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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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May 22, 2023

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1 Introduction & Motivation

2 The Implementation

3 Methods & Results

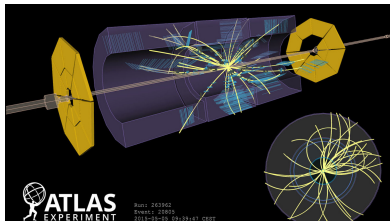
4 Conclusion & Outlook

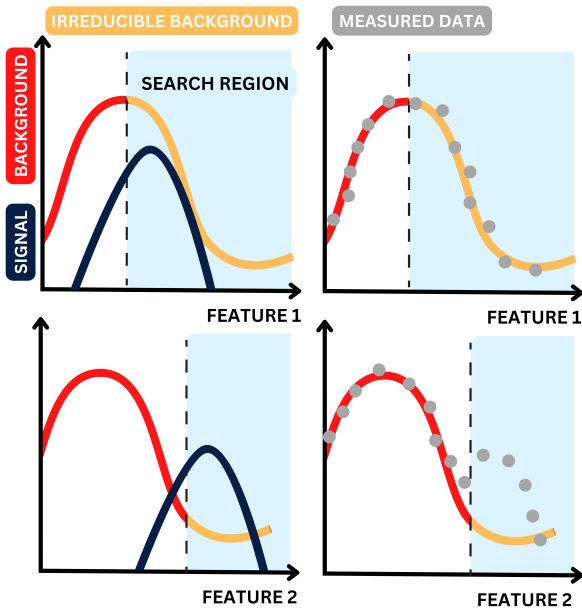
Why apply machine learning to HEP problems?

- 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?

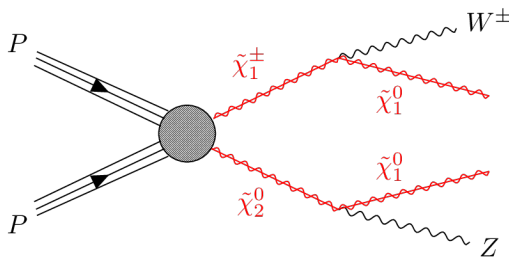
- Two data sets
 - Theory: Simulated based on Standard model physics
 - Experiment: Proton-proton collisions measured in particle detectors
- Data sets include information regarding collisions (momentum and mass of particles, collision angle etc.)
- Compare theory with experiment
 - Match: Standard model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





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?



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

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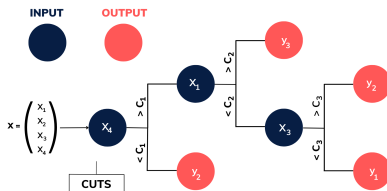
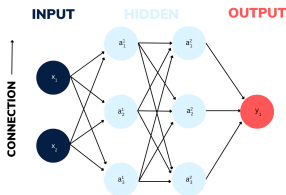
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A summary of the applied methods

- *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

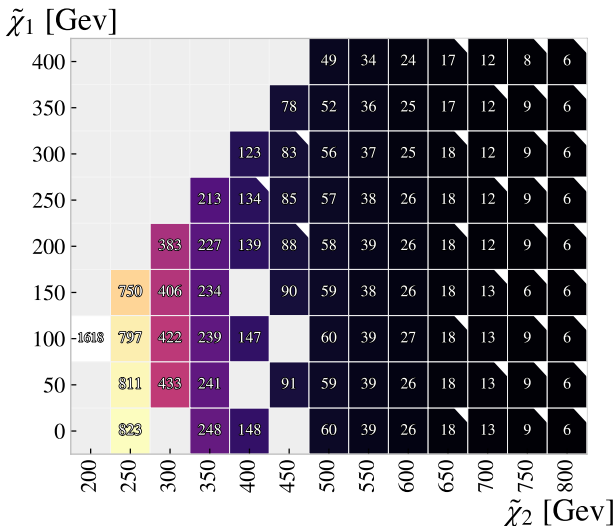


Training strategy

- 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



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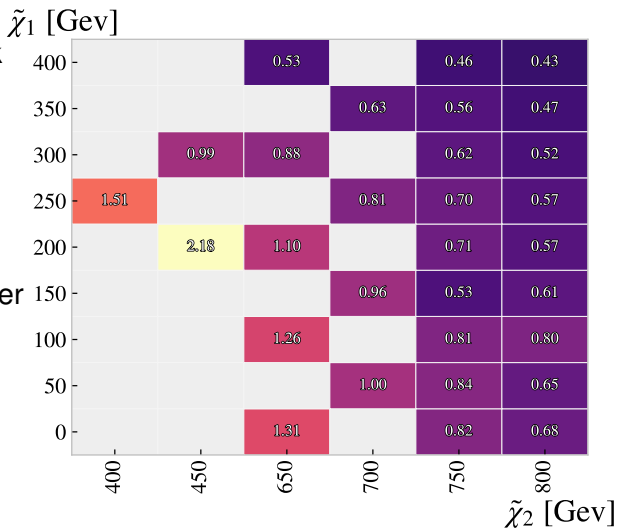
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Boosted decision trees - XGBoost

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

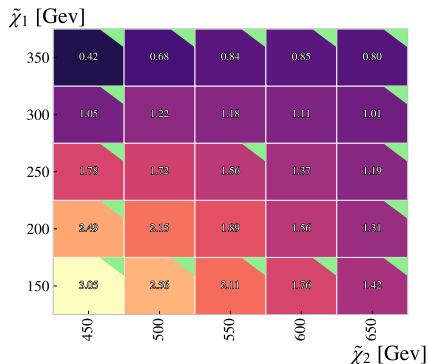
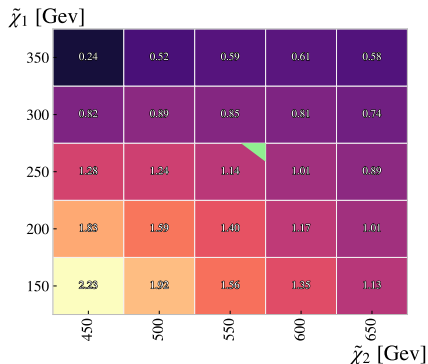


Ordinary dense neural network

NN:

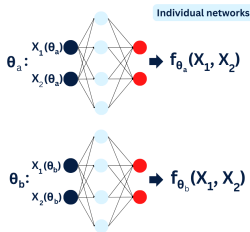


Compare one-mass approach to several-masses approach

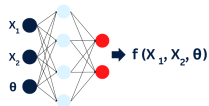


Parameterized neural network

- 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



Parametrized networks



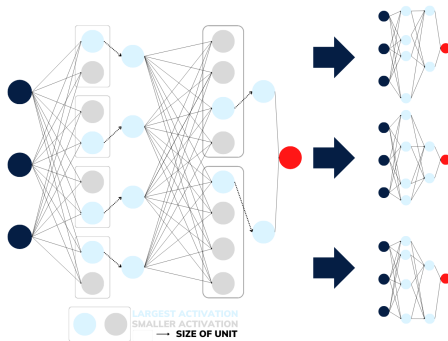
Study the effect of the parameters in the PNN

- 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 $\{50, 250\}_{\text{GeV}}$
- Second test: All events are given parameters $\{200, 300\}_{\text{GeV}}$

Parameters \ Channel	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%

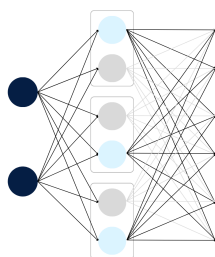
Ensemble methods - LWTA

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

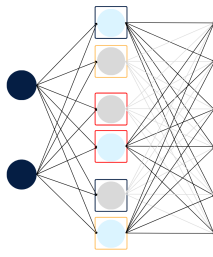


Channel-Out, SCO and Maxout

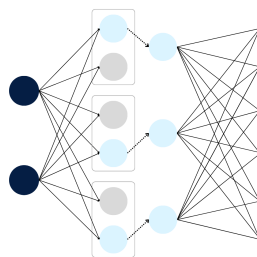
Layer	Separate weights	Static units
Channel-Out	✓	✓
SCO	✓	X
Maxout	X	✓



CHANNEL-OUT



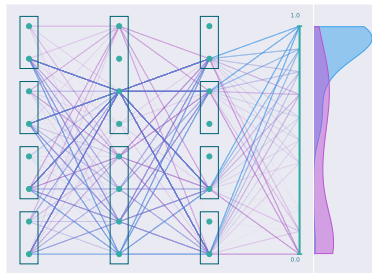
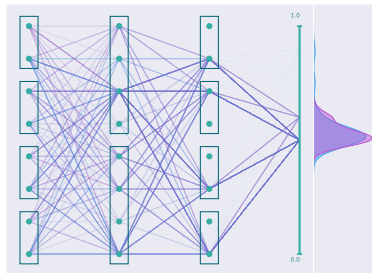
SCO



MAXOUT

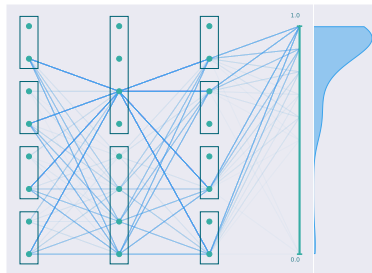
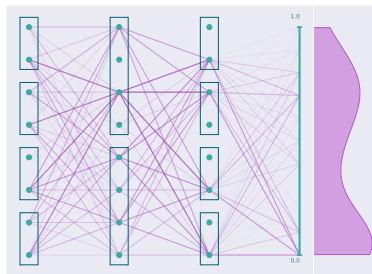
Visualization and study of sparse pathways

- 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.
- Color of lines
 - Pink: SM background
 - Blue: SUSY signal

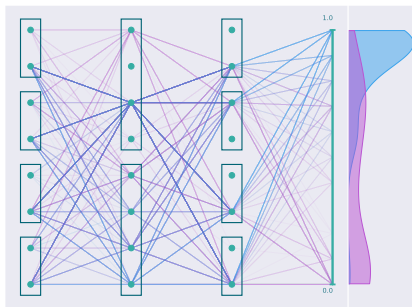


Visualization and study of sparse pathways

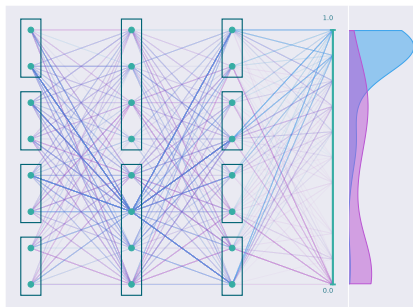
- A study of the implementation and effect of LWTA layers
 - Specifically maxout
- Visualize the activation and paths of 100 randomly sampled events
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 - 50 signal
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Comparing activation of Maxout with SCO



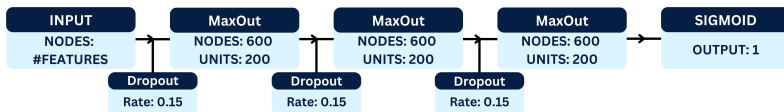
Maxout



SCO

Ensemble network architecture

MaxOut:

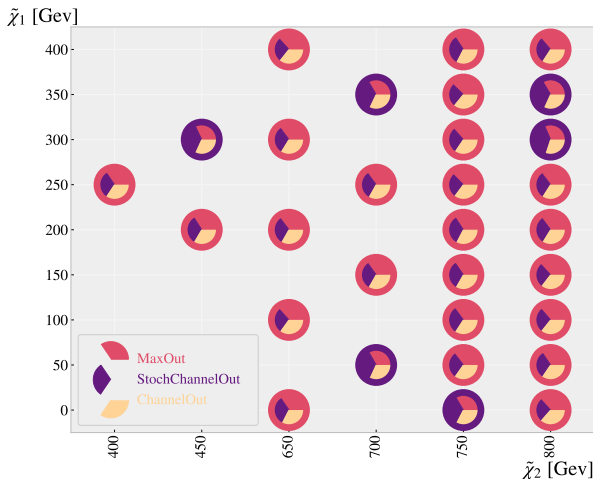


Comparing sensitivity of channel-out, SCO and maxout

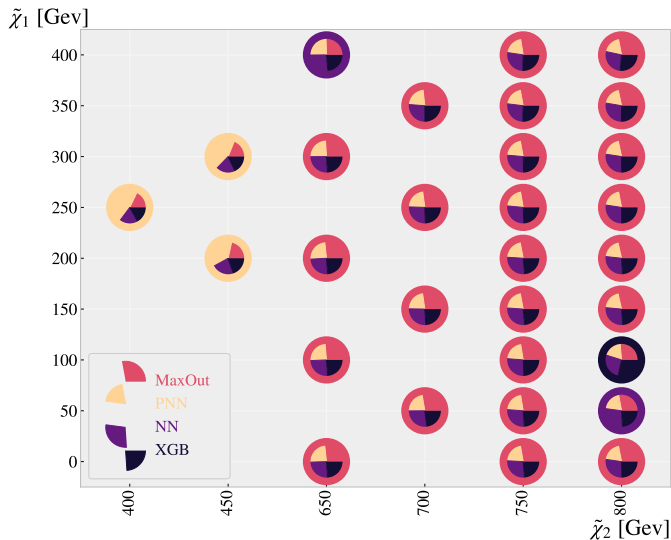
■ Maxout: 23/30

■ SCO: 7/30

- No trend for preferred masses
- Possibly improve without layer on prediction

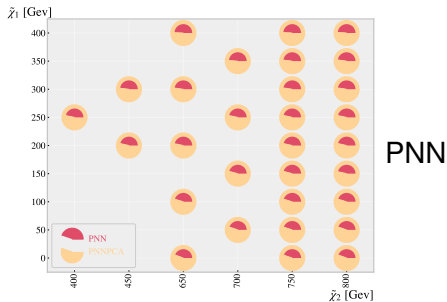
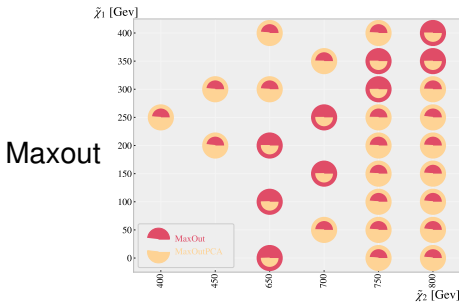


Comparing the sensitivity on a subset of the signal



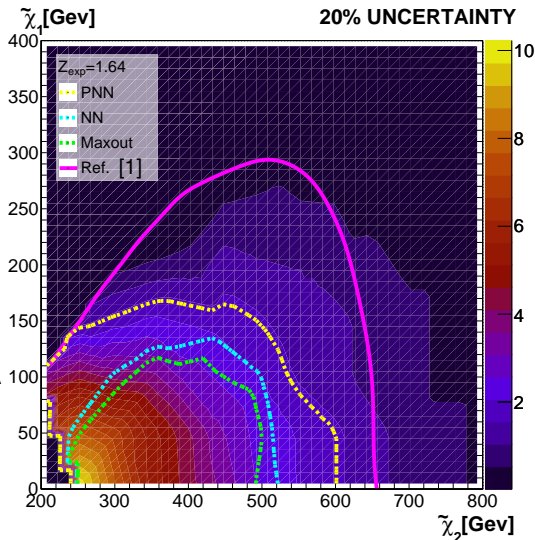
Increasing sensitivity through a PCA

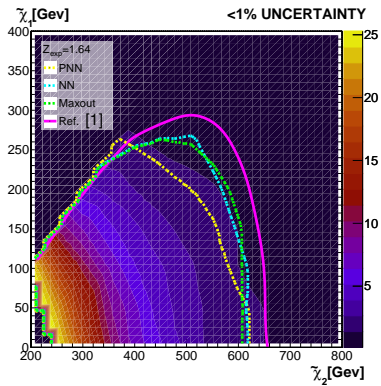
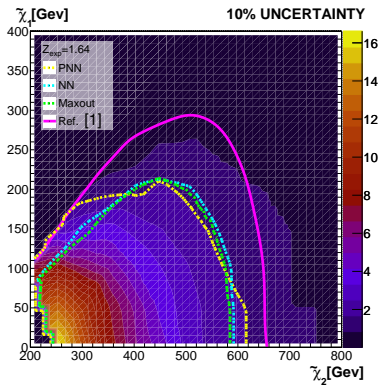
- Dimensionality reduction
- Creates new features using linear combination of original features
- Ranks from most to least variance
- This analysis
 - Demand conservation of 99.9% of variance/spread
 - 5 features removed



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





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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



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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