Advances in Machine Learning tools in High Energy Physics

David Rousseau

LAL-Orsay

rousseau@lal.in2p3.fr

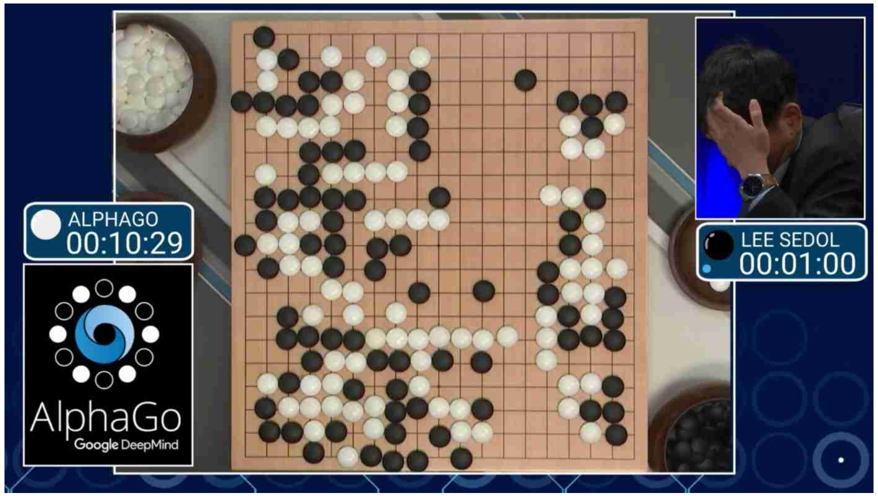
SPP Seminar, Monday 9th May

Outline

- Basics
- ML software tools
- ML techniques
- ML in analysis
- ML in reconstruction/simulation
- Data challenges
- Wrapping up

ML in HEP

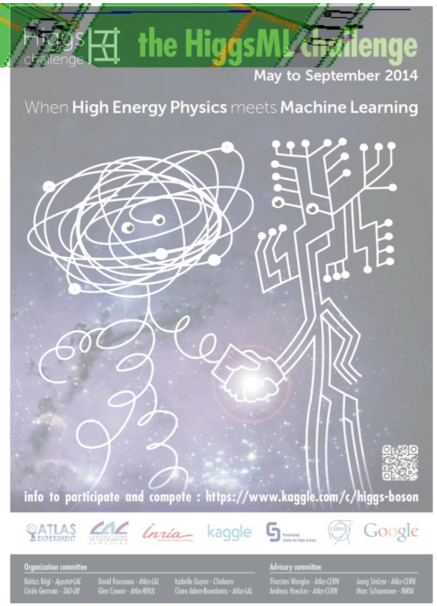
- Use of Machine Learning (a.k.a Multi Variate Analysis as we used to call it) already at LEP somewhat (Neural Net), more at Tevatron (Trees)
- At LHC, Machine Learning used almost since first data taking (2010) for reconstruction and analysis
- In most cases, Boosted Decision Tree with Root-TMVA
- Meanwhile, in the outside world :

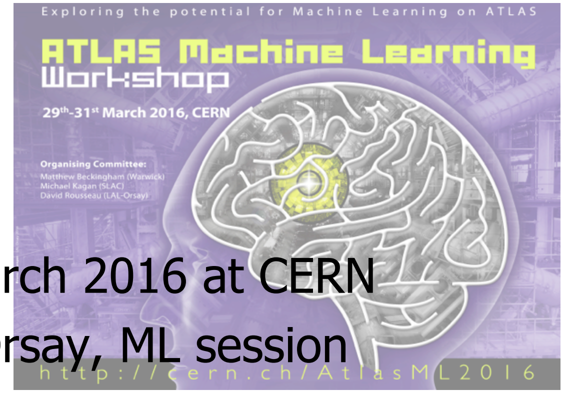


- “Artificial Intelligence” not a dirty word anymore!
- We’ve realised we’re been left behind! Trying to catch up now…

Multitude of HEP-ML events

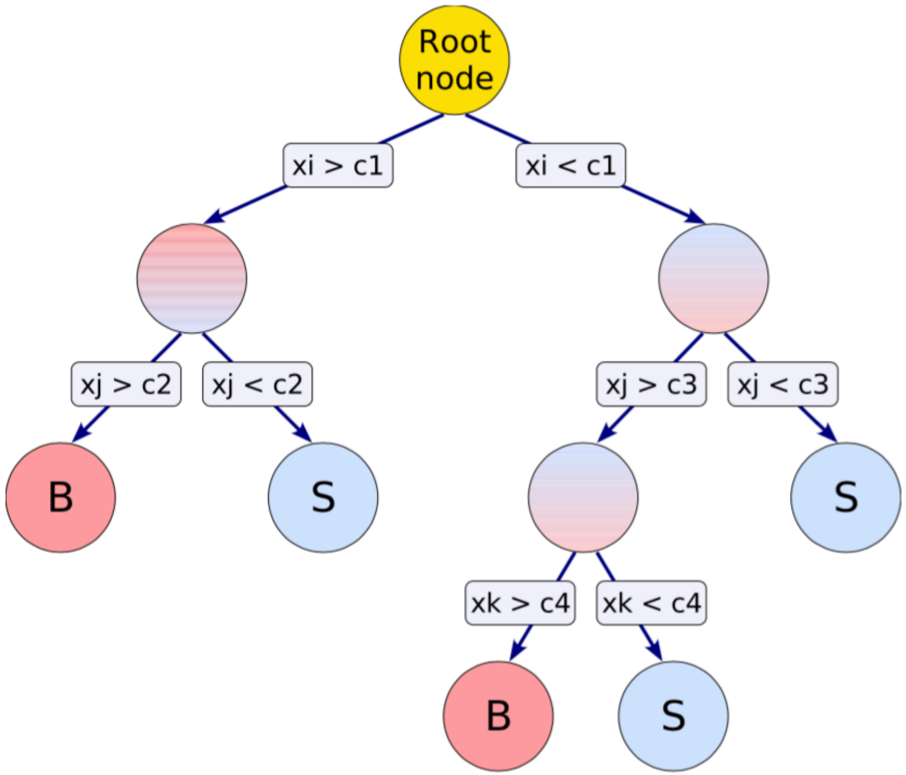
- HiggsML Challenge, summer 2014
  - ➔HEP ML NIPS satellite workshop, December 2014
- Connecting The Dots, Berkeley, January 2015
- Flavour of Physics Challenge, summaer 2015
  - ➔HEP ML NIPS satellite workshop, December 2015
- DS@LHC workshop, 9-13 November 2015
  - ➔future DS@HEP workshop
- LHC Interexperiment Machine Learning group
  - Started informally September 2015, gaining speed
- 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
- (internal) ATLAS Machine Learning workshop 29-31 March 2016 at CERN
- Hep Software Foundation workshop 2-4 May 2016 at Orsay, ML session
- TrackML Challenge, fall 2016





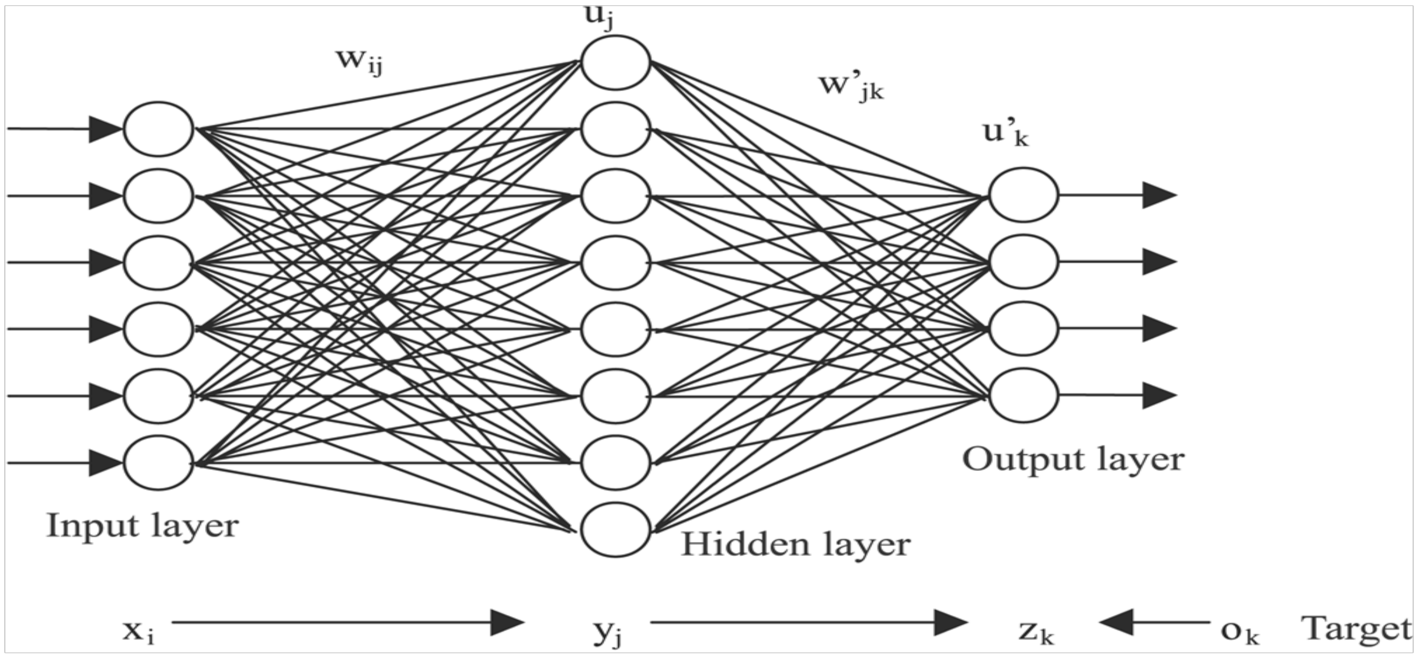
ML Basics

BDT in a nutshell



- Single tree (CART) <1980
- AdaBoost 1997 : rerun increasing the weight of misclassified entries ➔boosted trees

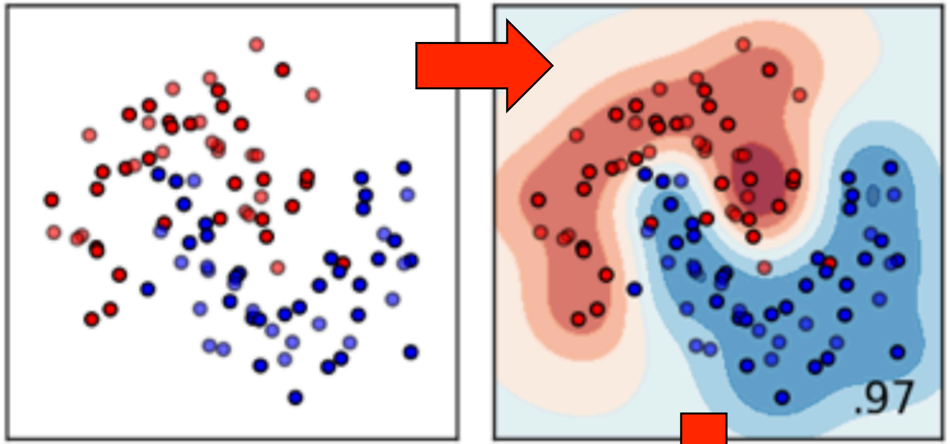
Neural Net in a nutshell

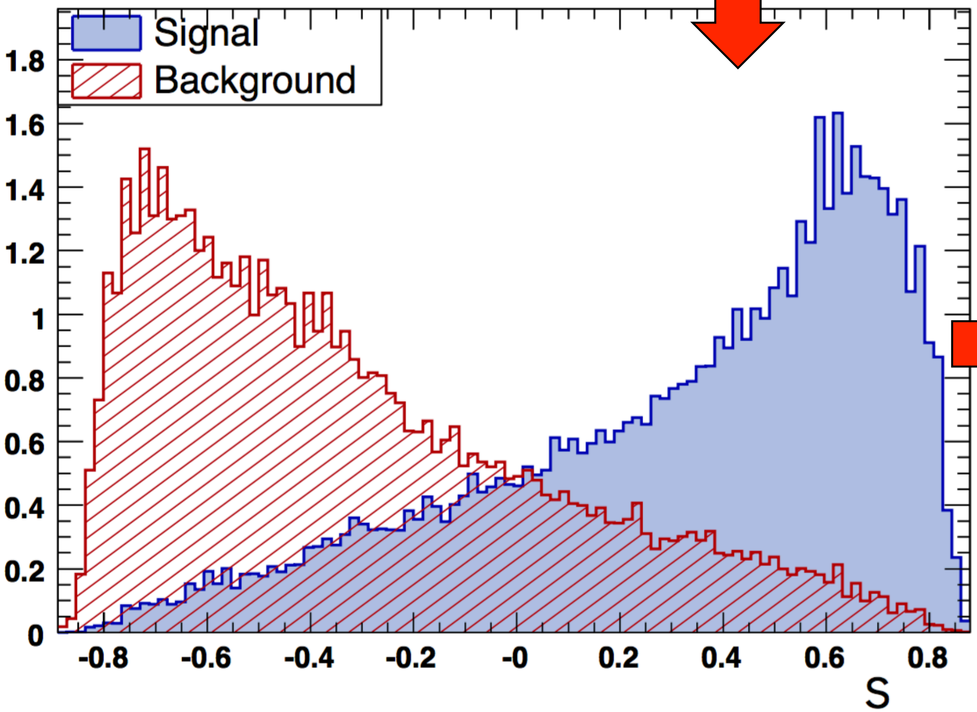


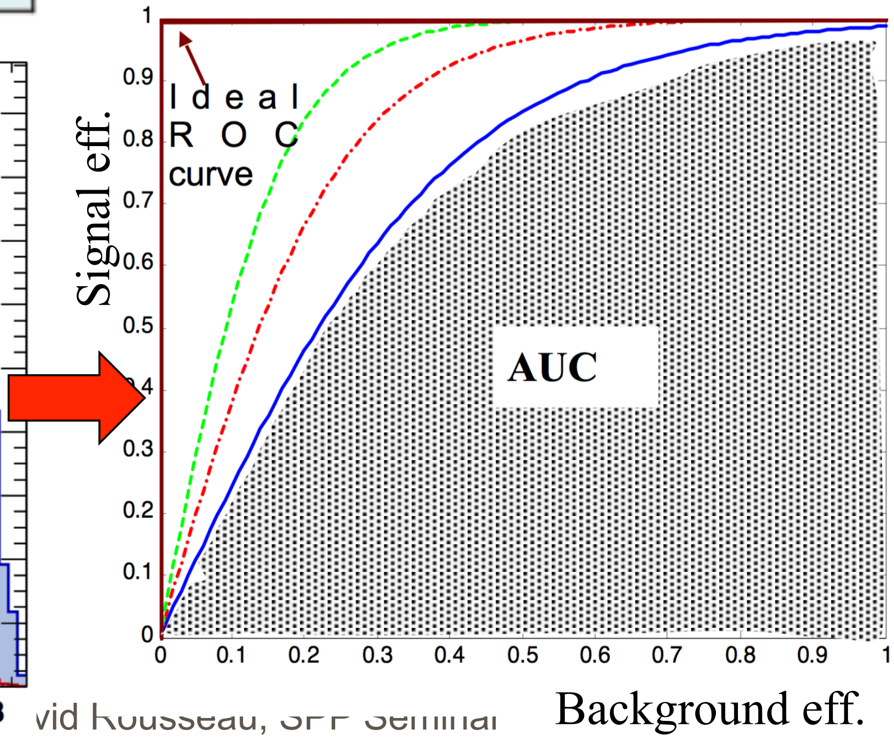
- Neural Net ~1950!
- But many many new tricks for learning, in particular if many layers (also ReLU instead of sigmoïd activation)
- Computing power (DNN training can take days even on GPU)

Any classifier

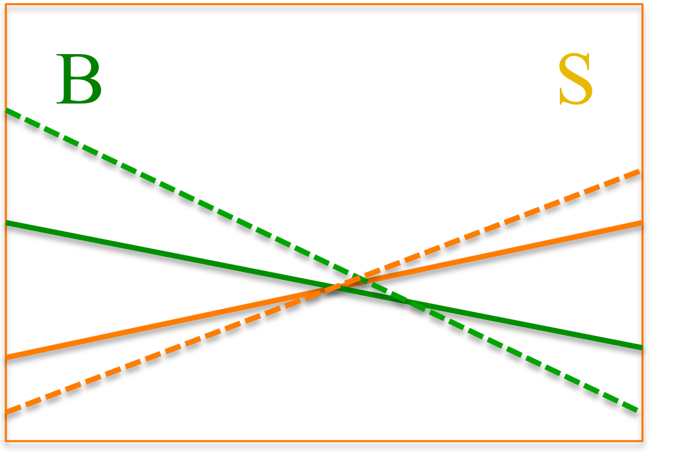
Classification : learn label 0 or 1
Regression : learn continuous variable

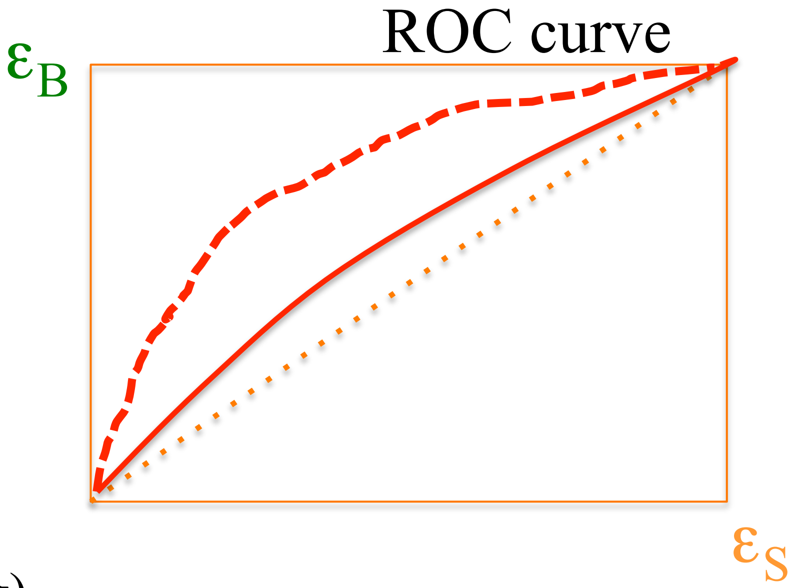






Overtraining



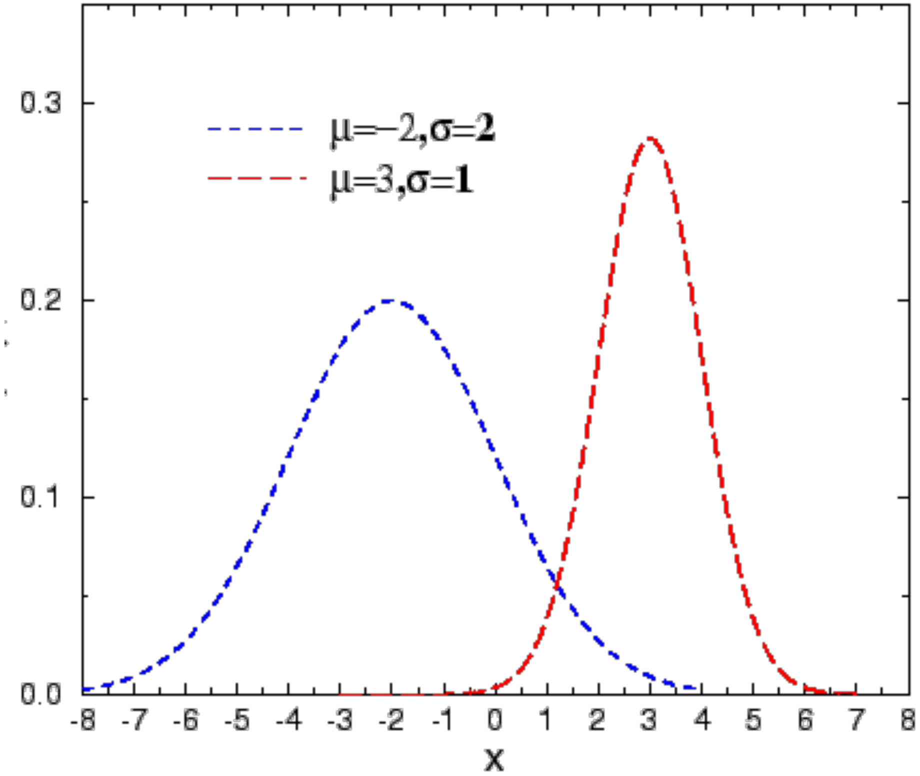


Evaluated on training dataset (wrong)

Evaluated on independent dataset (correct)

No miracle

- ML does not do miracles
- If underlying distributions are known, nothing beats Likelihood ratio! (often called "bayesian limit")
- ML starts to be interesting when there is no proper formalism of the pdf

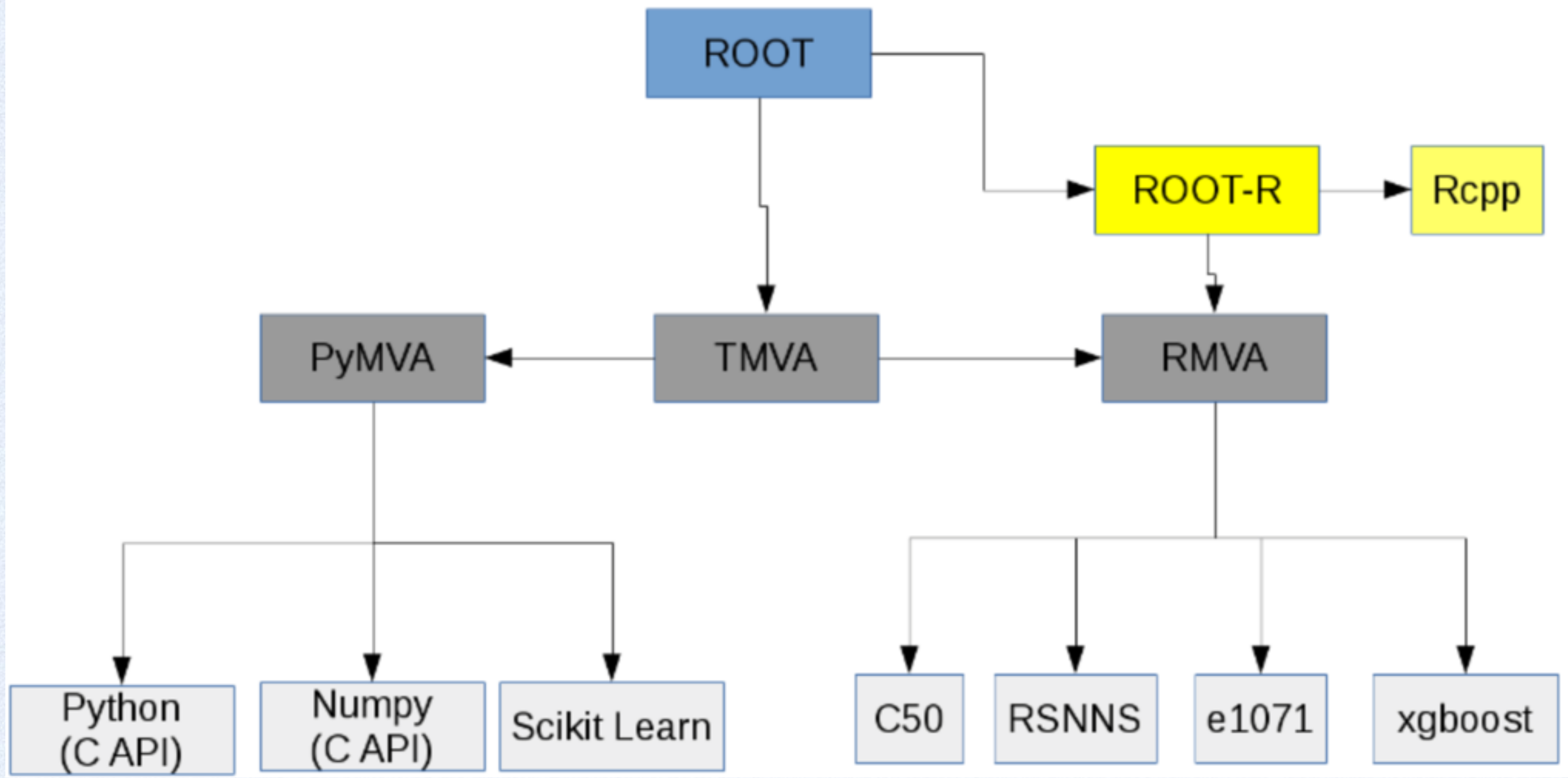


ML Tools

ML Tool : TMVA

- Root-TMVA de-facto standard for ML in HEP
- Has been instrumental into “democratising” ML at LHC (at least)
- Well coupled with Root (which everyone uses)
- But:
  - Has sterilized somewhat the creativity
  - Mostly frozen the last few years, left behind
- However:
  - Rejuvenating effort since summer 2015
  - Revise structure for more flexibility
  - Improve algorithms
  - Interface to the outside world
- See talk Lorenzo Moneta at Hep Software Fondation workshop at LAL last week

TMVA interfaces ROOT v>= 6.05.02



ML Tool : XGBoost

- XGBoost : Xtreme Gradient Boosting :
  https://github.com/dmlc/xgboost, arXiv:1603.02754
- Written originally for HiggsML challenge
- Used by many participants, including number 2
- Meanwhile, used by many other participants in many other challenges
- Open source, well documented, and supported
- Best BDT on the market, performance and speed
- Classification and regression

ML Tool : SciKit-learn

- SciKit-Learn : Machine Learning in python
- Modern Jupyter interface (notebook à la Mathematica)
- Open source (several core developers in Paris-Saclay)
- Built on NumPy, SciPy, and matplotlib
- (very fast, despite being python)
- Install on any laptop with Anaconda
- All the major ML algorithms (except deep learning)
- Superb documentation
- Quite different look and fill from Root-TMVA
- Short demo (Navigator should be started)

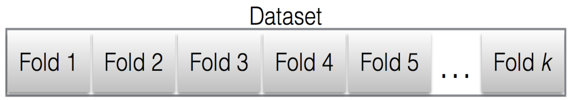
ML platforms

- Training time can become prohibitive (days), especially Deep Learning, especially with large datasets
- With hyper-parameter optimisation, cross-validation, number of trainings for a particular application large ~100
- Emergence of ML platforms :
  - Dedicated cluster (with GPUs)
  - Relevant software preinstalled (VM)
  - Possibility to load large datasets (GB to TB)

ML Techniques

Cross Validation

- Cross Validation (CV) are techniques to measure MVA performance independently of the training
- Goal is to build an optimisation curve (e.g. significance, ROC,..) with the smallest variance (despite lack of data), for a better optimisation of hyper parameters or choice of techniques
- Default TMVA CV (one fold CV):
  - o split sample in two halves A and B.
  - o train on A, test on B
- Two-fold CV (e.g. ATLAS Htautau analysis)
  - o Split sample in two halves A and B
  - o Train on A, test on B; train on B test A
  - o ➔test statistics = total statistics➔double test statistics wrt one fold CV (double training time of course)
- n-fold CV (very standard technique in ML)
  - o Split sample in n e.g. 5 equal pieces A,B,C,D and E
  - o Train on ABCD, test on E;train on ABCE, test on D; etc…
  - o ➔same test statistics wrt two-fold CV, but larger training statistics 4/5 over ½ (larger training time as well)
  - o bonus: variance of the samples an estimate of the statistical uncertainty
- Nested CV : if hyper-parameters tuned using CV, need an independent measurement of the final performance
- Technique being integrated in TMVA



- Split the dataset into k randomly sampled independent subsets (folds).
- Train classifier with k-1 folds and test with remaining fold.
- Repeat k times.

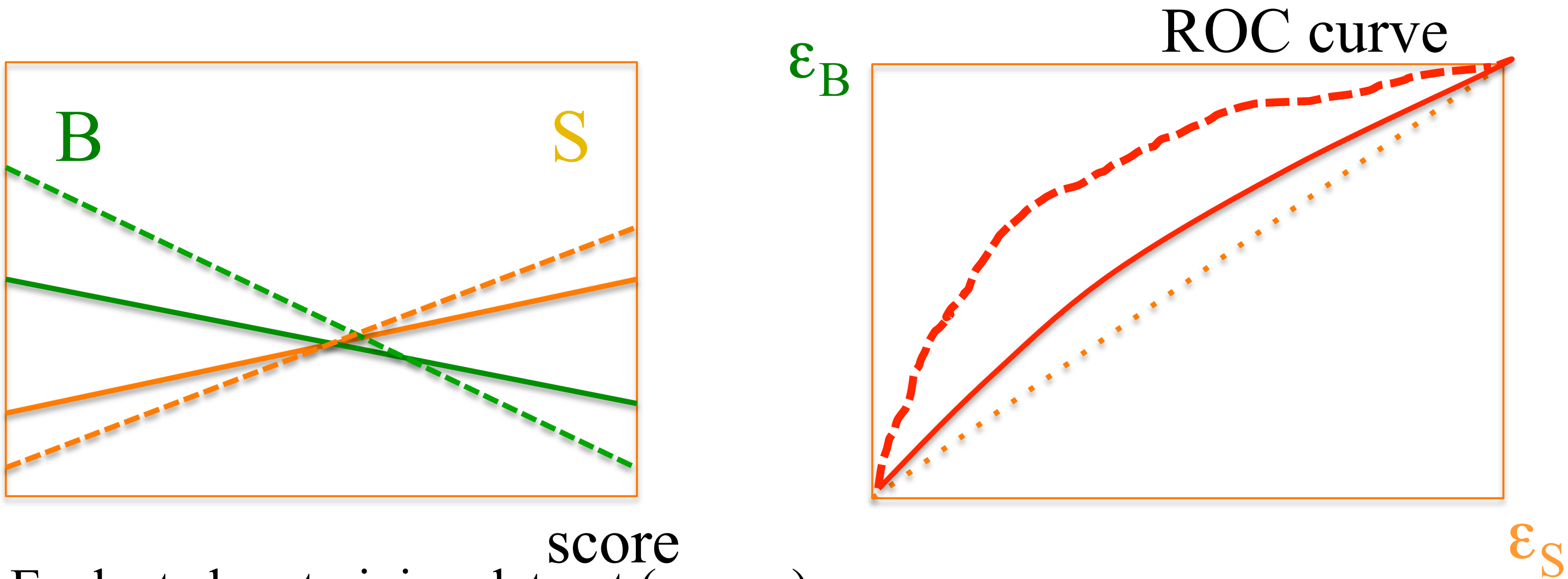
$$E = \frac{1}{k}\sum_{i=1}^{k} E_i.$$

CV, under/over training

Gilles Louppe, github

Some overtraining is good!

(reminder) Overtraining

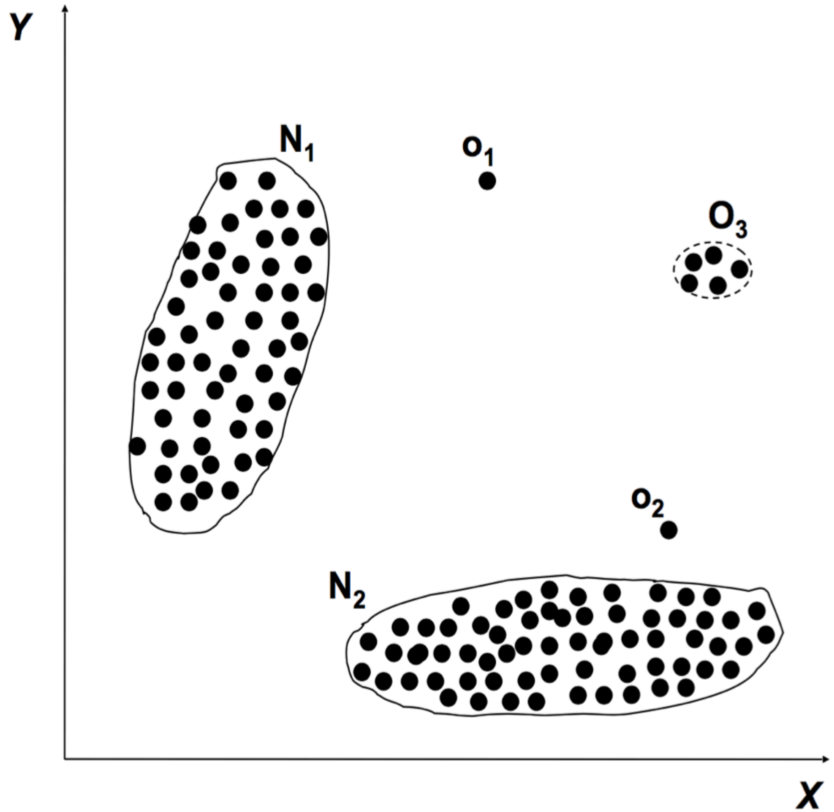


Evaluated on training dataset (wrong)

Evaluated on independent dataset (correct)

Anomaly : point level

- Also called outlier detection
- Two approaches:
  - Give the full data, ask the algorithm to cluster and find the lone entries : o1, o2, O3



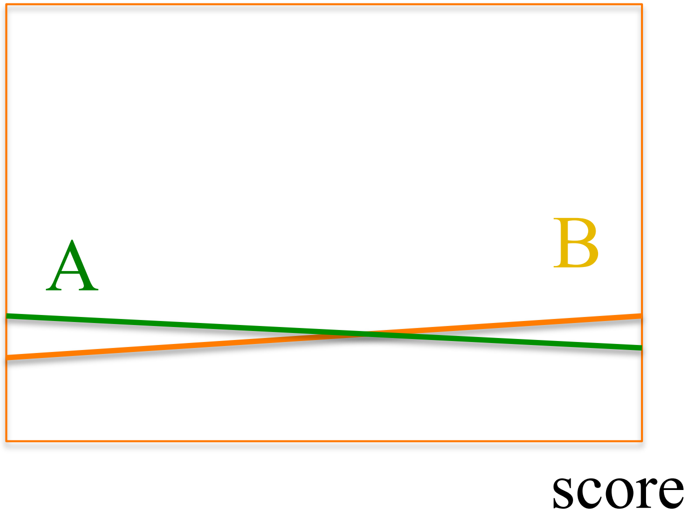
  - We have a training "normal" data set with N1 and N2. Algorithm should then spot o1,o2, O3 as "abnormal" i.e. "unlike N1 and N2" (no a priori model for outliers)
- Application : detector malfunction, grid site malfunction, or even new physics discovery...

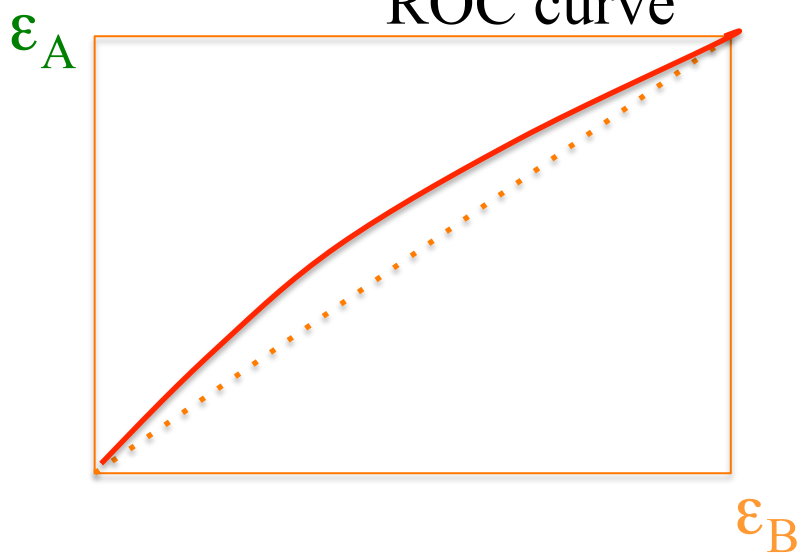
Anomaly : population level

- Also called collective anomalies
- 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
  - Derivation V12, Derivation V13
  - G4 Release 20.X.Y, release 20.X.Z
  - Production at CERN, production at BNL
  - 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)
- ML approach : ~~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

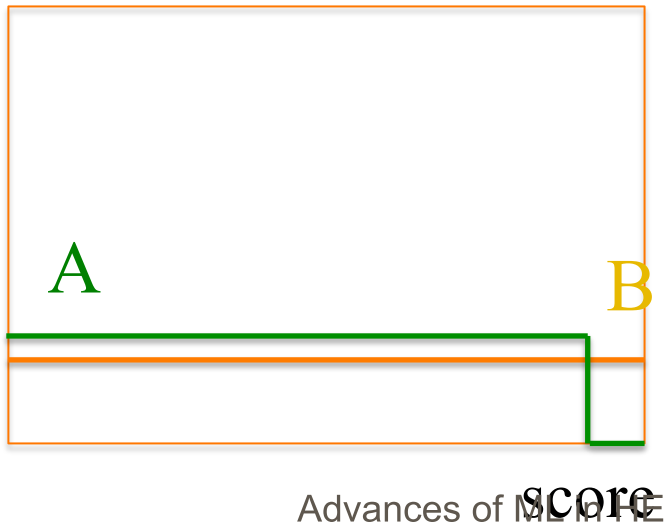
Small non-local difference

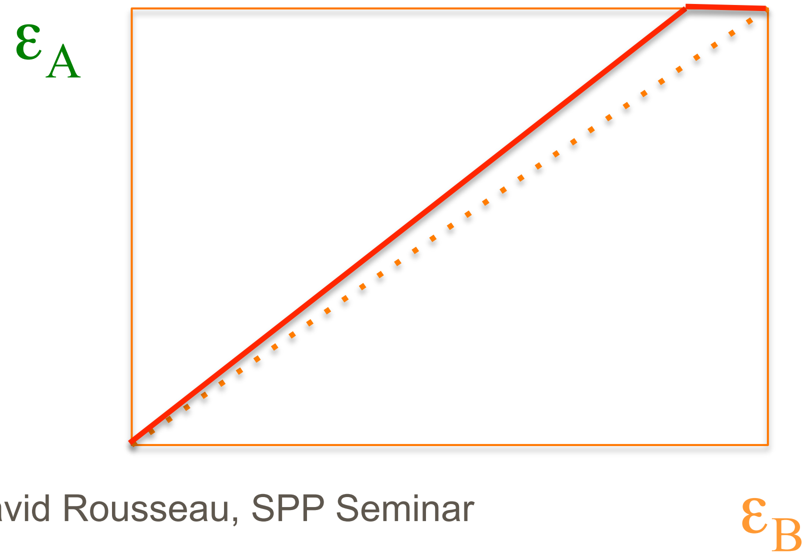
ROC curve





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

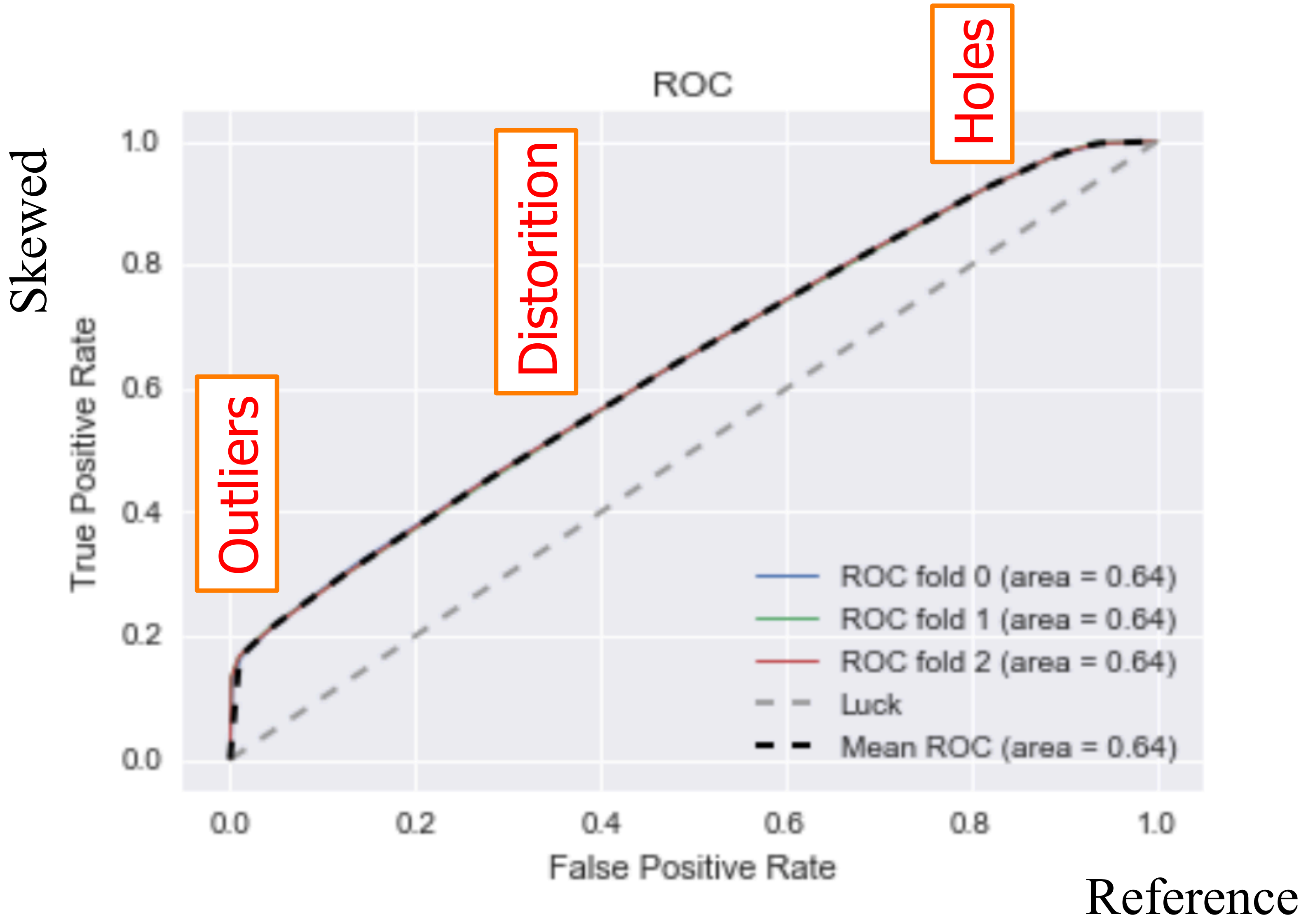




HSF ML RAMP on anomaly

- RAMP : collaborative competition around a dataset and a figure of merit. Organised by CDS Paris Saclay with HEP people. See agenda.
- Dataset built from the Higgs Machine Learning challenge dataset (on CERN Open Data Portal)
  - Lepton, and tau hadron 3 momentum, MET : PRImary variables
  - DERived variables (computed from the above) from Htautau analysis
  - Jet variables dropped
- ➔reference dataset
- "Skewed" dataset built from the above, introducing small and big distortions:
  - Small scaling of Ptau
  - Holes in eta phi efficiency map of lepton and tau hadron
  - Outliers introduced, each with 5% probability
    - Eta tau set to large non possible values
    - P lepton scaled by factor 10
    - Missing ET + 50 GeV
    - Phi tau and phi lepton swapped ➔ DERived variables inconsistent with PRImary one
- ➔skewed dataset

HSF ML RAMP on anomaly (2)



HSF RAMP (2)

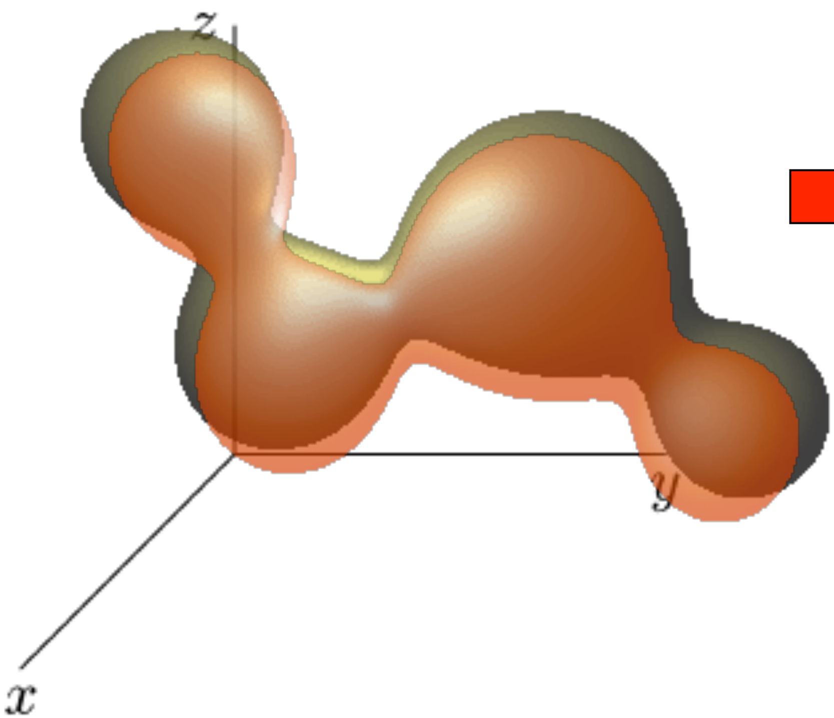
team	submission	accuracy
mcherti	adab2_mt1_calibrated	0.611
dhrou	adab2_mt1	0.611
kazeevn	GradientBoosting	0.596
glouppe	bags2	0.594
glouppe	boosting-duo	0.595
mcherti	adaboost2	0.594
glouppe	bags	0.593
mcherti	adaboost1	0.593
djabbz	beta tester	0.591
soobash	ExtraTreesClassifier	0.576
mcherti	extratrees1	0.562
dhrou	DRv0	0.553
calaf	starting_kit_paolo	0.526

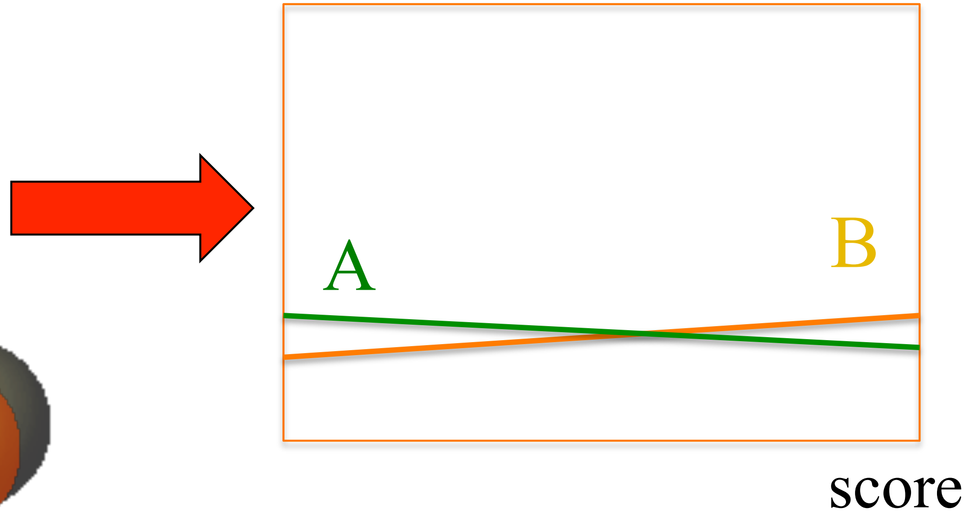
Breakthrough : add new variable:
$\Delta m_T=\sqrt{(2P_{lT}*MET*(1-\cos(\phi_l-\phi_{MET})))}-m_T$
Non zero for some outliers
➔classifiers were unable to guess it

Classifier optimisation

➔what functional form classifiers can learn ?

What does a classifier do?

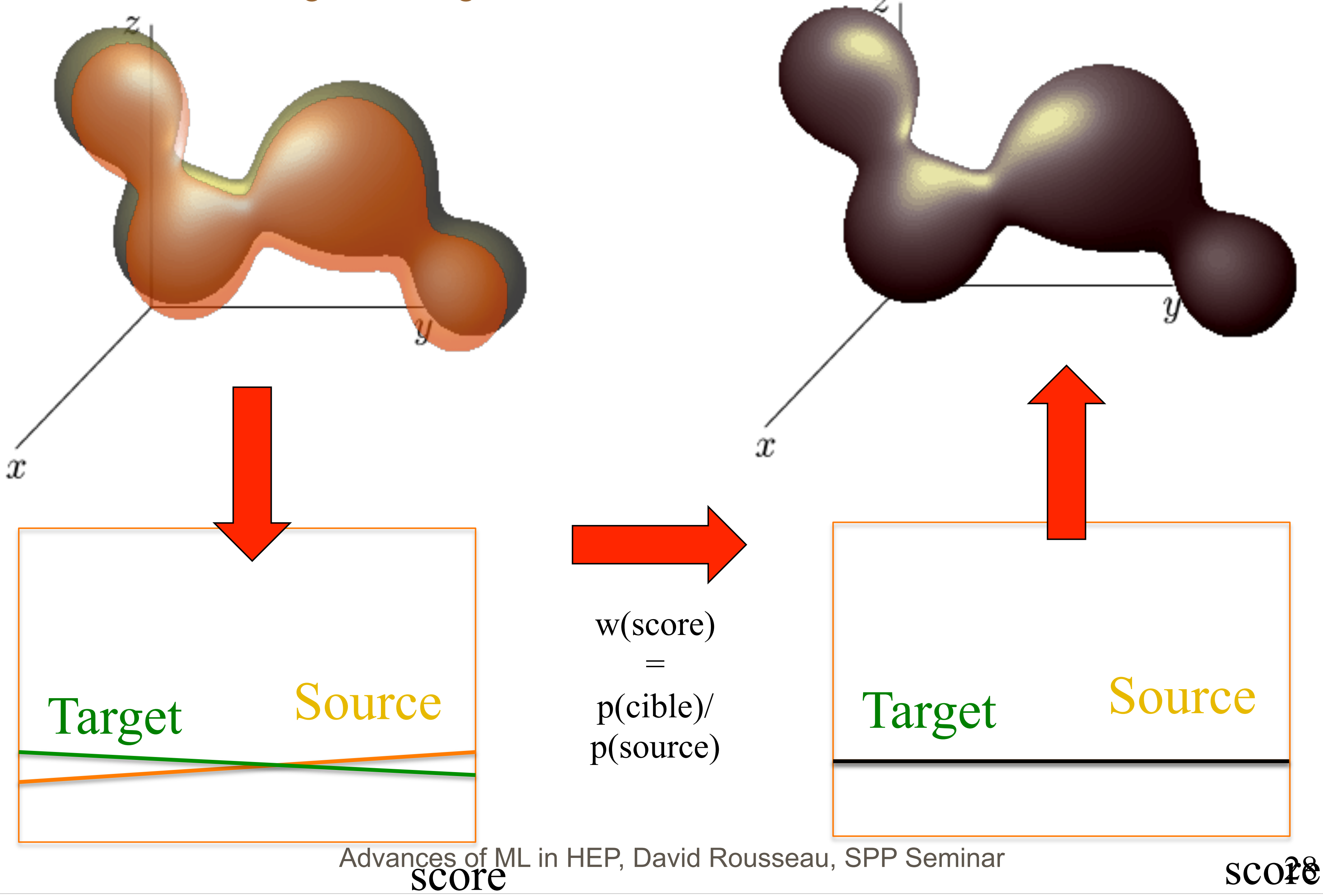




- The classifier "projects" the two multidimensional "blobs" maximising the difference, without (ideally) any loss of information

Multidimension reweighting

See demo on Andrei Rogozhnikov github



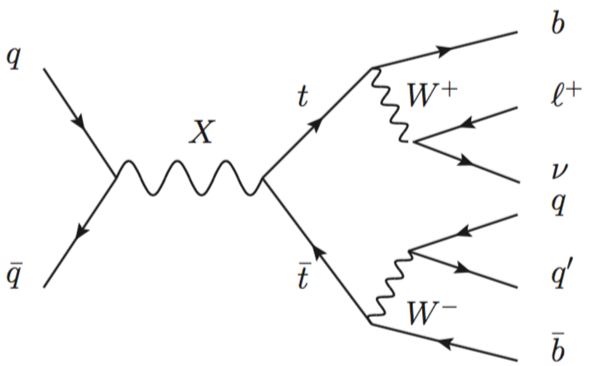
Multi dimensional reweighting (2)

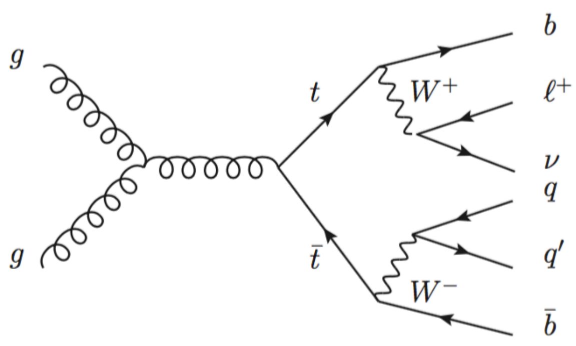
- Reweighting usually done one 1D projection, at best 2D, because of quick lack of statistics
- Reweighting the Source distribution on the score allows multidimensional reweighting without statistics problem
- Usual caveat still hold : Target support should be included in Source support, distributions should not be too different otherwise unmanageable very large or very small weights
- (Note : “reweighting” in HEP language <==> “importance sampling” in ML language)

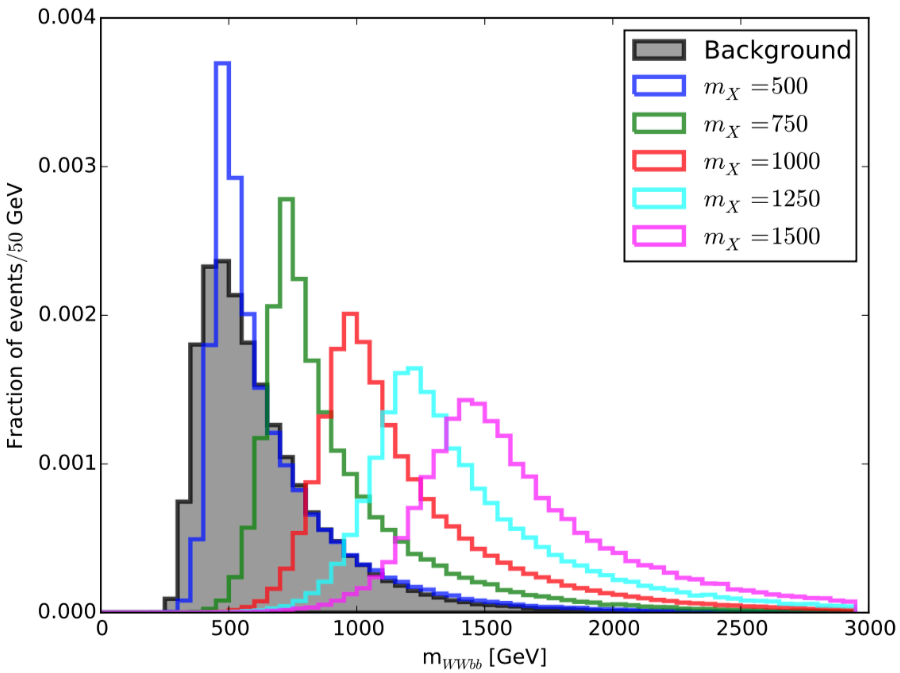
ML in analysis

Parameterised learning

1601.07913 Baldi, Cranmer, Faucett, Sadowksi, Whiteson

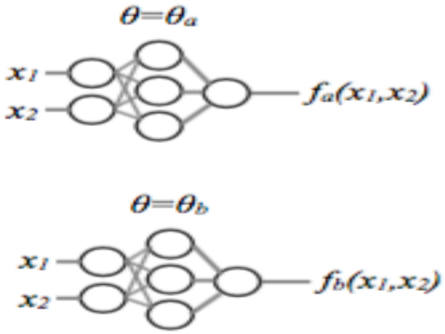


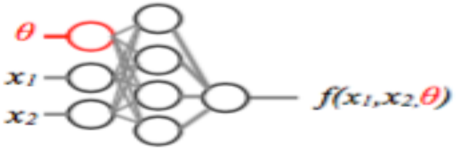


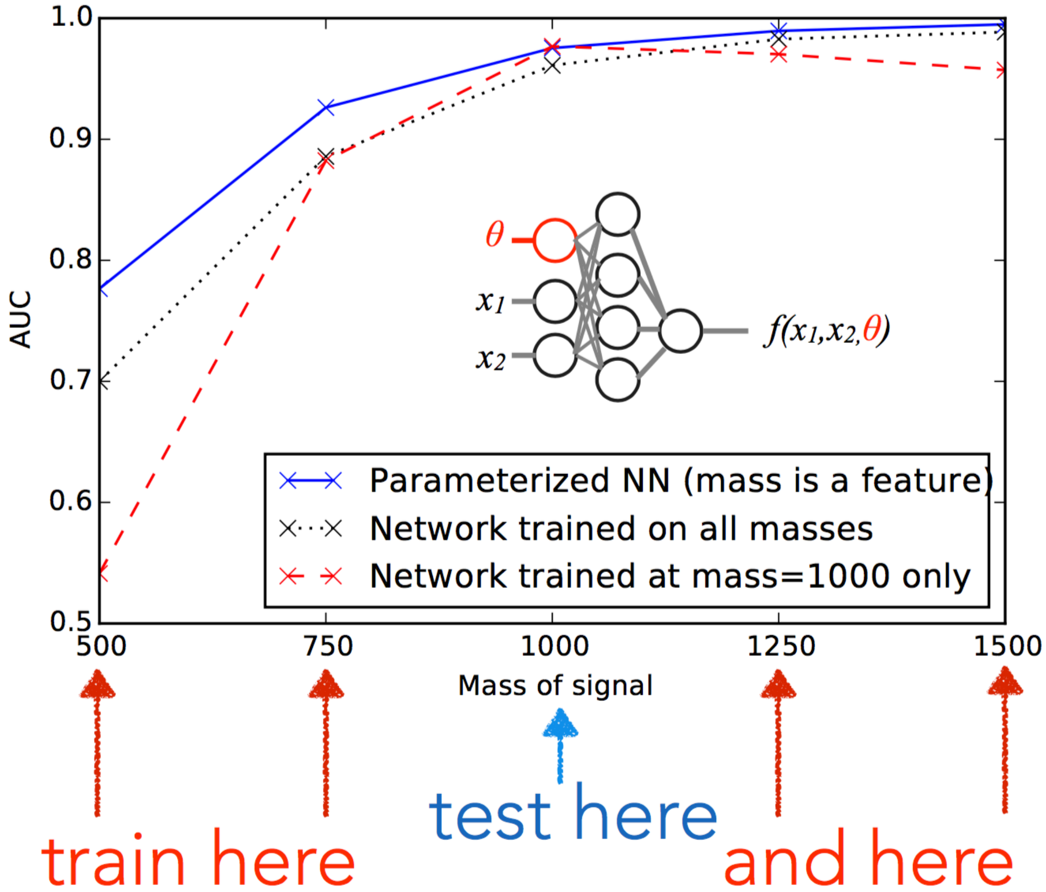


- Typical case: looking for a particle of unknown mass
- E.g. here tt decay

Parameterised learning (2)







- Train on 28 features plus mass
- Parameterised NN as good as single mass training
- ➔clean interpolation
- (mass just an example)

Systematics

- Our experimental 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)

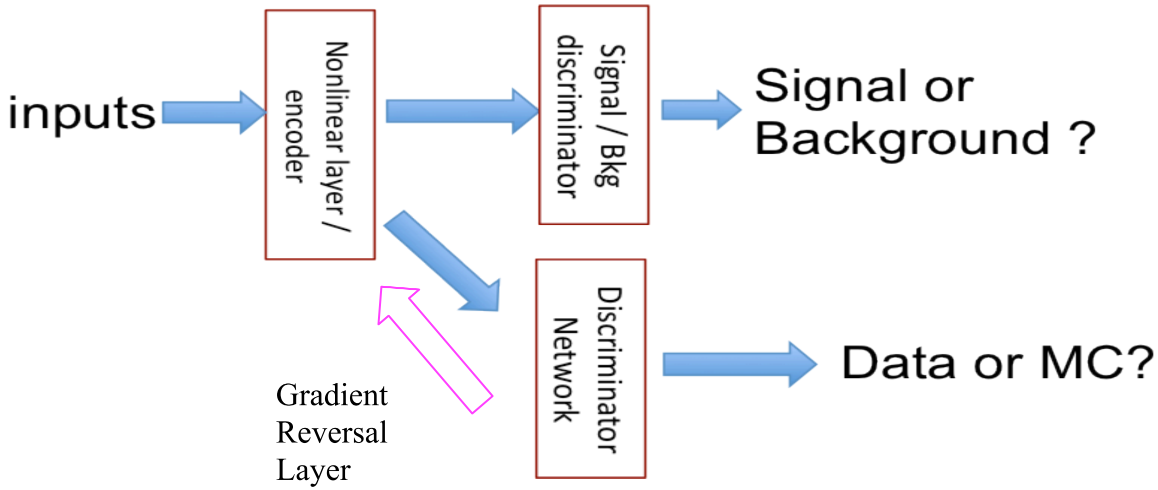
- ML techniques used so far to minimise σ(stat)
- Impact of ML on σ(syst) or even better global optimisation of σ(stat) ± σ(syst) is an open problem
- Worrying about σ(syst) untypical of ML in industry

Systematics (2)

- 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
- One possible approach:

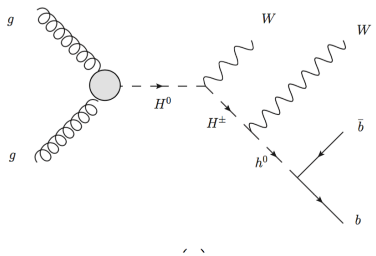
Adversarial neural networks

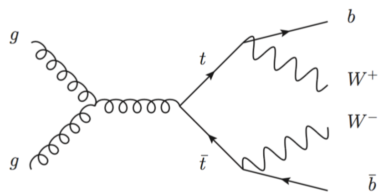
Adapted from : 1505.07818 Ganin, Ustinova, Ajakan, Germain, Larochelle, Laviolette, Marchand, Lempitsky

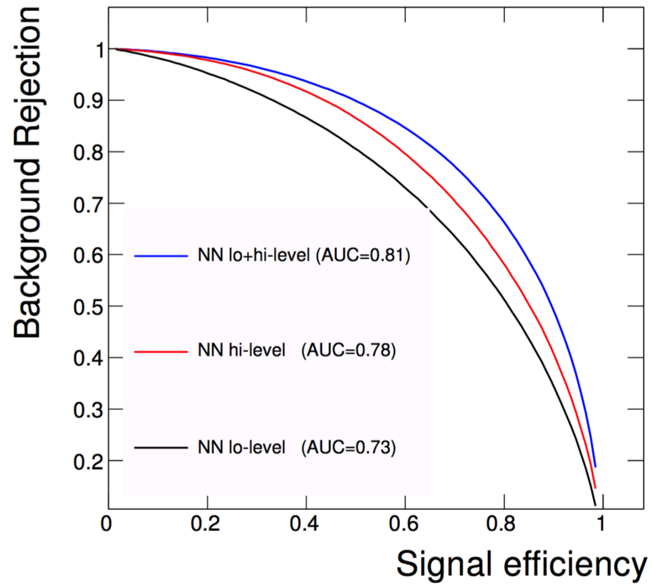


Deep learning for analysis

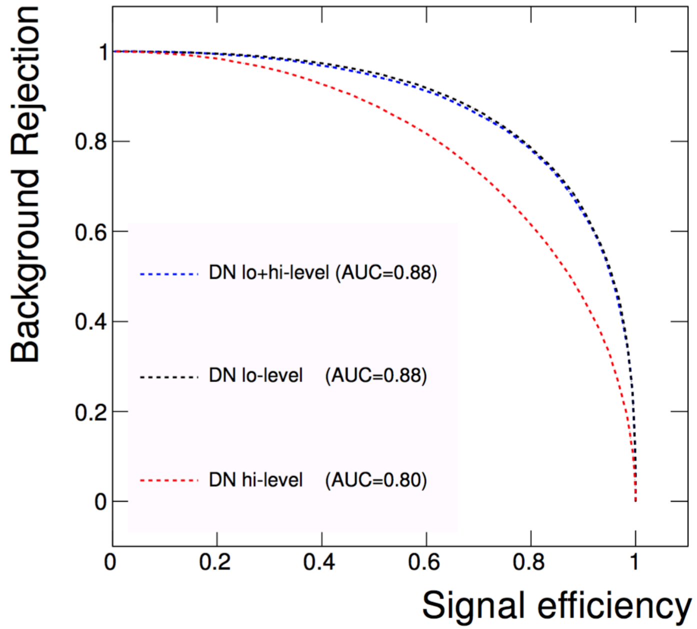
1402.4735 Baldi, Sadowski, Whiteson







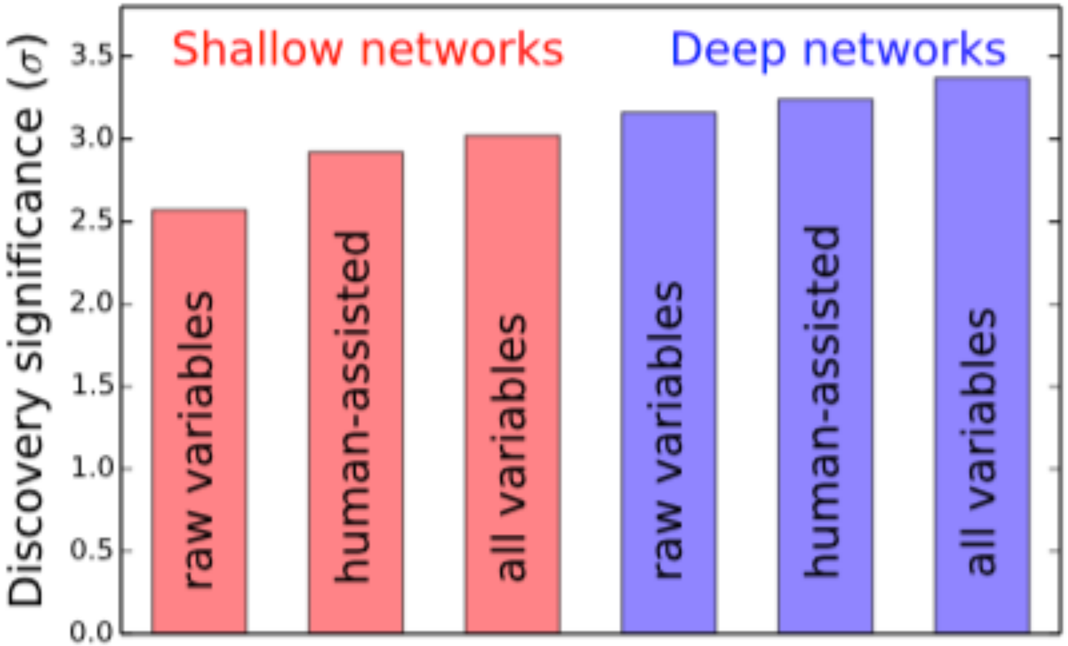
- MSSM at LHC : $H^0 \rightarrow WWbb$ vs $tt \rightarrow WWbb$
- Low level variables:
  - 4-momenta
- High level variables:
  - Pair-wise invariant masses
- Deep NN outperforms NN, and does not need high level variables
- DNN learns the physics ?



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
- ~10M events used for training (>10 full G4 simulation in ATLAS)

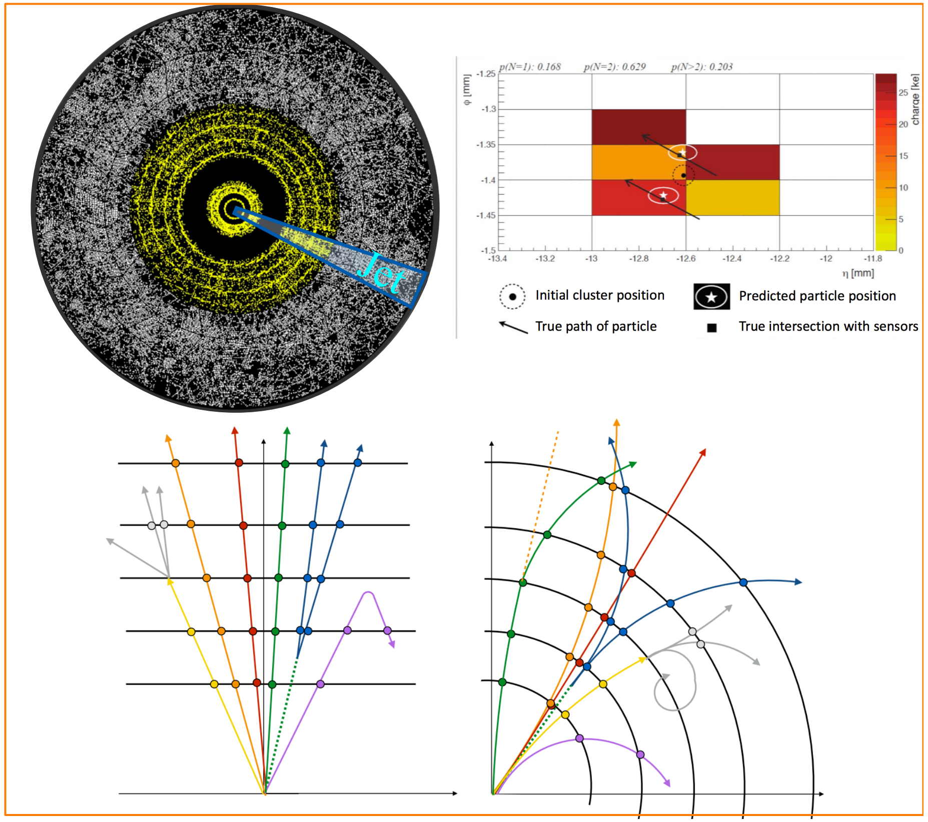
ML in reconstruction

Reconstruction

- Clear upcoming challenges as we approach HL-LHC

- Generally, making everything robust to increased pileup, and resource usage will be vital
  - New techniques needed

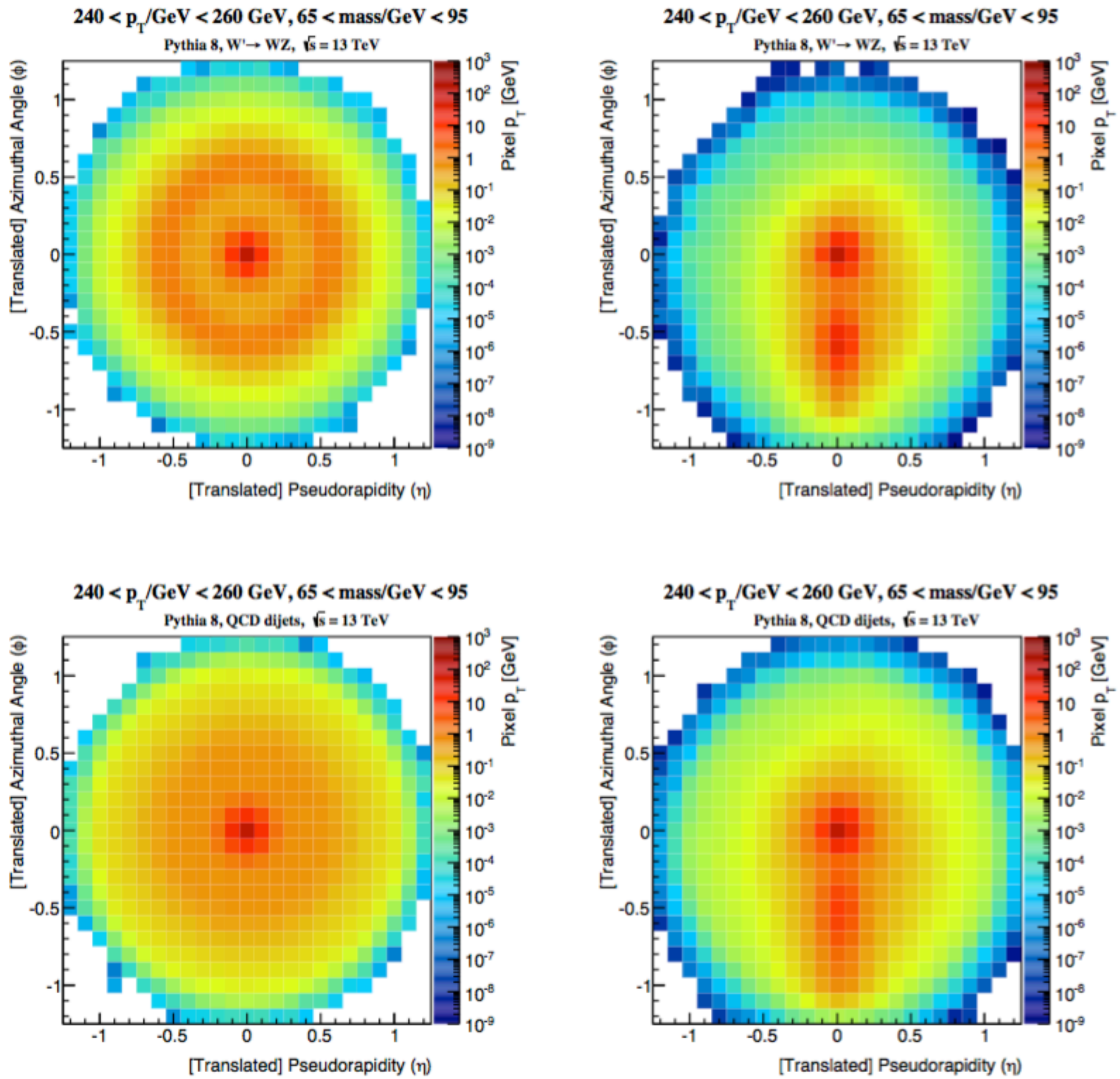
  (e.g. TrackML challenge, end of this talk)



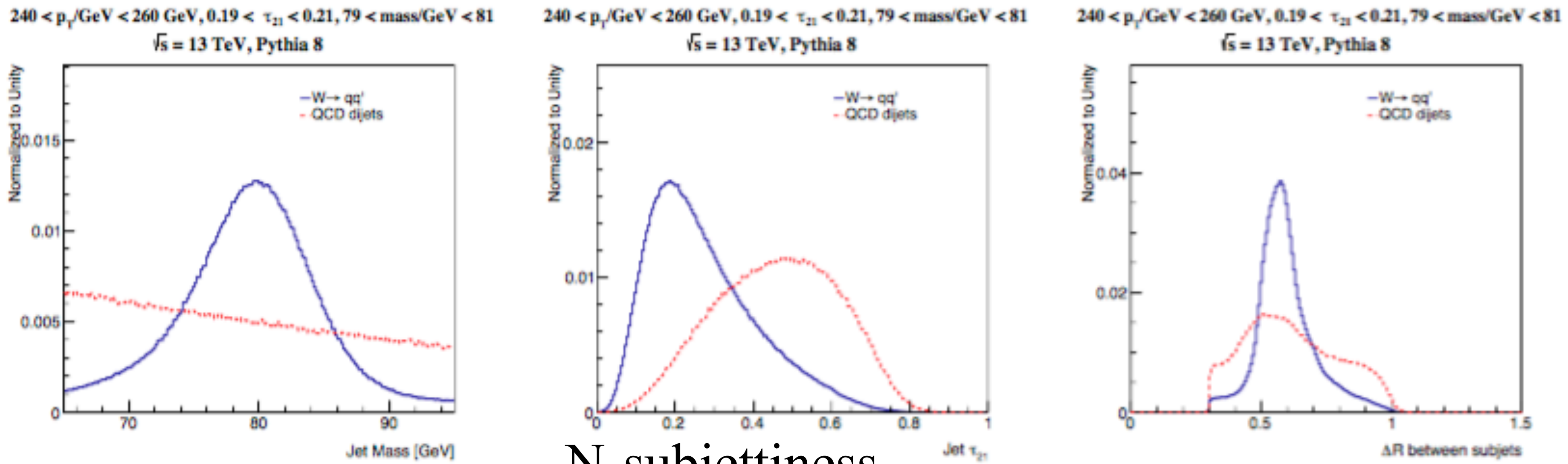
Jet Images

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

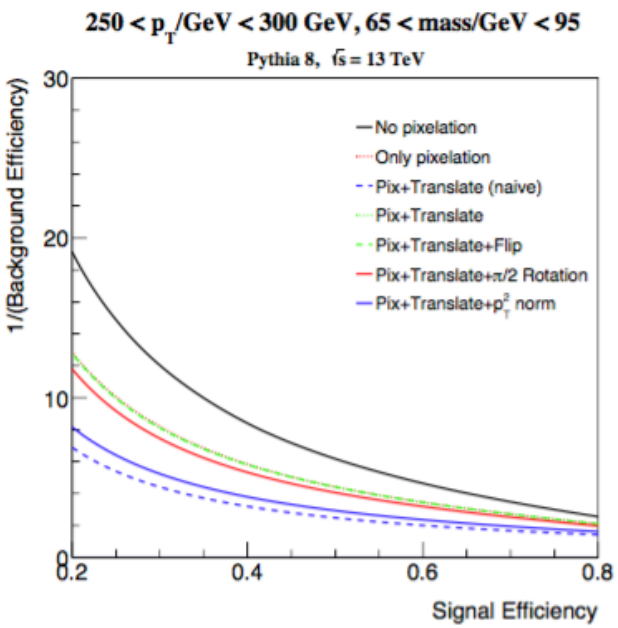
- Distinguish boosted W jets from QCD
- Particle level simulation
- Average images:



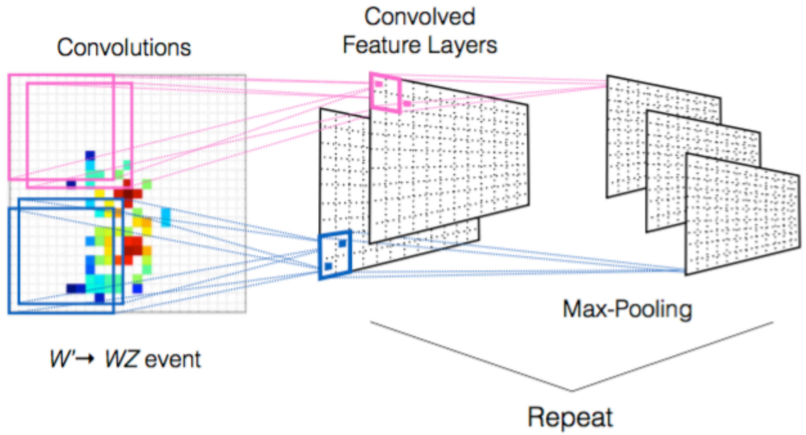
Boosted jets : standard variables

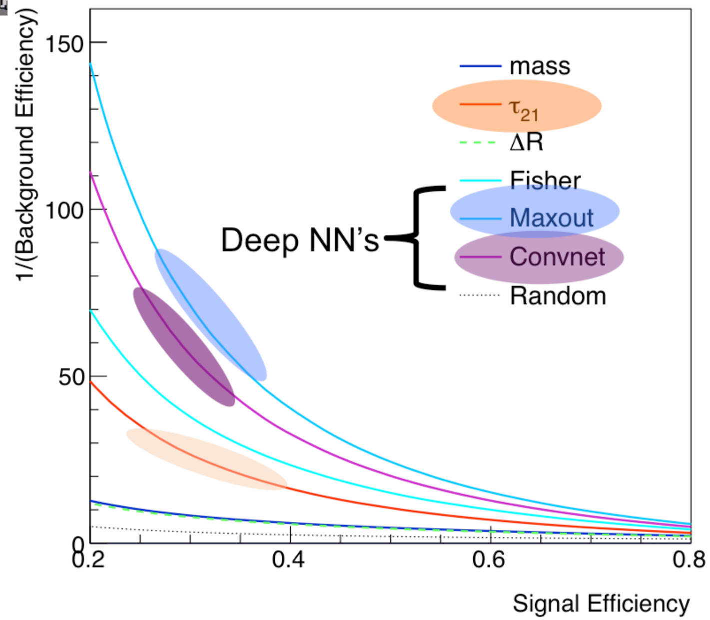


N-subjettiness

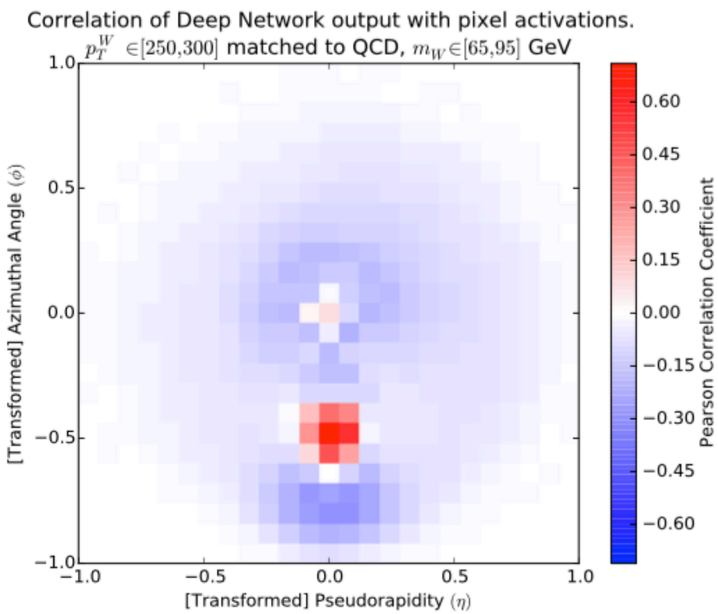


Jet Images : Convolution NN

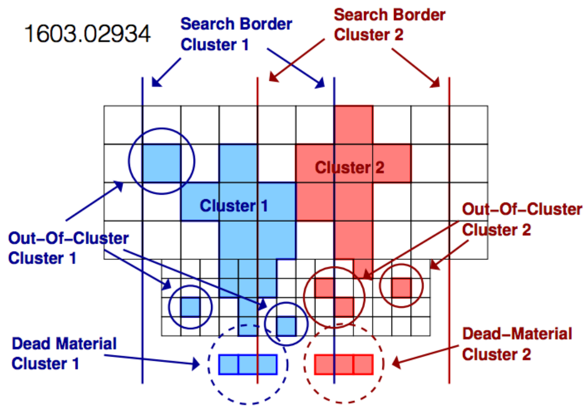




- Variables build from CNN outperform the more usual ones



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



ML in Simulation

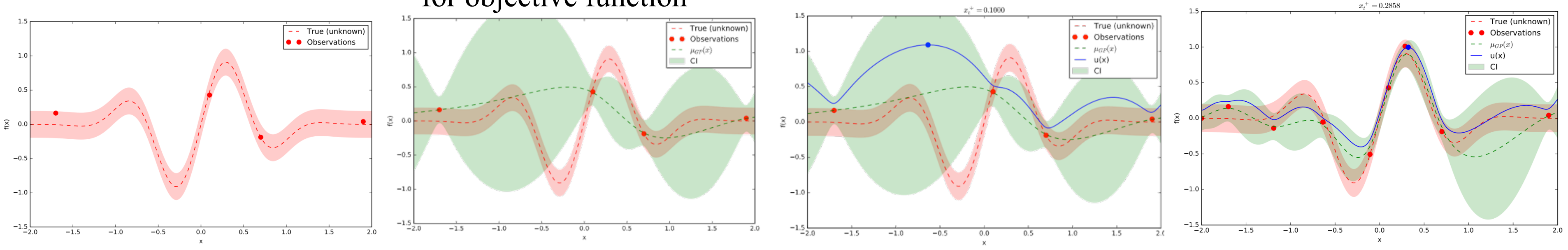
- We invest a lot of resources (CPU: ~100k cores/experiment *year, human) on very fine tuned simulations:
  - so far very manual optimisation by super experts
  - optimisation in many dimensions parameter space, with costly evaluation
- Now turning to more modern techniques e.g.:
  - Bayesian Optimization and Gaussian Processes

Gilles Louppe, DIANA meeting

Build probabilistic model for objective function

Sample new point

Repeat until convergence



This gives a posterior distribution over functions that could have generated the observed data.

$x_{t+1} = \arg\max_x \mathrm{UCB}(x)$

- Another avenue : multivariable regression to parameterise detector response

Data Challenges

Challenges (competition)

- Challenges are essentially a way to create a buzz around an open dataset dressed with a benchmark
  - HiggsML (ATLAS) 2014
  - FlavourML (LHCb) 2015
  - future TrackML (ATLAS+CMS) 2016?
- Buzz in non-HEP world to get the attention of ML specialists

HiggsML in a nutshell

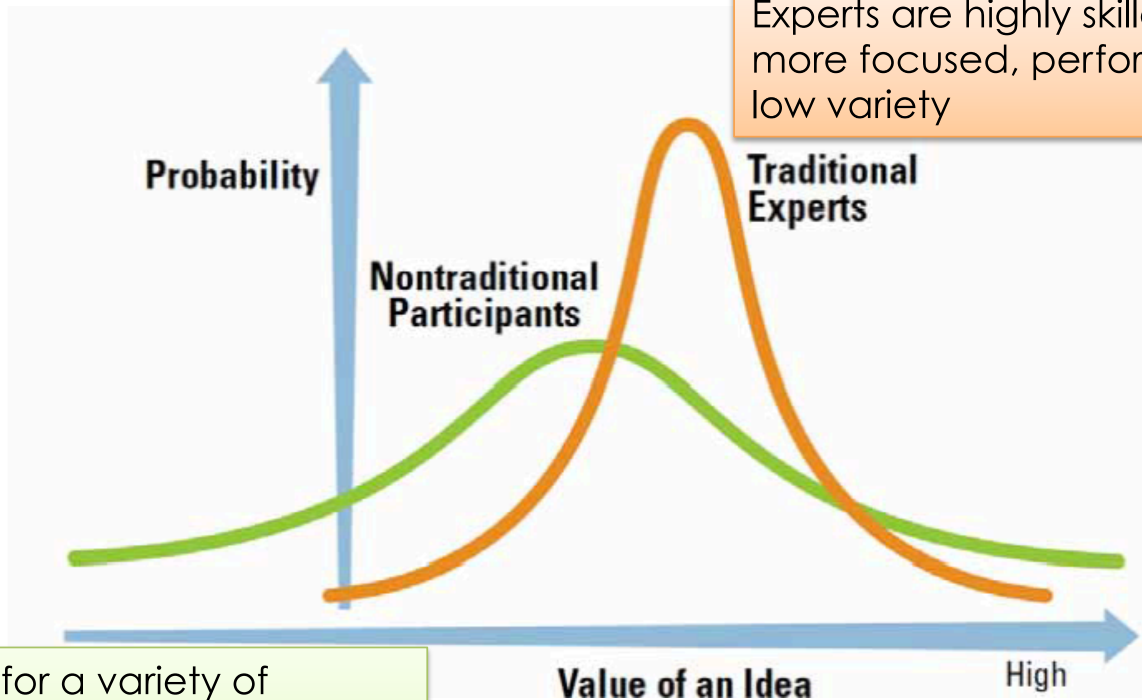
- Why not put some ATLAS simulated data on the web and ask data scientists to find the best machine learning algorithm to find the Higgs ?
  - Instead of HEP people browsing machine learning papers, coding or downloading possibly interesting algorithm, trying and seeing whether it can work for our problems
- Challenge for us : make a full ATLAS Higgs analysis simple for non physicists, but not too simple so that it remains useful
- Also try to foster long term collaborations between HEP and ML
- Do not underestimate the time to learn common languages (e.g. hand waving explanation of S/sqrt(B) not enough)
- Do not underestimate the percolation time :
  - 1) New ML ideas ➔ 2) Demo on toy data set ➔ 3) Demo in real ATLAS analysis➔4) published ATLAS analysis ==> we're still between 1 and 2 for most new ideas

Why challenges work ?

MOTIVATION OF ORGANIZING CONTESTS: EXTREME VALUE

Courtesy : Lakhani 2014

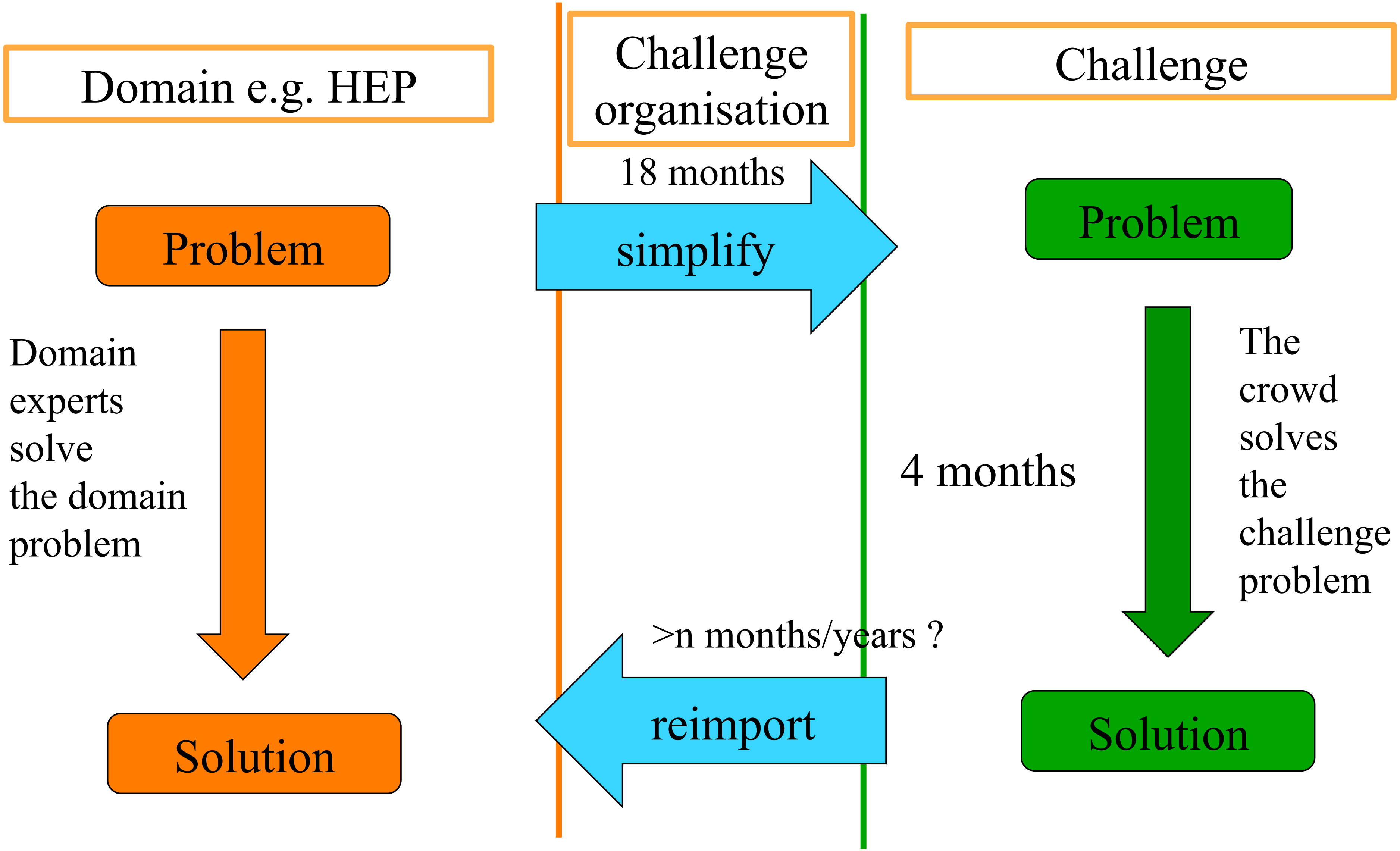
Experts are highly skilled, trained - > more focused, performed solution, low variety



OI is suitable for a variety of nonconvential surprising ideas that are « far » from traditional expertise - > high volatility

Not just ML, but a general trend: Open Innovation

From domain to challenge and back

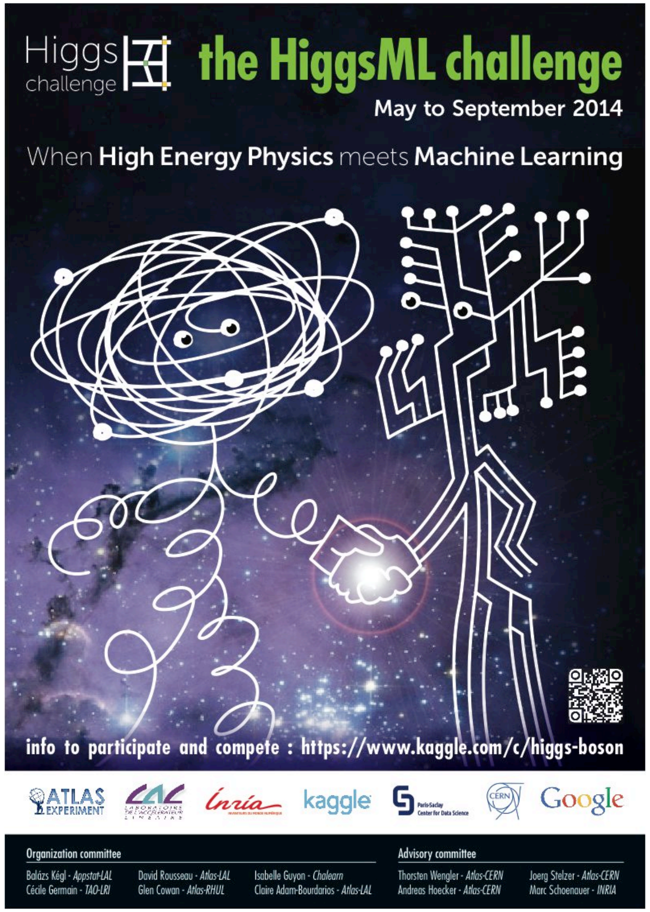


HiggsML : Committees

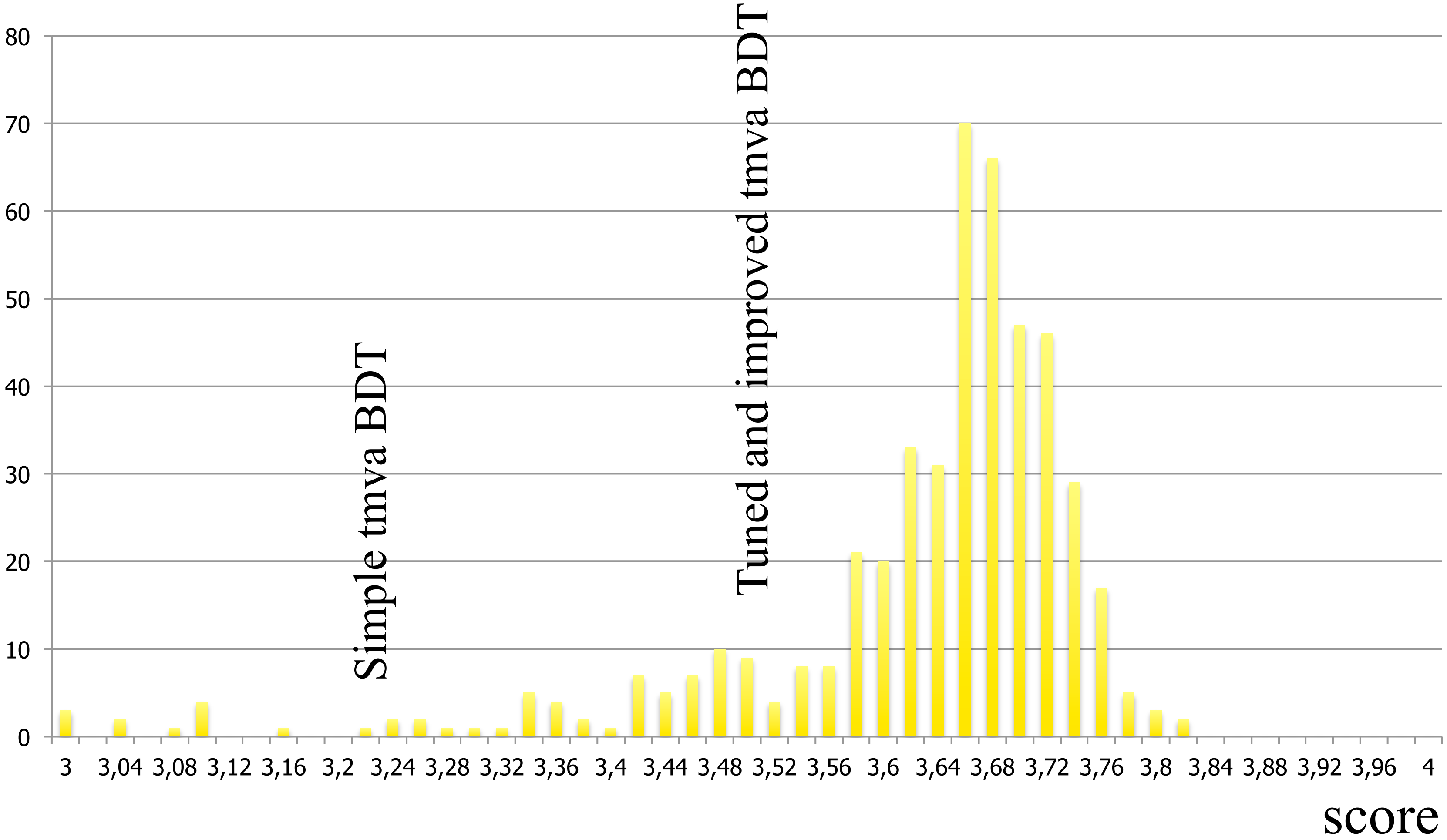
- Organization committee:
  - ATLAS
    - David Rousseau : Atlas-LAL
    - Claire Adam-Bourdarios : Atlas-LAL (outreach, legal matter)
    - Glen Cowan : Atlas-RHUL (statistics)
  - Machine Learning
    - Balazs Kegl : Appstat-LAL
    - Cécile Germain : TAO-LRI
    - Isabelle Guyon : Chalearn (now chaire Paris Saclay) (challenges organisation)
- Advisory committee:
  - Andreas Hoecker : Atlas-CERN (PC,TMVA)
  - Joerg Stelzer : Atlas-CERN (TMVA)
  - Thorsten Wengler : Atlas-CERN (ATLAS management)
  - Marc Schoenauer : INRIA

Higgs Machine learning challenge

- See [talk DR CTD2015 Berkeley]
- An ATLAS Higgs signal vs background classification problem, optimising statistical significance
- Ran in summer 2014
- 2000 participants (largest on Kaggle at that time)
- Outcome
  - Best significance 20% than with Root-TMVA
  - BDT algorithm of choice in this case where number variables and number of training events limited (NN very slightly better but much more difficult to tune)
  - XGBoost best BDT on the market (quite wide spread nowadays)
  - Wealth of ideas, documented in [JMLR proceedings v42]
  - Still working on what works in real life what does not
  - Raised awareness about ML in HEP
- Also:
  - Winner Gabor Melis hired by DeepMind
  - Tong He, co-developper of XGBoost, winner of special "HEP meets ML" price got a PhD grant and US visa



Best private scores

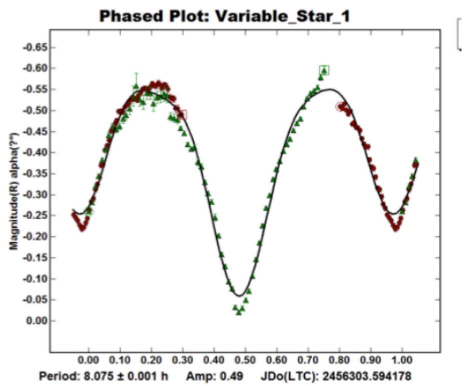


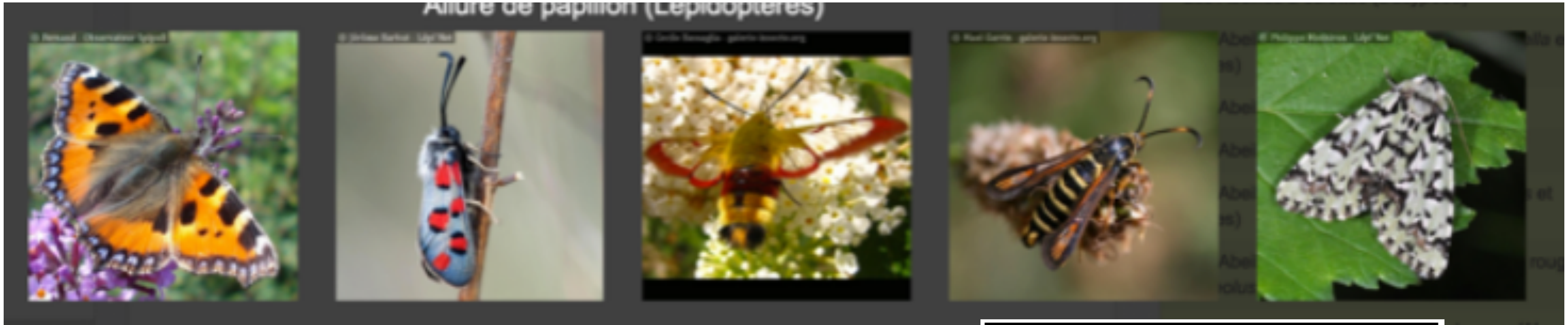
LHCb : flavour of physics

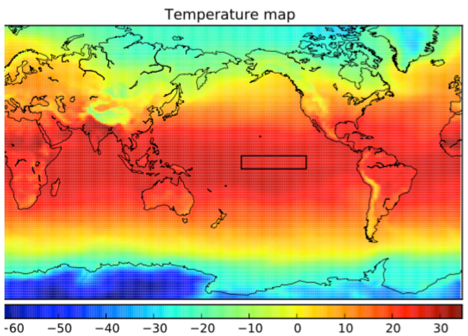
- LHCb organised in summer 2015 another challenge "flavour of physics": search for LFV decay $\tau \rightarrow \mu\mu\mu$
- similar to HiggsML, with a big novelty:
  - some variables known to be poorly described by MC
  - algorithm had to behave similarly on data and MC in a control region $D0 \rightarrow K\pi\pi$
- ➔Nice idea, however, never underestimates the machine learners: They devised an algorithm which
  - was able to distinguish control region from signal region
  - was behaving well (data=MC) in the control region
  - but was recklessly abusing the data/MC difference in the signal region
- ➔rules had to be changed in the middle of the challenge to disallow this
- Anyway, this does show that systematics is tricky to handle

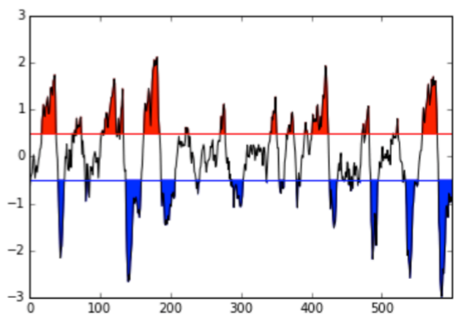
Beyond challenges : RAMP

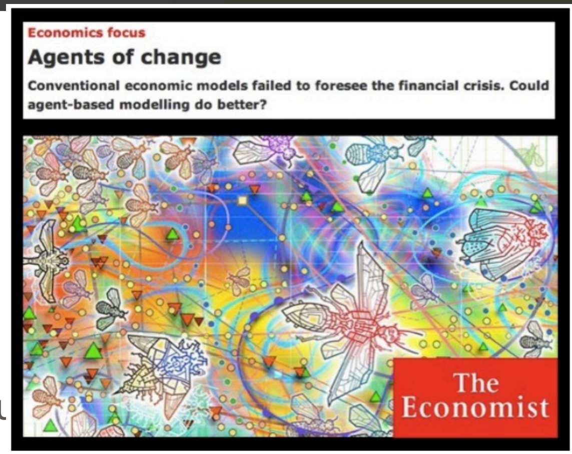
- (Already mentioned for Anomaly Detection)
- Run by CDS Paris Saclay
- Main difference wrt to HiggsML:
  - participants post their software, which is run by the RAMP platform
  - one day hackathon
  - participants are encouraged to re-use other people's software
- Can adapt to all domains:





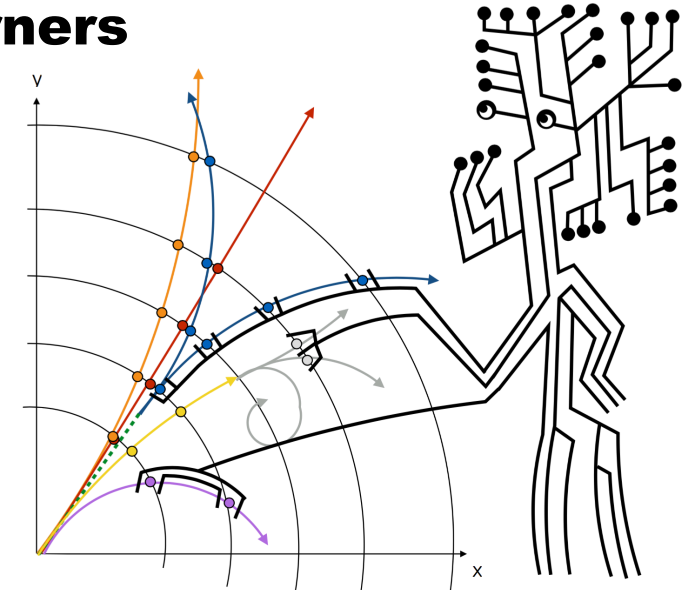






Towards a Future Tracking Machine Learning challenge

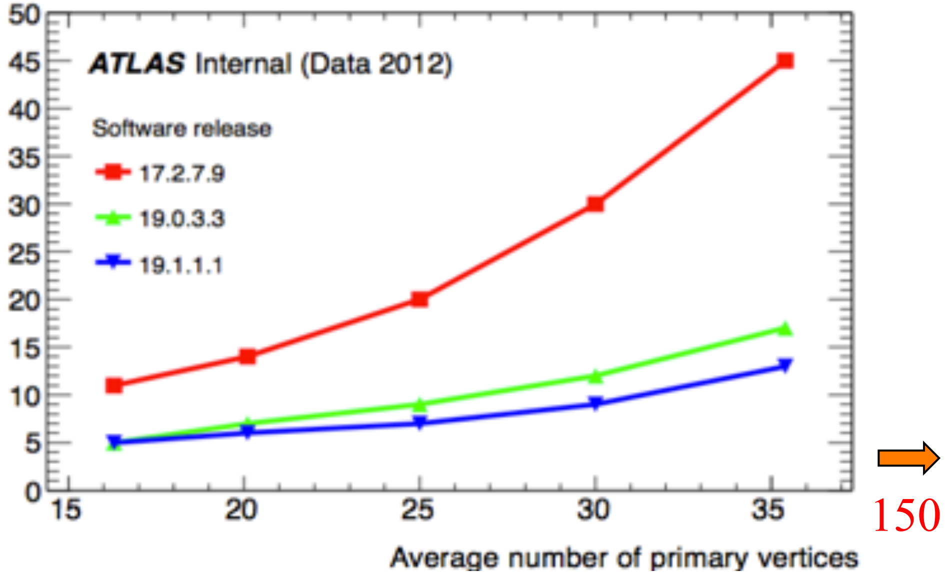
A collaboration between ATLAS and CMS physicists, and Machine Learners

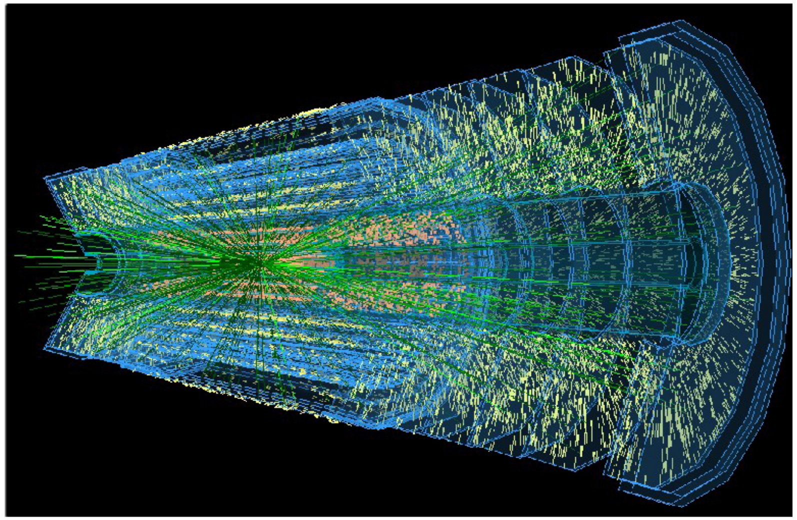


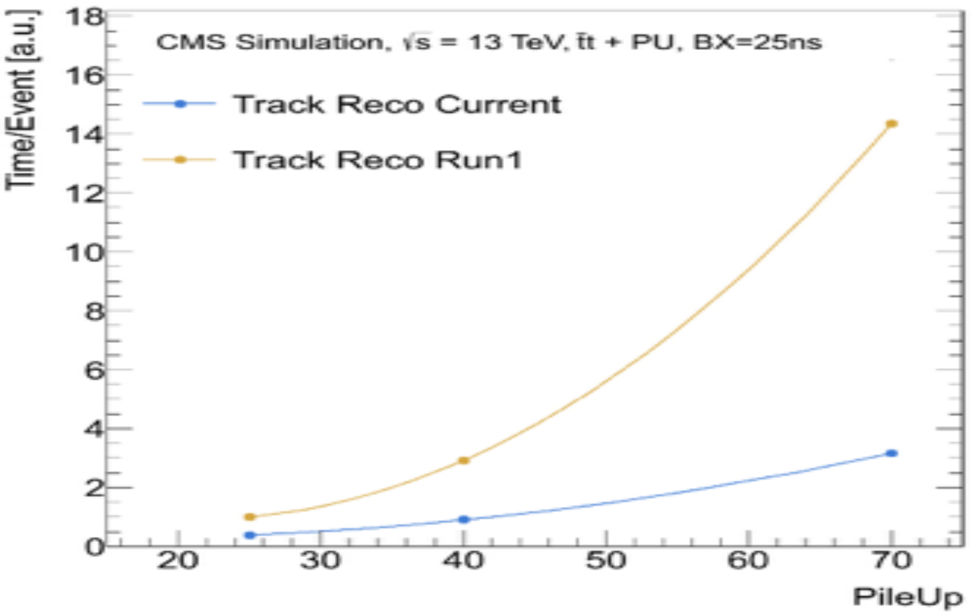
TrackML : Motivation 1

Graeme Stewart ECFA HL-LHC workshop 2014

- See details DR talk at CTD2016
- 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)







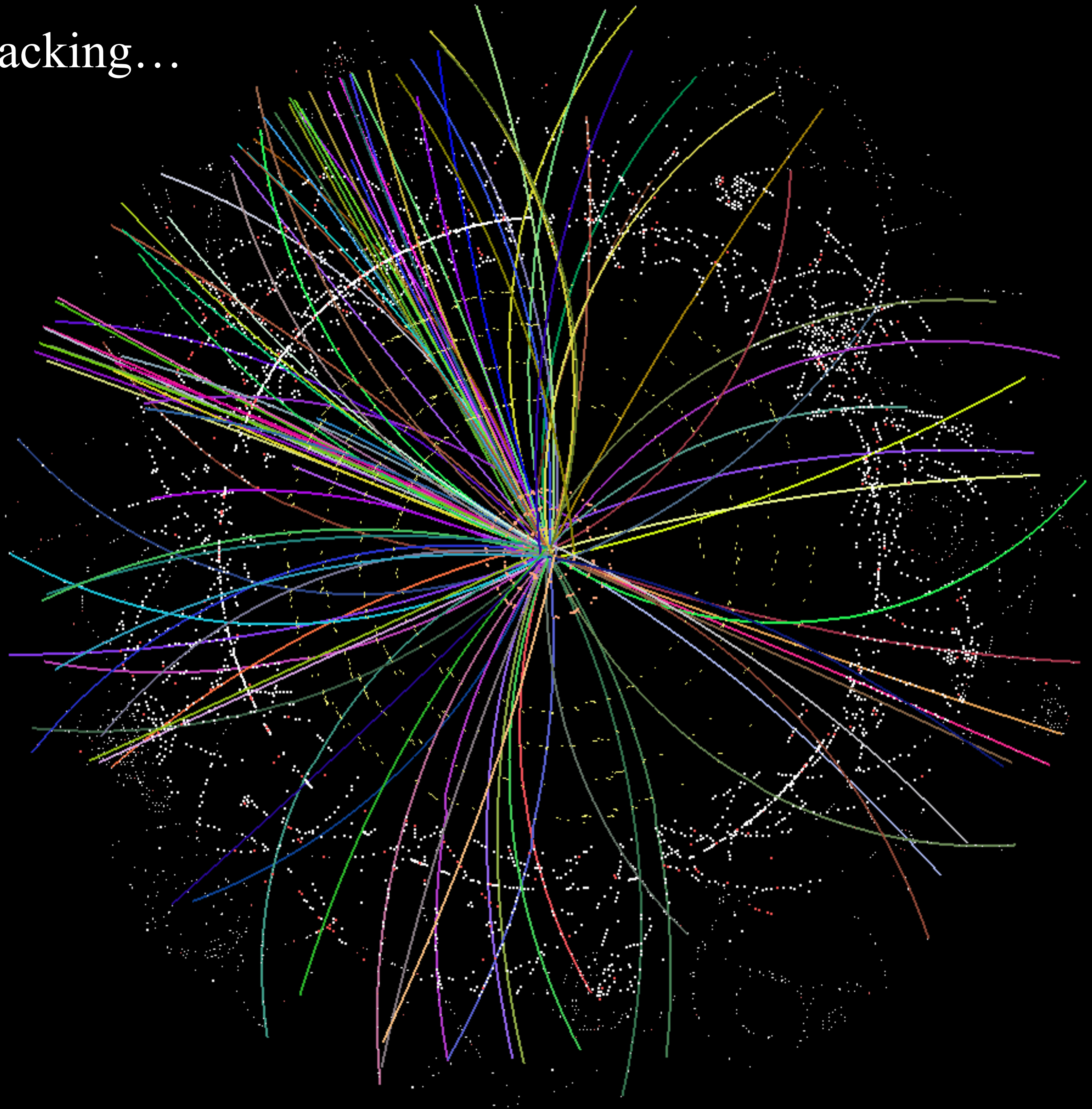
TrackML : Motivation 2

- LHC experiments future computing budget flat (at best)
- Installed CPU power per \$==€==CHF expected increase factor ~10 in 10 years
- Experiments plan on increase of data taking rate ~10 as well (~1kHz to 10kHz)
- ➔HL reconstruction at mu=150 need to be as fast as Run1 reconstruction at mu=20
- ➔requires very significant software improvement, factor 10-100
- 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)
- Need to engage a wide community to tackle this problem

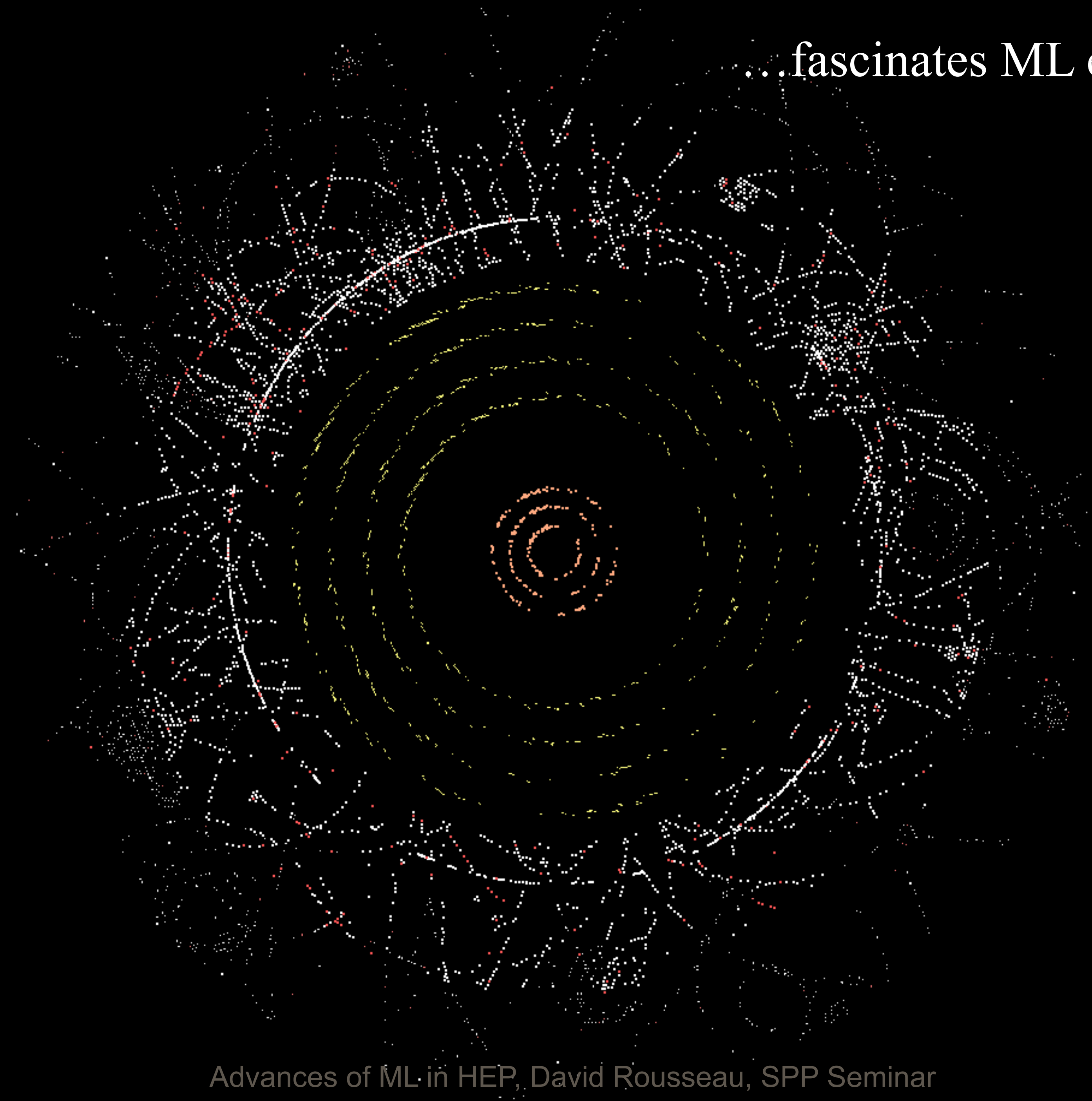
TrackML : engaging Machine Learners

- Suppose we want to improve the tracking of our experiment
- We read the literature, go to workshops, hear/read about an interesting technique (e.g. ConvNets, MCTS…). Then:
  - Try to figure by ourself what can work, and start coding➔traditional way
  - Find an expert of the new technique, have regular coffee/beer, get confirmation that the new technique might work, and get implementation tips➔better
- …repeat with each technique...
- Much much better:
  - Release a data set, with a benchmark, and have the expert do the coding him/herself
  - ➔ he has the software and the know-how so he'll be (much) faster even if he does not know anything about our domain at the beginning
  - ➔engage multiple techniques and experts simultaneously (e.g. 2000 people participated to the Higgs Machine Learning challenge) in a comparable way
  - ➔even better if people can collaborate
  - ➔a challenge is a dataset with a benchmark and a buzz
  - Looking for long lasting collaborations beyond the challenge
- Focus on the pattern recognition : release list of 3D points, challenge is to associate them into tracks fast. Use public release of ATLAS tracking (ACTS) as a simulation engine and starting kit.

HEP tracking…

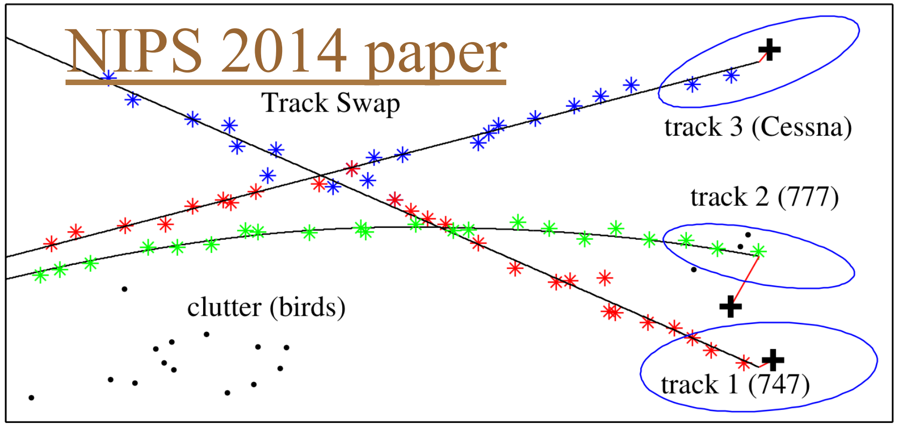


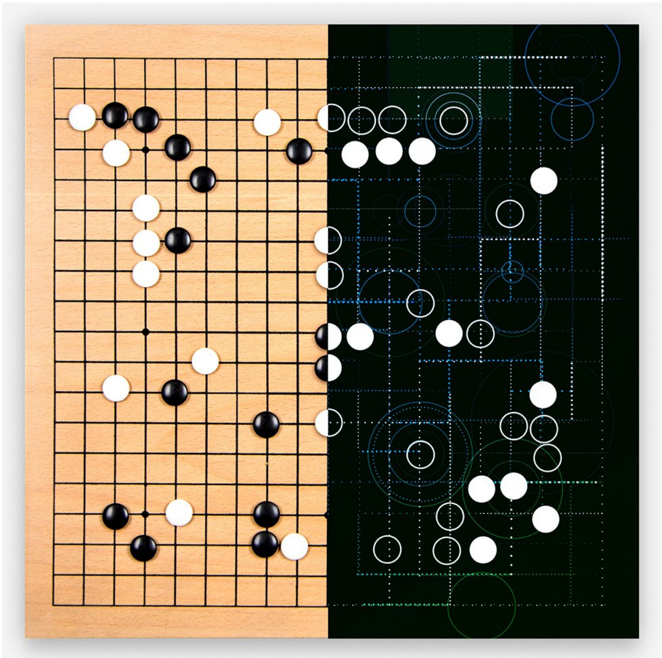
…fascinates ML experts

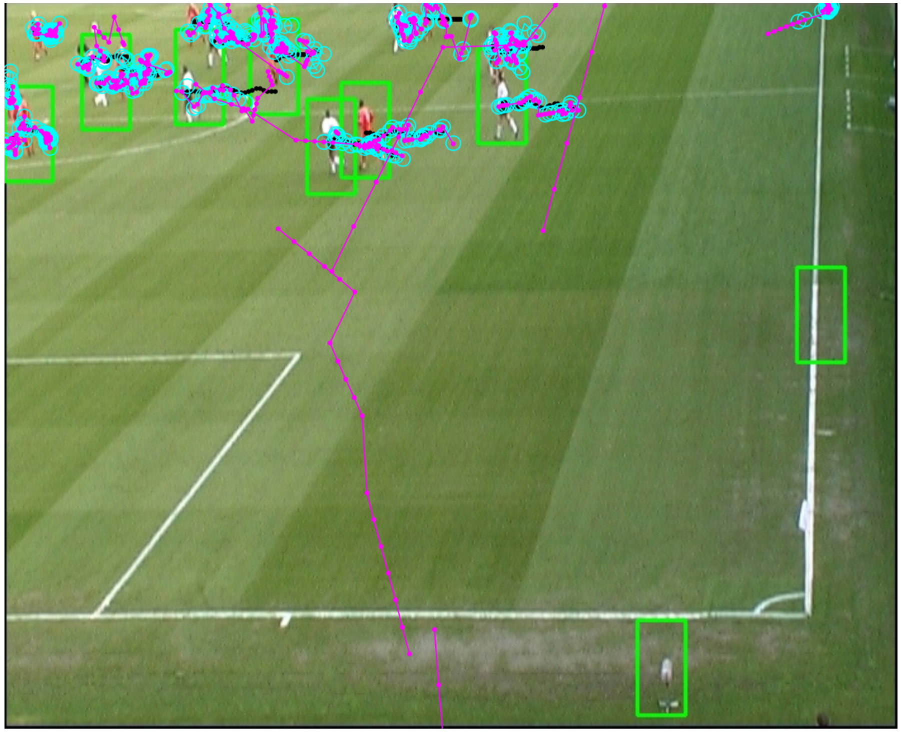


Pattern recognition

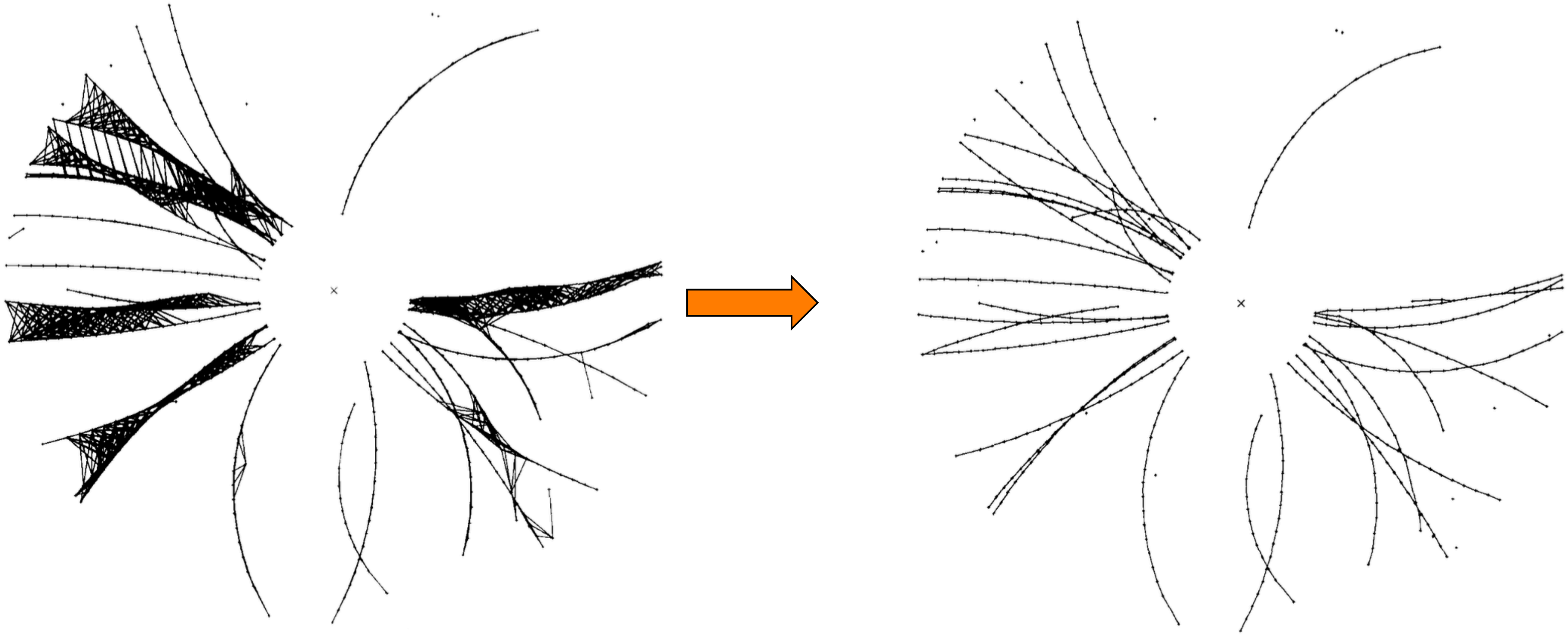
- Pattern recognition is a very old, very hot topic in Artificial Intelligence
- Note that these are real-time applications, with CPU constraints







TrackML : An early attempt



- Stimpfl-Abele and Garrido (1990) (ALEPH)
- All posssible neighbor connections are built, the correct ones selected by the NN (not used in production)
- Also PhD Vicens Gaitan 1993, winner of Flavour of Physics challenge

Wrapping-up

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 (see later)
- Note : Yandex Data School of Analysis (with ~10 ML scientists) now a bona fide institute of LHCB
- Very useful/essential to build HEP - ML collaborations (study on shared dataset, thesis (Computer Science or HEP)
- Successful collaborations often within one campus
- Center for Data Science Paris-Saclay 'role is precisely to favour these collaborations
- Most likely within CEA too…

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 NDA
- 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
- Role of CERN Open Data portal:
  - We (ATLAS) initially saw its use for outreach purposes (CMS has been more open on releasing 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.
- An internal ATLAS ML group will start by June. Probably also in CMS ?
- https://www.kaggle.com/c/higgs-boson
- 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/
- http://cern.ch/higgsml-visit mini workshop at CERN
- Mailing list opened to any one with an interest in both Data Science and High Energy Physics : HEP-data-science@googlegroups.com

Conclusion

- Machine Learning techniques widely used in HEP
- 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: collaboration between HEP and ML scientists are needed
- More and more open datasets/simulators to favour the collaborations
- More and more HEP and ML workshops, forums, group, challenges etc…
- Never underestimate the time for :
  - (1) Great idea➔
  - (2) demonstrated on toy dataset➔
  - (3) demonstrated on real experiment dataset ➔
  - (4) experiment publication using the great idea