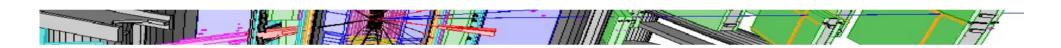
Advances in Machine Learning in experimental High Energy Physics



David Rousseau LAL-Orsay

rousseau@lal.in2p3.fr

IPHC seminar 16th Oct 2017

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



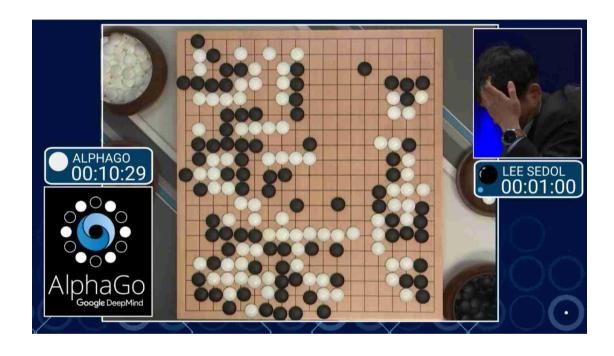
- ☐ Use of Machine Learning (a.k.a Multi Variate Analysis as we call it) already at LEP somewhat, much more at Tevatron (Trees)
- At LHC, Machine Learning used almost since first data taking (2010) for reconstruction and analysis
- ☐ In most cases, Boosted Decision Tree with Root-TMVA, on ~10 variables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

| analysis | data | no ML | ${ m ML}$ | ML |
|--|-------------|-------------|-------------|-----------|
| | taking year | sensitivity | sensitivity | data gain |
| ATLAS H $\rightarrow \gamma \gamma$ [16] | 2011-2012 | 4.3 | - | - |
| CMS H $\rightarrow \gamma \gamma$ [17] | 2011-2012 | ? | 2.7 | ? |
| ATLAS H $\rightarrow \tau^+ \tau^-$ [18] | 2012 | 2.5 | 3.4 | 85% |
| CMS H $\rightarrow \tau^+ \tau^-$ [19] | 2012 | 3.7 | - | - |
| ATLAS VH \rightarrow bb [20] | 2012 | 1.9 | 2.5 | 73% |
| ATLAS VH \rightarrow bb [21] | 2015-2016 | 2.8 | 3.0 | 15% |
| CMS VH \rightarrow bb [22] | 2012 | 1.4 | 2.1 | 125% |
| $CMS VH \rightarrow bb [23]$ | 2015-2016 | - | 2.8 | - |

→~50% gain on LHC running

ML in HEP

Meanwhile, in the outside world :

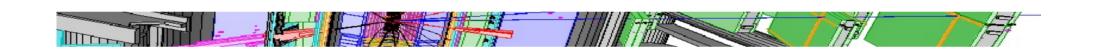


- "Artificial Intelligence" not a dirty word anymore!
- We've realised we're been left behind! Trying to catch up now...

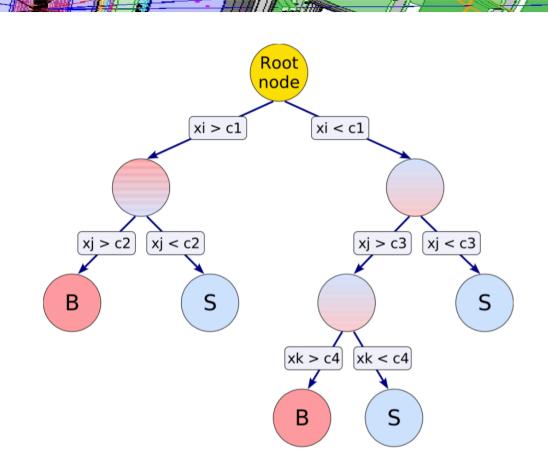
Multitude of HEP-ML events



ML Basics

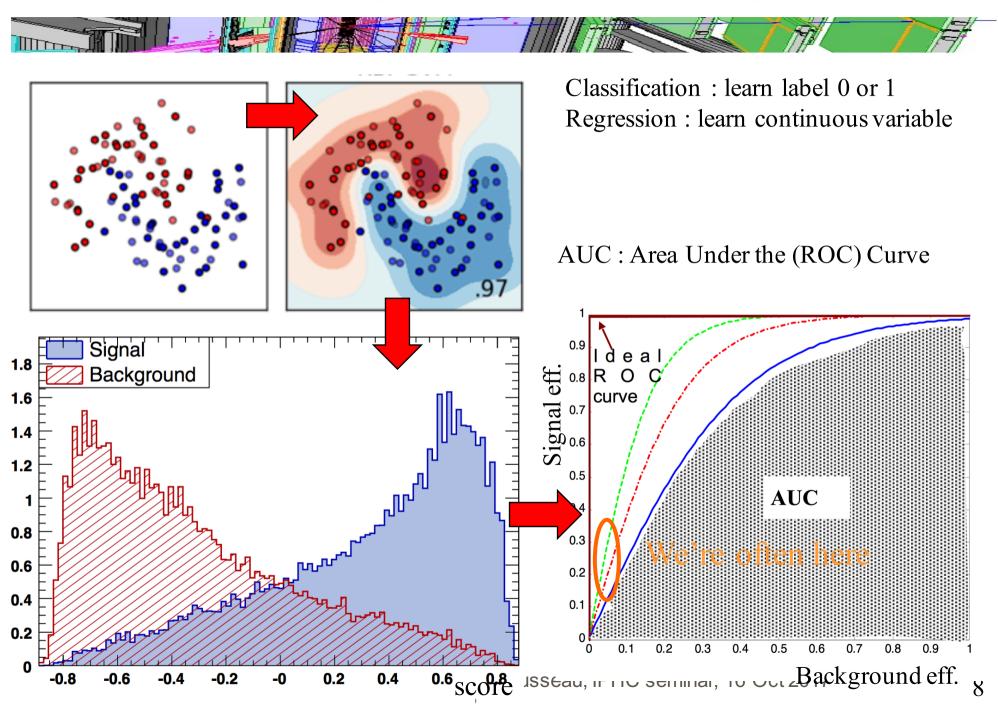


BDT in a nutshell

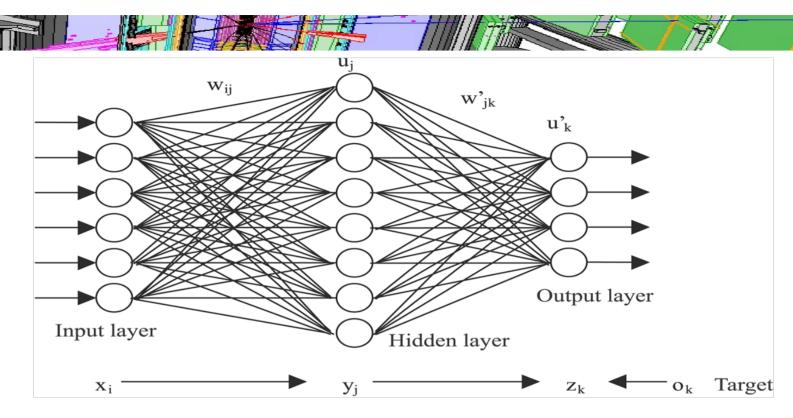


- ☐ Single tree (CART) <1980
- □ AdaBoost 1997: rerun increasing the weight of misclassified entries → Boosted Decision Trees (Gradient BDT, random forest...)

Classifier basics

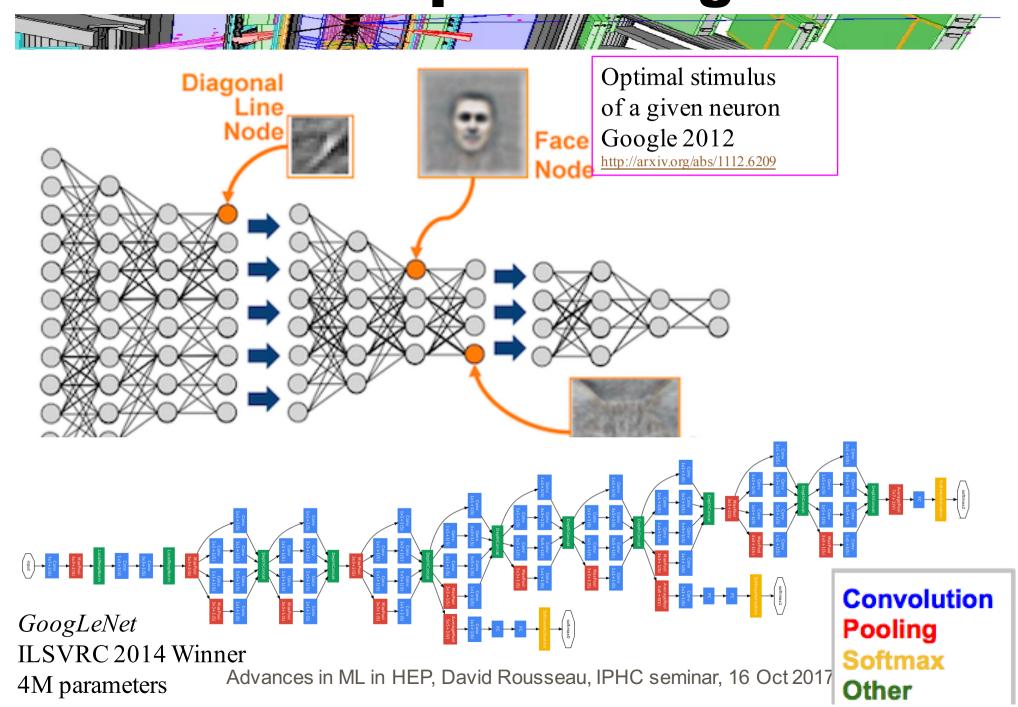


Neural Net in a nutshell



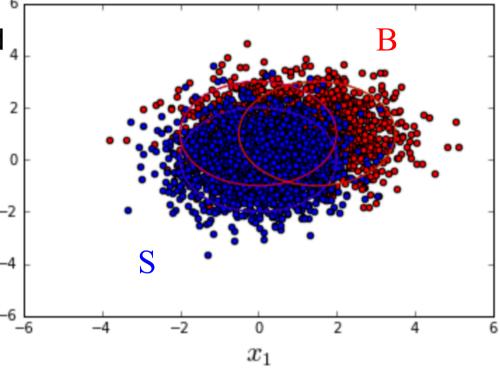
- Neural Net ~1950!
- But many many new tricks for learning, in particular if many layers (also ReLU instead of sigmoïd activation)
- "Deep Neural Net" up to 100 layers
- □ Computing power (DNN training can take days even on GPU)
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Deep learning



No miracle

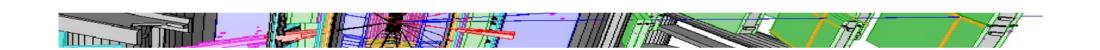
- ML (nor Artificial Intelligence) does not do any miracles
- For selecting Signal vs Background and underlying distributions are known, nothing beats Likelihood ratio! (often called "bayesian limit"):
 - $_{\rm O}$ $L_{\rm S}(x)/L_{\rm B}(x)$
- OK but quite often L_S L_B are unknown
 - + x is n-dimensional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



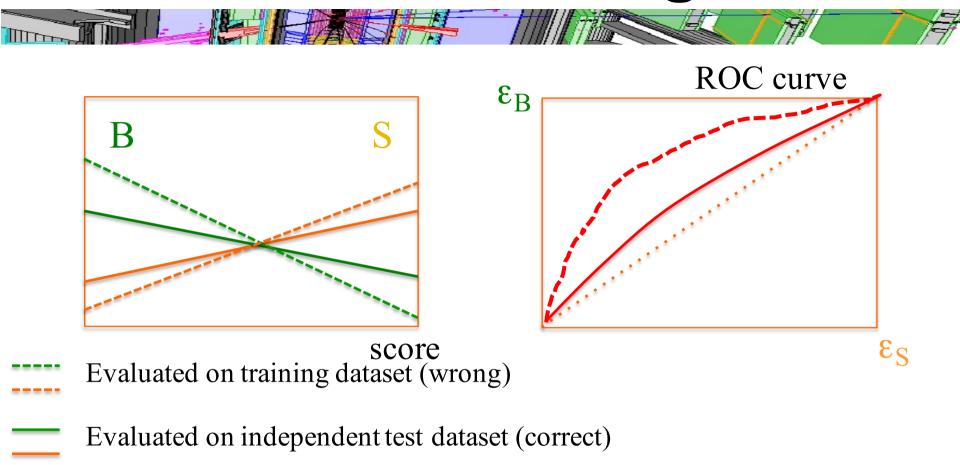
Some vocabulary

- "Features"
 - variables
- "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

ML Techniques



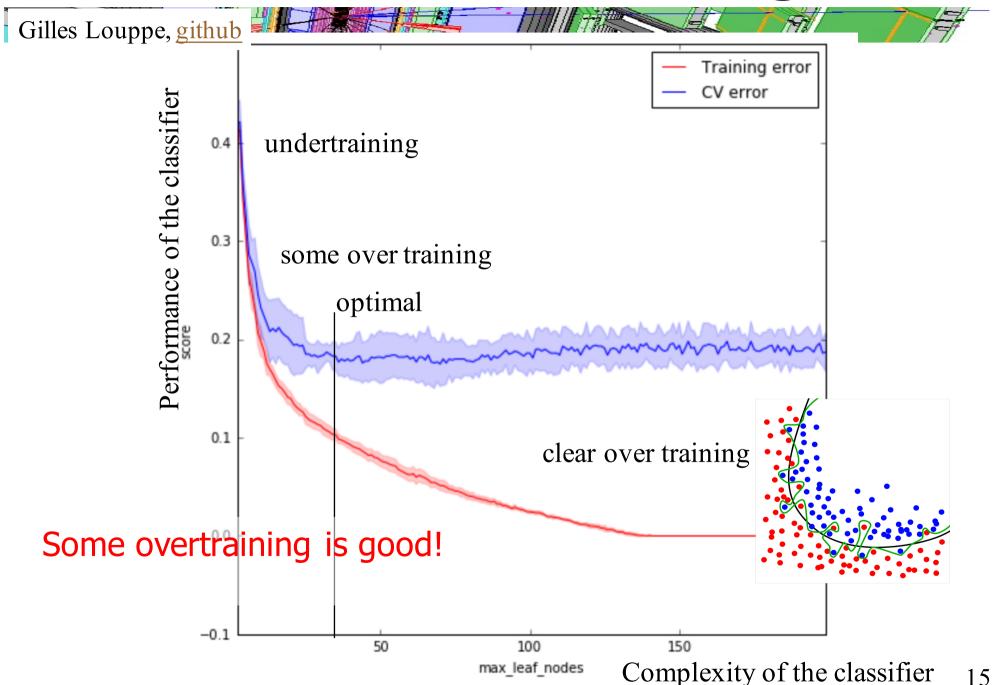
Overtraining

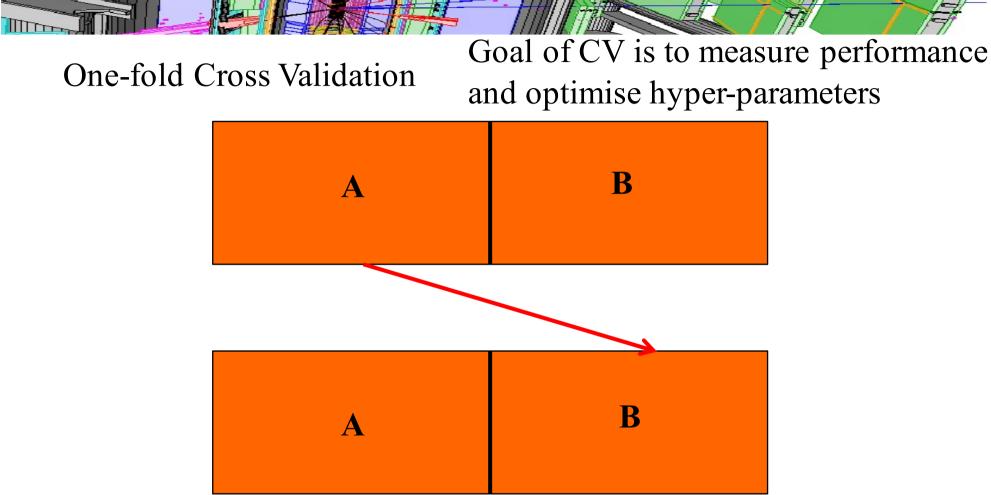


Score distribution different on test dataset wrt training dataset

"Overtraining" == possibly excessive use of statistical fluctuation

under/over training

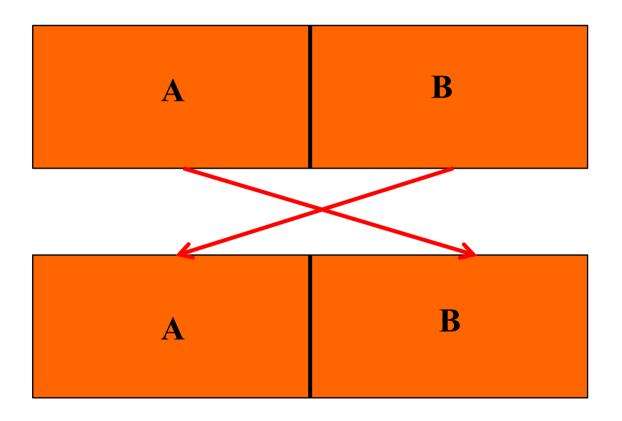




Standard basic way (default TMVA until recently)



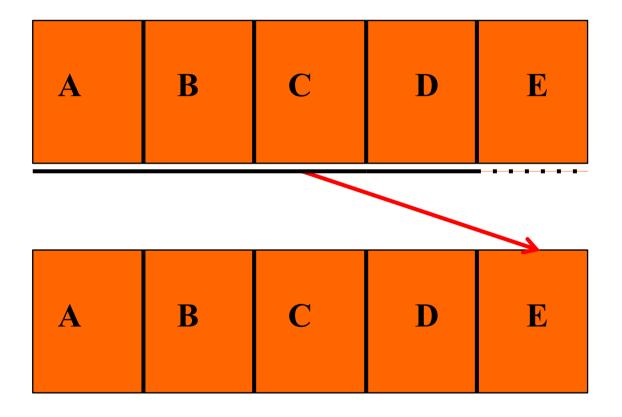
Two-fold Cross Validation



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



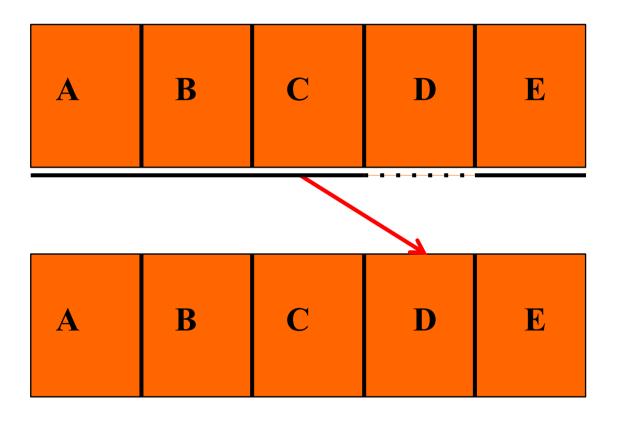
5-fold Cross Validation



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 in ML in HEP, David Rousseau, IPHC seminar, 16 Oct 2017

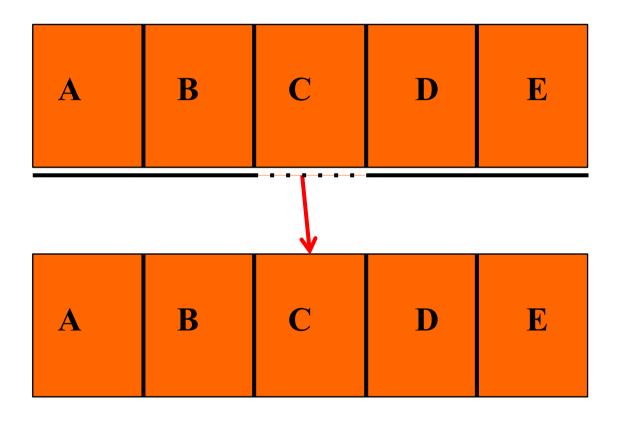


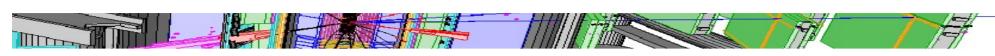
5-fold Cross Validation



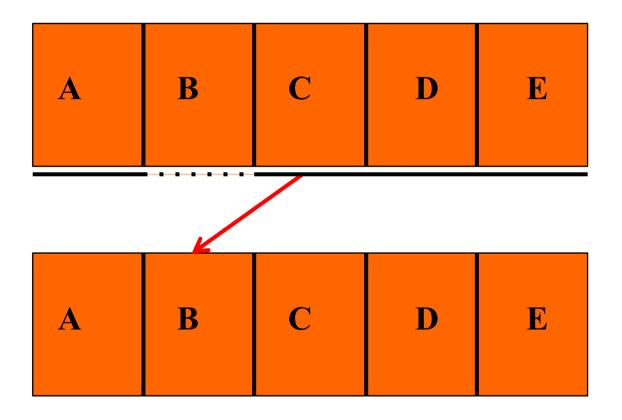


5-fold Cross Validation



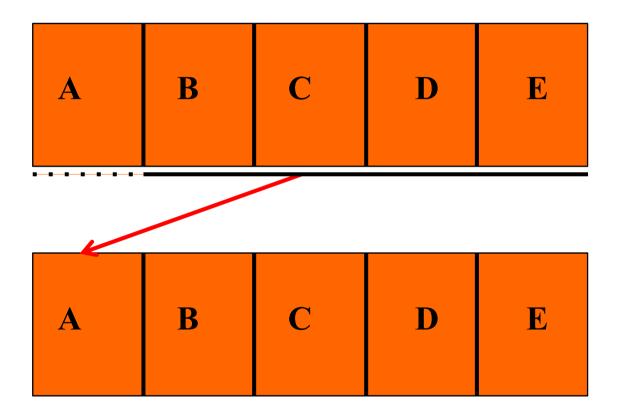


5-fold Cross Validation





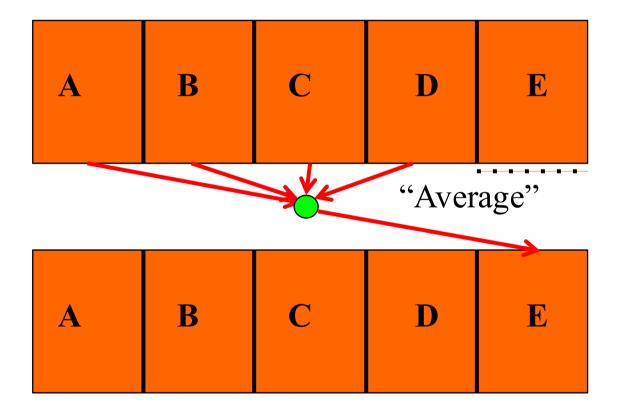
5-fold Cross Validation



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



5-fold Cross Validation "à la Gabor"



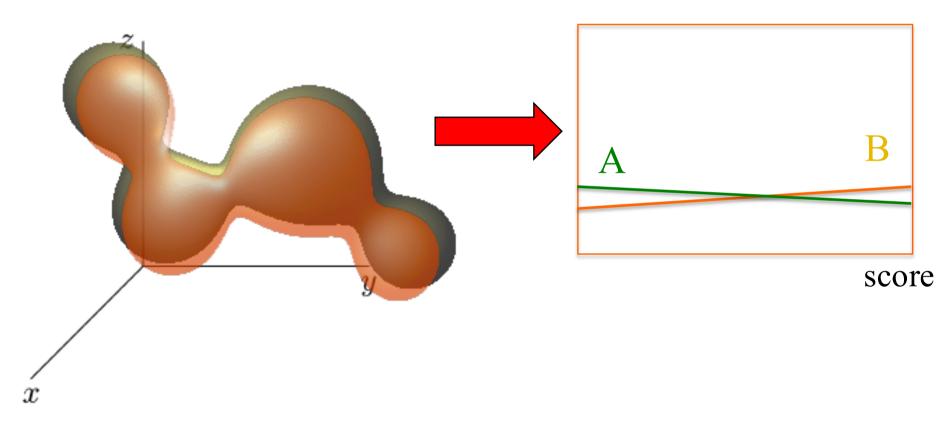
Average of the scores on A B C D is

often better than the score of one training ABCD

(also save on training time)

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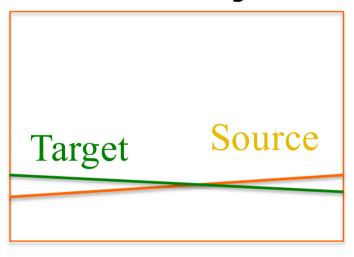
What does a classifier do?

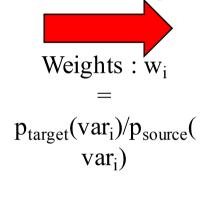


□ The classifier "projects" the two multidimensional "blobs" maximising the difference, without (ideally) any loss of information

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



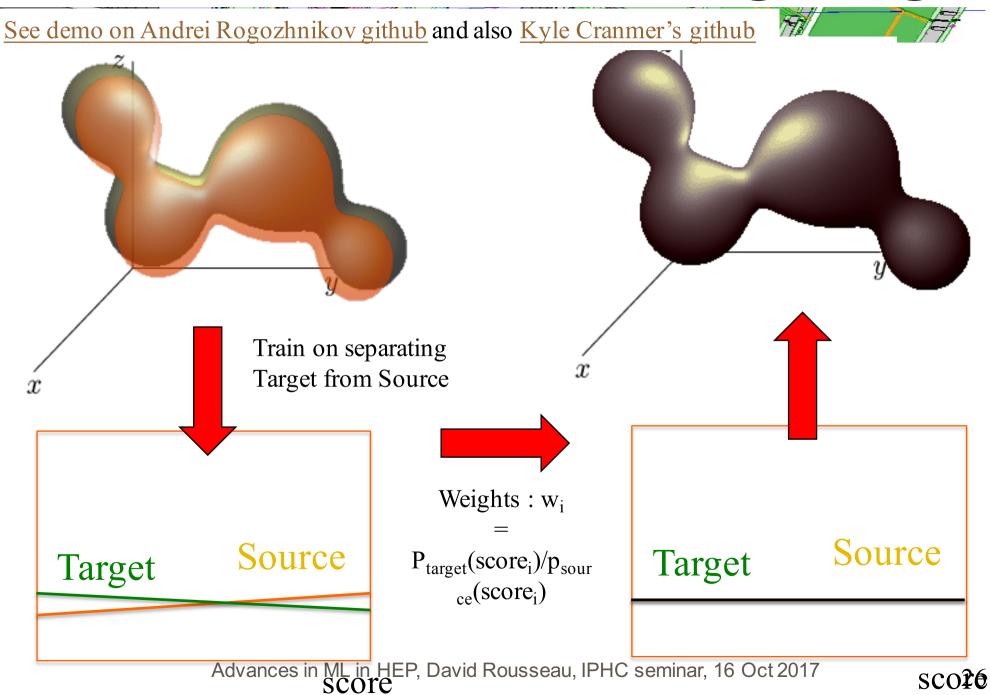




var

- 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



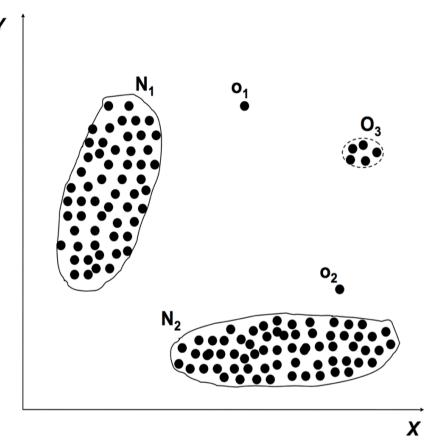
Multi dimensional reweighting (2)



- 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)

Anomaly: point level

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

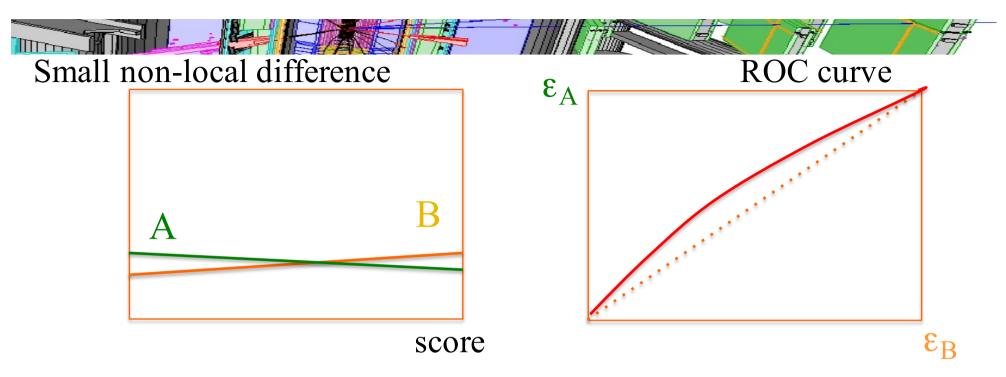


- Supervised: we have a training "normal" data set with N1 and N2.
 Algorithm should then spot o1,o2, O3 as "abnormal" i.e. "unlike N1 and N2" (no a priori model for outliers)
- Application: detector malfunction, grid site malfunction, or even new physics discovery...

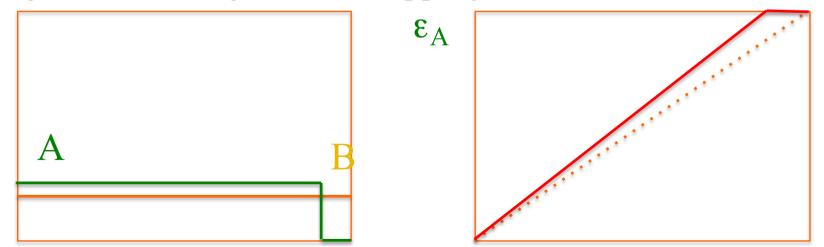
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Anomaly: population level

- 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
 - o 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)
- 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



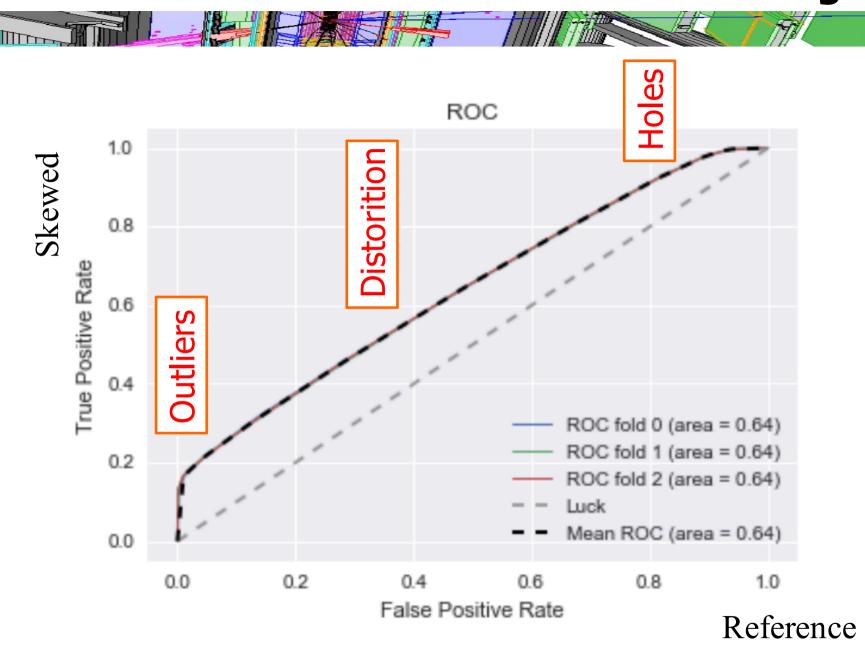
Local big difference (e.g. non overlapping distribution, hole)



HSF ML RAMP on anomaly

- Rapid Analysis Model Prototyping: collaborative competition around a dataset and a figure of merit. Organised in June 2016 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 e.g various invariant masses (computed from the above) from Htautau analysis
 - o → reference dataset
- "Skewed" dataset built from the above, introducing small and big distortions:
 - Change of tau energy scale (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)

| eam | submission | accuracy | |
|---------|----------------------|----------|--|
| ncherti | adab2_mt1_calibrated | 0.611 | |
| dhrou | adab2_mt1 | 0.611 | |
| cazeevn | GradientBoosting | 0.596 | |
| glouppe | bags2 | 0.594 | |
| glouppe | boosting-duo | 0.595 | |
| ncherti | adaboost2 | 0.594 | |
| louppe | bags | 0.593 | |
| ncherti | adaboost1 | 0.593 | |
| ljabbz | beta tester | 0.591 | |
| oobash | ExtraTreesClassifier | 0.576 | |
| ncherti | extratrees1 | 0.562 | |
| hrou | DRv0 | 0.553 | |
| alaf | starting_kit_paolo | 0.526 | |

Breakthrough : add new variable: $\Delta m_T = \sqrt{(2P_{lT}^*MET^*(1-cos(\varphi_l - \varphi_{MET})))} - m_T$ Non zero for some outliers

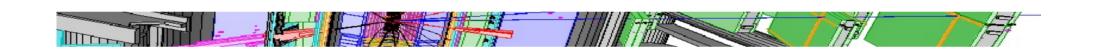
→ classifiers were unable to guess it

→ what functional form

classifiers can learn?

Classifier optimisation

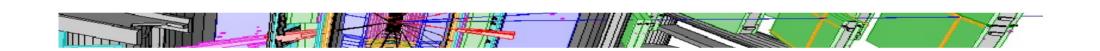
ML Tools

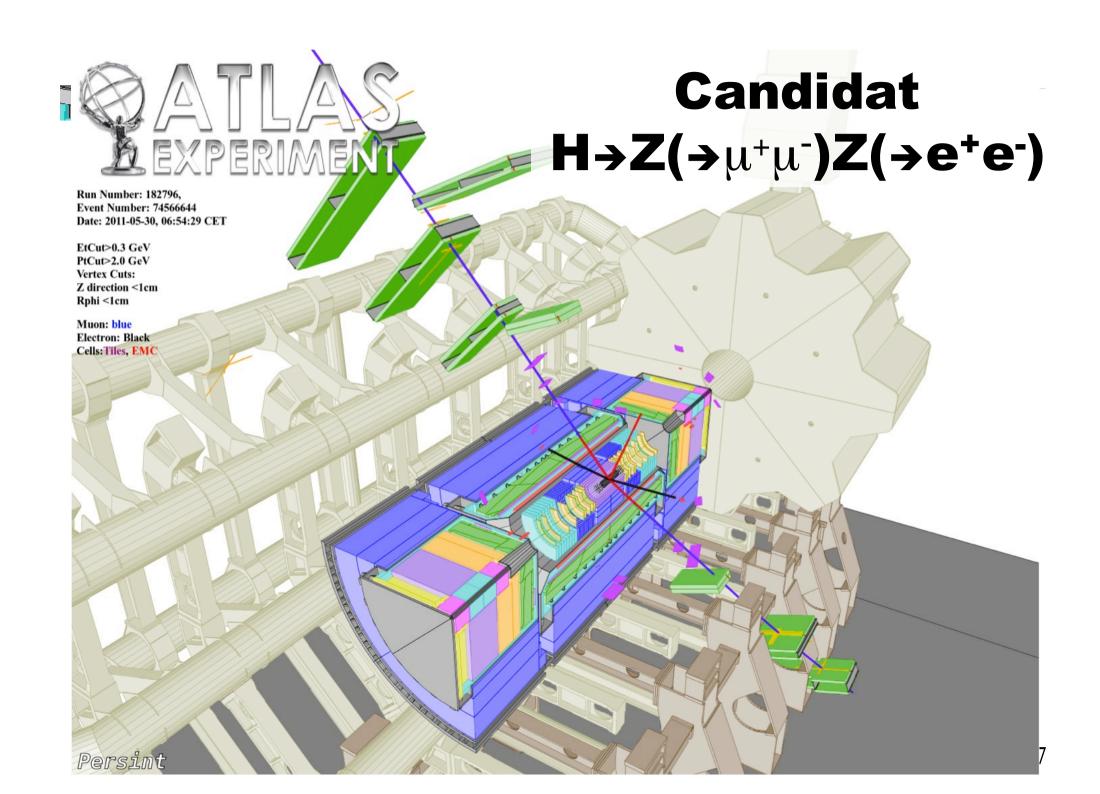


Modern Software and Tools

- New version of TMVA (root 6.0.8 on beyond) (see talk <u>Lorenzo Moneta, Sergei Gleyzer IML</u> workshop CERN March 2017)
 - Jupyter interface
 - Hyper-parameter optimisation
 - Cross-validation
 - o (...unfortunately not so well documented yet)
- Non HEP software
 - Sci-kit learn : de facto standard toolbox ML (except Deep Learning) (python, but fast)
 - Theano + Keras : NN toolbox (build a NN in a few lines of python)
 - XGBoost best BDT on the market, both speed and performance (c++ with python interface)
- \square Note: for ~ 10 variable classification/regression task 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)
 - 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

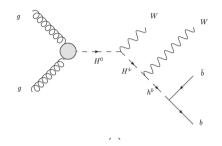
ML in analysis

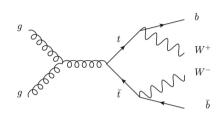


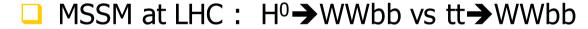


Deep learning for analysis

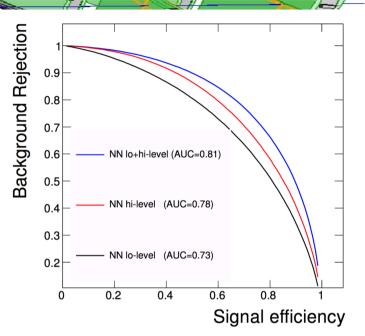
1402.4735 Baldi, Sadowski, Whiteson

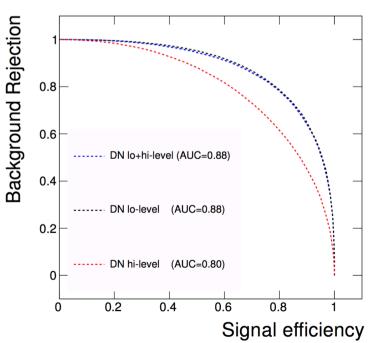






- Low level variables:
 - 4-momentum vector
- High level variables:
 - Pair-wise invariant masses
- Deep NN outperforms NN, and does not need high level variables
- DNN learns the physics ?

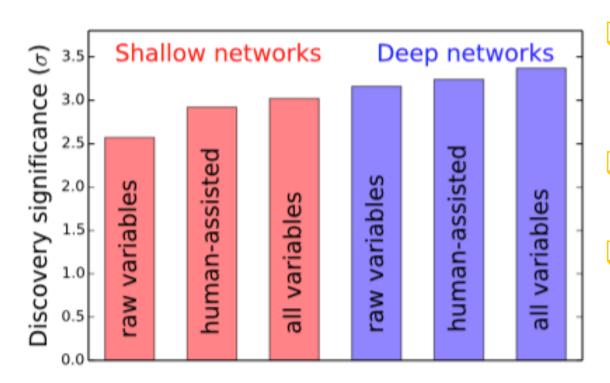




Deep learning for analysis (2)

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...)

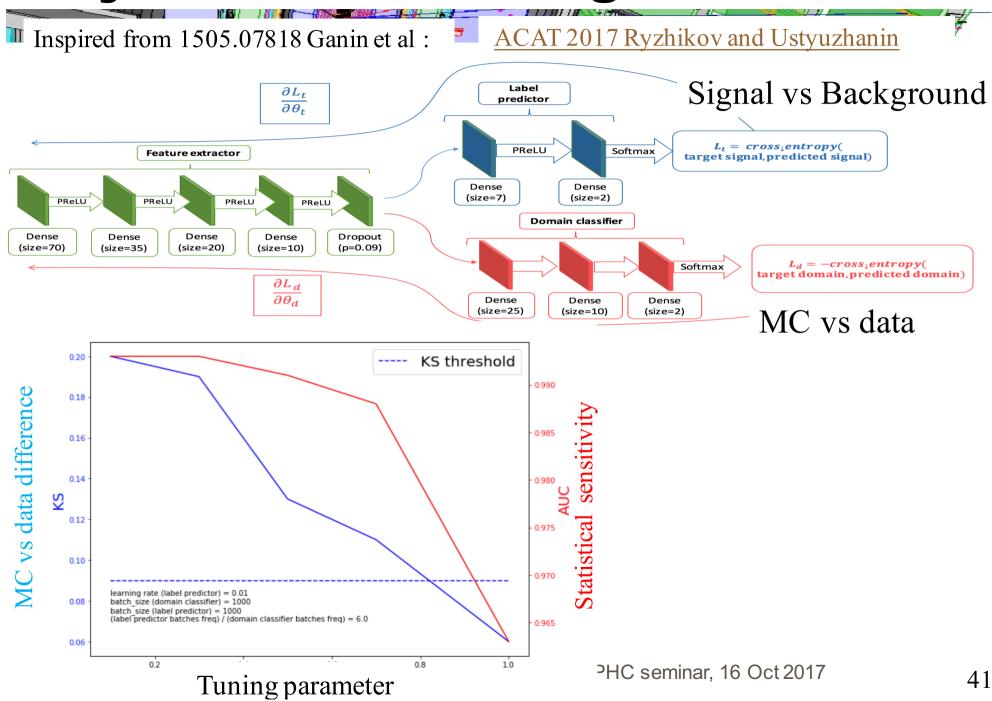


- Here, the DNN improved on NN but still needed high level features
- Both analyses withDelphes fast simulation
- ~10M events used for training (>>10* full G4 simulation in ATLAS)

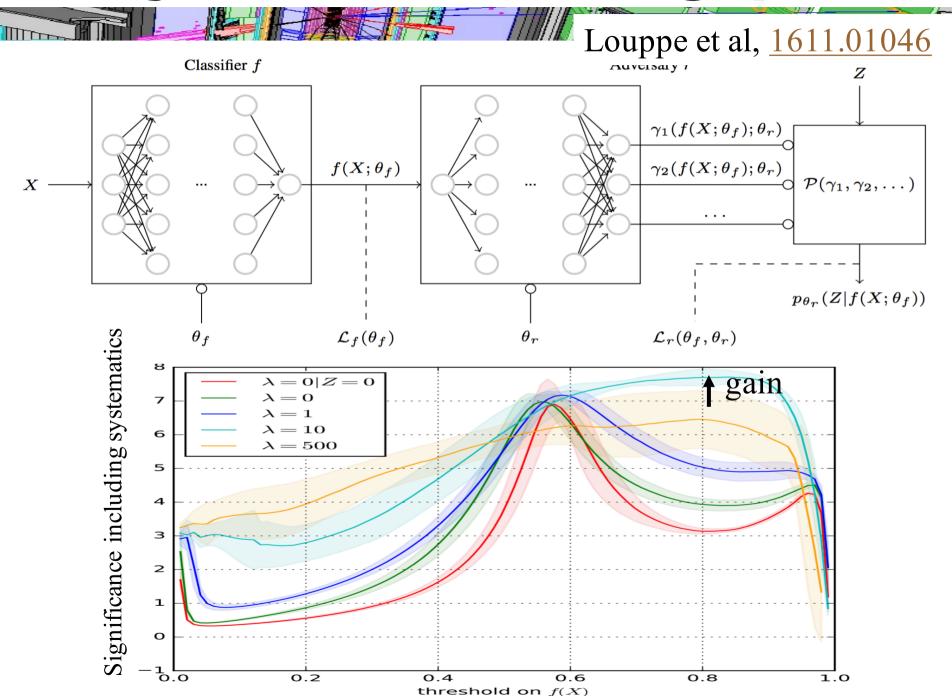
Systematics-aware training

- Our experimental measurement 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 $\sigma(\text{stat})$
- □ Impact of ML on σ (syst) or even better global optimisation of σ (stat) $\pm \sigma$ (syst) is an open problem
- \square 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 Advances in ML in HEP, David Rousseau, IPHC seminar, 16 Oct 2017

Syst Aware Training: adversarial

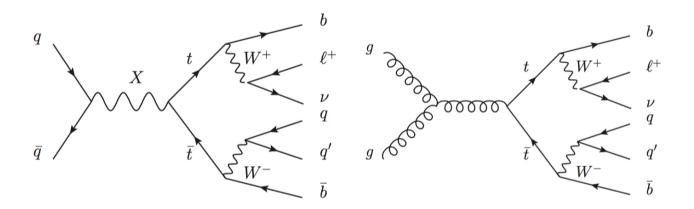


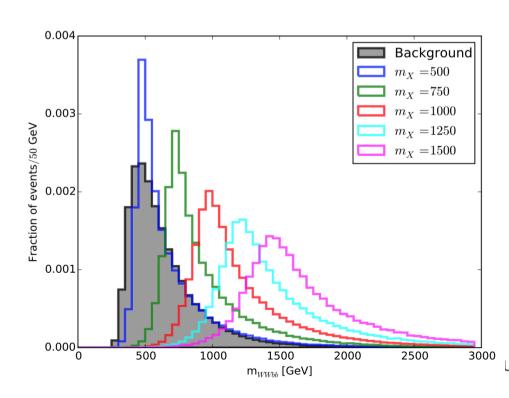
Syst Aware training: pivot



Parameterised learning

1601.07913 Baldi, Cranmer, Faucett, Sadowksi, Whiteson

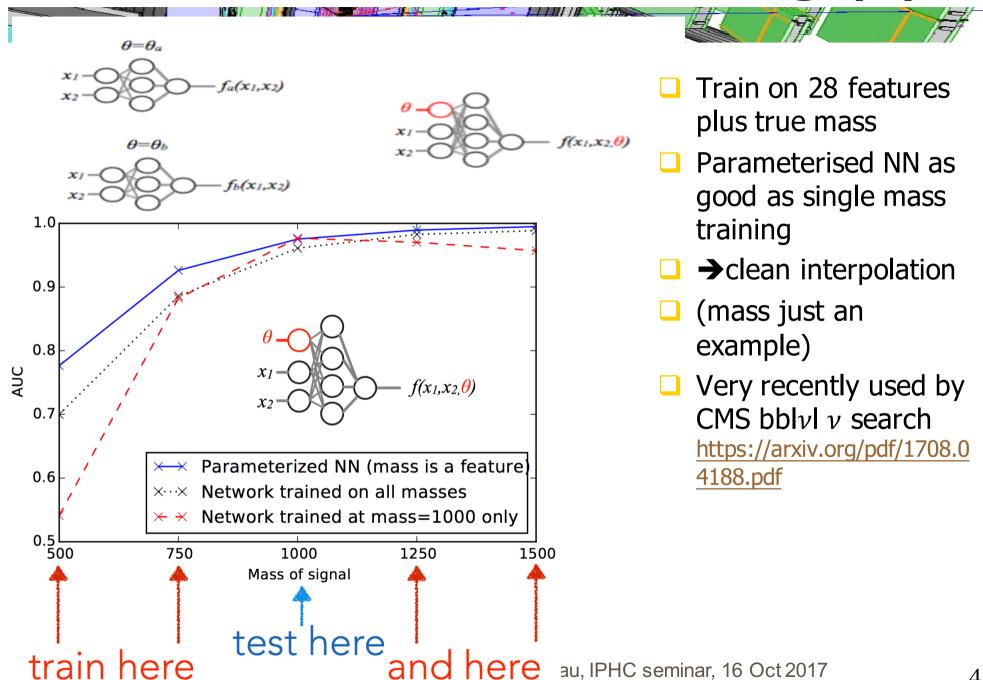




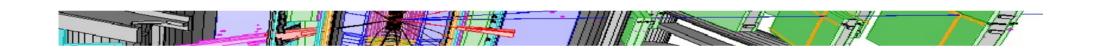
- Typical case: looking for a particle of unknown mass
- □ E.g. here tt decay

usseau, IPHC seminar, 16 Oct 2017

Parameterised learning (2)



ML in reconstruction



Jet Images

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



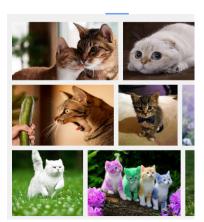
Distinguish boosted W

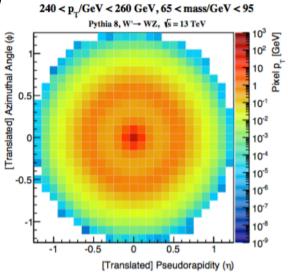
jets from QCD

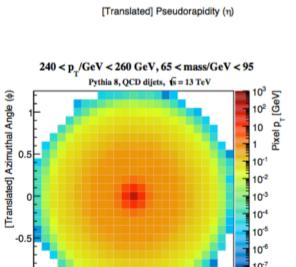
Particle level simulation

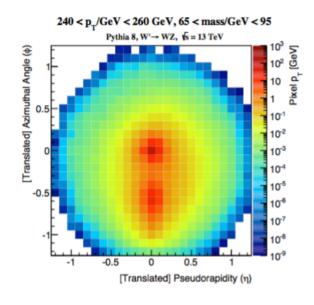
Average images:

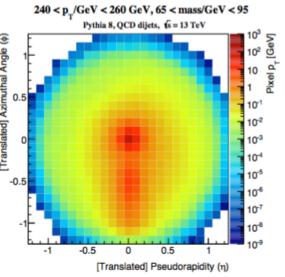










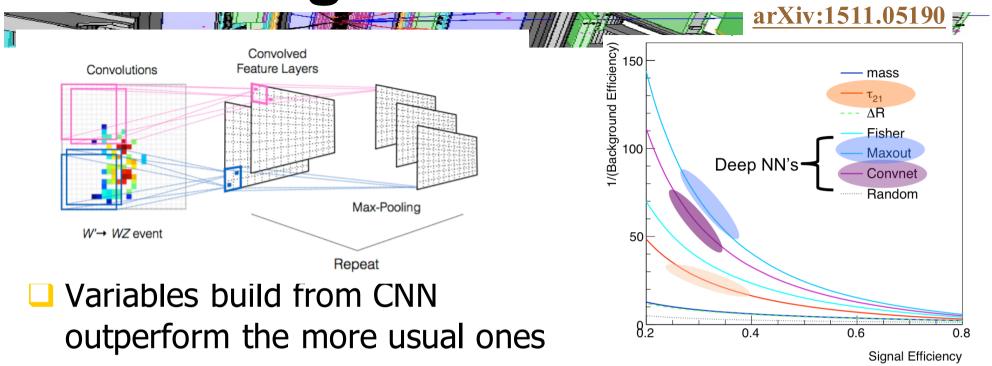


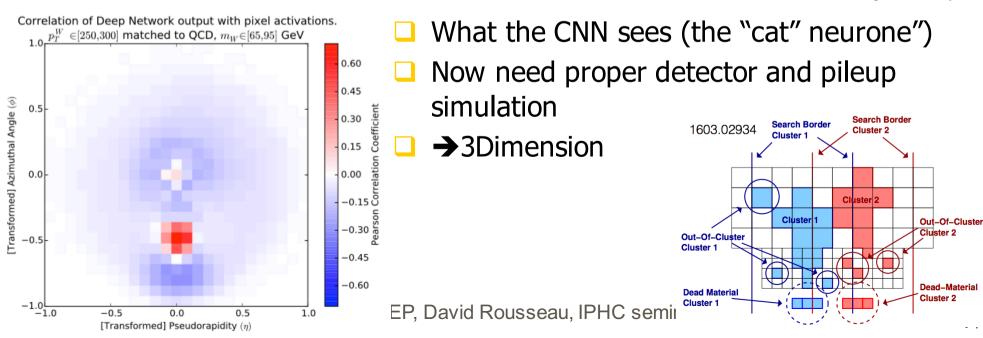
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0.5

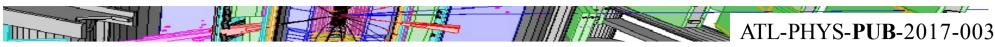
[Translated] Pseudorapidity (n)

Jet Images: Convolution NN

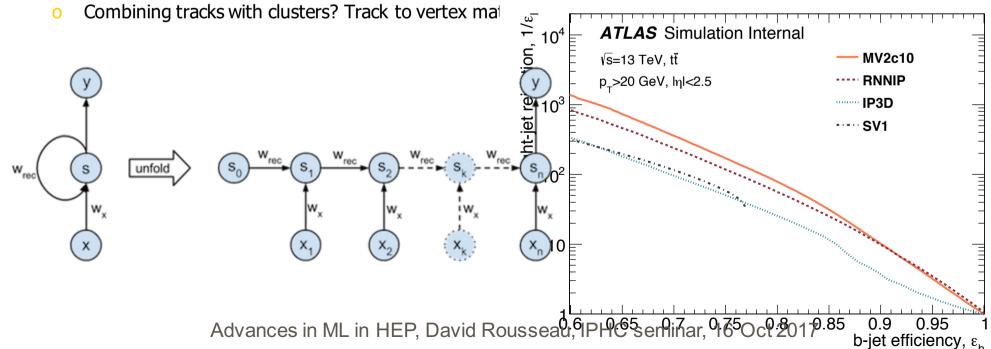




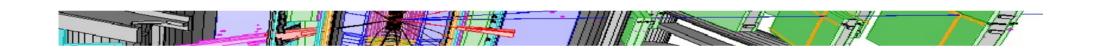
RNN for b tagging



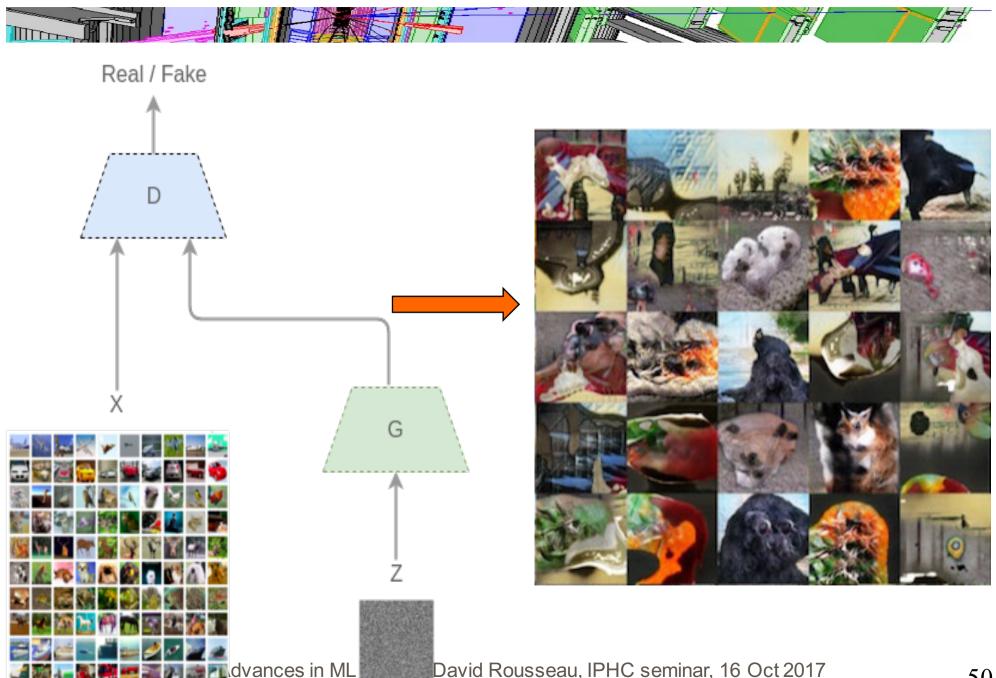
- BDT and usual NN expect a fix number of input. What to do when the number of inputs is not fixed like the tracks for b-quark jet tagging?
- Recurrent neural networks have seen outstanding performance for processing sequence data
 - o Take data at several "time-steps", and use previous time-step information 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!



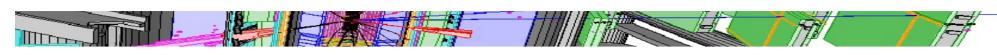
ML in simulation



Generative Adversarial Network



Condition GAN

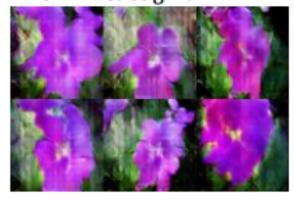


Text to image

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



the flower has petals that are bright pinkish purple with white stigma



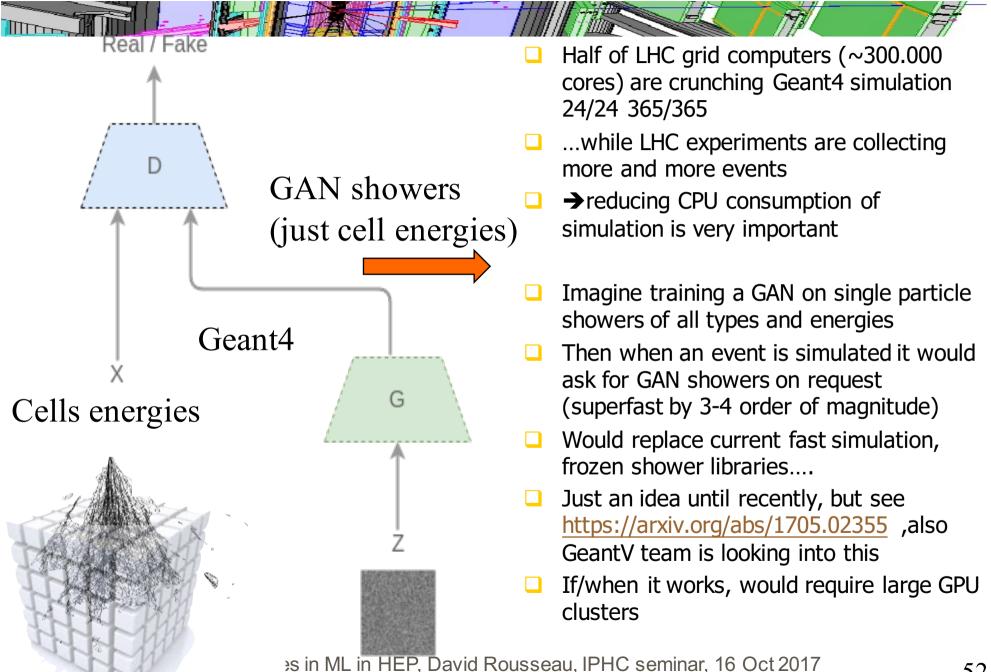
this magnificent fellow is almost all black with a red crest, and white cheek patch.



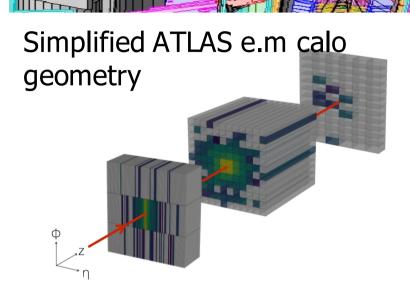
this white and yellow flower have thin white petals and a round yellow stamen



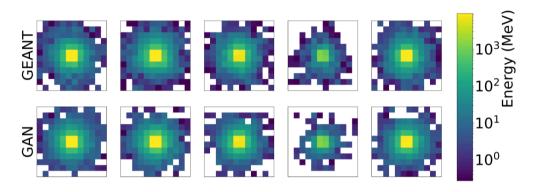
GAN for simulation

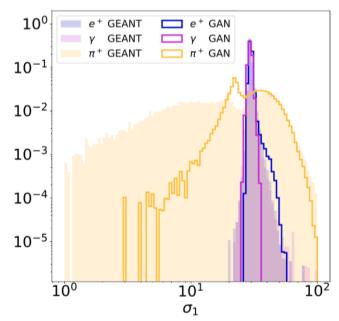


CaloGAN



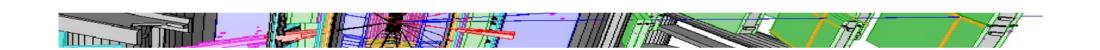






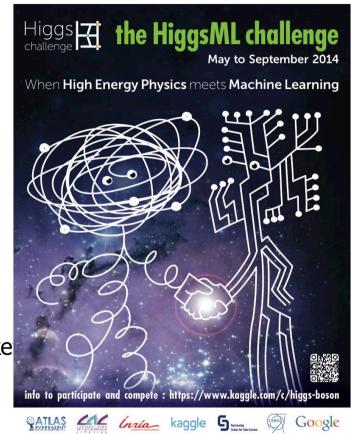
- One of many physics variable examined
- Pion more difficult
- very promising

Data Challenges



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 written for HiggsML, now best BDT on the marke
 - 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



Towards a Future Tracking Machine Learning challenge

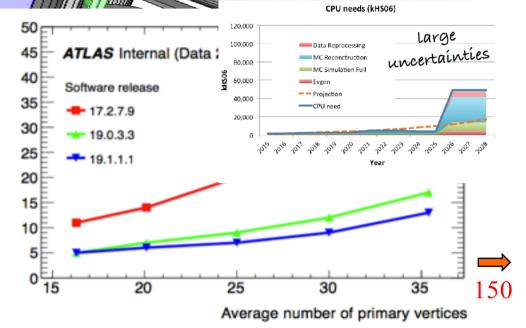


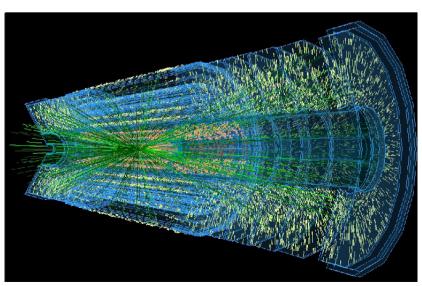
A collaboration between ATLAS and CMS physicists, and Machine Learners

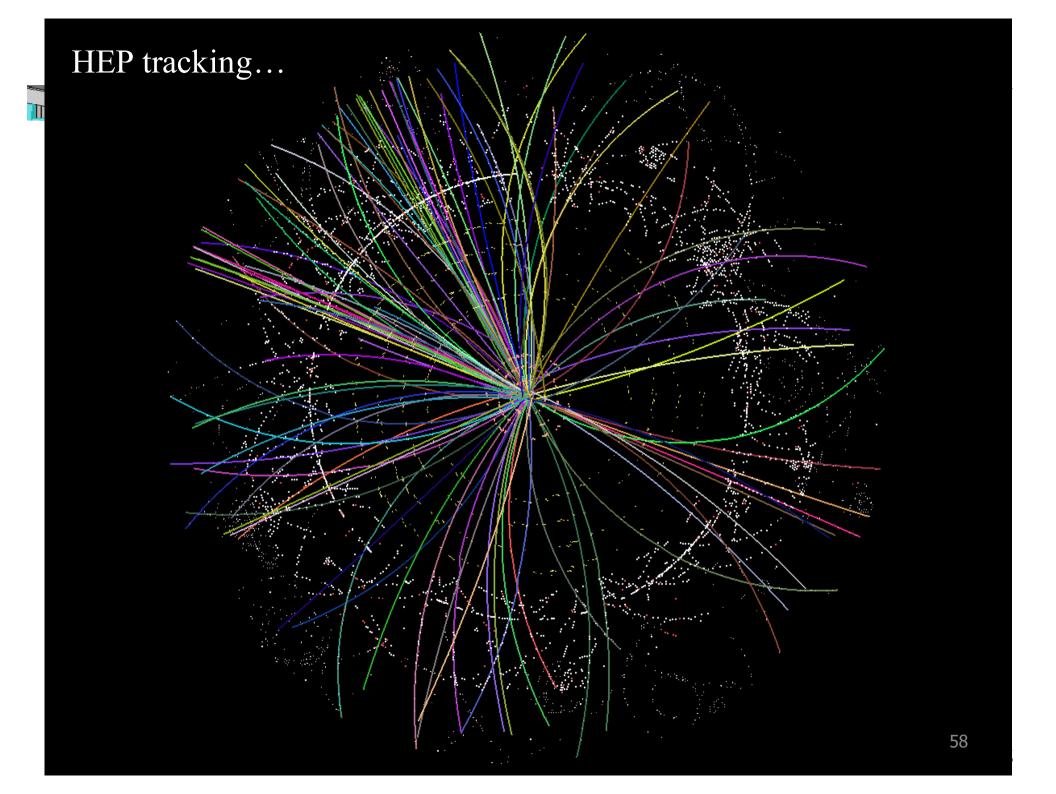
TrackML: Motivation



- ☐ 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)





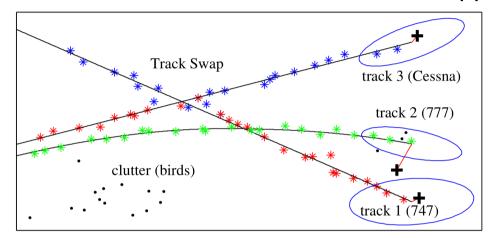


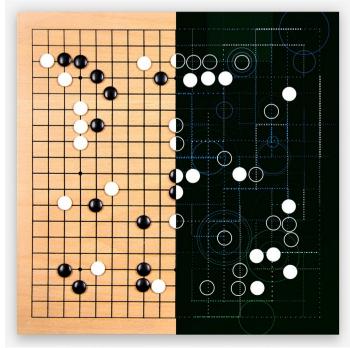
TrackML: engaging Machine Learners

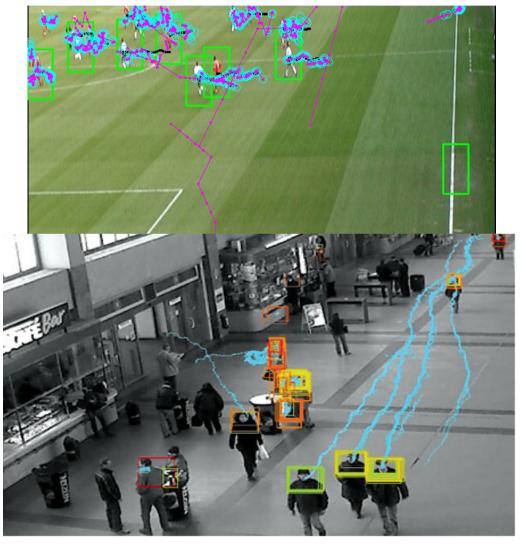
- □ Suppose we want to improve the tracking of our experiment
- We read the literature, go to workshops, hear/read about an interesting technique (e.g. ConvNets, MCTS...). Then:
 - Try to figure by ourself what can work, and start coding→traditional way
 - o Find an expert of the new technique, have 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
 - → 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
 - o →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
 - o →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 As weignesing in the many interesting in the seminar, 16 Oct 2017

Pattern recognition

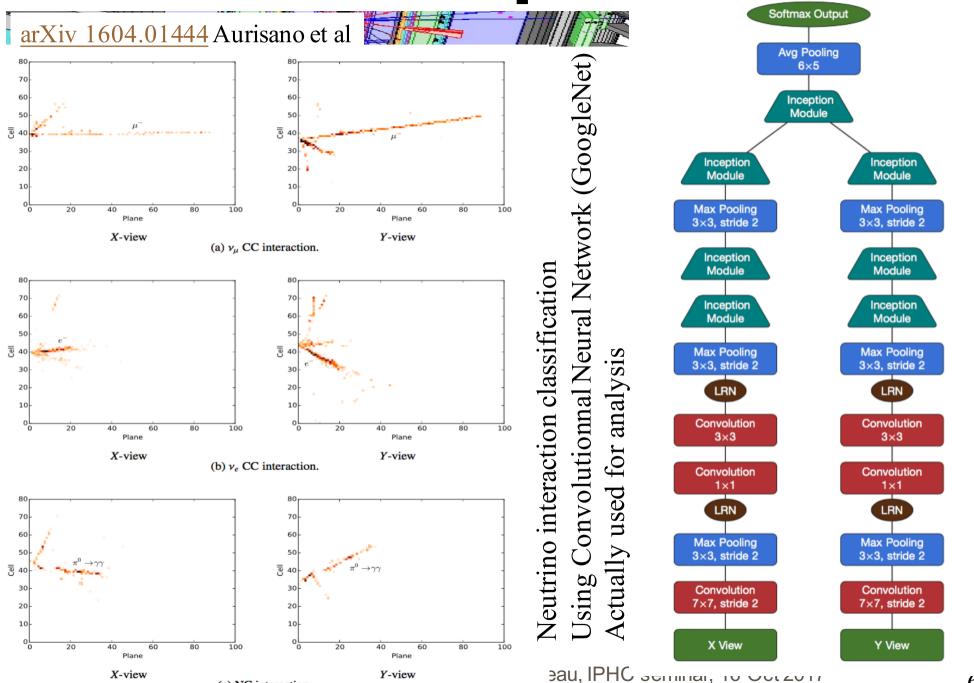
- □ Pattern recognition is a very old, very hot topic in Artificial Intelligence,
- □ Note that these are real-time applications, with CPU constraints







A recent attempt: NOVA

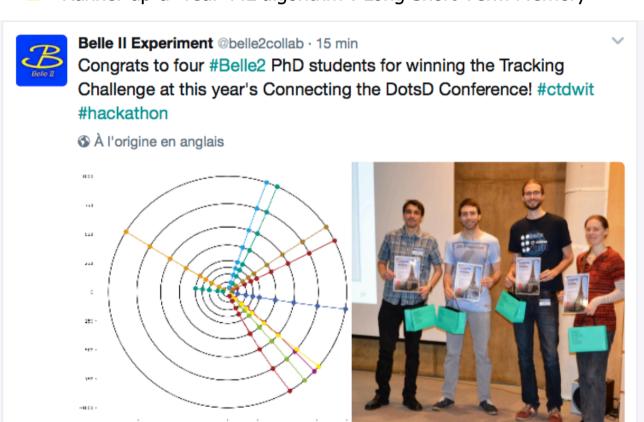


(c) NC interaction.

CTDWIT 2017 2D tracking Hackathon



- Very simplified 2D simulation with HL-LHC ATLAS layout (circular detectors, multiple scattering, inefficiency, stopping tracks)
 EPJ Web Conf., 150 (2017) 00015
- Run on RAMP platform
- 30 people (tracking experts mostly) for 2 hours in the same room, plus 36 hours till the end of the conference
- Winner is a Monte Carlo Tree Search algorithm (used in Go algorithms before and also by Alpha-Go)
- Runner-up a "real" ML algorithm : Long Short Term Memory



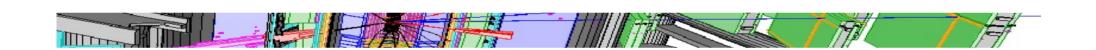


.@SteveAFarrell winner of #CTDWIT
TrackMLRamp 2D #hackathon at @LALOrsay in the ML category. Congrats!

À l'origine en anglais



Wrapping-up



More on ML in HEP history

- Very first ML in HEP paper known
- ML for tracking and calo clustering
- □ B. Denby still active outside HEP: analysis of ultrasonic image of the tongue

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

NEURAL NETWORKS AND CELLULAR AUTOMATA IN EXPERIMENTAL HIGH ENERGY PHYSICS

B. DENBY

Laboratoire de l'Accélérateur Linéaire, Orsay, France

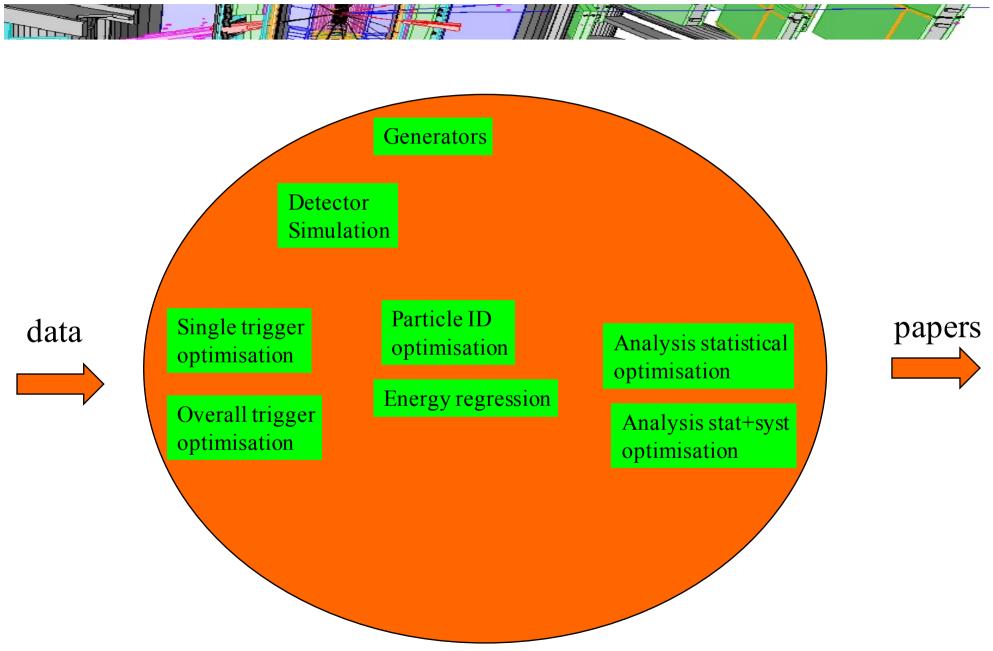
Received 20 September 1987; in revised form 28 December 1987

4494.1851 Energy Iteration $T = 0.5\tau$ Energy Iteration $T = 2.0\tau$

b

Advances in ML in HEP, David Rousseau, IPHC semi

ML playground



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: <u>HEP-data-science@googlegroups.com</u> and <u>Ihc-machinelearning-</u> 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)
- □ IN2P3 School of Statistics 28 May 1 June 2018 To be Confirmed (see SoS 2016)

ML Collaborations



- Many of the new ML techniques are complex→difficult for HEP physicists alone
- ML scientists (often) eager to collaborate with HEP physicists
 - o 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
- □ 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)
- There is probably a friendly Machine Learner on your 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
 - o 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 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

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→
 - o (2) ...demonstrated on toy dataset→
 - (3) ...demonstrated on real experiment analysis/dataset →
 - o (4) ...experiment publication using the great idea