Advances in Machine Learning tools in High Energy Physics



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LPSC Seminar, Tuesday 4th October 2016

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 :

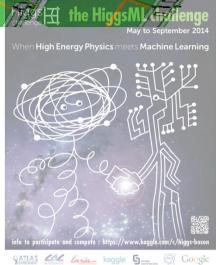


- "Artificial Intelligence" not a dirty word anymore!
- ☐ We've realised we're been left behind! Trying to catch up now...

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, summer 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, summer 2017?

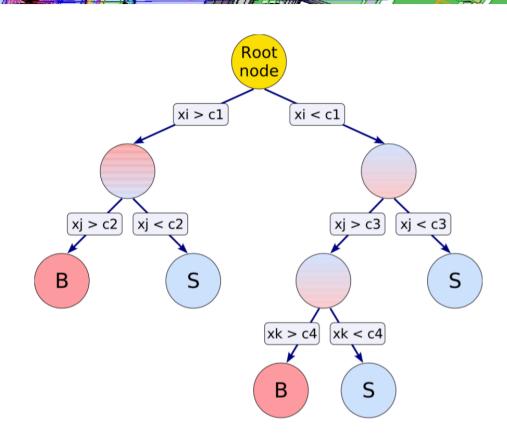




ML Basics

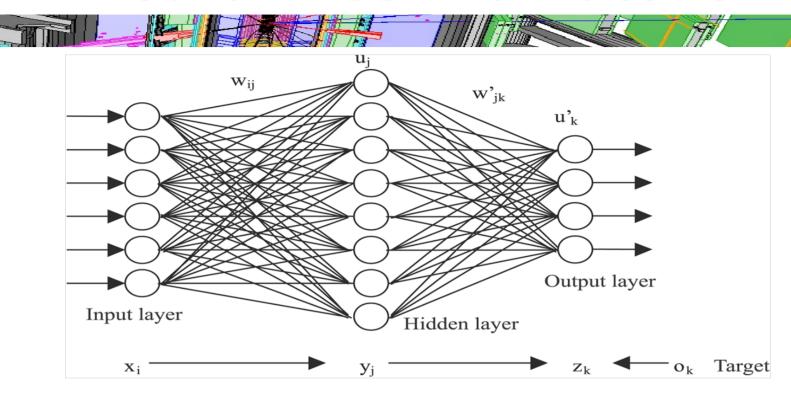


BDT in a nutshell



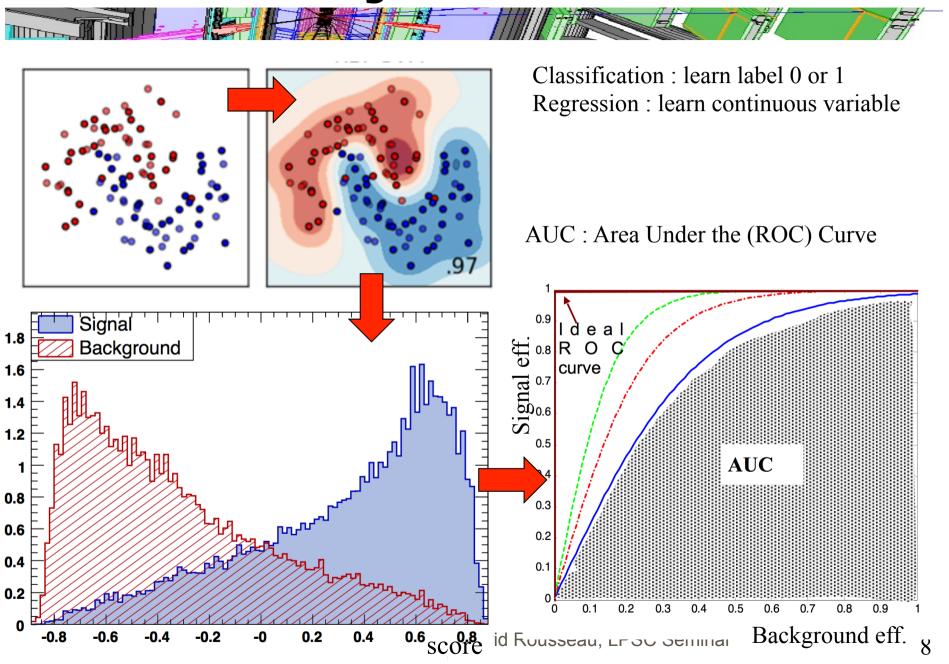
- ☐ Single tree (CART) < 1980
- □ AdaBoost 1997 : rerun increasing the weight of misclassified entries → boosted trees

Neural Net in a nutshell

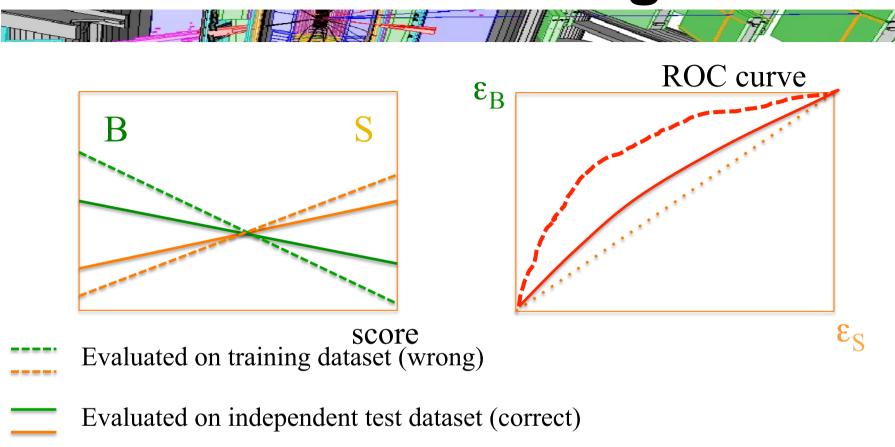


- Neural Net ~1950!
- But many many new tricks for learning, in particular if many layers (also ReLU instead of sigmoïd activation)
- "Deep Neural Net" up to 50 layers
- Computing power (DNN training can take days even on GPU)
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Any classifier



Overtraining



Score distribution different on test dataset wrt training dataset

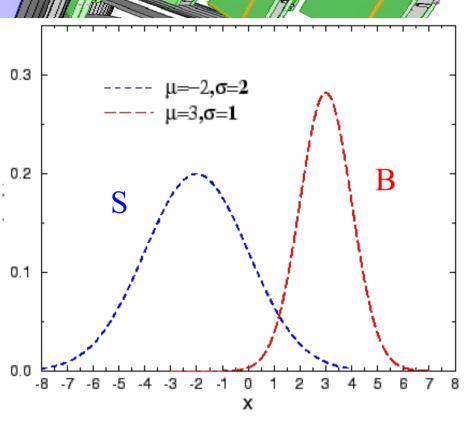
"Overtraining" == possibly excessive use of statistical fluctuation

More vocabulary

- "Hyper-parameters":
 - These are all the "knobs" to optimize an algorithm, e.g.
 - number of leaves and depth of a tree
 - number of nodes and layers for NN
 - and much more
 - "Hyper-parameter tuning/fitting"== optimising the knobs for the best performance
- "Features"
 - variables

No miracle

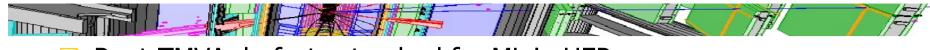
- ML does not do miracles
- ☐ If underlying distributions are known, nothing beats Likelihood ratio! (often called bayesian limit"):
 - $_{\rm O}$ $L_{\rm S}(x)/L_{\rm B}(x)$
- OK but quite often L_S L_B are unknown
 - + x is n-dimensional
- ML starts to be interesting when there is no proper formalism of the pdf



ML Tools

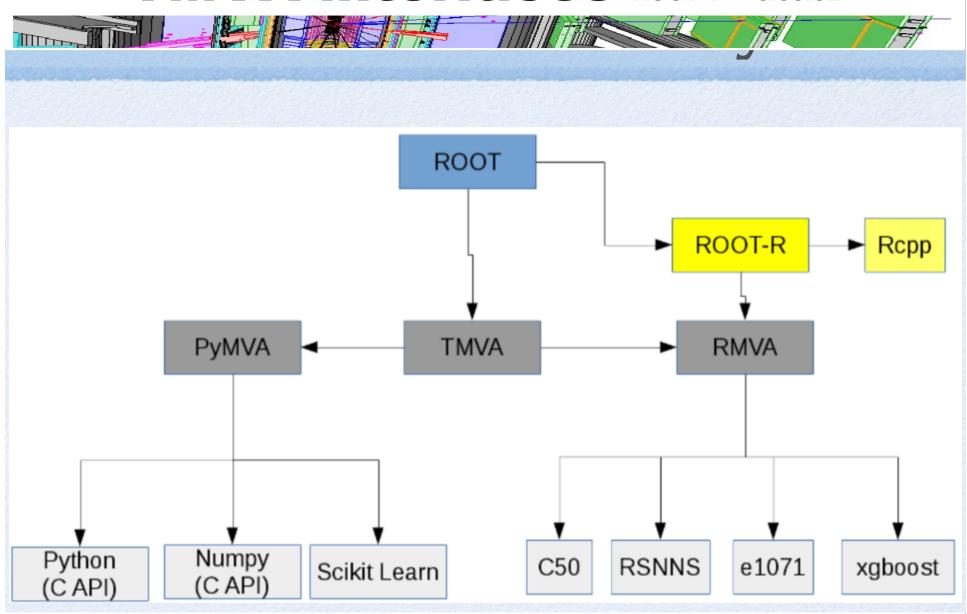


ML Tool: TMVA



- 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
 - Jupyter interface
 - Improve algorithms
 - "Envelope methods" for automatic hyper parameter tuning, crossvalidation
 - Interface to the outside world (R, scikit-learn)
- ☐ See <u>talk Lorenzo Moneta</u> at Hep Software Fondation workshop at LAL in June 2016

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
 - Has won many challenges meanwhile
 - Best BDT on the market, performance and speed
- Classification and regression

ML Tool: SciKit-learn

- Coikit Loarn : Machino Loarning in nython
 - 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 <u>Anaconda</u>
 - 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

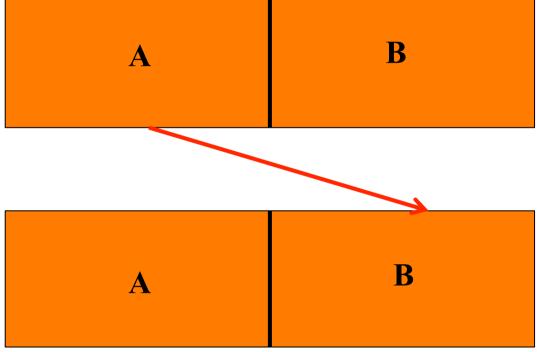
- ☐ Training time can become prohibitive (days), especially Deep Learning, especially with large datasets
- With hyper-parameter optimisation, cross-validation, number of trainings for a particular application large ~100
- Emergence of ML platforms :
 - Dedicated cluster (with GPUs)
 - Relevant software preinstalled (VM)
 - Possibility to load large datasets (GB to TB)
- At CERN SWAN now in production
 - Jupyter interface
 - Access to your CERNbox or to eos

ML Techniques



One-fold Cross Validation

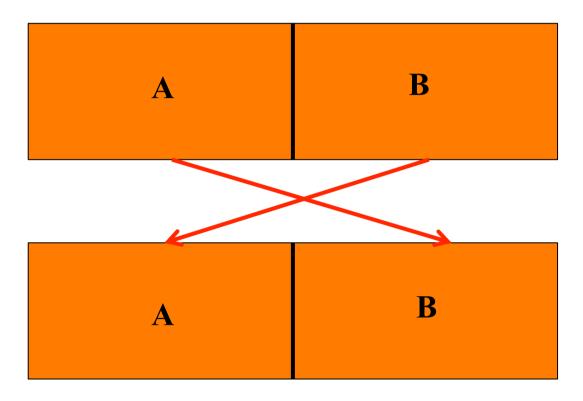
Goal of CV is to measure performance and optimise hyper-parameters



Standard basic way (default TMVA)



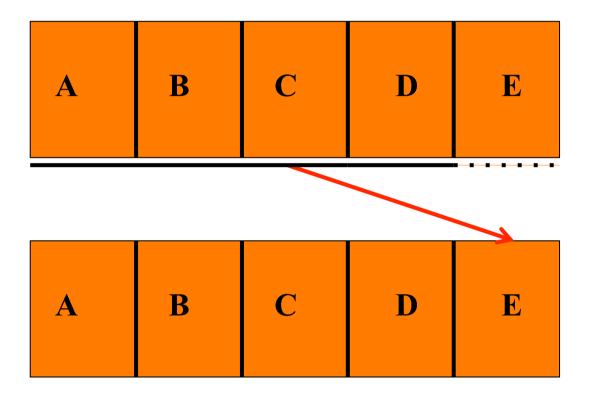
Two-fold Cross Validation



- → test statistics = total statistics
- → double test statistics wrt one fold CV
- → (double training time of course)



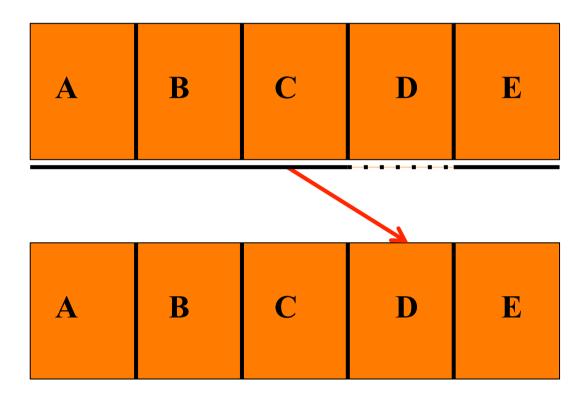
5-fold Cross Validation



same test statistics wrt two-fold CV, larger training statistics 4/5 over ½ (larger training time as well) bonus: variance of the samples an estimate of the statistical uncertain Advances of ML in HEP, David Rousseau, LPSC Seminar

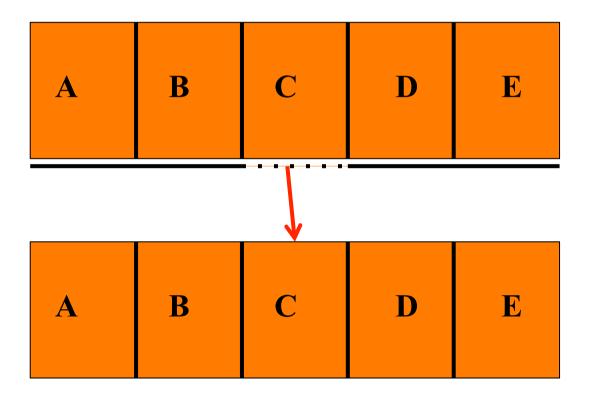


5-fold Cross Validation



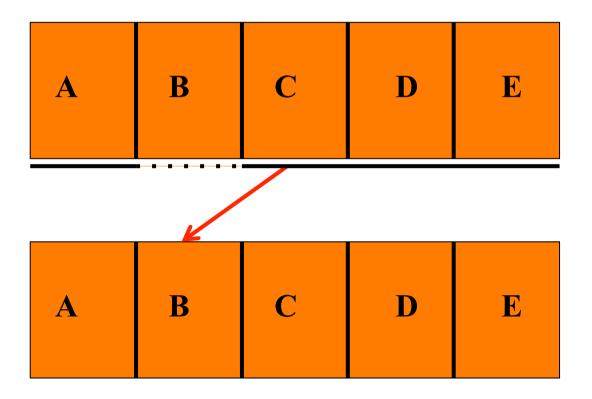


5-fold Cross Validation



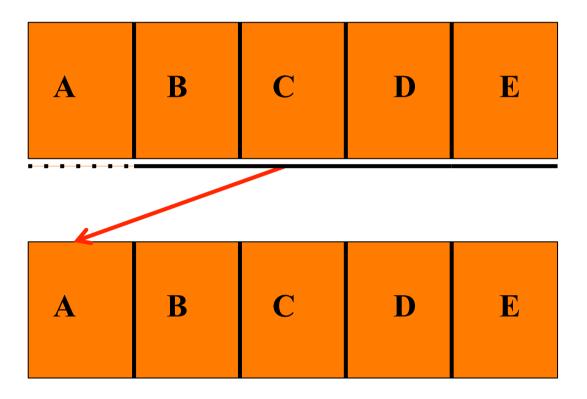


5-fold Cross Validation





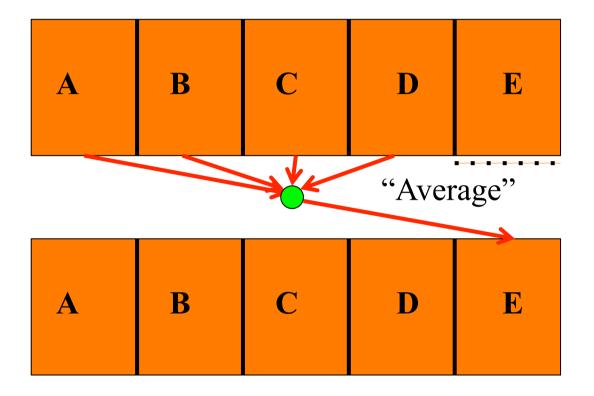
5-fold Cross Validation



Note: if hyper-parameter tuning, need a third level of independent sample "nested CV"



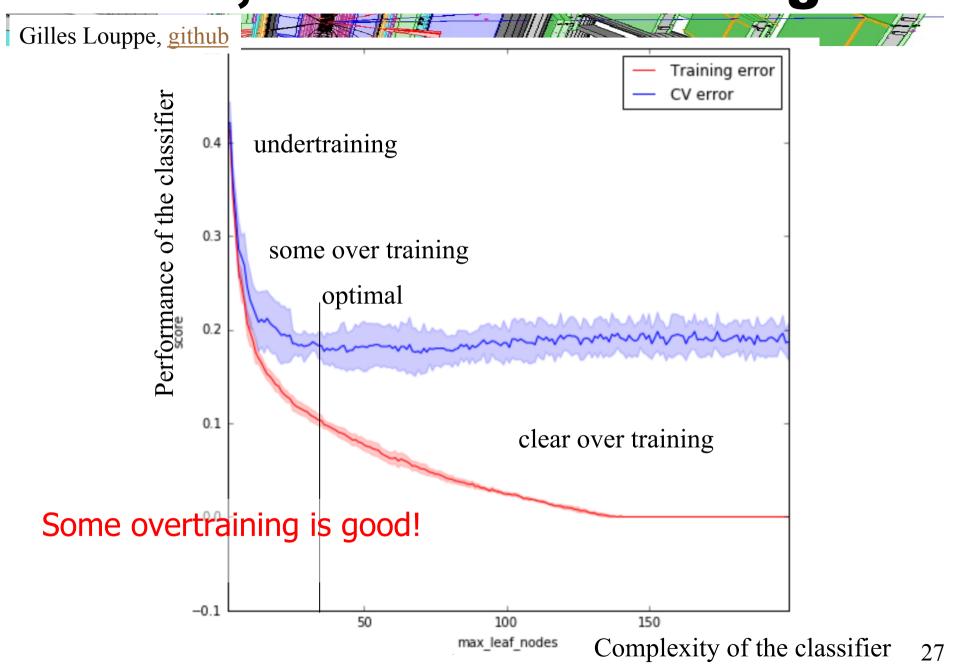
5-fold Cross Validation "à la Gabor"



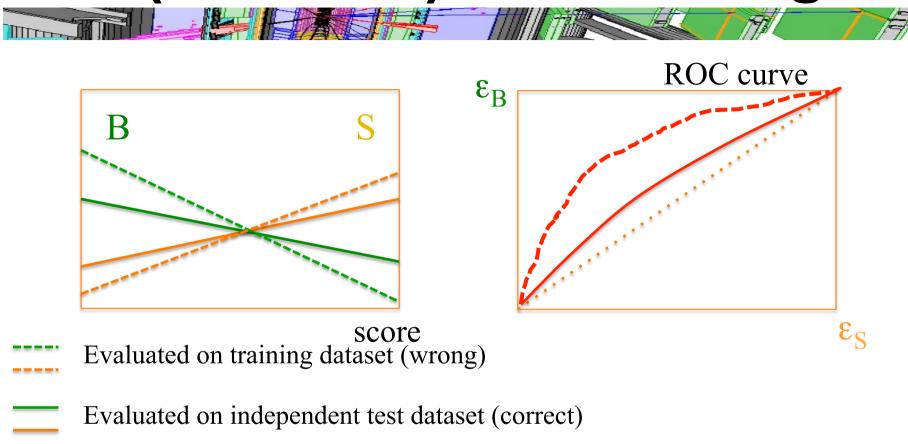
Average of the scores on A B C D is **often** better than the score of one training ABCD (also save on training time)

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CV, under/over training



(reminder) Overtraining

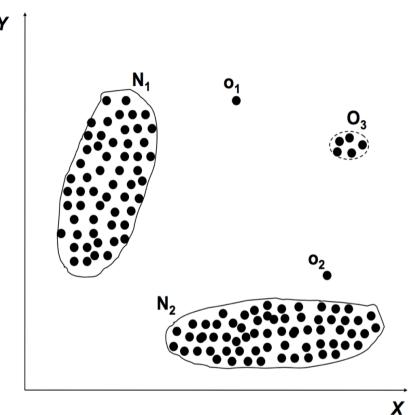


Score distribution different on test dataset wrt training dataset

"Overtraining" == possibly excessive use of statistical fluctuation

Anomaly: point level

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

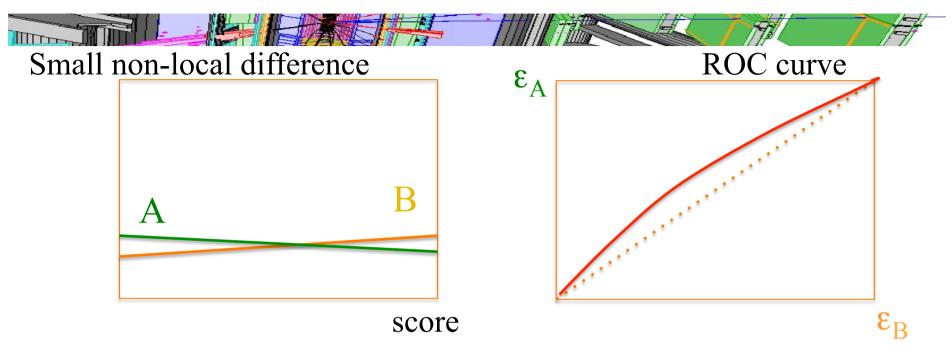


- We have a training "normal" data set with N1 and N2. Algorithm should then spot o1,o2, O3 as "abnormal" i.e. "unlike N1 and N2" (no a priori model for outliers)
- Application : detector malfunction, grid site malfunction, or even new physics discovery...

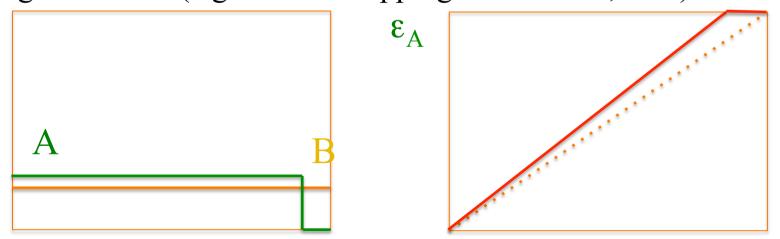
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Anomaly: population level

- 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
 - Geant4 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



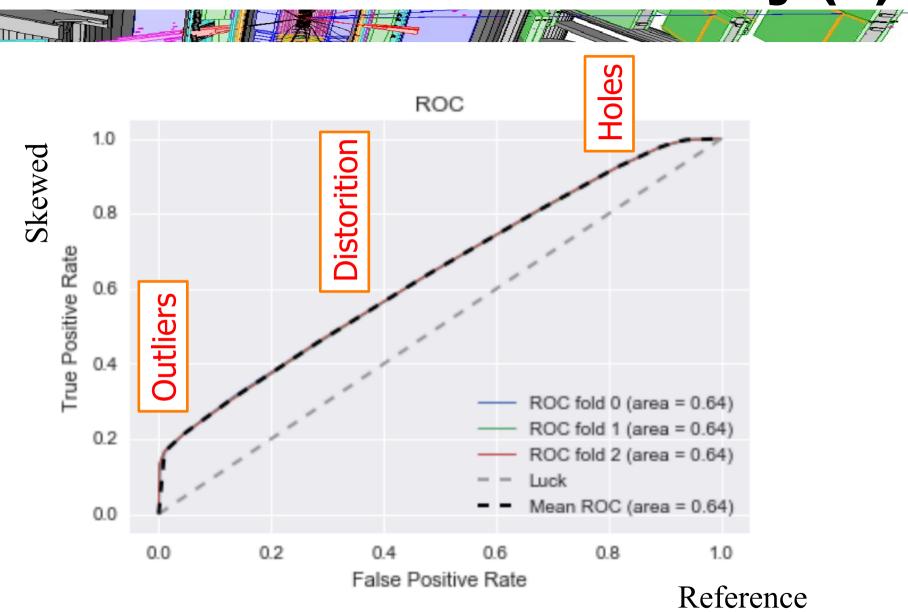
Local big difference (e.g. non overlapping distribution, hole)



HSF ML RAMP on anomaly

- RAMP: collaborative competition around a dataset and a figure of merit. Organised in June 2016 by CDS Paris Saclay with HEP people. See <u>agenda</u>.
- 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 Advances of ML in HEP, David Rousseau, LPSC Seminar

HSF ML RAMP on anomaly (2)



HSF RAMP (2)

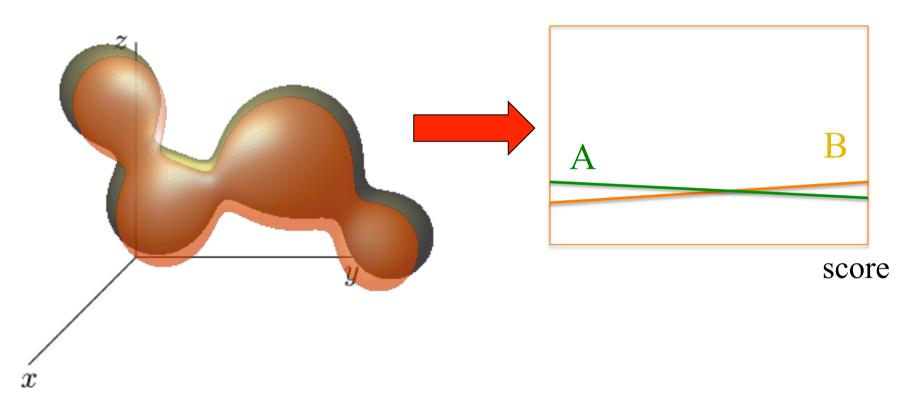
team	submission	accuracy
mcherti	adab2_mt1_calibrated	0.611
dhrou	adab2_mt1	0.611
kazeevn	GradientBoosting	0.596
glouppe	bags2	0.594
glouppe	boosting-duo	0.595
mcherti	adaboost2	0.594
glouppe	bags	0.593
mcherti	adaboost1	0.593
djabbz	beta tester	0.591
soobash	ExtraTreesClassifier	0.576
mcherti	extratrees1	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 \rightarrow classifiers were unable to guess it

→ what functional form classifiers can learn?

Classifier optimisation

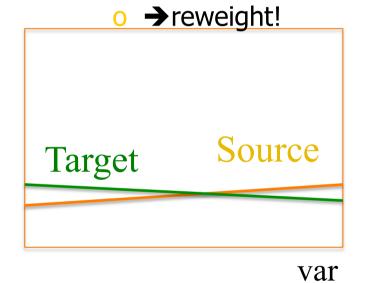
What does a classifier do?

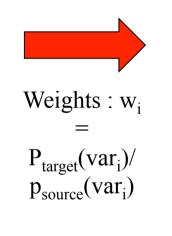


The classifier "projects" the two multidimensional "blobs" maximising the difference, without (ideally) any loss of information

Re-weighting

□ Suppose a variable distribution is slightly different between a Source (e.g. Monte Carlo) and a Target (e.g. real data)

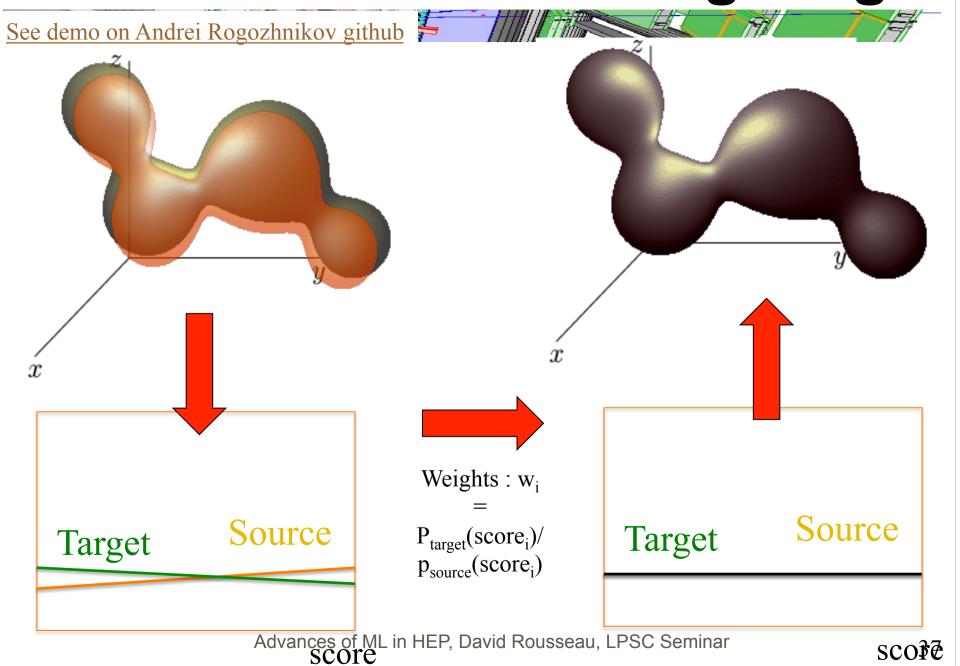






- What if multi-dimension ?
- Usually: reweight separately on 1D projections, at best 2D, because of quick lack of statistics
- Can we do better ?

Multidimension reweighting



Multi dimensional reweighting (2)

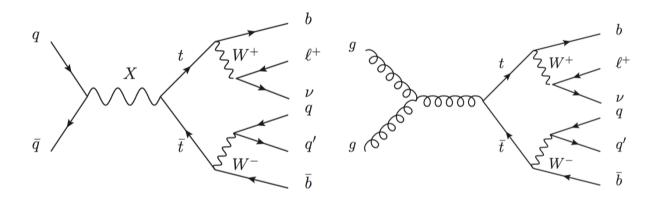
- Reweighting the Source distribution on the score allows multidimensional reweighting without statistics problem
- ☐ Usual caveat still hold: Target support should be included in Source support, distributions should not be too different otherwise unmanageable very large or very small weights
- (Note: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

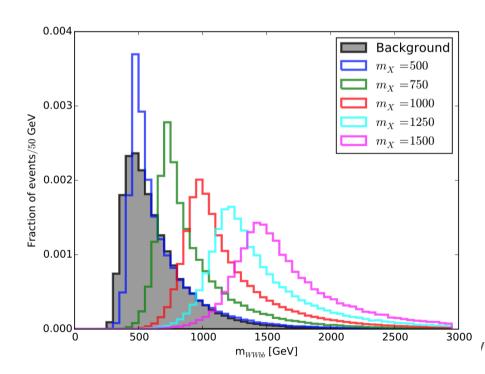
ML in analysis



Parameterised learning

1601.07913 Baldi, Cranmer, Faucett, Sadowksi, Whiteson

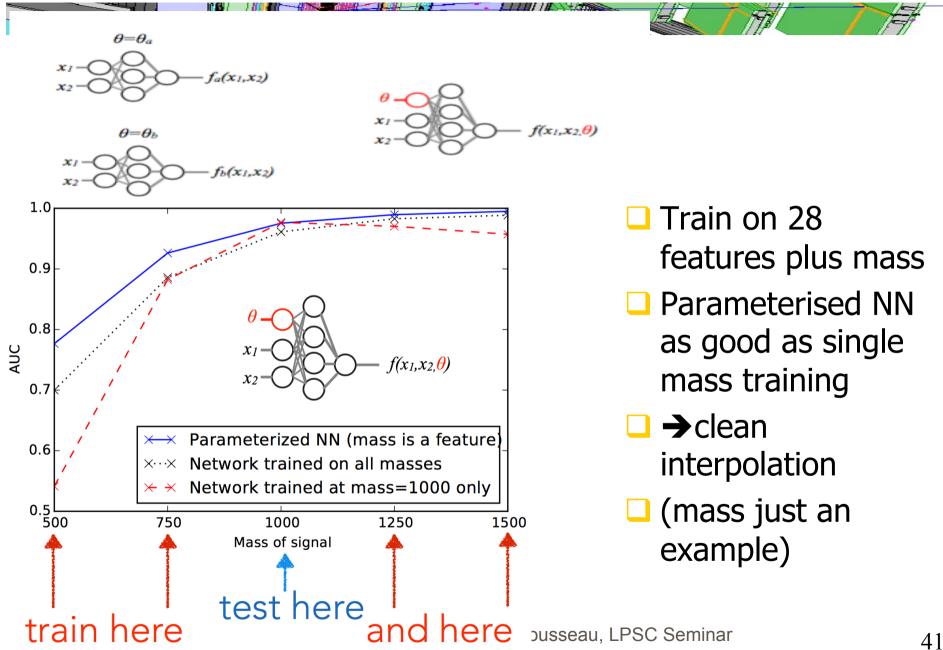




- Typical case: looking for a particle of unknown mass
- E.g. here tt decay

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Parameterised learning (2)



Systematics

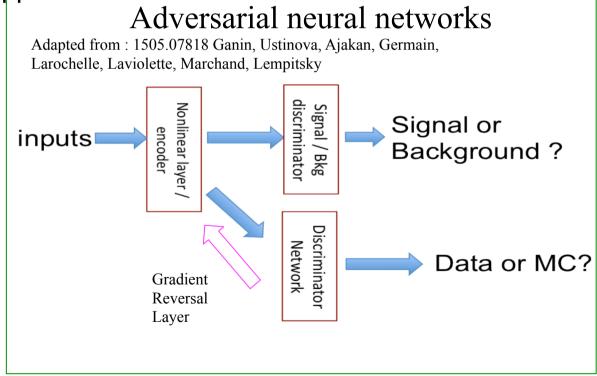


- Our experimental papers typically ends with
 - o measurement = m $\pm \sigma(stat) \pm \sigma(syst)$
 - o σ(syst) systematic uncertainty: known unknowns, unknown unknowns...
- □ Name of the game is to minimize quadratic sum of : $\sigma(\text{stat}) \pm \sigma(\text{syst})$
- \square ML techniques 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
- \square Worrying about σ (syst) untypical of ML in industry

Systematics (2)

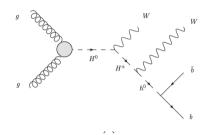
- ☐ However, a hot topic in ML in industry: *transfer learning*
- □ E.g.: train image labelling on a image dataset, apply on new images (different luminosity, focus, angle etc...)
- □ For HEP: we train with Signal and Background which are not the real one (MC, control regions, etc...) source of systematics

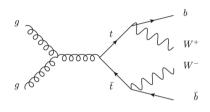
One possible approach:

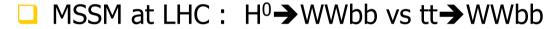


Deep learning for analysis

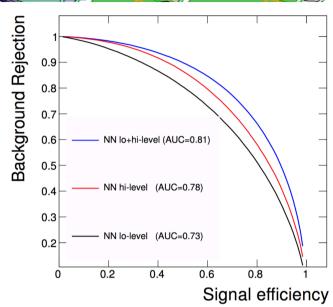
1402.4735 Baldi, Sadowski, Whiteson

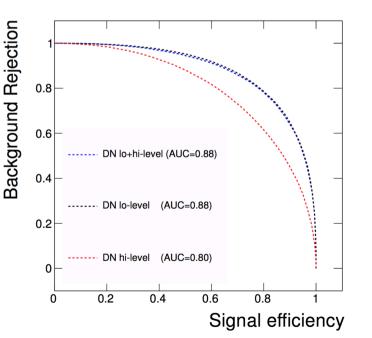






- Low level variables:
 - 4-momenta
- High level variables:
 - Pair-wise invariant masses
- Deep NN outperforms NN, and does not need high level variables
- DNN learns the physics ?

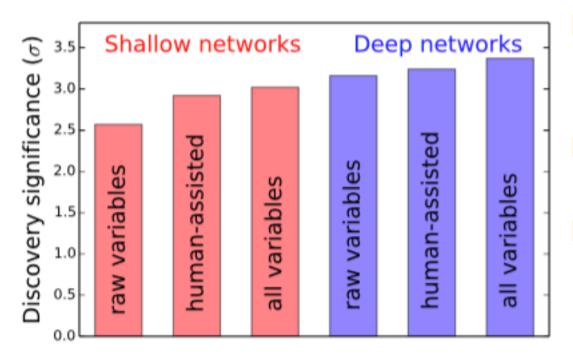




Deep learning for analysis (2)

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

ML in reconstruction



Jet Images

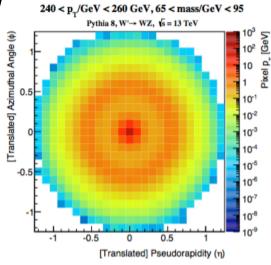
arXiv 1511.05190 de Oliveira, Kagan, Mackey, Nachman, Schwartzman

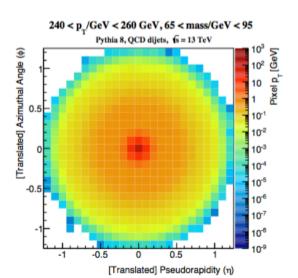


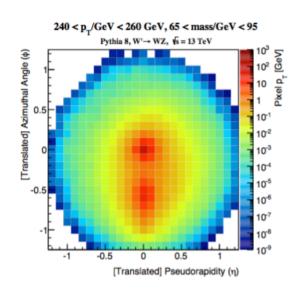
- Distinguish boosted W jets from QCD
- Particle level simulation
- Average images:

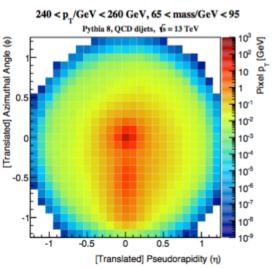






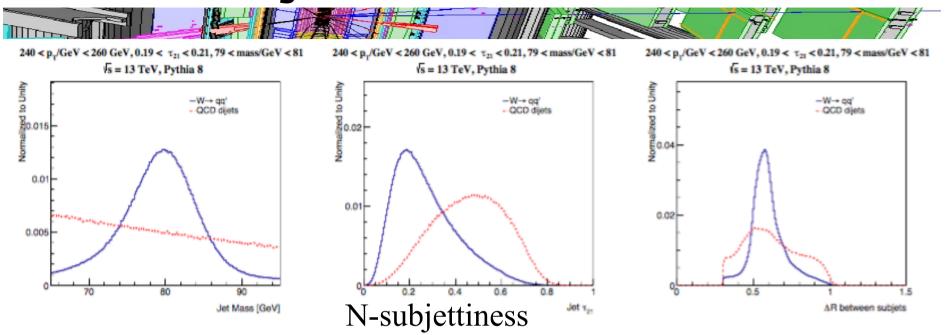




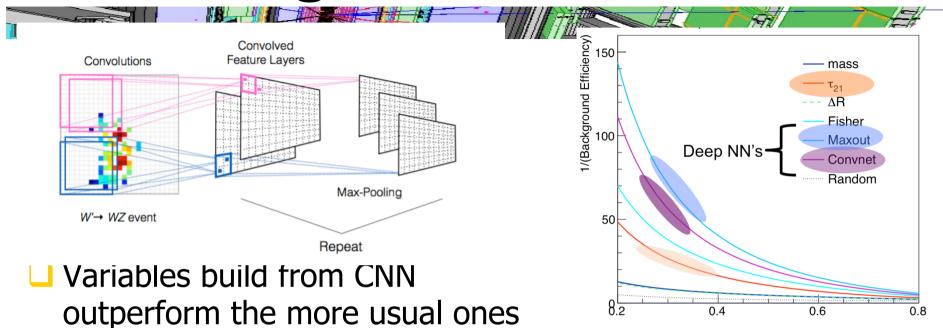


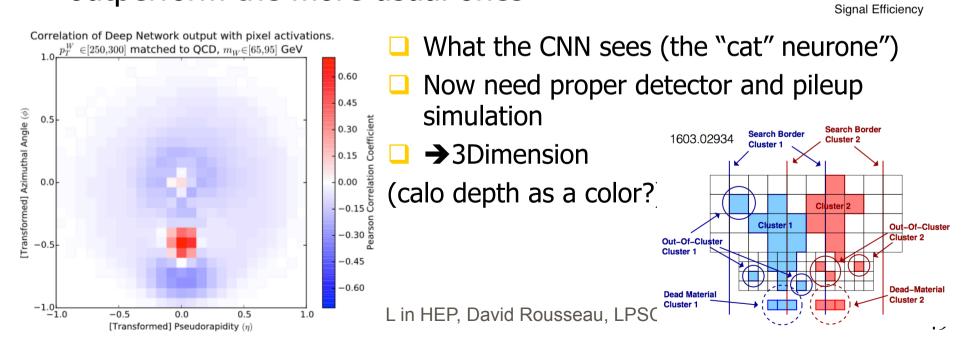
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Boosted jets: standard variables



Jet Images: Convolution NN

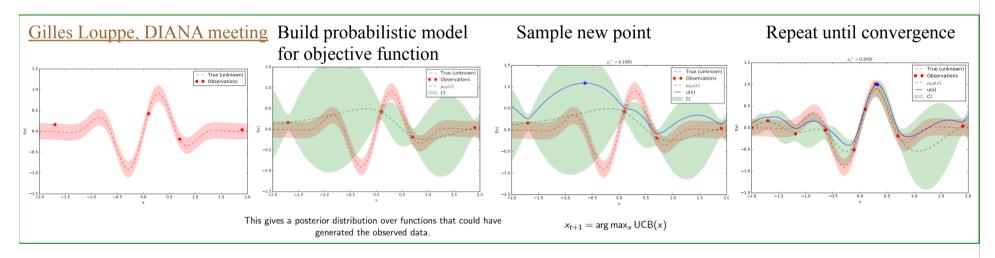




ML in Simulation



- 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
 - o optimisation in many dimensions parameter space, with costly evaluation
- Now turning to more modern techniques e.g.:
 - Bayesian Optimization and Gaussian Processes



- Another avenue : multivariable regression to parameterise detector response
- By the way: Bayesian Optimisation can also be used to optimised analysis

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Data Challenges



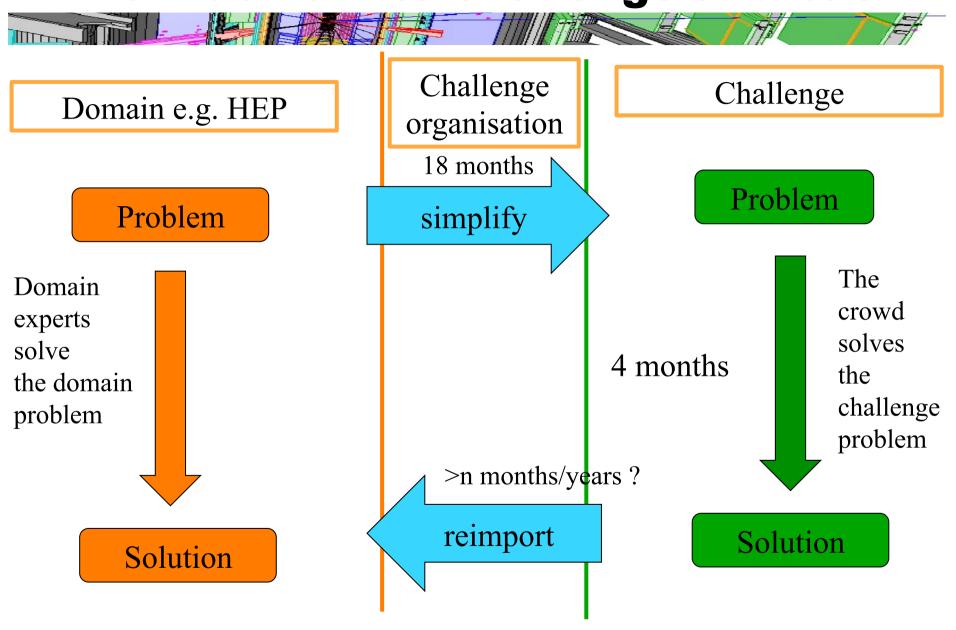
Challenges (competition)

- Challenges are essentially a way to create a buzz around an open dataset dressed with a benchmark
 - o HiggsML (ATLAS) 2014
 - FlavourML (LHCb) 2015
 - o future TrackML (ATLAS+CMS) 2017
- 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

From domain to challenge and back

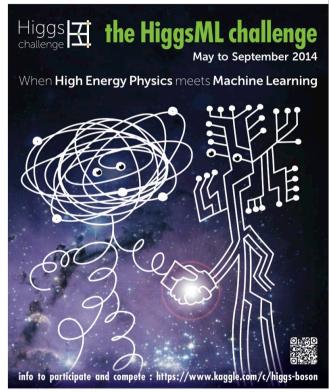


HiggsML: Committees

- Organization committee:
- 🚰 🌈 o David Rousseau : Atlas-LAL
 - Claire Adam-Bourdarios : Atlas-LAL (outreach, legal matter)
 - Glen Cowan: Atlas-RHUL (statistics)
 - Balazs Kegl: Appstat-LAL
 - o 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)
 - O Marc Schoenauer: INRIA Advances of ML in HEP, David Rousseau, LPSC Seminar

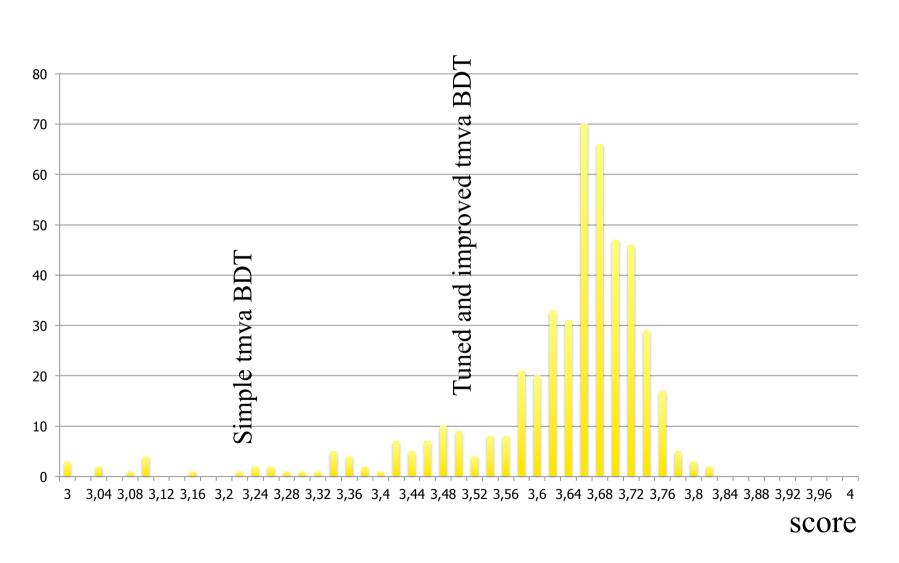
Higgs Machine learning challenge

- 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 <u>JMLR proceedings v42</u>
 - 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

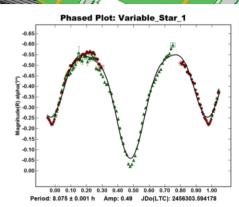


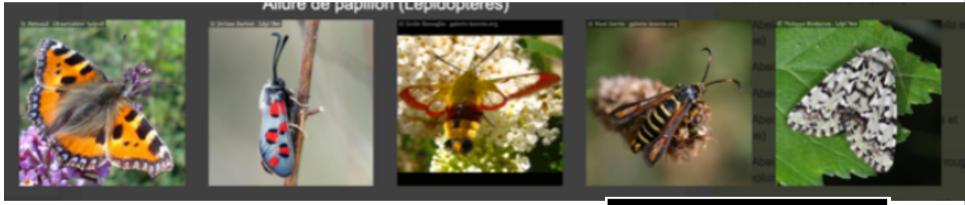
LHCb: flavour of physics

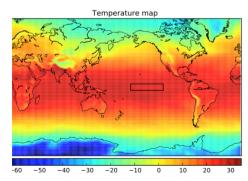
- □ LHCb organised in summer 2015 another challenge "flavour of physics": search for LFV decay τ→μμμ
- similar to HiggsML, with a big novelty:
 - some variables known to be poorly described by MC
 - o algorithm had to behave similarly on data and MC in a control region D0 \rightarrow K $\pi\pi$
- → Nice 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

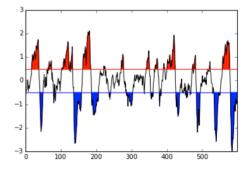
Beyond challenges: RAMP

- ☐ (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
 - o one day hackathon
 - o participants are encouraged to re-use other people's software
- Can adapt to all domains:

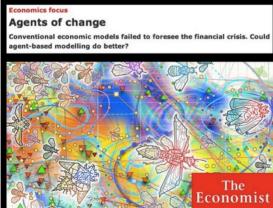








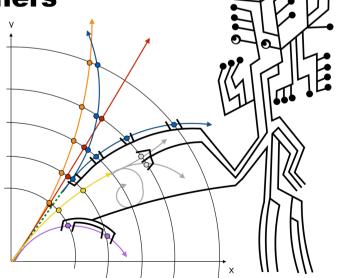
Advances of ML in HEP, David Rousseau



Towards a Future Tracking Machine Learning challenge



A collaboration between ATLAS and CMS physicists, and Machine Learners

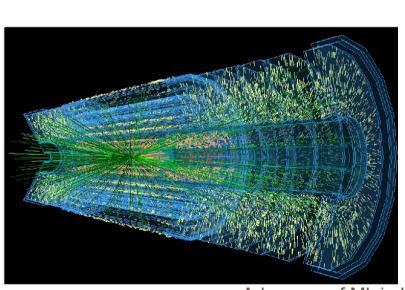


TrackML: Motivation 1

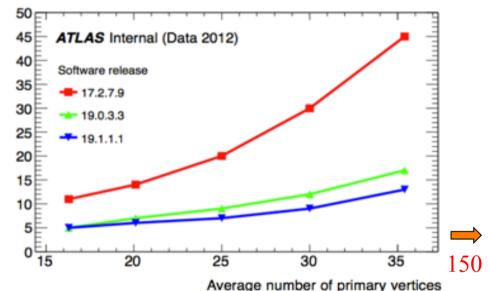


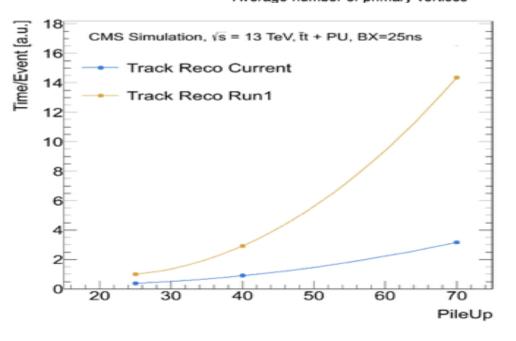
Graeme Stewart ECFA HL-LHC workshop 2014

- ☐ See details DR talk at CTD2016
- Tracking (in particular pattern recognition) dominates reconstruction CPU time at LHC
- HL-LHC (phase 2) perspective : increased pileup :
 - o Run 1 (2012): <>~20
 - o Run 2 (2015): <>~30
 - o Phase 2 (2025): <>~150
- CPU time quadratic/exponential extrapolation (difficult to quote any number)



Advances of ML in HE



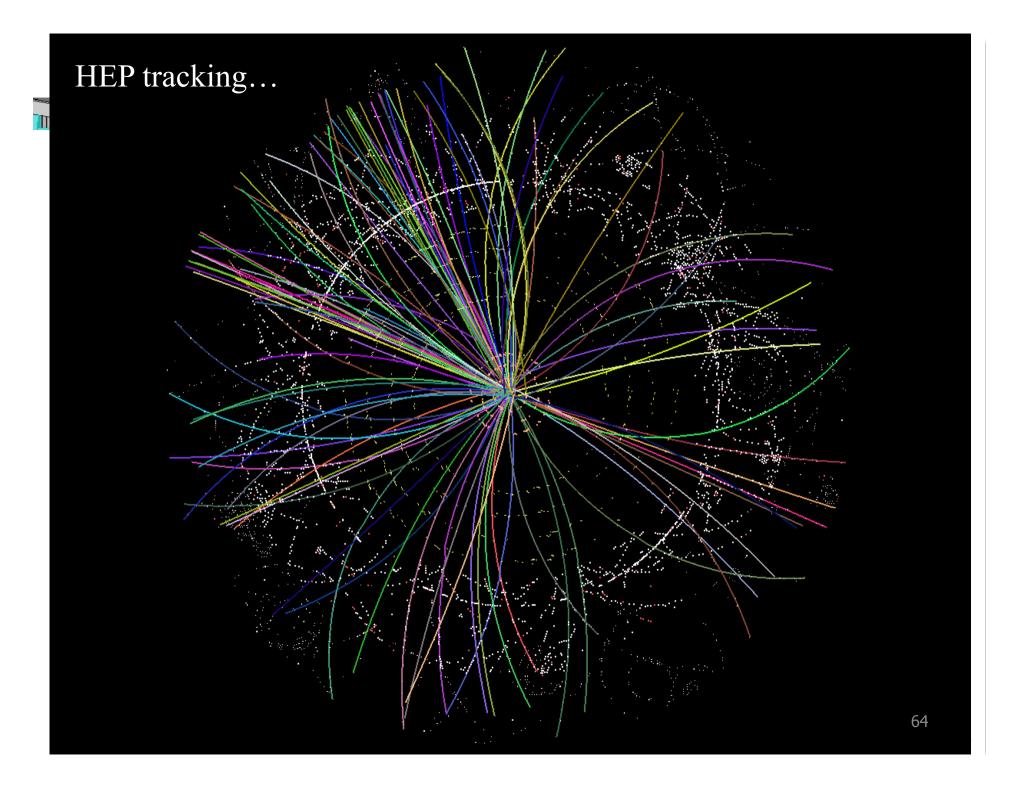


TrackML: Motivation 2

- - ☐ 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

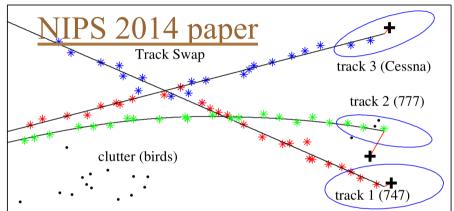
TrackML: engaging Machine Learners

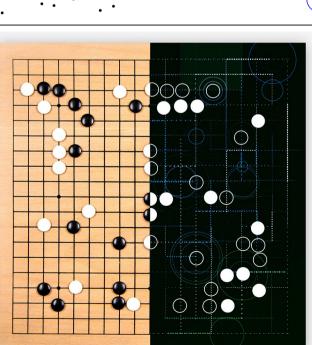
- Suppose we want to improve the tracking of our experiment
- We read the literature, go to workshops, hear/read about an interesting technique (e.g. ConvNets, MCTS...). Then:
 - o Try to figure by ourself what can work, and start coding→traditional way
 - o Find an expert of the new technique, have 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
 - o → 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, LPSC Seminar

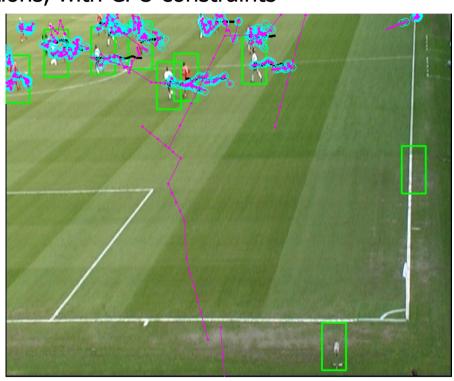


Pattern recognition

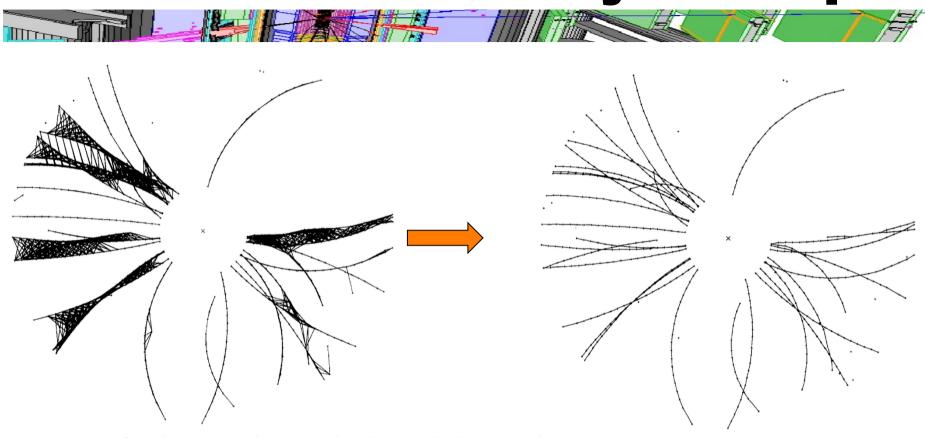
- Pattern recognition is a very old, very hot topic in Artificial Intelligence
- □ Note that these are real-time applications, with CPU constraints





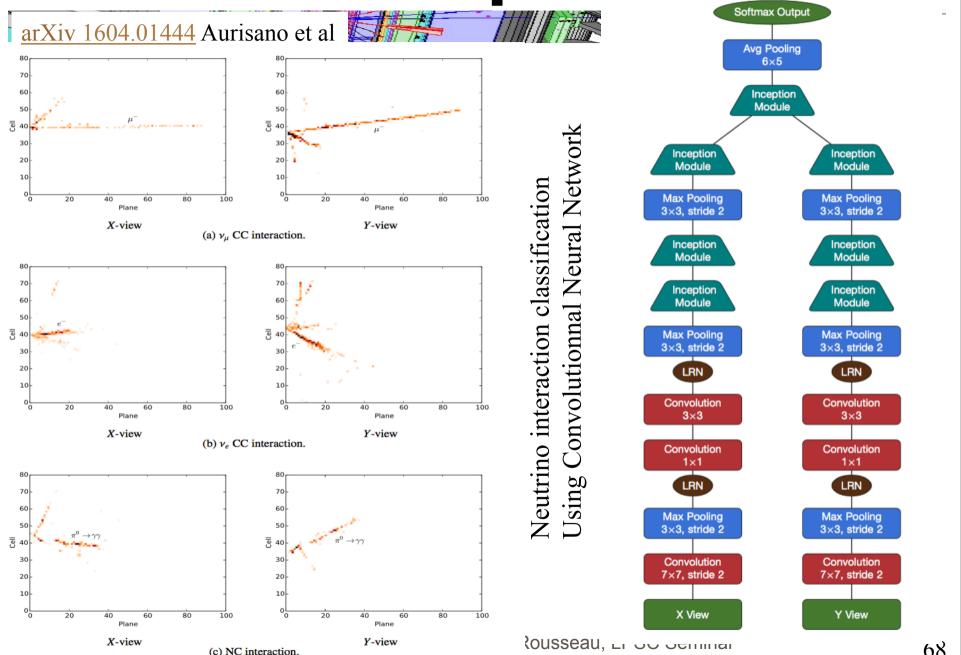


TrackML: An early attempt



- ☐ 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

A recent attempt: NOVA



Wrapping-up



ML Collaborations



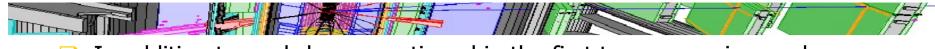
- Many of the new ML techniques are complex→difficult for HEP physicists alone
- ML scientists (often) eager to collaborate with HEP physicists
 - prestige
 - o new and interesting problems (which they can publish in ML proceedings)
- ☐ Takes time to learn common language
- Access to experiment internal 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
- Most likely there are friendly ML scientists in Grenoble

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)
 - o 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
 - o good for a start, but inaccurate
- Effort to have better open simulation engine (e.g. Delphes 4-vector detector simulation, ACTS for tracking)
- ☐ <u>UCI dataset repository</u> 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 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
- ☐ <u>Interexperiment Machine Learning group (IML)</u> is gathering speed (documentation, tutorials, etc...). Topical monthly meeting.
- An internal ATLAS ML group has started in June 2016. Probably also in CMS?
- □ IN2P3 School Of Statistics http://sos.in2p3.fr very good introduction
- 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/
- 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:
 - o software tools are ~easy to get, but still need know-how
 - o forum, workshops etc....
 - collaboration between HEP and ML scientists are often needed
- More and more open datasets/simulators to favor the collaborations
- More and more HEP and ML workshops, forums, group, challenges etc...
- Never underestimate the time for :
 - o (1) Great (or small) ML idea→
 - (2) ...demonstrated on toy dataset→
 - (3) ...demonstrated on real experiment analysis/dataset →
 - (4) ...experiment publication using the great (or small) idea