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Application of Supervised Machine Learning to the Search for New Physics in ATLAS data

A Study of Ordinary Dense, Parameterized and Ensemble Networks and their Application to High Energy Physics

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Outline

Overview

Shed some light on the application of supervised learning in HEP by experimenting and studying a set of ML methods as they search for a set of SUSY signals.

1. Study individual attributes of a set of supervised methods
2. Compare expected sensitivity between methods on a subset of data
3. Attempt to increase sensitivity via feature reduction (PCA)
4. Compare the expected limits achieved by best performing methods to previous ATLAS analysis

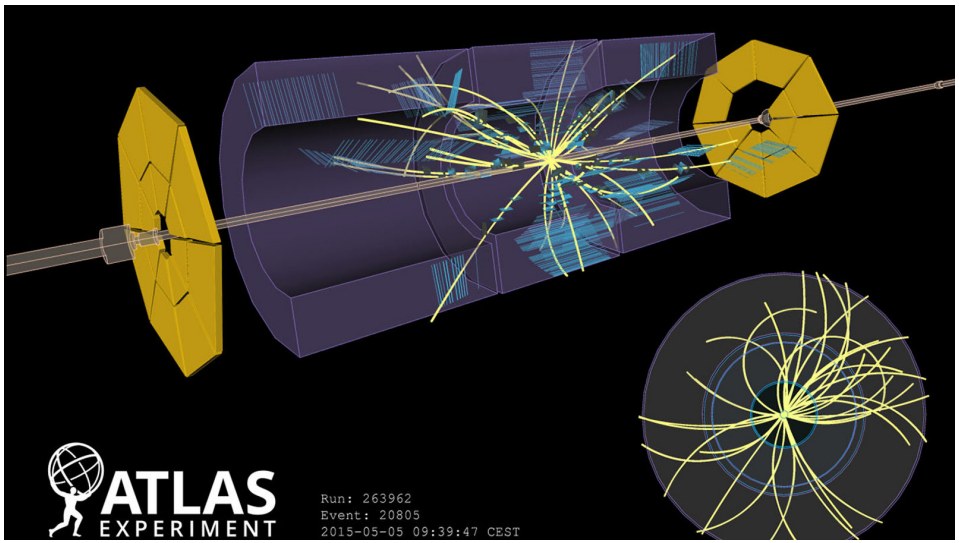
Outline

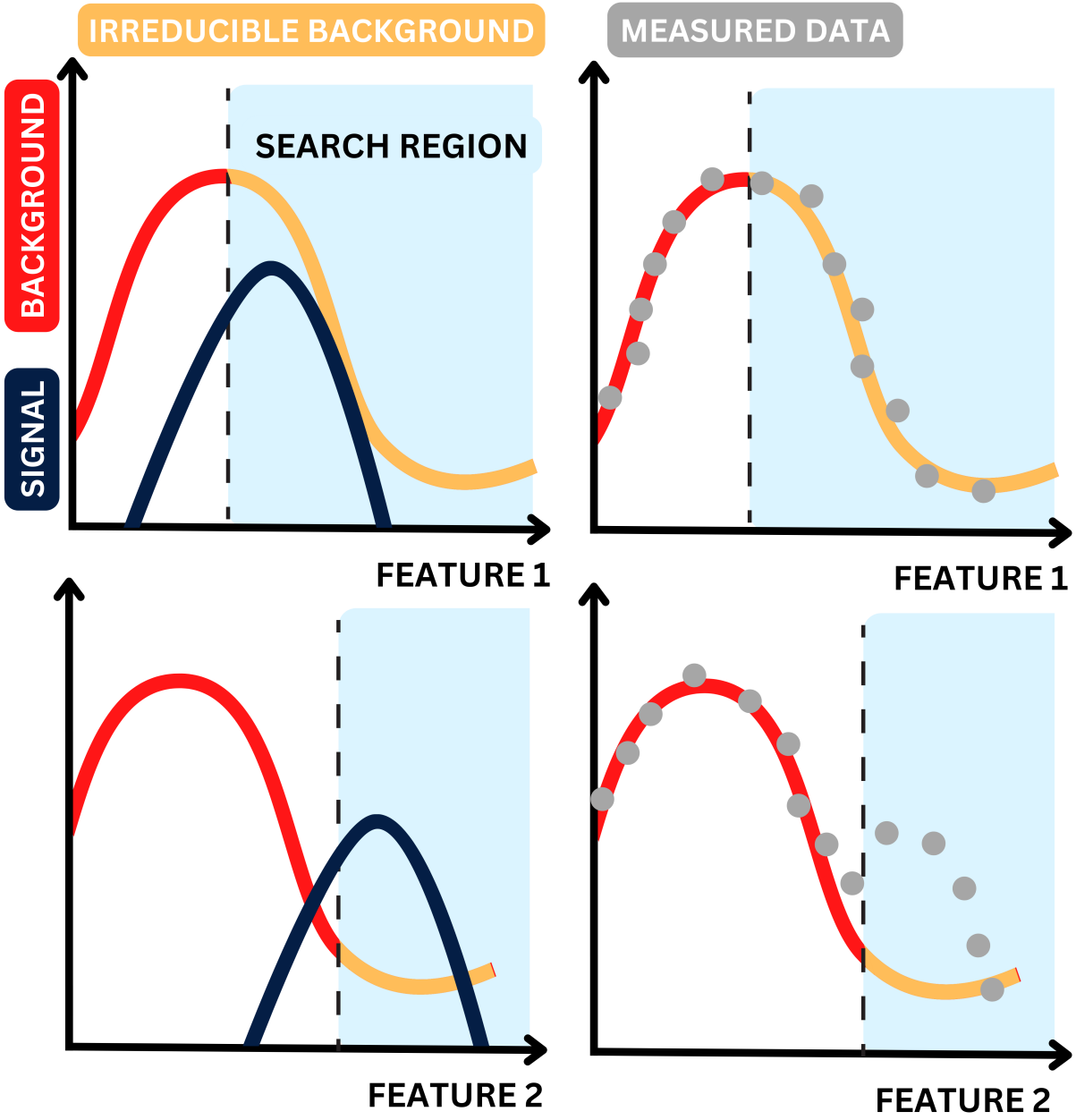
Why apply machine learning to HEP problems?

- The standard model of particle physics is one of the most successful theories of all time
- Some aspects of the universe are currently not described by the standard model
  - Neutrino masses
  - Hierarchy problem
  - Energy-matter density in the universe
- To precisely test extensions of the standard model we produce progressively larger amounts of data
- Upholding the quality of analysis demands advanced tools
  - Machine learning

How do we search for new physics?

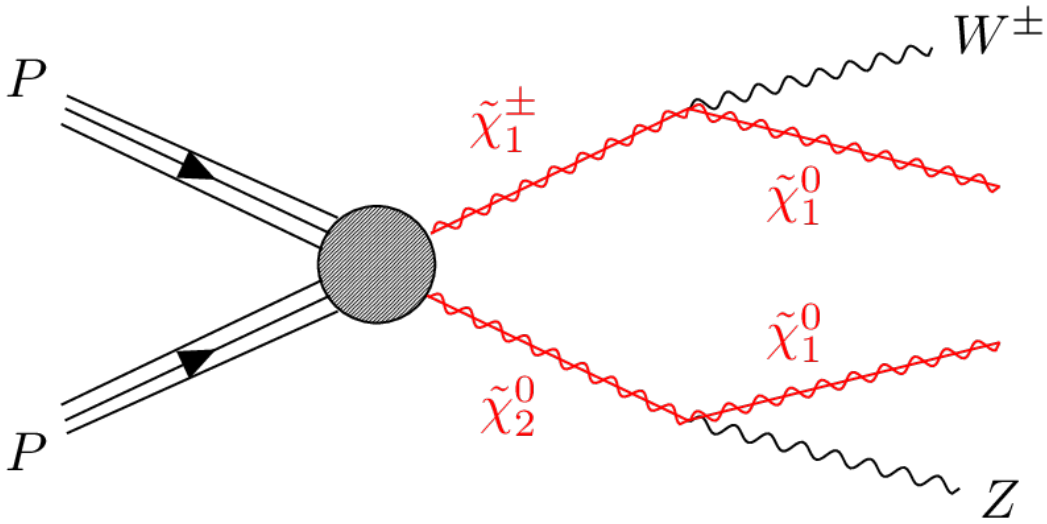
- Two data sets
  - Theory: Simulated based on Standard model physics
  - Experiment: Proton-proton collisions measured in particle detectors
- Data sets include information regarding collisions (momentum and mass of particles, collision angle etc.)
- Compare theory with experiment
  - Match: Standard model adequately explain collision
  - Deviations: New physics, or statistical fluctuations
- Create search region
  - Traditional: Cut-and-Count
- Measure deviation in significance, Z
  - $Z \approx \frac{n_{obs} - bkg}{\sqrt{bkg}} = \frac{signal}{\sqrt{background}}$




IRREDUCIBLE BACKGROUND
MEASURED DATA
BACKGROUND
SIGNAL
SEARCH REGION
FEATURE 1
FEATURE 1
FEATURE 2
FEATURE 2

The search

- Study application of supervised learning as it searches for SUSY signal
  - Chargino-neutralino production
  - 2 free parameters: masses of the chargino and neutralino
- Measure sensitivity of an analysis
  - Expected significance
  - How many collisions do we expect to find in search region?



Outline

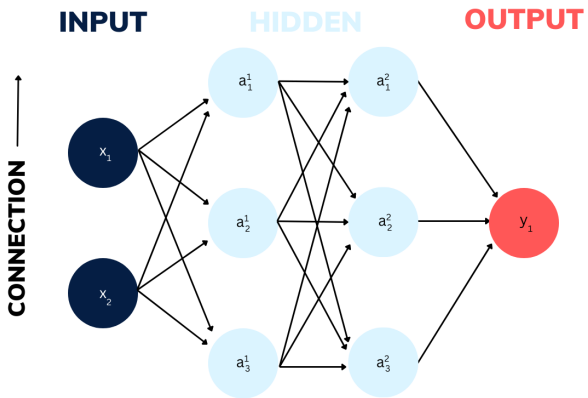
A summary of the applied methods

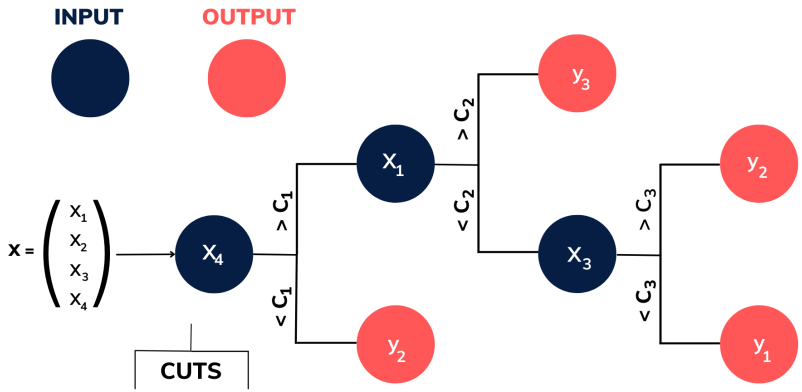
Three neural network variants

- Ordinary dense neural network
- Ensemble networks utilizing Local-Winner-Takes-All (LWTA) layers
- Parameterized neural networks (PNN)

One boosted decision tree method

- XGBoost using default settings



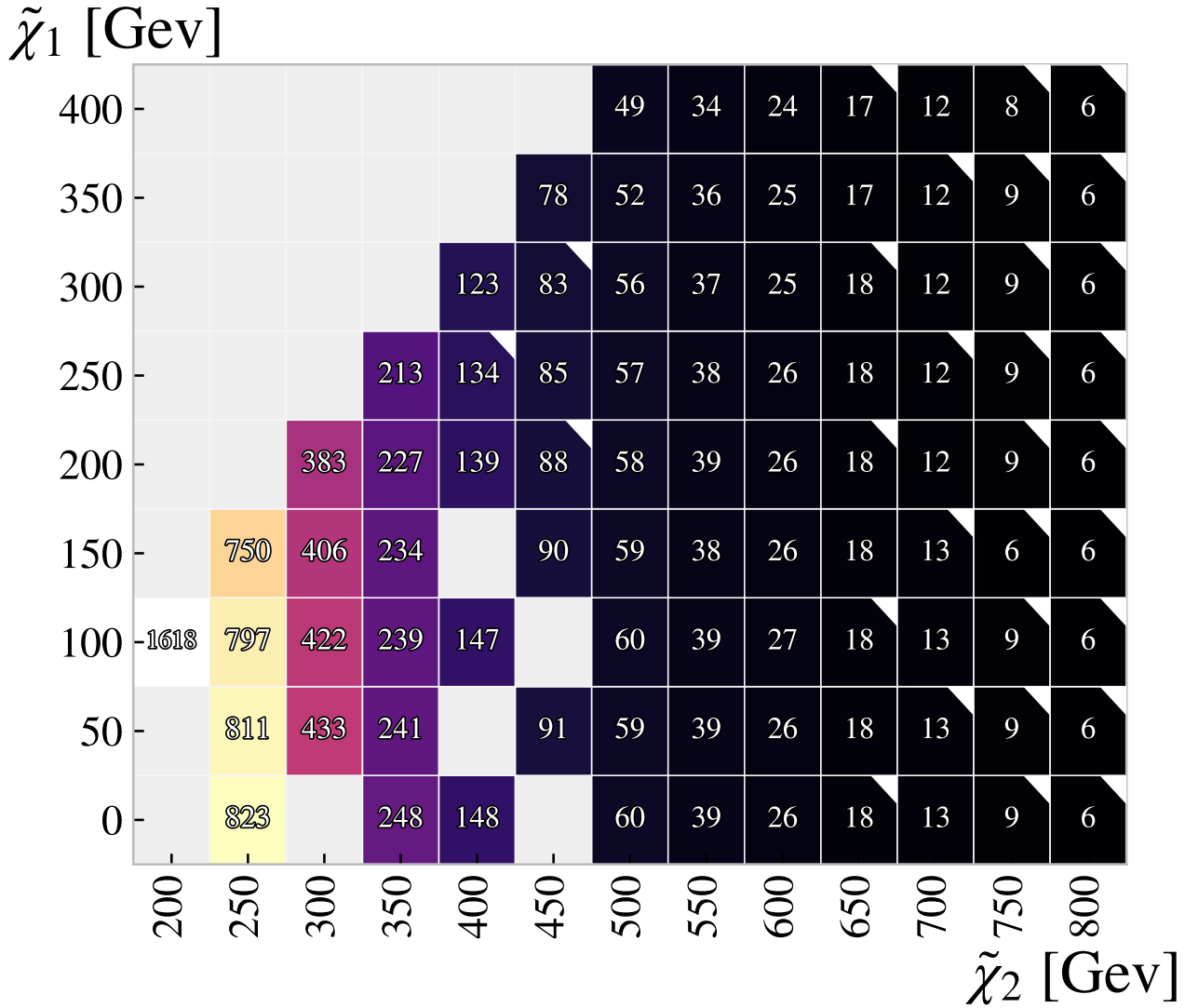


Training strategy

- Train using simulated data
- Objective: Classify standard model background as 0, and SUSY signal as 1
- 80% training and 20% validation
- Early stopping criteria
  - Train as long as performance on validation set improves
  - Patience 10 epochs
  - Reset weights to best epoch

Mass combinations of the chargino-neutralino pair

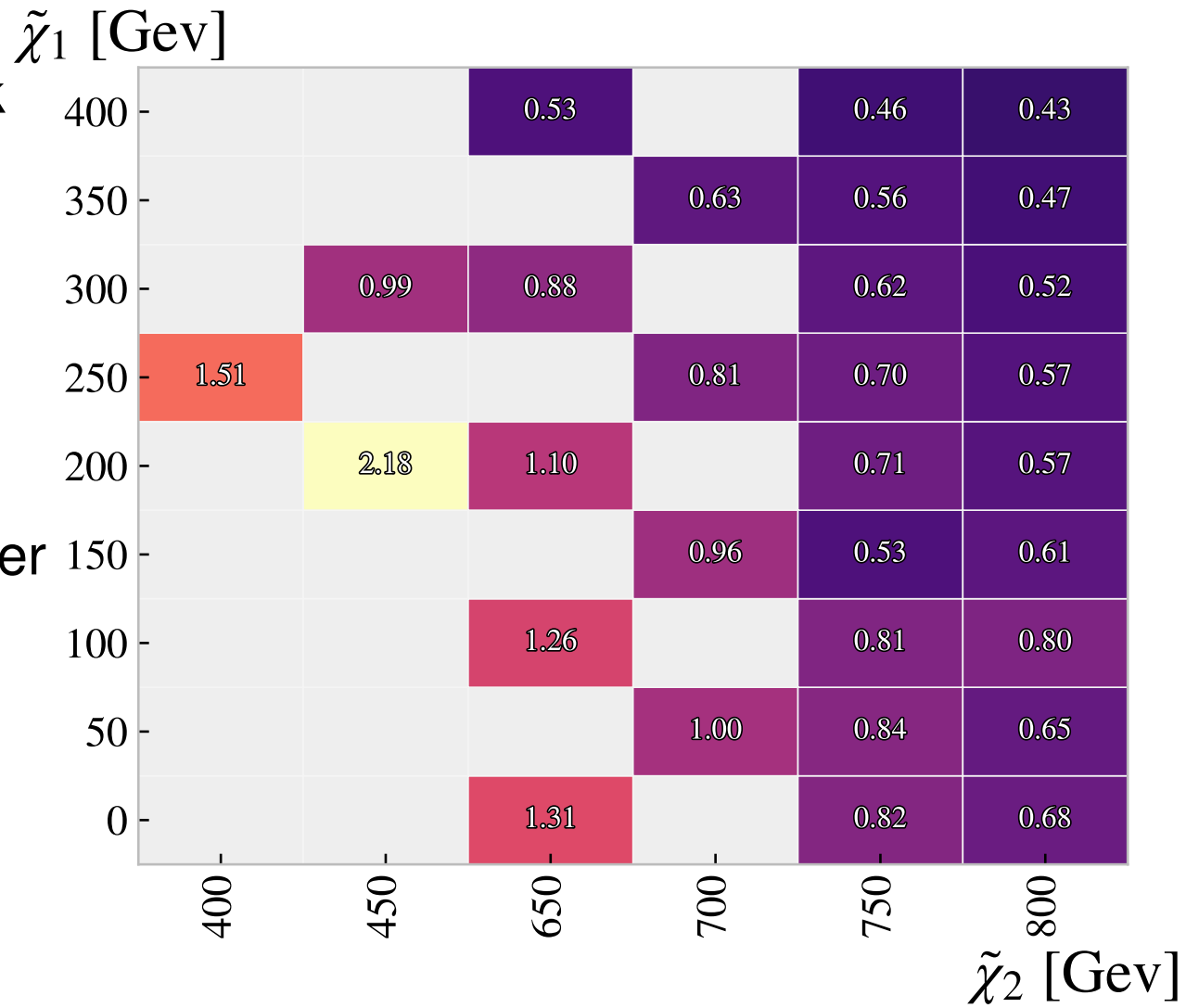
- Full signal grid
  - 89 mass combinations
- Original signal set: white corners
  - 30 mass combinations
- The smaller the masses, the larger the contribution



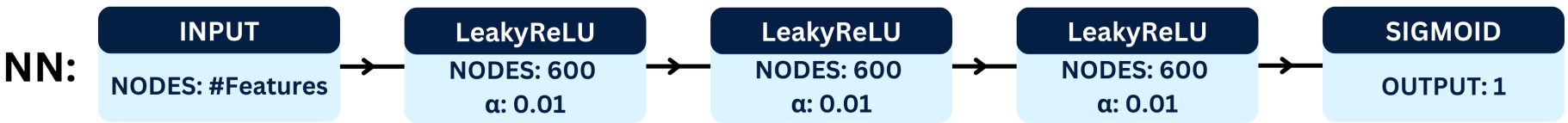
Outline

Boosted decision trees - XGBoost

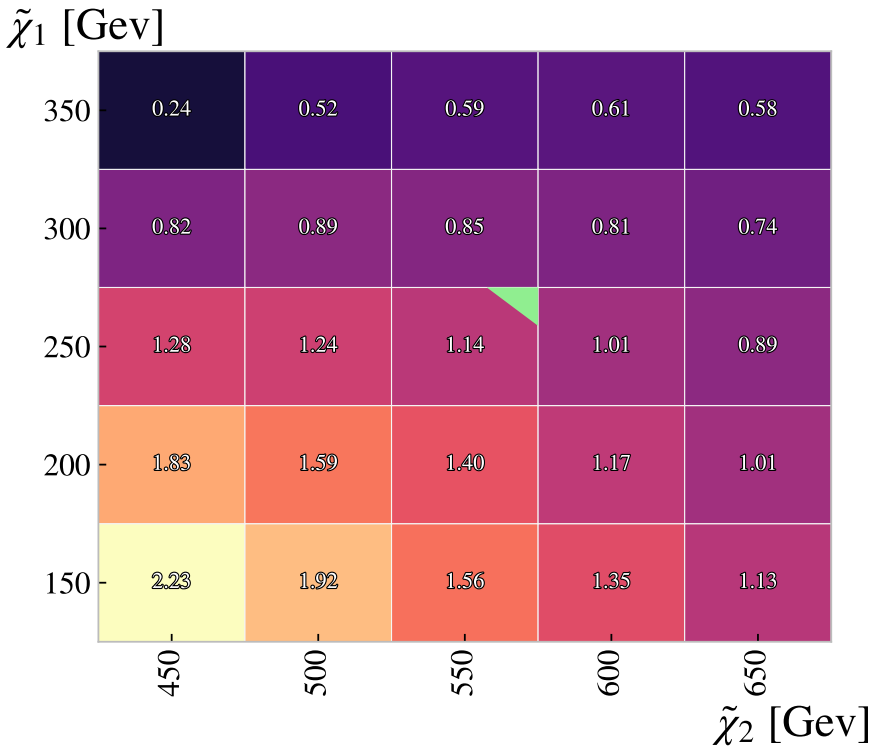
- Used as benchmark
- Minimal time spent tuning BDT
- Trained on original signal set
- Displayed better performance on lower masses

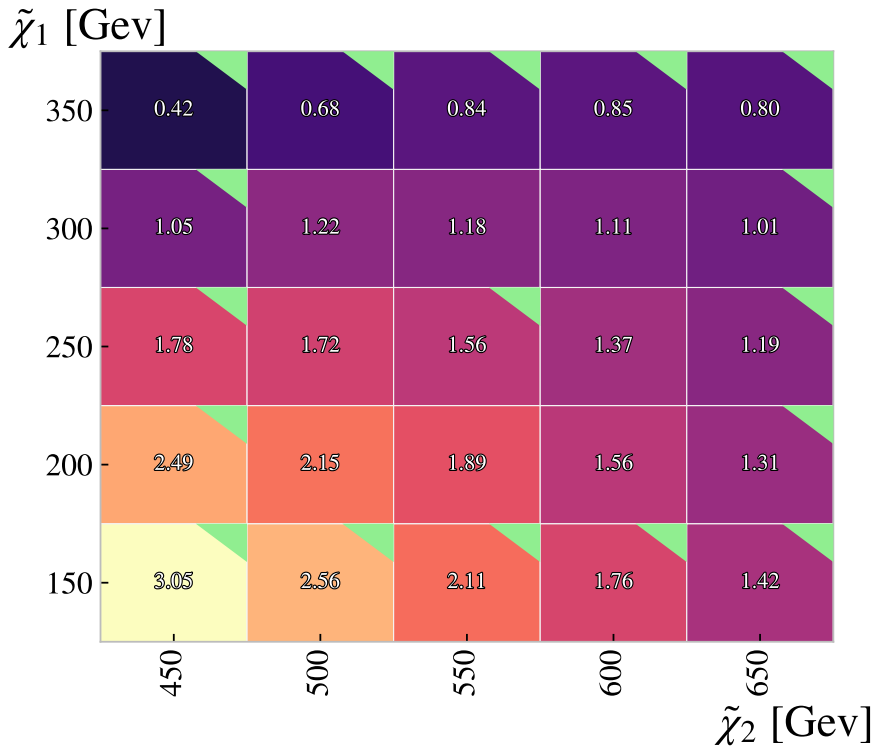


Ordinary dense neural network



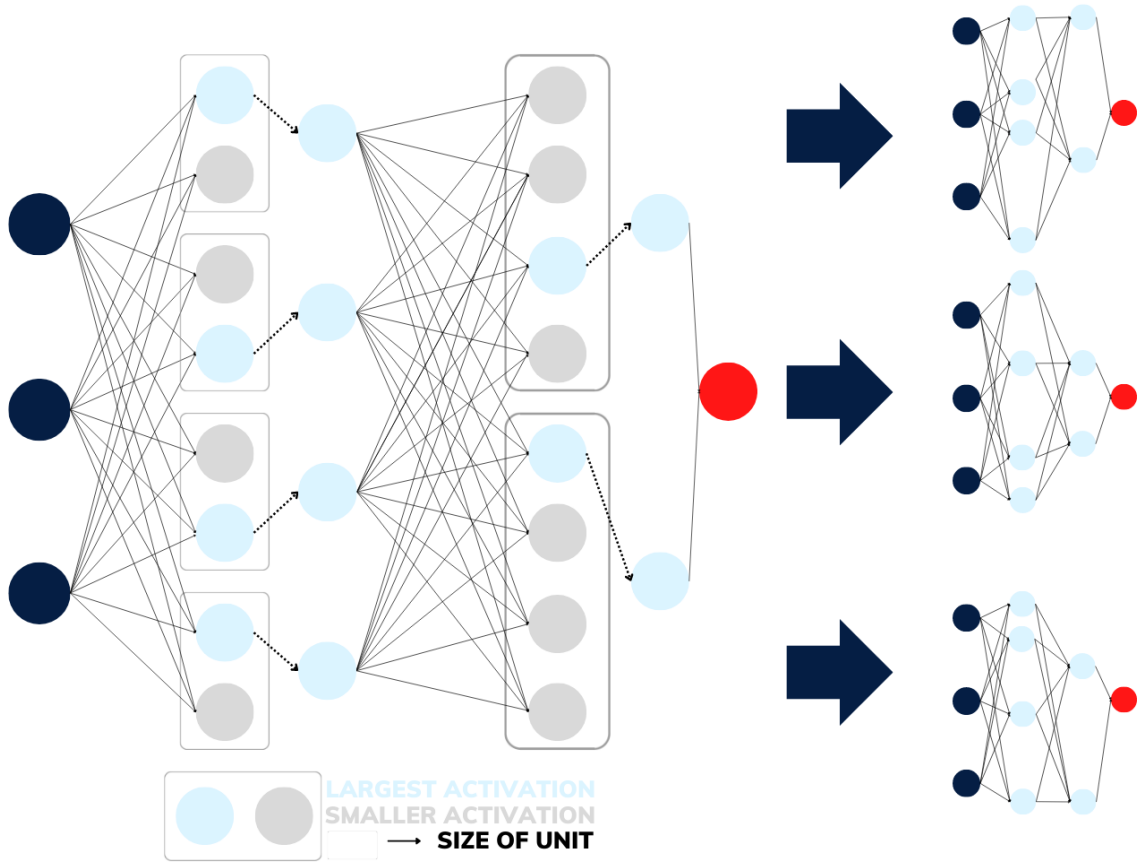
Compare one-mass approach to several-masses approach





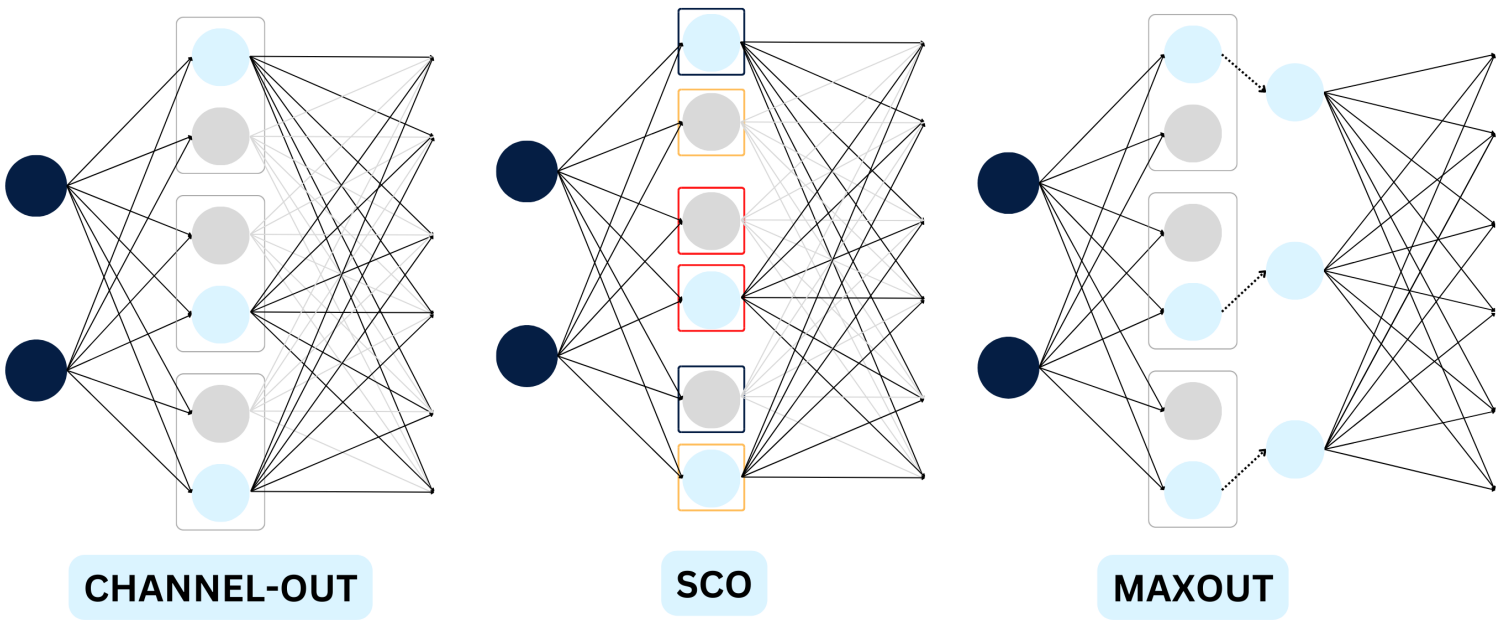
Ensemble methods - LWTA

- Dropout
- What is LWTA?
- Competing nodes - Units
- Encode information in pattern specific pathways



Channel-Out, SCO and Maxout

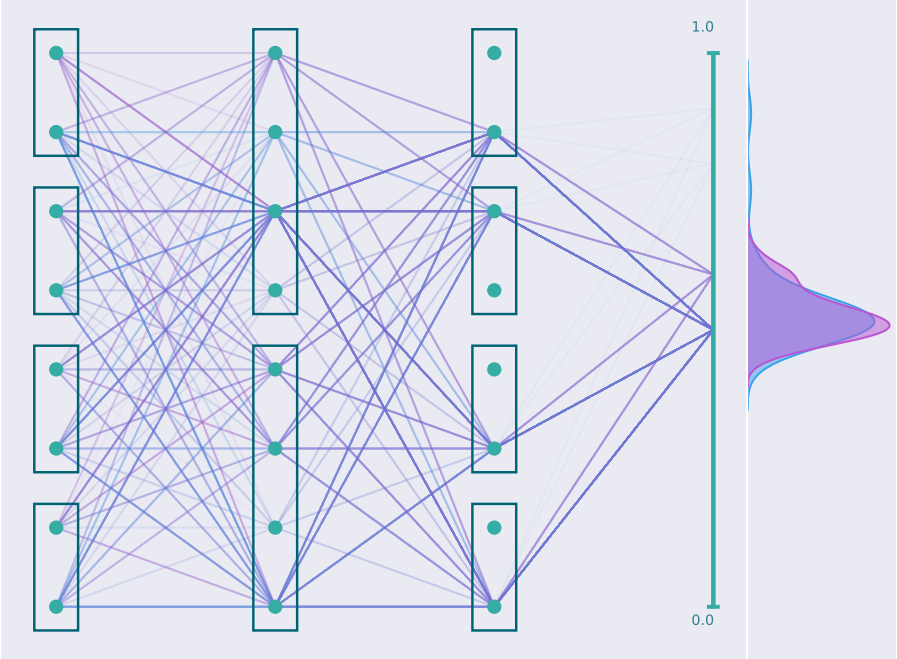
Layer	Separate weights	Static units
Channel-Out	*Yes*	*Yes*
SCO	*Yes*	*No*
Maxout	*No*	*Yes*



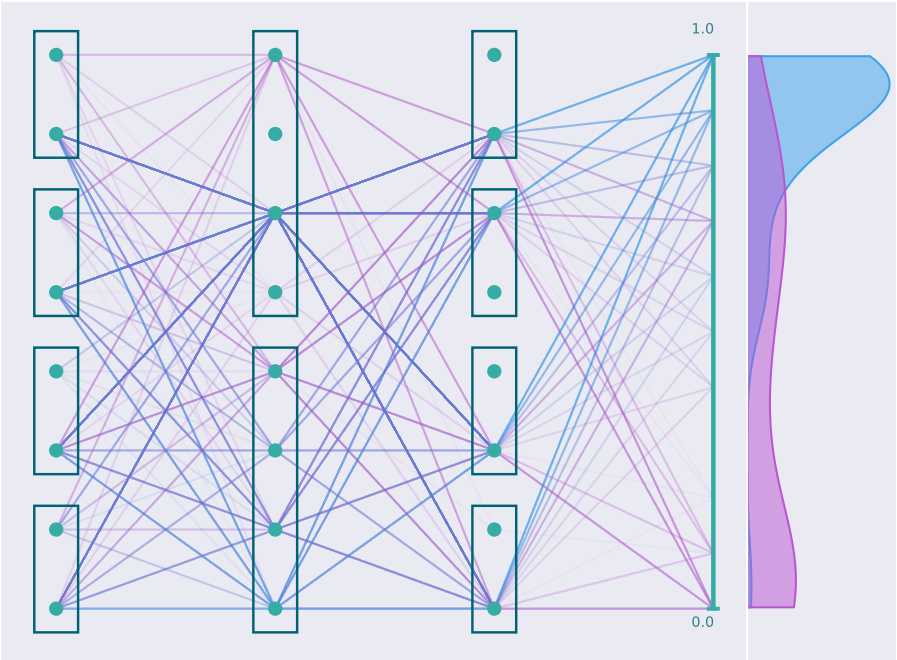
Visualization and study of sparse pathways

- A study of the implementation and effect of LWTA layers
- Visualize the activation and paths of 100 randomly sampled events
  - 50 background
  - 50 signal
- The bolder the line the more frequently the path is used.

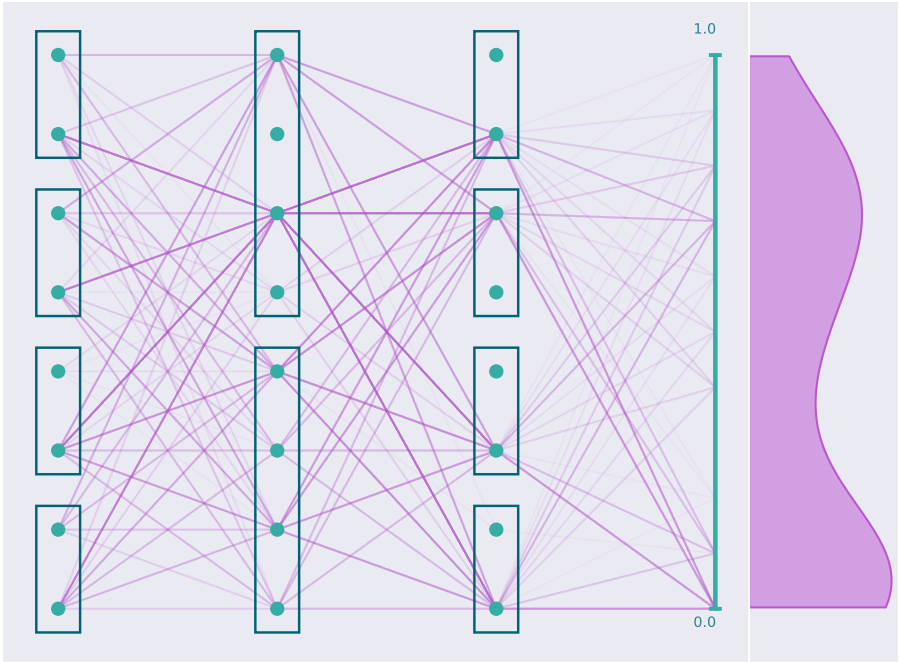
Before training



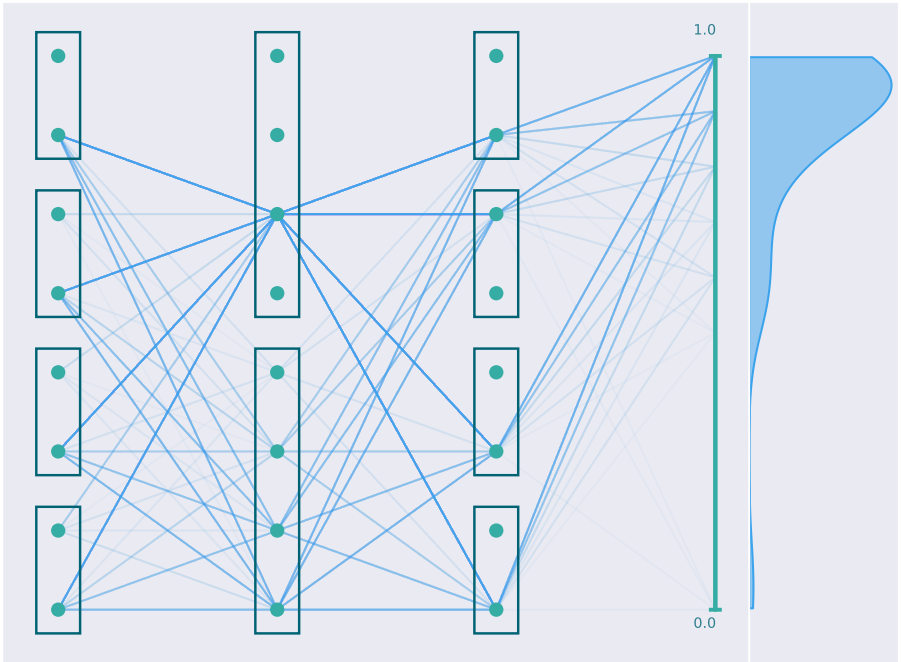
After training



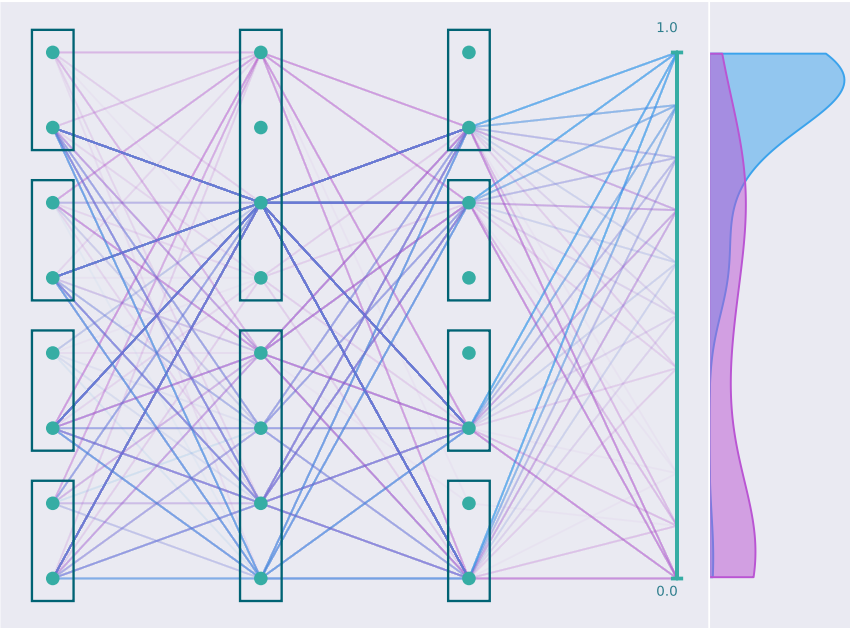
Background



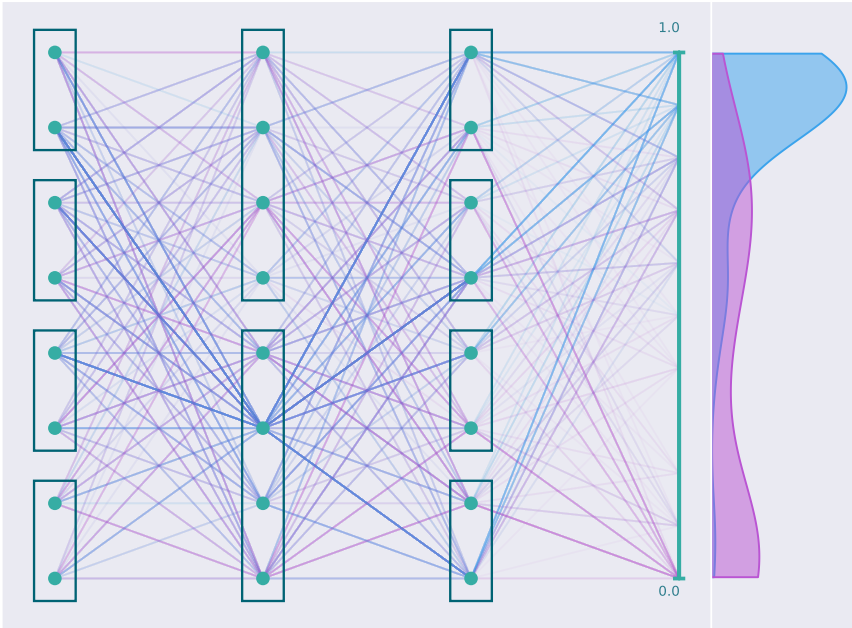
Signal



Comparing activation of Maxout with SCO

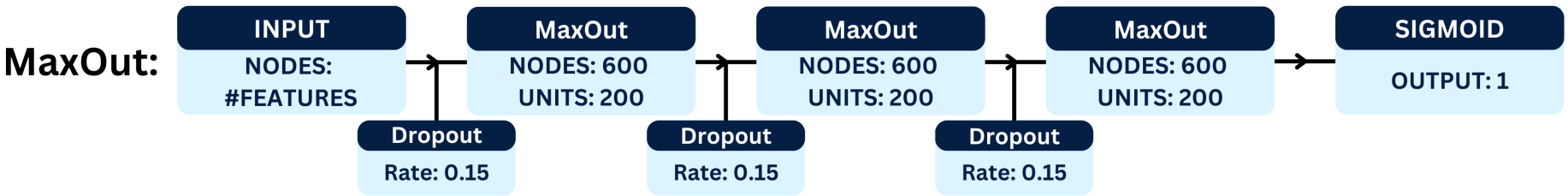


Maxout



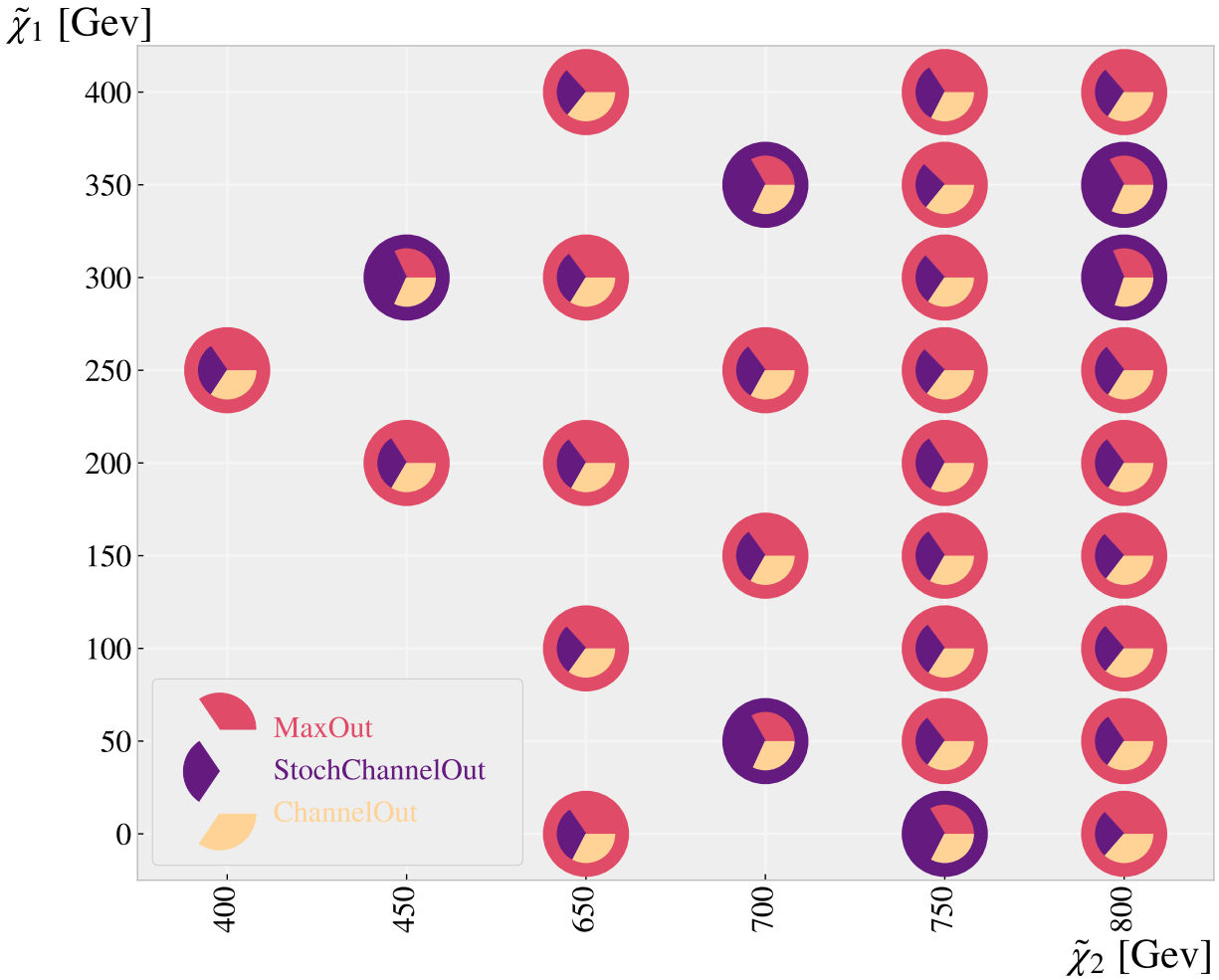
SCO

Ensemble network architecture



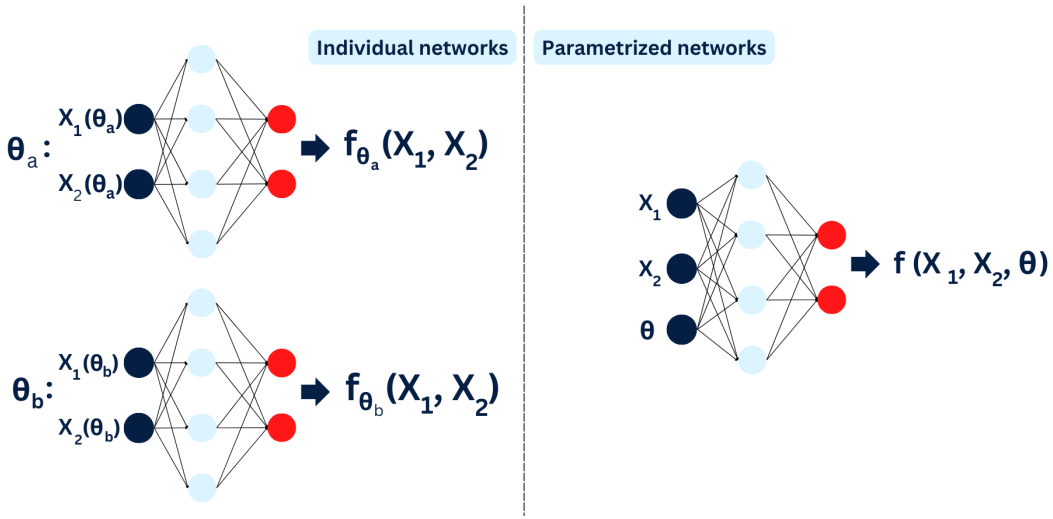
Comparing sensitivity of channel-out, SCO and maxout

- Maxout: 23/30
- SCO: 7/30
  - No trend for preferred masses
  - Possibly improve without layer on prediction

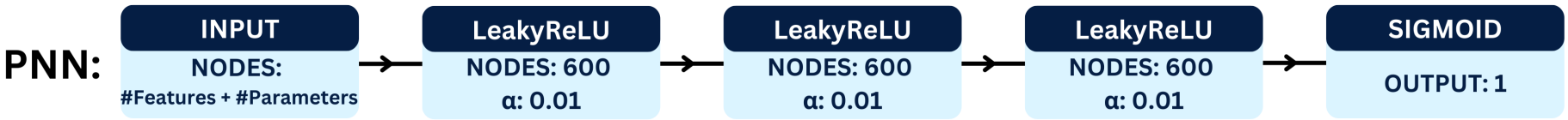


Parameterized neural network

- For diverse data set, X, dependent on a parameter, $X(\theta)$
  - Classical approach: One model for each parameter
  - PNN approach: Include θ as feature in feature set
- Signal events using masses $\{A, B\}_{GeV}$ to generate event during simulation will include the parameters A and B in feature set
- Background assigned parameters randomly using same distribution as signal
- Motivation
  - Network will associate parameters with trends in the data



PNN architecture

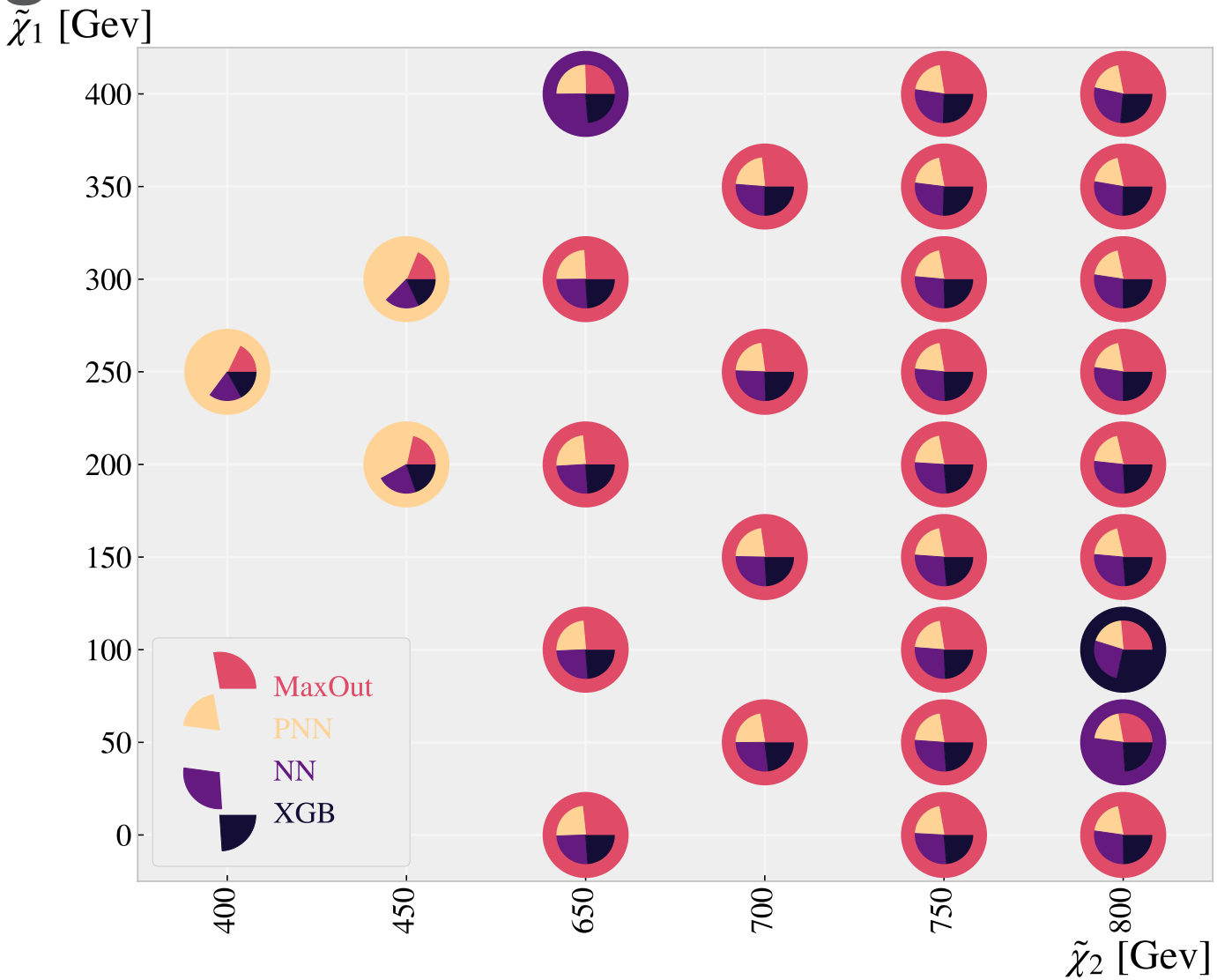


Study the effect of the parameters in the PNN

- Study if the parameters effect the training as intended
- Test: Manually assign all the events, both background and signal, the same parameters (mass combinations) thereby assigning most of the signal the wrong parameters
- Hypothesis: PNN performs better when events are assigned correct parameters
- First test: All events are given parameters $\{50, 250\}_{GeV}$
- Second test: All events are given parameters $\{200, 300\}_{GeV}$

Parameters \ **Channel**	(50, 250)	(100, 200)	(150, 300)	(200, 300)	(*Background*)
(50, 250)	**80.8**%	45.8%	**77.5**%	50.1%	2.4%
(200, 300)	77.3%	**54.6**%	76.3%	**59.0**%	**2.7**%

Comparing the sensitivity on a subset of the signal

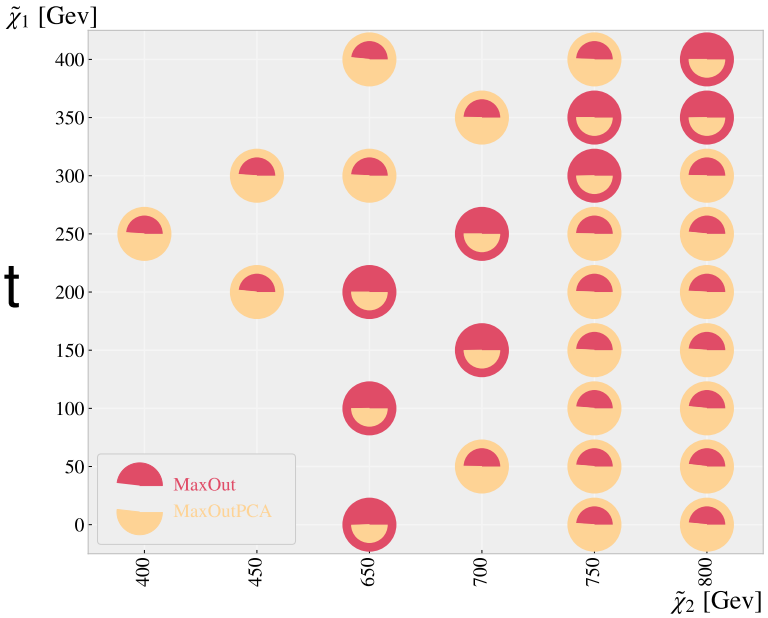


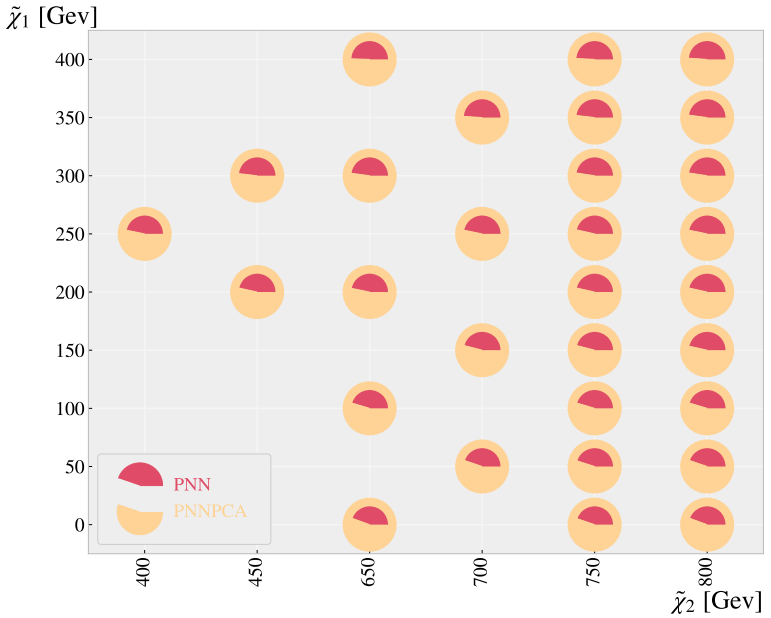
Increasing sensitivity through a PCA

- Dimensionality reduction
- Creates new features using linear combination of original features
- Ranks from most to least variance
- This analysis
  - Demand conservation of 99.9% of variance/spread
  - 5 features removed

Compare methods with and without PCA

Maxout



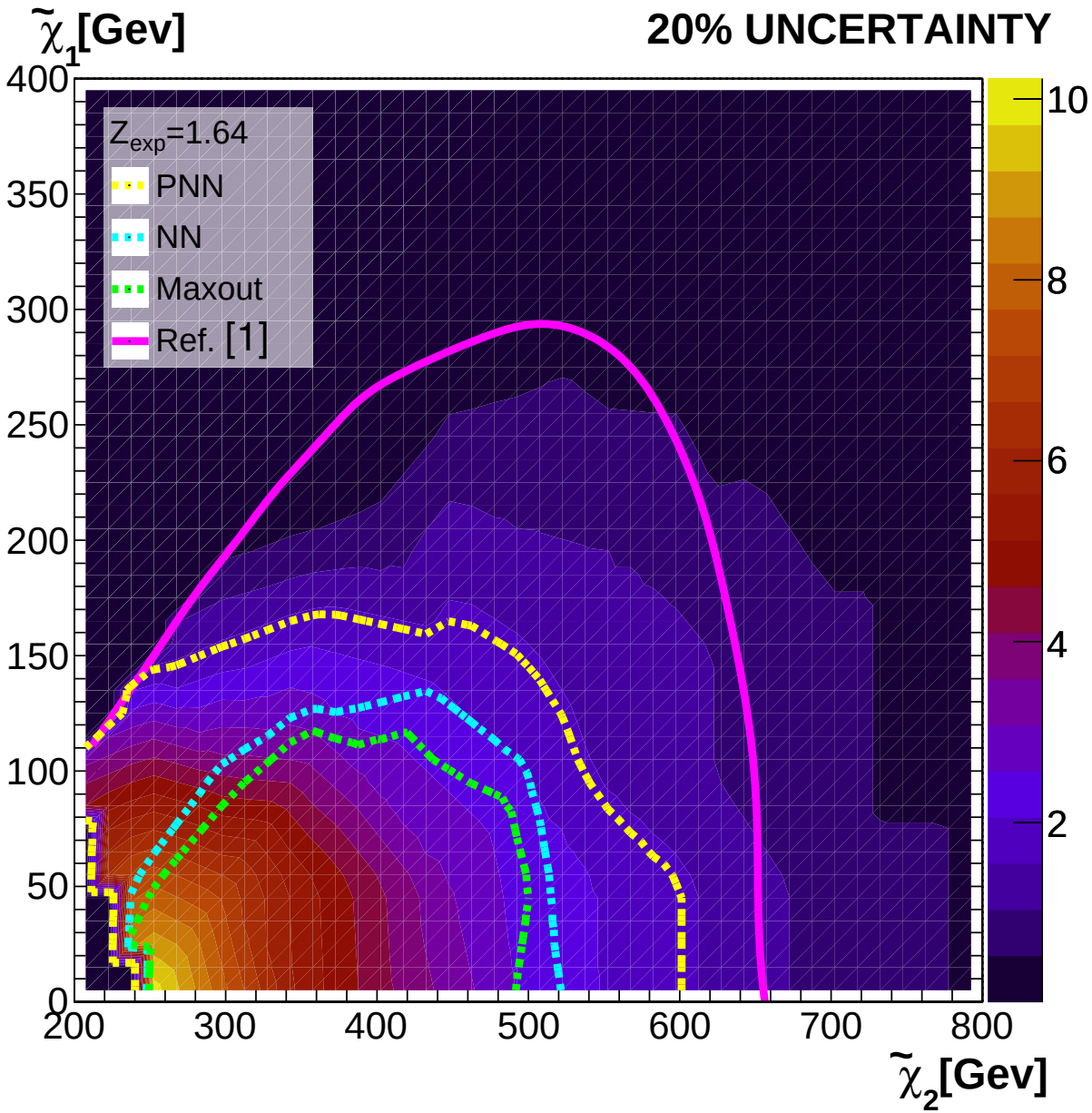


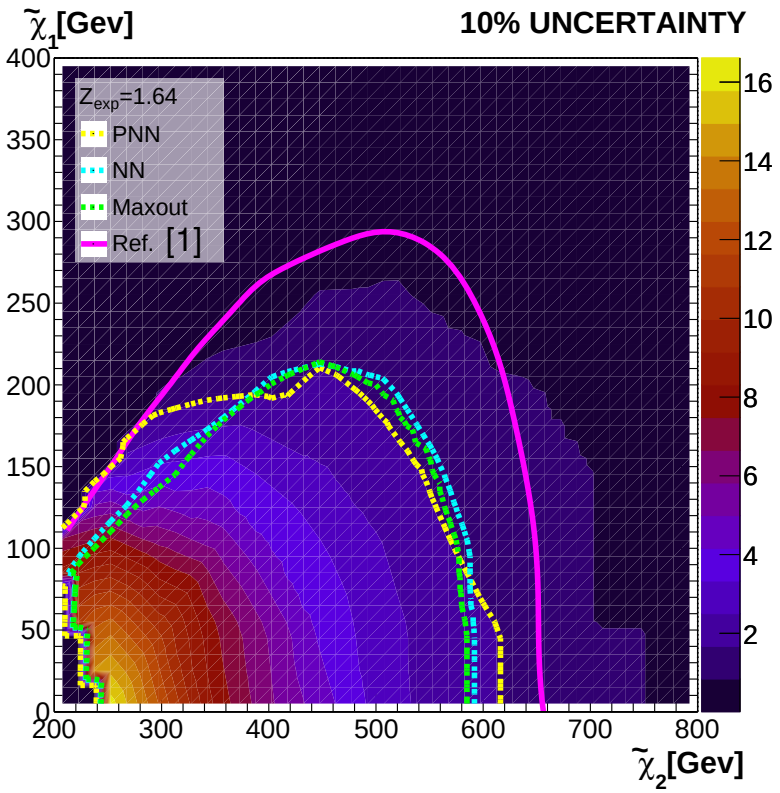
PNN

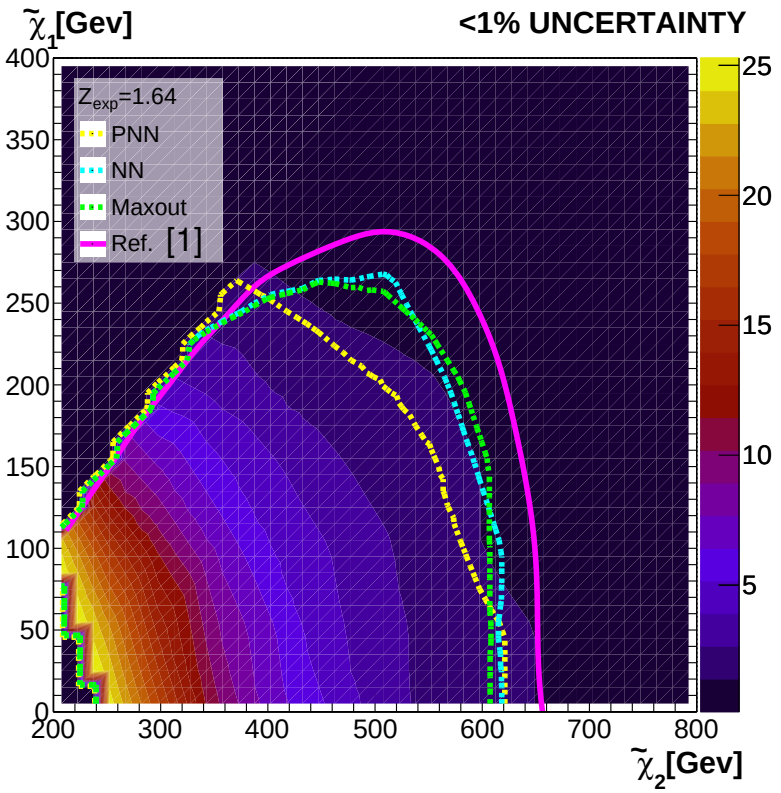
NN

Comparing the methods to previous analysis

- Compare the expected limits of three best models to analysis made by ATLAS in 2021 [1]
- Introduce flat uncertainty for realistic comparison (20%, 10%, $< 1\%$)
- Include top performing methods
  - Maxout model with PCA
  - PNN with PCA
  - Ordinary dense neural network without PCA


$\tilde{\chi}_1$[Gev]
20% UNCERTAINTY
Z_{exp}=1.64
PNN
NN
Maxout
Ref. [1]
400
350
300
250
200
150
100
50
0
200
300
400
500
600
700
800
10
8
6
4
2
$\tilde{\chi}_2$[Gev]


$\tilde{\chi}_1$[Gev]
10% UNCERTAINTY
Z_{exp}=1.64
PNN
NN
Maxout
Ref. [1]
$\tilde{\chi}_2$[Gev]


$\tilde{\chi}_1$[Gev]
<1% UNCERTAINTY
Z_{exp}=1.64
PNN
NN
Maxout
Ref. [1]
$\tilde{\chi}_2$[Gev]

Outline

Conclusion & Outlook

1. Including a diverse signal set can improve performance
2. The LWTA layers improve long-term memory via pattern specific pathways
3. All network variants outperformed default settings of XGBoost
4. PCA increased sensitivity of PNN and maxout model in original signal set
5. None of the networks extended expected limit past previous ATLAS analysis
6. PNN exhibited bias towards lower masses, whereas maxout model achieved a more balanced sensitivity
7. LWTA layer's increase in long-term memory is promising in future analysis where higher masses are studied

References I

ATLAS Collaboration.
'Search for chargino–neutralino pair production in final states with three leptons and missing transverse momentum in $\sqrt{s}$ = 13 TeV pp collisions with the ATLAS detector'.
http://arxiv.org/abs/2106.01676

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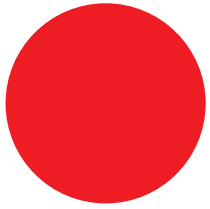

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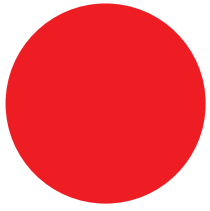

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