idea➔
  - (2) …demonstrated on toy dataset➔
  - (3) …demonstrated on real experiment analysis/dataset ➔
  - (4) …experiment publication using the great idea