

Evolution of Al approaches at the LHC P. Harris (MIT,IAIFI,A3D3)





Overview of this talk

Origins of Deep Learning at LHC Where Algorithms are Going

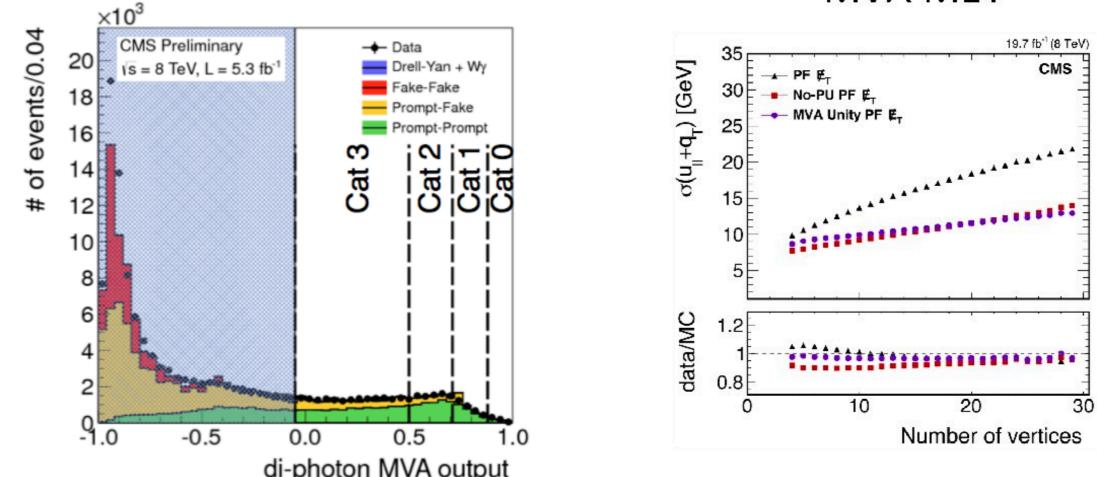
Where Experiments are Going Deep Learning For Others (LIGO/Neut)

Anomaly Detection

Power of ML

- The LHC has long kept up with trends from ML
 - In the era of BDTs, many big advancements came
 - Many were critical for the observation of the Higgs boson

MVA MET



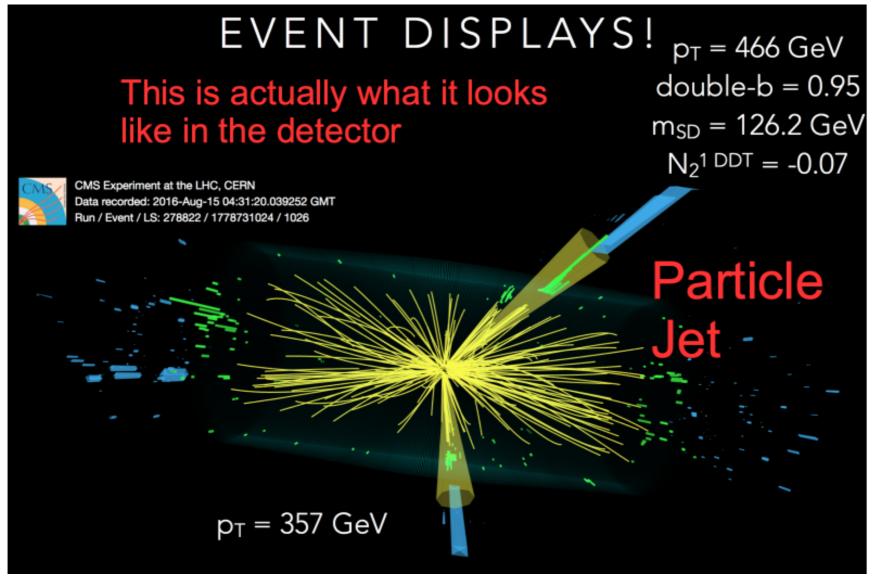
A Change in Past 5 years

- Deep Learning has heavily push progression to other arch
- Why was this case?
 - New DL frameworks dramatically changed flexibility
 - We can now train for arbitrary loss functions
- DL frameworks are very effective with GPUs
 - GPUs allow us to have many inputs > 100! (BDTs capped at 40-50)

TMVA Loss Regression(MSE) Classier(CCE)

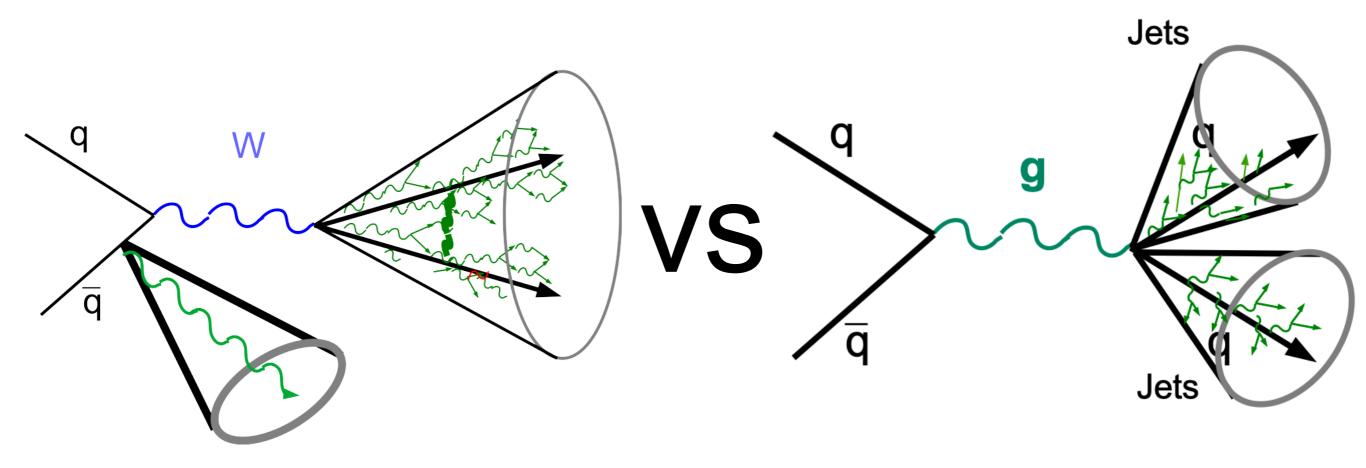


For Jets



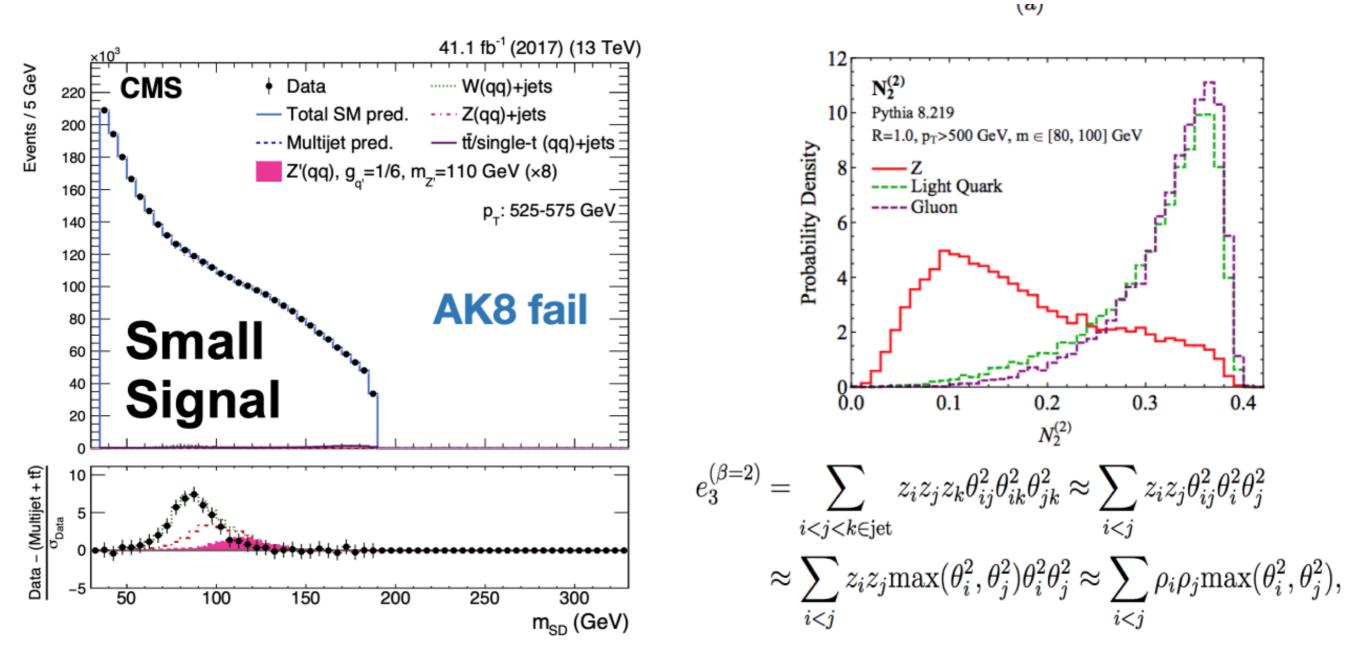
- Jets have the chance to benefit greatly from Deep Learning
 - There is a large variety of variables that we can construct

Selecting a Jet in data



- If you select a jet in data and look at the mass
- There is an enormous amount of background
- But, you can potentially find a W boson or a Higgs boson

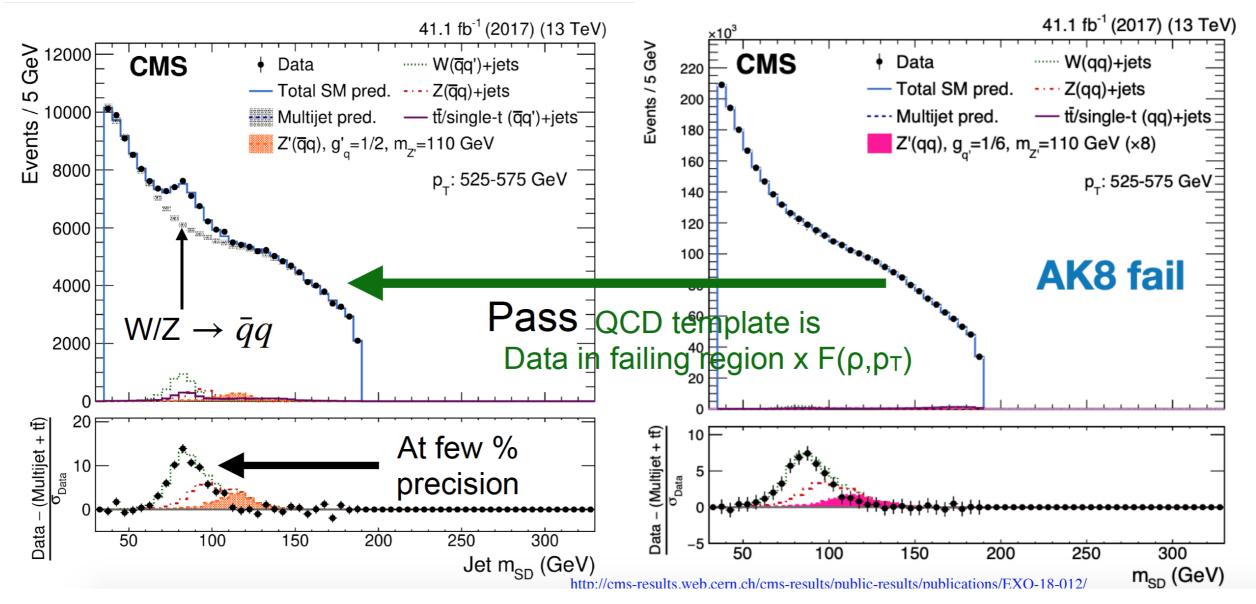
Jets have 100s of particles



Large backgrounds and many particles good ML problem

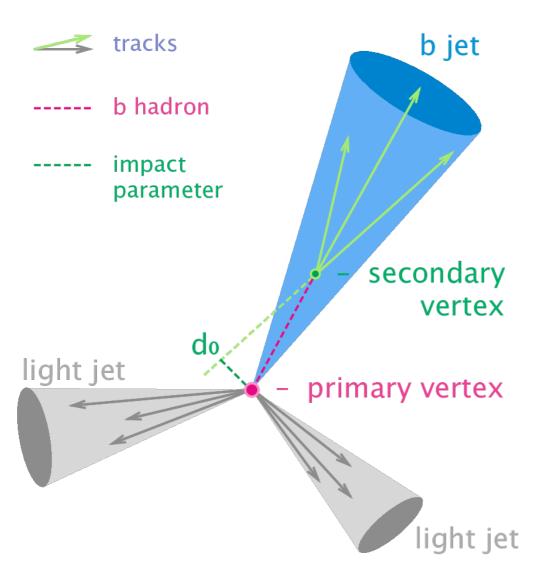
• To see anything we need to reduce bkg by x10-100

Without Deep Learning



- Already with jet substructure we can start to see resonances
- But these analyses set the stage for a great deep learning

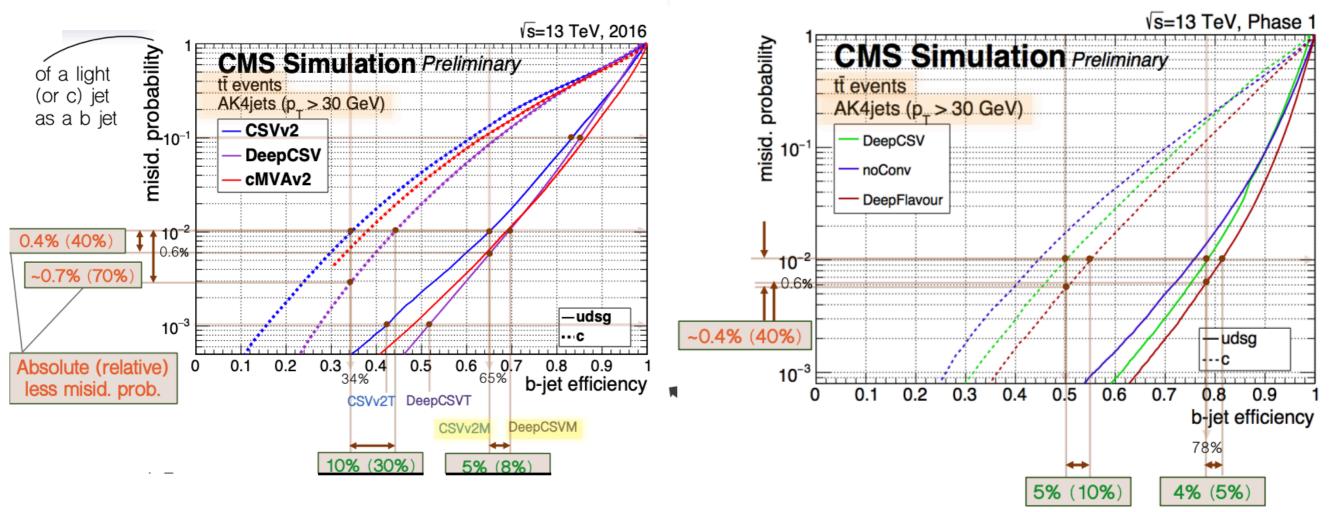
Where Deep Learning really started to help



B-tagging has lots of handles Also there is lots of background Discrimination is key!

- For b-quark tagging Deep Learning brought a lot of gains
 - Part of these gains was from the fact that things were not tuned

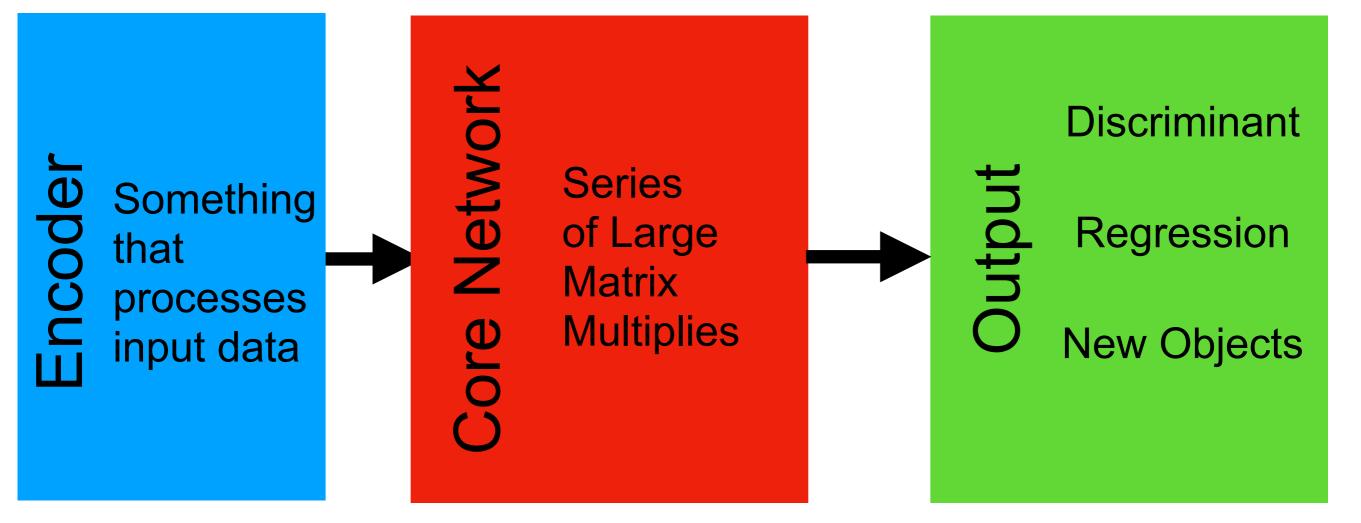
Where Deep Learning really started to help



- For b-quark tagging Deep Learning brought a lot of gains
 - Part of these gains was from the fact that things were not tuned

Neural Network Arch

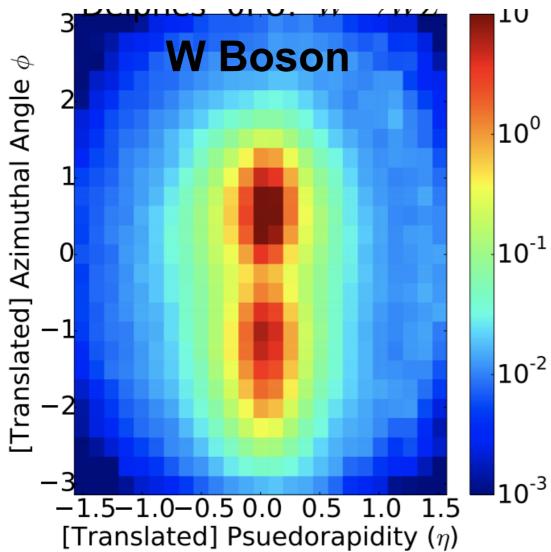
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- Encoders capture much of the physics to all for standard DL tools
 - Responsible for much of the big gains over the past few years

So what has happened?

- Big gains in deep learning have come from embedded data
- How can we take a complex object like a jet and process it



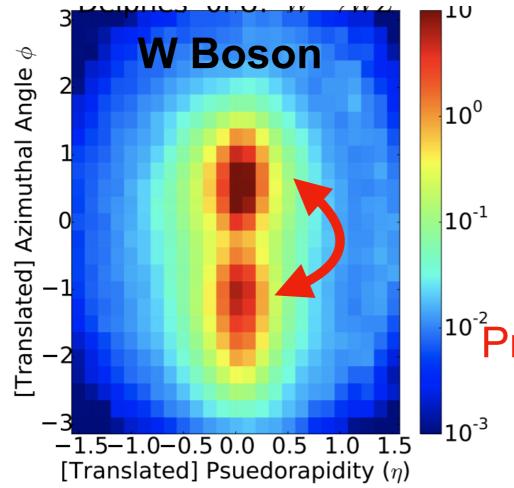
Jet Image

Take a jet and do an energy weighted sum of the particles centered about the jet axis

 ^{10⁻¹} When we first tried this Convolutional Neural Networks
 ^{10⁻²} for Imag Id were the new big thing!

So what has happened?

- Big gains in deep learning have come from embedded data
- How can we take a complex object like a jet and process it



Jet Image

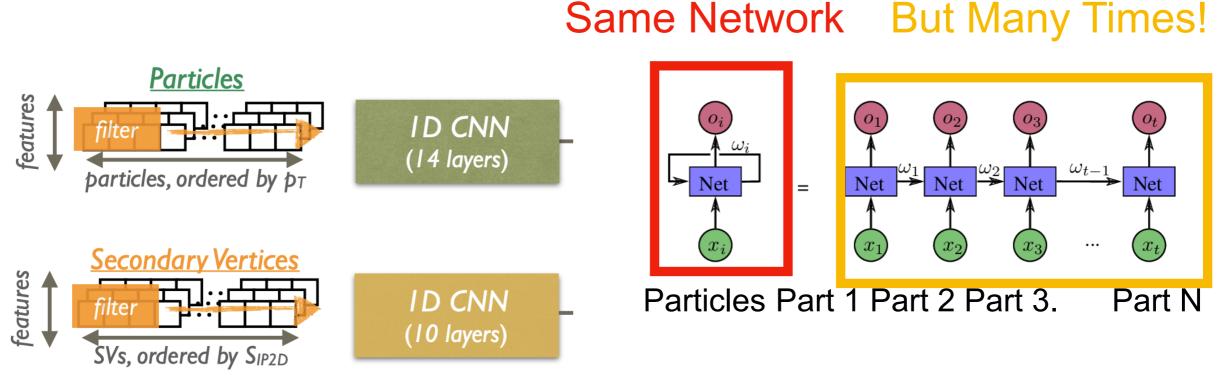
Take a jet and do an energy weighted sum of the particles centered about the jet axis

^{o*}Problem! Image Not Lorentz Invariant

Jet p_T will change the overall position!

Improving the idea

- Instead we can consider sending in 4 vectors
 - Utilizing 4-vectors gives us a notion of lorentz invariance

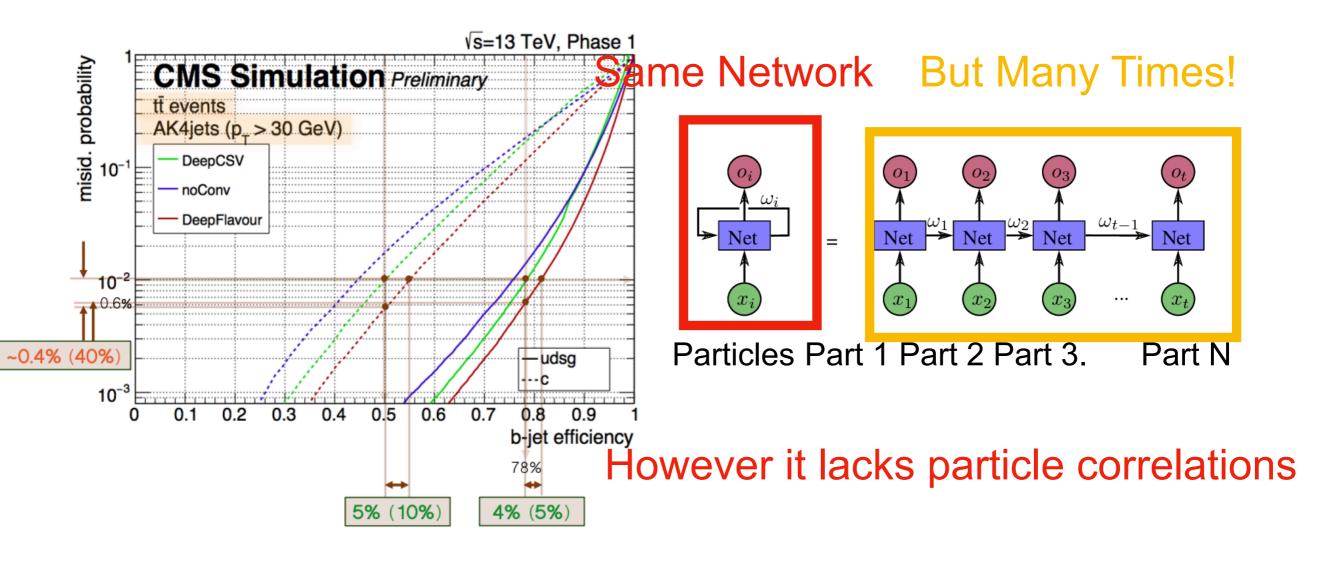


Take's a single Particle in at a time

Popular in 2018 when Recurrent Neural Networks were the crazy

Improving the idea

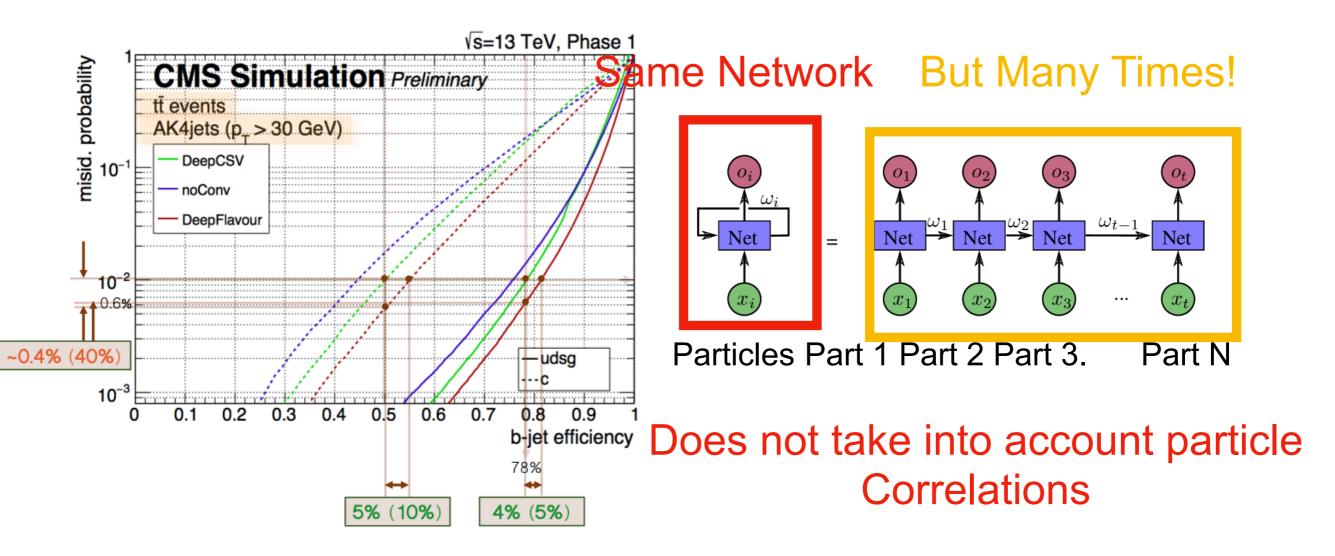
- Instead we can consider sending in 4 vectors
 - Utilizing 4-vectors gives us a notion of lorentz invariance



Lack or particle correlations limits Jet Identification ability

Improving the idea

- Instead we can consider sending in 4 vectors
 - Utilizing 4-vectors gives us a notion of lorentz invariance

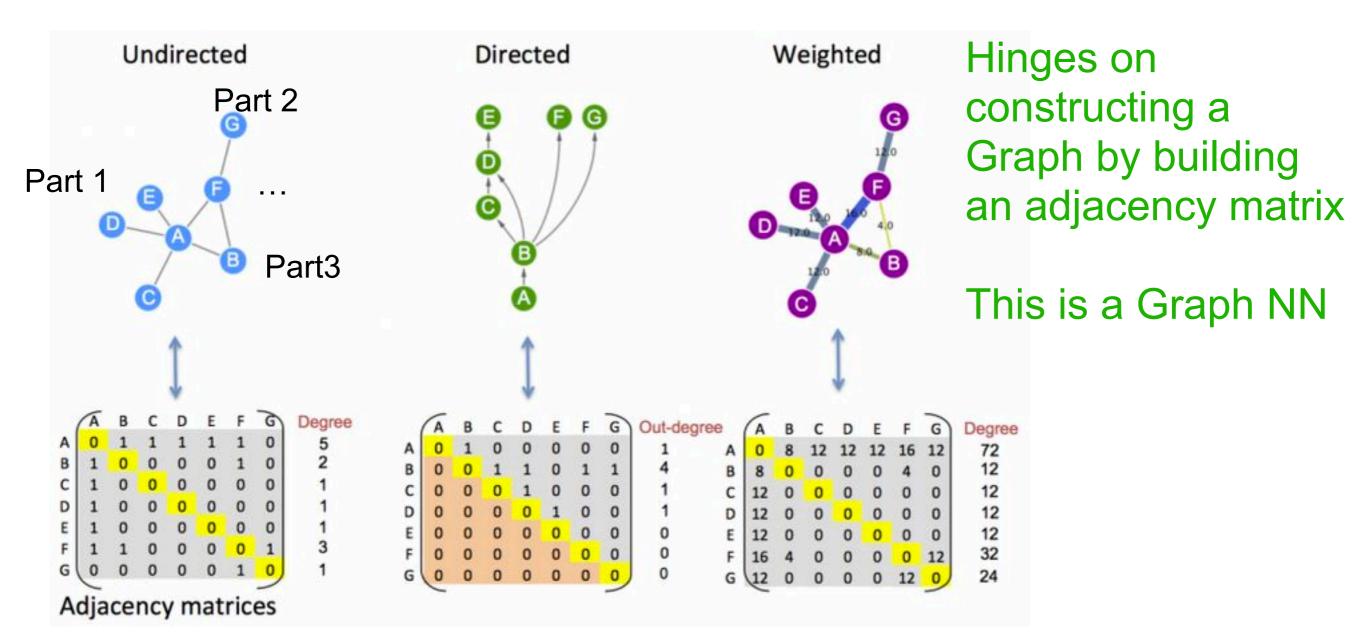


Gain from DeepCSV to DeepFlavor is from the Architecture choice

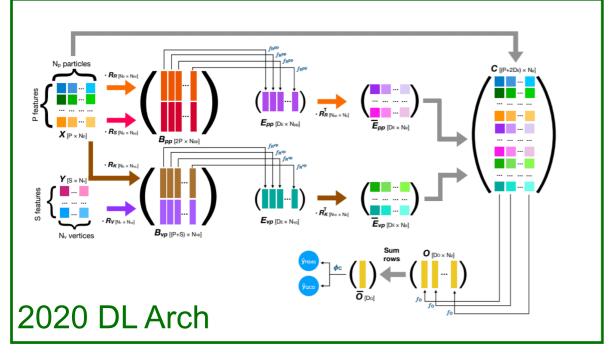
Current State of the Art

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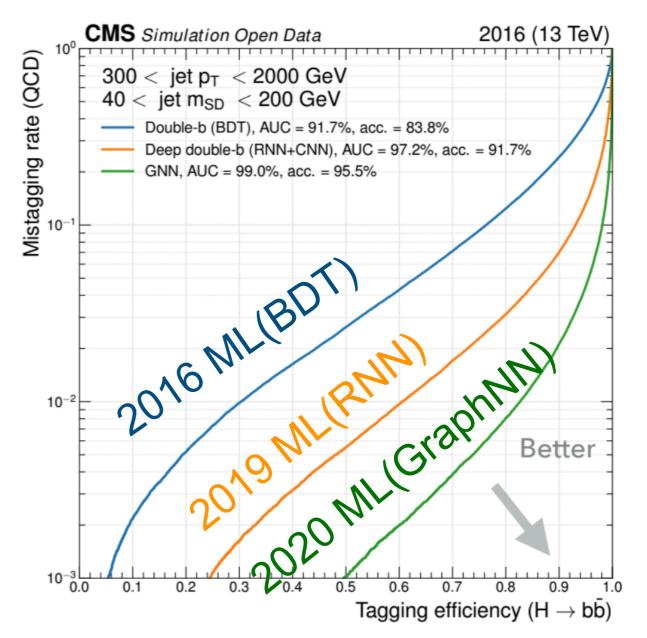
- We can take the same 4-vectors and features
 - Instead construct an NN that takes particles and correlations



Observing Big gains

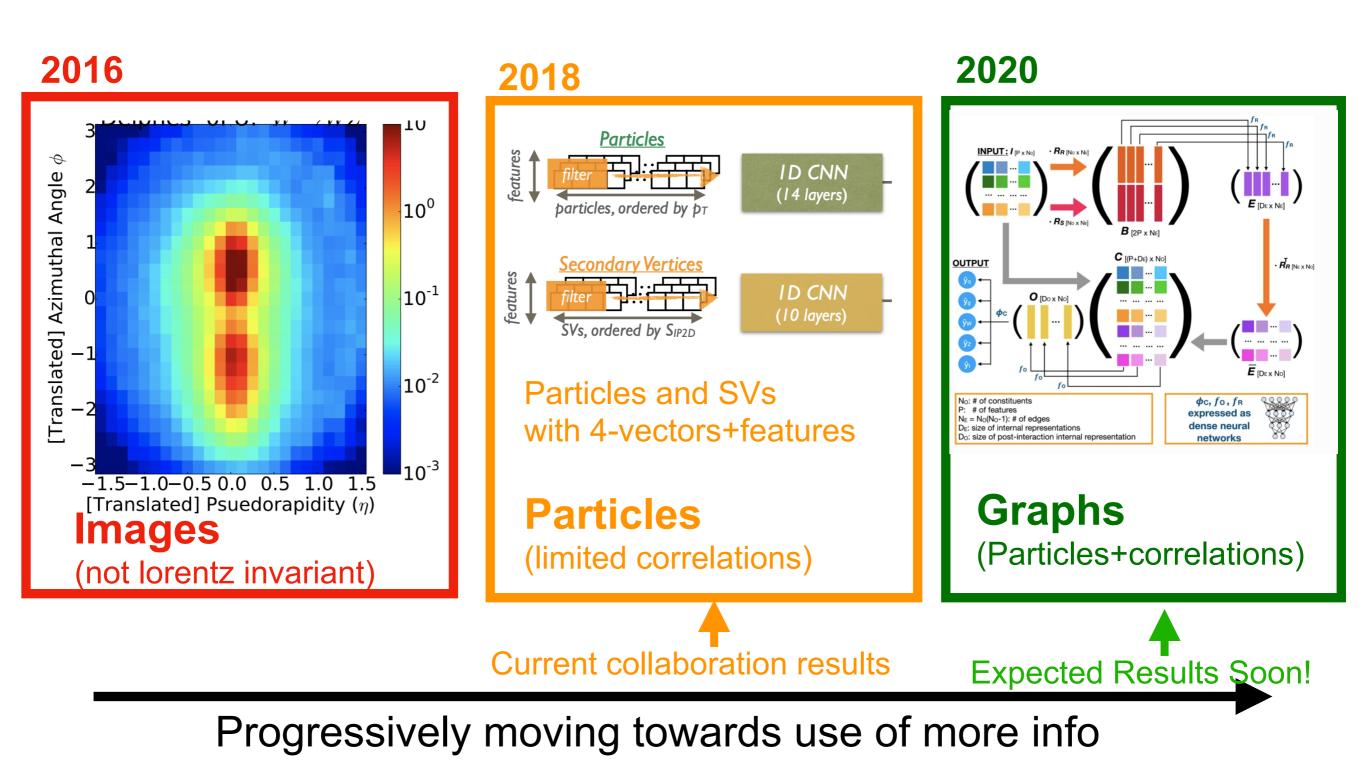


- For a Higgs boson at high energy
 - We have to rely on deep learning



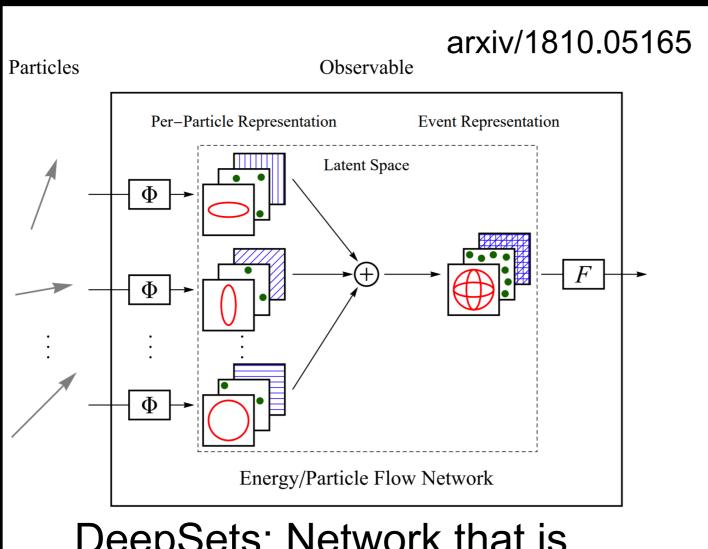
- Deep learning is quickly leading to a major transformation
- We can measure processes that we didn't think possible arxiv:1909.12285

Encoder Progression

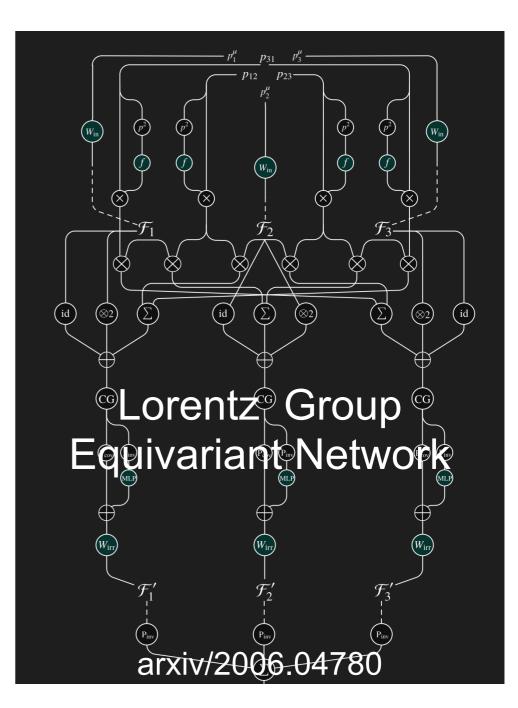


Extensions of these Ideas

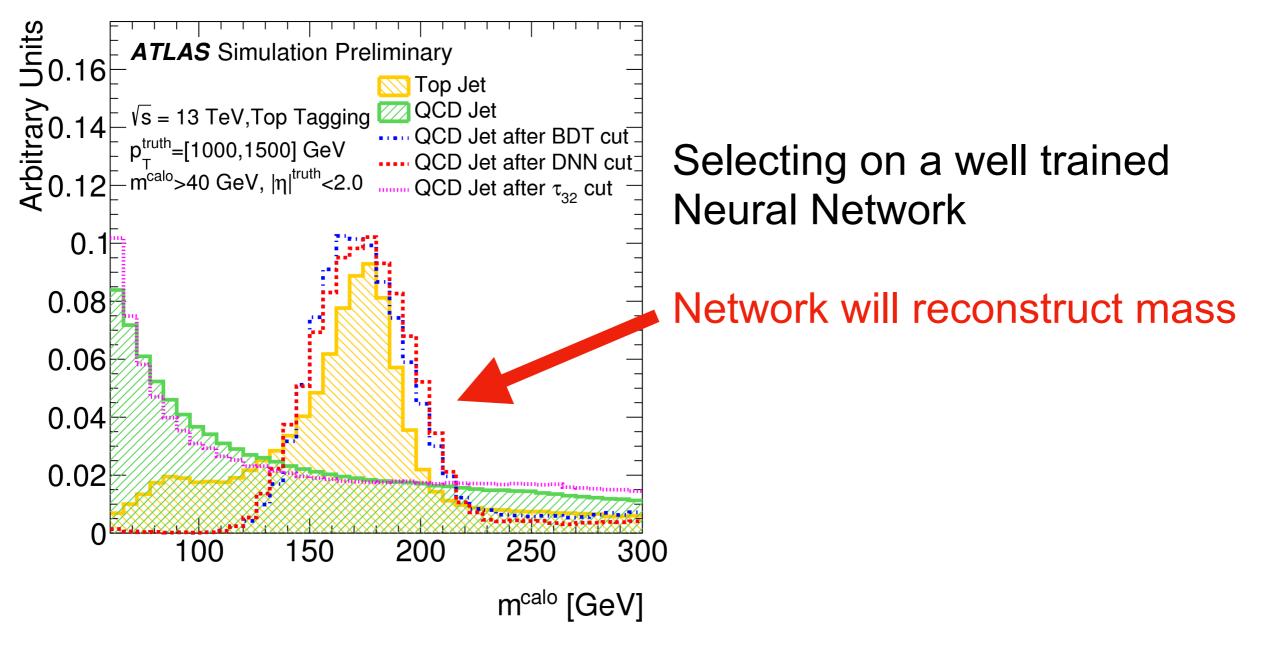
There are many ways to make encoders better



DeepSets: Network that is IR and Collinear safe Encoder

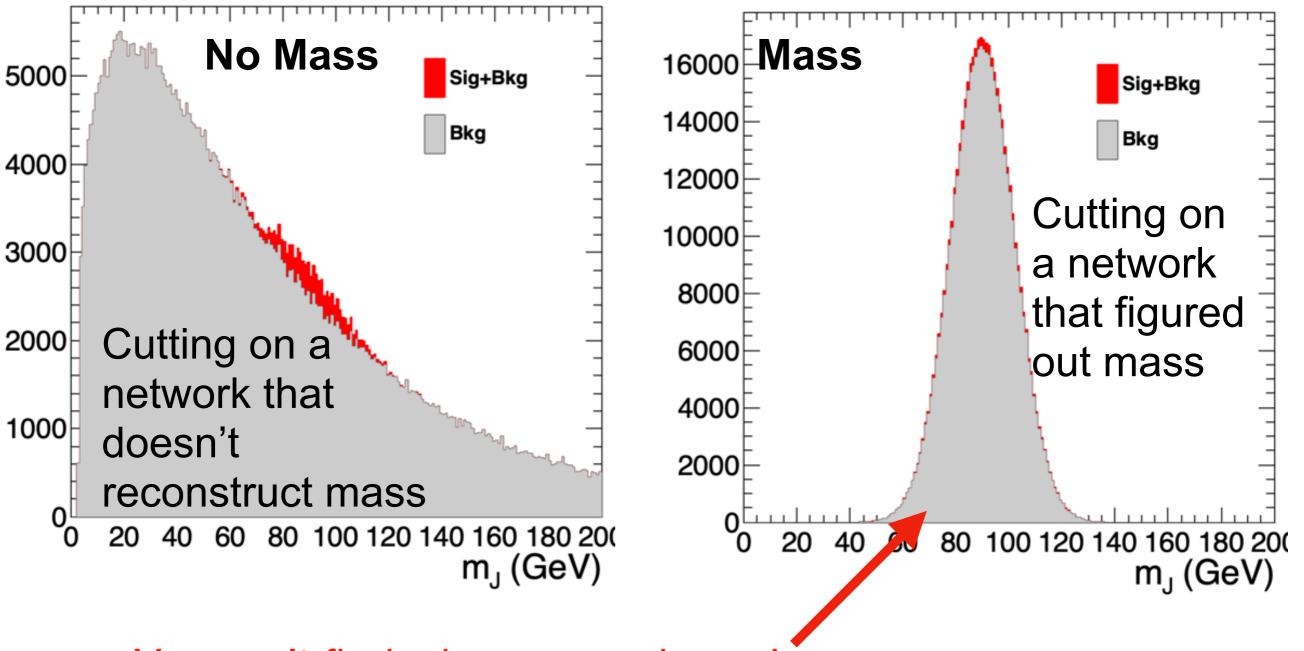


Finding a resonance



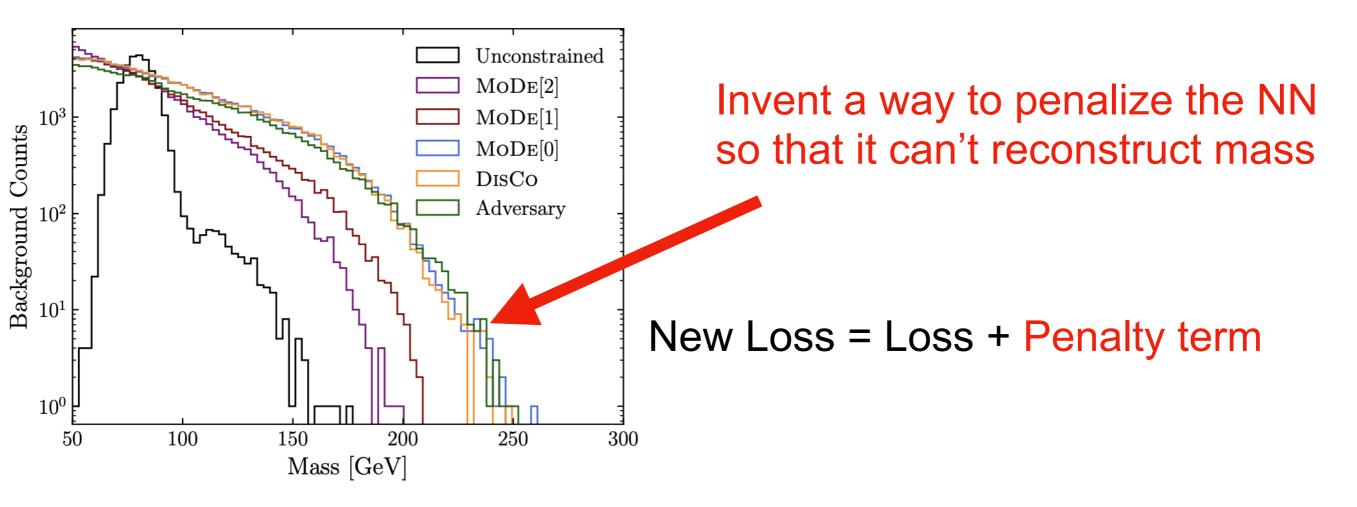
- To find a resonance, we don't just need a good DNN
 - We also need a way to extract it

Finding a resonance



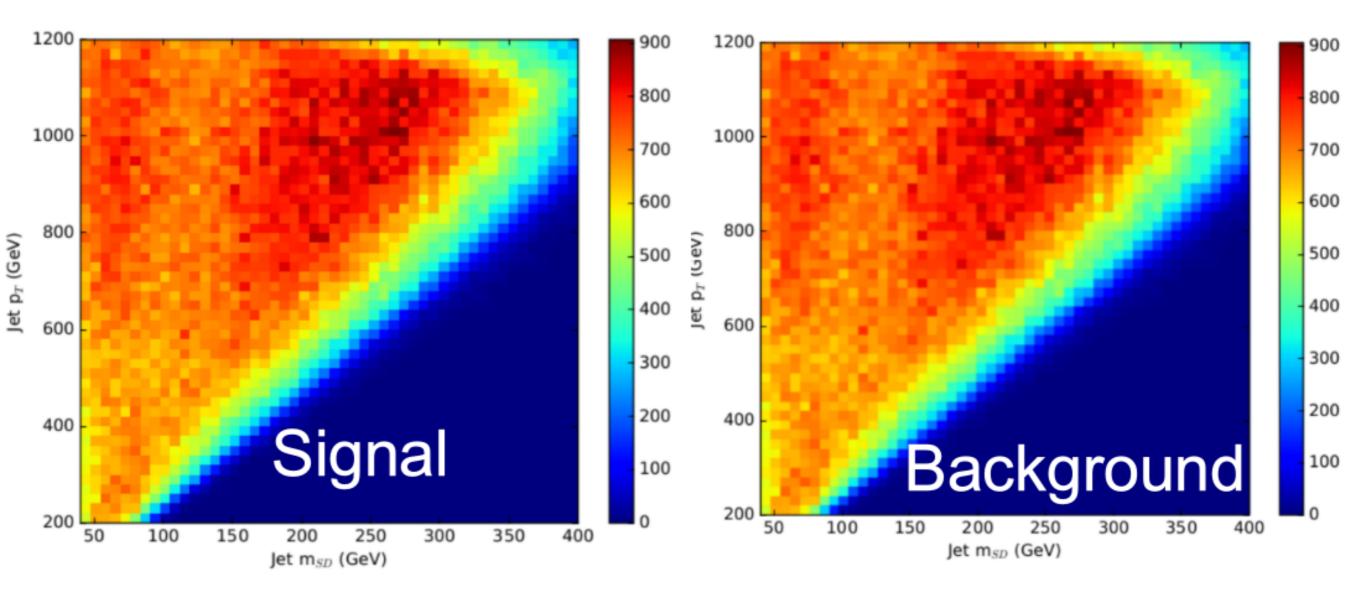
- You can't find a bump on a bump!
 - Being able to control background is essential in data

One Method To Control



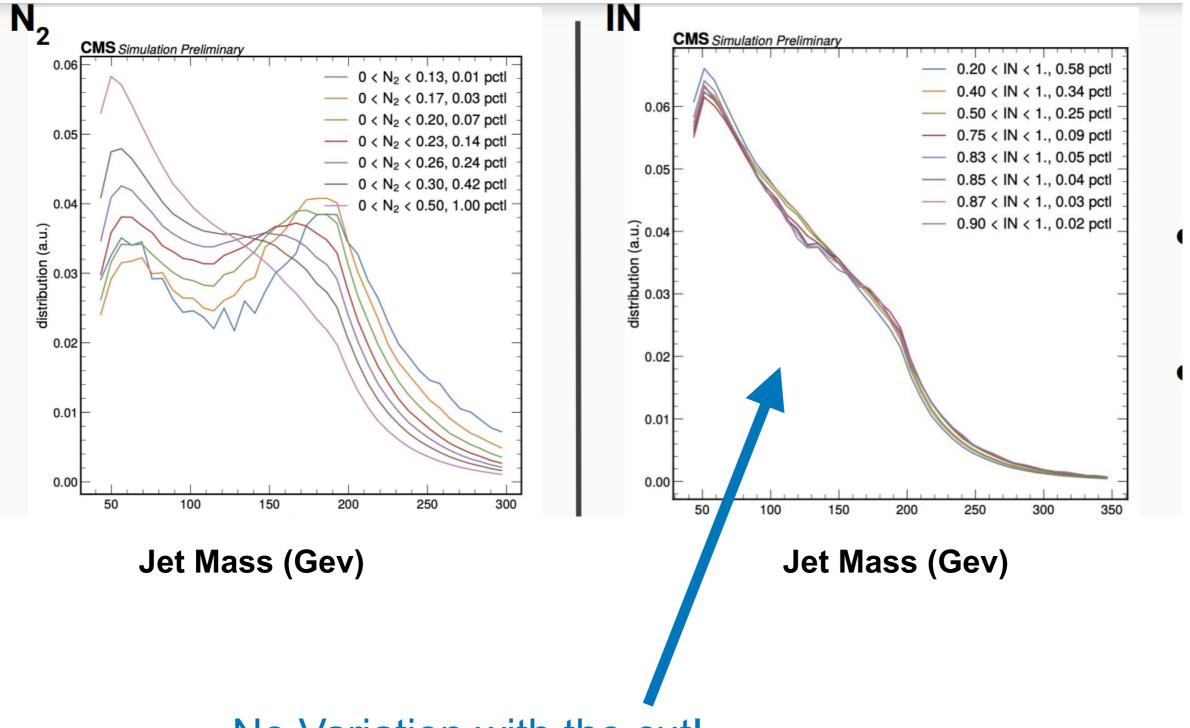
- Adding a penalty can force the network to go the other way
- This requires a bit of tuning
- However there is lots of literature doing this

A More Robust Approach



- Modifying Matrix elements so signal and background are the same
- This solution turns out to be very powerful, but "Old School"

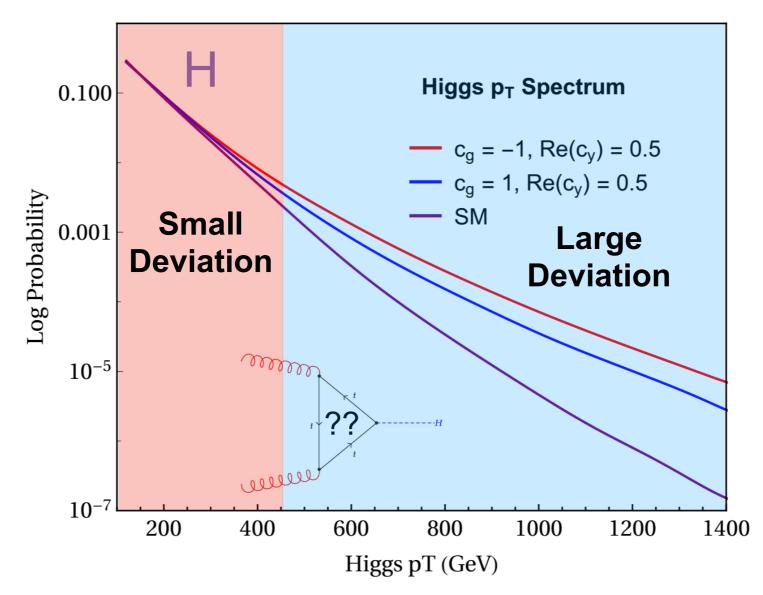
A More Robust Approach



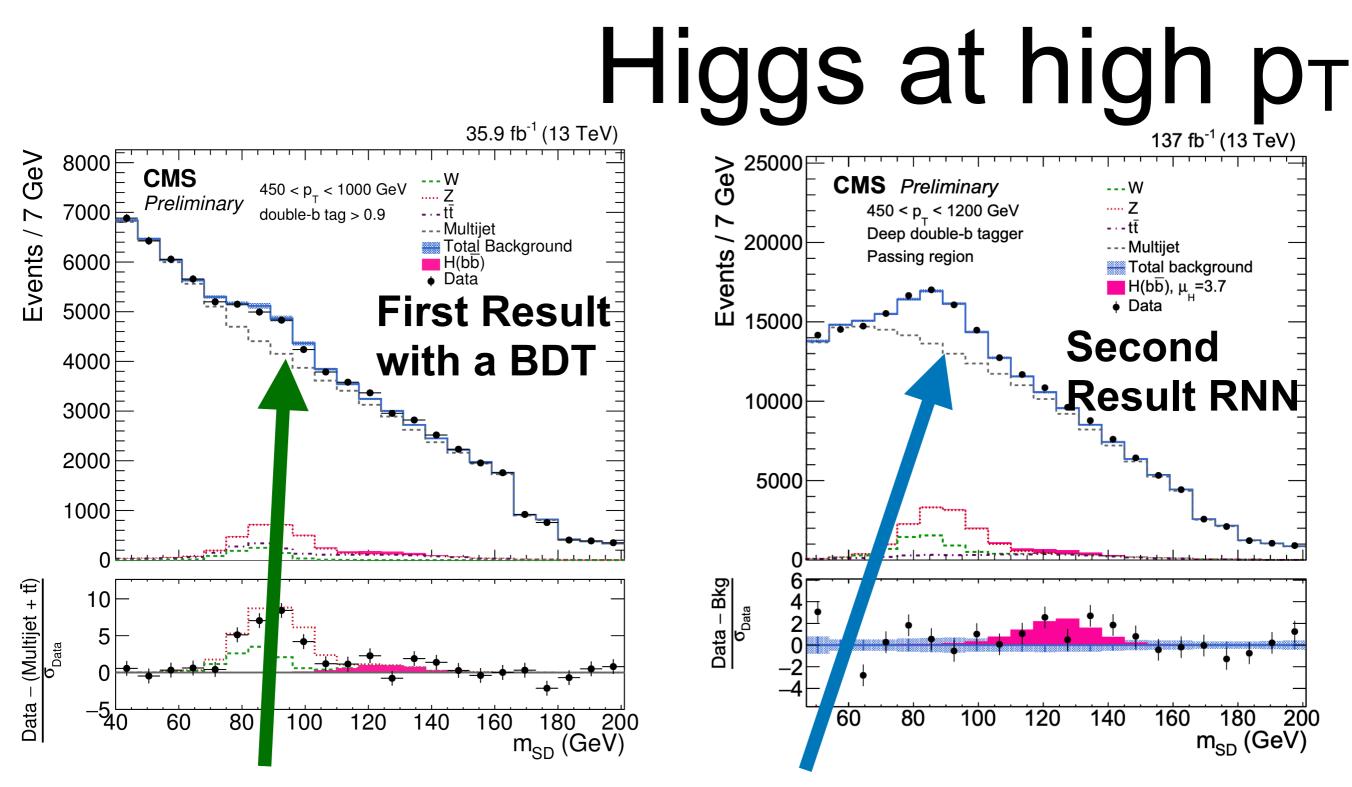
No Variation with the cut!

Boosted Higgs Result

Can we build a new Higgs boson result with deep learning?

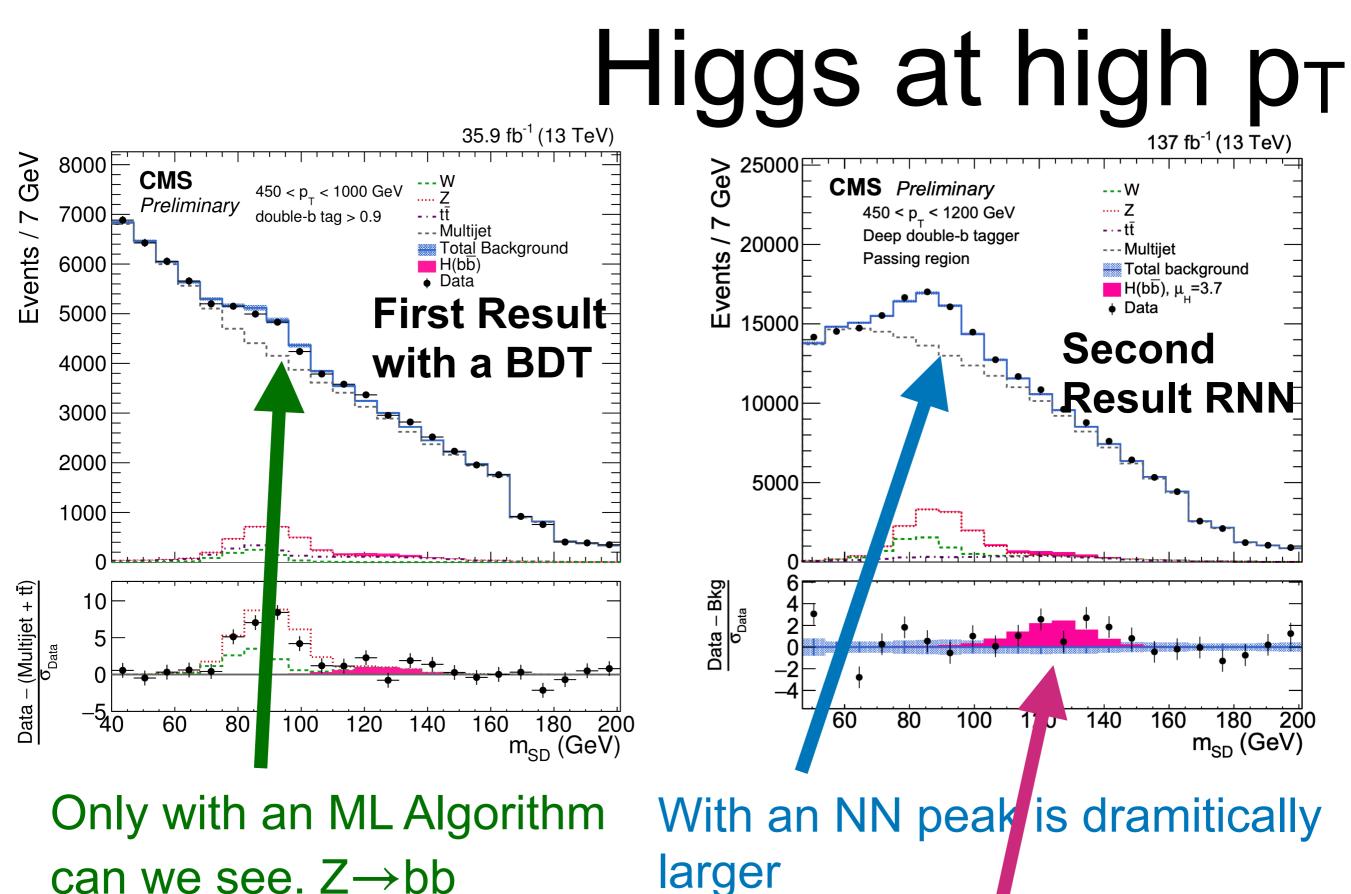


Deep learning is effective at isolating overlapping b-quarks With deep learning we were able to reduce background by 2



Only with an ML Algorithm can we see. $Z \rightarrow bb$

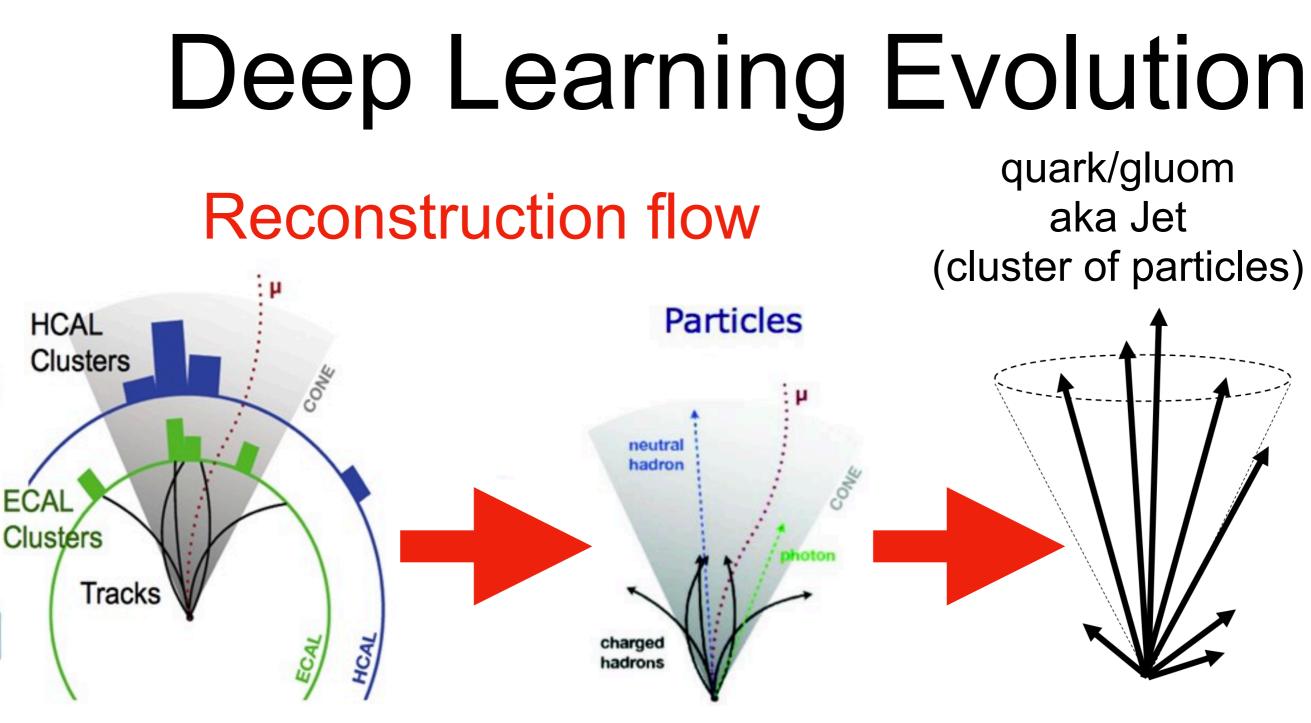
With an NN peak is dramitically larger

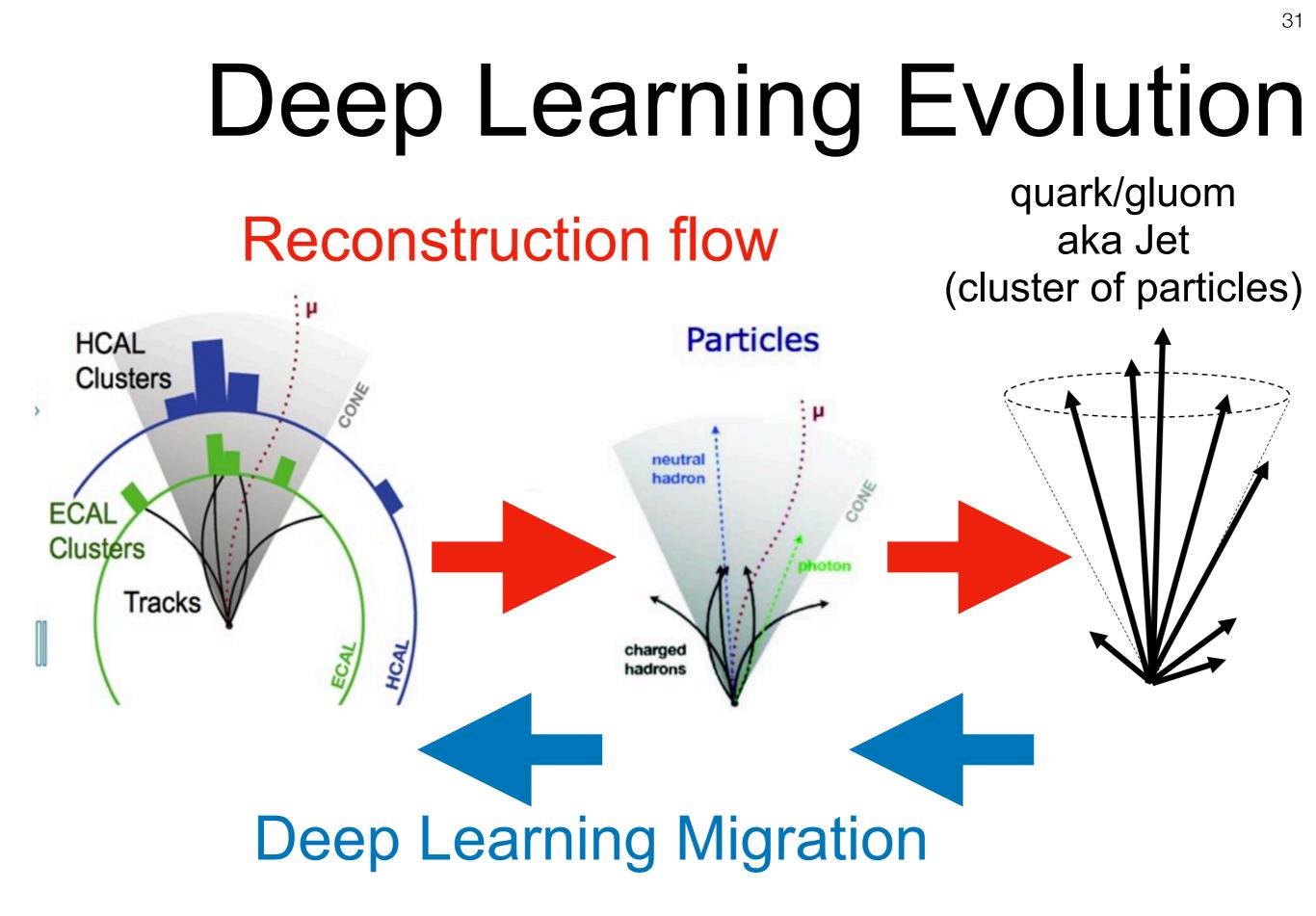


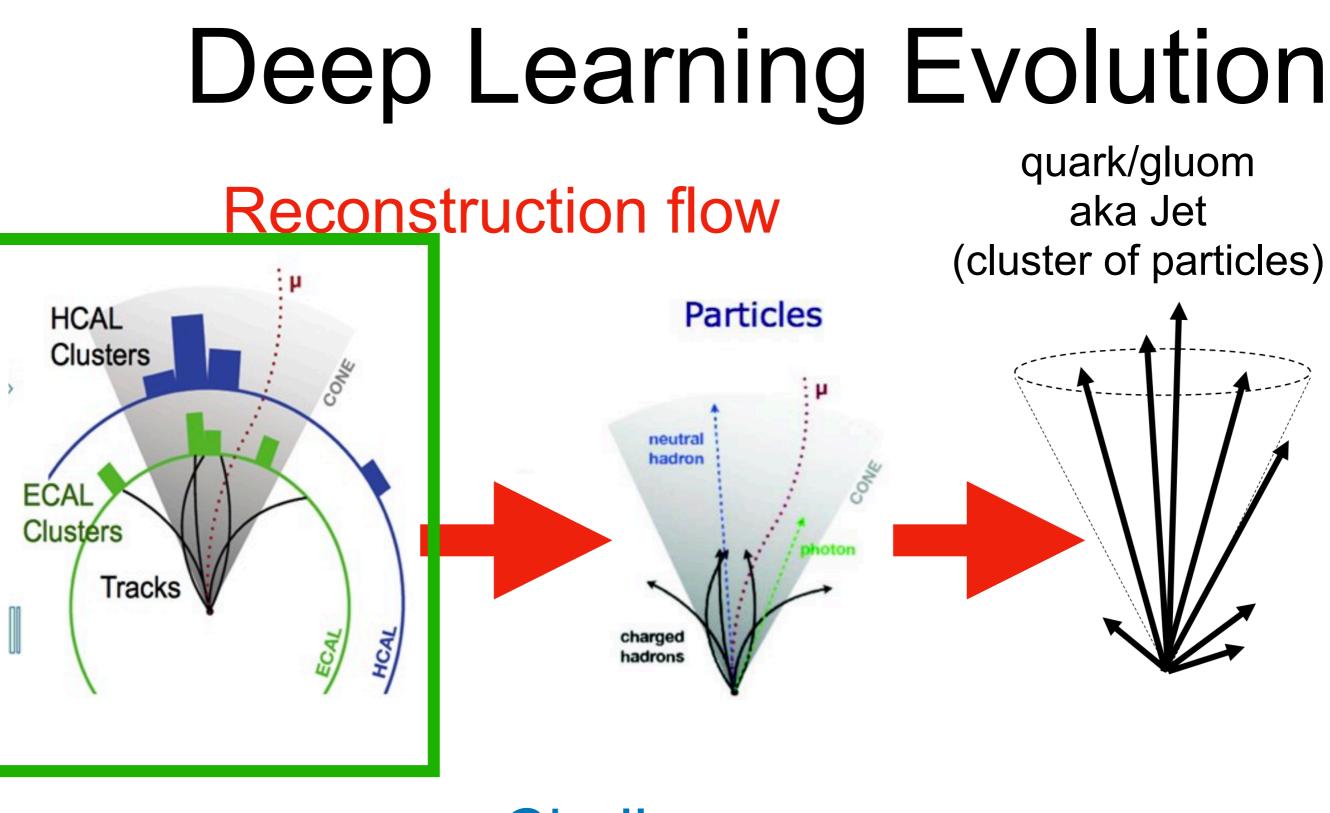
And there are signs of a Higgs Peak



What LHC physicists have been doing during COVID



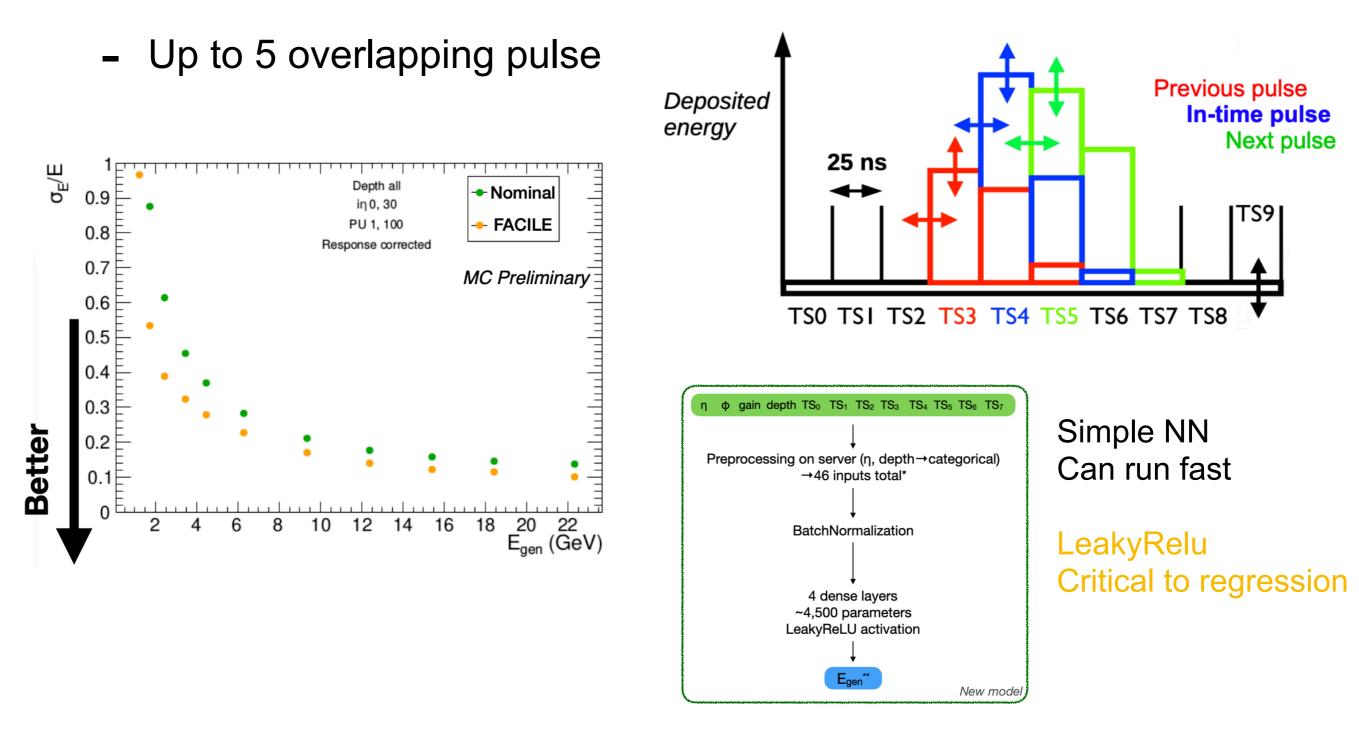




Challenge: Can you go from Raw inputs to reco?

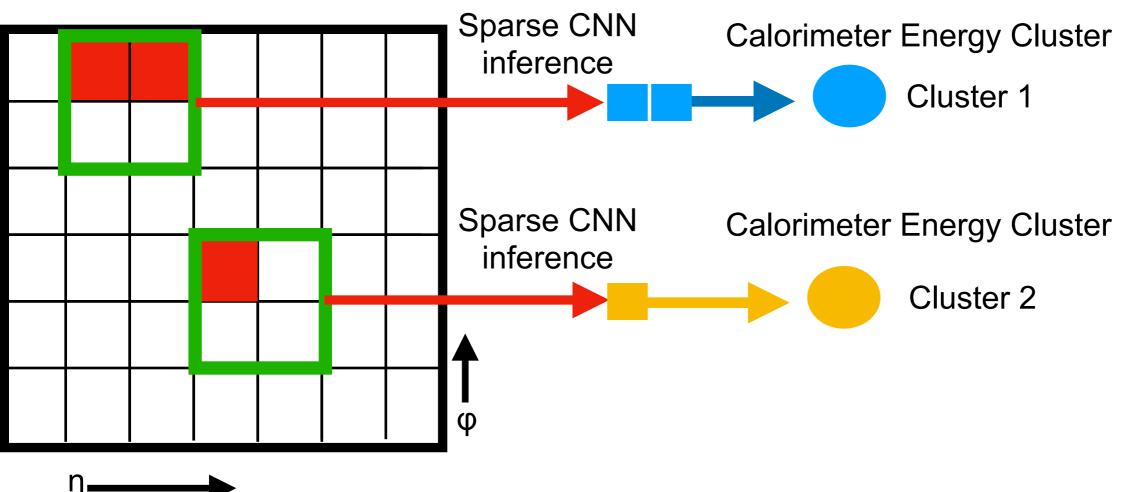
Simple Example

- Reconstructing a single calorimeter tower
 - FACILE Algorithm: Reconstruct integral of in-time pulse



From Single to Collection

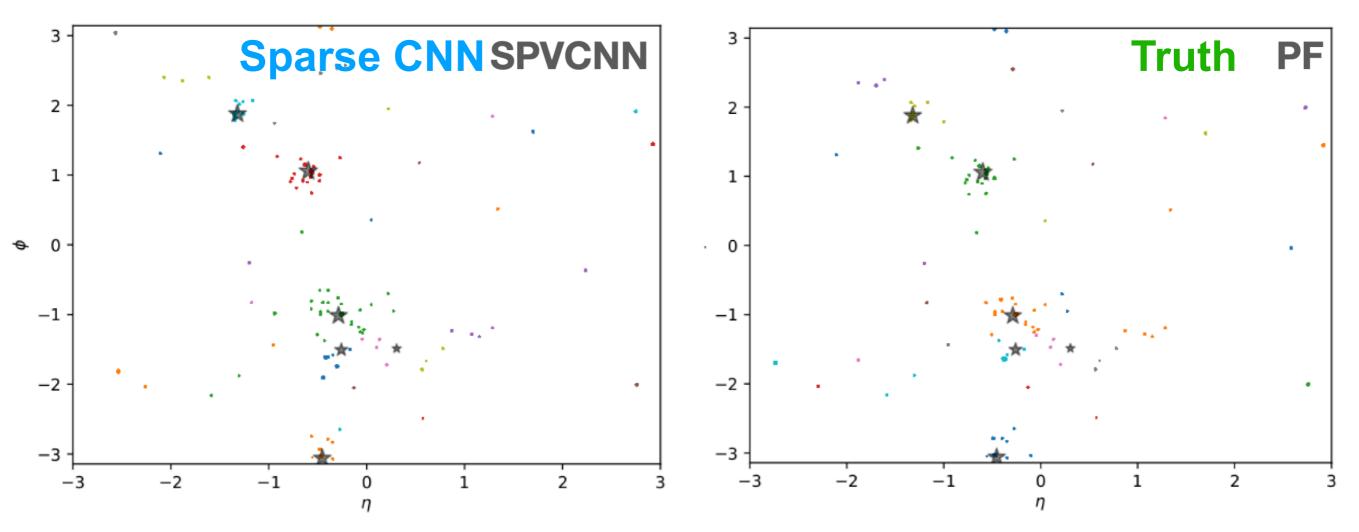
- Facile runs reconstruction on a single channel
 - We can envision an algorithm that takes in all channels
 - One way is to use a sparse CNN for graph-like inputs



By taking the grid geometry of calorimeter can deploy Sparse CNN to Infer whole calo at once

Can compare to Reality

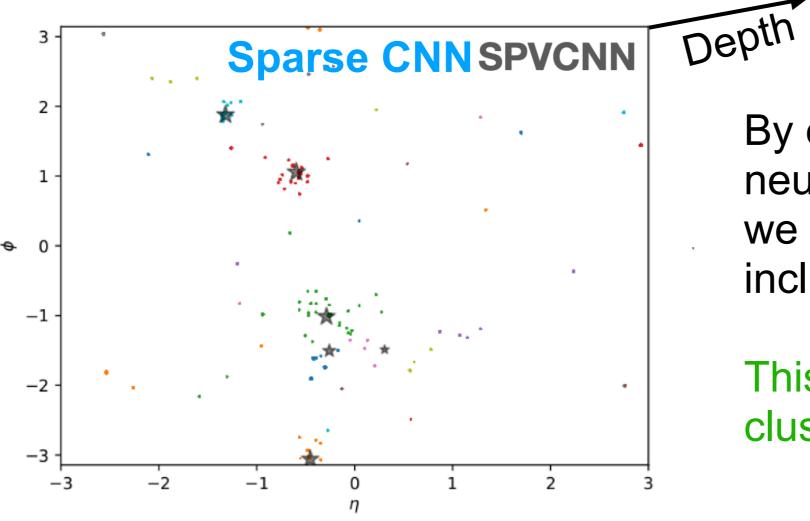
• A single algorithm is doing all of the clustering



- Clustering algorithm produces very similar results to truth
 - Single algorithm that takes in whole detector at once

So what do we gain?

• A single algorithm is doing all of the clustering



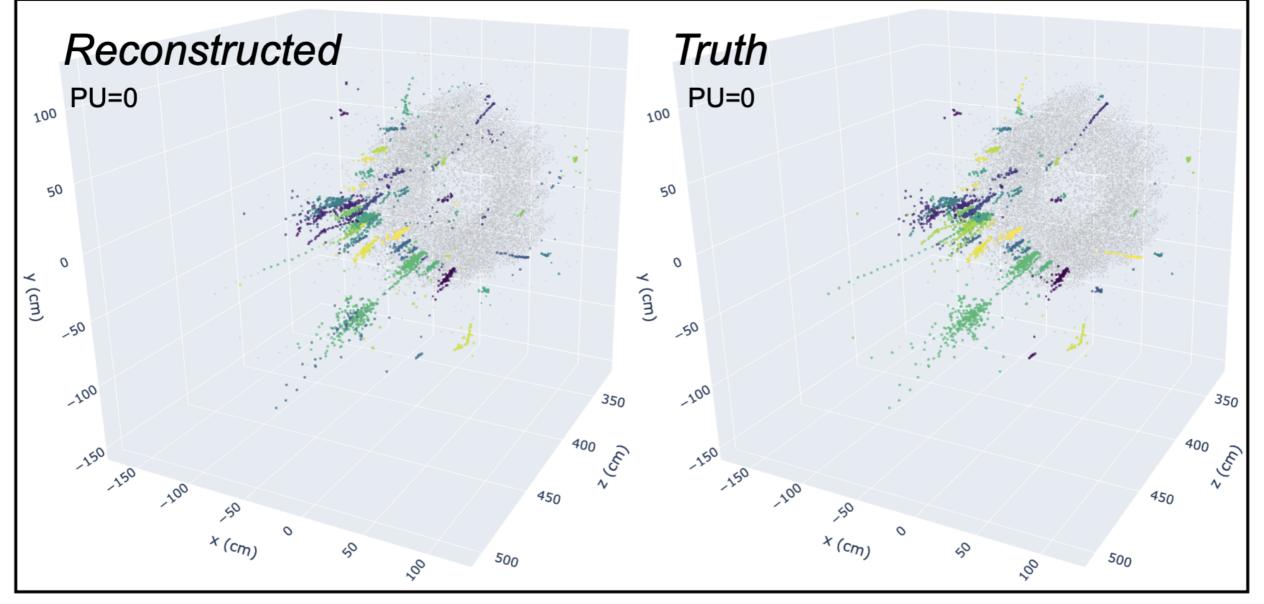
By embedding this in a neural network we can extend algo to include more info

This is 1st algorithm to cluster with depth info

- Moreover this algorithm can now look at whole event to perform clustering
 - Awarness of the event can allow for dynamic thresholds/interpretations
- Finally, this algorithm is highly parallelize \rightarrow Can Run it Fast!

A more Extreme Example

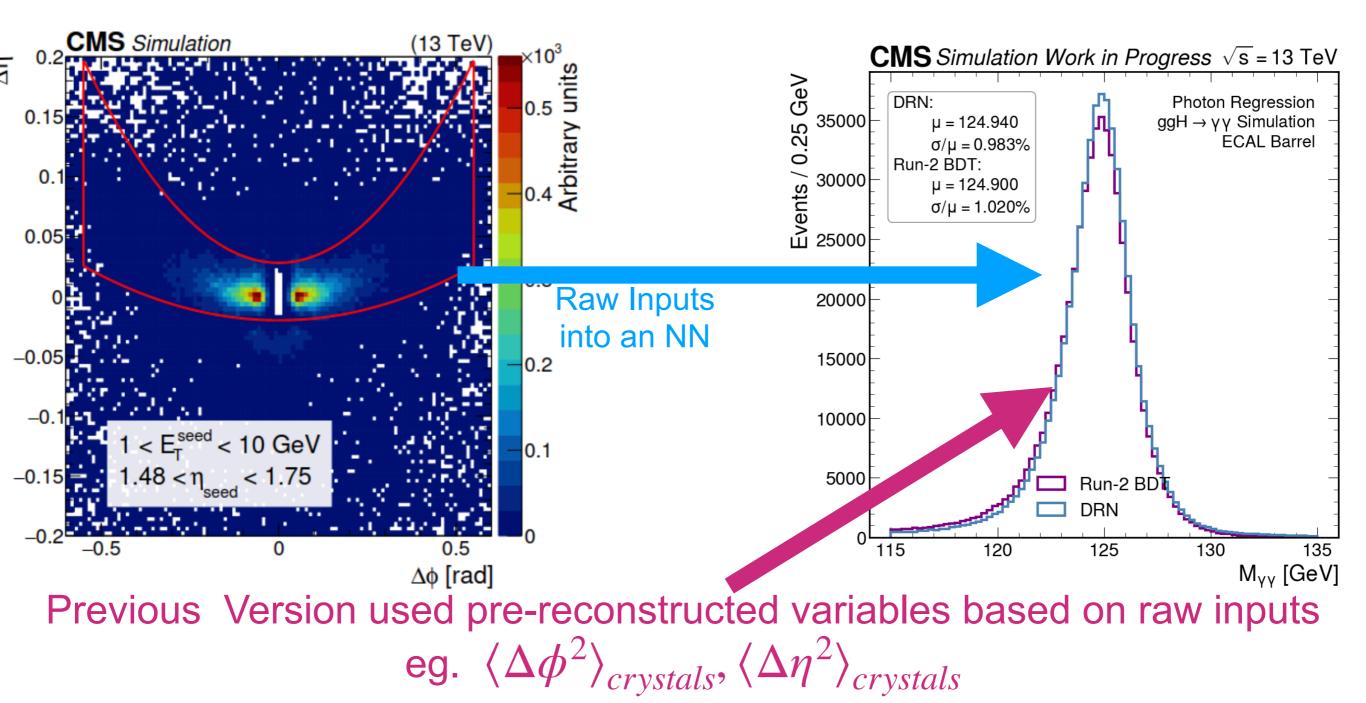
CMS Simulation Preliminary



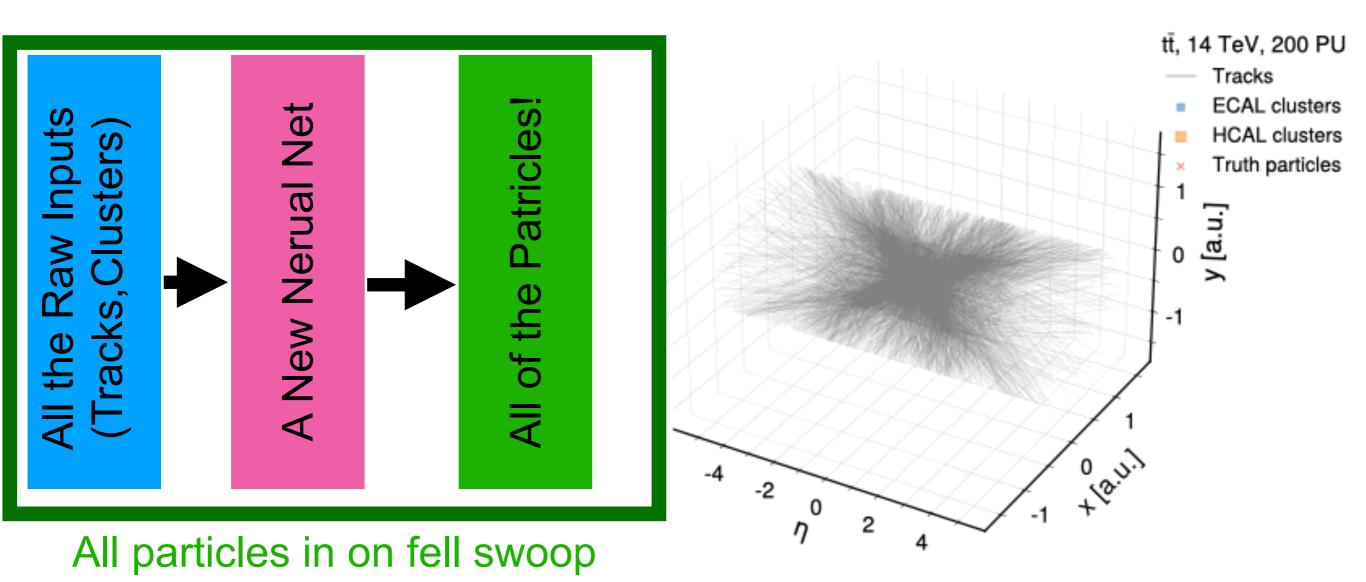
• Algorithm effective a reconstructing new complex topologies

Another Example

- Electron and Photon energy regression with an NN
 - Raw inputs to make an NN gives significant improvements

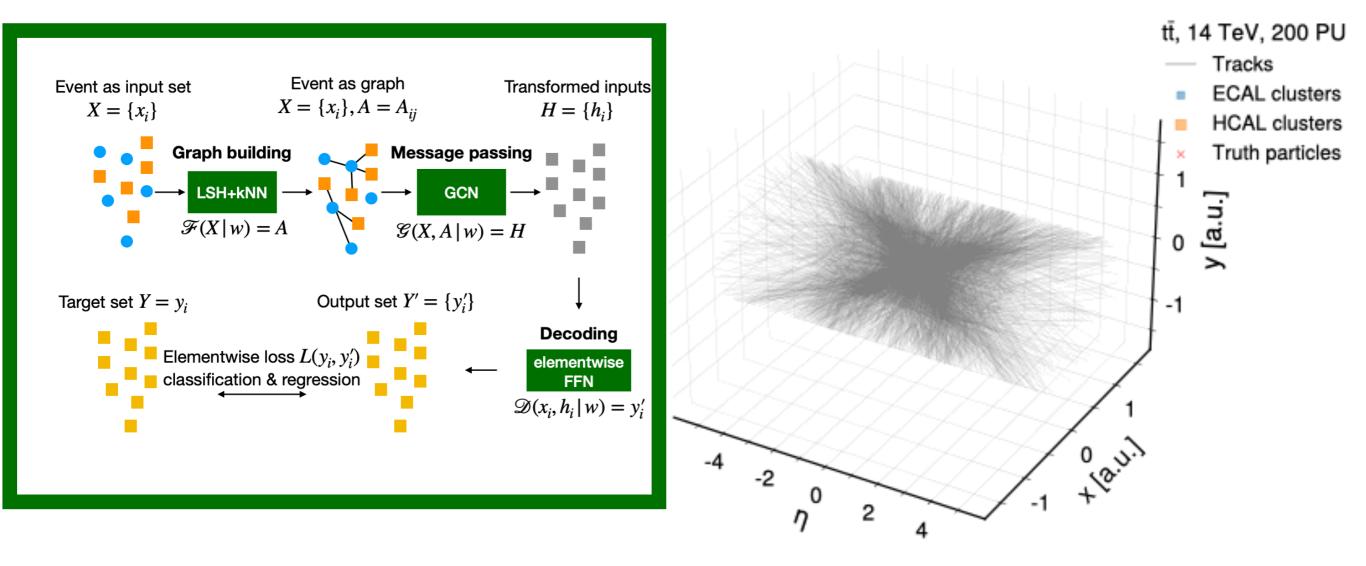


Success of Deep Learning



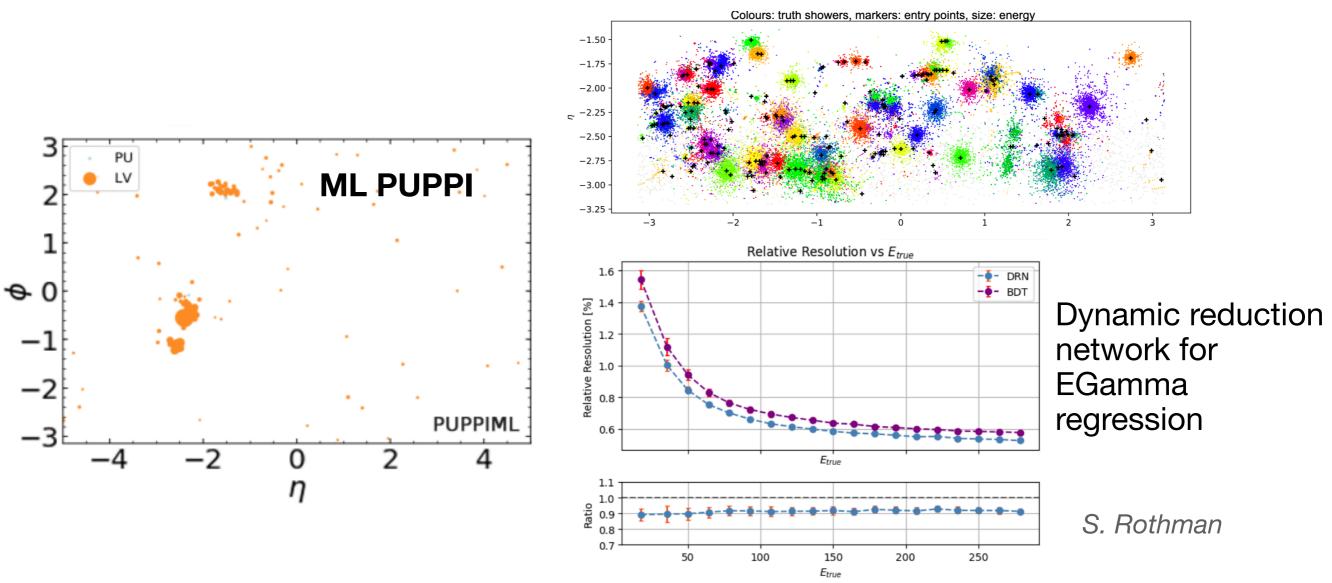
- First ideas of full particle based reconstruction are emerging
- Tools are emerging to do particle reconstructeion in one go arxiv:2101.08578

Success of Deep Learning



- First ideas of full particle based reconstruction are emerging
- LHC is a great place for DL because we have fantastic simulation arxiv:2101.08578

Success of Deep Learning

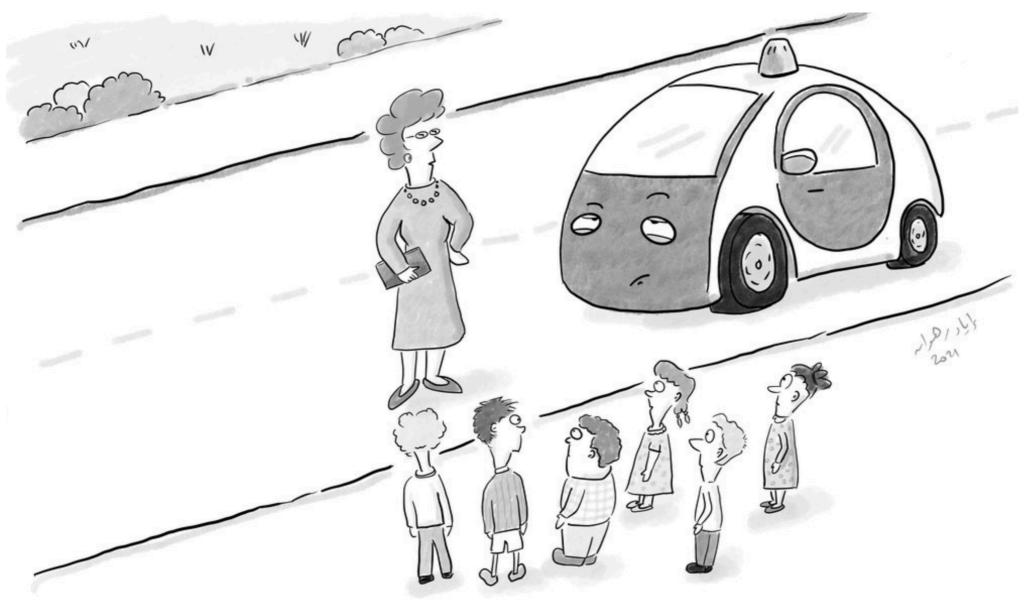


Clustering: Graph NNs for HGCAL

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- Networks are emerging to do calorimeter clustering
- Additionally networks are emerging to identify all objects

Taking a Leap of Faith



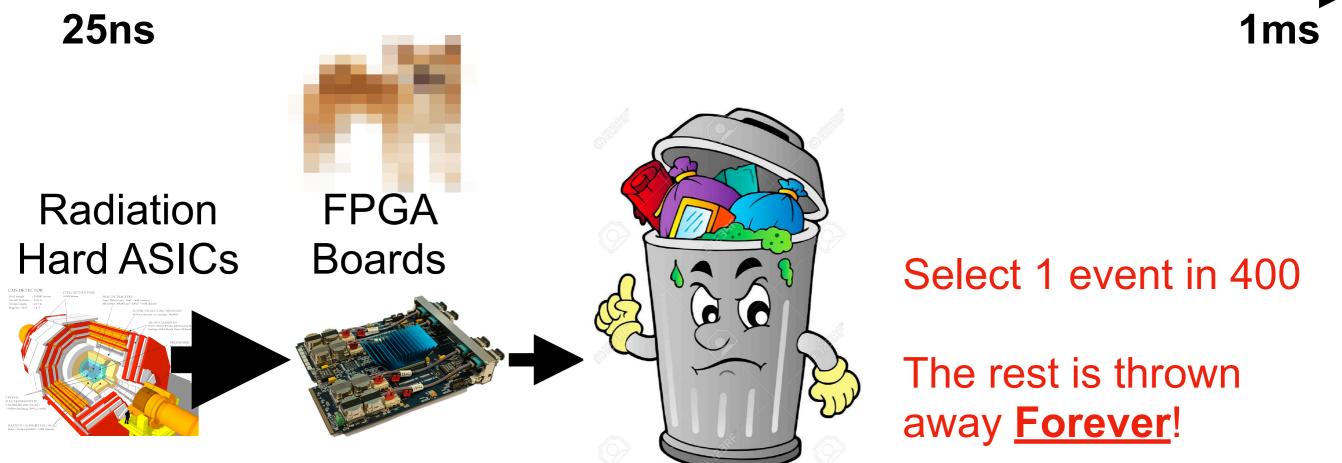
"Remember kids, you should <u>never</u> look before you cross, because driverless cars will always stop for you!"

Can we really trust AI to work from scratch well? always?



and Thinking Fast! (NN Inference)

40 MHz Spanning Frequencies



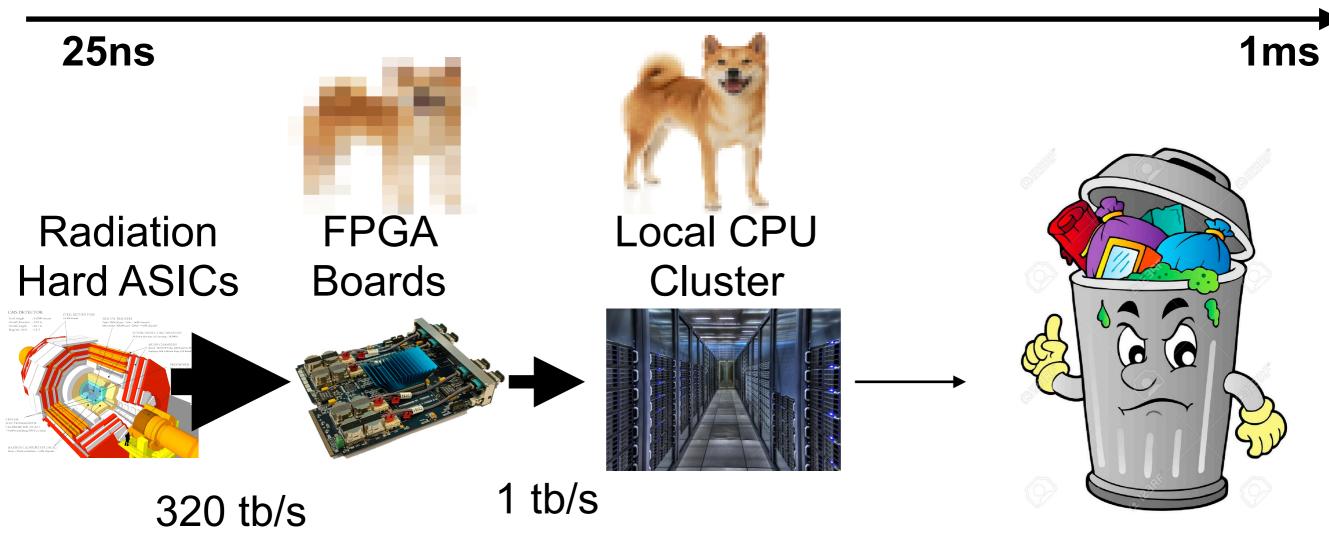
320 tb/s

Fast 40 MHz Collisions 10 µs window

L1Trigger

Spanning Frequencies 1 kHz



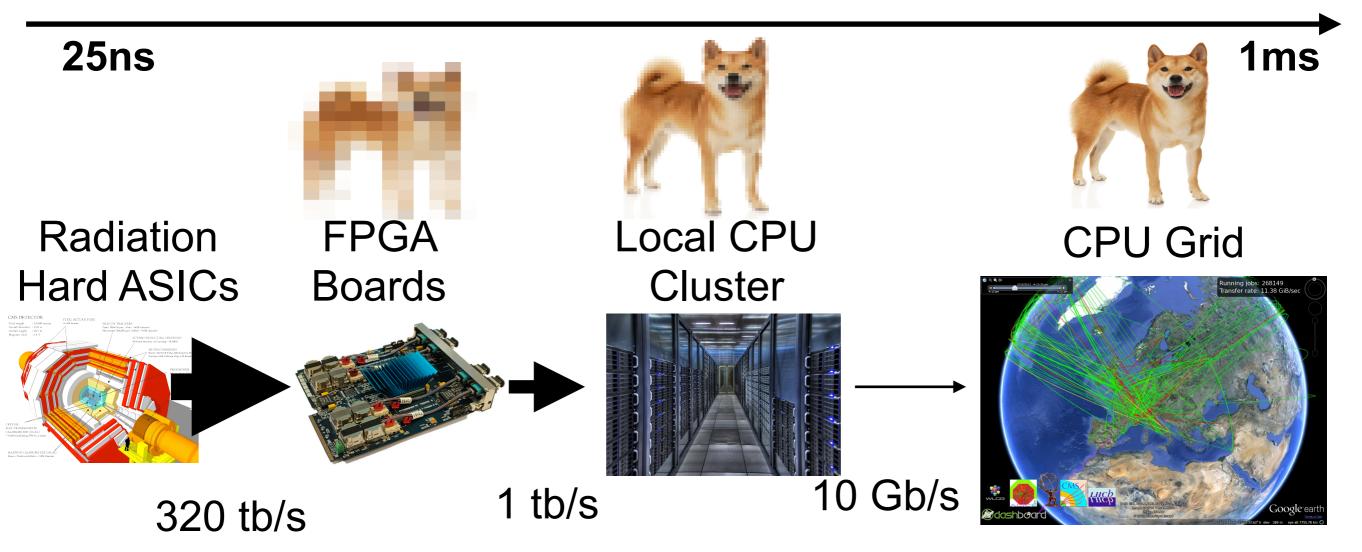


Fast 10 µs window L1Trigger

Intermediate 40 MHz Collisions 100 kHz Collisions <500 ms window **High Level Trigger**

Select 1 in 100

Spanning Frequencies 1 kHz



Fast 10 µs window L1Trigger

40 MHz

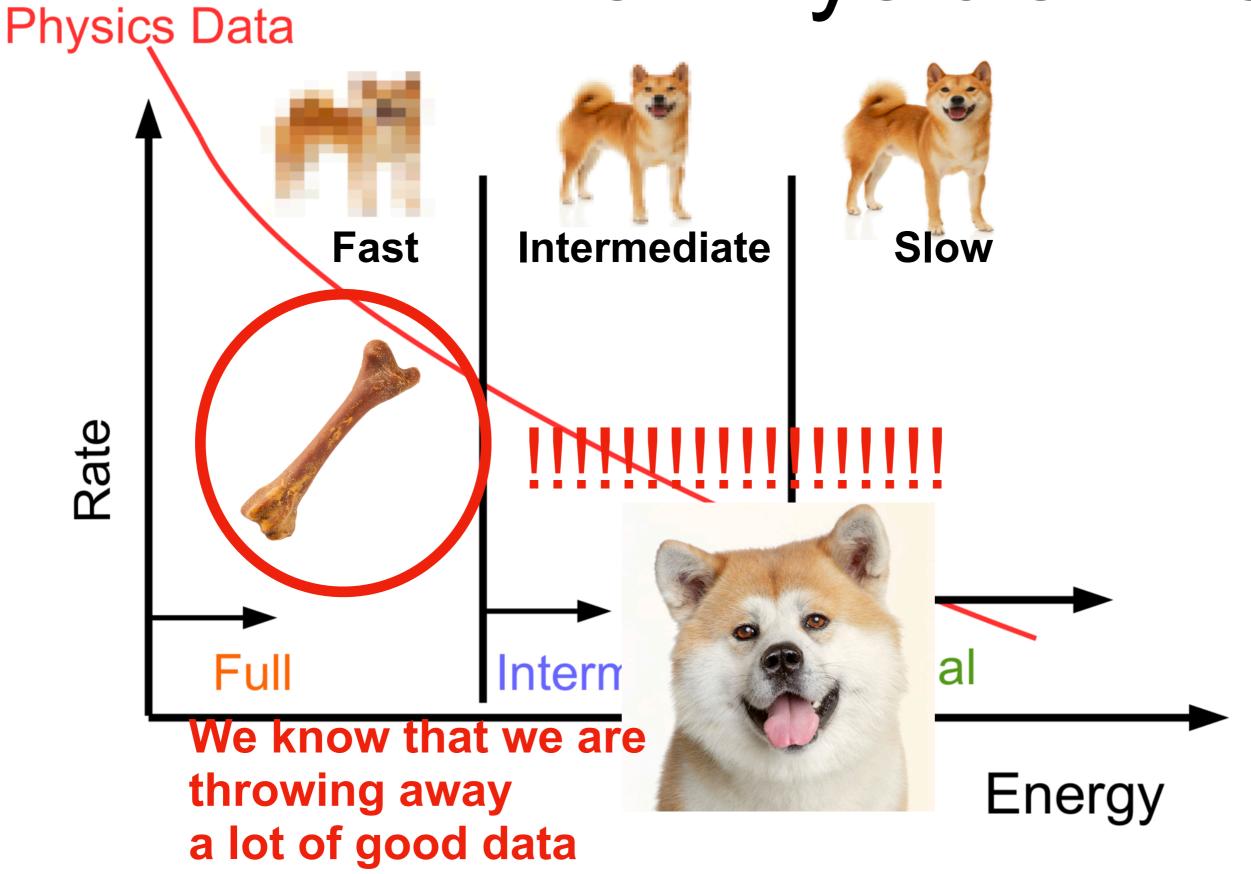
Intermediate 40 MHz Collisions 100 kHz Collisions <500 ms window High Level Trigger

Slow 1 kHz Collisions 10 s window **Offline Cluster**

The Physicist View **Physics Data** Intermediate Fast Slow Rate Keep All data Keep **Final** Full Intermediate

Energy

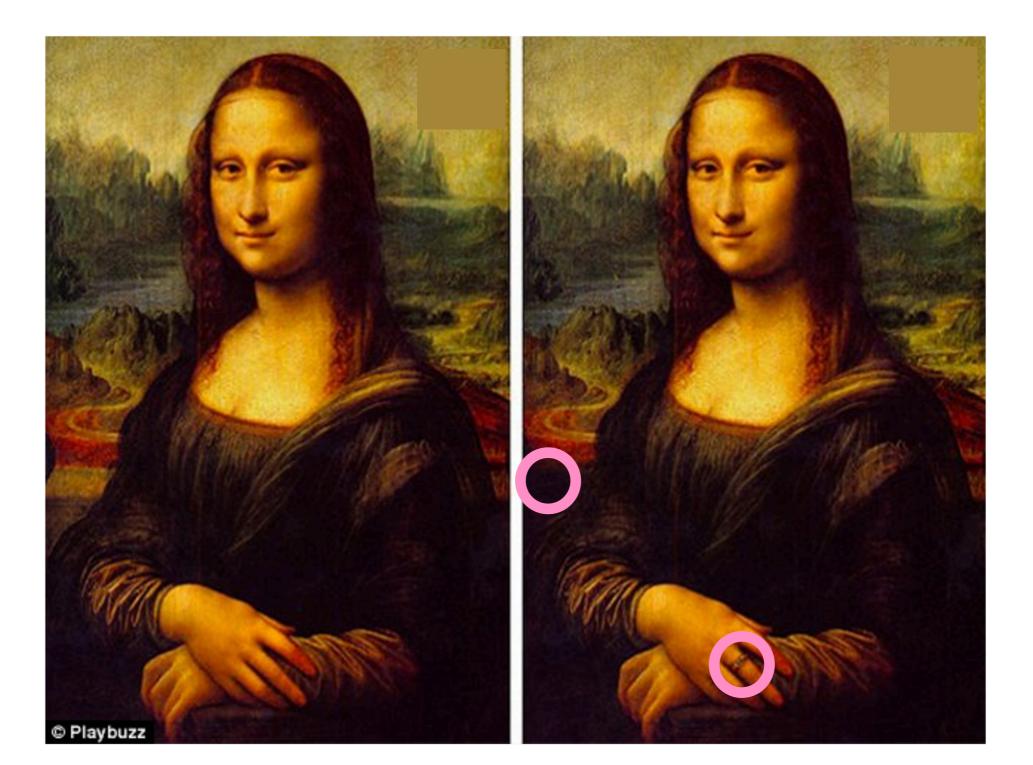
The Physicist View



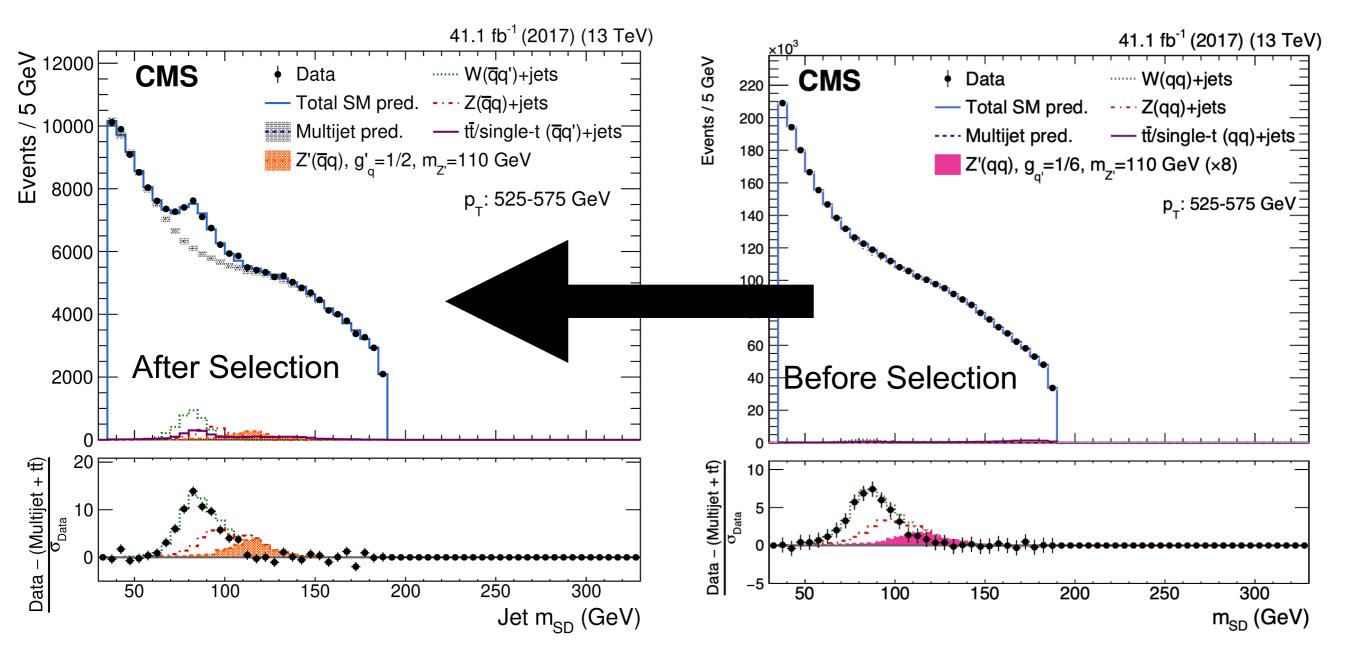
What is different w/Left and Right?



The Need for Subtlety

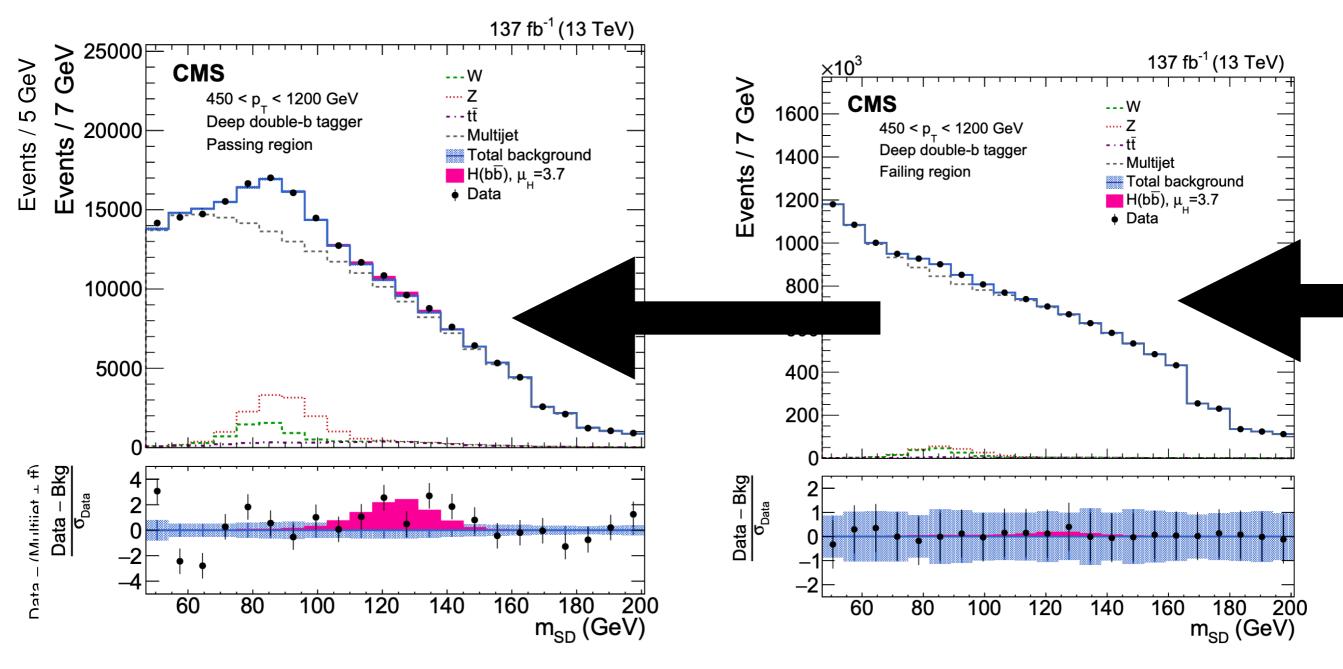


Looking for small signals



There is still a wealth of unexplored physics at the LHC Its just a bit harder to find

Looking for small signals

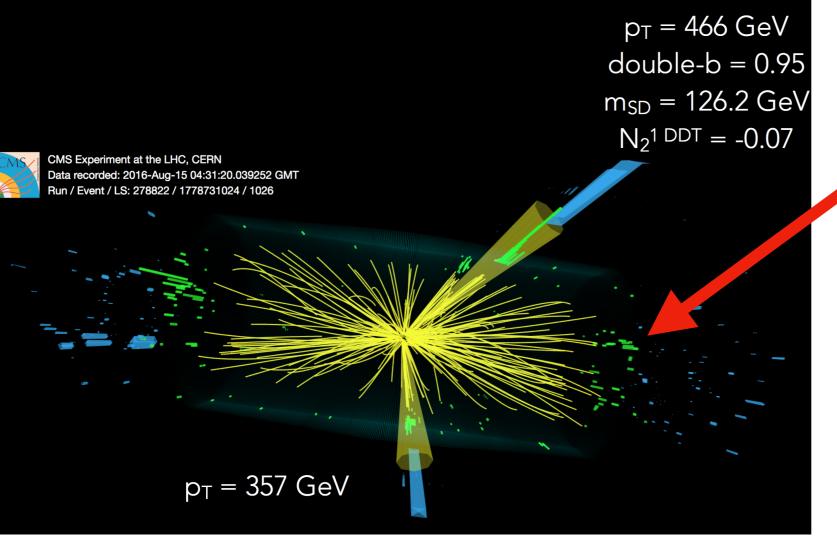


There is still a wealth of unexplored physics at the LHC Its just a bit harder to find



Hidden gems?

There is a plethora of physics that we throw out



Higgs boson right on the cusp of being thrown out

The dream

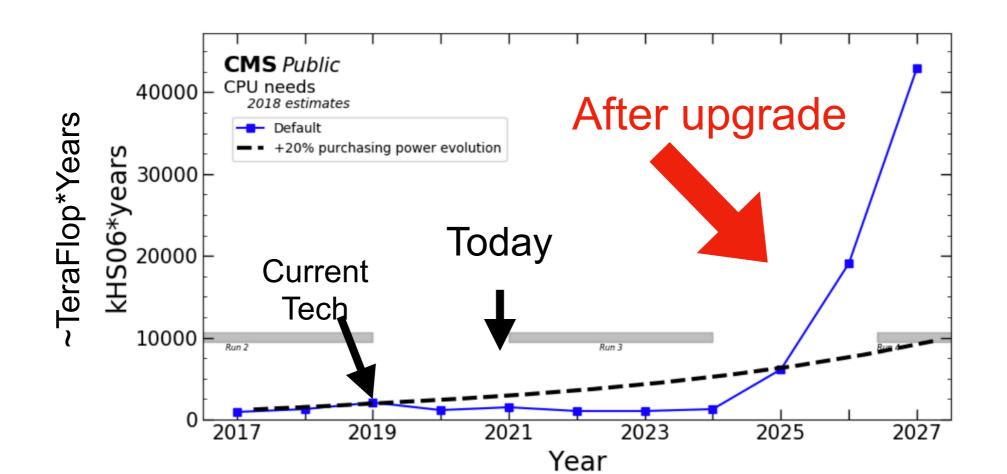
- At the moment:
 - We only get a full data of one in 40,000 collisions
 - There is interesting physics that we have to throw away

- We would like to analyze every collision at the LHC
 - To deal with this we need to increase our throughput
 - Ultimately this means going to 100s of Tb/s

The Challenge

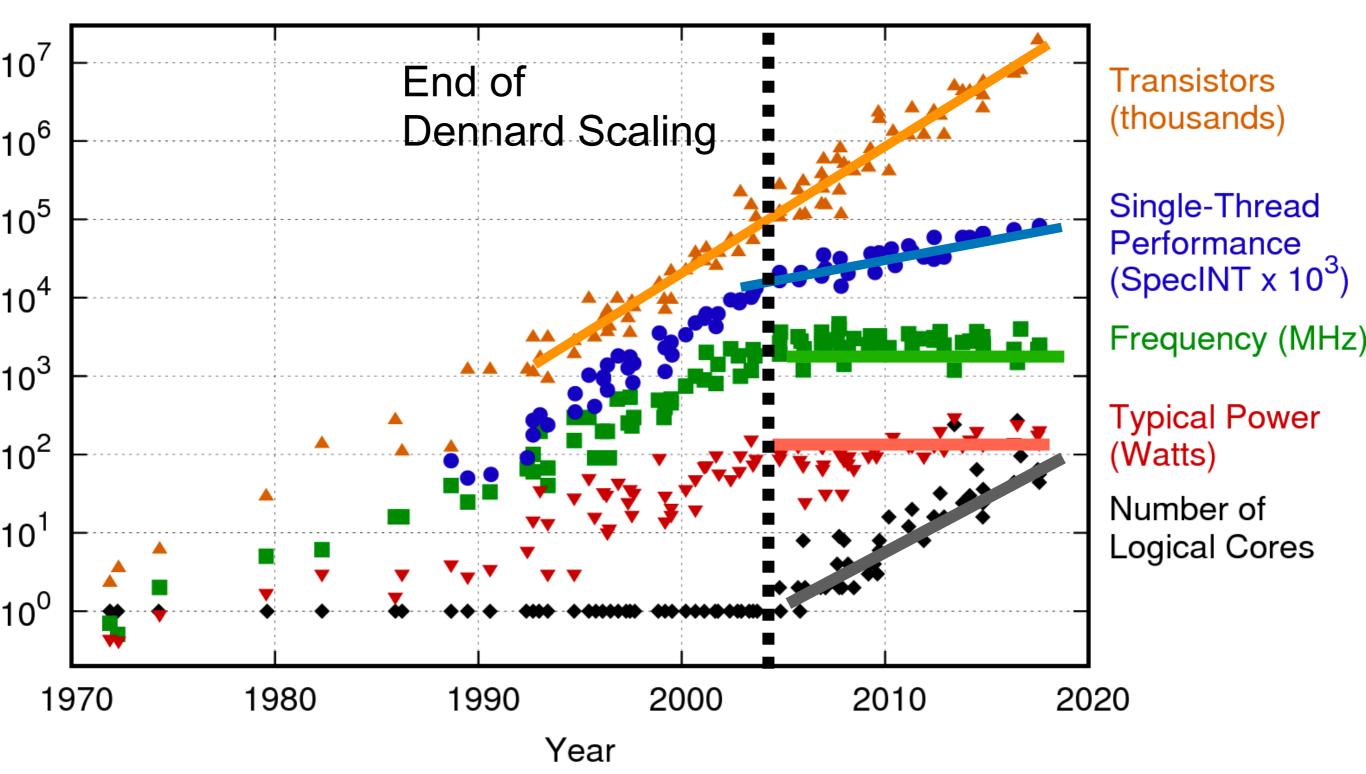
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- To deal with the upgraded LHC intensity
- To preserve current physics we are upgrading the system
 - Our event size will have to be 10x larger
 - We will have to take data at 5 times the current rate



The Crises

42 Years of Microprocessor Trend Data



Original data up to the year 2010 collected and plotted by M. Horowitz, F. Labonte, O. Shacham, K. Olukotun, L. Hammond, and C. Batten New plot and data collected for 2010-2017 by K. Rupp

Processor Technology

Will we be able to handle the future upgrades?



Modern Processing

- Your standard CPU with split all up (you know this)
- GPU :

Multi cores CPU:

- Effectively many multi-cores with simplified instructions
 - Many cores in parallel (O(500)) with addition and mult.
- Power hungry (better, but not too different from a CPU)
- FPGA:
 - Pre-programed the chip to do the operation you want
 - Every switch and multiplier assigned to a fixed patter
 - Energy efficient and hyper parallel (5000 parallel)
- ASIC:
 - FPGA but with inability to be programmed

Processing Tech





1 player





A few at same time

A soloist A group

Whatever Main theme and some freedom to improv



The whole chip

An orchestra

Score has to be known perfectly beforehand

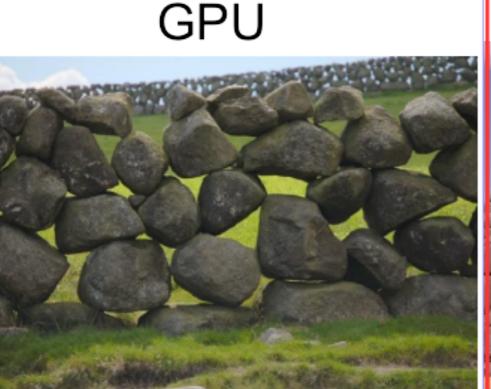
Processing Tech

Past Present

CPU

Past







Speed: 1

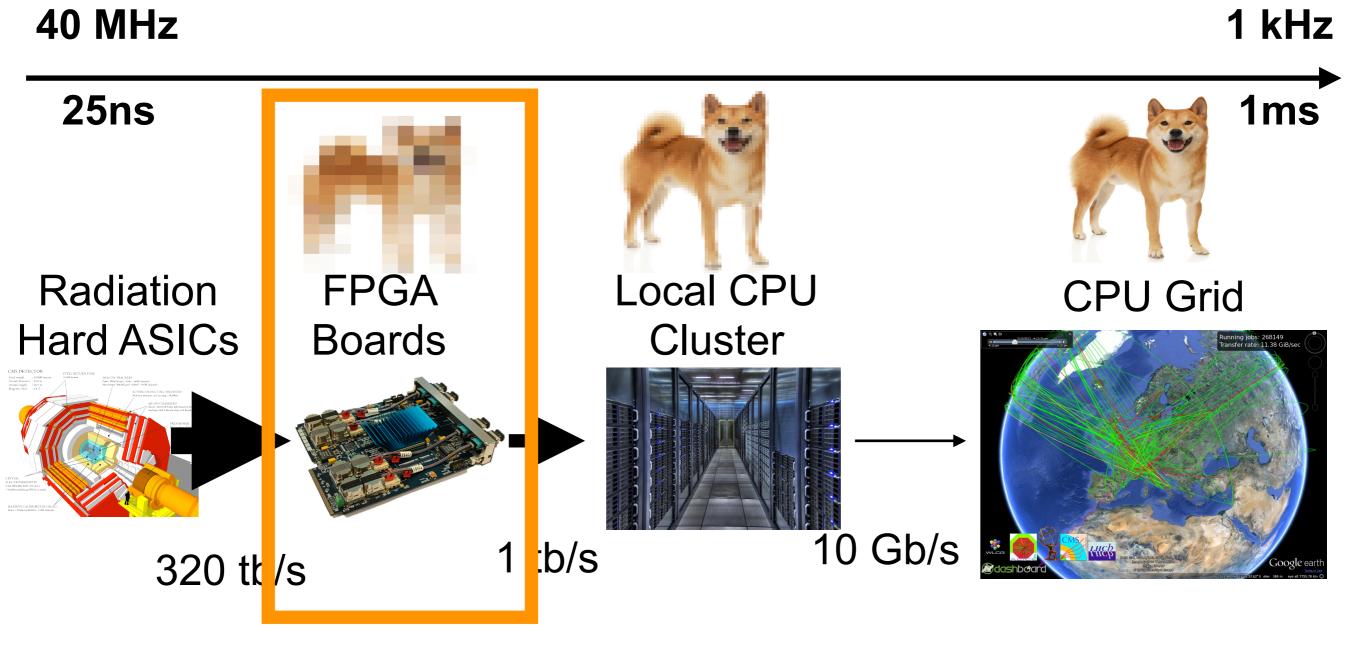
Speed: 20-50

Single complex operation per clock

Multiple simpler operations in parallel commonly available

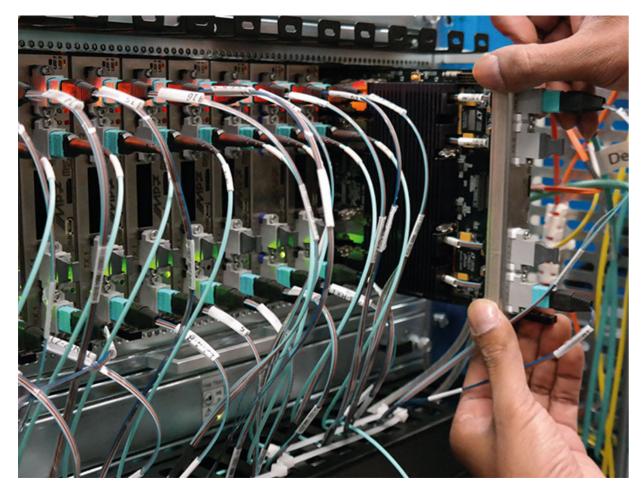
Speed: 200-1000

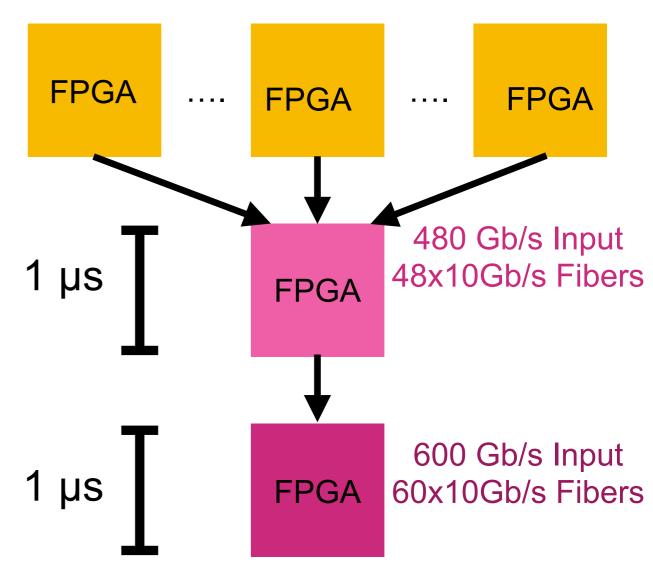
Efficient packing of operations highly parallelized (low power)

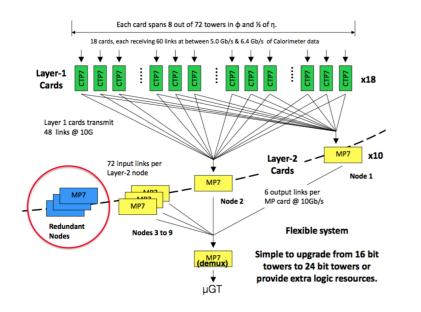


Real-time AI on every LHC Collisions To process this data we need Deep Neural Networks on FPGAs in Nanoseconds!

Current (Old) Tech







Current System is roughly 100 Virtex7 FPGAs interconnected with Fibers

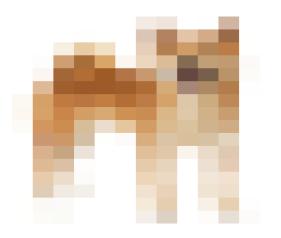


Algo

Current Algos

Simultaneously scan over calorimeter region a very simple algorithm

FPGA is essential to parallelize & deal w/ enormous bandwidth



Region

Algorithms have traditionally been simple due to the size of the FPGAs + RTL code

Region

Phi

←iEta→ +

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 25 27
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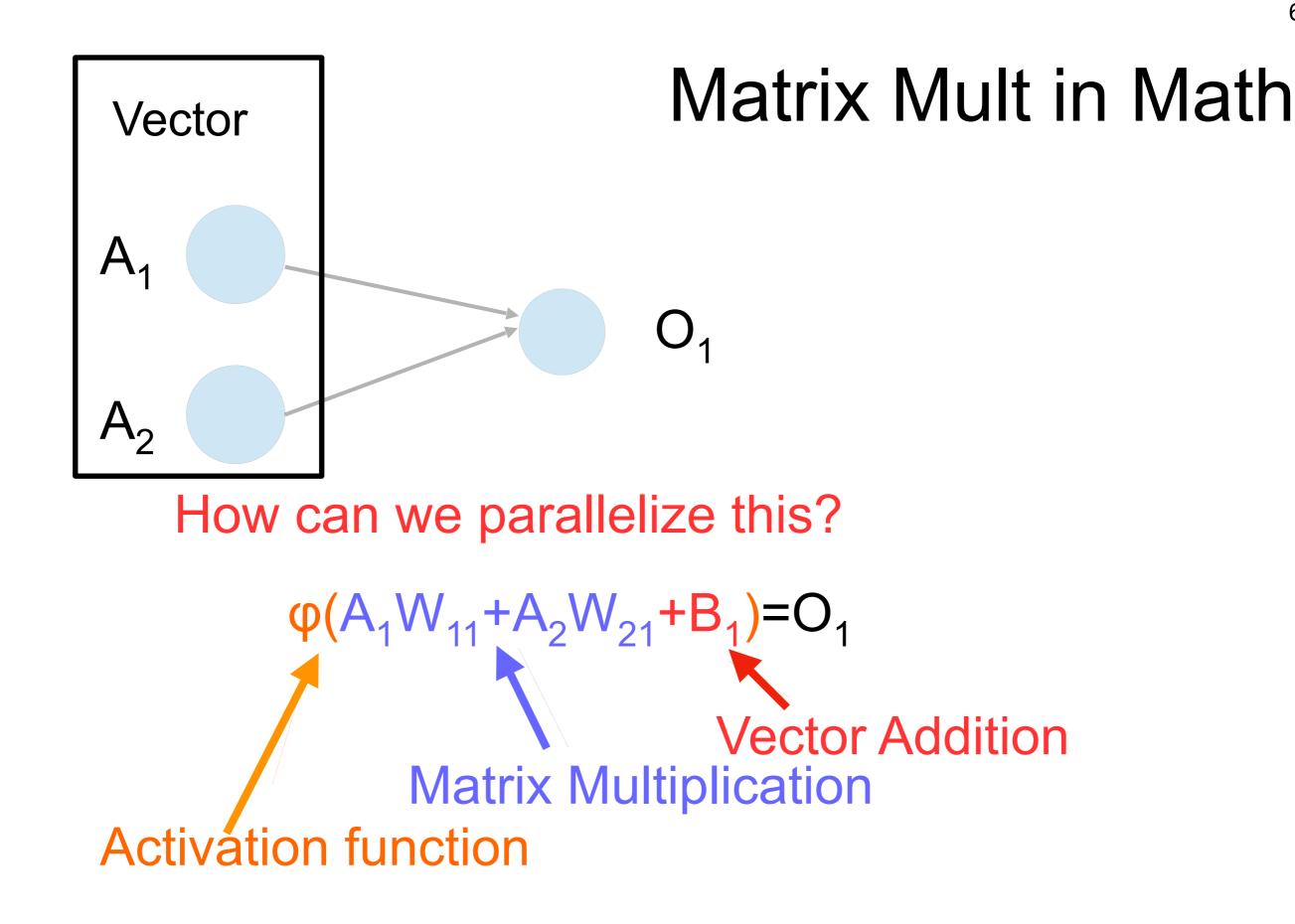
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Real-Time Deep Learning

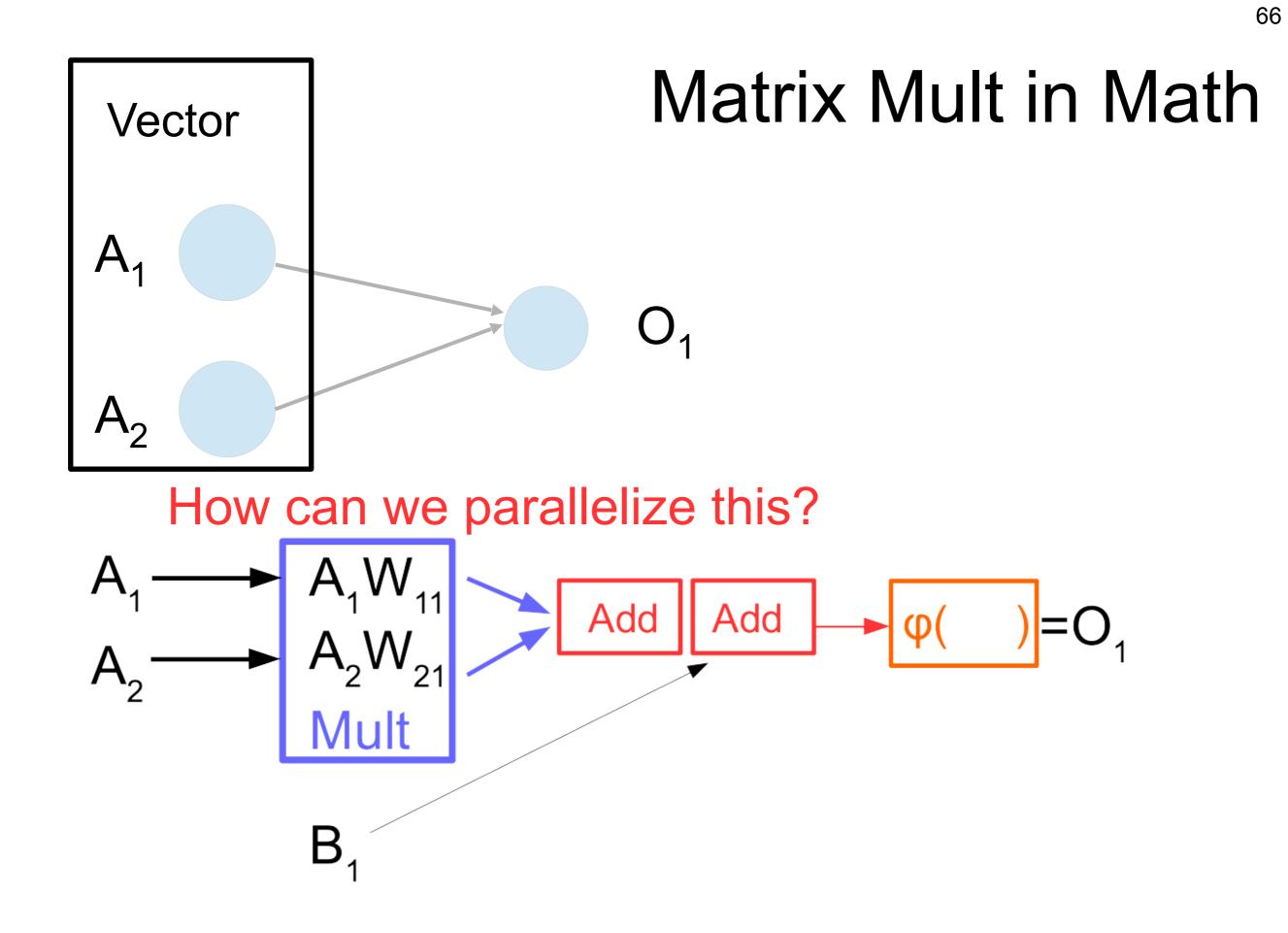
64

- We only have 1µs or less for the inference time
 - We need to run the networks at a rate > 40 MHz (II < 25ns)
 - Forced us to re-think DNN hardware implementations
- This work led us to the project:

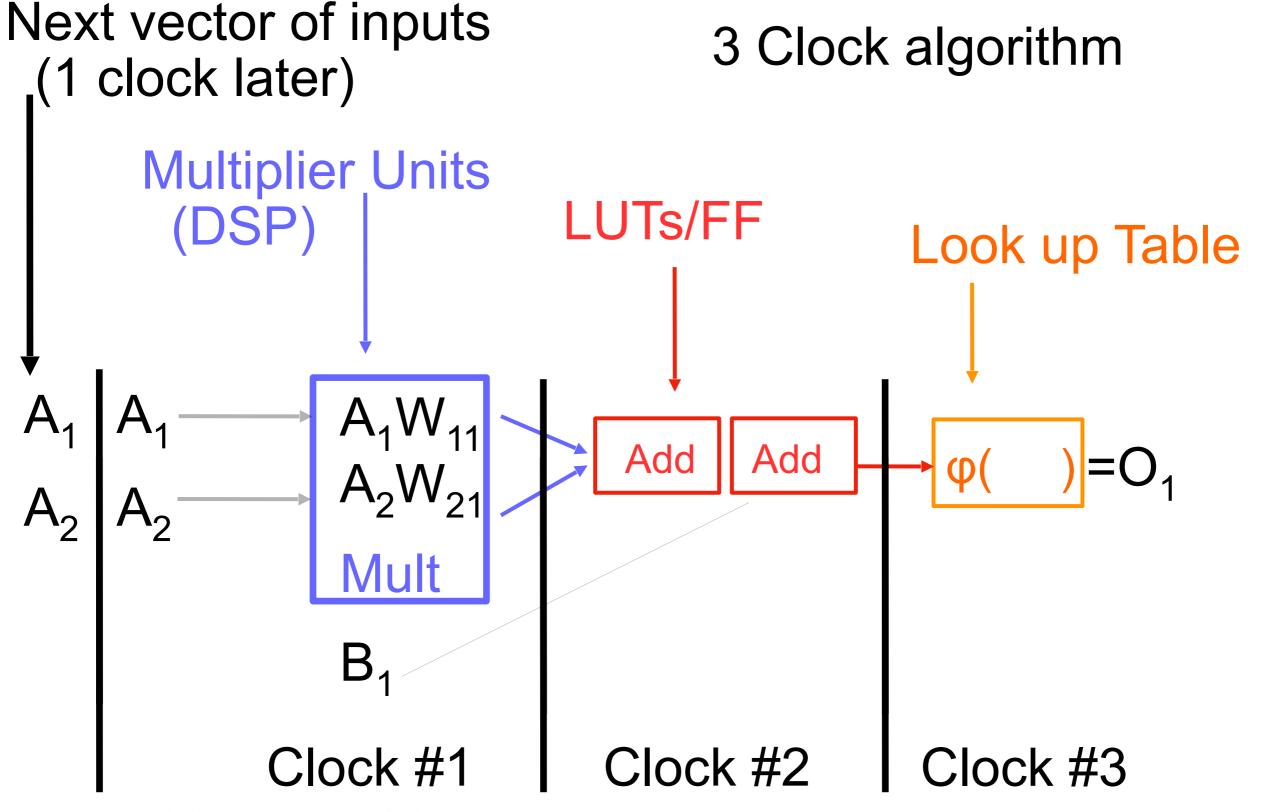




arxiv:1804.06913



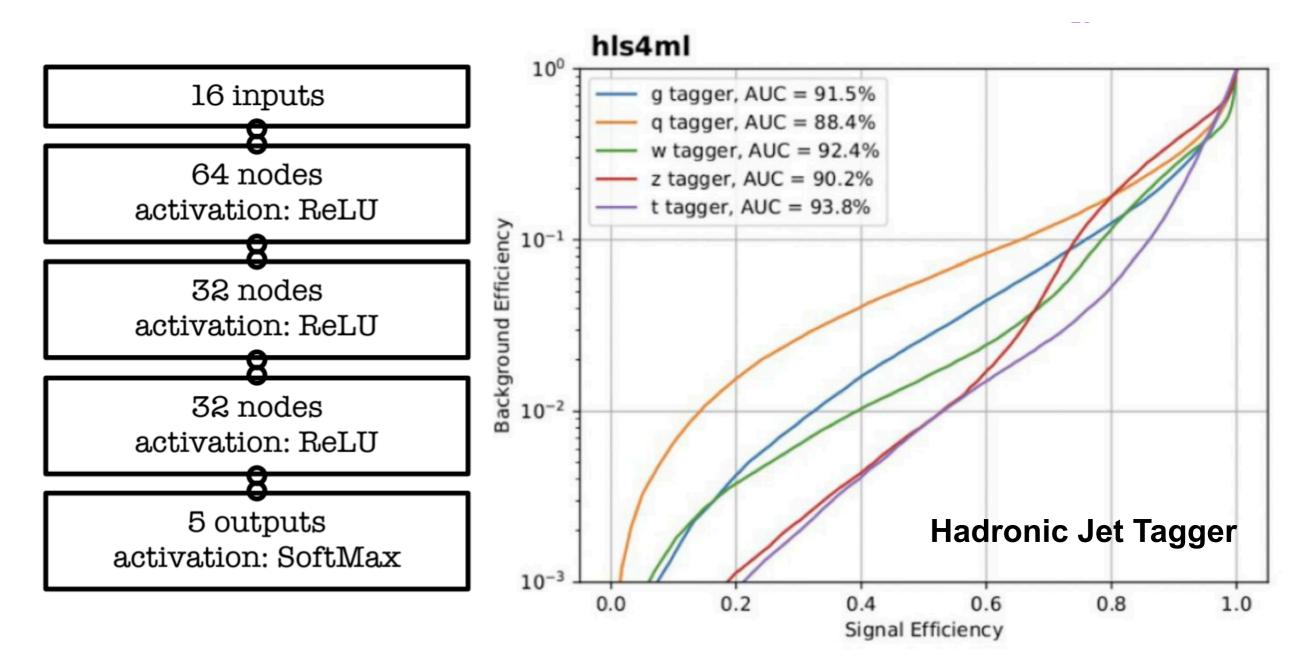
Matrix Mult in an FPGA



Results subject to precision outputs

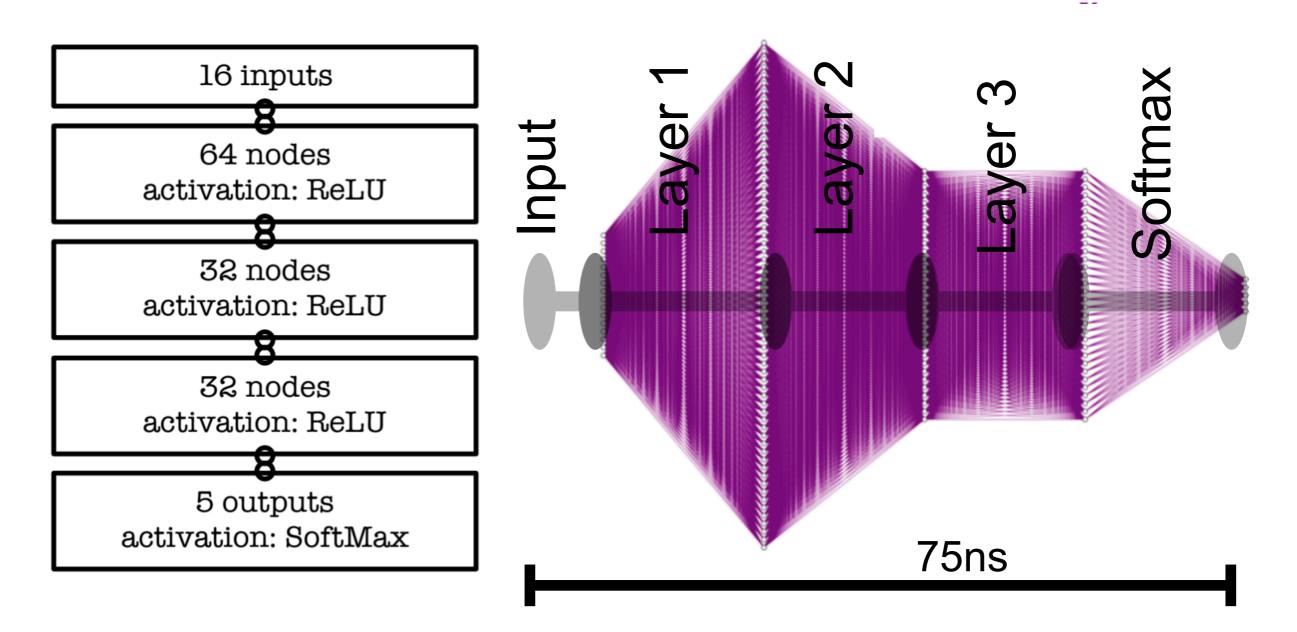
A full benchmark example

68



This network has an II of 1 clock, being run constantly It has 4.3k weights and 4.3k DSPs at II=1

A full benchmark example



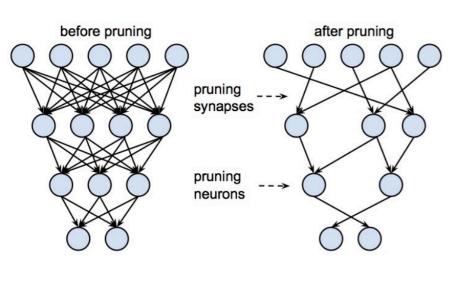
This network has an II of 1 clock, being run constantly It has 4.3k weights and 4.3k DSPs at II=1

How can we reduce resources?

Focus on 3 ways to cut down resources

Is our algorithm overly complex?

Algorithmic Compression



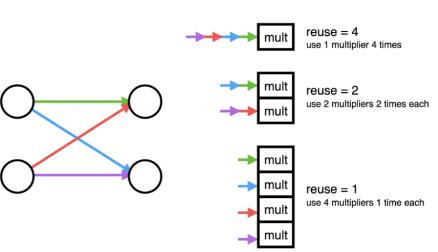
Are we too precise?

Quantization

ap_fixed<width,integer>
0101.1011101010
integer fractional
width

Does it really need to be this fast?

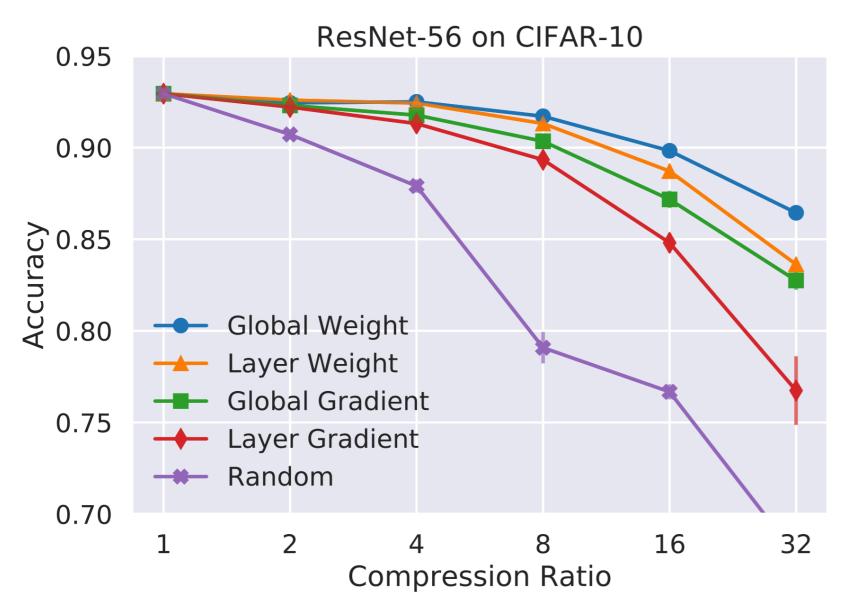
Reuse Factor



arxiv:1804.06913

Algorithm Compression

- Compression is a critical aspect to reduce ML
- A suprising amount of weights in an NN are irrelevant

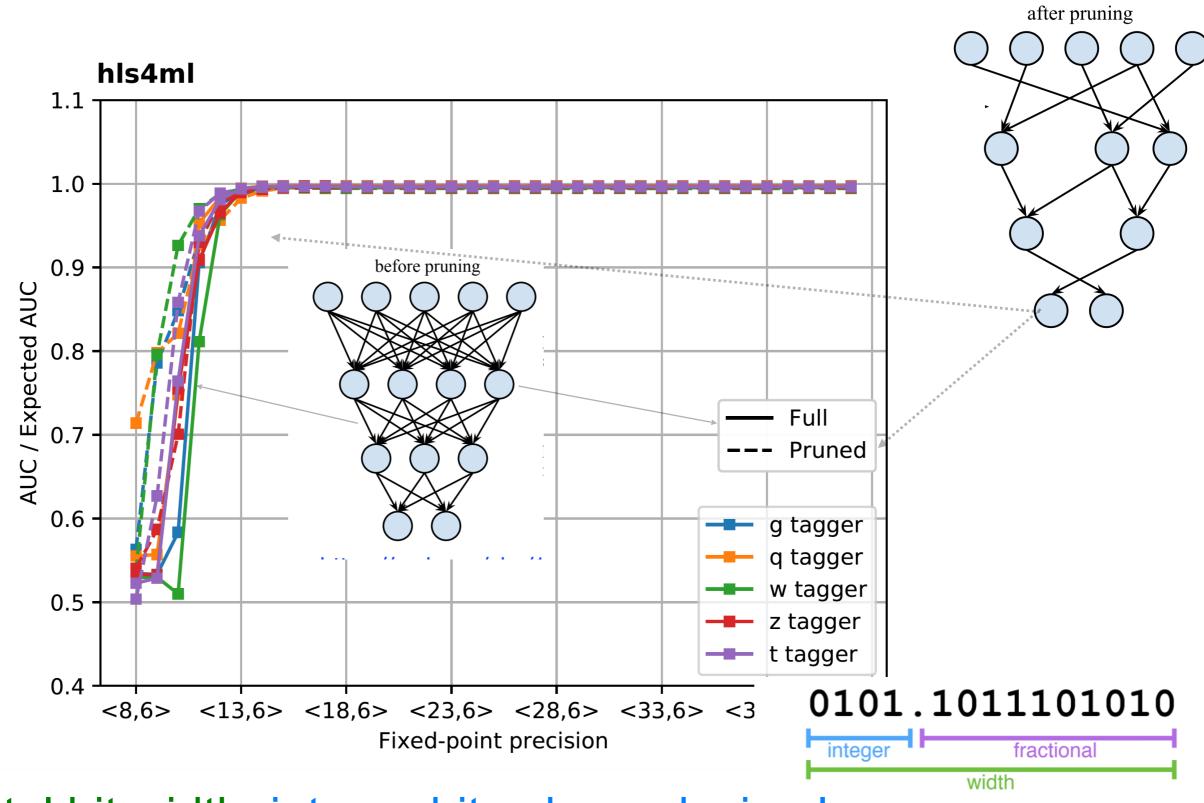


Model	Mult(DSP)	LUTs
Before	15%	13%
After	0%	1%

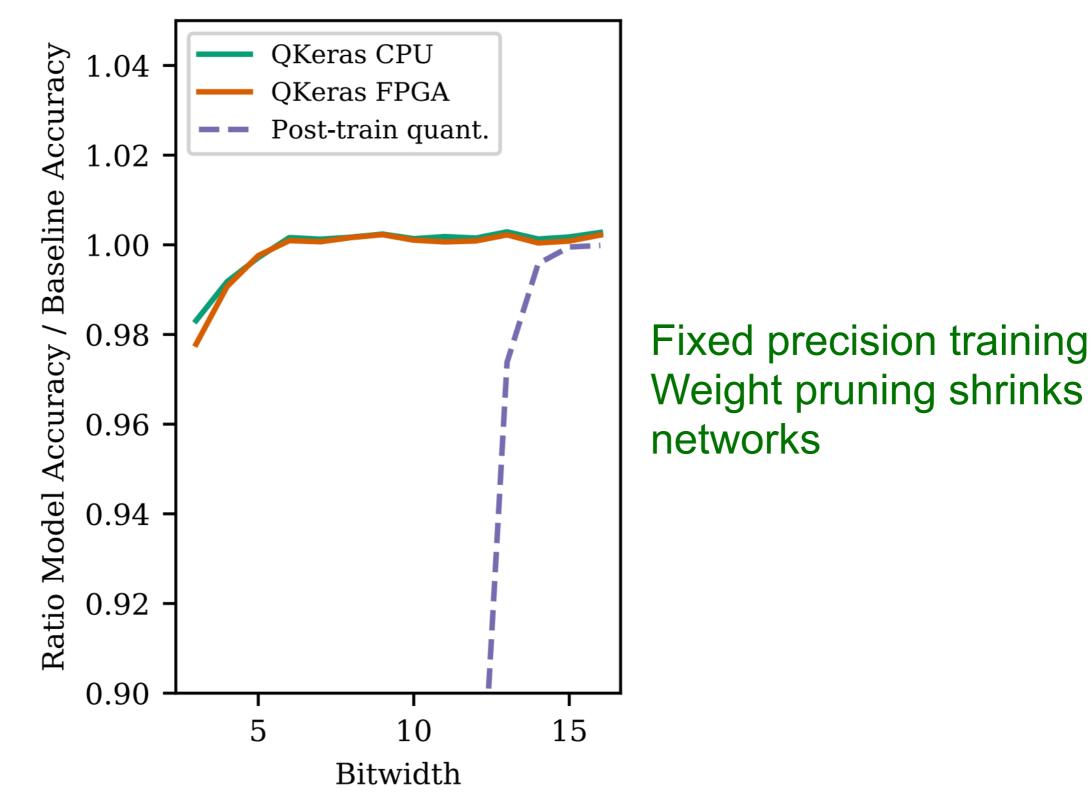
Same Performance Smaller Latency (50→40ns) Dramatic Compression

arxiv:1804.06913

Quantization

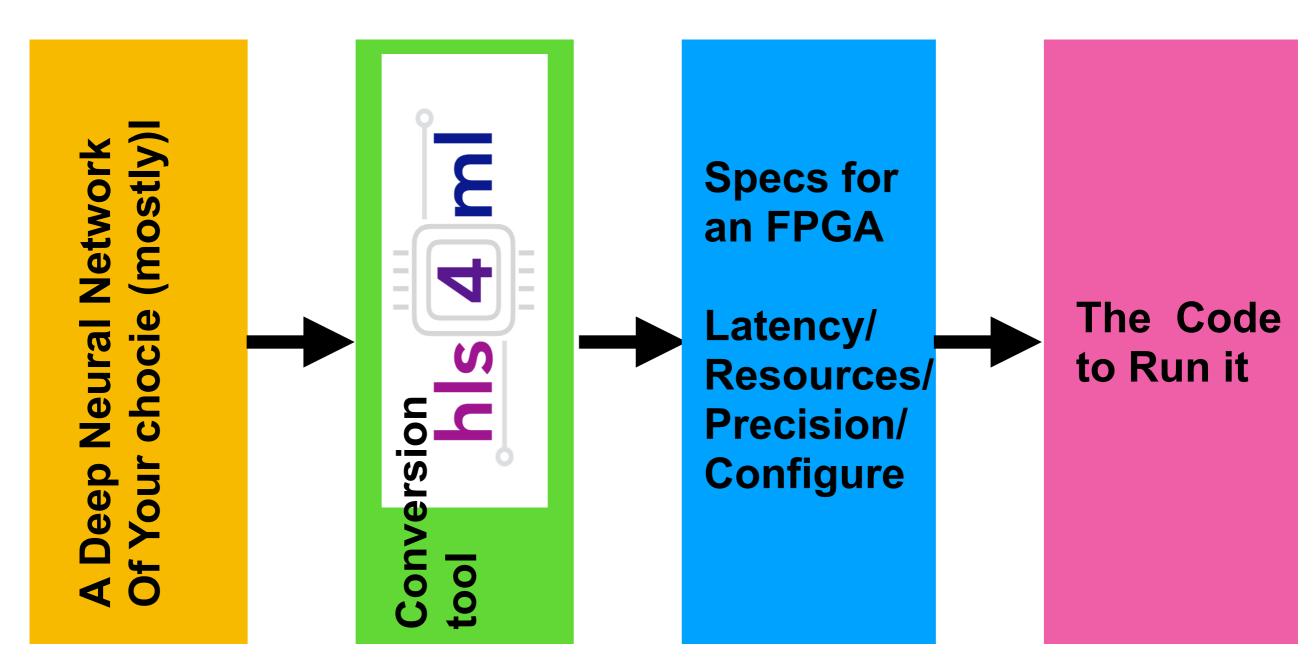


Algorithm Compression



arxiv:2103.05579

A Compiler than can do it

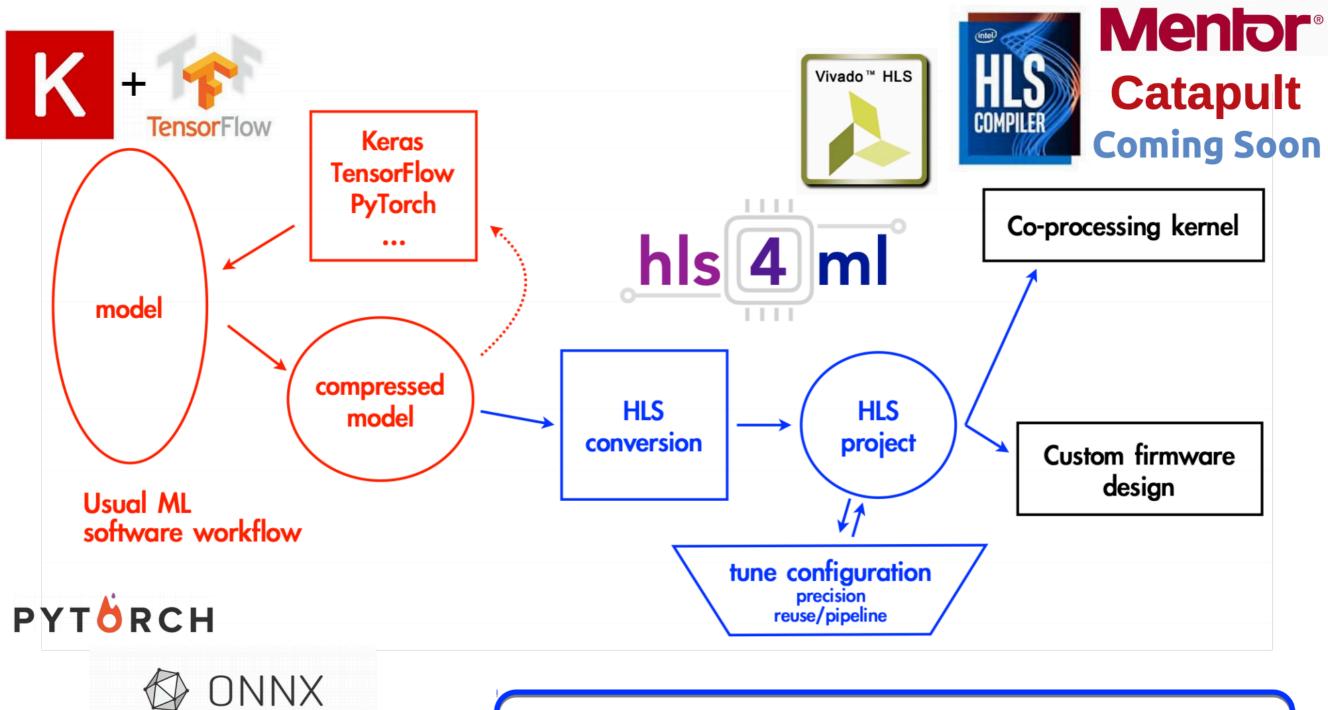


There are now a few tools See Tae Min's Talk for another tool!

https://fastmachinelearning.org/hls4ml/

A Compiler than can do it

python keras-to-hls.py -c keras-config.yml



https://fastmachinelearning.org/hls4ml/

Flexibility

- Many different types of collisions are analyzed at LHC
 - A diverse set of algorithms are required
 - There is no one size fits all NN that will solver our problems
- With HLS4ML we have continued to expand options
 - HLS has allowed for quick development

A	lgo	ritl	hm	S

MLPs arxiv:2003.06308 arxiv:2002.02534 arxiv:2008.03601 arxiv:2006.10159 RNNs(LSTM/GRU) Binary & Ternary NNs Graph NNs(MPNN/GravNet/GarNet) BDTs Not yet in official release

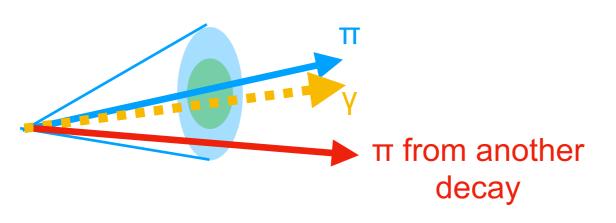
Backends

Xilinx Vitis HLS Intel HLS Quertus Mentor Catapult HLS Intel OneAPI

Not yet in official release

Example #1 Tau Tagging

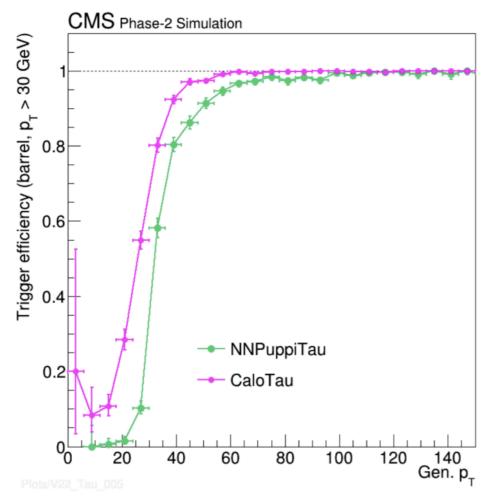
Tau Leptons have complex final states

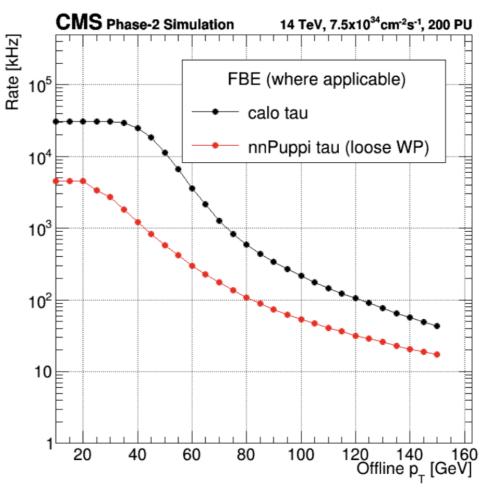


Tau Lepton can decay to as many as 10 different particles

Background can decay to many more

Neural Network has long been the algorithm of choice to identify Taus

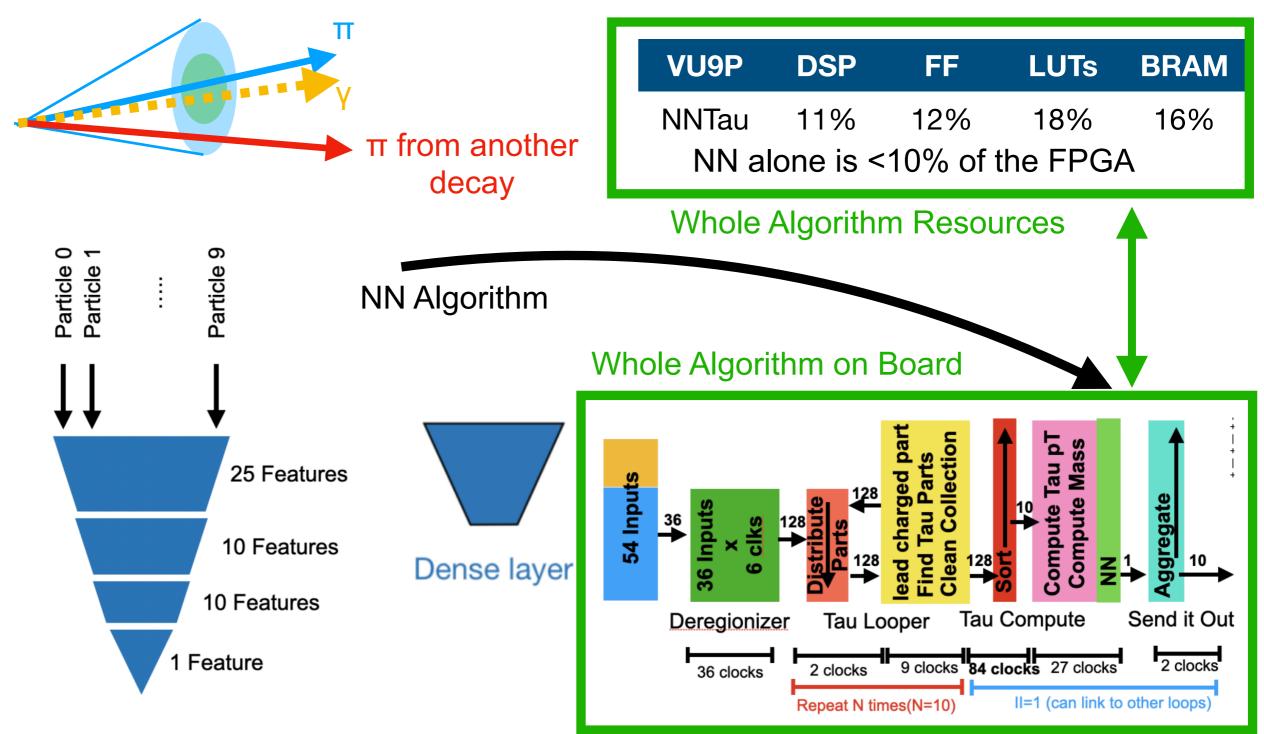




Example #1 Tau Tagging

Algorithm Takes 10 top particles in a cone and runs NN

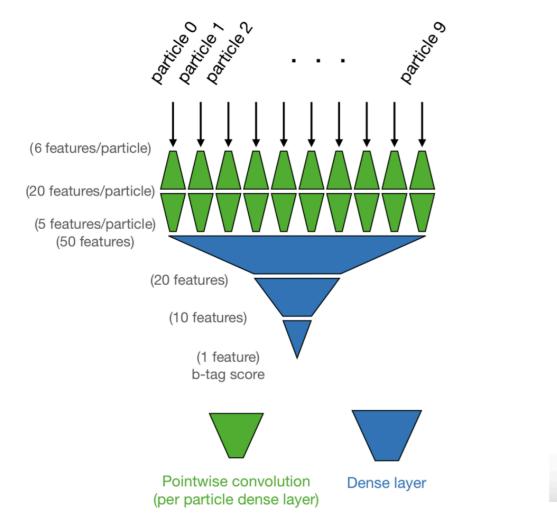
With HLS4ML we can run this algorithm in 70ns



Example #2 BTagging

In addition to taus B-tagging good ML candidate

Not obvious CMS Trigger vertex resolution is large

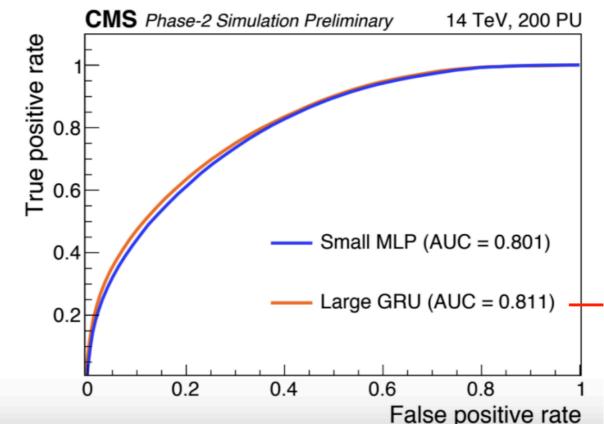


 π from another

decay

BJet is

displaced



Example #2 BTagging

In addition to taus B-tagging good ML candidate

π from another decay

Not obvious CMS Trigger vertex resolution is large

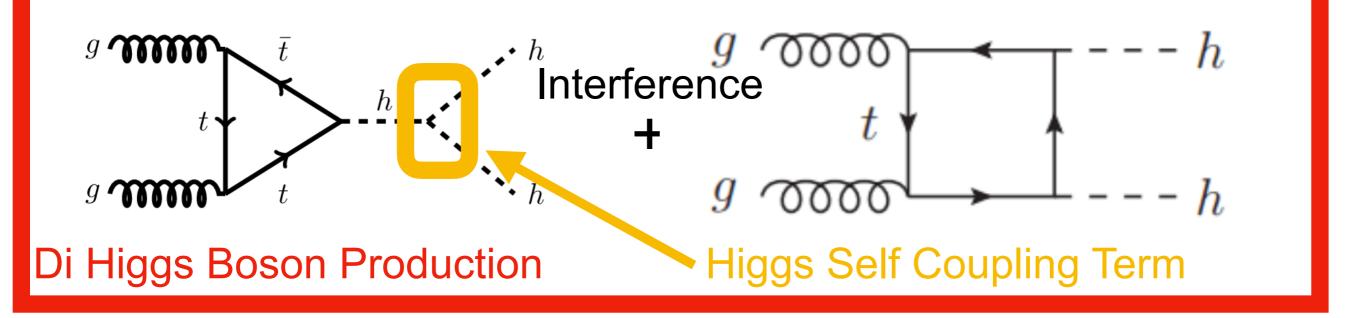
Resolution in Trigger is worse

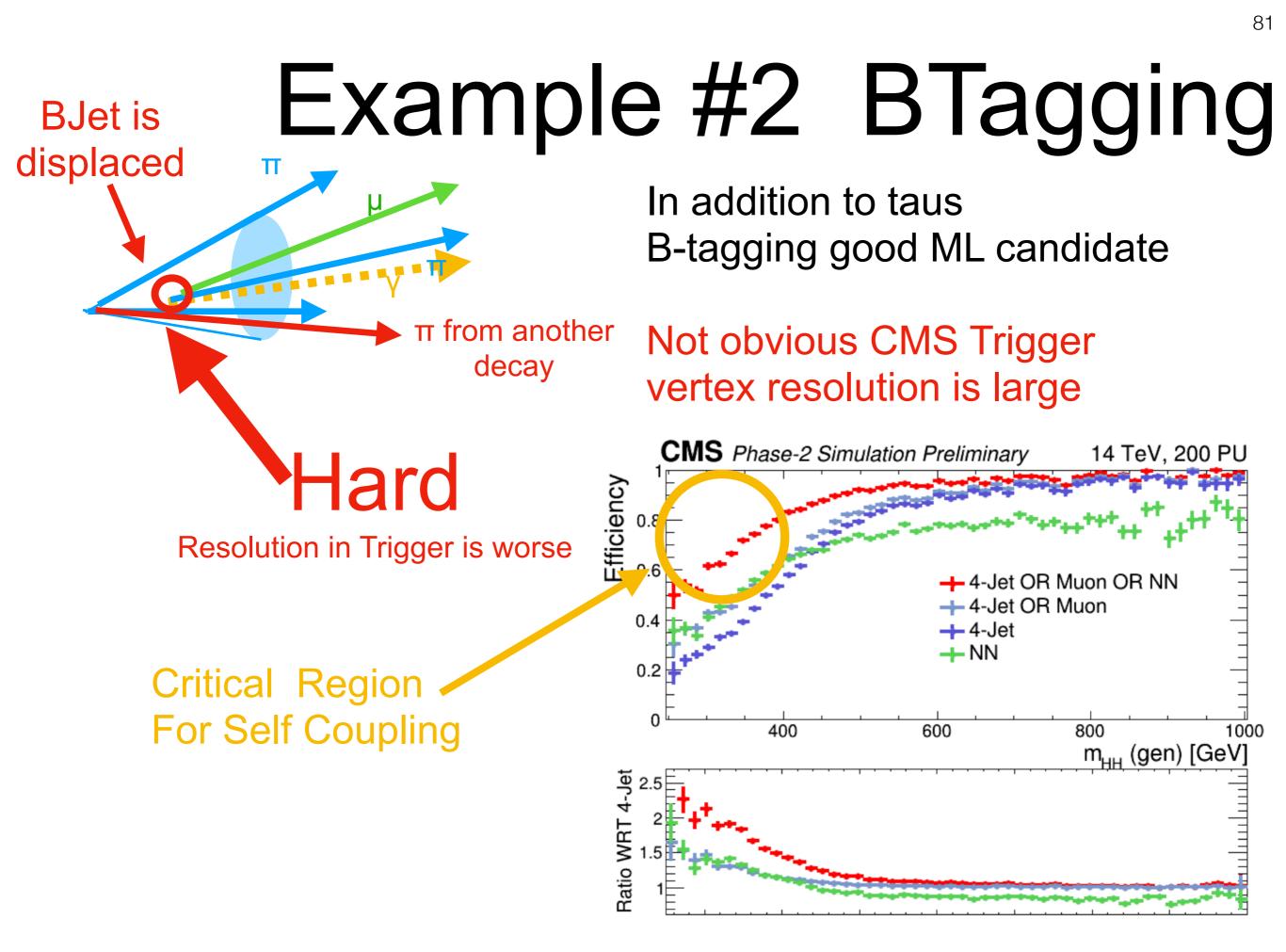
ard

BJet is

displaced

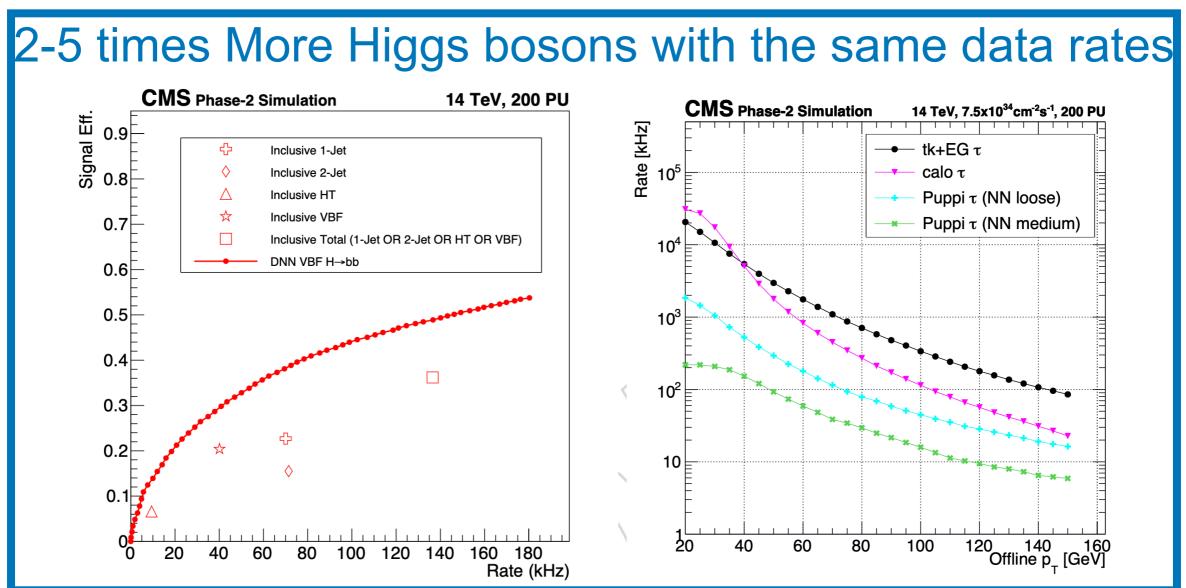
Π





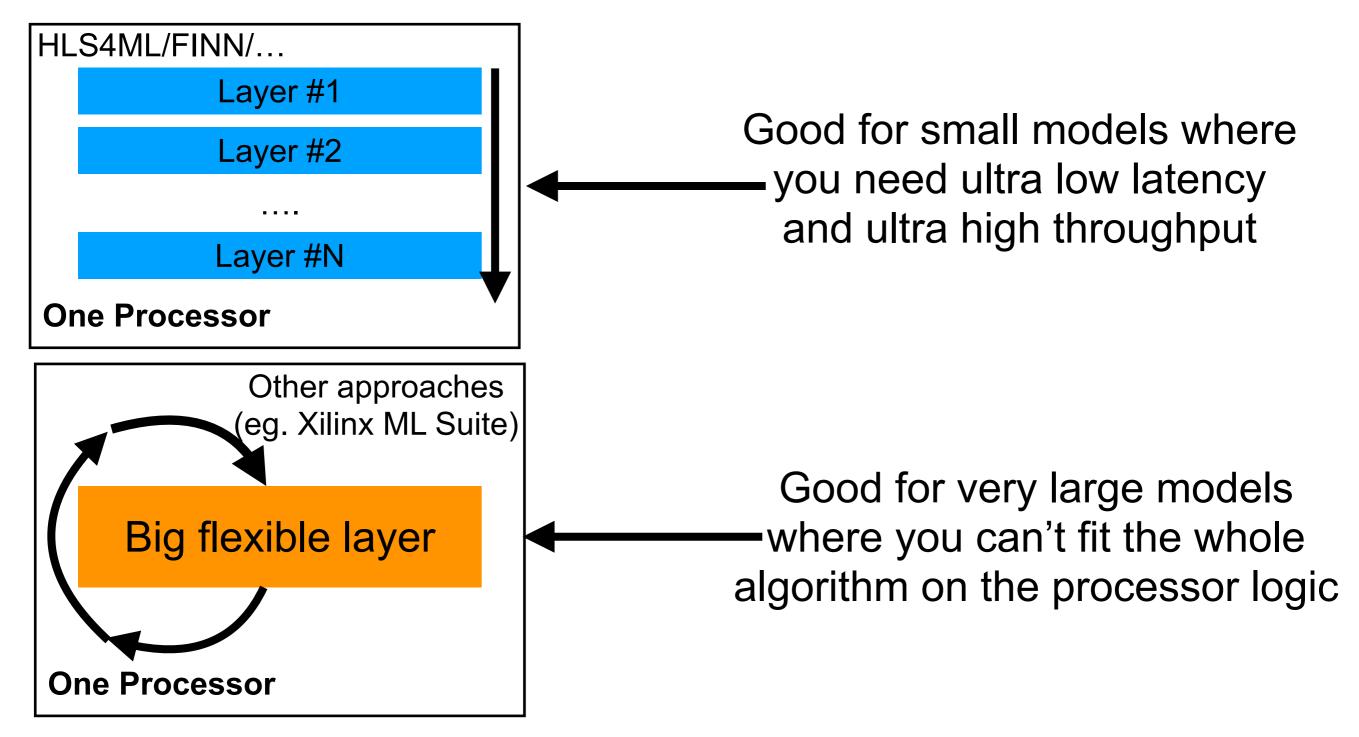
Accomplishments

- HLS4ML is rapidly being adopted in our trigger system
 - Will be used in the next running at the LHC
- We already see a number of substantial improvement



Other Deep Learning Models

HLS4ML differs from other ML models



How does a GPU do this?

evaluations of a big network Layer Code Layer Code Layer Code Not Great for a small network **One Processor One Processor One Processor** Layer Code Layer Code Layer Code **One Processor One Processor One Processor**

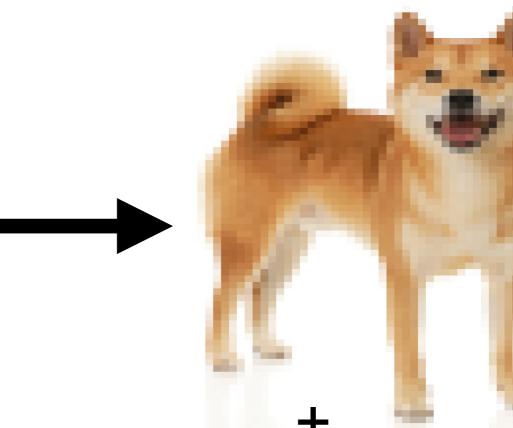
GPU is about even more standardization

Great for many

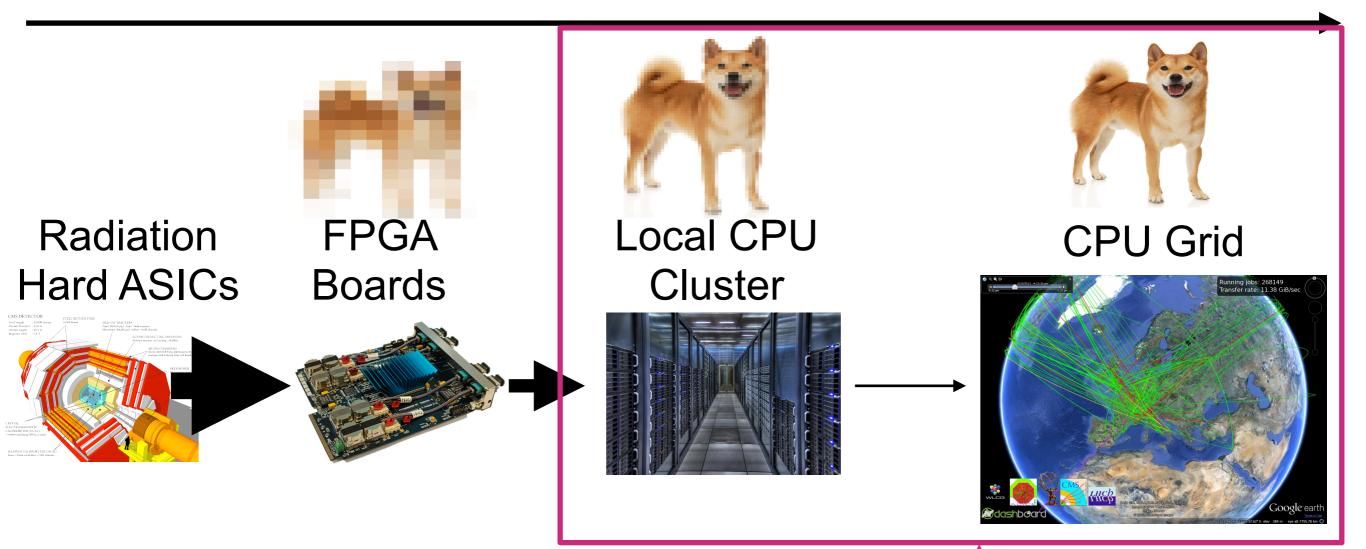
many

Running @ Longer latencies



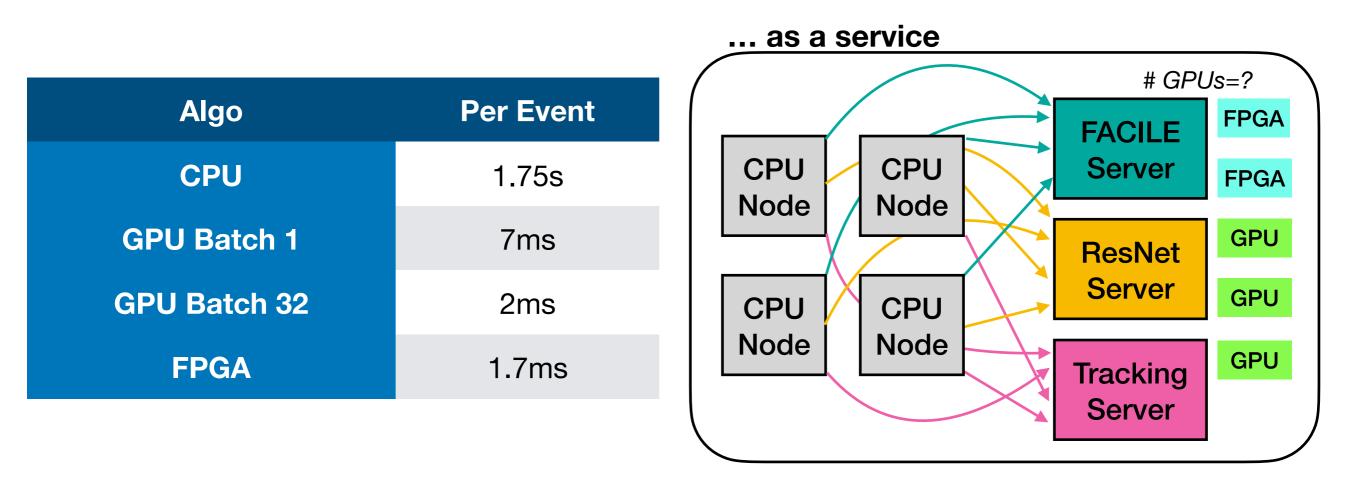


40 MHz HLT Trigger+Offline Reco



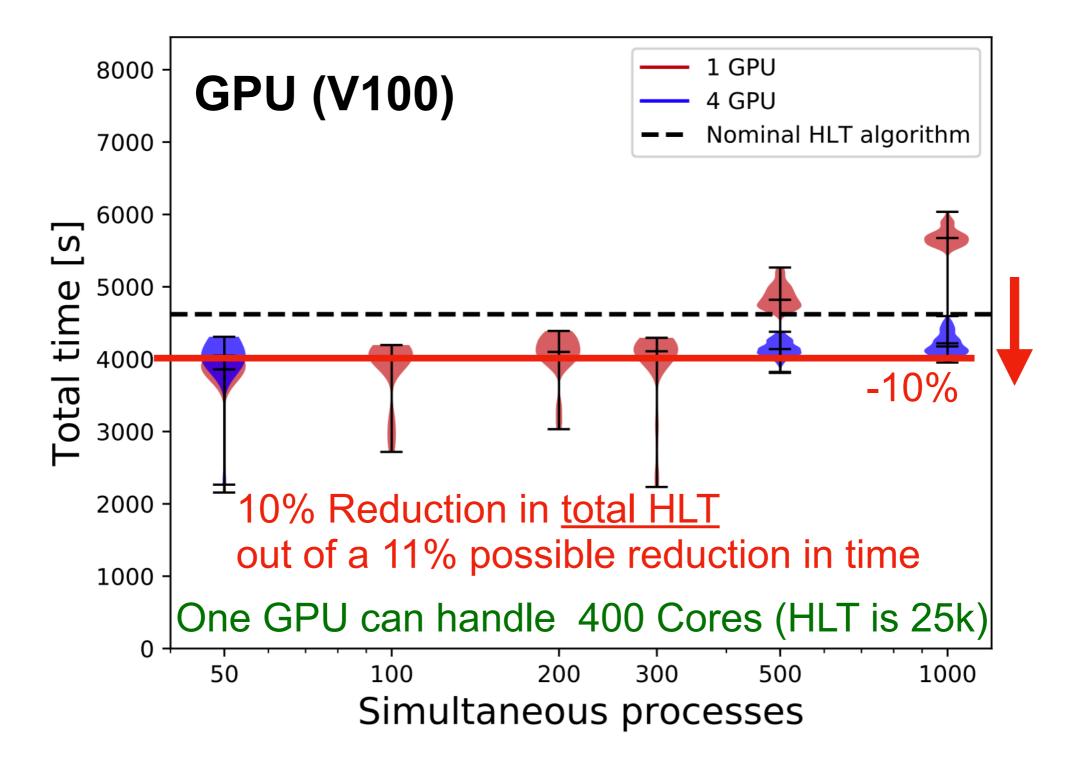
Both Tiers are CPU similar algos(different scales)

Talking to GPUs



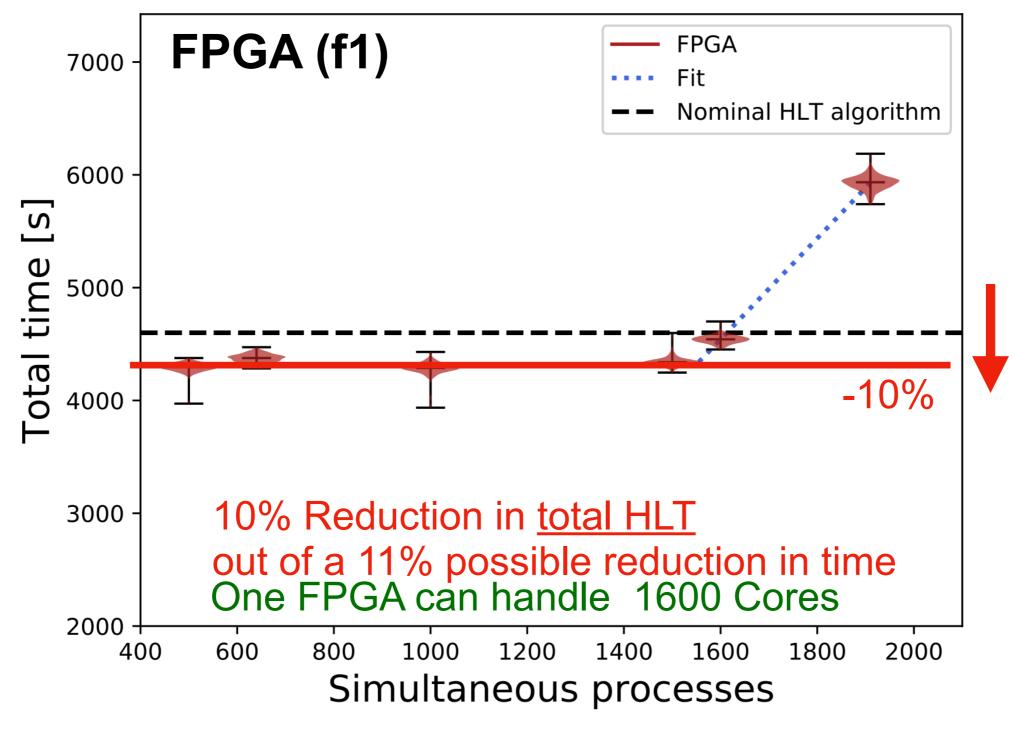
- Deep learning + GPUs or FPGAs can help to speed up systems
 - Deep Learning's regular arch makes GPU/FPGA speedups large
- There are a few ways to integrate these systems
 - My preference is to the right (some connect GPUs directly)

4 GPUs can reduce a 1000 CPUs systems time by 10%



arxiv:2007.10359

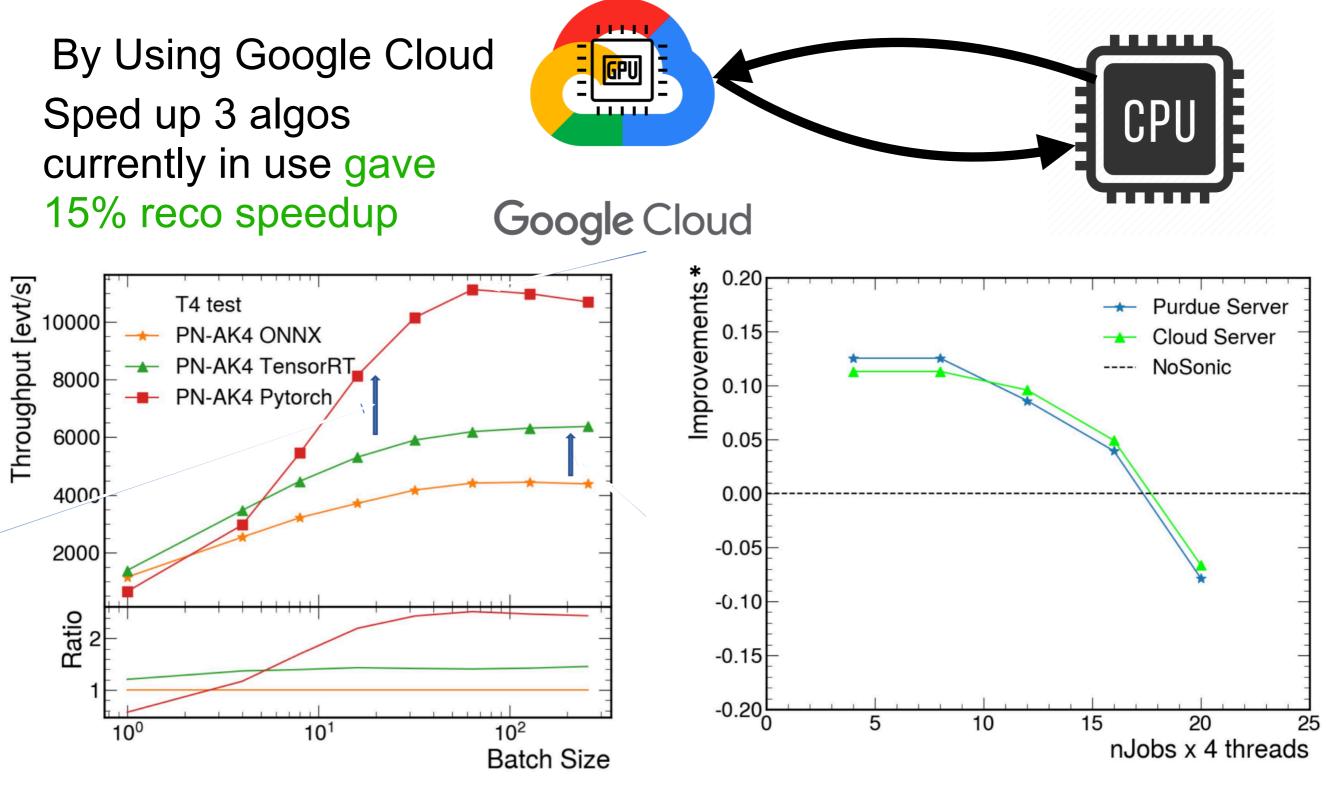
1 FPGA can reduce a 1500 CPU systems time by 10%



In fact the limit here is not from the FPGA its network (25 Gbps) arxiv:2010.08556

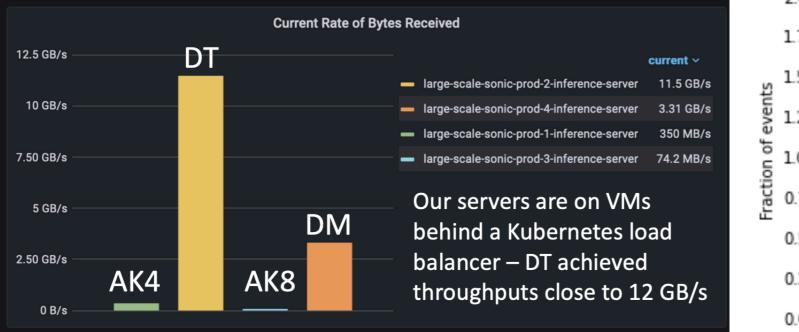
Running To Scale

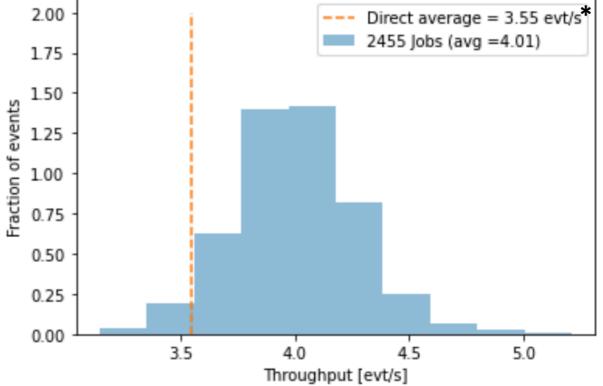
In addition we have been able to run this work to scale



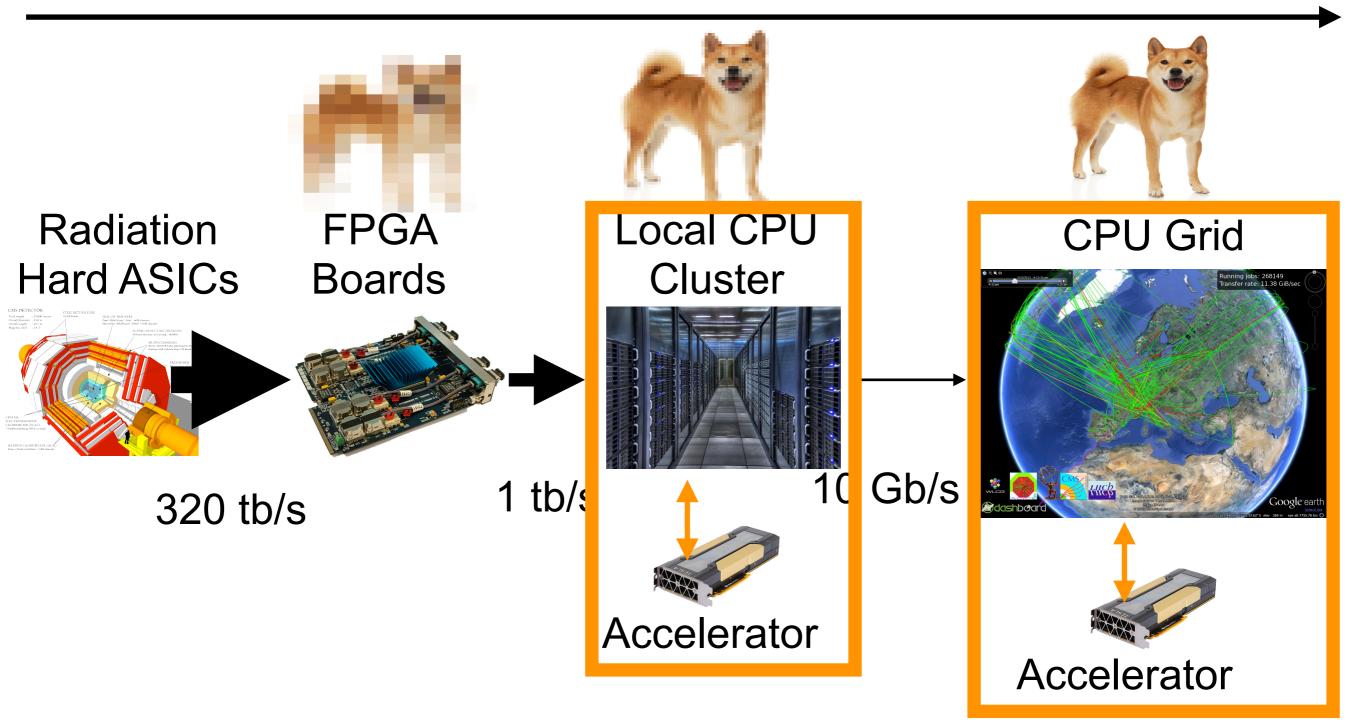
Running To Scale

- In addition we have been able to run this work to scale
 - Ran a test with 10000 CPU cores and 150 GPUs
 - Processes a realistic 150 TB sample
 - Demonstrated this paradigm works to scale!

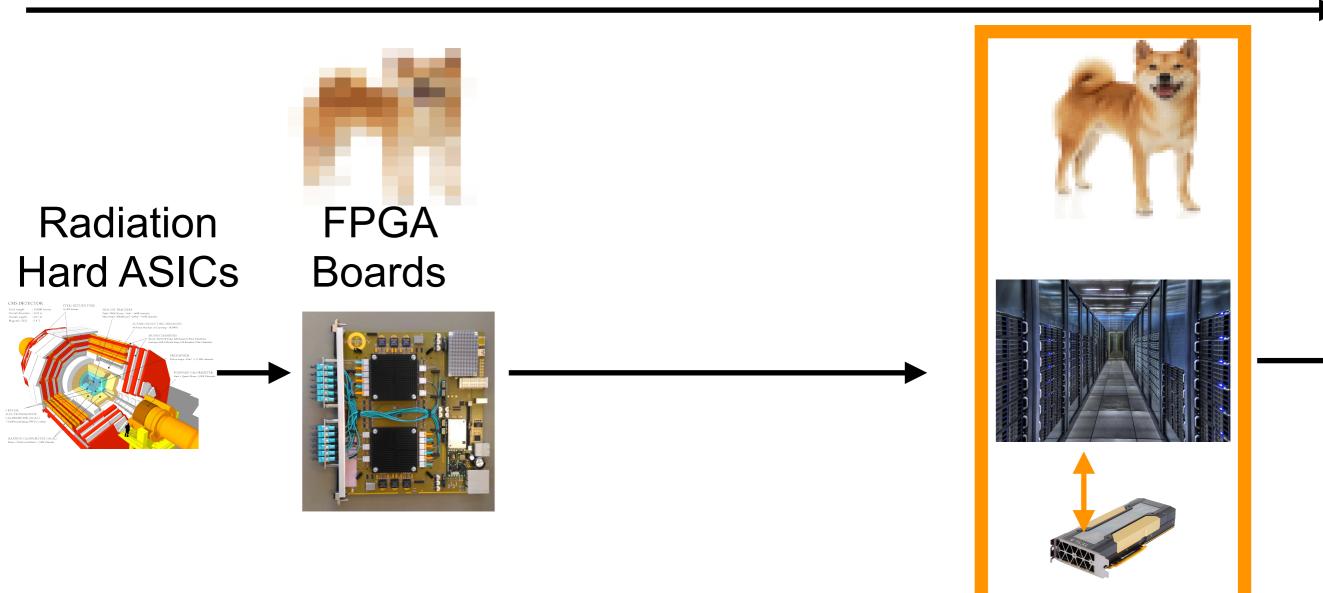




A Broader Vision of DAQ ^{40 MHz}

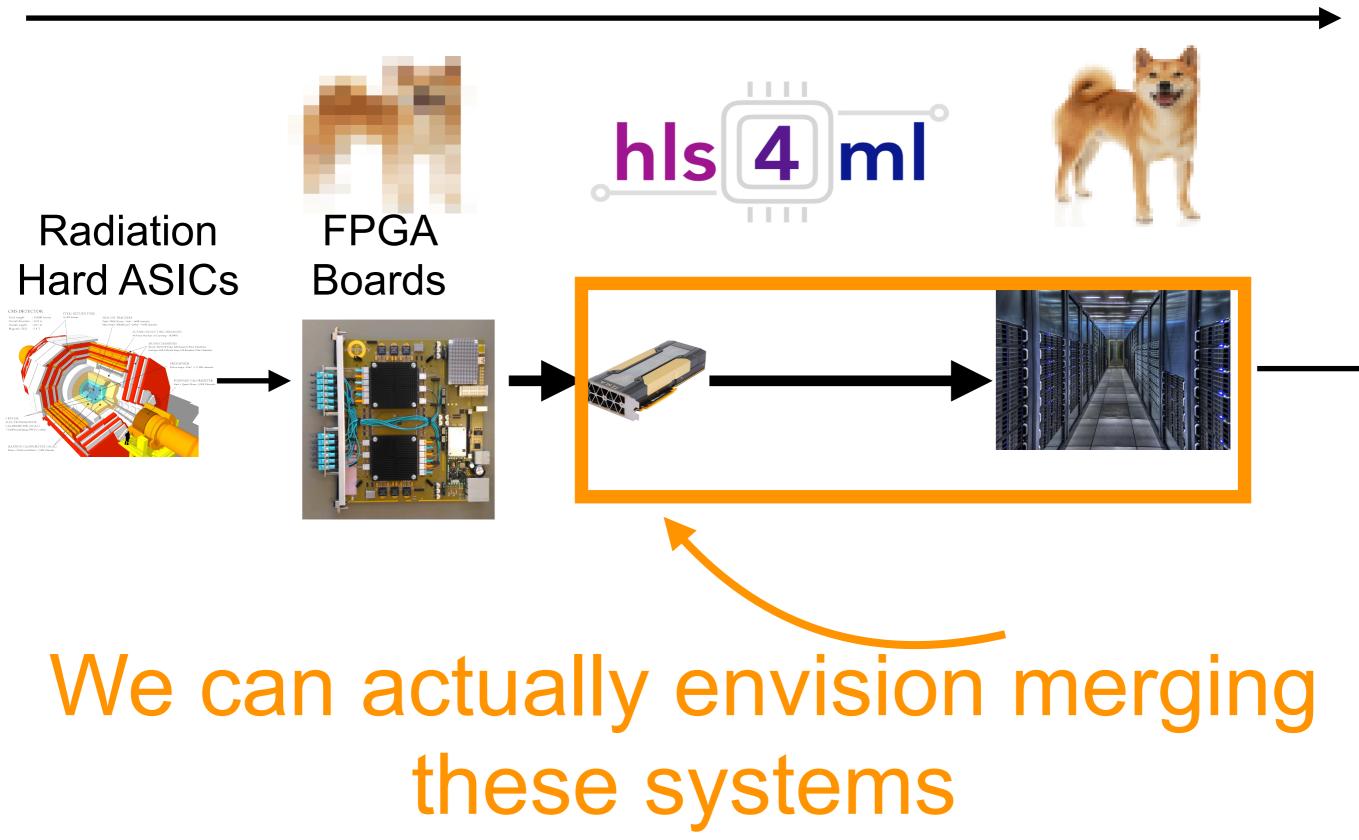


40 MHz A Broader Vision of DAQ 100 kHz

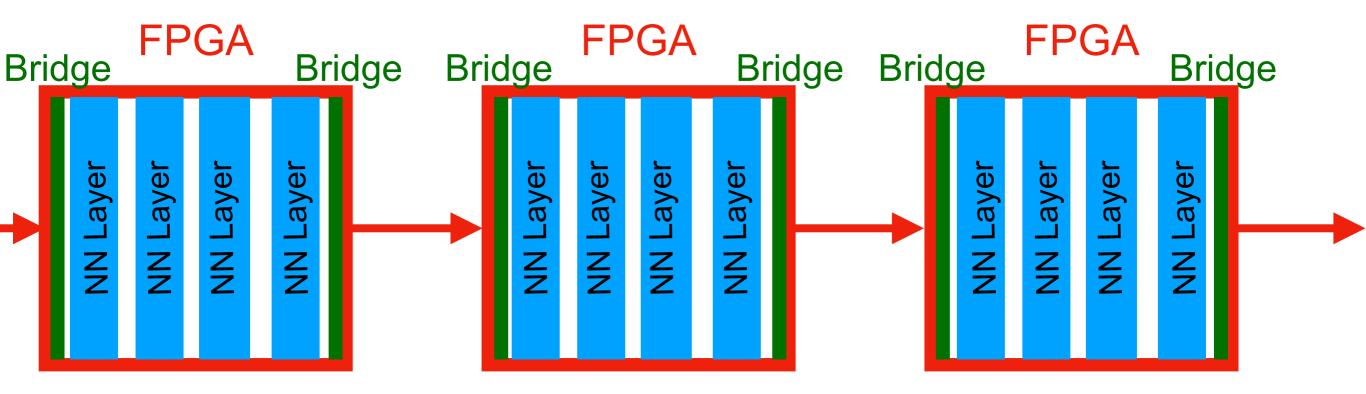


Now Lets Zoom In on our system

40 MHz A Broader Vision of DAQ 100 kHz



Algean



With Algean we can stretch out networks across many FPGAs 100 Gb/s protocol between FPGAs (can go to CPUs)

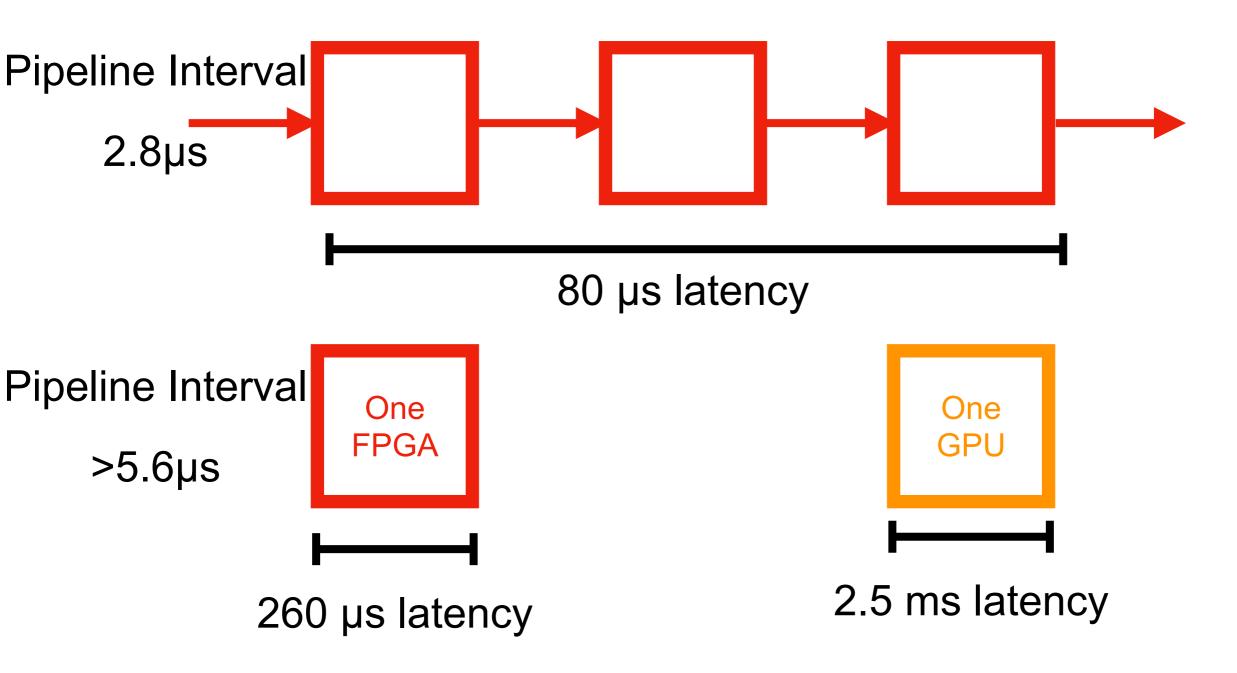
This allows us to run inference for very large networks

Very Fast

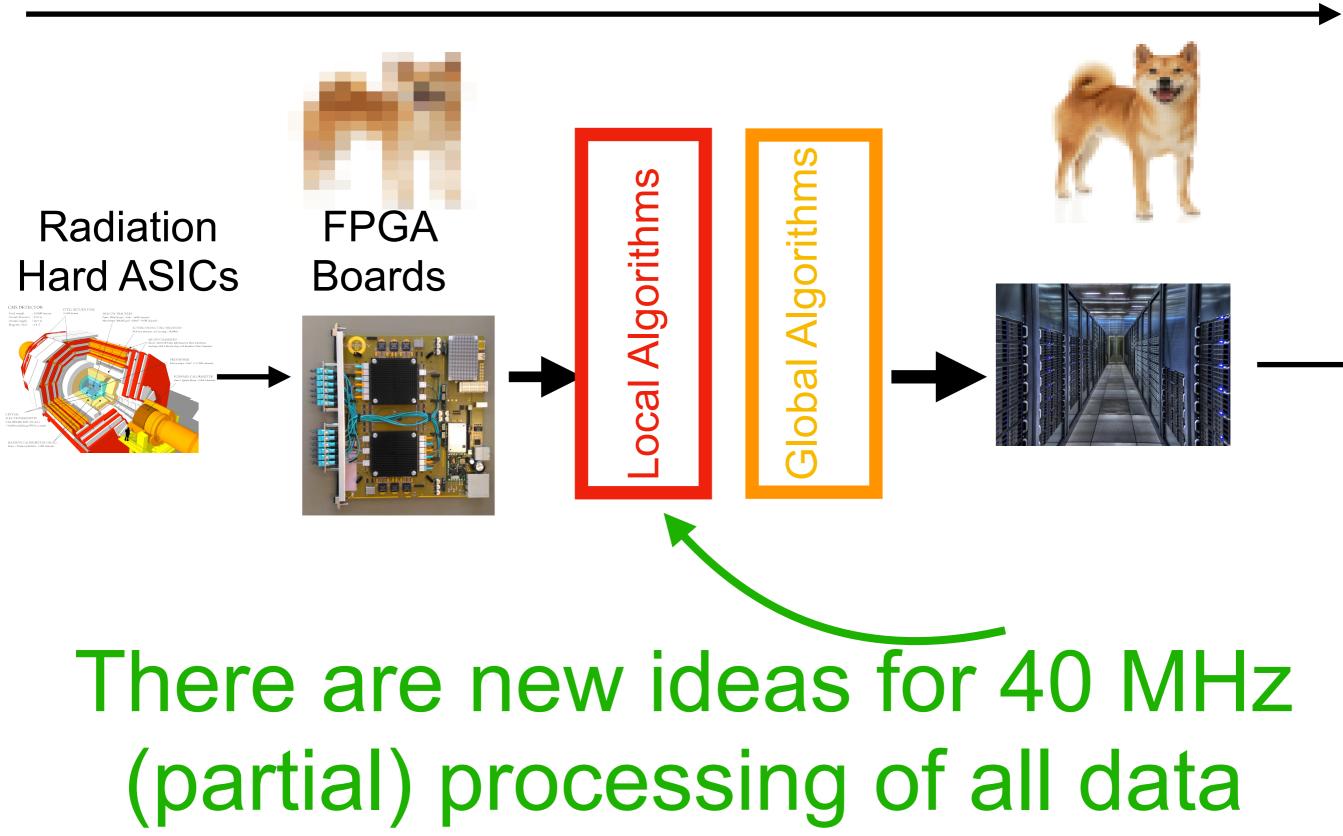
Tune our network to the resources we have

Example Autoencoder

Anomaly detection algorithm

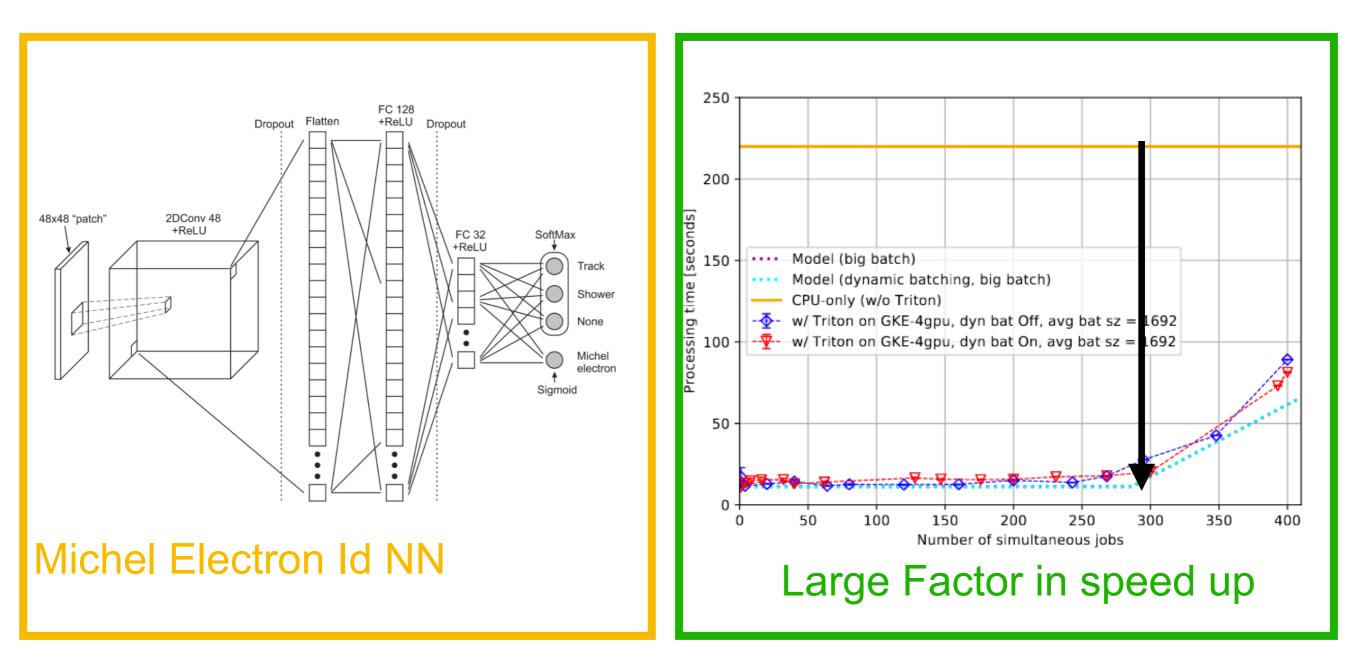


40 MHz A Broader Vision of DAQ 100 KHz



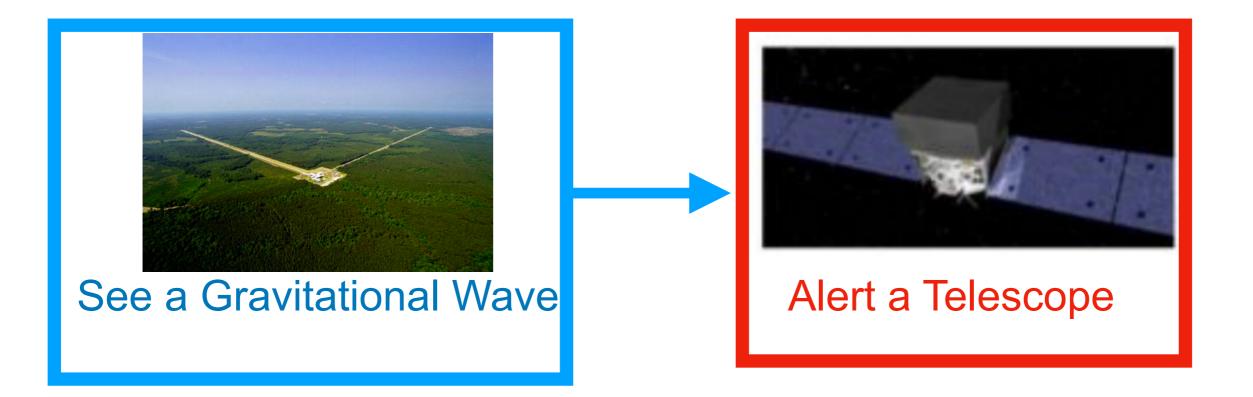
Neutrino Physics

• We are pursuing the same idea in Neutrino physics



Gravitational Waves

- Aiming to identify Gravitatoinal waves fast to do MMA
 - Correlating GW and Optical observations is powerful

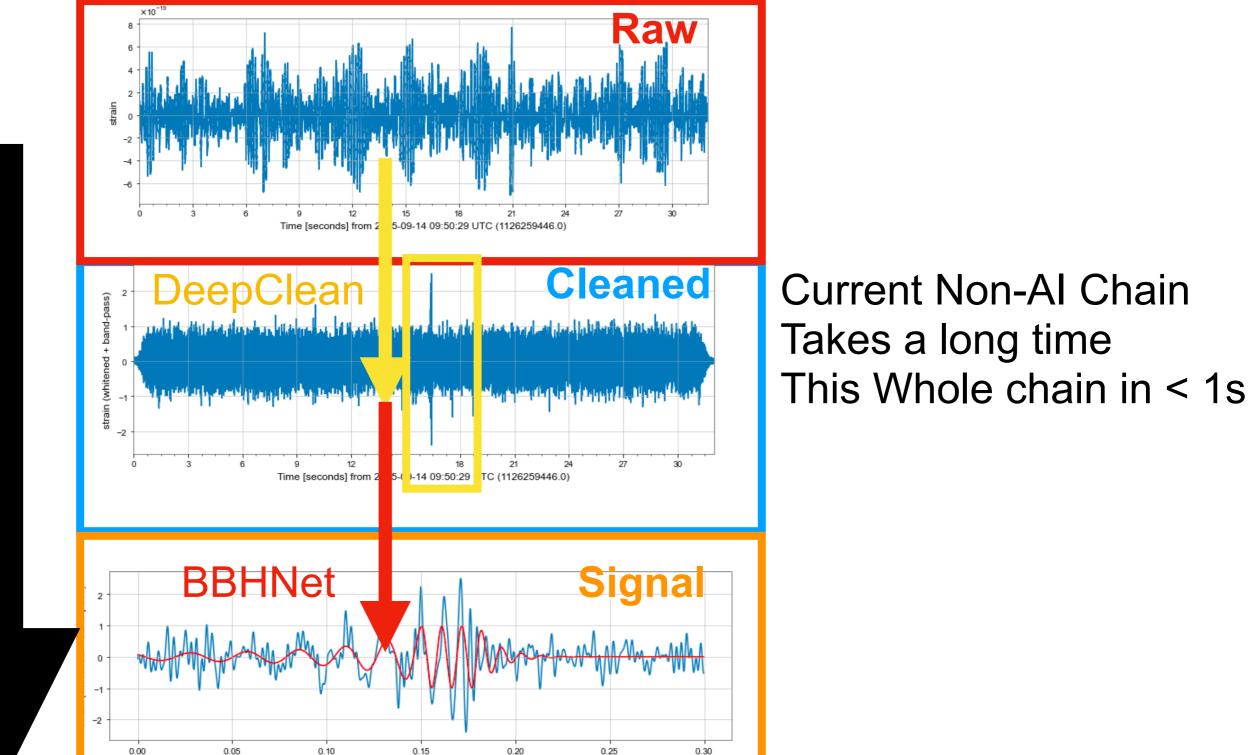


Can we make the GW reconstruction fast enough to be real-time?

Gravitational Waves

• Aiming to identify Gravitatoinal waves fast to do MMA

AI System



Arsenal of telescopes



Once you have found the GW event have to send the coordinates to a huge network

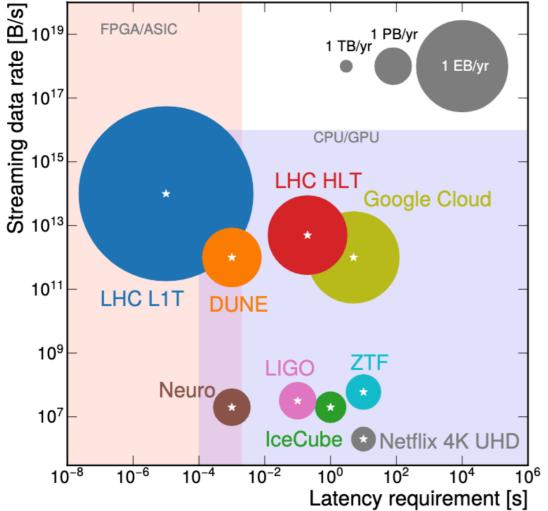
A3D3

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- An institute to unite real-time AI
 - Quickly looking for people to be part of extended team



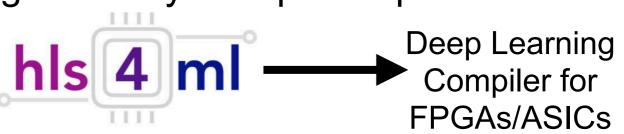
Fast ML and now A3D3





- We make AI run fast :
 - Our goal is to use AI to speed up processing of experiments
 - Additionally we are developing new ways to speed up AI

IAIFI Colloquium FPGA Keynote Talk

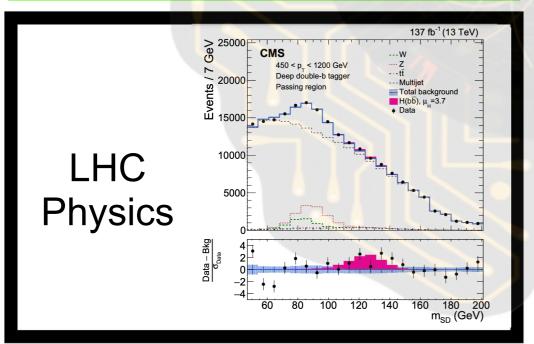


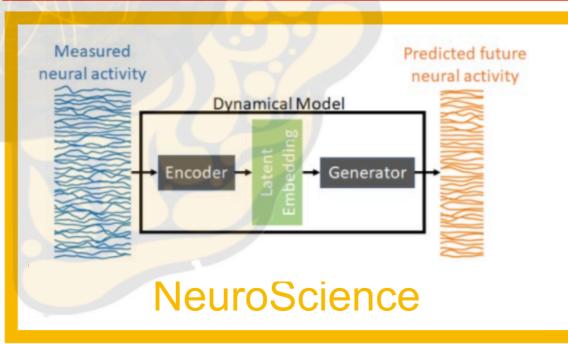
A New Institute: A3D3

- We have been awarded a new institute to explore real-time AI
- Accelerated AI Algorithms for Data Driven Discovery (A3D3) New Types of Computing

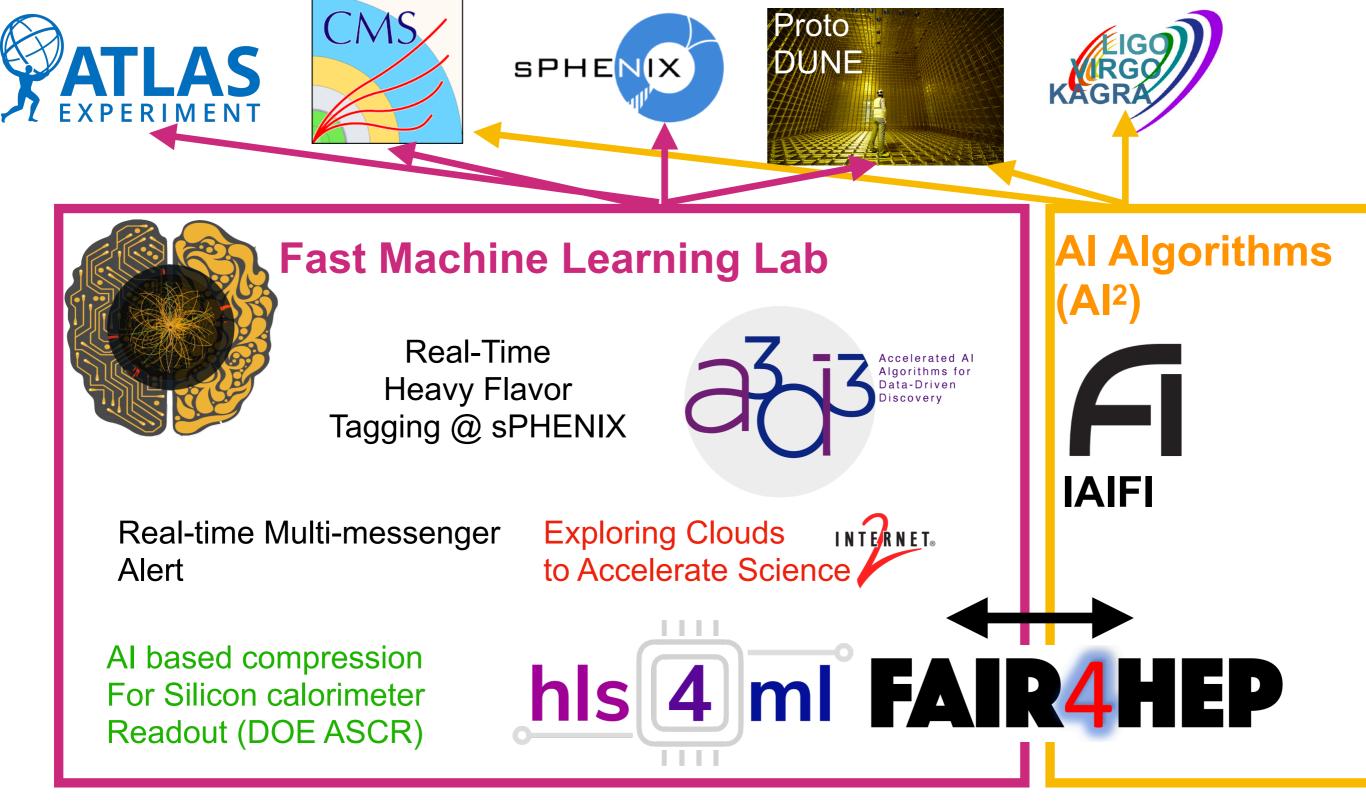




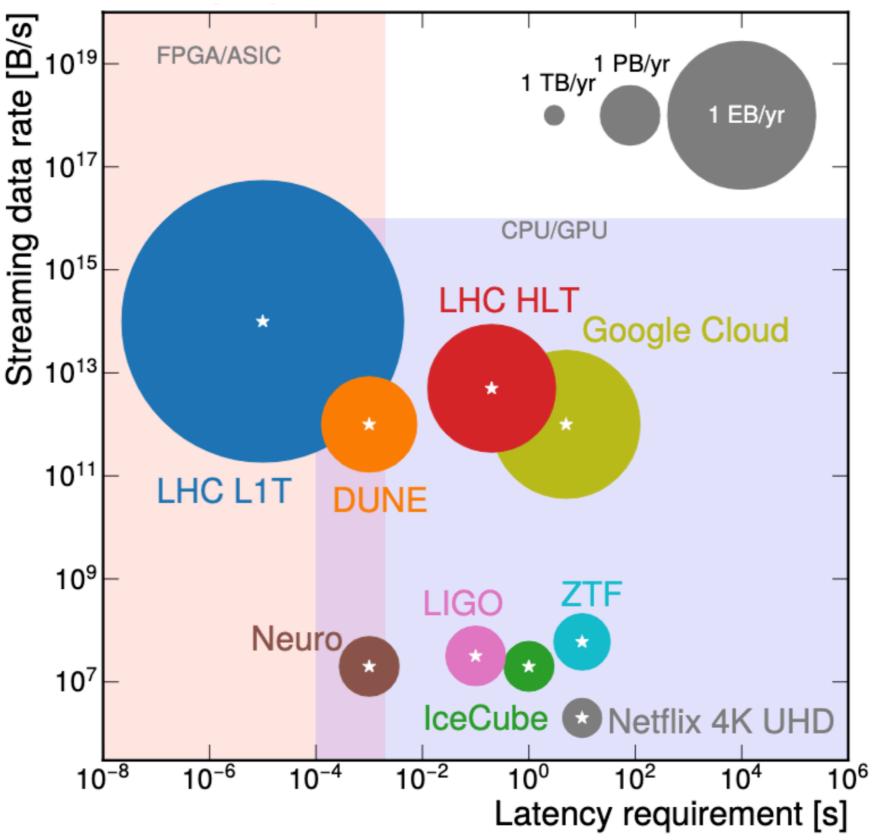


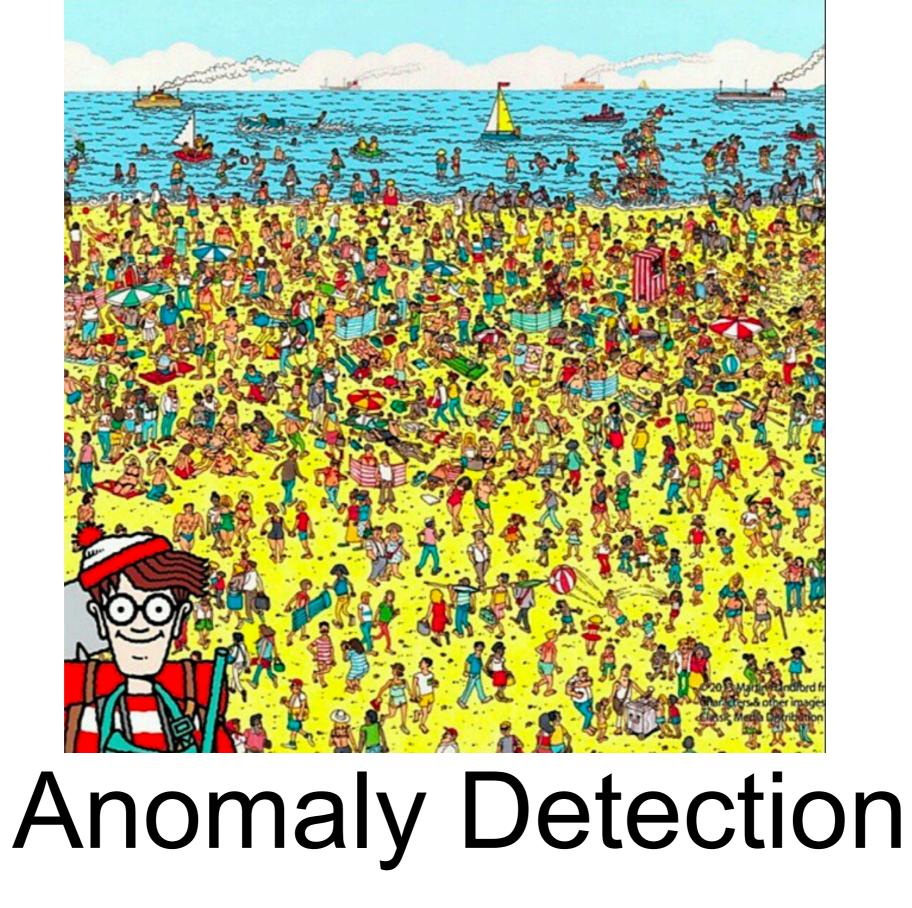


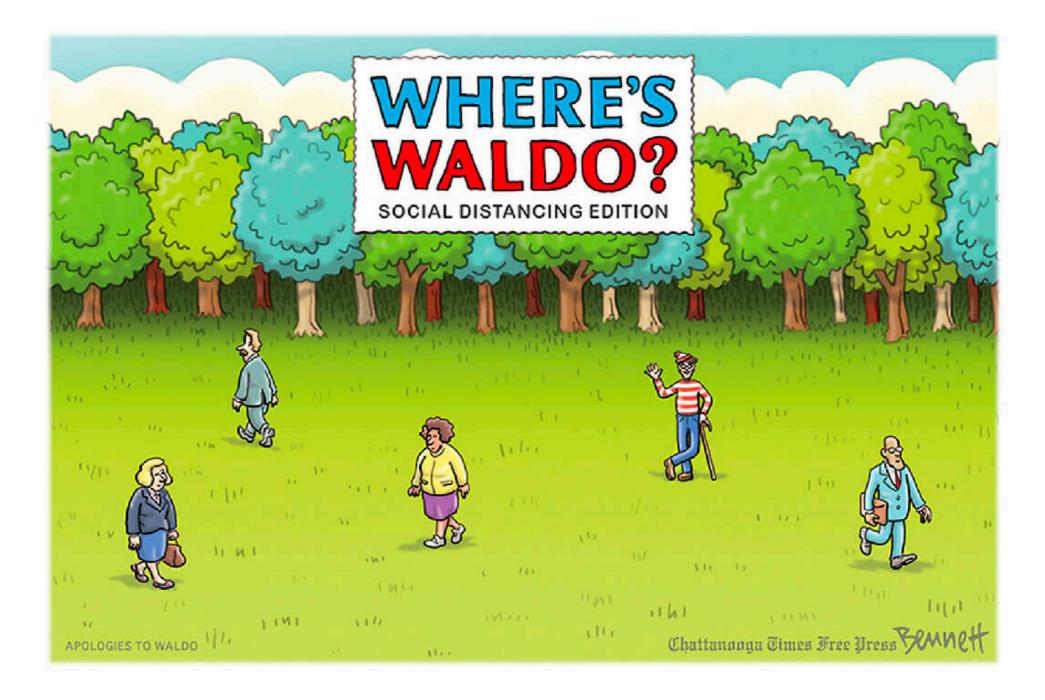
Overview Venn Diagram



Preparing for the future





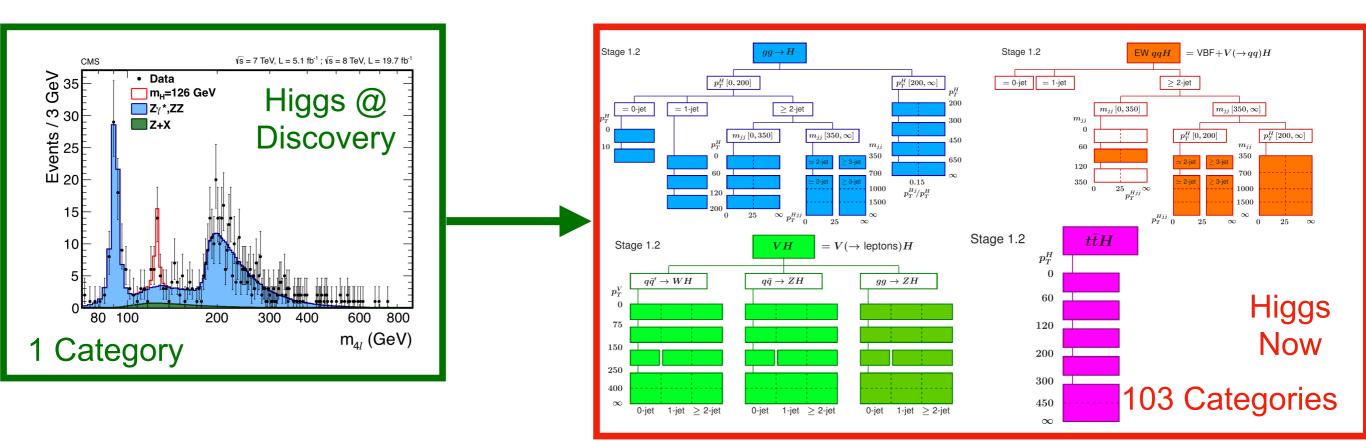


Anomaly Detection Another Fun thing to do during COVID

Ageing Analyses @LHC

109

- Data analyses at the LHC are changing
 - Analyses are becoming much more complex
 - Many categories and many final states
- General trend towards more complicated analyses



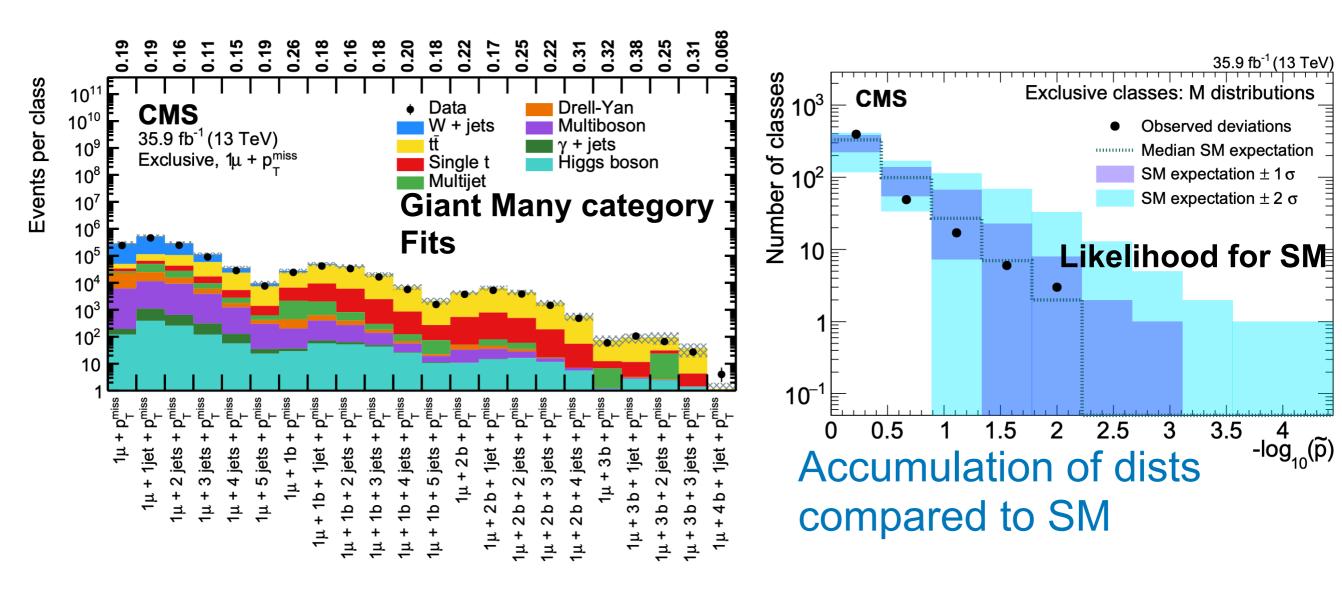
What has caused trend?

- The power of computing
 - Complex many parameter fits run much faster these days
 - Newer optimization strategies that are proven to be robust
 - Along with the ease of use of complex fitting tools
 - Many tools now auto build likelihood and minimize
- A better understanding of our simulation
 - Many processes are understood
 - Steps to making categories has become progressively simpler
- Encroaching on a general philosophy to do more at the same time

From this trend

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- Some old ideas are starting to be taken more seriously
 - Can we perform analyses on a broad range of data at once

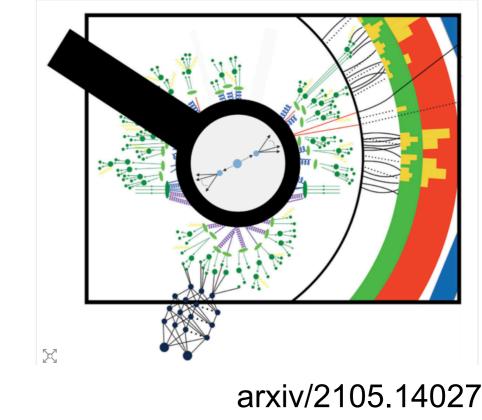


Two Anomaly Challenges LHC Olympics 2020 Dark Machines



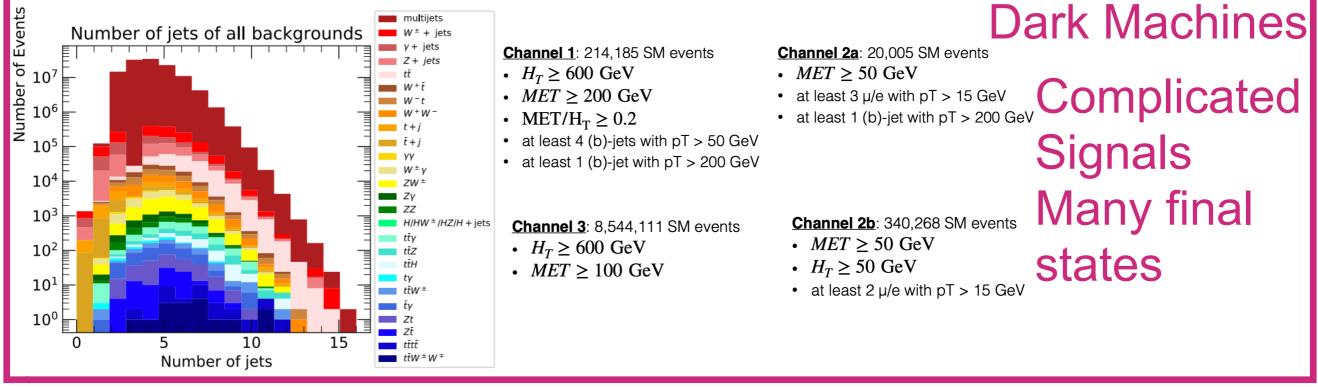
arxiv/2101.08320

David Shih, Ben Nachman, Gregor Kasieczka



Challenge: Hide signal(s) in a lot of data See if the community can find it

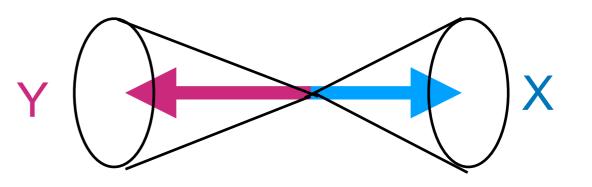
Anomaly Data

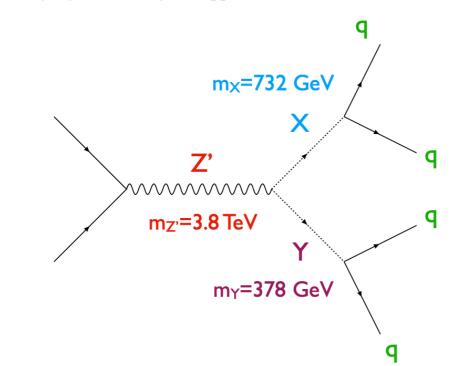


Black Box #1

LHC Olympics



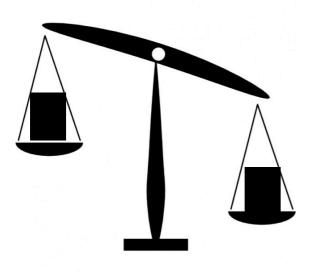




Anomaly Strategies@LHC

Anomaly Strategies at LHC fall into two categories

I know regions where new physics does not exist



I want to leverage those regions against other parts of the data to find differences

I know how to predict all collisions

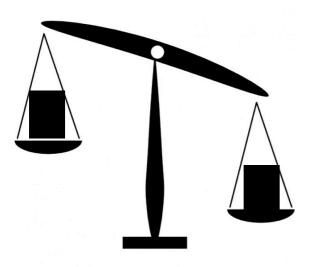


Are there any collisions that I cannot predict?

Anomaly Strategies@LHC

Anomaly Strategies at LHC fall into two categories

Weakly-Supervised I know regions where new physics does not exist

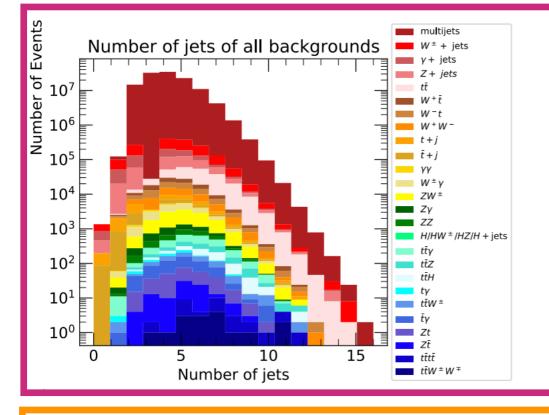


I want to leverage those regions against other parts of the data to find differences Autoencoders I know how to predict all collisions



Are there any collisions that I cannot predict?

Anomaly Data Dark Machines

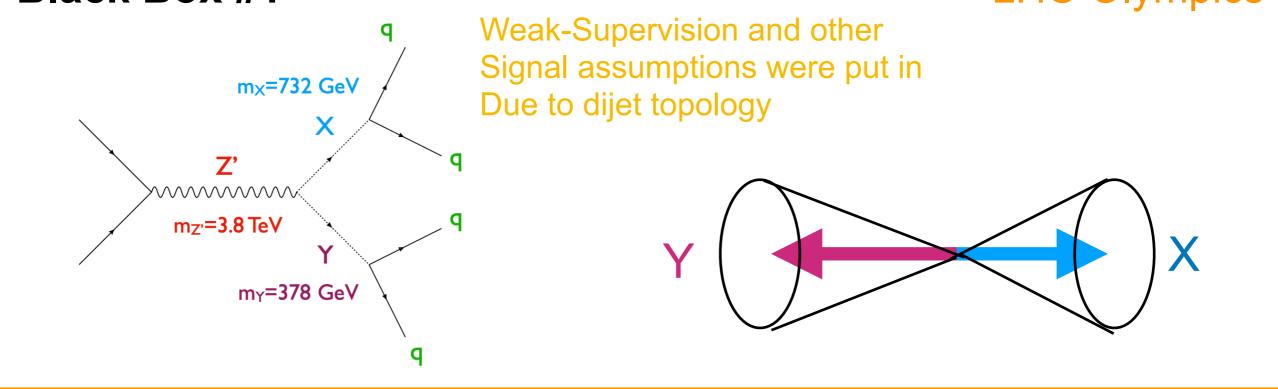


General emphasis was on Signal Prior free approaches

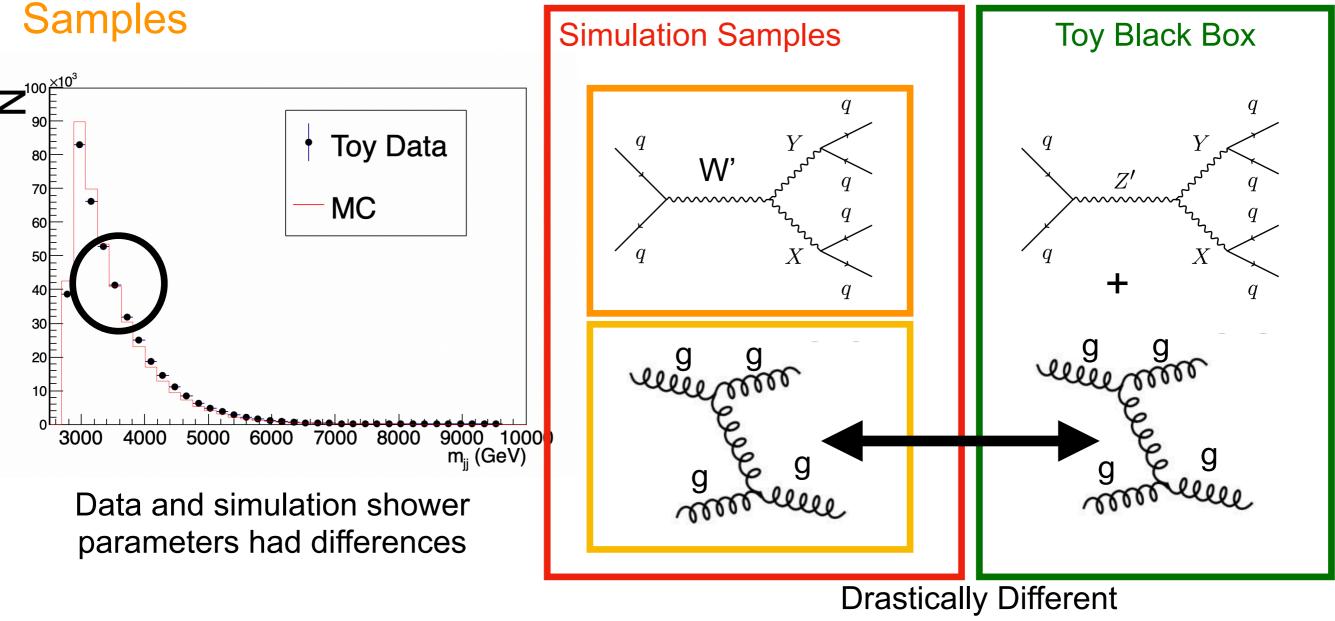
Many different types of Autoencoders

Black Box #1

LHC Olympics



Simulation



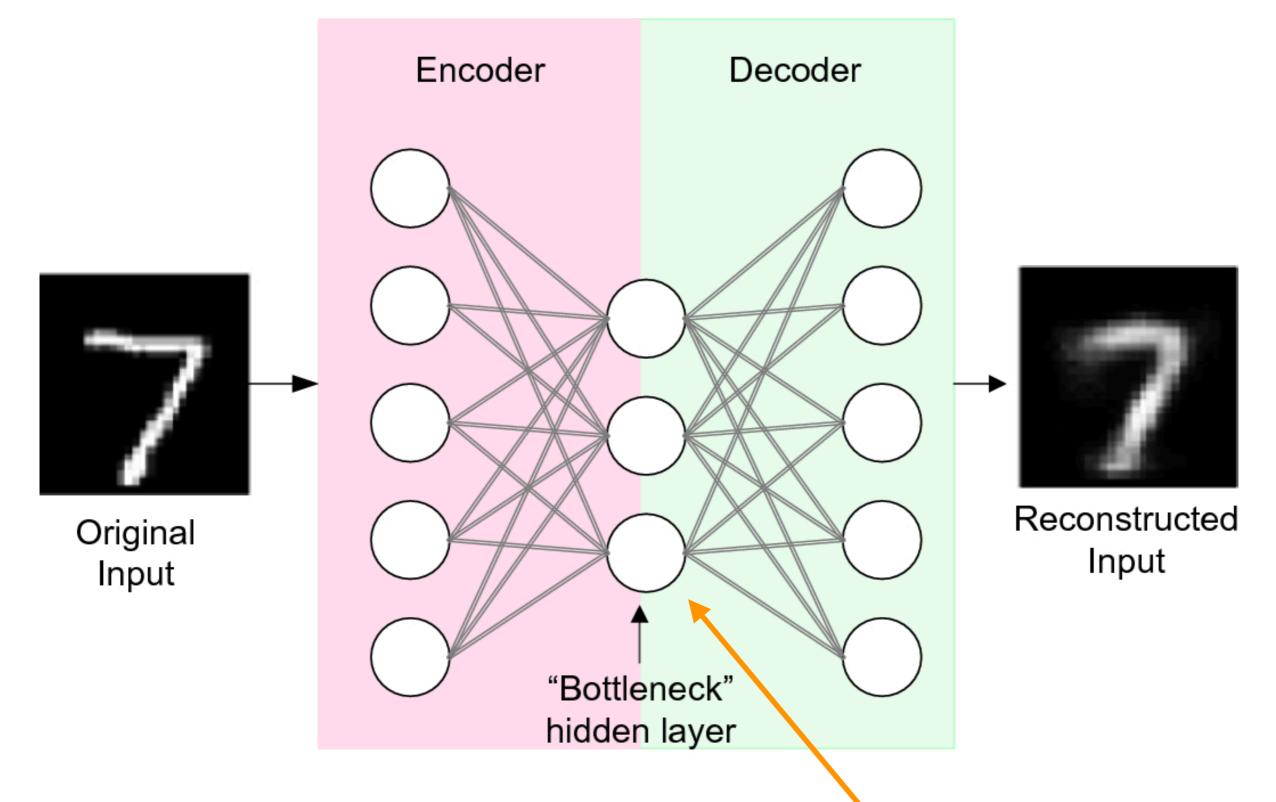
Simulation Parameters

- Aim was to emulate a real search as much as as possible
 - Simulation and Toy Data are released (Sim and Data different)



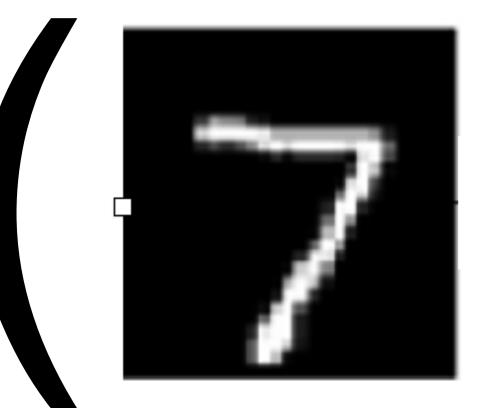
What are people thinking about to find anomalies?

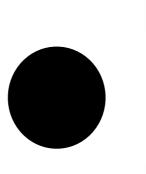
Autoencoders



Strategy is to create a space in the middle that embodies all features of physics

Autoencoders







Original Input Reconstructed Input

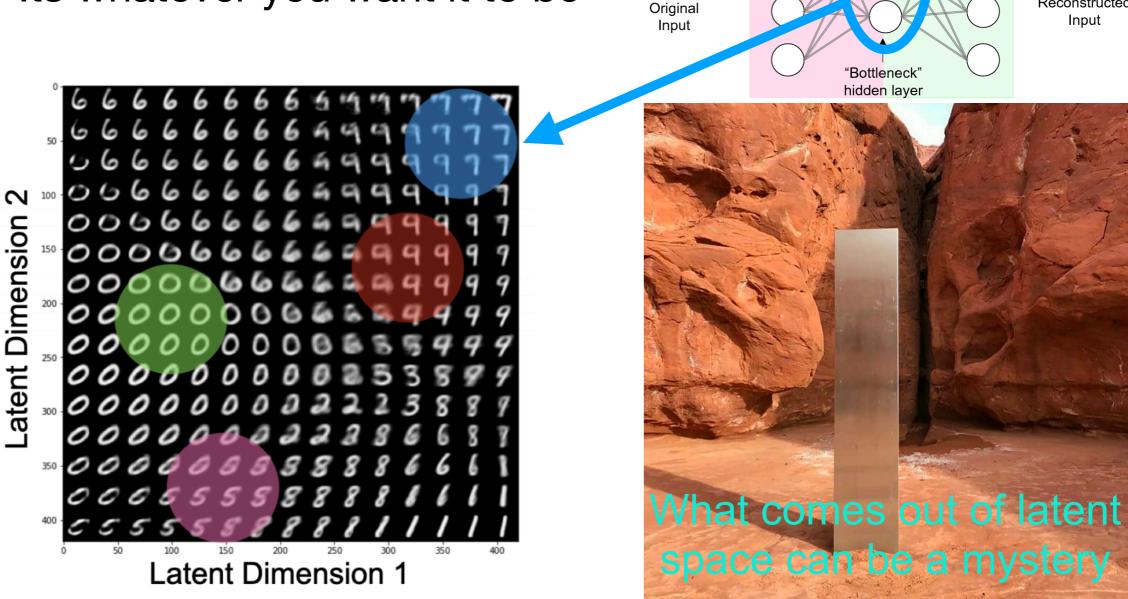
Dot product the input and output Large Value : Good Small Value : Anomaly

The Latent Space

Encoder

Decoder

- Deep learning algos tend to focus on the latent space
- What is the latent space?
 - Its whatever you want it to be



Reconstructed

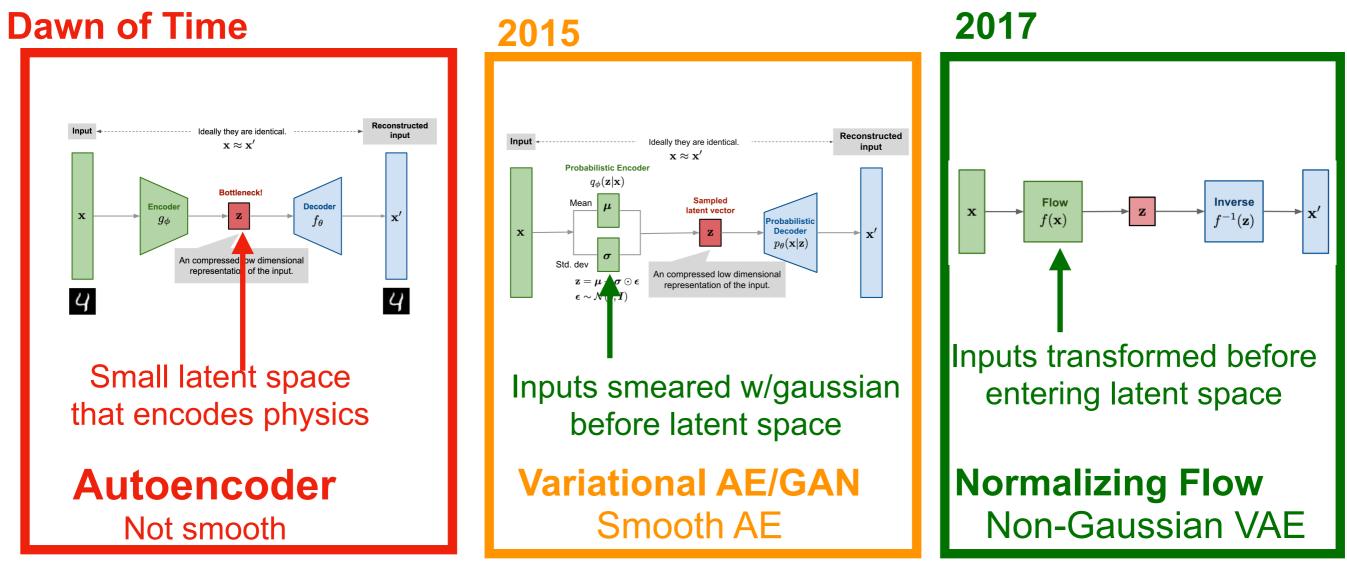
Encoder Progression

2020 2016 2018 τu **Particles** features Φ ID CNN [Translated] Azimuthal Angle (14 layers) 10⁰ particles, ordered by pT C [(P+DE) x No] Secondary Vertices OUTPUT · RR [NE X No] features 10⁻¹ ID CNN O [Dox No (10 layers) SVs, ordered by SIP2D E [DE X NO] 10⁻² Particles and SVs No: # of constituents $\phi_{c, fo, fR}$ # of features expressed as = No(No-1): # of edges with 4-vectors+features dense neura DE: size of internal representations o: size of post-interaction internal representation 10^{-3} -1.5-1.0-0.5 0.0 0.5 1.0 1.5 [Translated] Psuedorapidity (η) Graphs **Particles** Images (Particles+correlations) (limited correlations) (not lorentz invariant) **Current collaboration results**

Progressively moving towards use of more info

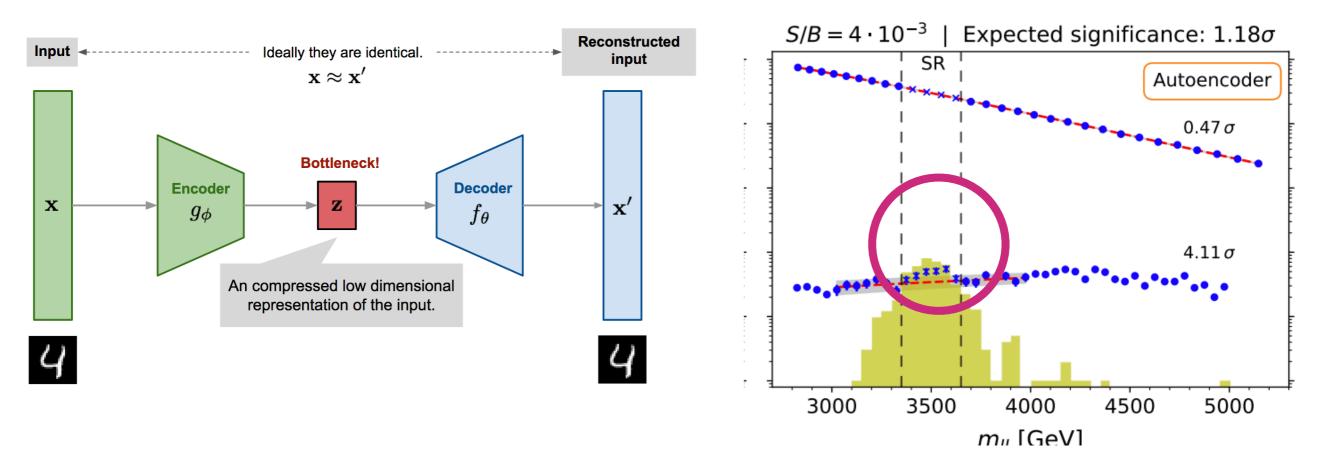
Autoencoder Progression

Autoencoders are gaining popularity in HEP just now



We started with AEs

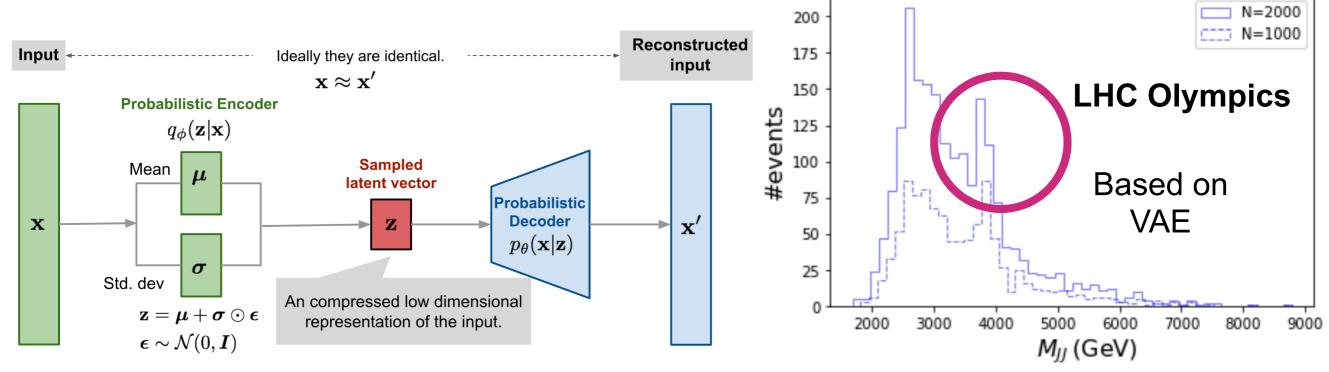
Try to repeat the inputs with the outputs



Anomaly Defined by how well reproduced the input is An anomaly will not reconstruct the input well

We updated with VAEs

- Try to repeat the inputs with the outputs
 - but Smear with gaussians before you repeat outputs

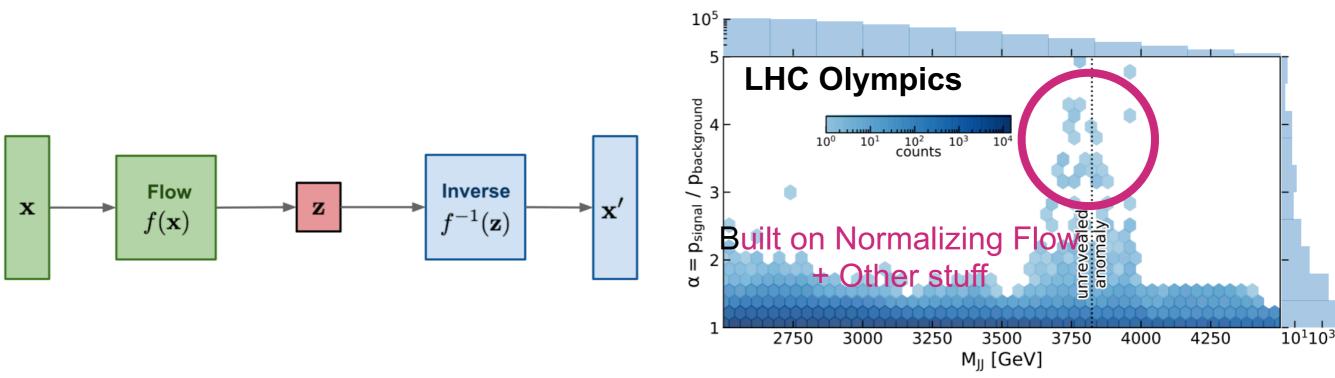


VAE makes latent space continuous which improves performance

Found to be very effective (dark machines) Particularly when adding tight constraints on μ and σ

added Normalizing Flows

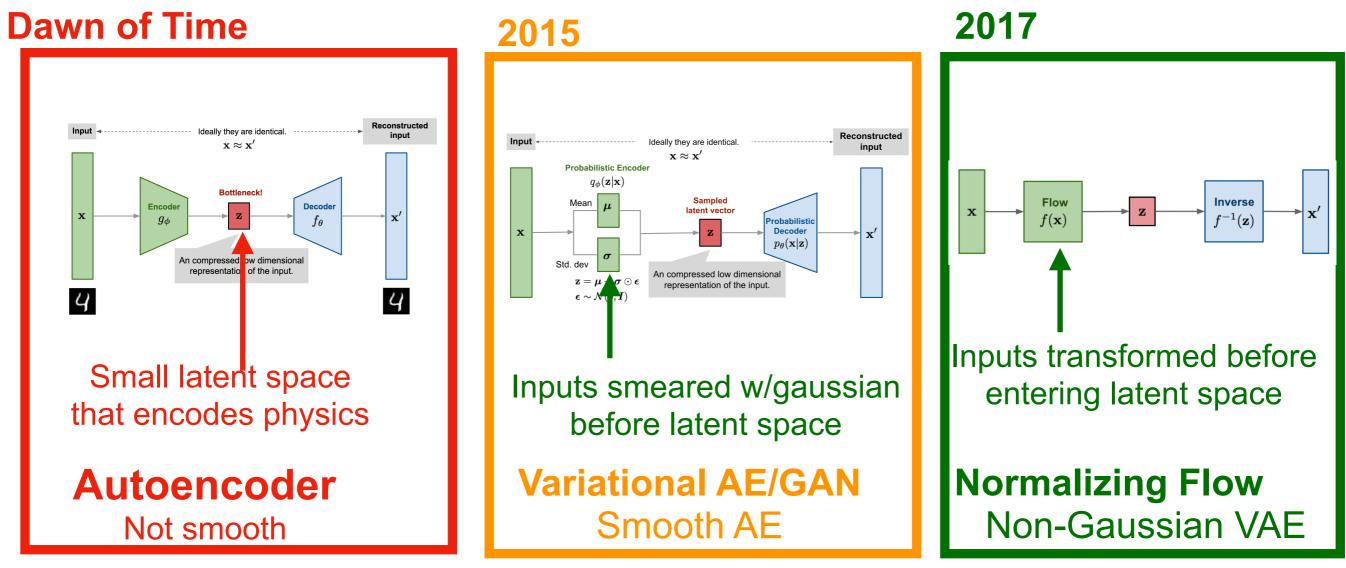
- Try to repeat the inputs with the outputs
 - But transform (and smear) outputs



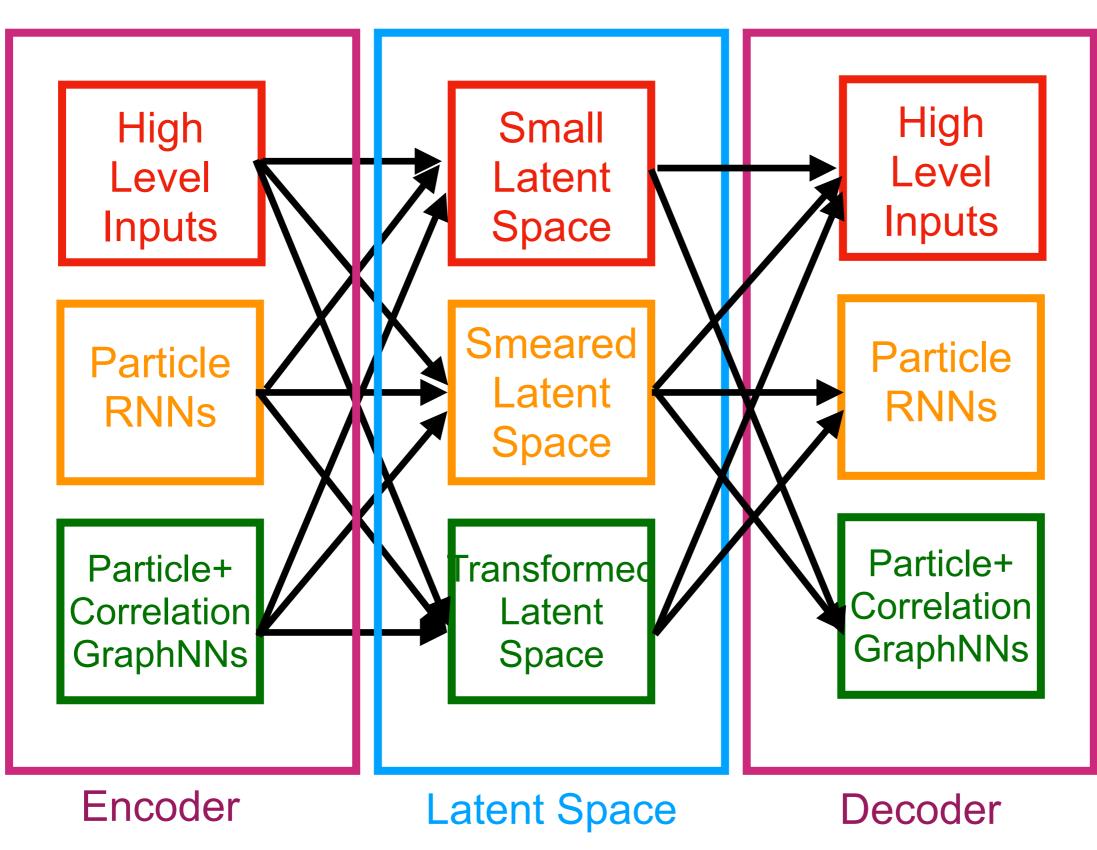
NF transforms the latent space so it has a lot more fexibility Gaussian smearing and motion in space can capture physics These tend to perform the best in terms of anomaly detection

Autoencoder Progression

Autoencoders are gaining popularity in HEP just now



Combinations



Weak Supervision

How do we separate two samples (one with anomalies)

VS

Sample A



Sample B



Difference:

Strategy: Train the data in A agains B Challenge: Must all be same in A and B

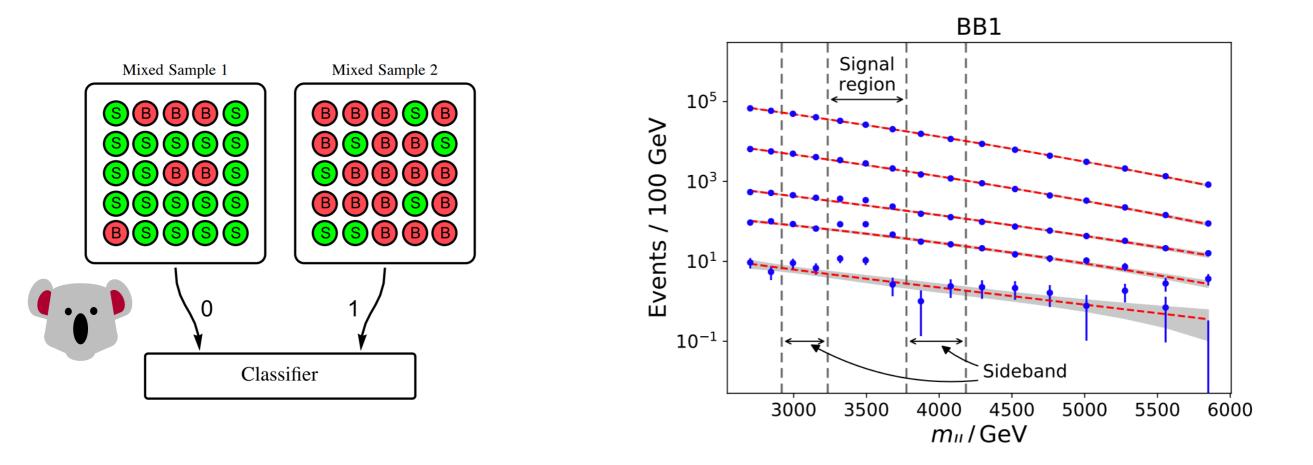
More realistic example



How do we train samples with variations of populations of an anomaly

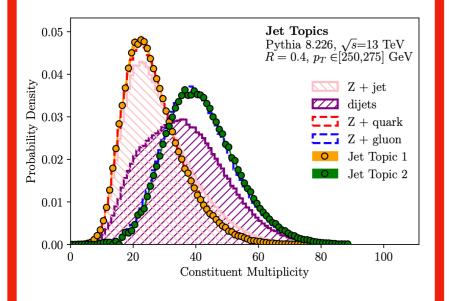
Classification w/o Labels

- CWoLA approach aims to exploit differences in datasets
 - Can play one region of data off the other
 - Provided you can separate out the two approaches



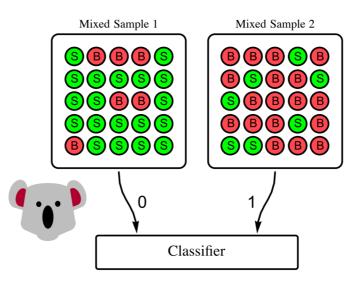
Training Strategies

Topic Modeling/ Clustering



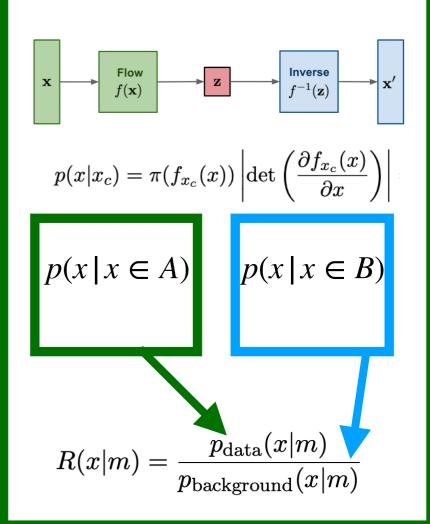
Split a histogram into multiple distributions by looking for separate regions

Classification W/O Labels

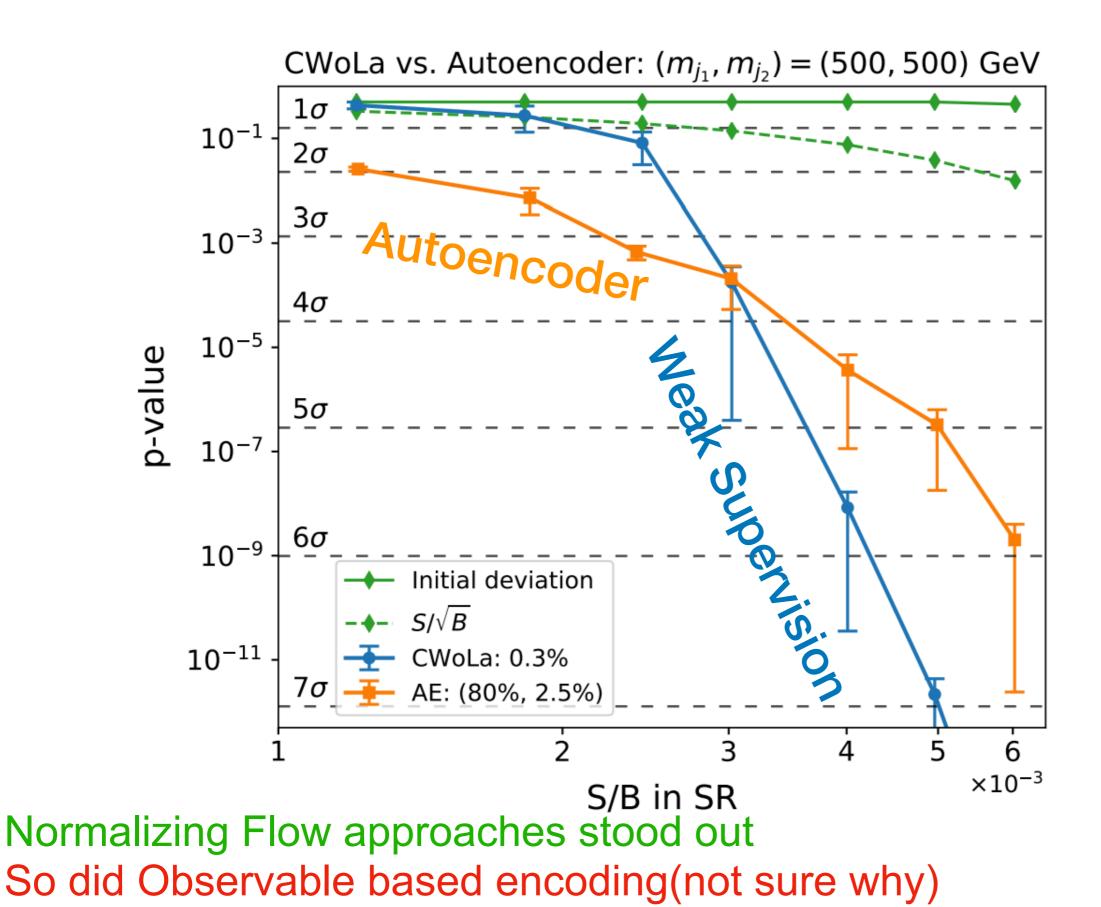


Separate out Sample 1 from Sample 2 by hidden signal

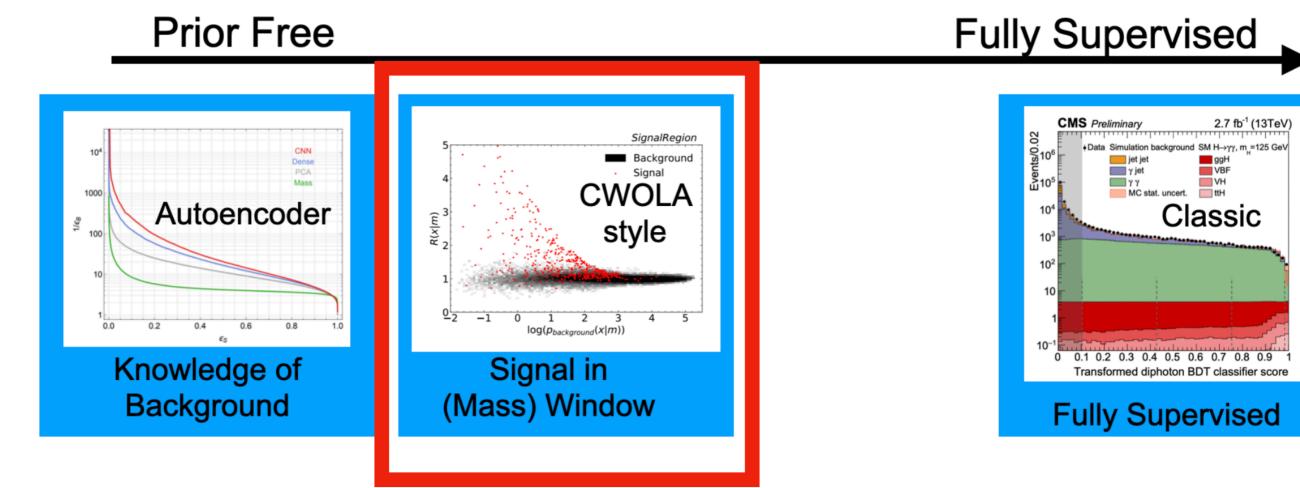
Likelihood Discrimination



Performance Observations



Anomaly Searches Spectrum

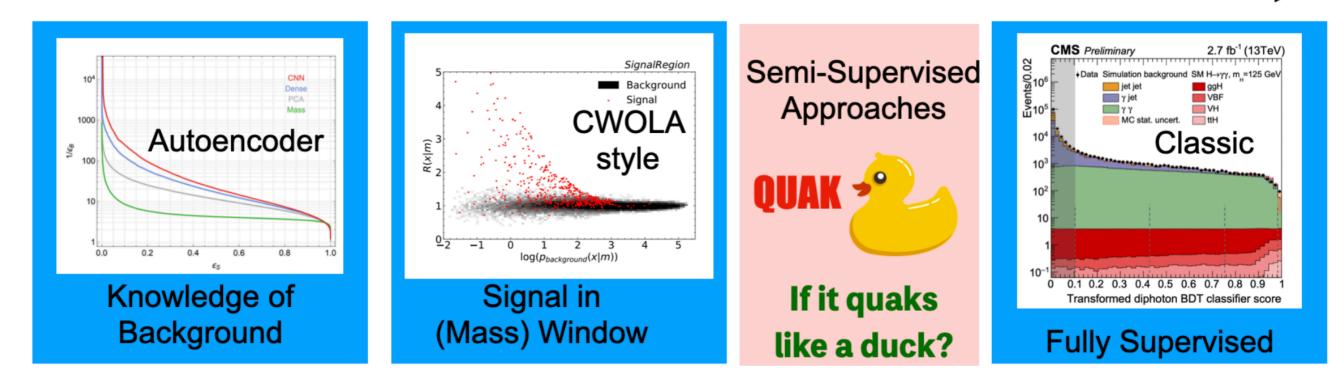


Gain in sensitivity by assuming a mass peak Adding assumptions about the signal

Playing with Prior

Prior Free

Fully Supervised

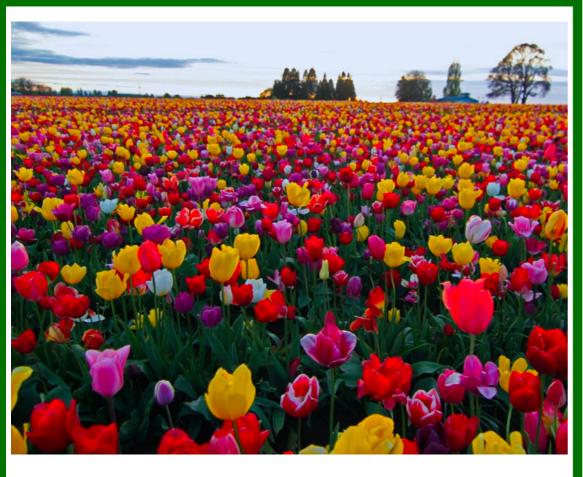


Gain in sensitivity by assuming a mass peak Adding assumptions about the signal

What if we decide to add more signal assumptions? Can we make a robust construction?

Semi-Supervision

Autoencoder



Supervised Training



A small amount labeled data

A large amount of unlabelled data

• Use supervised training to catch

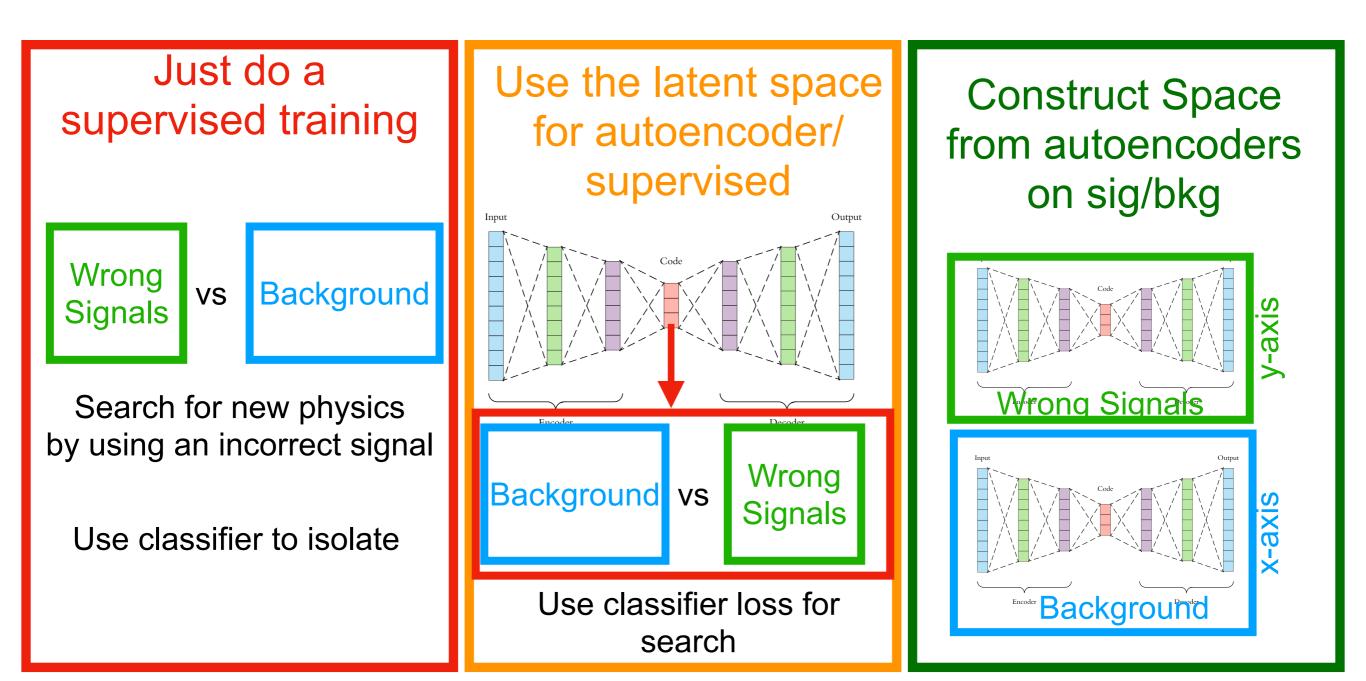




(i.e. Find anamalous tulips not anomalous something else in LHC a detector glitch)

Training Strategies

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One-Shot Learning

Normalizing

Flow

One-shot learning aims to build a space of similar objects



Our idea: Normalizing Flow to build a latent space of physics objects

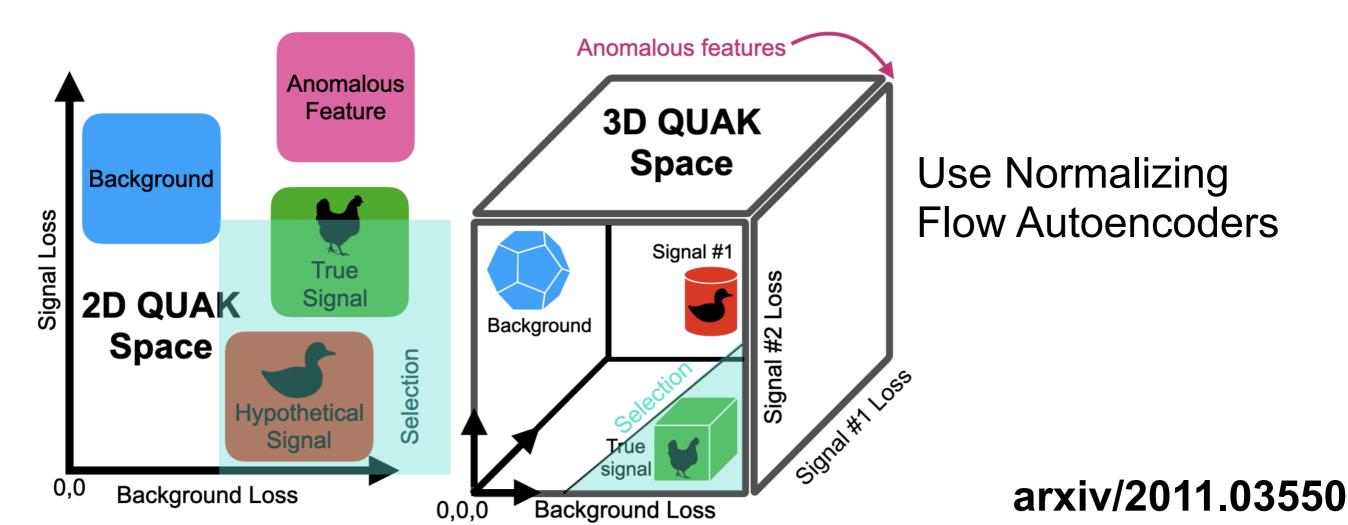
➡Similar

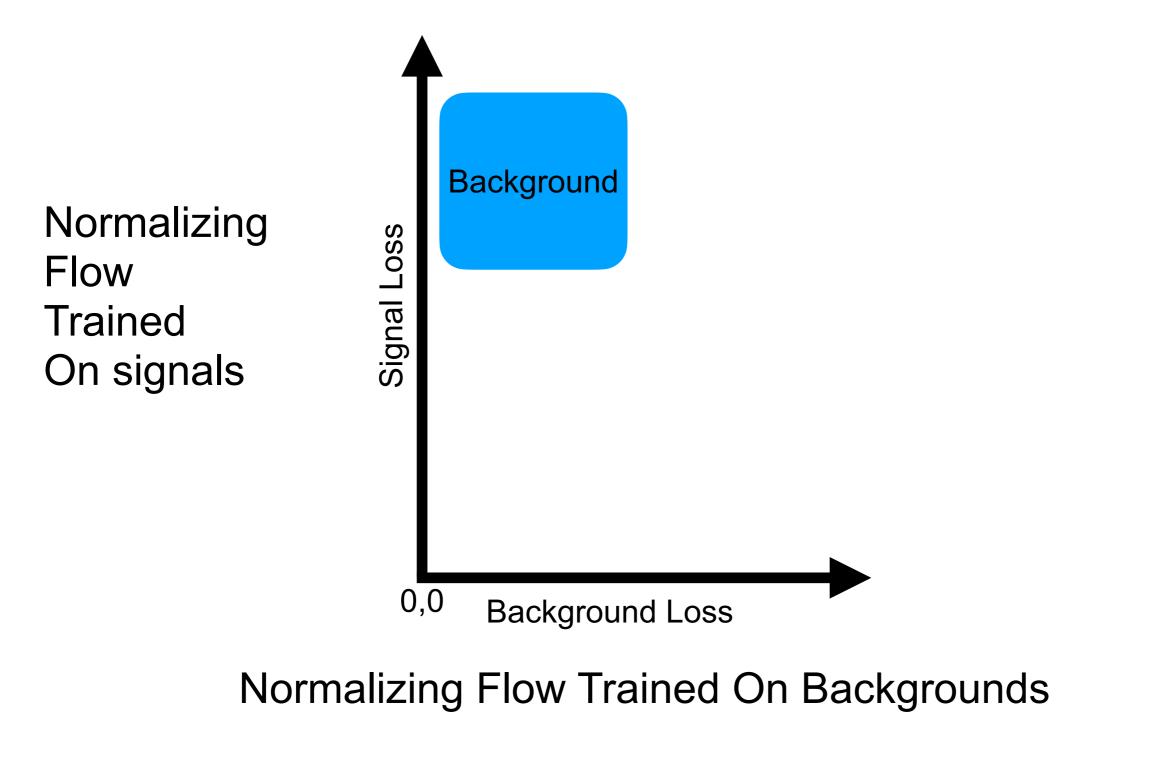
QUasi-Anomalous Knowledge(QUAK)

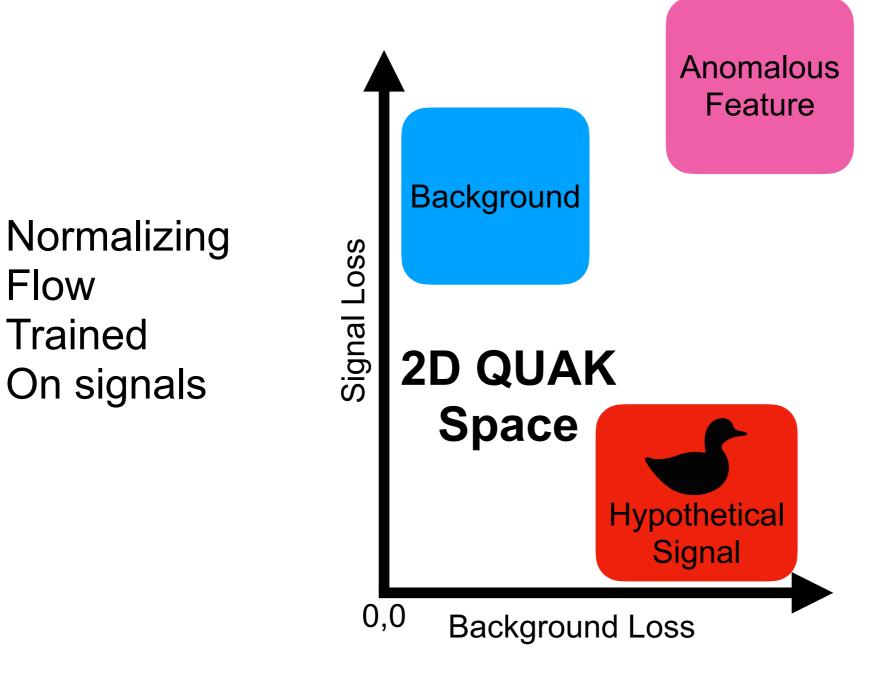
Strategy: Train autoencoders on background and Signals

Choose a broad range of signals that capture physics of interest

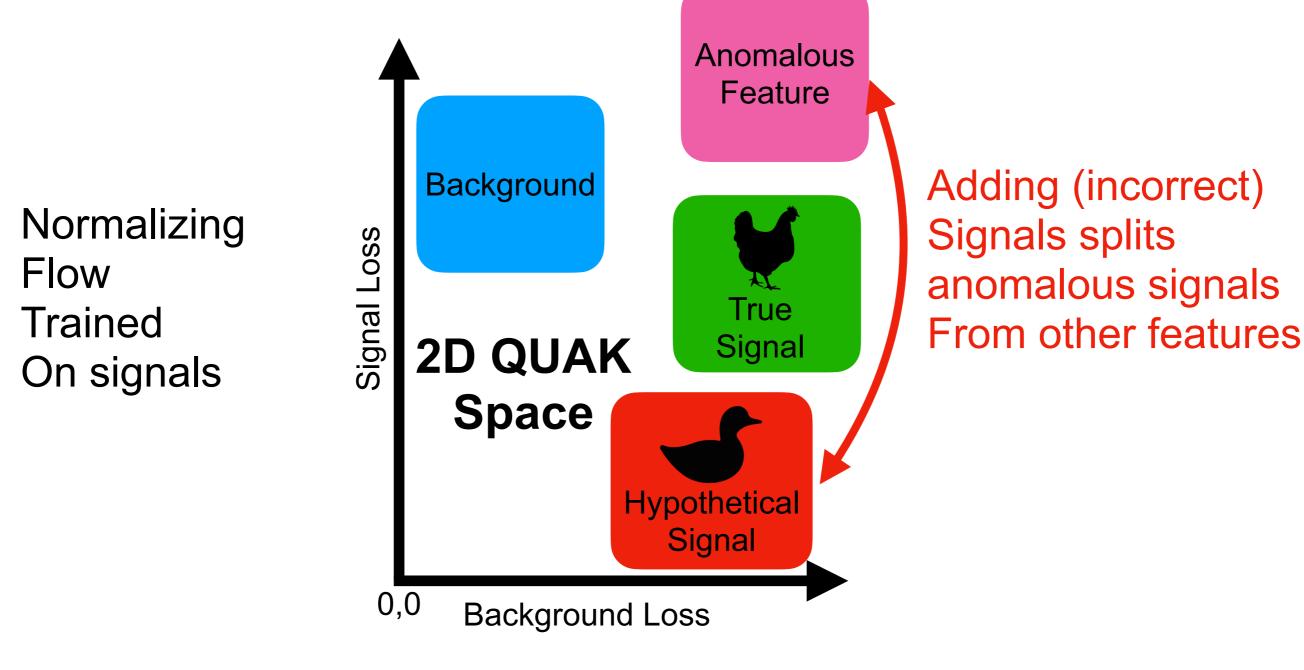
Probe the result space for physics-like anomalies



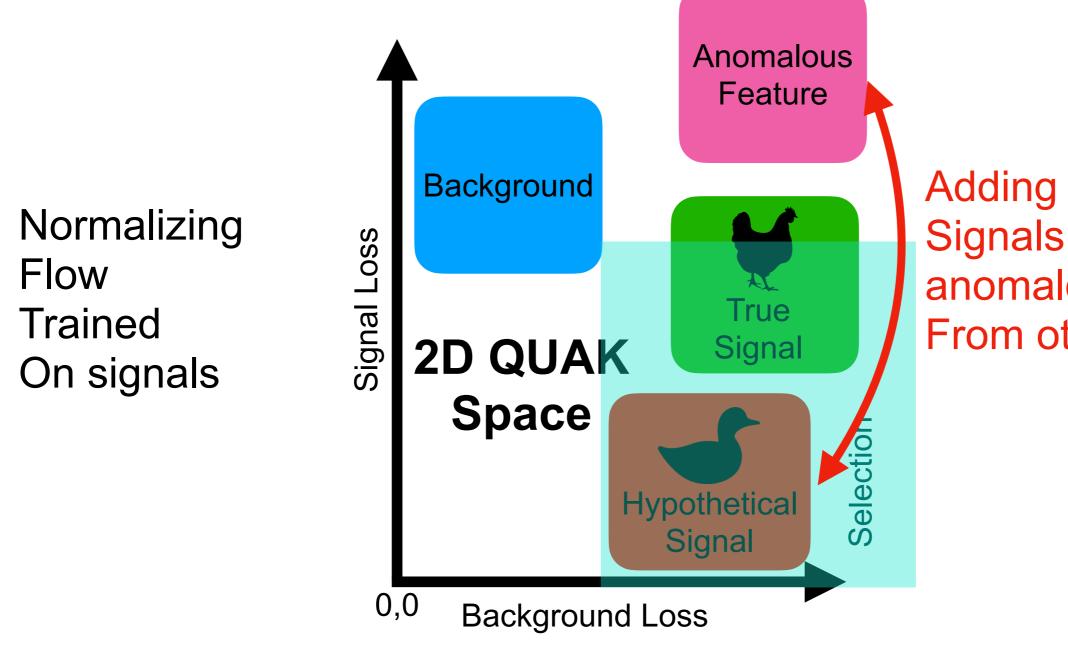




Normalizing Flow Trained On Backgrounds



Normalizing Flow Trained On Backgrounds

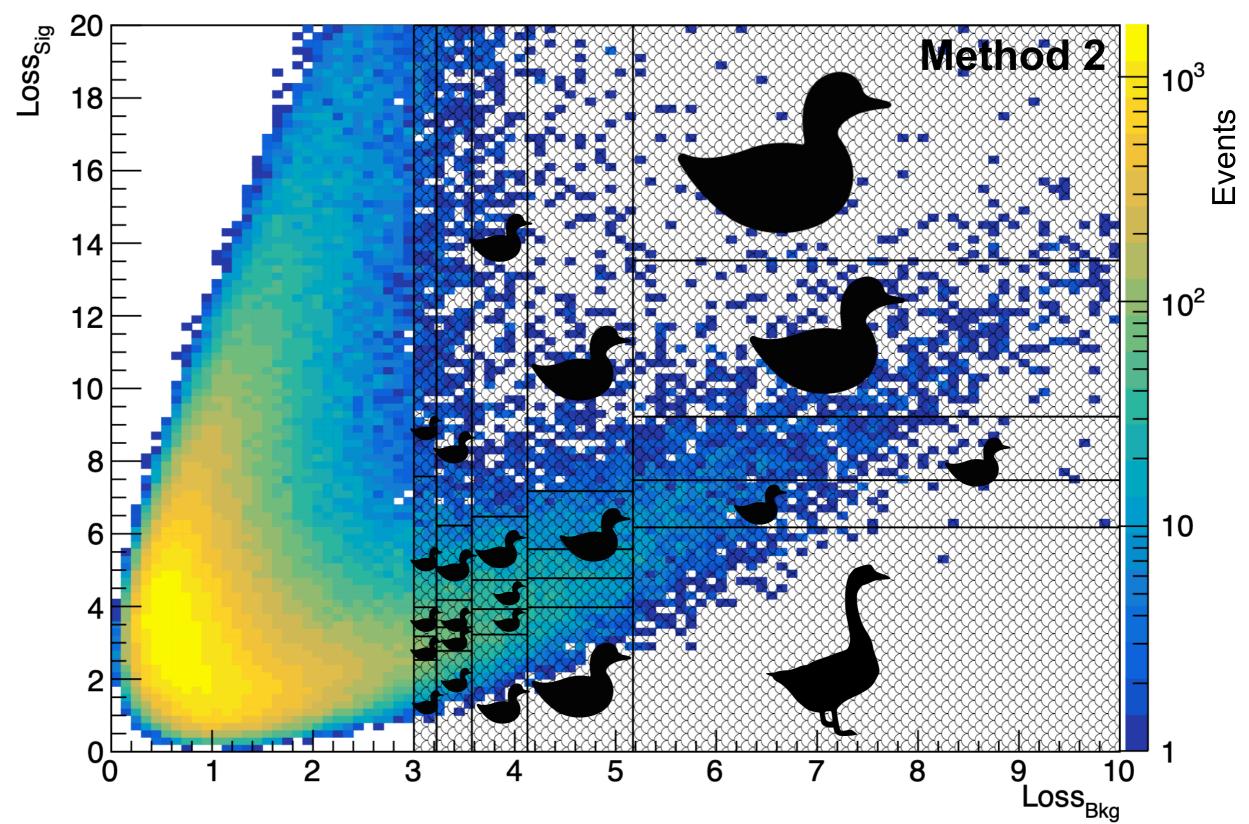


Adding (incorrect) Signals splits anomalous signals From other features

Normalizing Flow Trained On Backgrounds

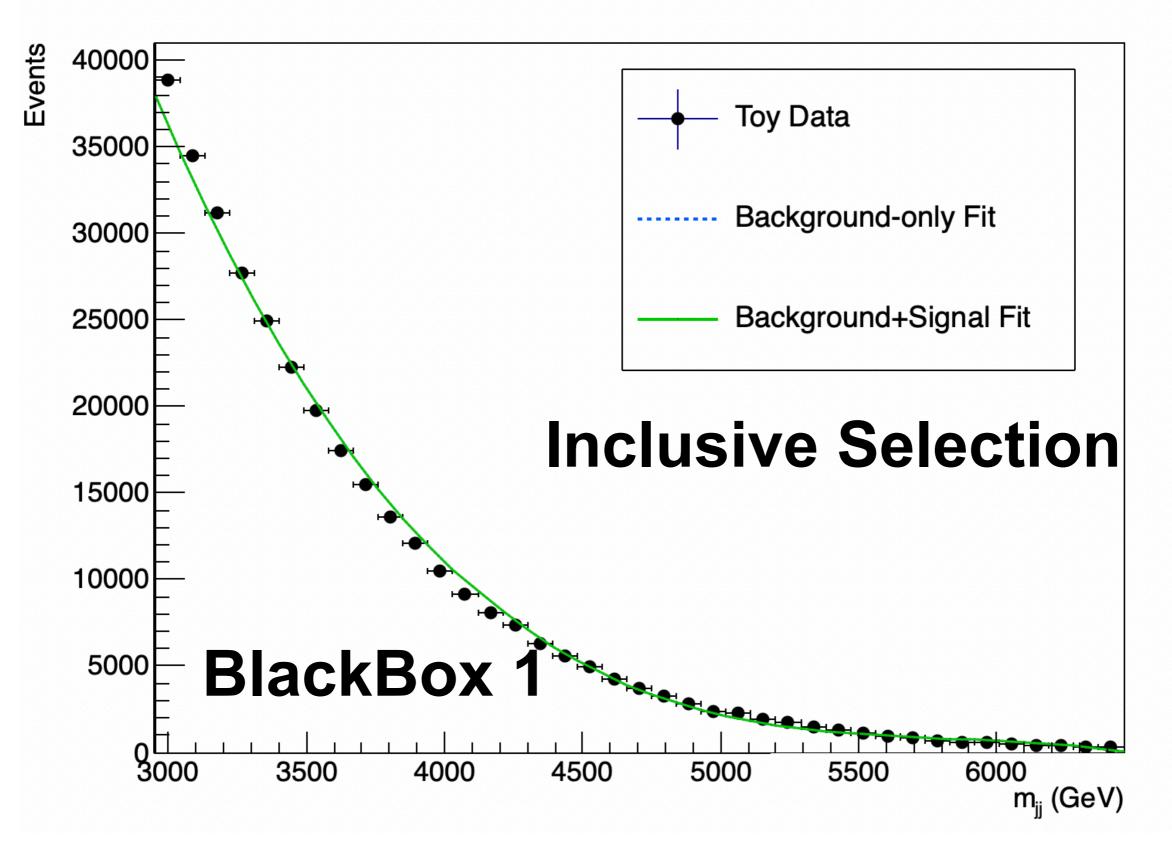
Duck Duck Goose!

Search all of the regions one big simultaneous fit

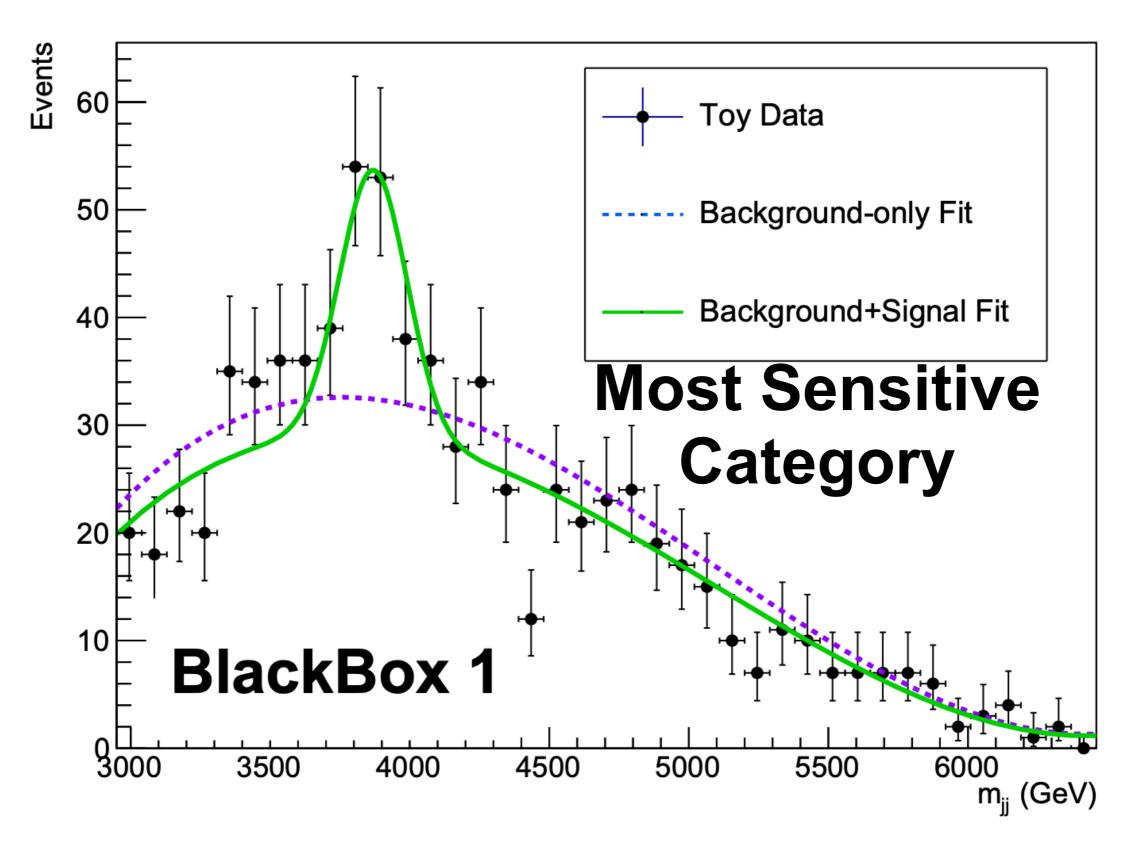


Seeing a Signal

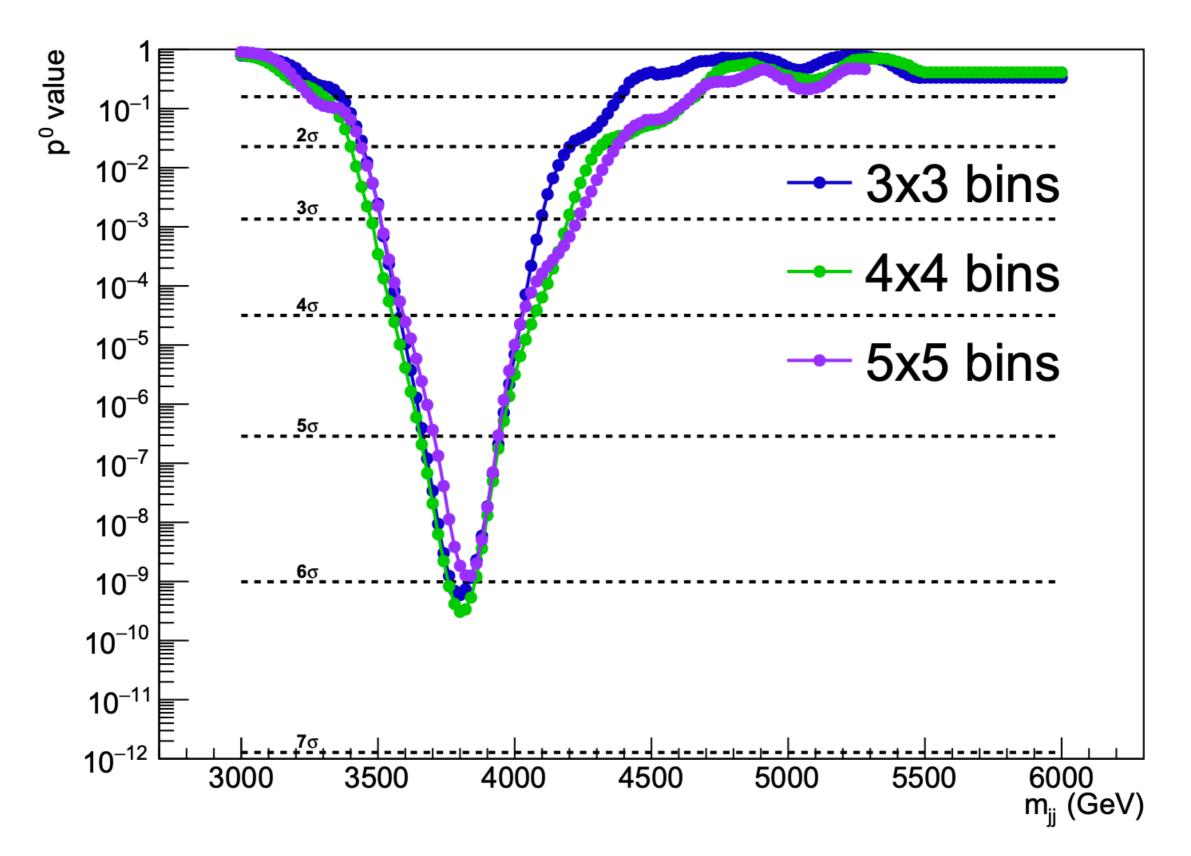
145



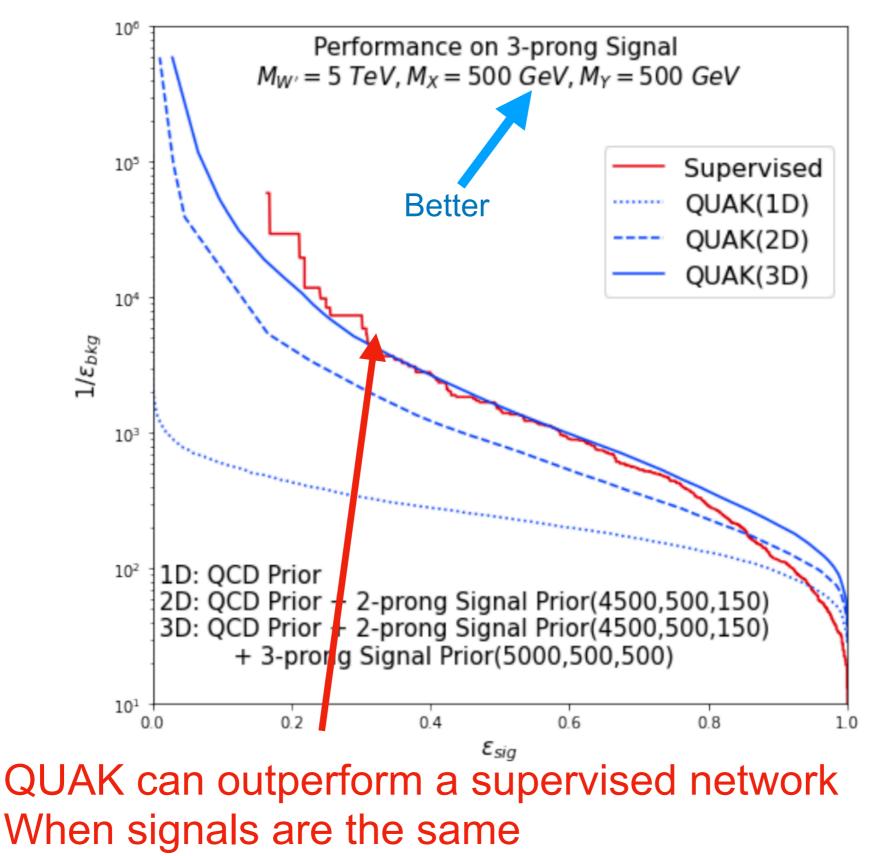
Seeing a Signal



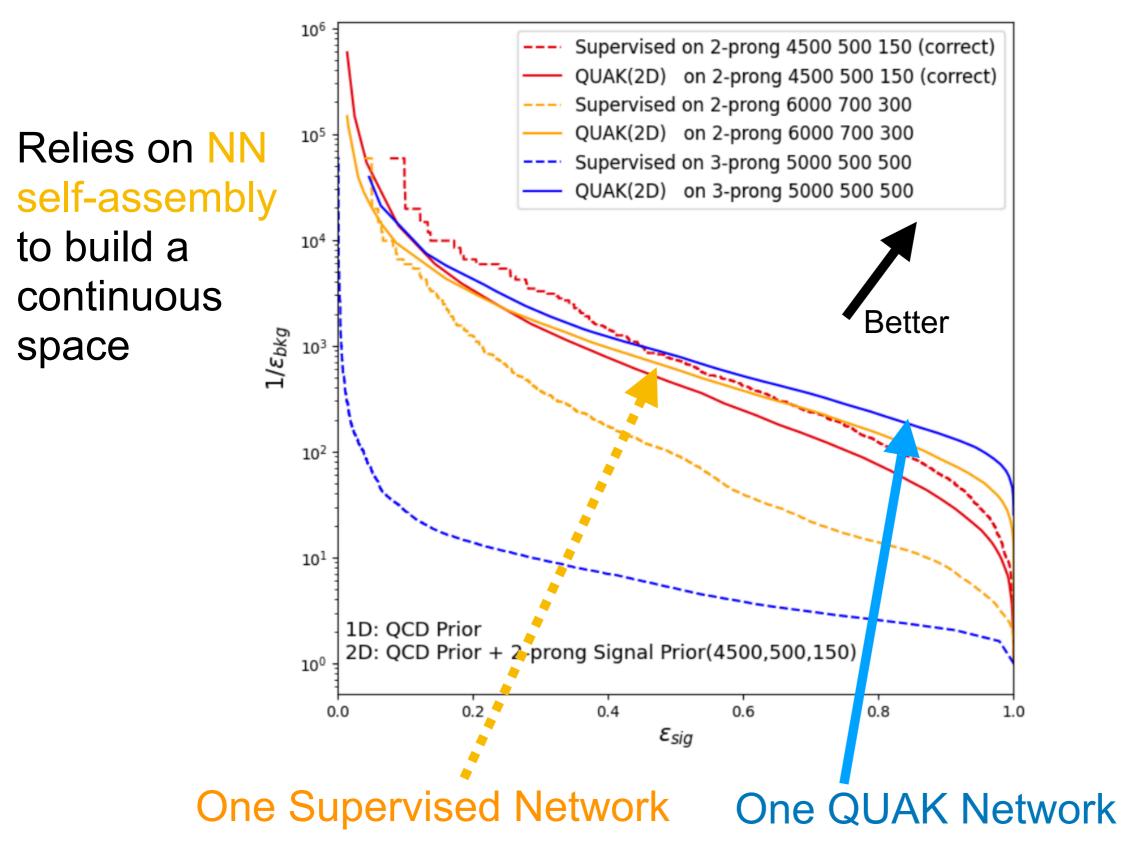
Applying to Anomaly



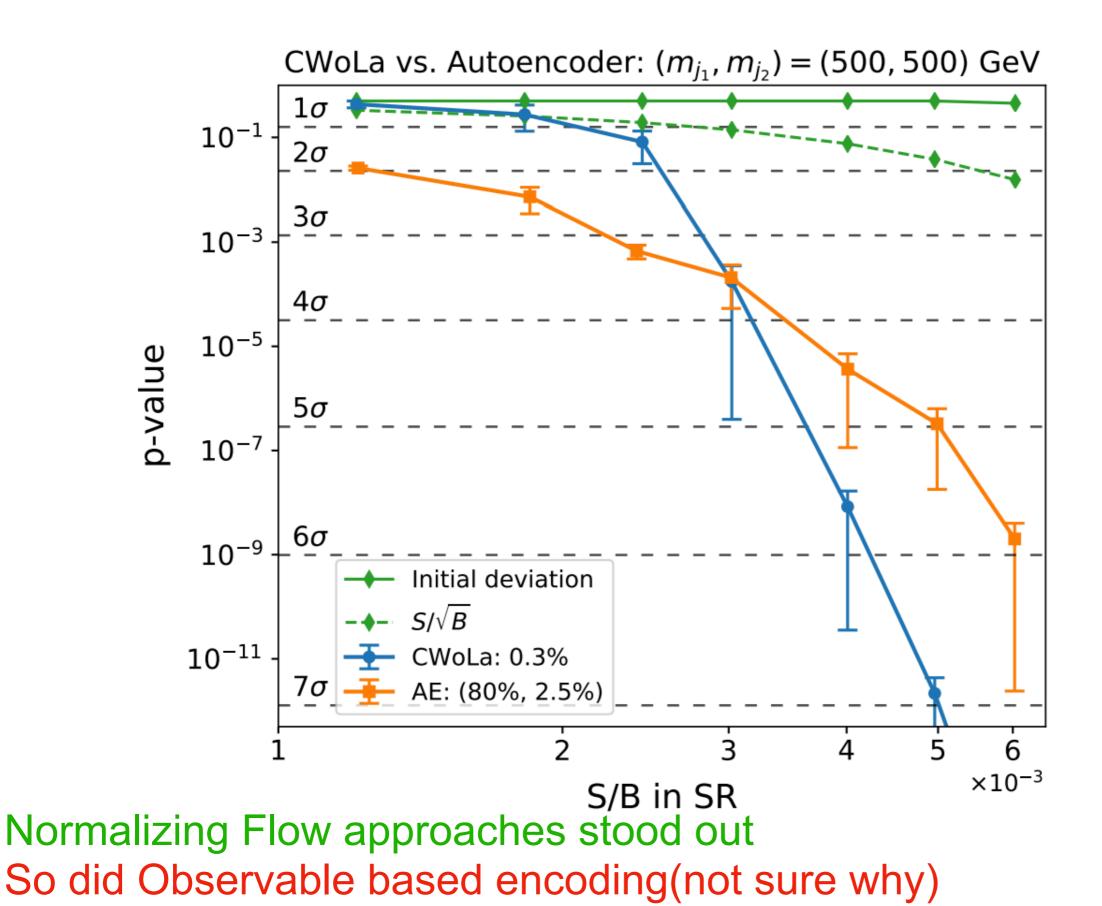
How Close to Optimal?



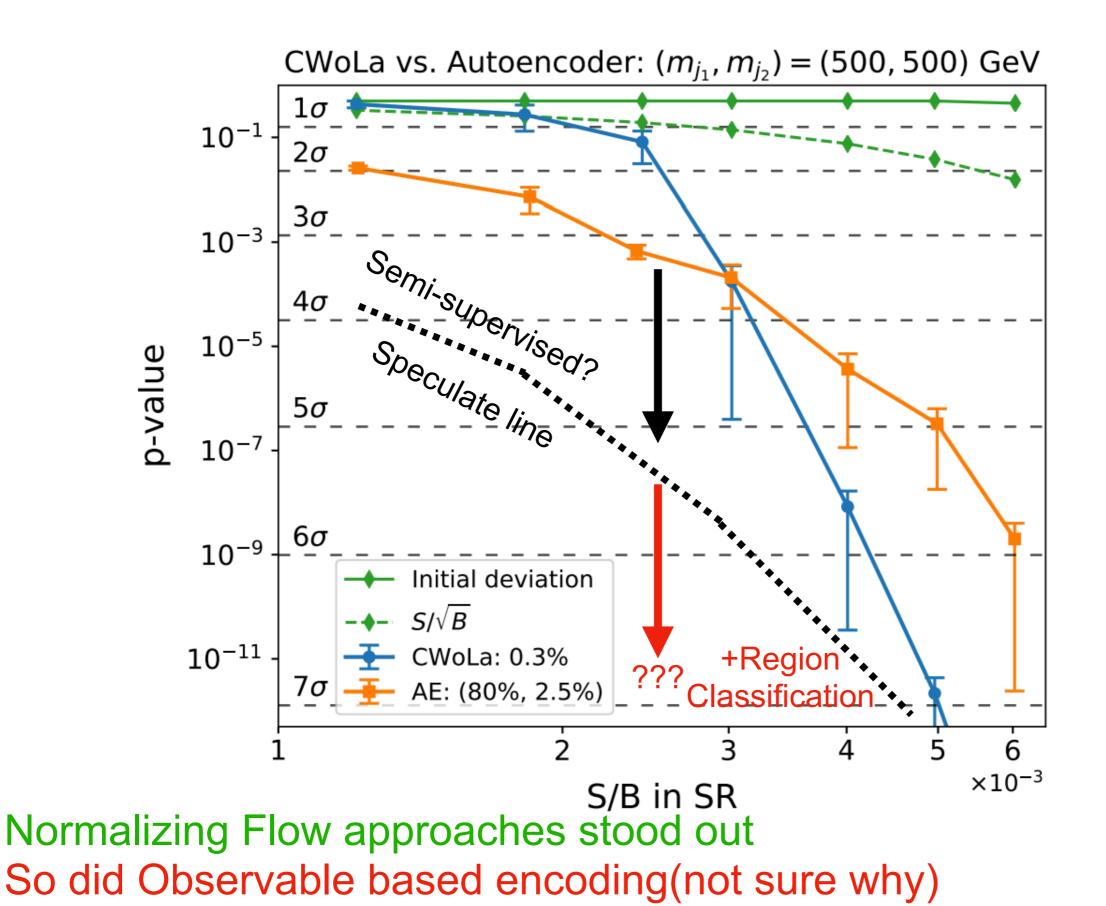
How Close to Optimal?



Performance Observations



Performance Observations



What will the future be?

- Deep learning is helping us to look at things in finer detail
 - It lets us go deeper and make sense of things



Did we find all the Higgs bosons in there?

Towards The Future 152

What are all the hidden signals in there?

Deep Learning can help¹⁵³ Elucidate

- Al is helping us to look at things in finer detail
 - It lets us go deeper and make sense of things



Did we find all the Higgs bosons in there?

Towards The Future

Perhaps there is a hidden Discovery

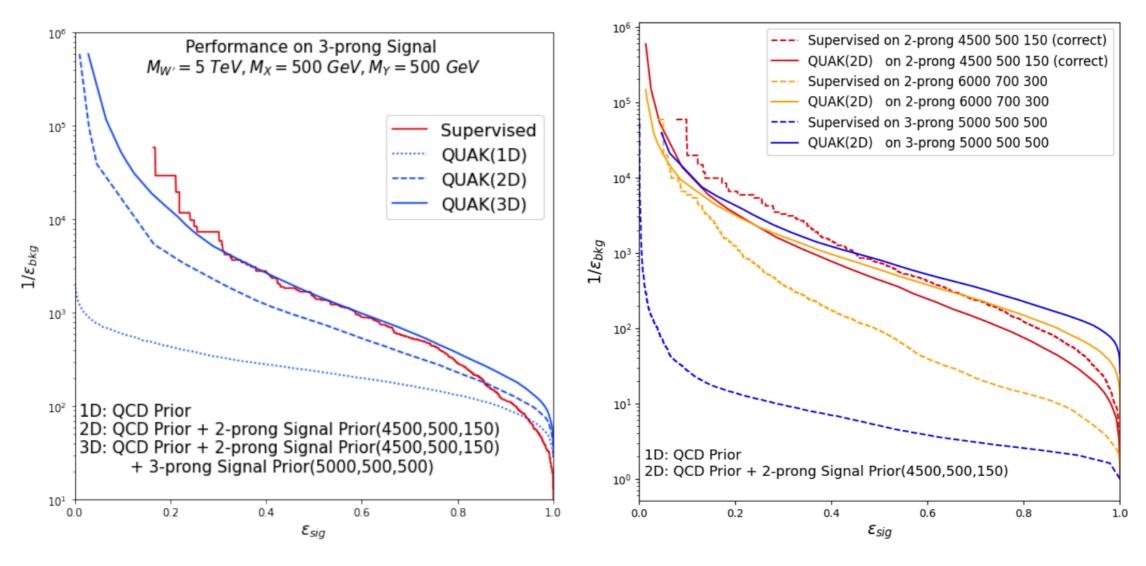
What are all the hidden signals in there?



Thanks to the organizers for inviting me!

QUAK

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QUAK approaches or beats supervised NNs when signal is similar

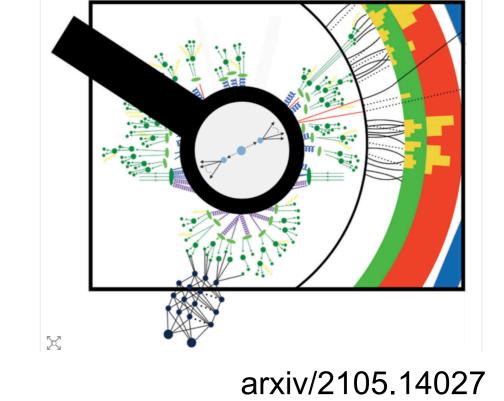
Has been observed in literature with similar type of constructions Relies on NN self-assembly to build a continuous space Space starts to classify regions of algorithms

Overview of this talk

- Strategy for this talk
 - I will do a broad overview of ideas about deep learnig
 - The idea is to discuss various general trends
 - Would like to tie this in to broad vision of AI
 - Mostly this will showcase work from my group
 - Don't consider this a full survey of methods
 - Even though title says LHC I will go beyond at times

Two Anomaly Challenges LHC Olympics 2020 Dark Machines





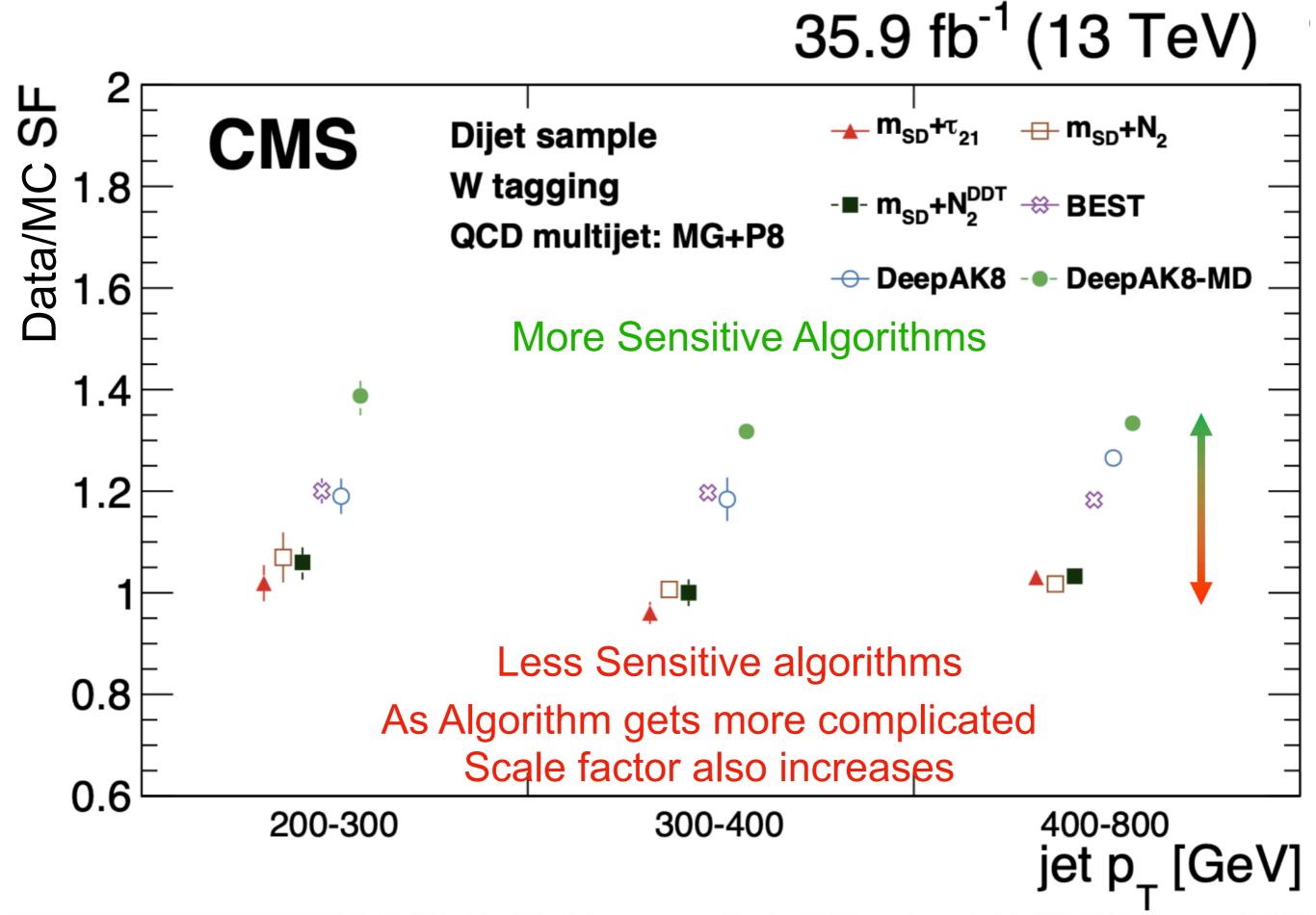
David Shih, Ben Nachman, Gregor Kasieczka

- LHC Olympics focused on find a single di-jet resonant model
- DarkMachines focused on searching for a broad range of models

LHC Olympics 2020

- Over the past year there were two competitions
- In each setup a signal/signals wer hidden in pseudo data
 - The challenge was to "Find the hidden signal"
 - Emulate a realistic analysis as much as possible
 - Challenge : use deep learning to find an anomaly
- A number of different strategies are used for this approach
 - We will review the core concepts of these strategies

hep-ph/2101.08320



Next generation of taggers would benefit from next generation of MC

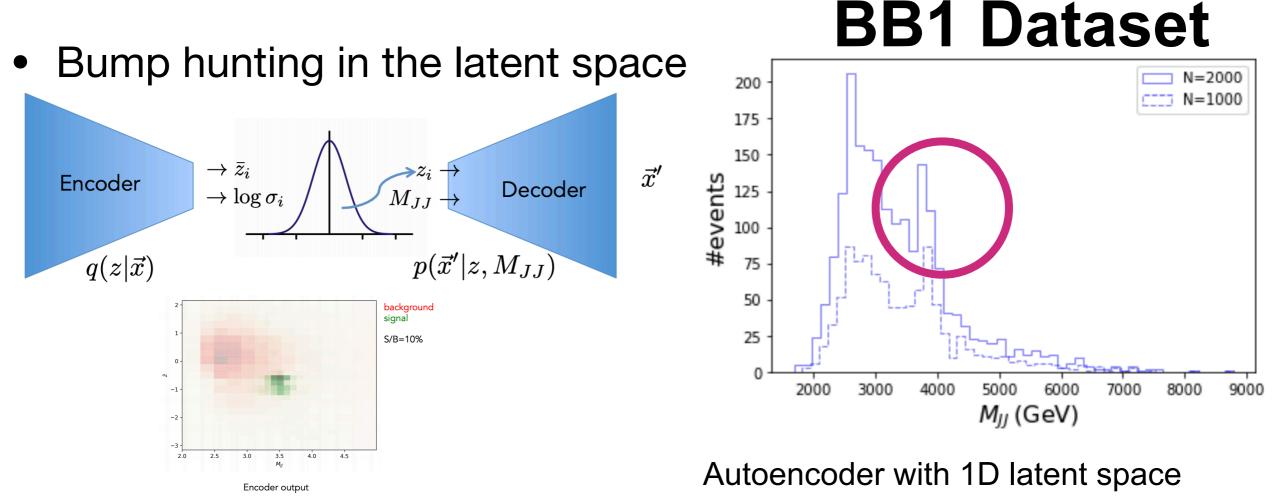
Training on Data

161

- Generally with anomaly approaches
 - There has been an emphasis to train on data
- Training on data simplifies our ability to process data
 - No need to correct for simulation/data disagreements
 - Regions where data/simulation don't agree can be probed
 - No fancy methods to probe these regions w/complicated fits
- Training on data throws away some interpretability of result
 - Not clear what features may drive an access

BuHuLaSpa

Inputs: High Level Features (Nsubjettiness/Jet masses/...)



Latent space forced to be decorrelated with mass

$$\mathcal{L} = -D_{\mathrm{KL}}(q_{\phi}(\vec{z}_i|\vec{x}_i)|p(\vec{z}_i)) + \beta_{\mathrm{reco}}\log p_{\theta}(\vec{x}_i|\vec{z}_i)$$

Signal Extraction : None

 \vec{x}

Take Away: Training is critical to ensure good performance

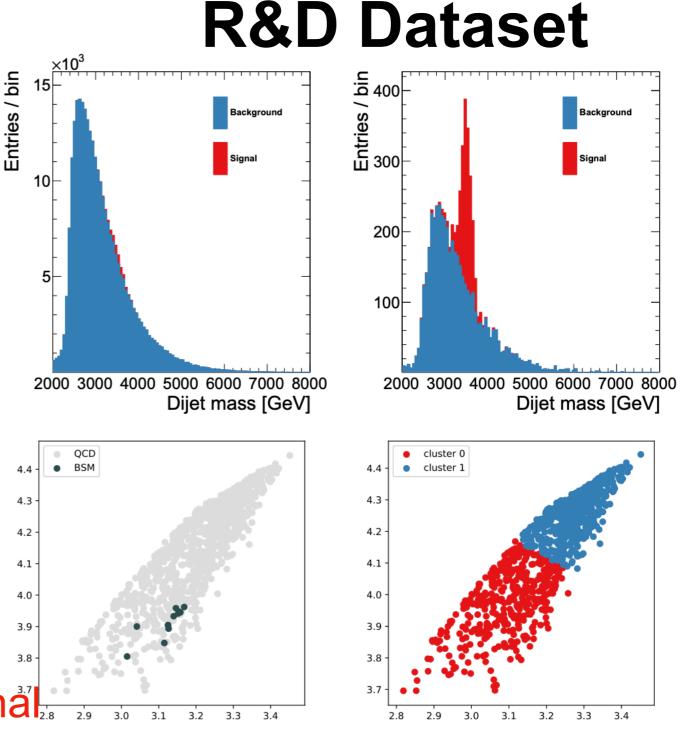
UCluster

Inputs: Particle Objects

Train a supervised network for jet classification

Cluster in the latent space Scan clusters for anomaly

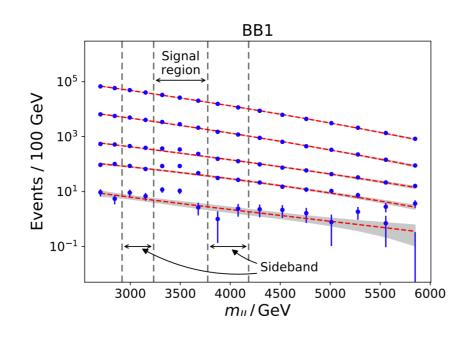
Signal Extraction : No signal Take Away: Hard with small signal <u>https://arxiv.org/abs/2010.07106</u>



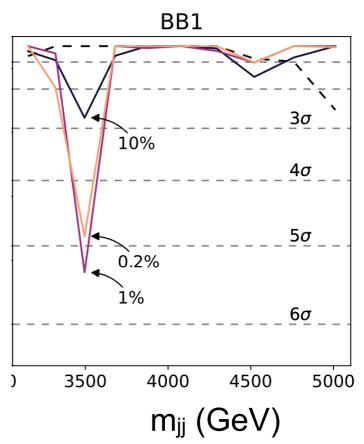
CWOLA

Inputs: High level features

- CWOLA modified from original paper
 - Mass inputs dimensionless



BB1 Dataset



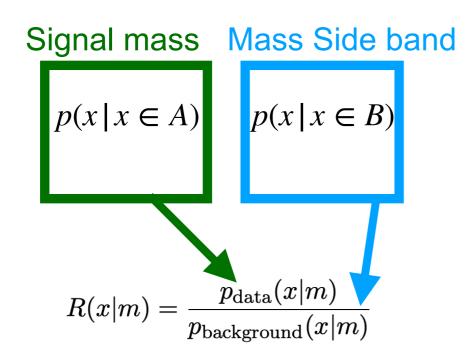
Signal Extraction : Bump fit(5σ)

Take Away: Works but needed to correct dimension

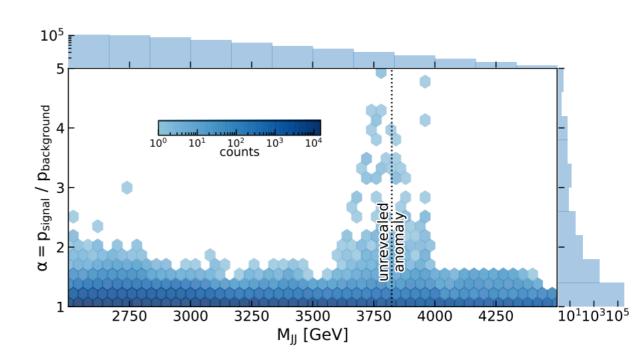
GIS(CWOLA+NF)

Inputs: High level features

GIS normalizing flows trained conditional on the mass distribution Scan mass window (250 GeV) Compute likelihood ratio (below)



BB1 Dataset



Large and significant signal

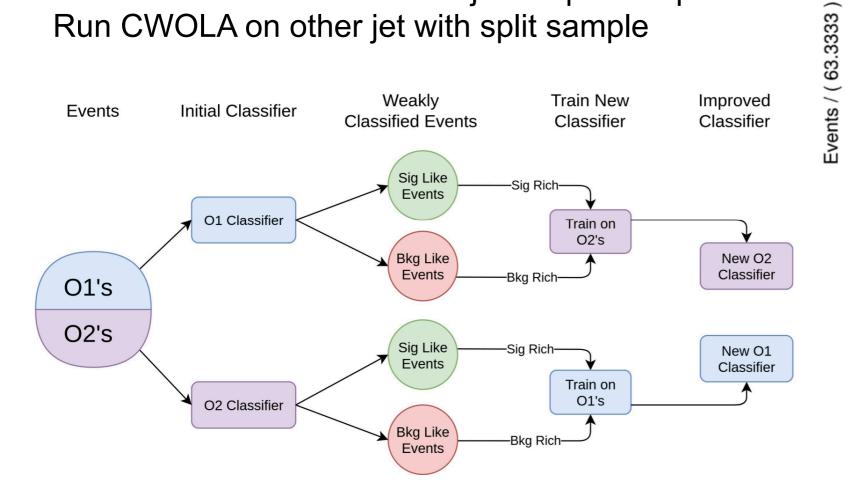
Signal Extraction : Note, but large signal

Take Away: Normalizing Flow can help CWOLA style approach https://arxiv.org/pdf/2001.04990.pdf

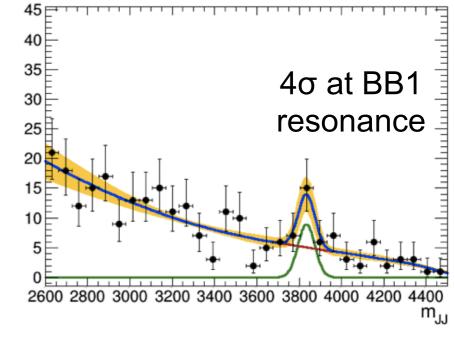
Tag N'Train

Inputs: High level features

Use dijet signature play one jet off the other Start with an autoencoder on jet to split sample Run CWOLA on other jet with split sample



BB1 Dataset



Would benefit more from mass decorrelation

Signal Extraction : Bump Fit

Take Away: Avoid mass windows by relying on the different jets https://arxiv.org/abs/2002.12376

GAN supported AE

Inputs: High Level Features (Nsubjettiness/Jet masses/...)

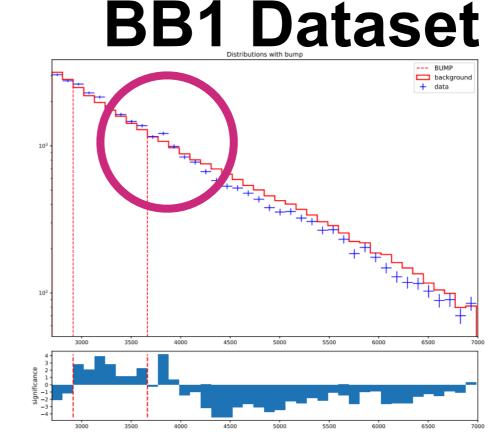
- Build an auto encoder (AE)
 - Add an GAN to help AE
 - Additionally decorrelate with mass

 $loss_{AE} = BC + \varepsilon \times MED + \alpha \times DisCo$

itent space forced to be decorrelated with mass

Signal Extraction : Bump Hunter (it Failed)

Take away: Mass Decorrelation+Good Simulation needed



Normalizing Flow

Inputs: High Level Features (Nsubjettiness/Jet masses/...) BB1 Dataset

0.0008

- Use a normalizing flow
 - Cut on high loss
 - Decorrelate loss with mass

$$\mathcal{R}_{m_{jj}}(x) = \frac{||x - g(g^{-1}(x))||^2}{1 + \frac{p_u(g^{-1}(x))}{p_{KDE}(m_{jj}^x)}}$$

Data cut (high R_{mii}) R_{mii} thrsh : 50th percentile 0.0007 R_{mii} thrsh : 70th percentile 0.0006 0.0005 0.0004 0.0003 0.0002 0.0001 0.0000 2000 4000 6000 8000 10000 m_{ii}

Cut is too loose (may actually work)

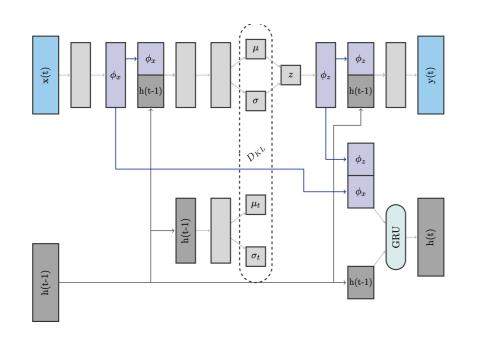
Signal Extraction : None (No signal)

Take Away: single auto encoder even with NF is not enough too many anomalies (no clear signal)

Particle VAE

Inputs: Particle four vectors of the jet

• VAE using particle inputs (RNN)

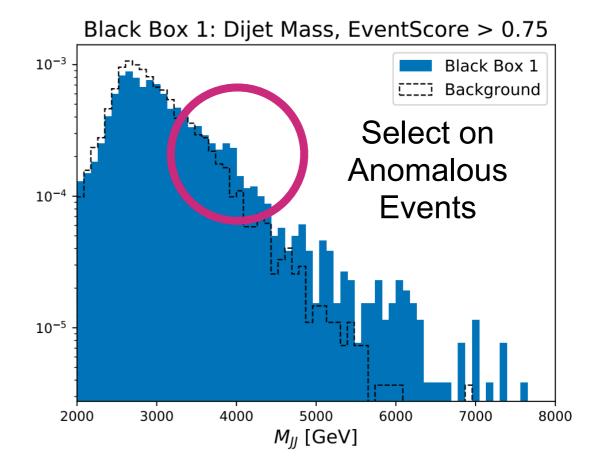


 $\mathcal{L}(t) = \text{MSE} + 0.1 \times \overline{p_T}(t) D_{\text{KL}}$

Anomaly Score = $1 - e^{-\overline{D_{\text{KL}}}}$ Signal Extraction : None

Take Away: Works but preparation of inputs is critical

BB1 Dataset

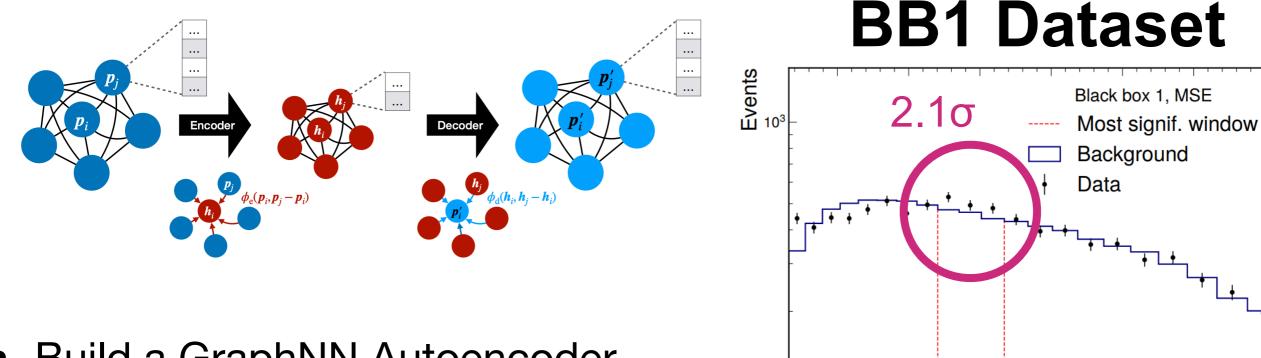


Particle Graph AE

Inputs: Particle four vectors of the jet (Graph w/correlations)

 10^{2}

Signif.



- Build a GraphNN Autoencoder
 - Try with mean squared error loss

Signal Extraction : Bump Hunter Algo Take Away: No good handle on loss

Just Training

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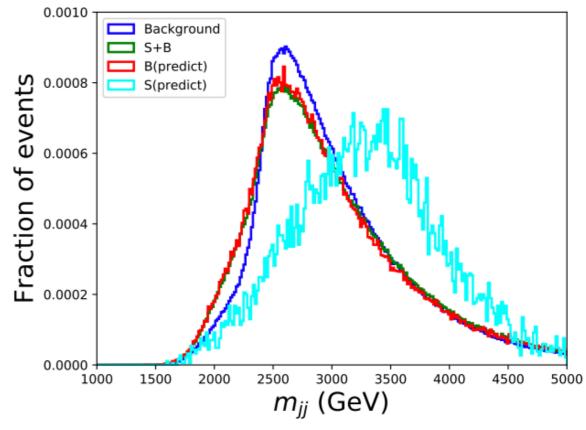
Inputs: High level features

Use R&D dataset and do a fully supervised training

Use the output discriminator

Try to see a signal from that

BB1 Dataset



Two submissions tried No Significant excess in either

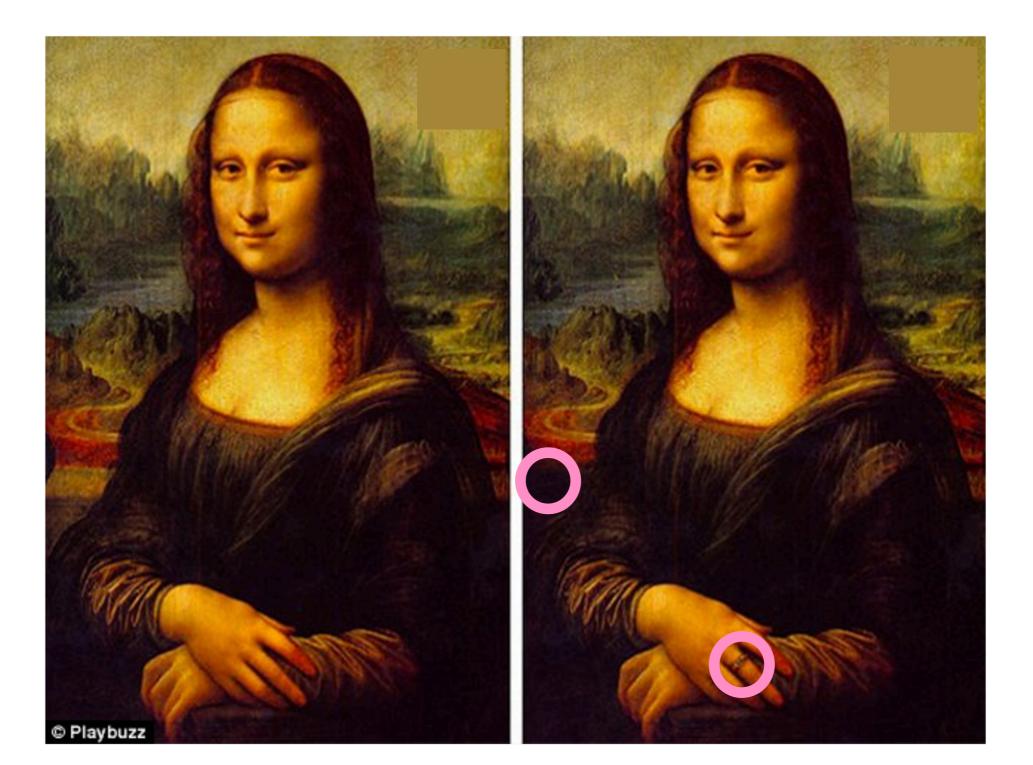
Signal Extraction : None

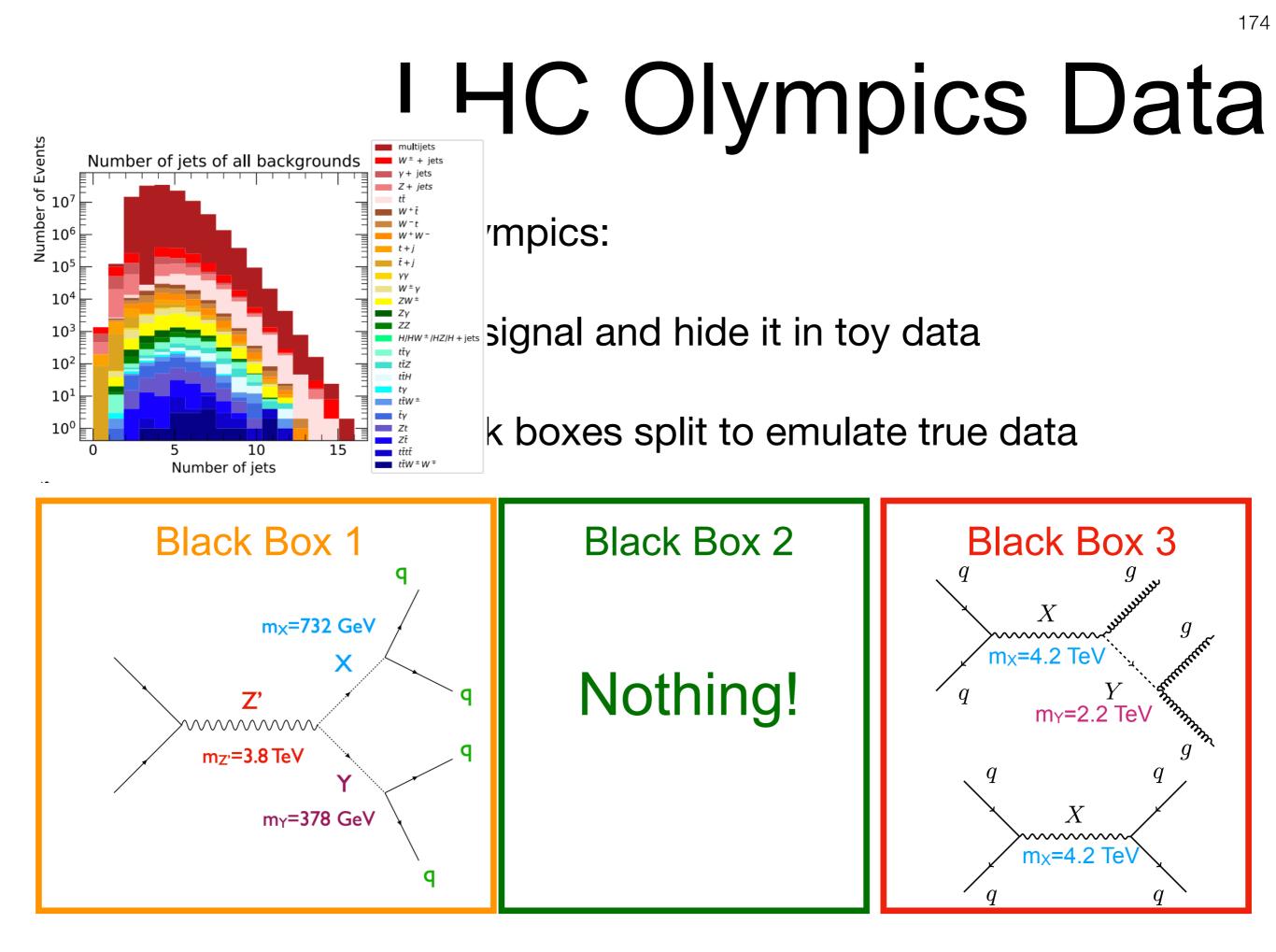
Take Away: Signal needs to be close to the hidden signal

What is different w/Left and Right?



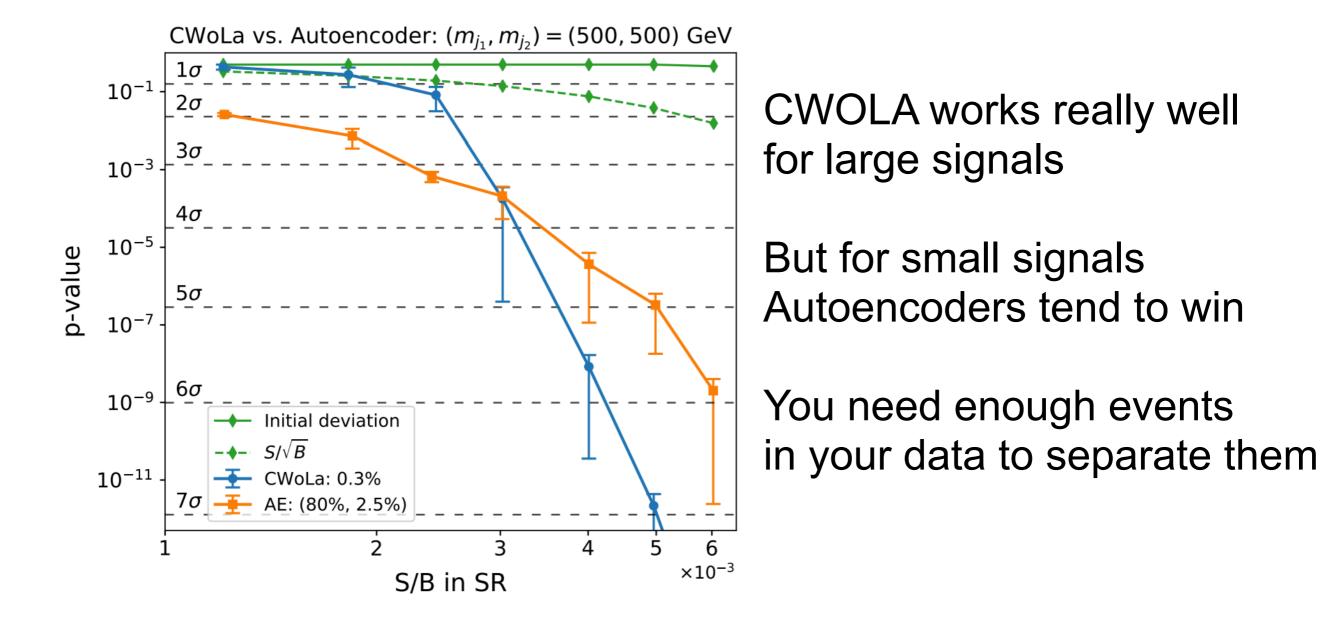
The Need for Subtlety





Observation

Inputs: High level features

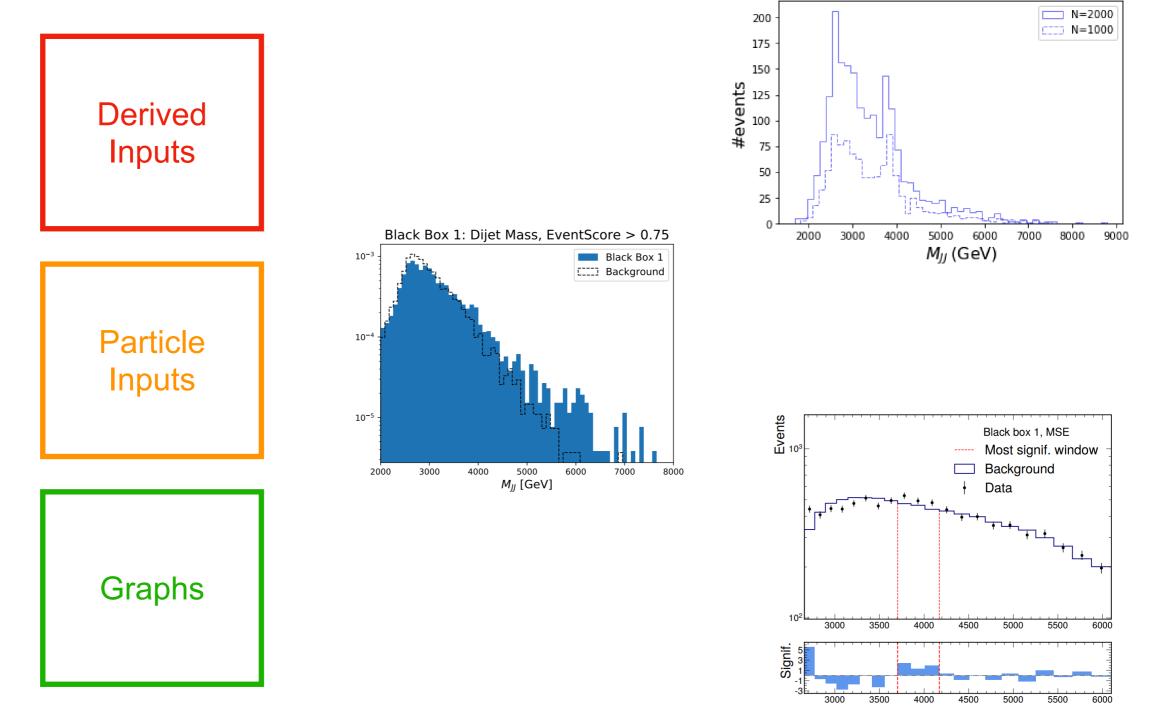


Signal Extraction : Bump fit

Take Away: Works but needed to correct dimension

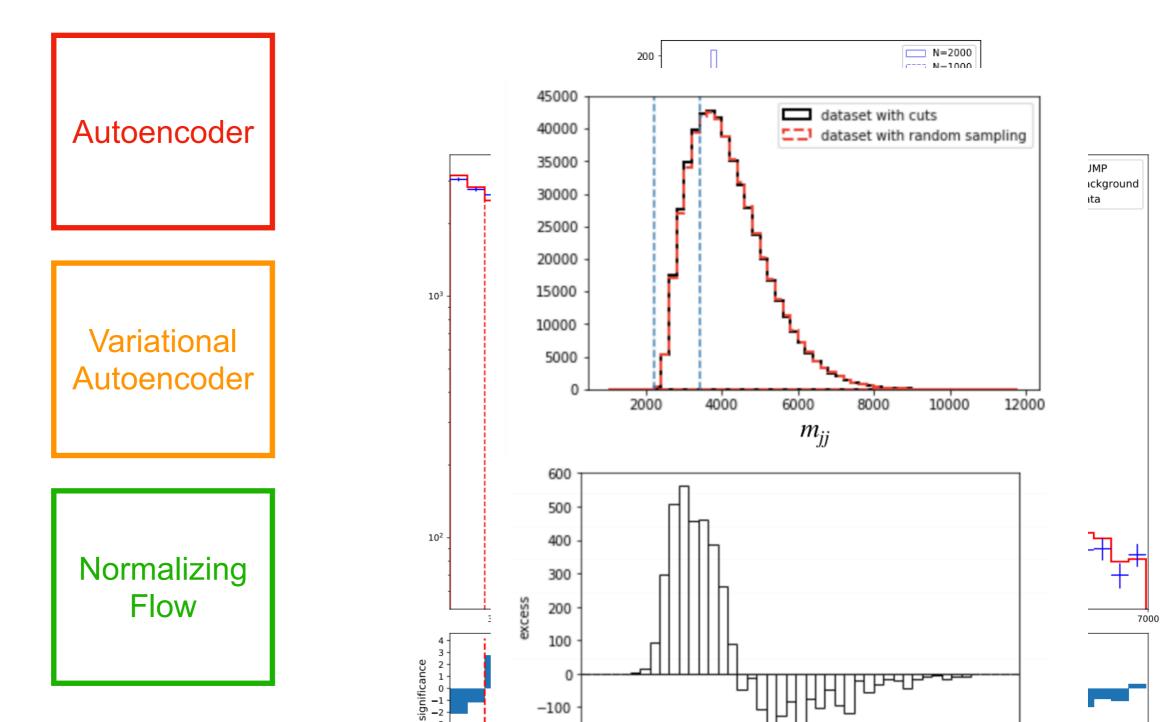
Variation of Encoder

Varying the encoder architecture can allow for a broad range of possibilities

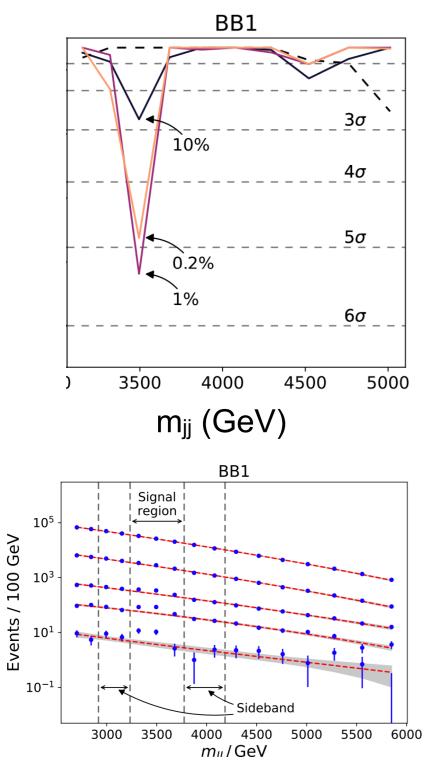


Variation of Architecture

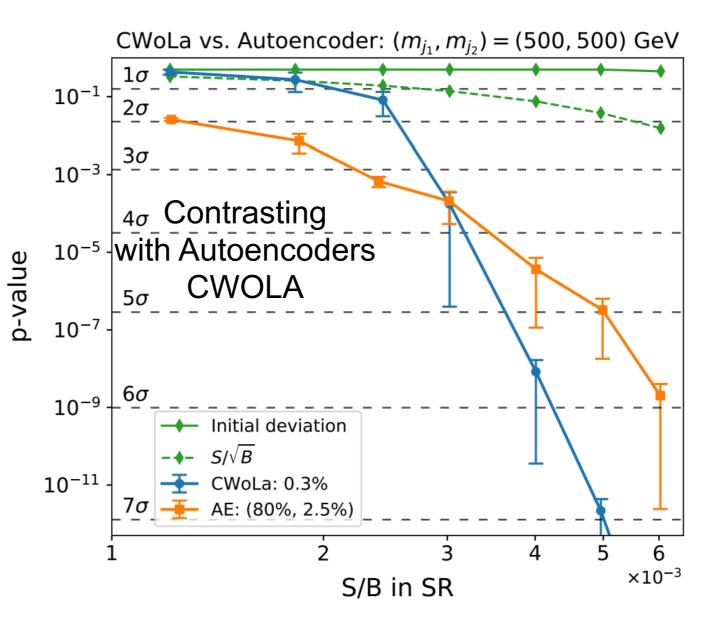
Varying the encoder architecture can allow for a broad range of possibilities



CWOLA style approach



- Running just a training got it to work
 - Was able to observe 5 standard deviations

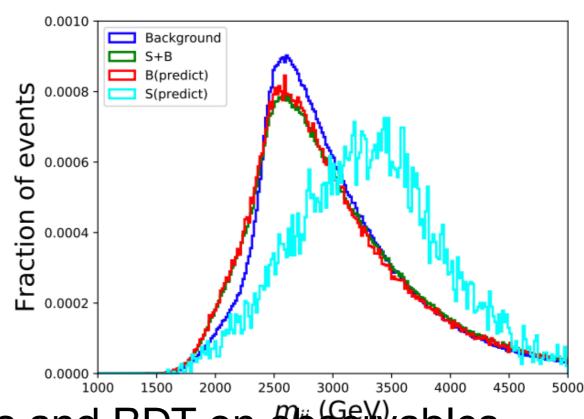


Excess at 3500 instead of 3800

Method 12:Deep Ensemble

- Use R&D dataset and do a fully supervised training
 - Use the output discriminator
 - Try to see a signal from that
 - Try with both a CNN on jet images and BDT on doservables

Observation:Low noise robust density estimation is key

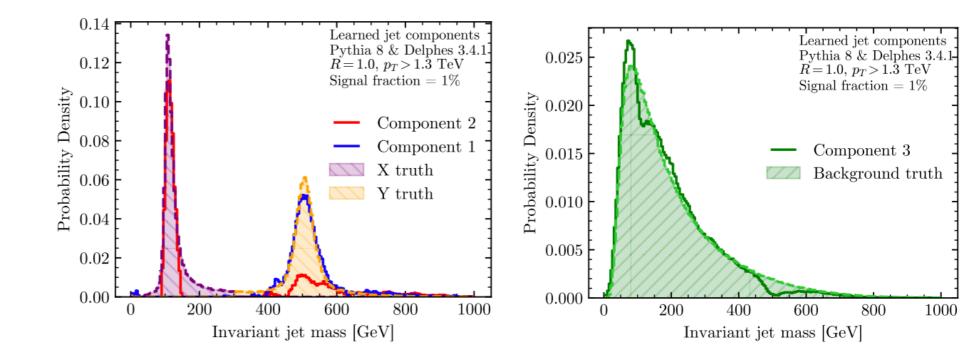


 m_{j_1} (Gev)

Method13:Factorized

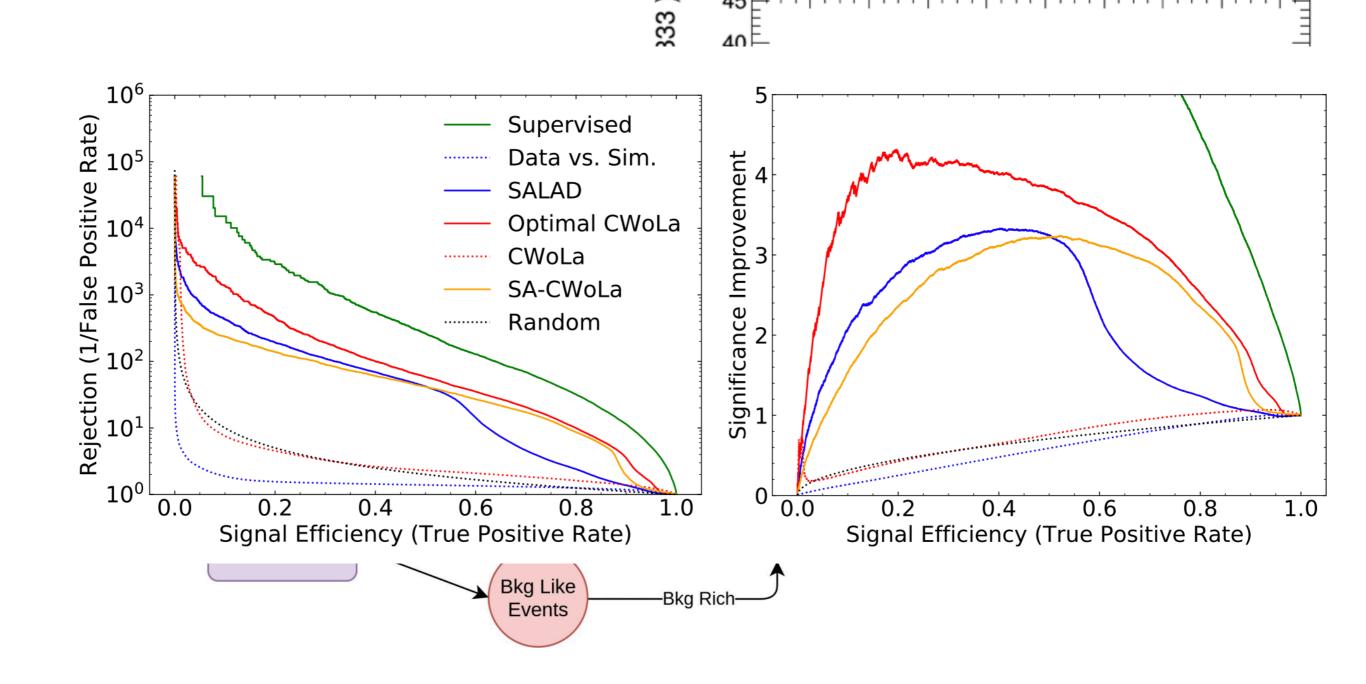
- Sample independence: each jet of a dijet can be treated as **Topics** independent and for QCD its composition is the same for leading and subleading
- Factorization: jet mass distributions can be factorized

$$\mathcal{L}(\mathbf{x}_{1}, \mathbf{x}_{2}) = \frac{f(\text{signal}) \cdot p_{\text{signal}}(\mathbf{x}_{1}, \mathbf{x}_{2})}{f(\text{background}) \cdot p_{\text{background}}(\mathbf{x}_{1}, \mathbf{x}_{2})}$$
$$= \frac{f(X, Y) p_{X}(\mathbf{x}_{1}) p_{Y}(\mathbf{x}_{2}) + f(Y, X) p_{Y}(\mathbf{x}_{1}) p_{X}(\mathbf{x}_{2})}{f(\text{QCD}, \text{ QCD}) p_{\text{QCD}}(\mathbf{x}_{1}) p_{\text{QCD}}(\mathbf{x}_{2})}$$



Method 10: Salad+CWOLA

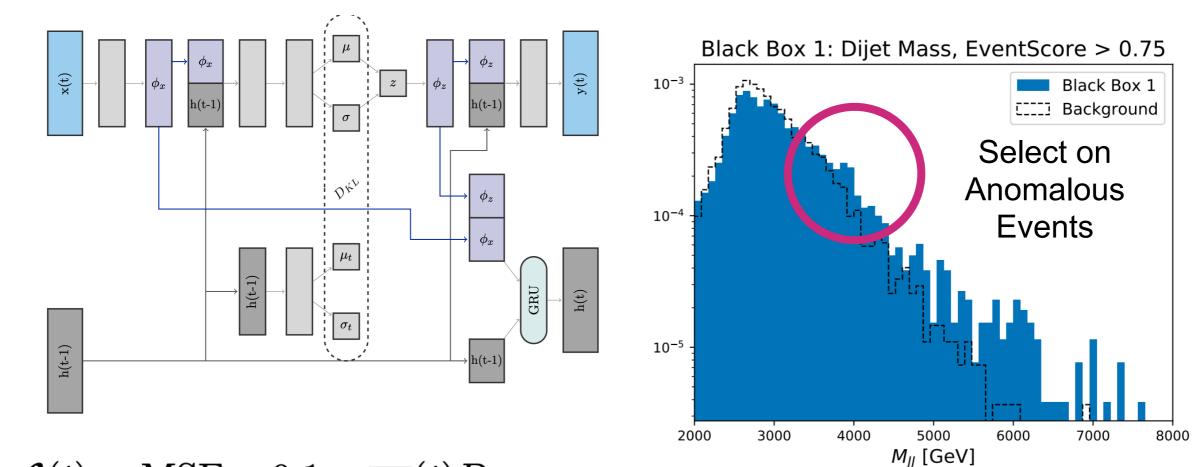
45



Observation:Works well on jets, some limiations from using jet images Would benefit more from mass decorrelation

Method1:VRNN

• Variational Autoencoder using particle inputs (RNN)



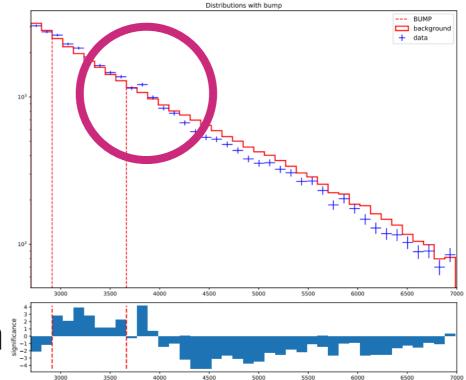
 $\mathcal{L}(t) = \text{MSE} + 0.1 \times \overline{p_T}(t) D_{\text{KL}}$

Anomaly Score = $1 - e^{-\overline{D_{\text{KL}}}}$

Observation: Works but preparation of inputs is critical

Method 3:GAN-AE

- Build an auto encoder (AE)
 - Add an GAN to help AE
 - Additionally decorrelate with mass
 - Compute a distance (ED) for anom



Autoencoder with 10D latent space Latent space forced to be decorrelated with mass

 $loss_{AE} = BC + \varepsilon \times MED + \alpha \times DisCo$

Observation: Mass Decorrelation+Good Simulation needed

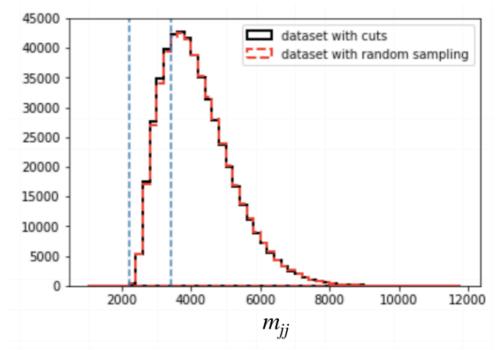
Method 4:LDA

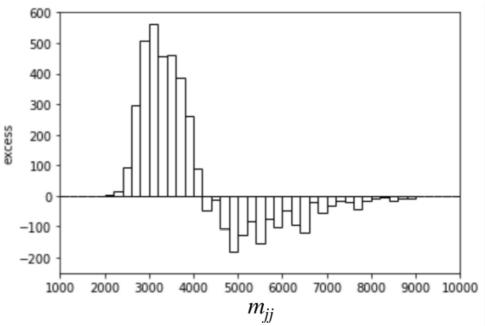
- Latent Dirichlet Allocation (LDA)
 - Decluster jet and use splitting info
 - Construct 2 hypotheses in data
 - Generated through LDA approach

Compute likelihood of two hypoth to be consistent

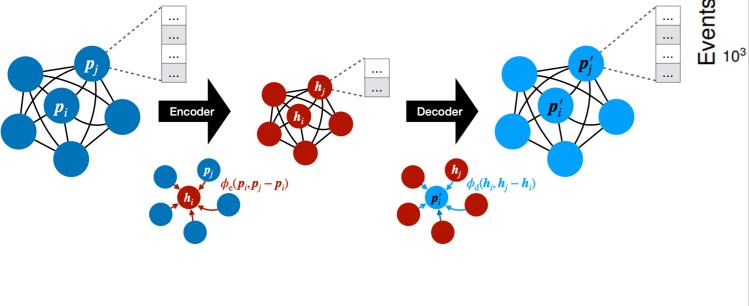
$$L(o_1,\ldots,o_N|\alpha) = \prod_{i=1}^N \frac{p(o_i|\hat{\beta}_1(\alpha))}{p(o_i|\hat{\beta}_2(\alpha))}.$$





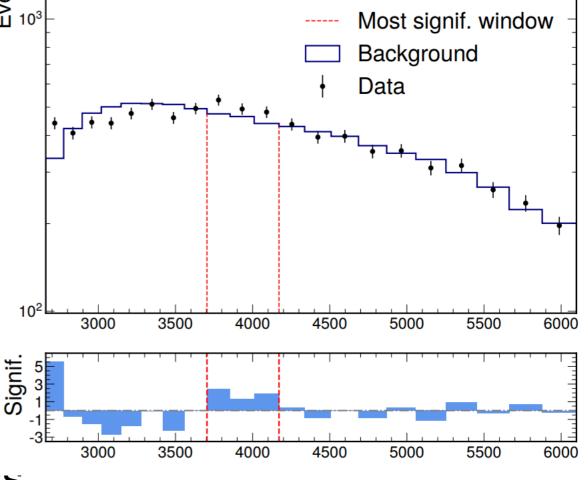


Method 5: Particle Graph AE



- Build a GraphNN Autoencoder
 - Try with mean squared error loss
 - Try with a permuation invariant loss (robust against physics)

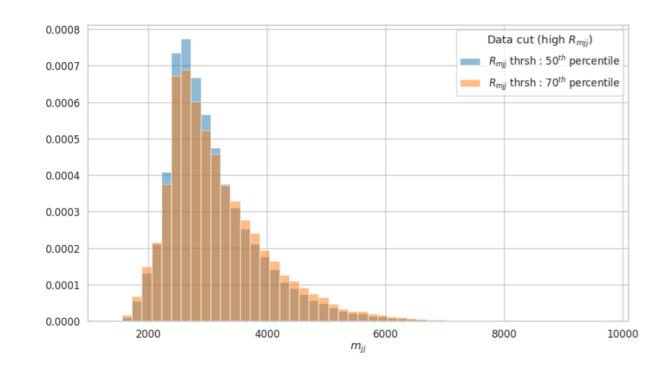
Observation: No good handle on loss

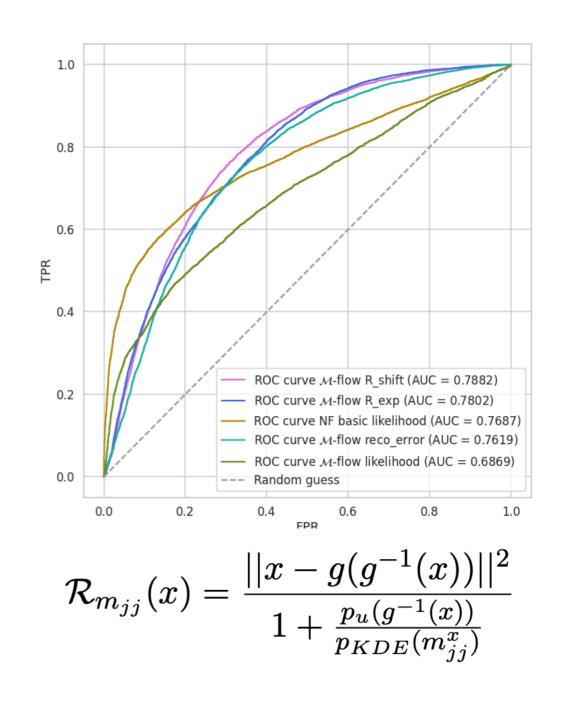


Black box 1, MSE

Method 6: Regularized Likelihood

- Use a normalizing flow
 - Cut on high loss
 - Decorrelate loss with mass

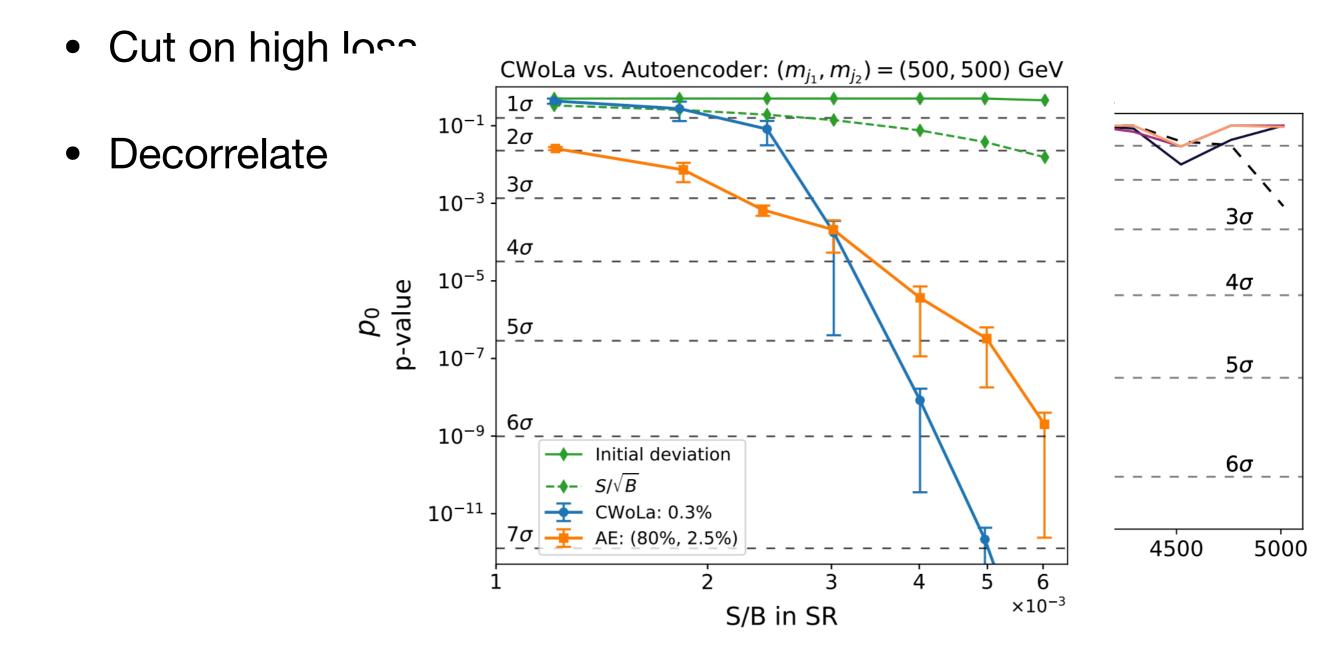




Observation: A single auto encoder even with NF is not enough too many anomalies (no clear signal)

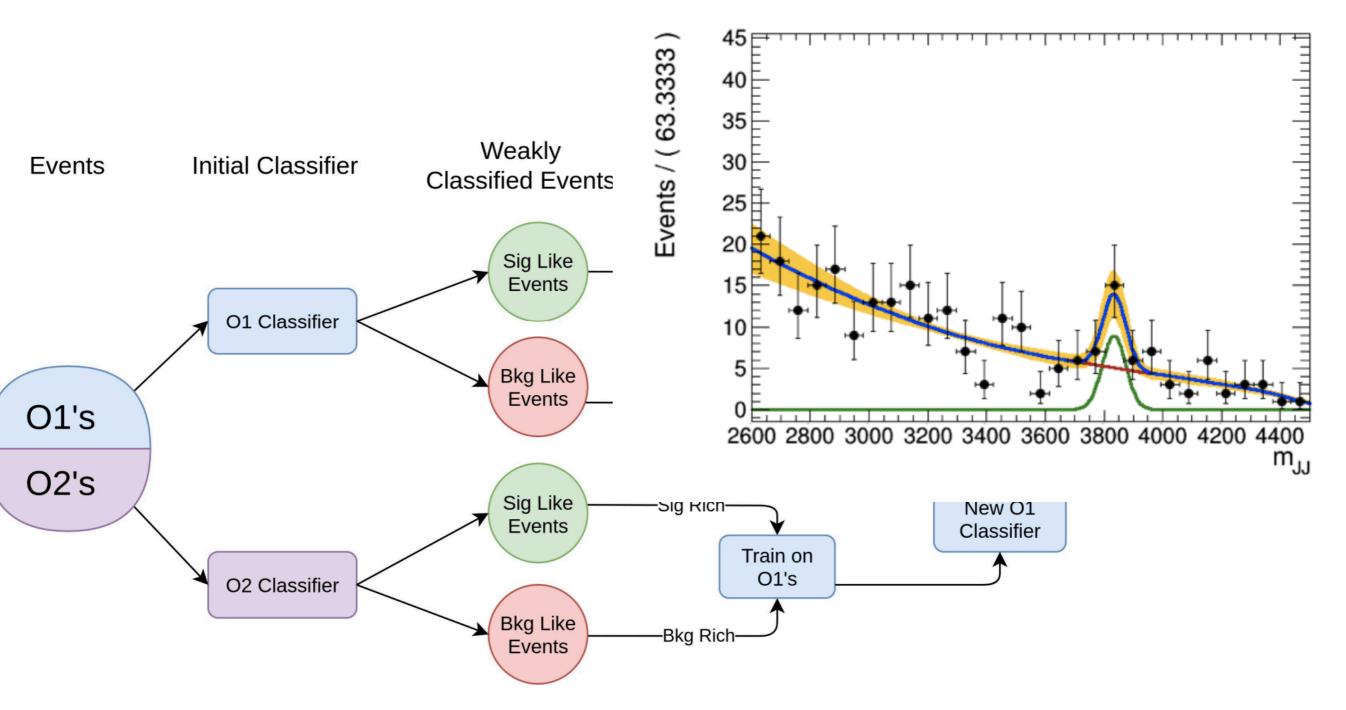
Method 8: CWoLa

• Use a normalizing flow



Observation: Approach works for single jet resonances

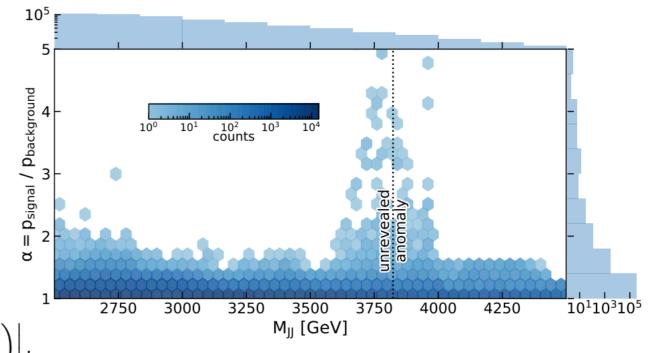
Method 9: Tag N'Train



Observation:Works well on jets, some limiations from using jet images Would benefit more from mass decorrelation

Method 11:GIS

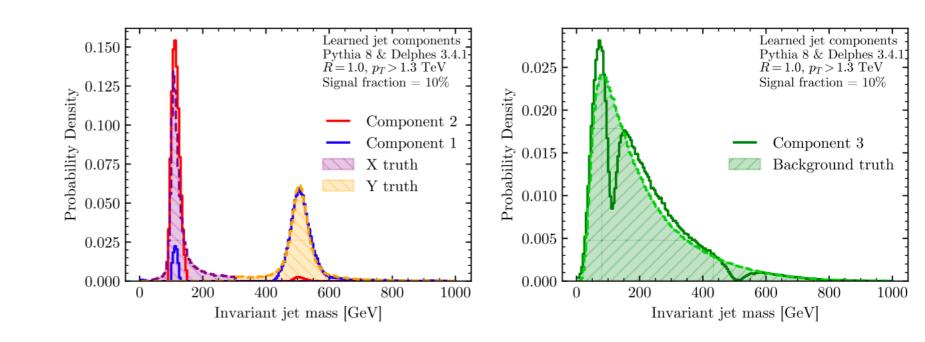
- Guassian Iterative Slicing
 - Cut on high loss
 - Decorrelate loss with mas



$$p(x|x_c) = \pi(f_{x_c}(x)) \left| \det\left(\frac{\partial f_{x_c}(x)}{\partial x}\right) \right| = \pi(f_{x_c}(x)) \prod_{i=1}^{i=N} \left| \det\left(\frac{\partial f_{x_c,i}(x)}{\partial x}\right) \right|.$$

Observation:Low noise robust density estimation is key

Method14:QUAK



Data Format

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- Data released in h5 format
 - Standard python format using h5py and pandas
 - Easy to process tools that allow for quick turnaround

```
Entrée [1]:
              import numpy as np
              import matplotlib.pyplot as plt
              import h5py
              import pandas as pd
Entrée [2]: file='events anomalydetection Z XY ggg.h5'
              #f sig = h5py.File(file,'r')
              pd.read hdf(file)
   Out[2]:
                                                                                           7
                          0
                                   1
                                             2
                                                      3
                                                               4
                                                                        5
                                                                                  6
                                                                                                     8
                                                                                                              9 ...
                                                                                                                   2091 2092 2093 2094 2095
                                                                                                                                              2096
                    18.283588 -0.903479
                                      0.060979
                                                 .316431 -0.784941 -0.008755
                                                                            9.464178 -0.812918 -0.037386
                                                                                                        4.578035 ...
                                                                                                                     0.0
                                                                                                                          0.0
                                                                                                                               0.0
                                                                                                                                     0.0
                                                                                                                                          0.0
                                                                                                                                               0.0
                   17.661003 -0.446288 -1.379160
                                                 .478683 -0.458125 -1.373650
                                                                            8.452606 -0.455308 -1.375457
                                                                                                       99.440353 ...
                                                                                                                     0.0
                                                                                                                          0.0
                                                                                                                               0.0
                                                                                                                                     0.0
                                                                                                                                          0.0
                                                                                                                                               0.0
                       Particle #1
                                                     Particle #2
                                                                                Particle #3
```

Search for Non-Standard Sources of Parity Violation in Jets at $\sqrt{s} = 8$ TeV with CMS Open Data

Christopher G. Lester^a Matthias Schott^{b,c}

^a Cavendish Laboratory, University of Cambridge, UK ^b Massachusetts Institute of Technology, Cambridge, USA ^c Johannes Gutenberg-University, Mainz, Germany

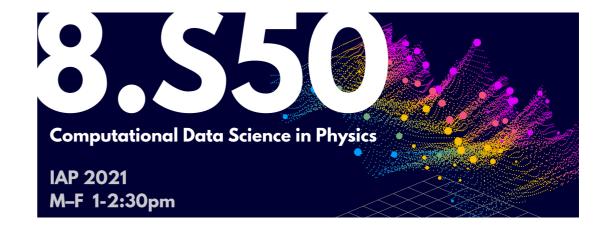
Opportunities and Challenges of Sta ^{cJohannes Gutenb} Production Cross Section Measuren ^{E-mail: lester} Proton–Proton Collisions at \sqrt{s} =8 TeV using CMS Open Data

E-mail: lester@hep.phy.cam.ac.uk, matthias.schott@cern.ch

Aram Apyan^a William Cuozzo^b Markus Klute^b Yoshihiro Saito^b Matthias Schott^{1b,c} Bereket Sintayehu^b

^a Fermilab, USA ^b Massachusetts Institute of Technology, Cambridge, USA ^c Johannes Gutenberg-University, Mainz, Germany

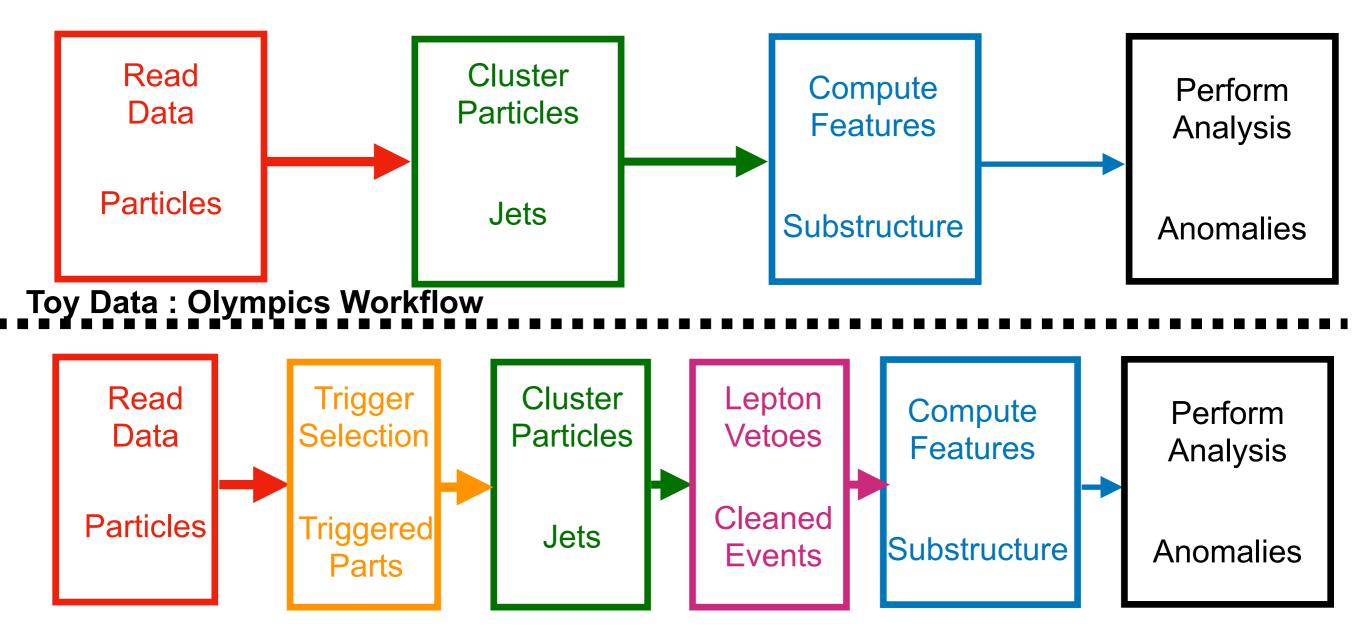
E-mail: matthias.schott@cern.ch



An Aside on Open Data

Processing Data

• To get from particles to analysis follow standard tool flow



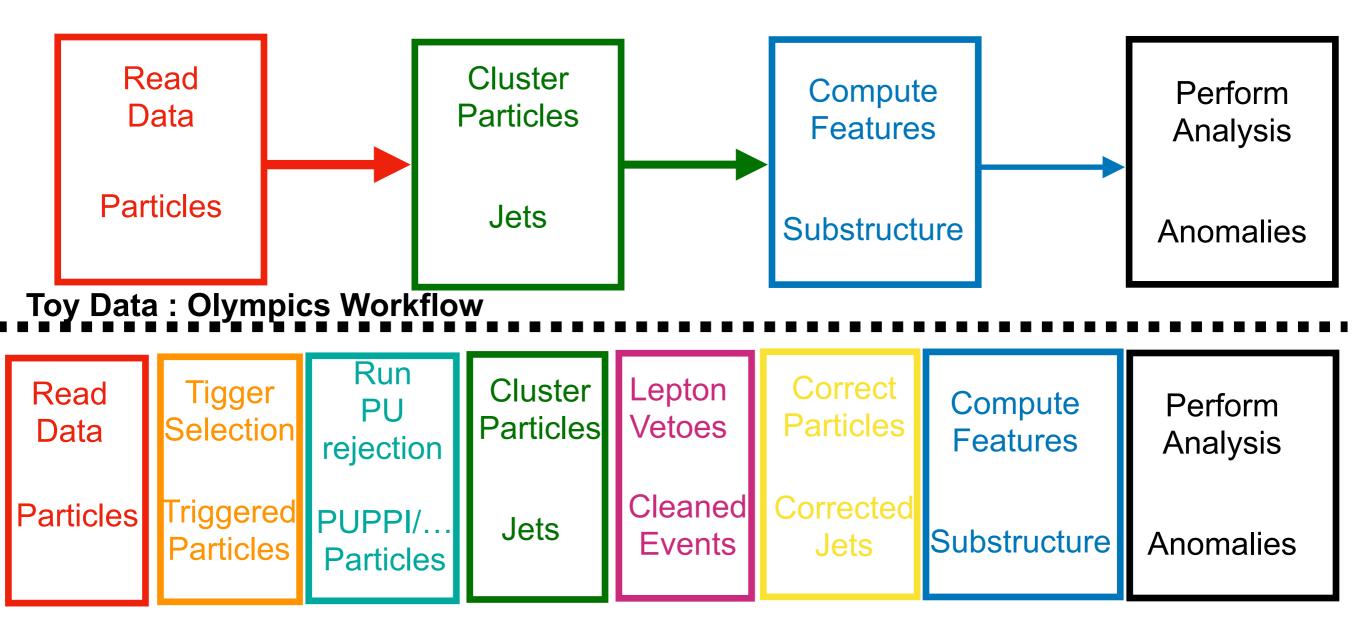
Real Data : Minimum Workflow

Why the extra steps?

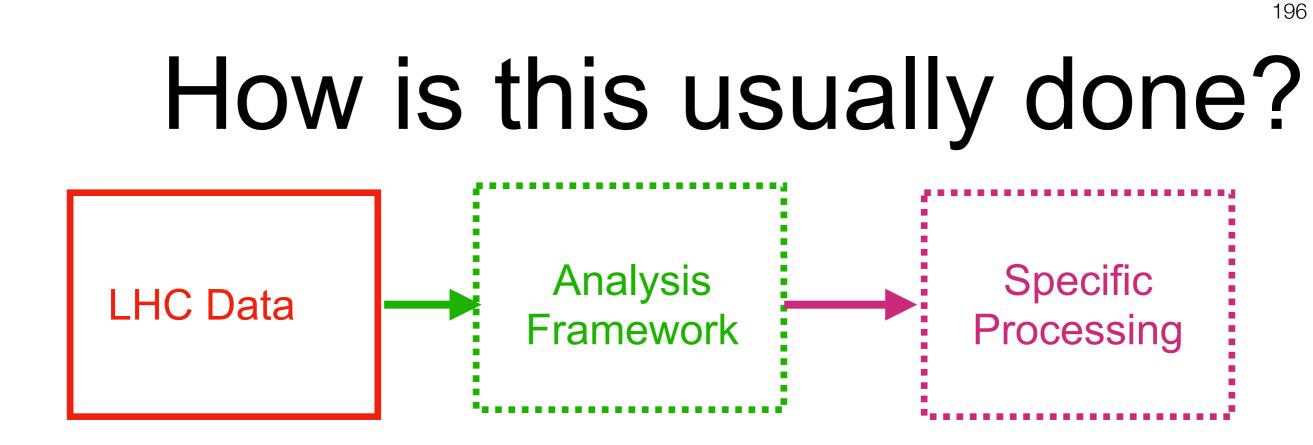
- Going to real data a number of effects need to be considered
 - Data needs to pass a well defined/measured trigger
 - Bias or inclusive selection can introduce peaks
 - Sample needs to be close to pure QCD to emulate toy data
 - Processes like ttbar, W+jets will contribute significantly
- In reality, there are several more steps
 - Above steps constitute a minimum to emulate olympics

Processing Data

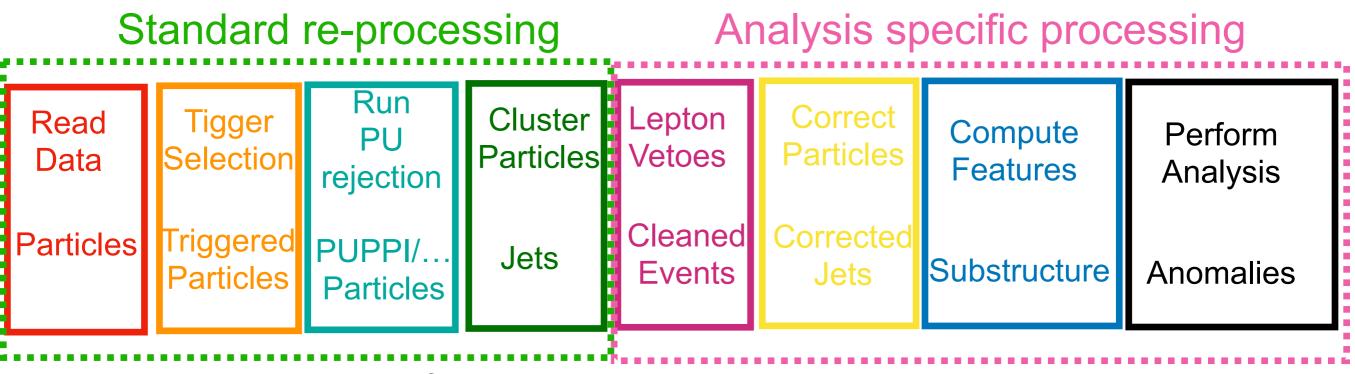
• To get from particles to analysis follow standard tool flow



Real Data : Minimum Workflow



Split is typically done to limit the amount of re-computing



Real Data : Minimum Workflow

Building an Analysis FWK

- Frameworks take a long time to build
 - Complicated steps to follow careful curation of the data
 - Many iterations to avoid bugs in code
 - Data formatting what to keep a complex decision
- When preparing data for open analysis worked to get flat ntuple
- Collaborations have taken steps to centralize this
 - Newer data formats embed standard corrections
 - These data formats starting to be available in open data

Towards Regularization

- Bigger biases/corrections eventually embedded in software
 - In CMS: MiniAOD => NanoAOD
 - These are light smaller frameworks that lead to fast analysis
 - Still don't solve all problems

	ш 🔽 Алан арр
	AK8Puppi
ີ່ ⊡່⊶ <u>ື</u> hg/tmp/Output_2.root	
– 🖗 Events;3	
	AK8Puppi.mass
	AK8Puppi.ptRaw
GenEvtInfo	
g 🛛 🦰 🦰 Gen Particle	
Electron	
	AK8Puppi.dz
a Muon	
🖉 🔤 📈 Tau	
o 🔁 Photon	
AK4CHS	
o 🚽 📈 AK4Puppi	
P AK8Puppi	- 🔖 AK8Puppi.vtxNtk
2 AddAK8Puppi	🛶 🔖 AK8Puppi.bjetcorr
o CA15Puppi	
> AddCA15Puppi	
⊃ <mark>X</mark> sv	
Events;2	- 🔖 AK8Puppi.deepcsvb
	🔉 AK8Puppi deepcmyab

Other things Lost

- Certain aspects in the data requires insider knowledge
 - Trigger preparation/Trigger biases
 - Which detectors were misfired
 - Details to address these issues are often complicated
- How do you deal with understanding inside knowledge?
 - Talk to others doing data analysis
 - Inside the collaboration many of these are well known

Examples Approaching

- Example sample approaching toy data
 - Special MC simulation sample used for Higgs tagging here
- Discussion on FAIRness of CMS open data here
 - Consensus is that this is close, but could be better
- Samples are are converted to h5 inputs

Variable	Туре	Description
event_no	UInt_t	Event number
npv	Float_t	Number of reconstructed primary vertices (PVs)
ntrueInt	Float_t	True mean number of the poisson distribution for this event from which the number of interactions in each bunch crossing has been sampled
rho	Float_t	Median density (in GeV/A) of pile-up contamination per event; computed from all PF candidates of the event
sample_isQCD	Int_t	Boolean that is 1 if the simulated sample corresponds to QCD multijet production

Dataset semantics

Future of Datasets is the FAIR convention

• Findable

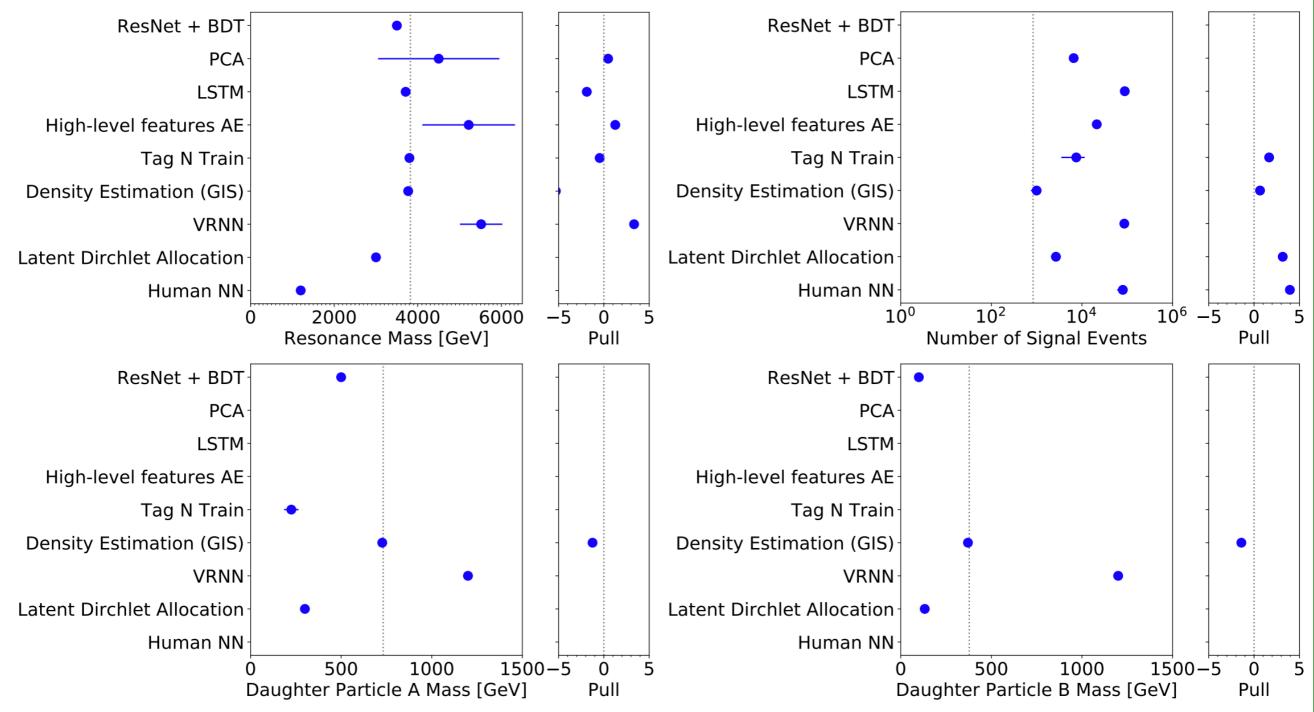
FAIR

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- Resources easy to find to by both humans+computers
- Metadata readily available; allows for the discovery of interesting data
- Accessible
 - Resource and metadata can be easily accessed and downloaded
 - Both locally by a human, but also machines using standard protocols
- Interoperability
 - Metadata should be ready to be exchanged, interepreted and combined in a semiautomated way with other datasets by humans and computers
- Reuseability
 - Data and metadata are sufficiently well described to allow data to be reused
 - Proper citation must be facilitated and conditions should be valid to machines

A fun look at results

Black Box 1



- Nobody found an excess in black box 3
- Black box 2 was empty

Black Box 2

Black Box 2 - Predictions

• PCA on high-level features (old):

A > BC with B > jj and C > jj m(A)=4800 +- 100 GeV, m(B)=725 GeV, m(C)=125 GeV p-value / Signal events: 0.00764 / 89

• VRNN (old):

A > BC with B > jj and C > jj m(A)=4422 +- 722 GeV p-Value: 0.229181609 / Signal events: < 12k

• Embedding clustering:

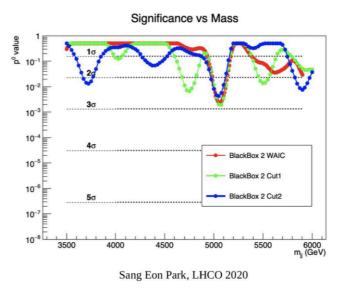
Z' resonance with mass **4600** GeV +- 17 GeV decaying to 2 jets p-Value: 0.0396 (1.8 sigma) / Event count: 76 +- 28

• Latent Dirichlet Allocation (old) Our method extracts signal descriptions which appear convincing, however the classifier does no identify a bump in the invariant mass spectra. Without this we were unable to determine that signal was present. The di-jet description extracted consisted of one jet of mass 350-400 GeV an another of mass 150-200 GeV. If the production of these states was non-resonant, we would b unable to find the signal with our method. Or if more than just di-jets were relevant to reconstruct the invariant mass, we would also not be able to find it. Otherwise, we determine that no signative was present in the data.

Reminder no signal

QUAK:

BB2 3sigma local evidence for resonance at $\sim 5~\text{TeV}$



• M-flows and GAN-AE:

work in progress (inconclusive)

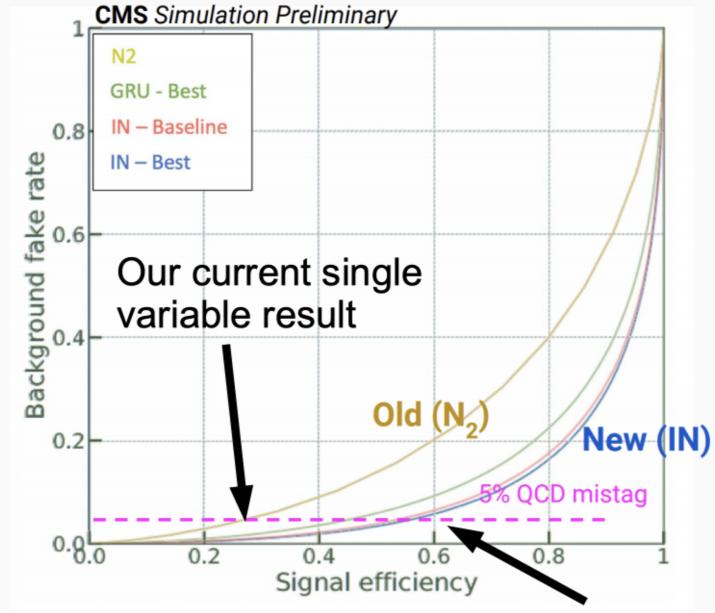
• VRNN (new):

Hint of an excess at 4.2 TeV

Observations²⁰⁴

- There is no catch all solution
 - Many of the best approaches combine multiple ideas
 - A diversity of approaches helps robustness
- LHC Olympics focused on resonant processes
 - Non-resonant processes make background extraction harder
 - Can we deal with complex topologies (such as black box 3)
- Data processing pipeline is assumed to be offline reconsturction
 - Could envision some approach in the triggers
- How can we actually compare sensitivities if we don't have a model?

Edit me

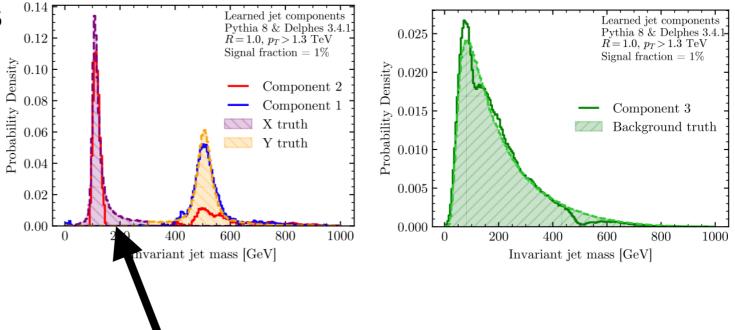


Factorized Topics

Inputs: Jet mass of each jet

- Factorization: each jet mass distributions can be factorized
- QCD composition is the same for leading and subleading

R&D Dataset



Use leading and trailing jet masses to make "topics"

Solve for the jet mass 1 and 2 that yield 3 distinct categories

Signal Extraction : None (did not work on BB1)

Take Away: Breaks down with small signal

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Inputs: Jet splittings from declustering

- Latent Dirichlet Allocation (LDA)
 - Decluster jet and use splitting info
 - Construct 2 hypotheses in data
 - LDA minimization to get 2

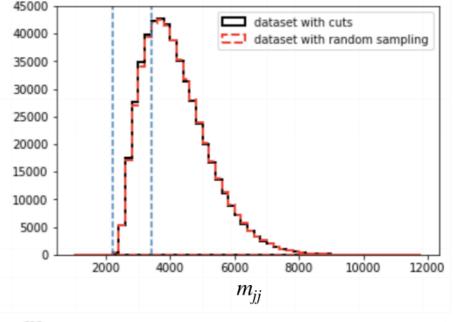
Compute likelihood of two hypothesis to be consistent

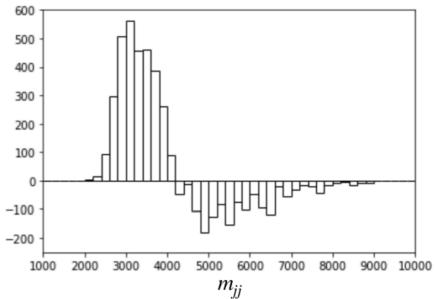
$$L(o_1,\ldots,o_N|\alpha) = \prod_{i=1}^N \frac{p(o_i|\hat{\beta}_1(\alpha))}{p(o_i|\hat{\beta}_2(\alpha))}.$$

Signal Extraction : None (did not work)

Take Away: LDA benefits from many event observables

BB1 Dataset





excess