# Common ground in classification (and generation?)


Gregor Kasieczka
(gregor.kasieczka@uni-hamburg.de)


*IDT ErUM-C Meeting*

*2020-04-08*

CLUSTER OF EXCELLENCE
QUANTUM UNIVERSE

Emmy Noether-Programm
Deutsche Forschungsgemeinschaft
DFG

UH
Universität Hamburg
DER FORSCHUNG | DER LEHRE | DER BILDUNG

PIER
Partnership of Universität Hamburg and DESY

Bundesministerium für Bildung und Forschung

# Introduction

- Research into ML applications to specific physics problems as part of task area C
- Chance for wider ranging developments:
  - methods generalise beyond specific problem
  - recommendations and strategies
- Two common problems:

**Classification**

- Distinguish different observations, particles, galaxies,…
- Supervised - need labelled training data from simulation
  (or controlled observation)
- Straightforward to train and benchmark

**Generative models**

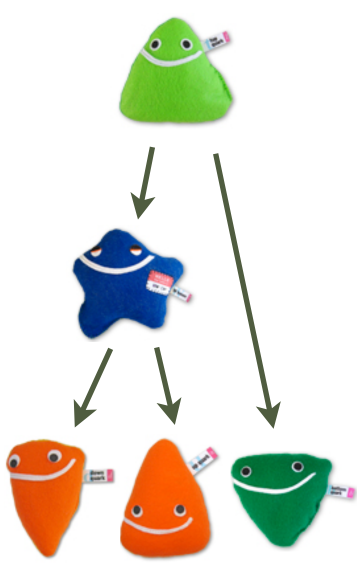
- Accelerate simulation of physics processes and detector responses
- Unsupervised - can train directly from data
- More difficult train, unclear how to benchmark
- *Of course this does not mean that it is not an interesting problem, only potentially more difficult to generalise for us*

# Example:
# Top Tagging Challenge

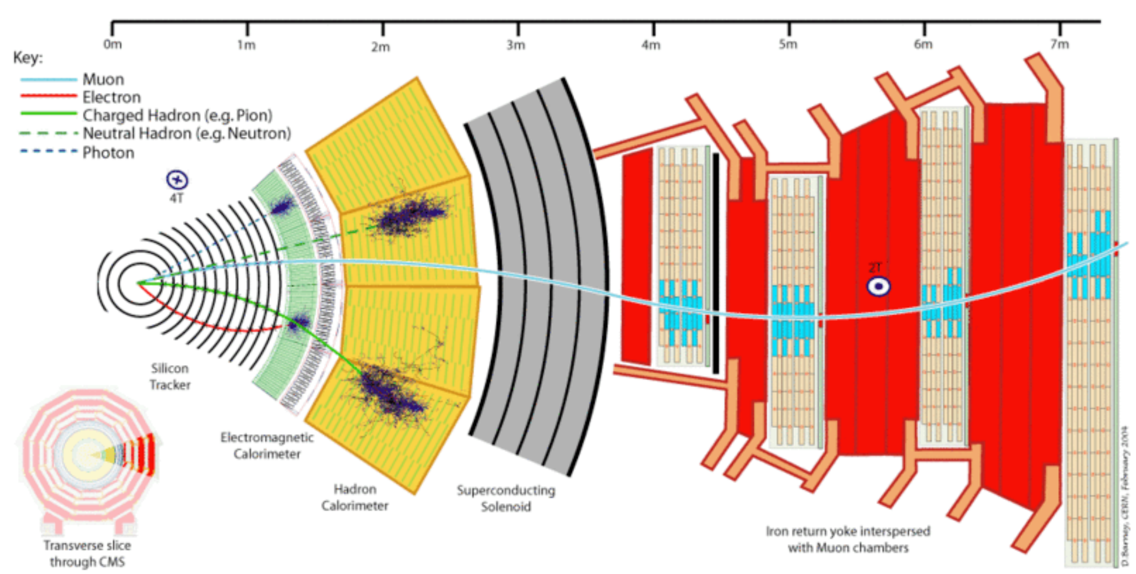
# Heavy Resonance Tagging

- **Goal**: Distinguish decay products of heavy resonance (top quark, W/Z boson, Higgs boson) from other particles (light quark/gluon jets)
- Achieve by looking at substructure of jets in the detector

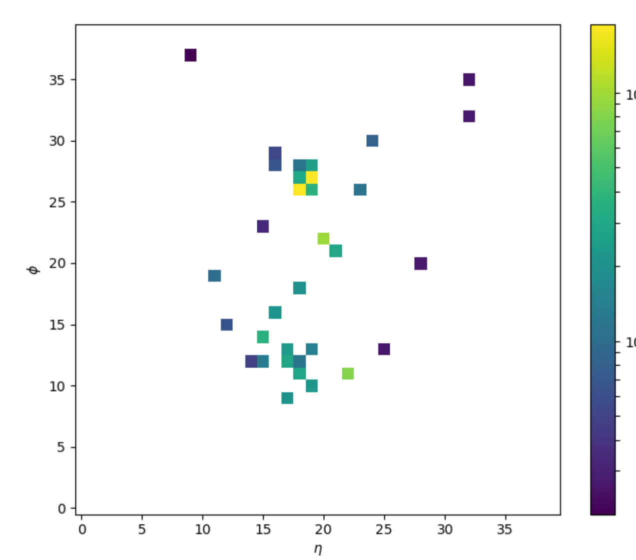
*Top Quark* | *(Simulated) Detector* | *Jet Image*



+




=

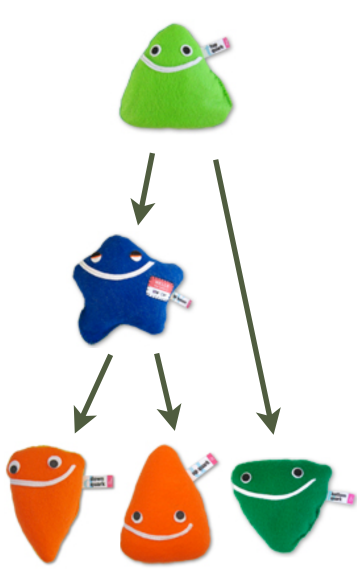



***(ignoring parton shower, hadronisation,...)***

# Heavy Resonance Tagging

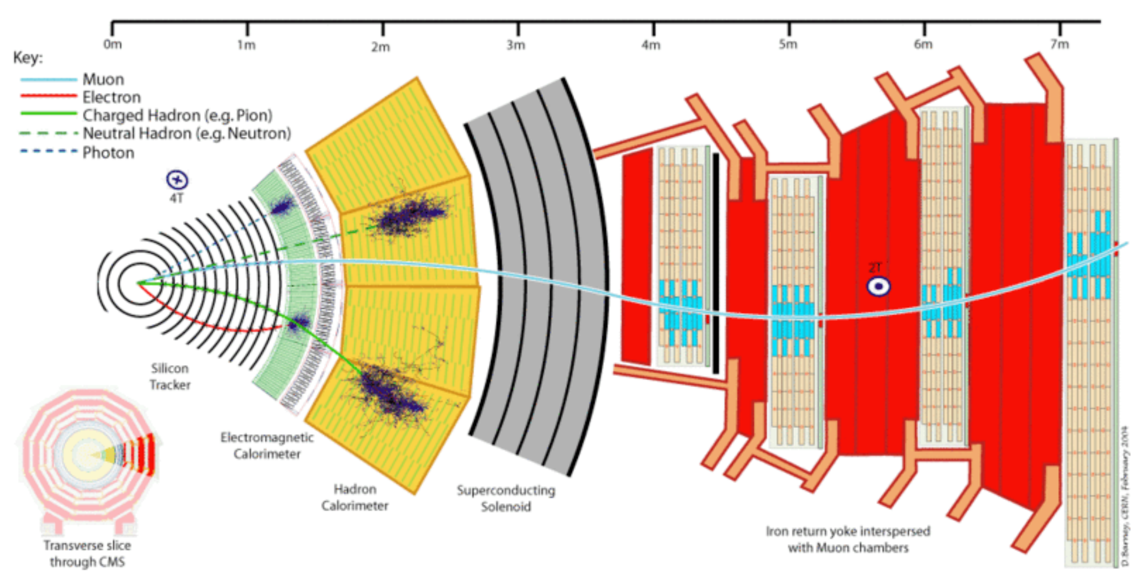
- **Goal**: Distinguish decay products of heavy resonance (top quark, W/Z boson, Higgs boson) from other particles (light quark/gluon jets)
- Achieve by looking at substructure of jets in the detector

*Top Quark*



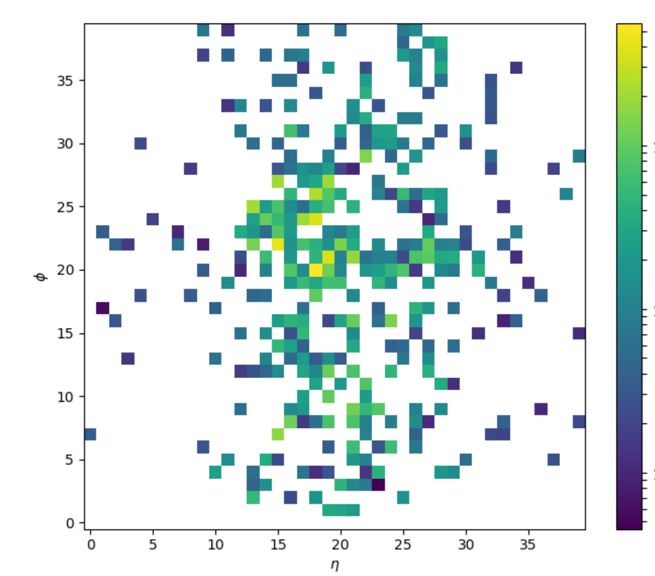
\+

*(Simulated) Detector*




=

*10 Images*

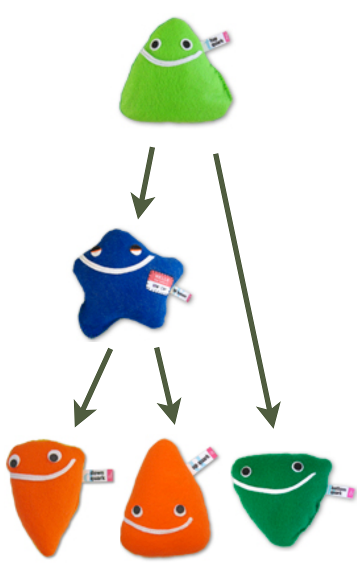



***(ignoring parton shower, hadronisation,...)***

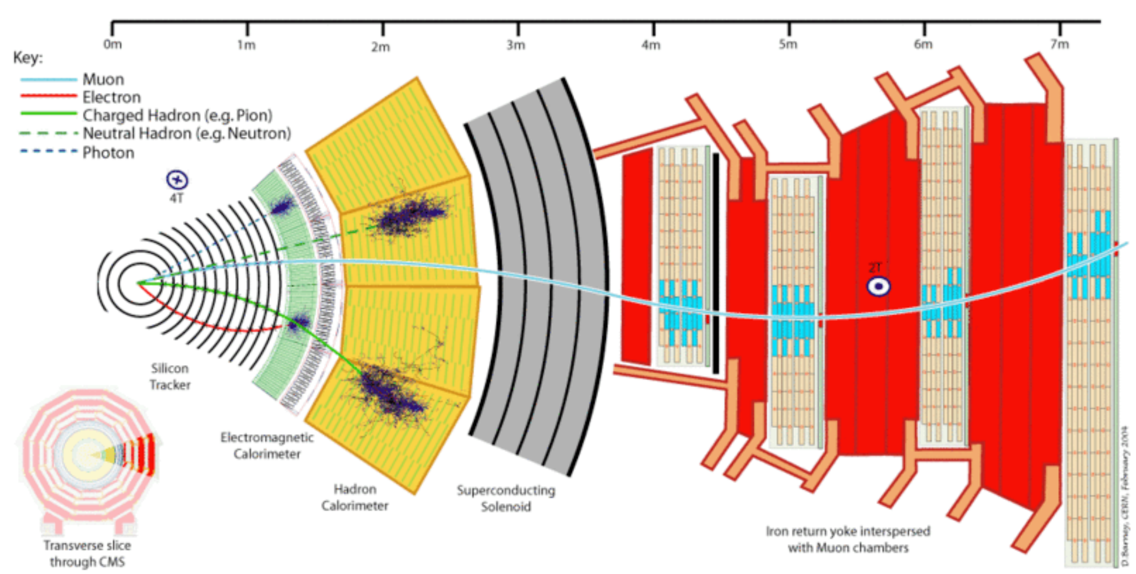
# Heavy Resonance Tagging

- **Goal**: Distinguish decay products of heavy resonance (top quark, W/Z boson, Higgs boson) from other particles (light quark/gluon jets)
- Achieve by looking at substructure of jets in the detector

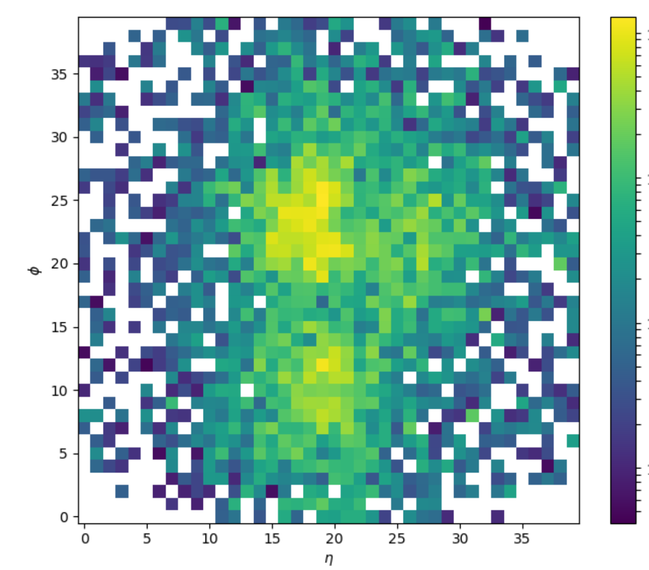
*Top Quark* *(Simulated) Detector* *100 Images*



+




=

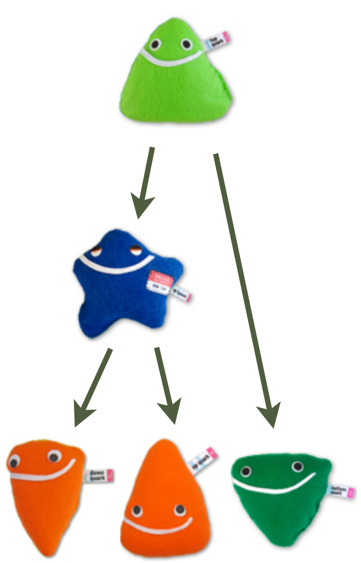



***(ignoring parton shower, hadronisation,…)***

# Heavy Resonance Tagging

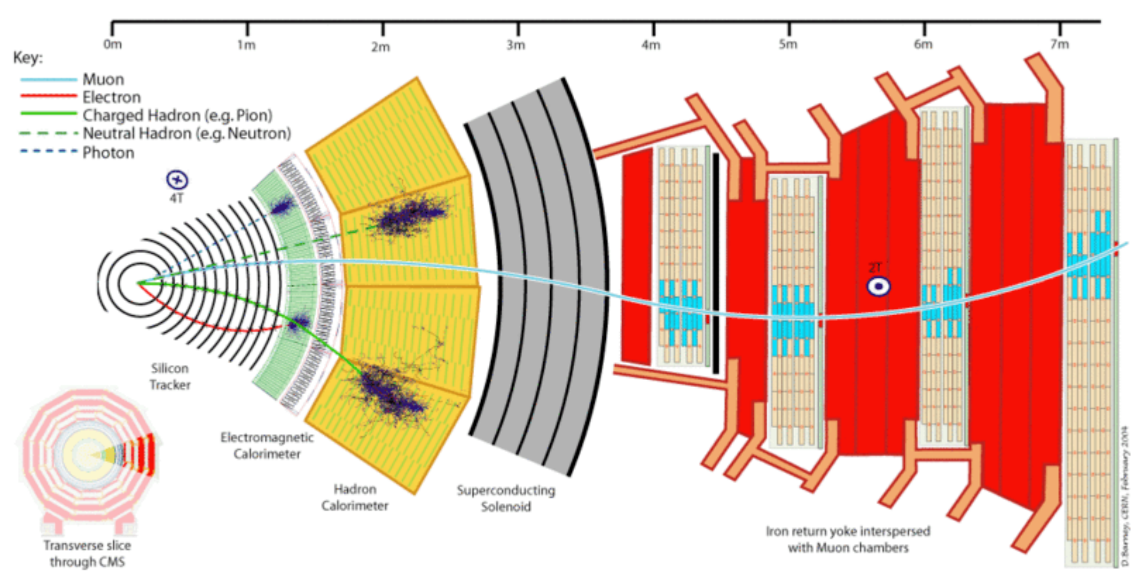
- **Goal**: Distinguish decay products of heavy resonance (top quark, W/Z boson, Higgs boson) from other particles (light quark/gluon jets)
- Achieve by looking at substructure of jets in the detector

*Top Quark*



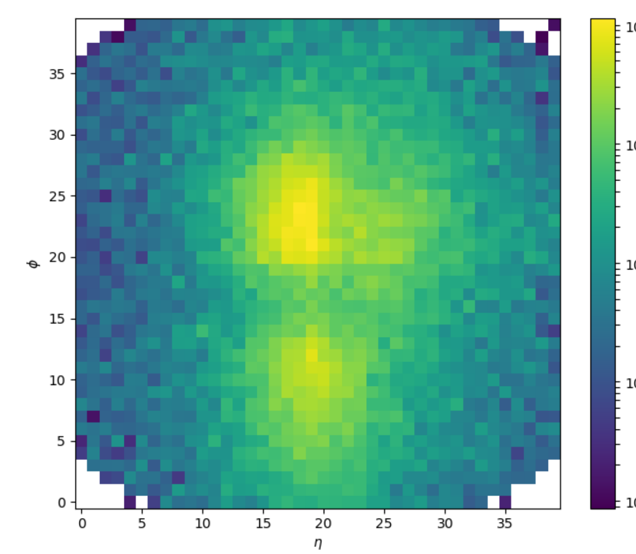
**+**

*(Simulated) Detector*




**=**

*1000 Images*

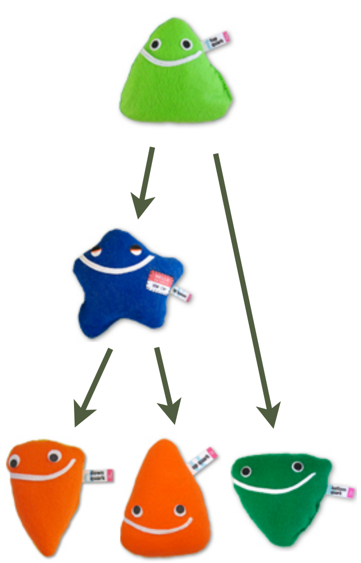



***(ignoring parton shower, hadronisation,…)***

# Heavy Resonance Tagging

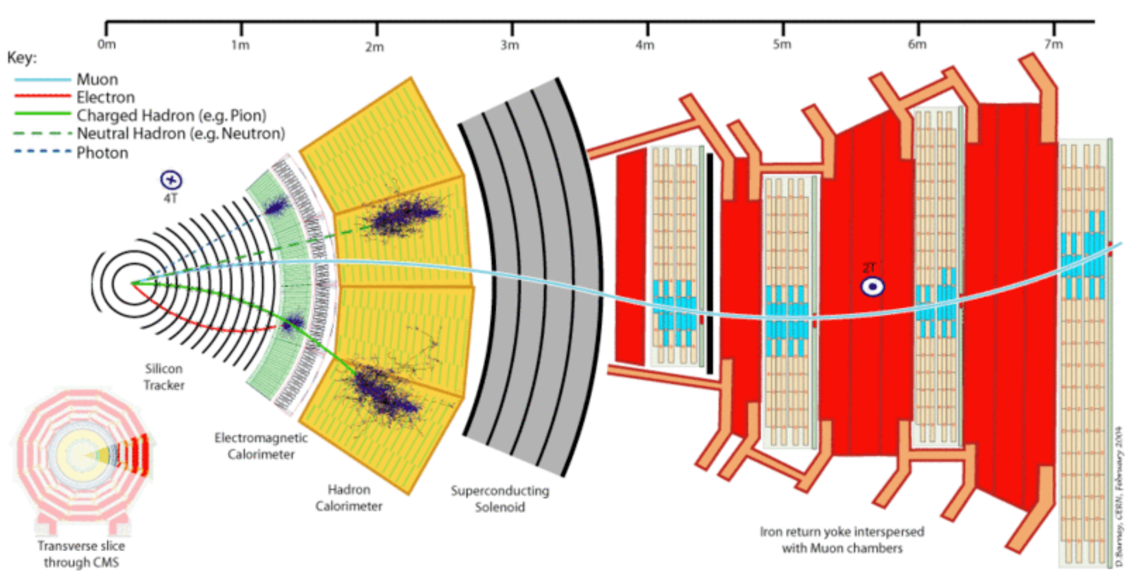
- **Goal**: Distinguish decay products of heavy resonance (top quark, W/Z boson, Higgs boson) from other particles (light quark/gluon jets)
- Achieve by looking at substructure of jets in the detector

*Top Quark*



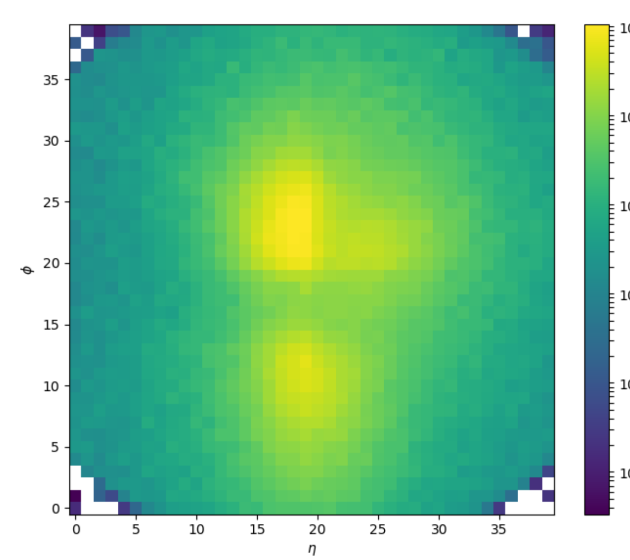
+

*(Simulated) Detector*



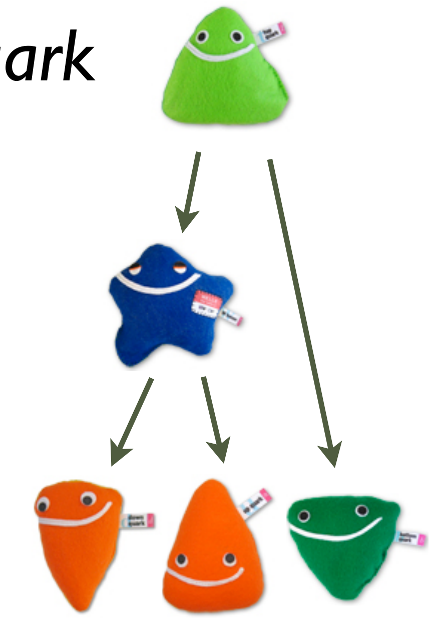

=

*10000 Images*

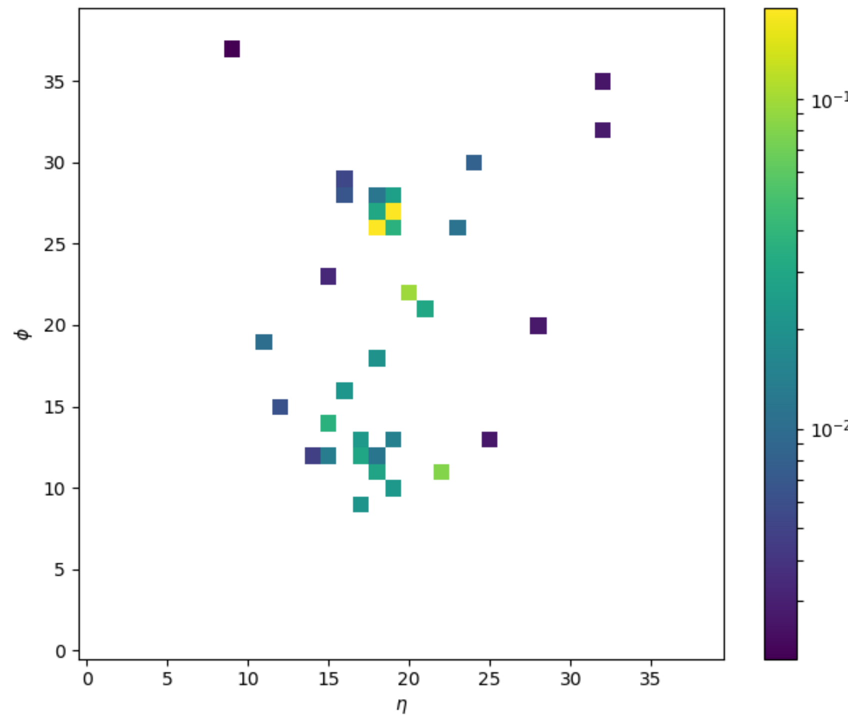


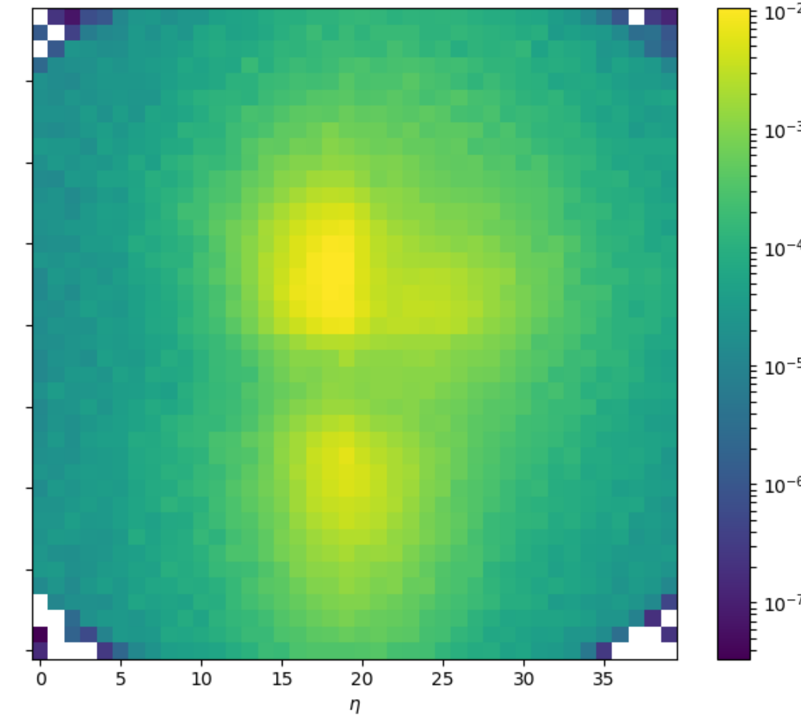
***(ignoring parton shower, hadronisation,...)***

*Top Quark Jet*



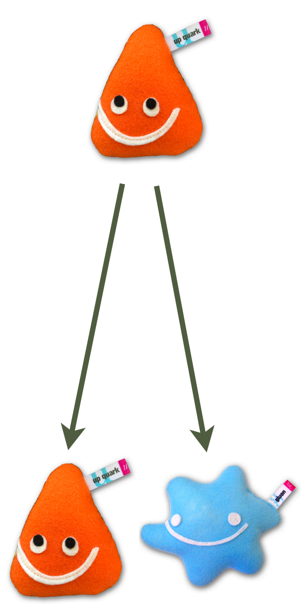
=



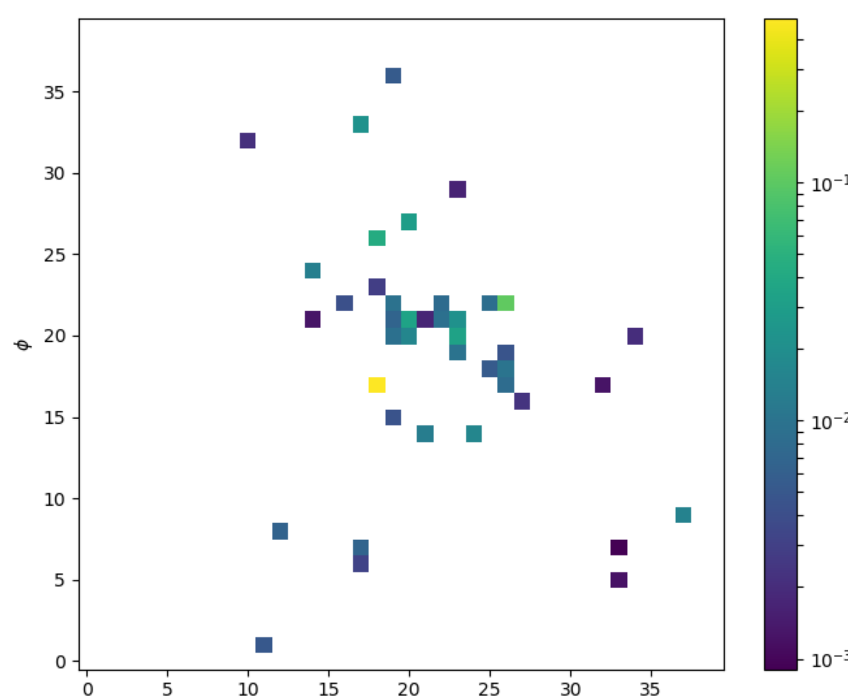


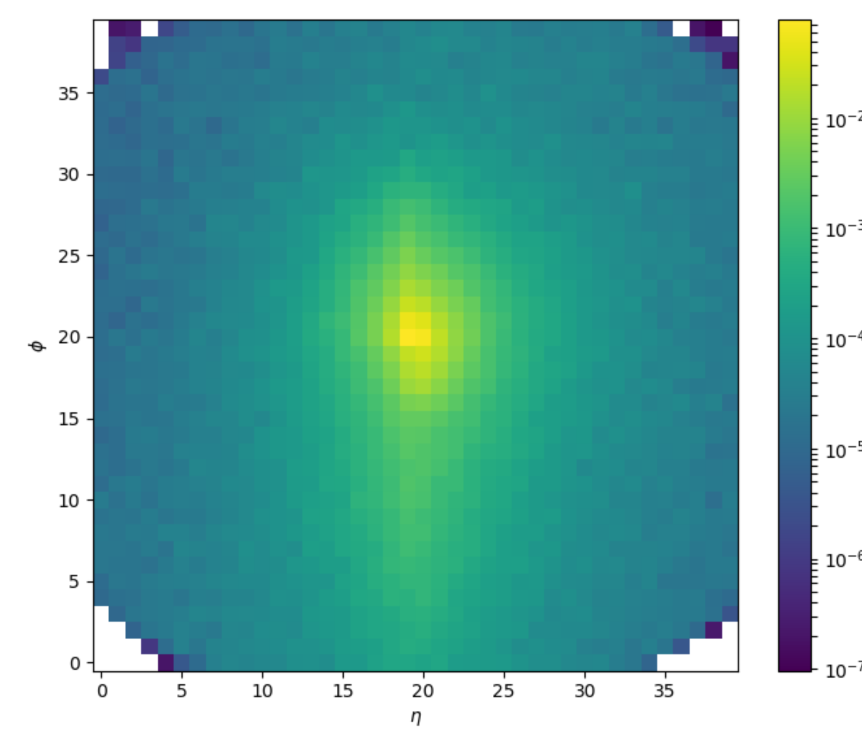
- *Binary classification task*
- *Fully supervised learning (using simulation)*
- *40x40 Pixels, $E_T$*
- *Perfectly suited for deep learning algorithms*

*QCD Jet*



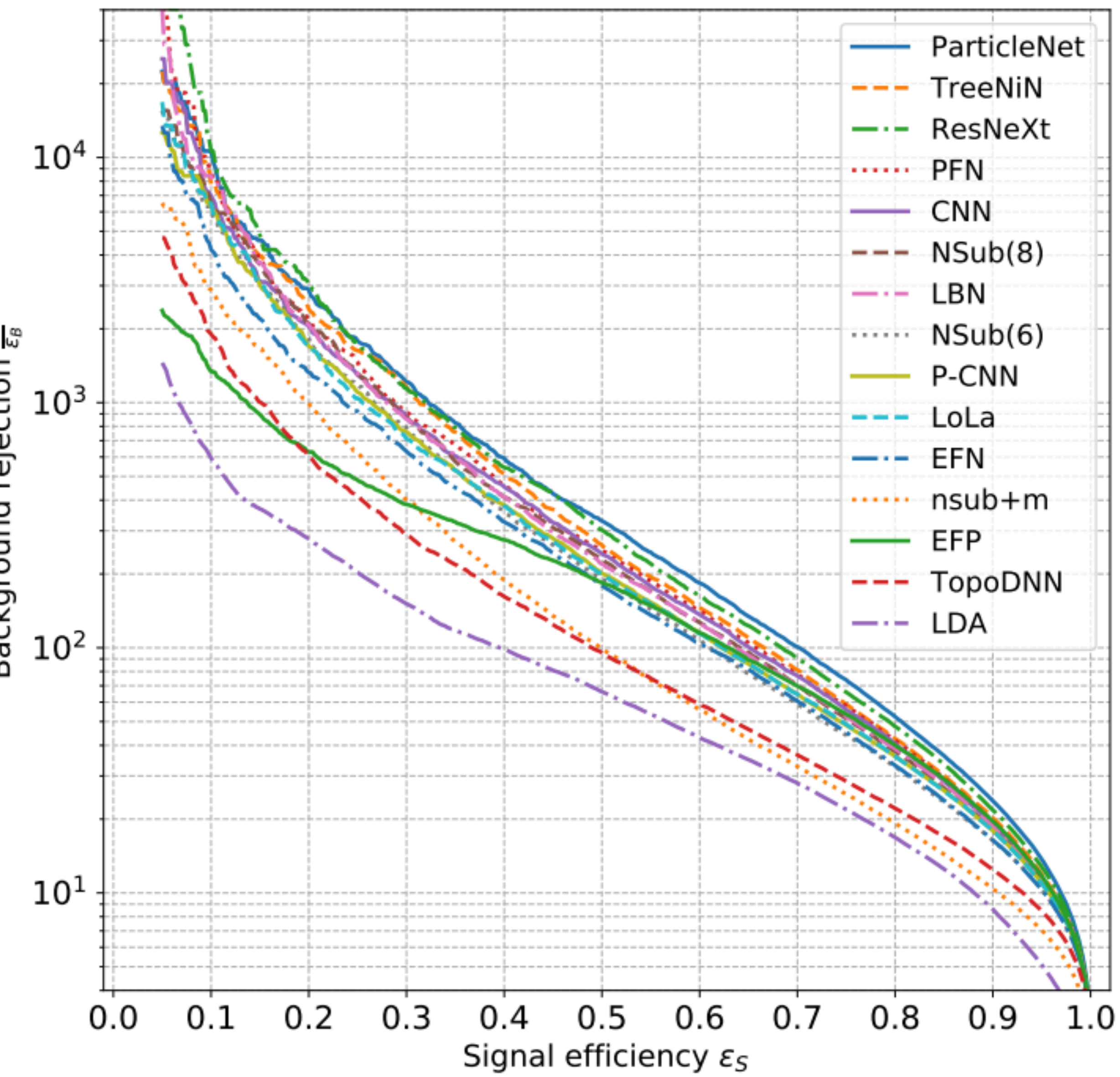
=





# Architecture Comparison

**Community performance comparison (toy dataset public): 1902.09914**




- 1.2M simulated top quark and background events
- Great test-bed to compare different data representations
    - (and, of course, useful for new physics searches, top/Higgs measurements)
- Still surprising gains in performance
    - Although it needs to be seen how well these translate to data
- (Also developments in flavour tagging, not covered here)

# Technical details

- Samples hosted on DESYCloud as .hdf5 files
- Up to 200 4-vectors per top-jet
  - Can also represent as images
- Total of ~1.6 GB
- Groups had access to all datasets - including final test
  trust that people do not abuse this
- Shared performance results and classification output on test-sample

| | AUC | Acc | $1/\epsilon_B$ ($\epsilon_S = 0.3$) single | mean | median | #Param |
|---|---|---|---|---|---|---|
| CNN [16] | 0.981 | 0.930 | 914±14 | 995±15 | 975±18 | 610k |
| ResNeXt [31] | 0.984 | 0.936 | 1122±47 | 1270±28 | 1286±31 | 1.46M |
| TopoDNN [18] | 0.972 | 0.916 | 295±5 | 382± 5 | 378 ± 8 | 59k |
| Multi-body $N$-subjettiness 6 [24] | 0.979 | 0.922 | 792±18 | 798±12 | 808±13 | 57k |
| Multi-body $N$-subjettiness 8 [24] | 0.981 | 0.929 | 867±15 | 918±20 | 926±18 | 58k |
| TreeNiN [43] | 0.982 | 0.933 | 1025±11 | 1202±23 | 1188±24 | 34k |
| P-CNN | 0.980 | 0.930 | 732±24 | 845±13 | 834±14 | 348k |
| ParticleNet [47] | 0.985 | 0.938 | 1298±46 | 1412±45 | 1393±41 | 498k |
| LBN [19] | 0.981 | 0.931 | 836±17 | 859±67 | 966±20 | 705k |
| LoLa [22] | 0.980 | 0.929 | 722±17 | 768±11 | 765±11 | 127k |
| LDA [54] | 0.955 | 0.892 | 151±0.4 | 151.5±0.5 | 151.7±0.4 | 184k |
| Energy Flow Polynomials [21] | 0.980 | 0.932 | 384 | | | 1k |
| Energy Flow Network [23] | 0.979 | 0.927 | 633±31 | 729±13 | 726±11 | 82k |
| Particle Flow Network [23] | 0.982 | 0.932 | 891±18 | 1063±21 | 1052±29 | 82k |
| GoaT | 0.985 | 0.939 | 1368±140 | | 1549±208 | 35k |

**Can use as template for a first IDT-ErUM overview**

# Challenges

- ErUM domains work with a diverse set of data representations
  - Different detector geometries, different types of experiments, theory calculations…
- But: several approaches should be flexible enough:
  - Fully connected
  - 1D convolutions
  - Graphs
  - (Images)
  - …?
- Developing a first set of general recommendations for non-ML-expert ErUM practitioners already would be valuable
  - ‘Physics’ performance
  - ‘Computational’ performance
  - Examples shared, eg on Vispa

# What do we have?

- Datasets:
  - Top tagging reference sample
    1902.09914
    (Can either use directly or provide a slimmed version)
  - **FIAS (Jan Steinheimer, Kai Zhou): Spinodal vs. Maxwell classification**
    arXiv: 1906.06562
    160k 20x20 Grayscale images
  - **FIAS (Jan Steinheimer, Kai Zhou): QCD transition: EOSL/EOSQ**
    arXiv: 1910:11530
    24x24 2D histograms of pion spectra
  - Aaachen (Jonas Glombitza):
    Air shower classification: Proton vs Iron
    https://doi.org/10.1016/j.astropartphys.2017.10.006
    100k examples, ~7k channels
  - **Upcoming: LMU (James Kahn)**
    Belle II
- Algorithms:
  - Fully connected
  - Images
  - 1D Convolution
  - Graph Convolution
  - Spectral Graph Networks