

# Diving into Deep Learning with keras using your ntuples

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tutorial envisioned and designed by  
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ATLAS Software Tutorial at CERN



UNIVERSITY OF CALIFORNIA  
**SANTA CRUZ**

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# I'm not an expert

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- I'm just starting to learn this stuff too. I'm an enabler.
- I guess I've drunk the coolaid, or I am interested enough to evangelize some because I think we, physics experimentalists, should think more about what is happening in ML *right now*.
- I am also *skeptical* about how quickly physicists will adapt to new techniques, as we are careful and good at reconstruction/analysis. But the gains could be important.
- In addition to Amir Farbin, I've learned a lot from David Rousseau and Michael Kagan, who run the new ML group in ATLAS. We had a workshop last March that brought a lot of this to my attention:  
<https://indico.cern.ch/event/483999/>

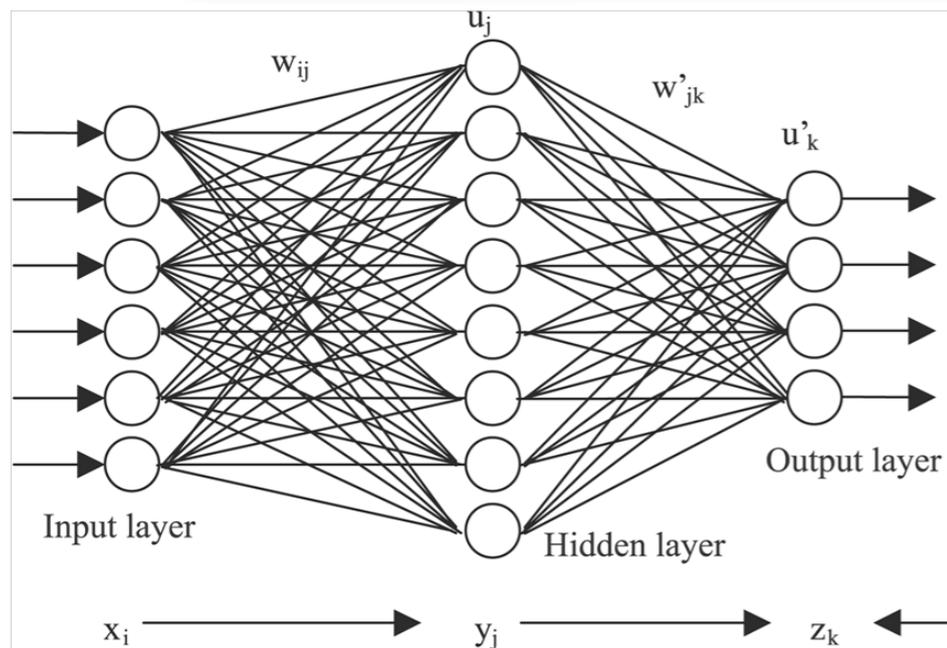
# Computing setup

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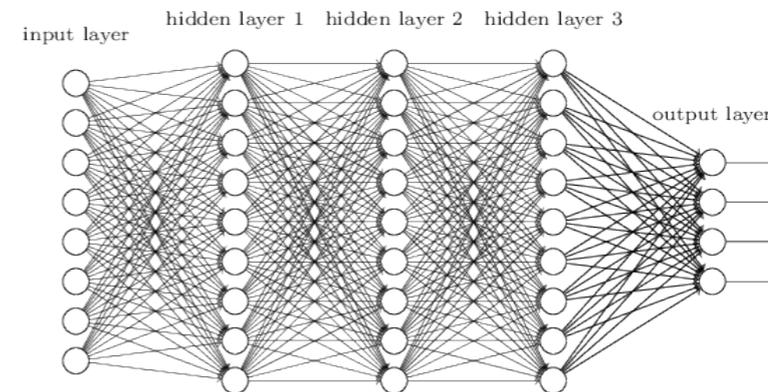
- We are following the tutorial here:  
<https://twiki.cern.ch/twiki/bin/view/AtlasComputing/SoftwareTutorialDeepLearning>
- Got to the **Setup on Ixplus** section and add to the PATH and source activate to setup my (Ryan's) installation on afs.
- You can follow the Installation instructions to install the full environment on your own machines on your own time.
- Try running the test out of the box:  

```
python -m EventClassificationDNN.Experiment --cpu
```
- Assuming that is ok for you, let's pause the walkthrough on the twiki to finish the introduction to DL in these slides.  
Then back to the TWiki.

# Neural Nets



“Deep” networks have multiple hidden layers



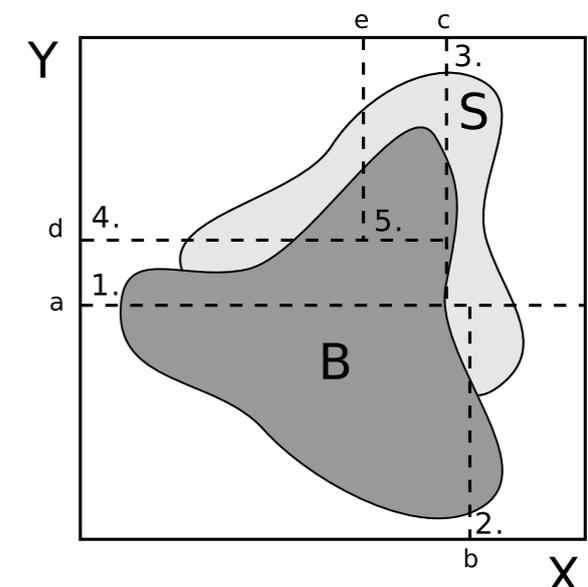
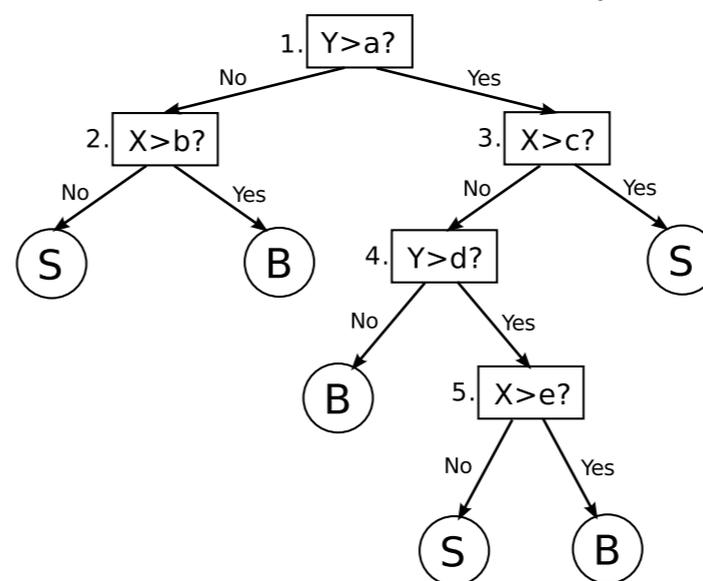
Can be used for *classification* or *regression*.

Similar to other multivariate techniques, cutting on a classifier makes some acceptance blob in parameter space.

Neural nets have:

- input variables,  $x_i$
- weights,  $w_{ij}$
- activation function (sigmoid, tanh, ...),  $u_j$
- output variables,  $y_j$
- a *learning rule* to update the weights.
- a learning step is called an “*epoch*.”
- Optimizing the weights is called “*training*.”

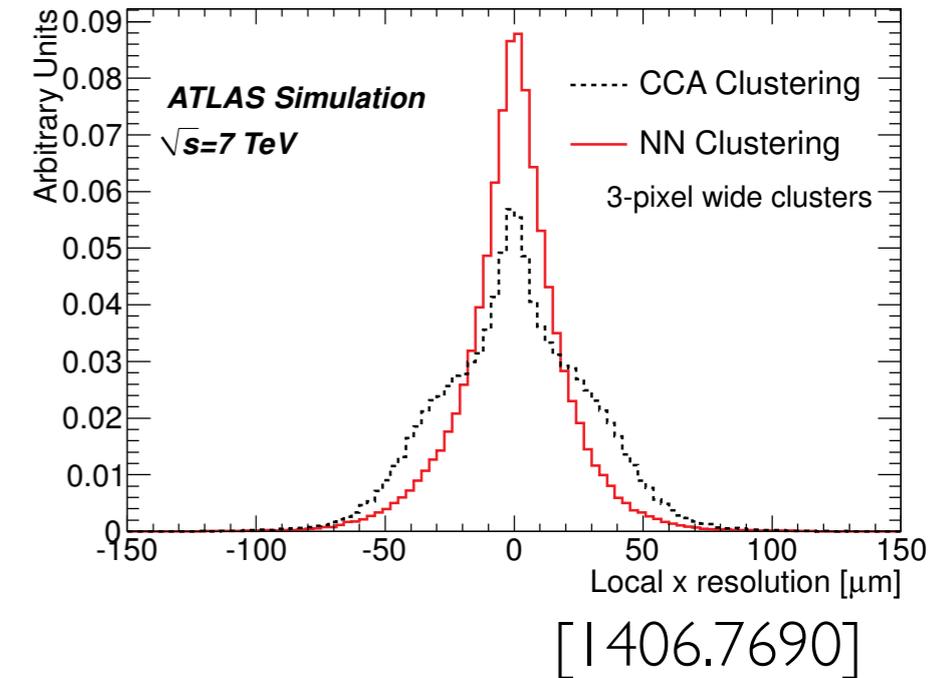
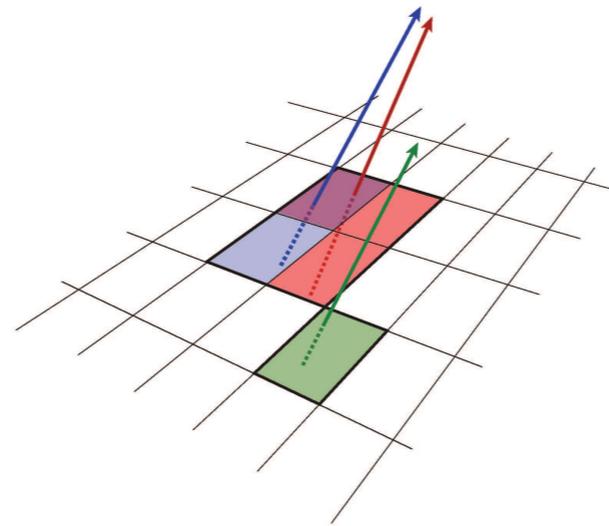
Boosted Decision Trees (BDT)



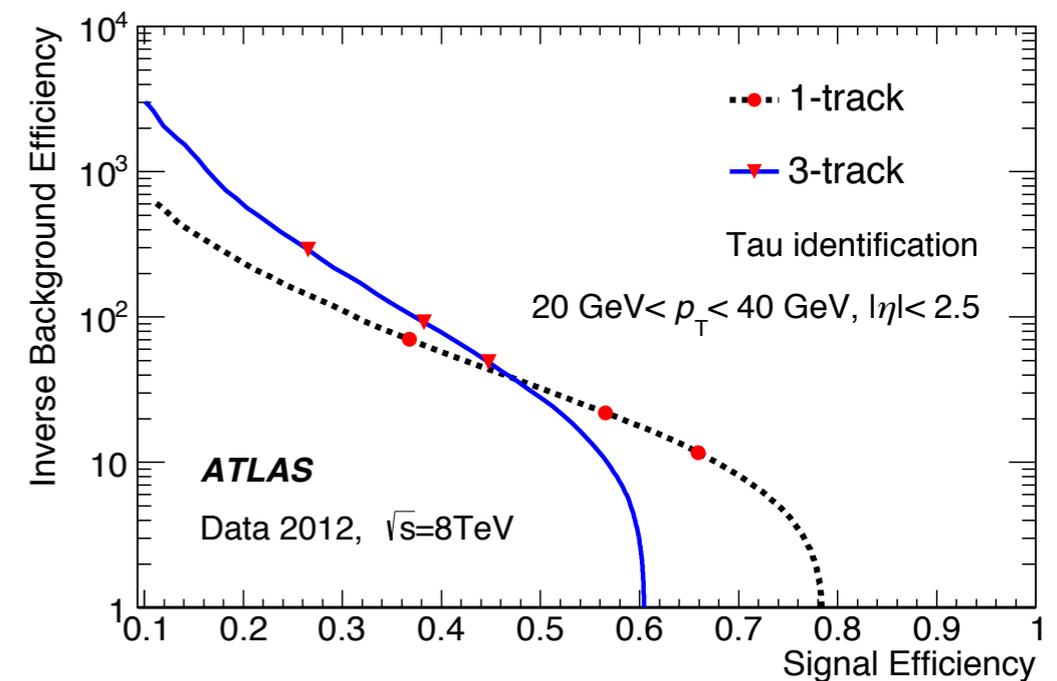
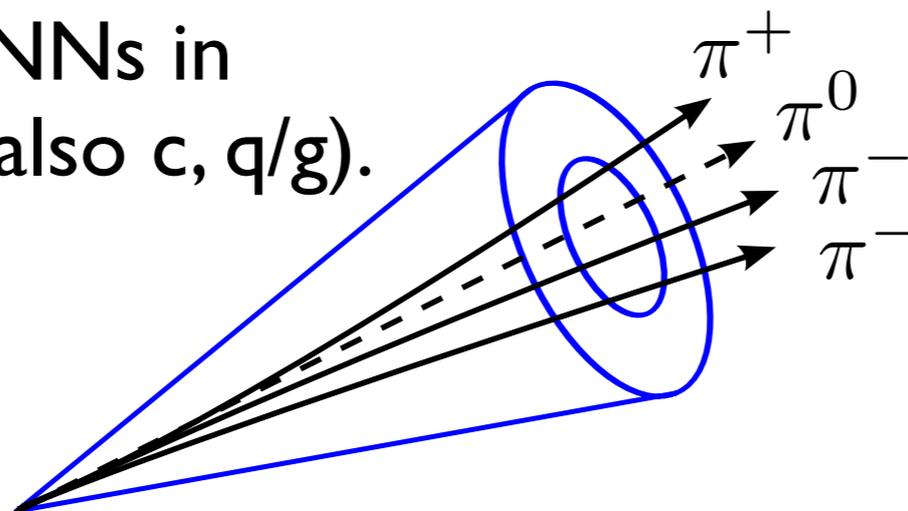
# NNs and BDTs in ATLAS

- Using NNs and other MVAs has been common in HEP for years, for pattern recognition, particle ID, event selection...
- In the past, always used *shallow* NNs.
- ATLAS uses NNs in many places, e.g. pixel clustering.
- Jet tagging for taus and b-quarks has used NNs in many iterations (also c, q/g).

## ATLAS pixel clustering with NNs

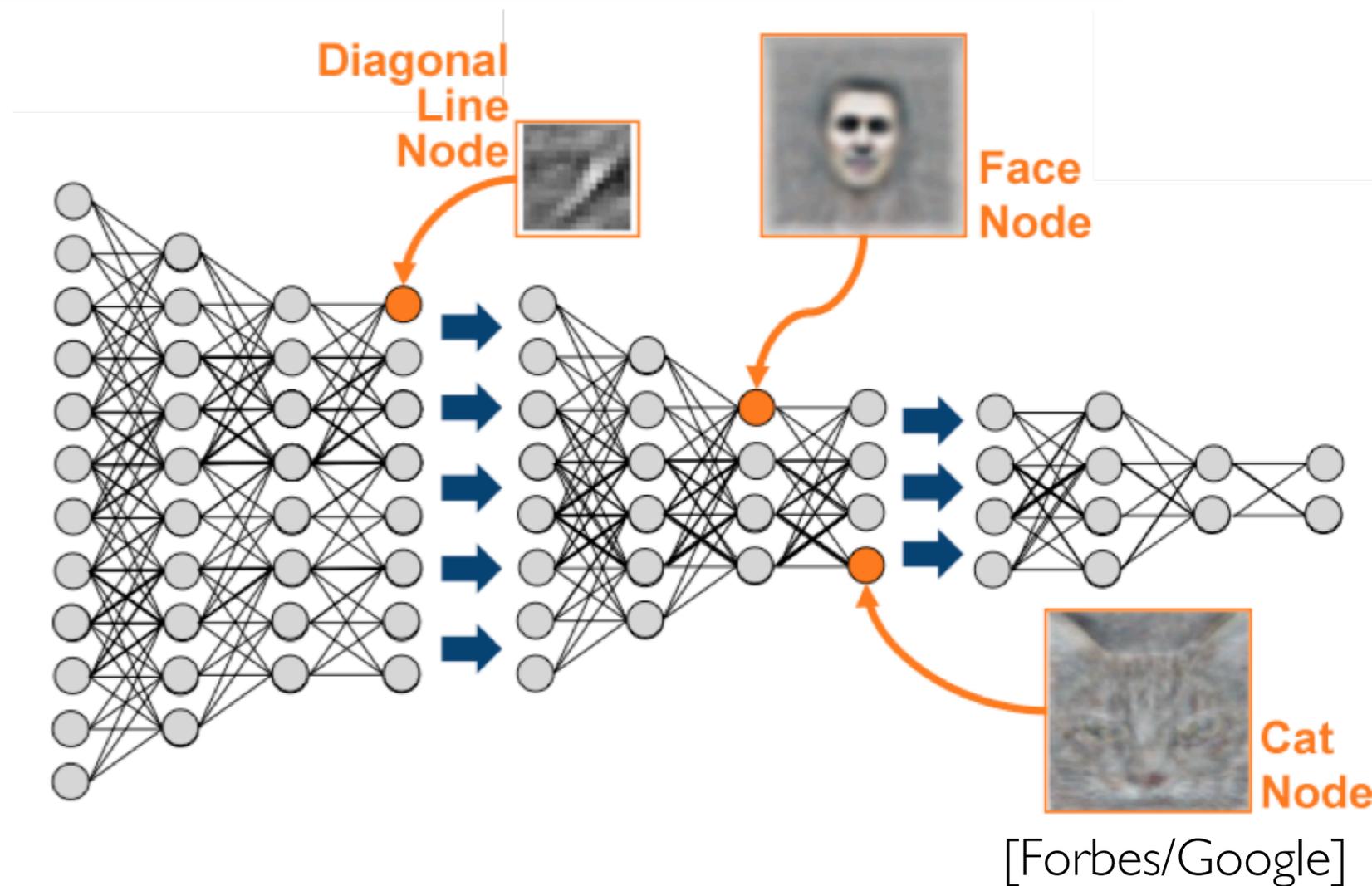


## ATLAS tau identification with BDTs



# Why go deep?

- “Vanishing gradient problem” → hard to train many layers.
- Multiple layers allow for *feature extraction*.
- Allow us to better explore and understand our data.
- **Now in “Deep Learning Renaissance”**



1. Better training: techniques and tools (e.g. smarter NN structures).
2. Better hardware: multicore, GPUs, bigger data centers, cloud computing, coming: neuromorphic computing.
3. More training: bigger datasets, search, the internet, open science.

# Examples of CNNs

- In 1990s, Yann LeCun pioneered Convolutional Neural Nets (CNN) and used them for Optical Character Recognition.
- Inspired by animal cortex.
- Now it is standard in image recognition and captioning, NLP, computer vision, etc.



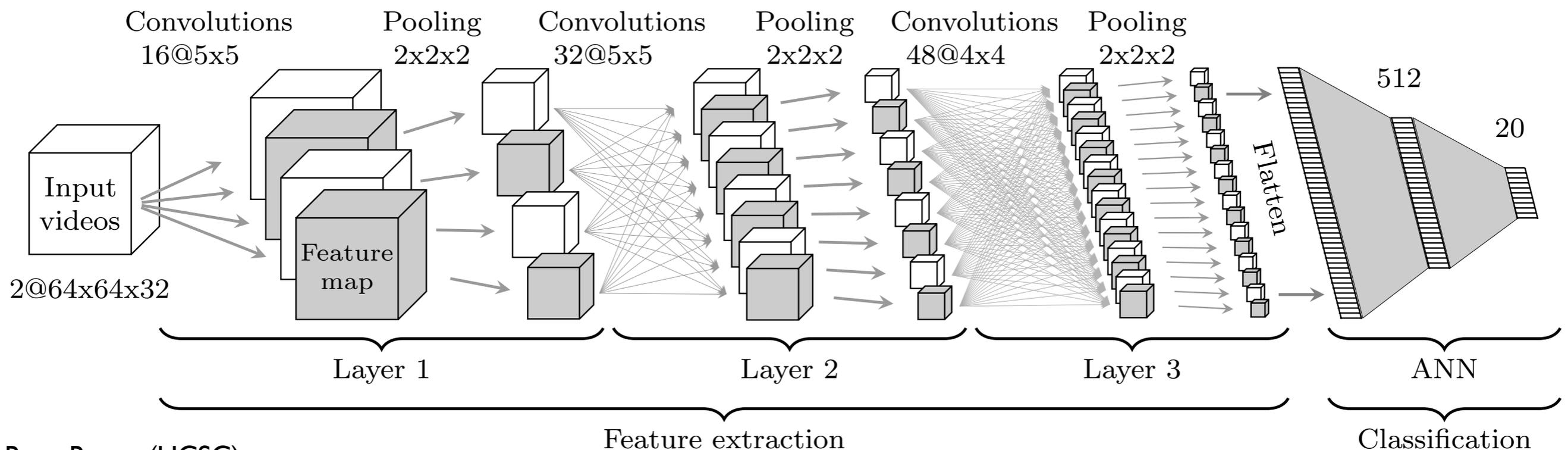
Pigou et al. (2014). Sign Language Recognition using Convolutional Neural Networks.



(a) RGB



(b) Depth map



# Deep Learning in HEP

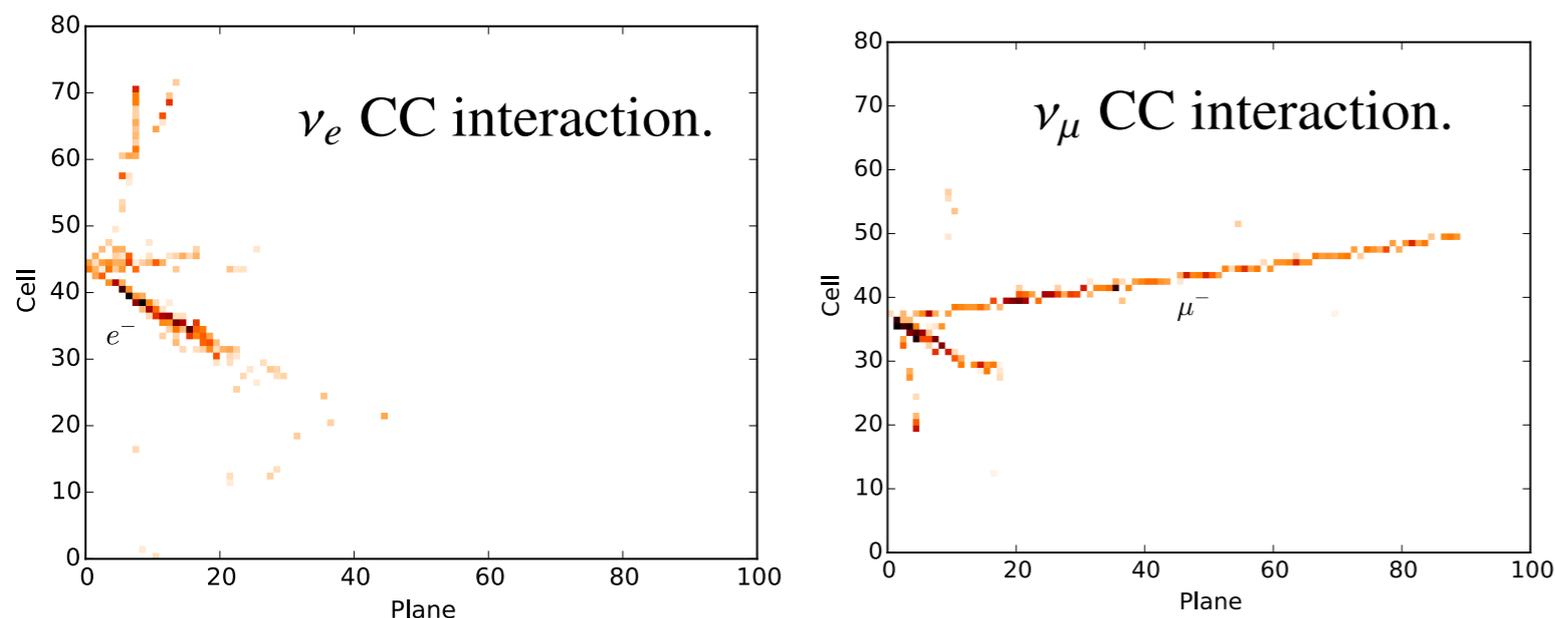
- Deep learning does best with raw data and when there are unexploited features.
- raw channels  $\rightarrow$  *tagging*
- basic kinematics  $\rightarrow$  *features*

- Baldi *et al.* (2014). Searching for Exotic Particles in High-Energy Physics with Deep Learning. [1402.4735]



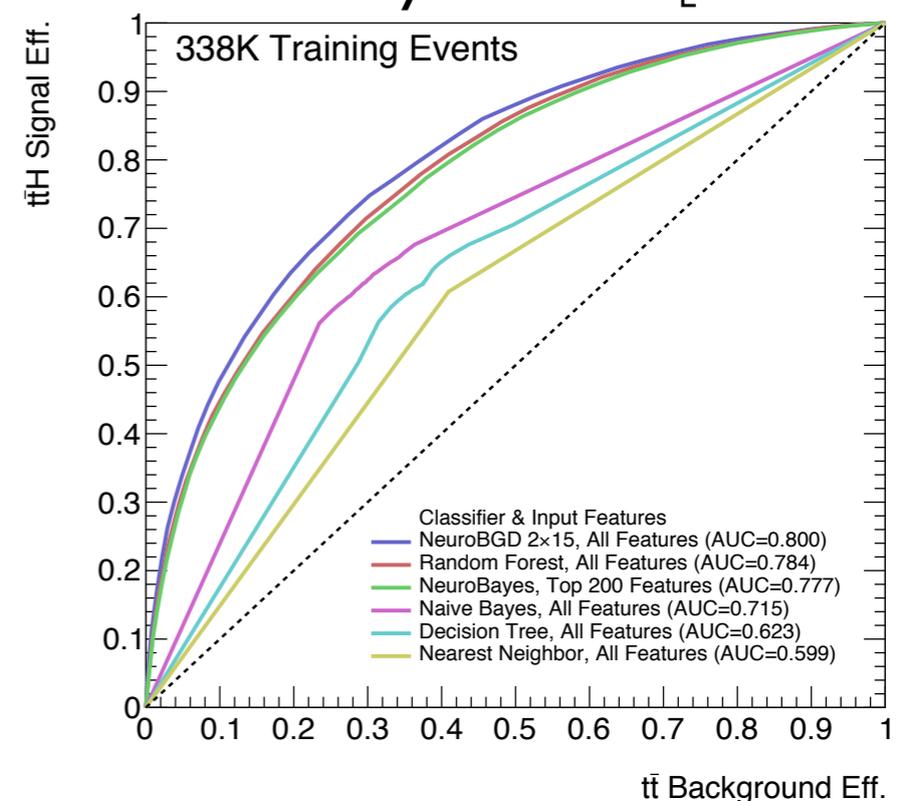
- Baldi *et al.* (2015). Enhanced Higgs to  $\tau^+\tau^-$  Search with Deep Learning. [1410.3469]

- Aurisano *et al.* (2016). A Convolutional Neural Network Neutrino Event Classifier. [1604.01444]



out performs NOvA's conventional reconstruction

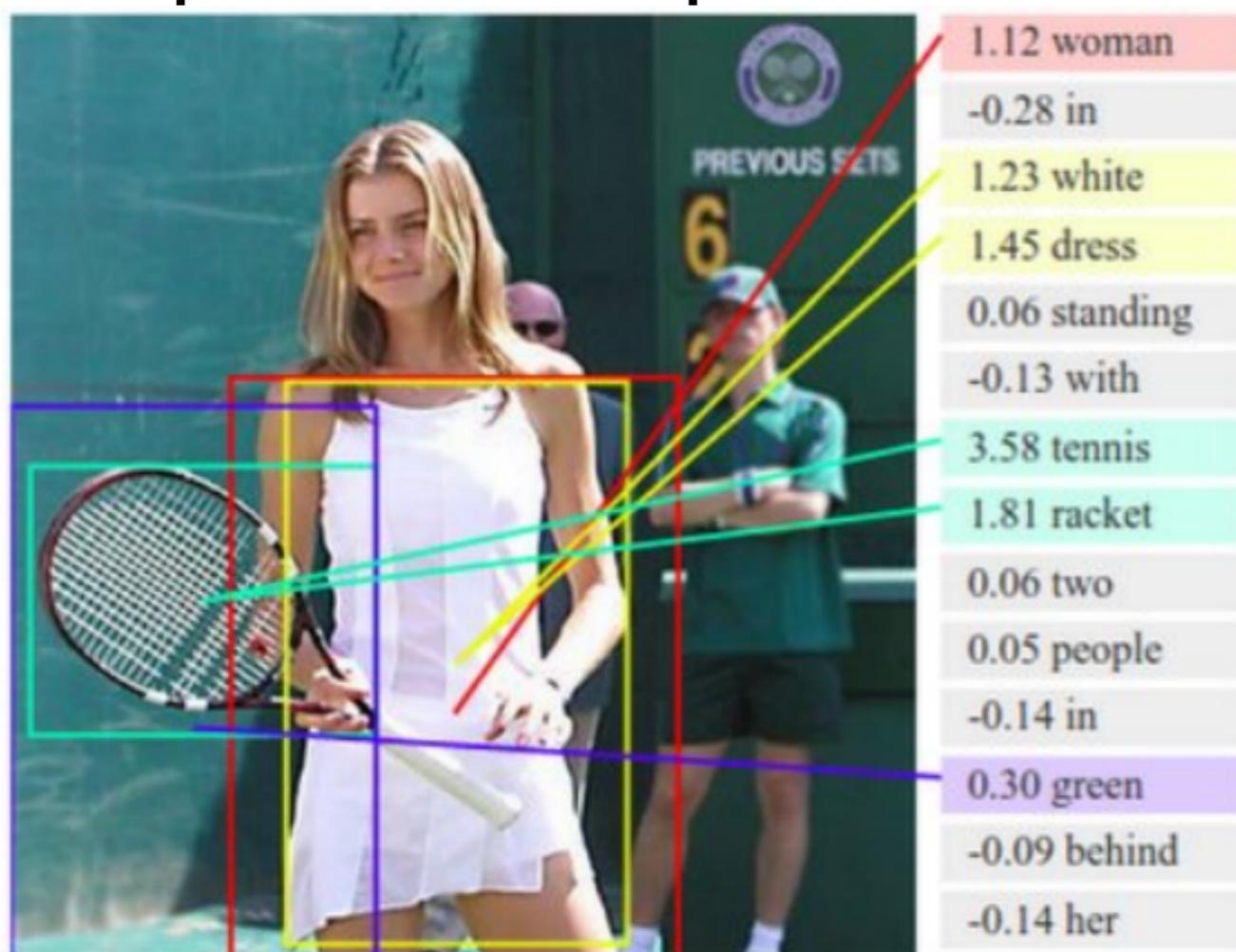
- Santos *et al.* (2016). Machine learning techniques in searches for  $t\bar{t}h$  in the  $h \rightarrow b\bar{b}$  decay channel. [1610.03088]



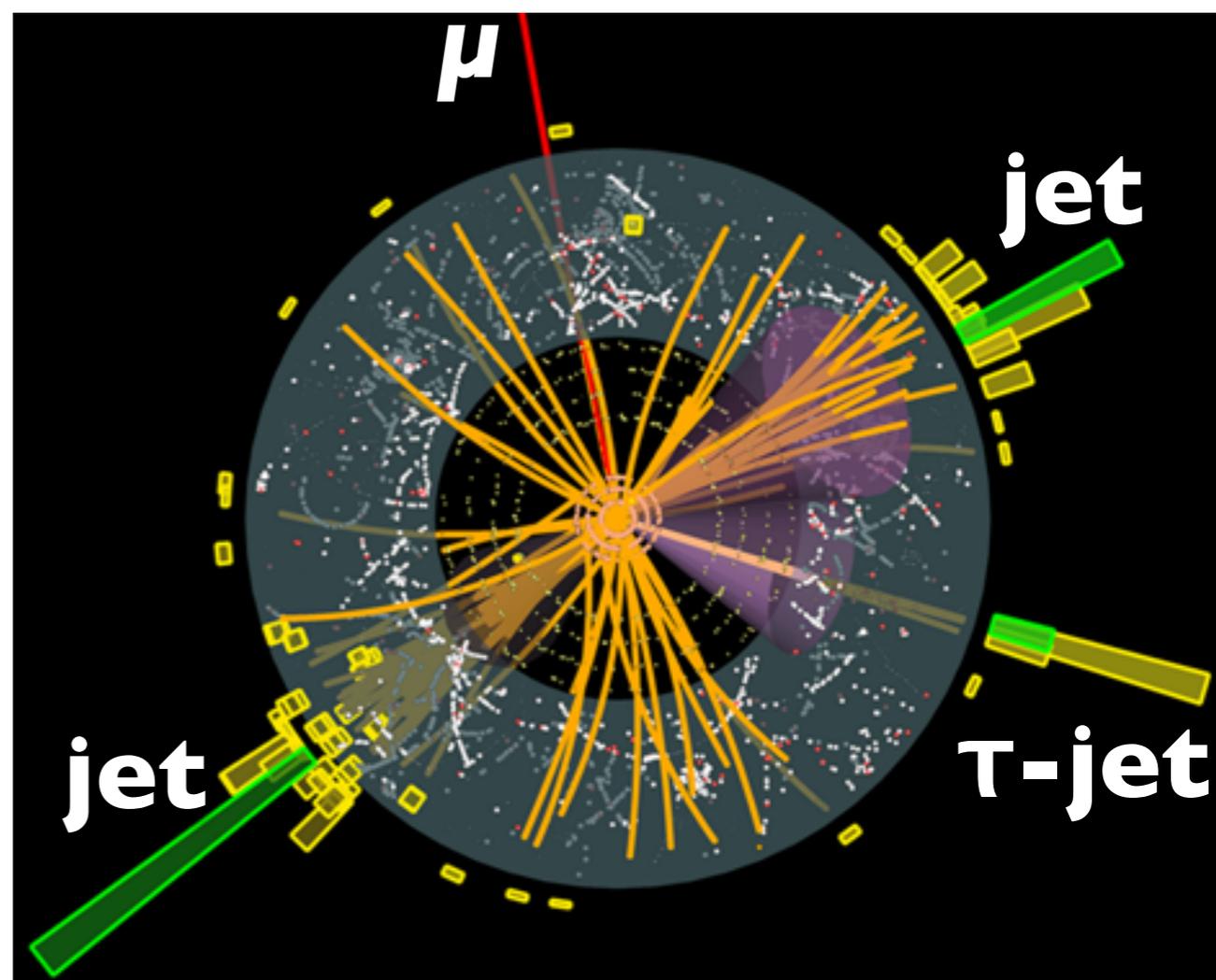
# Deep learn from *raw* inputs

*The vision as explained to me by Amir:*

ImageNet  
competition example



Future of ATLAS?



# Solutions to big problems in ATLAS?

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- Discover new features in the data and analysis techniques?
- Better particle and event classification?
- Faster, better pattern recognition and tracking for HL-LHC?
- Faster, better, data-driven simulations from generative models?

# Data Science & Deep Learning Tools

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- **scipy**

- ▶ matplotlib - common plotting library
- ▶ numpy - arrays and numerics in python
- ▶ pandas - library for reading/writing/plotting structured data

- **scikit-learn** - various ML and classification packages for python

- **tensorflow/theano** - computer algebra systems designed for machine learning

- **keras** - python ML framework wrapping calls to tensorflow or theano backends.

# Amir's DLKit

- DLKit is Amir's toolkit built around keras for handling datasets/models/results. As you learn keras, you'd probably build something like it.

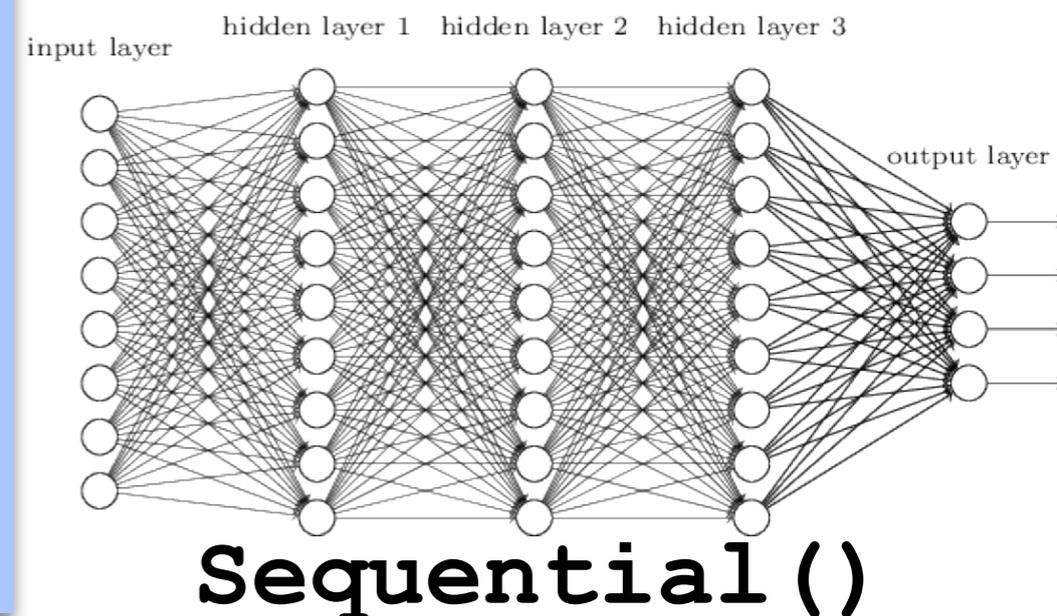
- In the top-level file:

DLKit/EventClassificationDNN/Experiment.py

```
# Build the Model
from EventClassificationDNN.Classification import FullyConnectedClassification
```

- The Build function actually constructs the NN using keras:

```
def Build(self):
    model = Sequential()
    model.add(Dense(self.width,
                    input_dim=self.N_input,
                    init=self.init))
    model.add(Activation('tanh'))
    for i in xrange(0, self.depth):
        model.add(BatchNormalization())
        model.add(Dense(self.width, init=self.init))
        model.add(Activation('tanh'))
        model.add(Dropout(0.5))
        model.add(Dense(1, input_dim=self.width))
    self.Model=model
```



# Amir's DLKit

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- You need to convert TTrees to hdf5.

- Specify your input files in

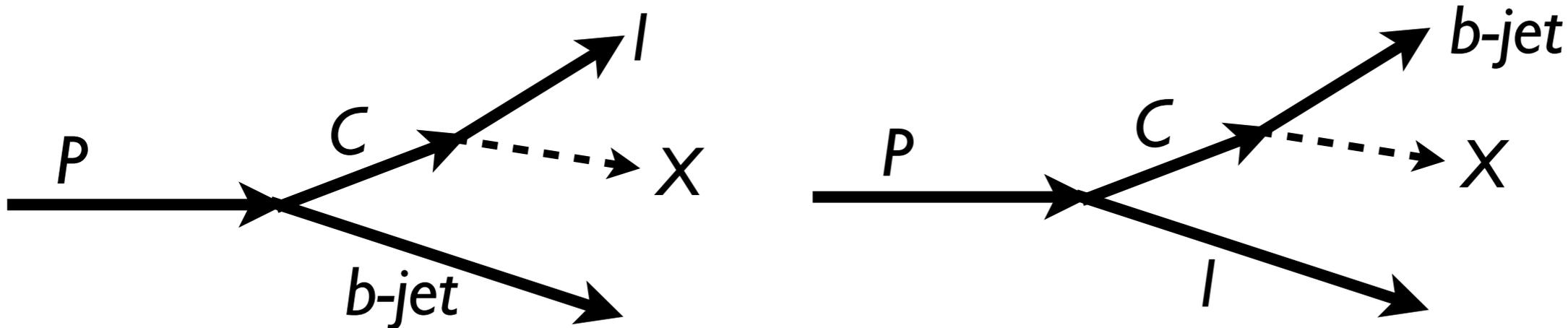
`EventClassificationDNN/InputFiles.py`

- The lines like:

`[InputData, "AA_Gen"],`

are labeling InputData as being of true class "AA\_Gen"

*Goal: discriminate A-type from B-type decays.*

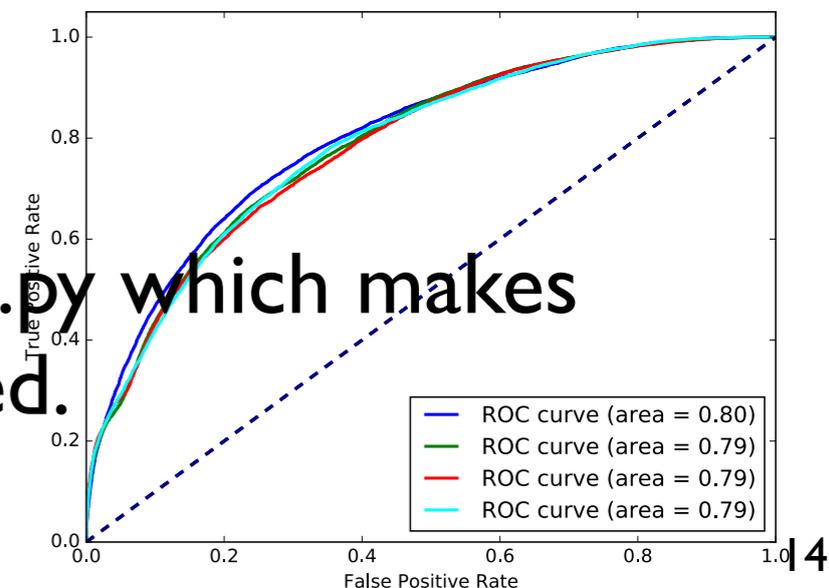


This example developed by Chris Rogan and Amir Farbin.

# Amir's DLKit

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- Also specify the input variables from your data in:  
`EventClassificationDNN/InputVars.py`
- The list `FieldGroups` groups together variables of common normalizations, like  $0-1$ ,  $-\pi$  to  $+\pi$ , energies, etc.
- `SelectedFields` selects which variables to use as input to the NNs. You can change these with:
  - v --varset e.g. -v 0 (everything)
  - v 1 ("jigsaw")
  - v 2 (four-vectors)
- Also note the file `EventClassificationDNN/ScanConfig.py` which is meant to sample the depth/width structure of the NN for study and optimization.
- Running the Experiment should also run `Analysis.py` which makes some ROC plots and could be further customized.



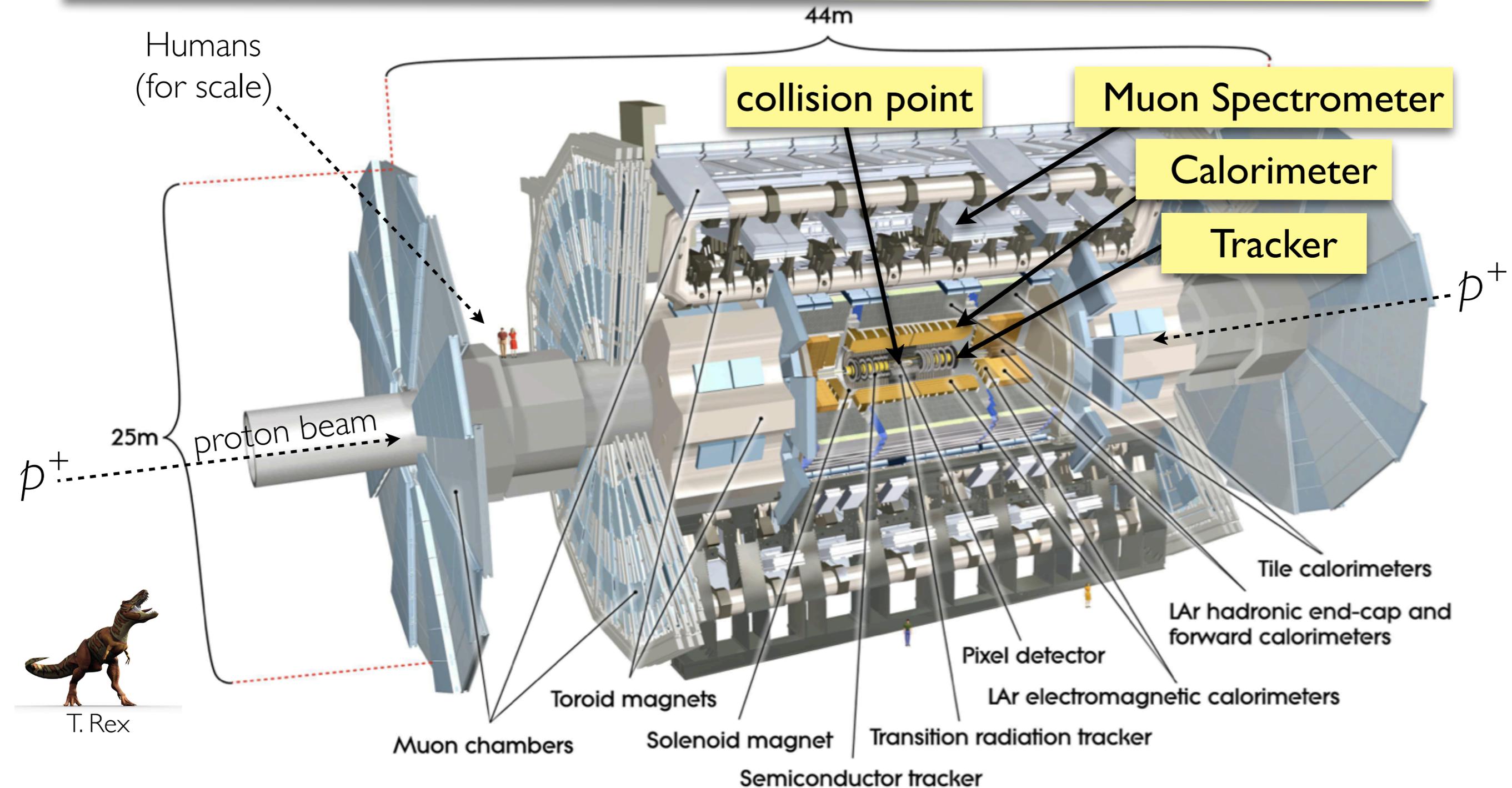
**Back-up  
slides**



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# ATLAS Detector

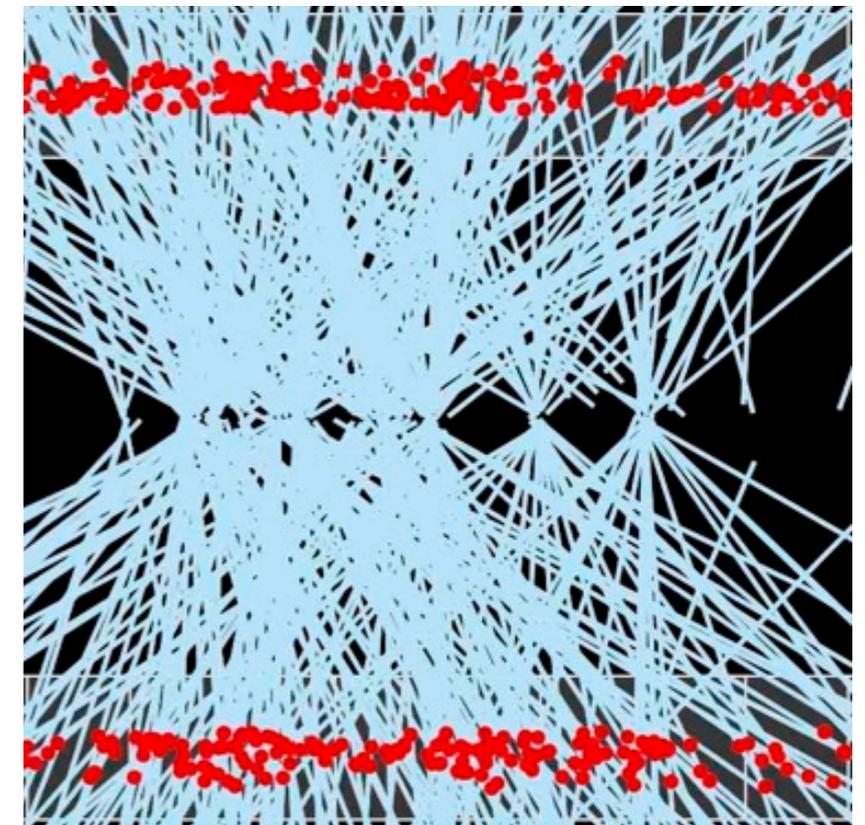
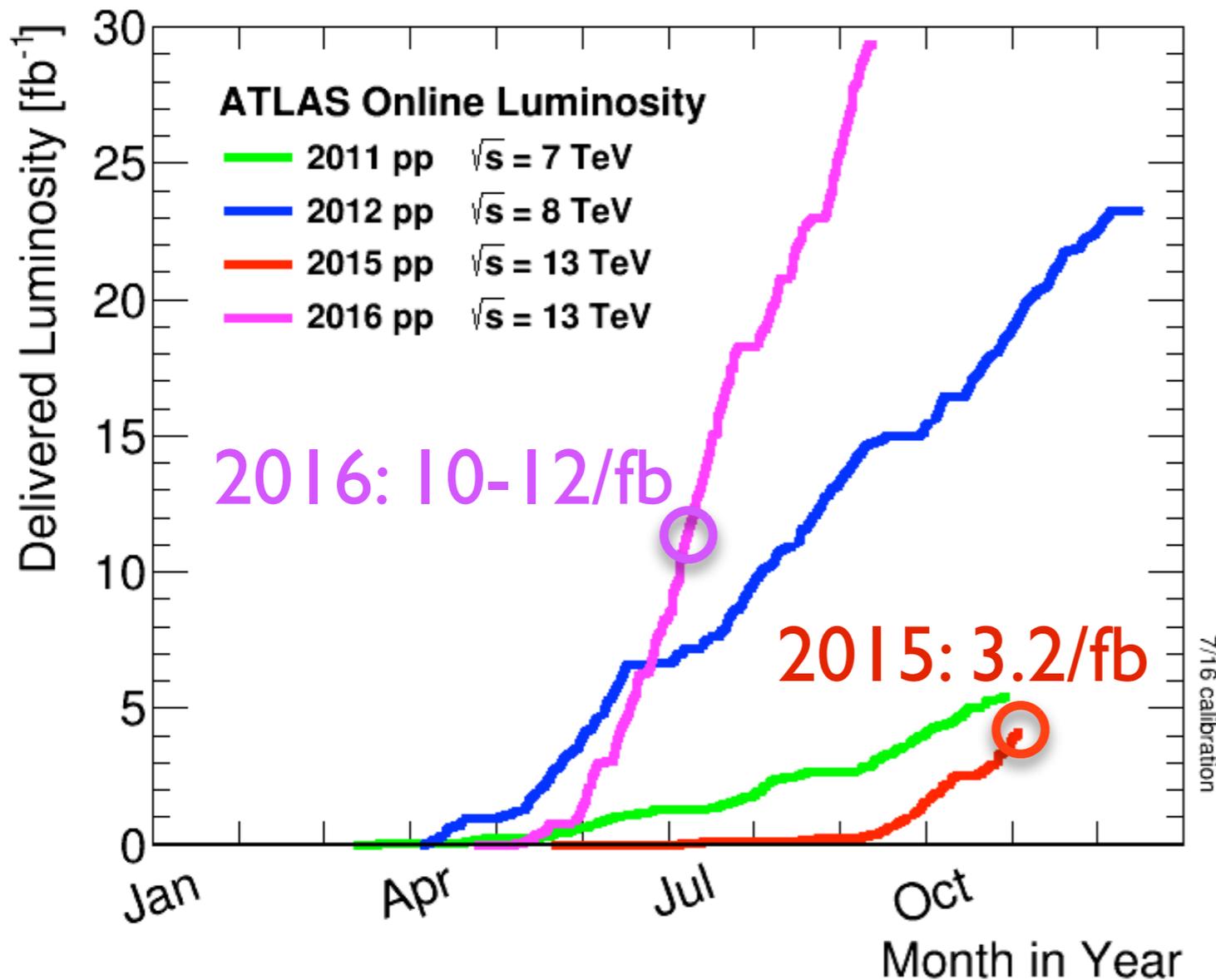
ATLAS is a 7 story tall, 100 megapixel “camera”, taking 3-D pictures of proton-proton collisions 40 million times per second, saving 10 million GB of data per year, using a world-wide computing grid with over 100,000 CPUs. The collaboration involves more than 3000 scientists and engineers.



# Datasets

The LHC has performed extremely well!!

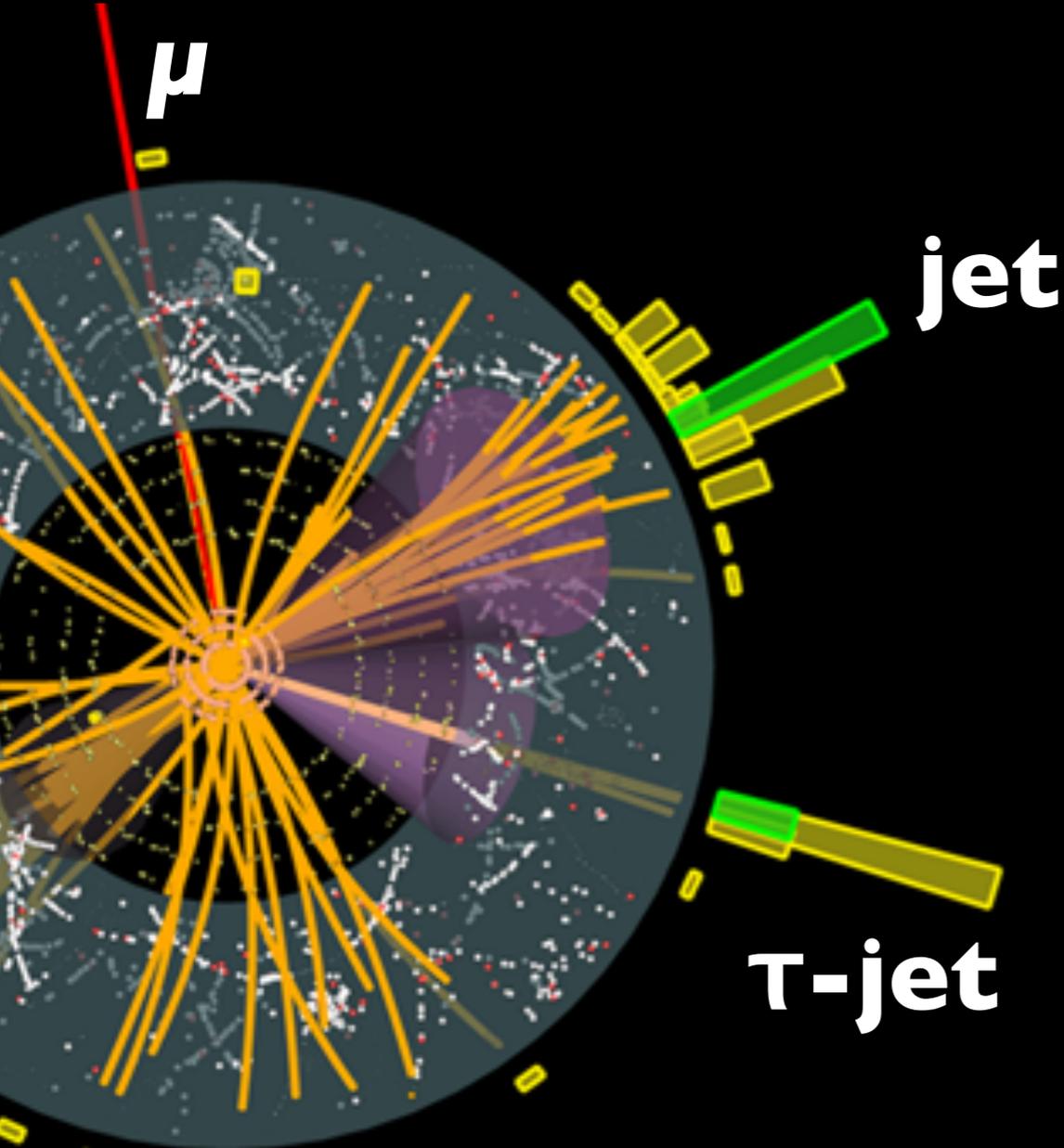
Recently broke inst. lumi. records  $> 10^{34} \text{ cm}^{-2}\text{s}^{-1}$



Typically 20-40 vertices per bunch crossing

Latest analyses combine collision data at  $\sqrt{s}=13\text{TeV}$  collected in the years 2015 and 2016, giving a total integrated lumi  $\approx 13\text{-}15 \text{ fb}^{-1}$ .

# What do we reconstruct?



- muons (main objects)
- electrons & photons
- jets of hadrons
- $\tau$ - and  $b$ -tagged jets
- missing energy

# How do we search?

**ATLAS Physics Groups**

**SM**

$W, Z, \text{top}, \dots$

**Higgs**

$H \rightarrow \gamma\gamma, ZZ, WW, \dots$

**SUSY**

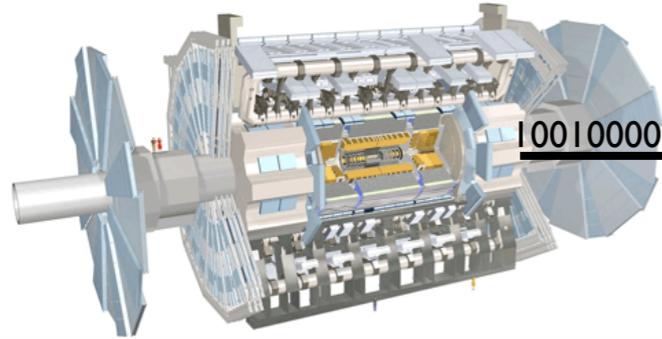
$l + \text{jets}, \gamma + \text{jets}, \dots$

**Exotics**

$Z', W', \dots$

**Currently ATLAS has published 579+ papers**

# ATLAS



## 3-level trigger

40 MHz → 100 kHz  
→ 10 kHz → 1 kHz



raw data



~ 10 PB/year

# ATLAS Data Flow

Worldwide LHC Computing Grid

Monte Carlo production

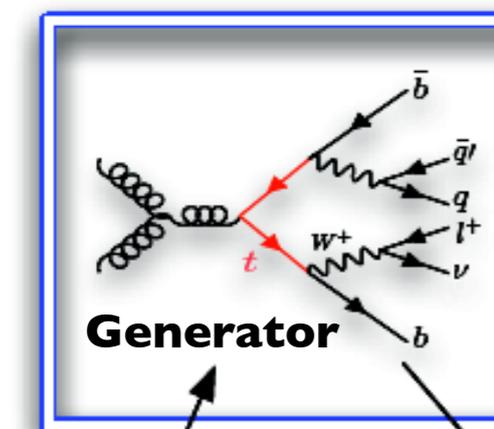
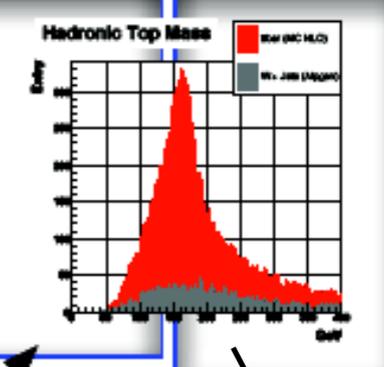
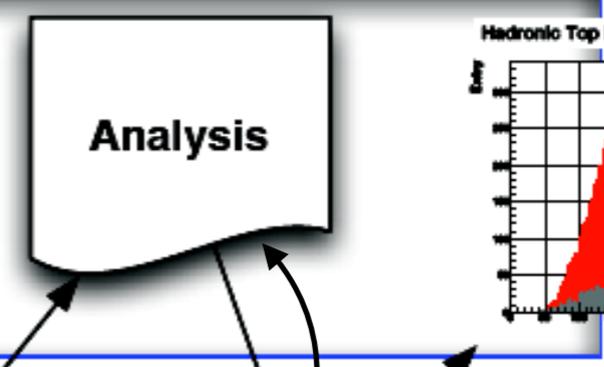
Local resources

~ 100k CPUs  
over 100 PB

Athena Framework

ROOT

### Detector Simulation



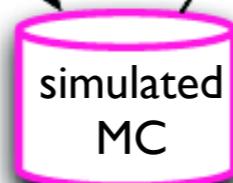
Generator



QFT matrix element



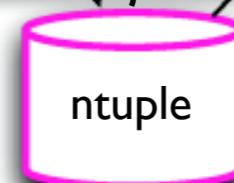
primary kinematics



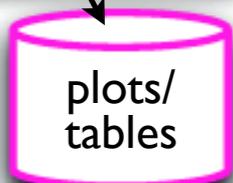
detector hits



tracks, clusters, jets



~GB-TB

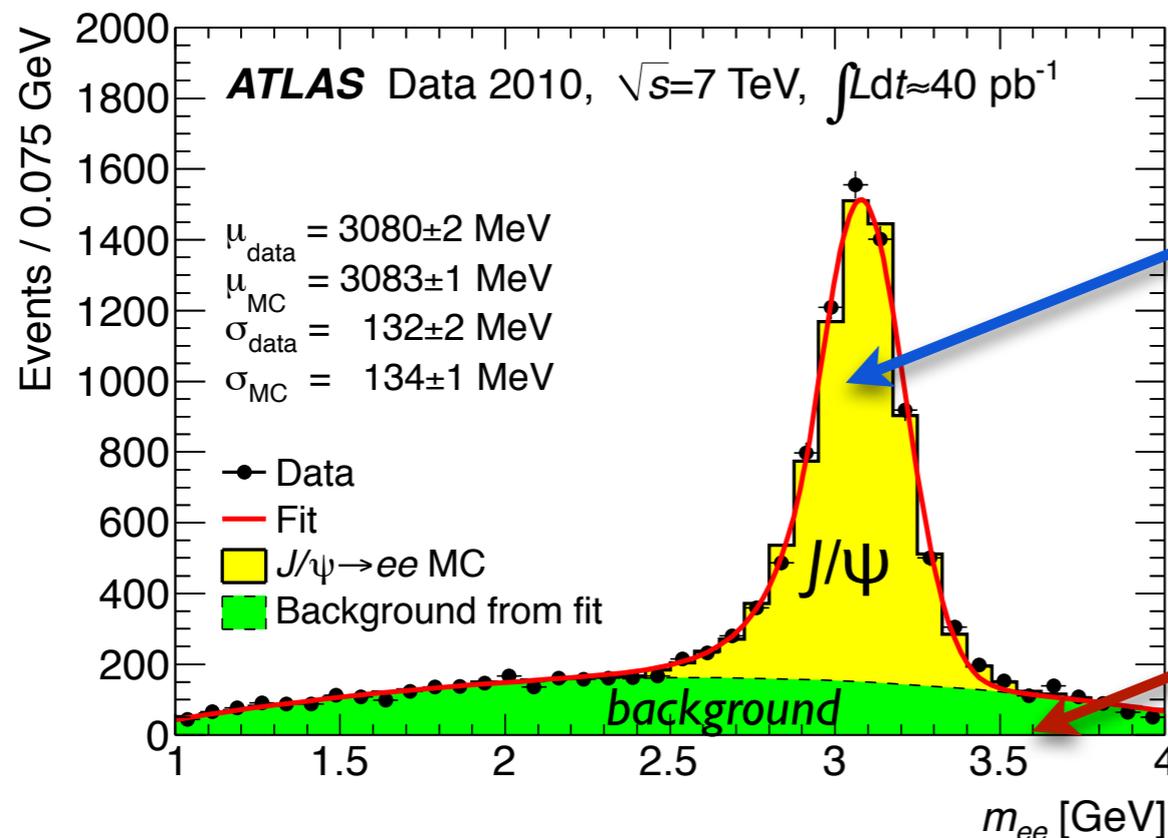


Results!

# Building a model

$$N(\text{expected}) = \underbrace{N(\text{correct-ID})}_{\text{Bottom-up}} + \underbrace{N(\text{fake})}_{\text{Top-down, "data-driven"}}$$

- **Bottom-up**
- well-identified objects have scale factors from control regions
- estimated with detailed Monte Carlo simulation
- **Top-down**, “**data-driven**”
- various magic with data depending on the analysis and your creativity
- side-band fit
- fake-factor method



**Bottom-up**  
**Monte Carlo**

**Data-driven**  
**side-band fit**

# Tau Reconstruction

- Tau candidates are seeded by anti- $k_t$  calorimeter jets ( $R=0.4$ ) formed from topological clusters with local hadronic calib.
- Tracks are matched to this calorimeter object and discriminating variables calculated from the combined tracking+calo information.
- Best vertex chosen from those matching tracks in core cone  $\Delta R < 0.2$ .
- Core track with  $\Delta R < 0.2$  associated to the tau.
- Annulus  $0.2 < \Delta R < 0.4$  used to calculate tracking and calorimeter isolation variables.
- *New in Run-2:*  $\pi^0$  counting using strips in EM calorimeter and subtracting charged energy matched to tracks. Improves jet rejection and energy resolution.

