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Search for new phenomena in two-body invariant mass distributions using unsupervised machine learning for anomaly detection at $\sqrt{s}$ = 13 TeV with the ATLAS detector

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Searches for new resonances in two-body invariant masses are performed using an unsupervised anomaly detection technique in events produced in collisions at a center-of-mass energy of 13 TeV recorded by the ATLAS detector at the LHC. An autoencoder network is trained with 1% randomly selected collision events. Anomalous regions are then defined which contain events with high reconstruction losses. Studies are conducted in data containing at least one isolated lepton. Nine invariant masses (m_{jX}) are inspected which contain pairs of one jet (b-jet) and one lepton (e,μ), photon, or a second jet (b-jet). No significant deviation from the background-only hypothesis is observed after applying the event-based anomaly detection technique. The 95% confidence level upper limits on contributions from generic Gaussian signals are reported for the studied invariant masses. The widths of the signals range between 0% and 15% of the resonance mass, and masses range from 0.3 TeV to 7 TeV. The obtained model-independent limits are shown to have a strong potential to exclude generic heavy states with complex decays.

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1. Introduction

Searches for new physics phenomena beyond those described by the Standard Model (SM) require advanced techniques to devise selections that involve a large number of variables characterizing collision events. The limited understanding of how new physics would manifest itself has inspired the design of model-independent searches [1]. Traditional methods optimize event selections for specific signatures of signals beyond the SM (BSM signals), maximizing their separation from SM background processes. Alternatively, event selection criteria can be relaxed to target more general signatures, but this reduces the ability to suppress background. Machine learning (ML) anomaly-detection methods [2–12] provide a new way to study collision events. One such approach uses an autoencoder (AE) [13–16], a neural network architecture that is commonly used in unsupervised learning. The AE is trained using mostly SM background events and is applied to identify events that display kinematic properties different from those of SM events.

This paper details a generic search for resonances in various two-body final states, applying an anomaly detection method to the event topology for the first time in ATLAS. Events are selected based on the presence of an isolated lepton, reducing contamination from QCD multijet events. The two-body final states consist of jet+Y, where the jet can be a light jet or a b-jet (containing a b-hadron decay) while Y can be a lepton (electron or muon), a photon, or another light jet or b-jet. In all, nine invariant mass distributions are studied in this analysis.

2. Anomaly detection

2.1 Rapidity-mass matrix (RMM)

Kinematic features of the final-state objects in the preselected events are structured in a matrix called the rapidity–mass matrix (RMM) which is proposed as an input for machine learning [17]. In this analysis, the reconstructed final-state objects are light jets, b-jets, muons, electrons, or photons. A maximum of ten light jets or b-jets are considered, along with up to five electrons, muons, and photons. Together with $E_{\mathrm{T}}^{\mathrm{miss}}$, a total number of 36 final-state objects are used to define the RMM. To ensure consistent input size for all events, zero-padding is applied if the number of available objects for a particular type is less than the maximum allowed. The nine invariant mass variables are excluded from the RMM to reduce biases in the jet+Y invariant mass spectra, resulting in an input dimension of 1287. The RMM matrix is then flattened to a one-dimensional input vector before being fed into the AE.

2.2 Training Autoencoder (AE)

The AE is implemented using TensorFlow [18], comprising an encoder and a decoder. The encoder compresses the input to a latent dimensional space, and the decoder decompresses it back to its original size. The network architecture includes two hidden layers in the encoder, with 800 and 400 neurons respectively, and a latent layer of 200 neurons. The decoder mirrors the encoder's structure. The leaky ReLU [19] activation function is applied to the output in all hidden and output layers. The reconstruction loss is defined as the mean squared error between the input and reconstructed values of the dataset. The logarithm of the reconstruction loss, log(Loss), is defined as the anomaly score for each event. To form the training and validation datasets, 1% of the collision events are randomly selected after the preselection with a 7:3 split.

The network is trained using the Adam optimizer [20], minimizing the logarithm of the reconstruction loss of the training sets. The training and validation sets are reshuffled at the beginning of each epoch, with training monitored via the reconstruction loss of the validation set and terminated if no improvement is observed within 30 epochs.

2.3 Anomaly regions (ARs)

The anomaly score distributions for collision data and several benchmark BSM models are shown in Figure 1. Three ARs are chosen based on the anomaly scores, defined by $\log(\text{Loss}) > -9.1$, > -8.0, and > -6.5 respectively.

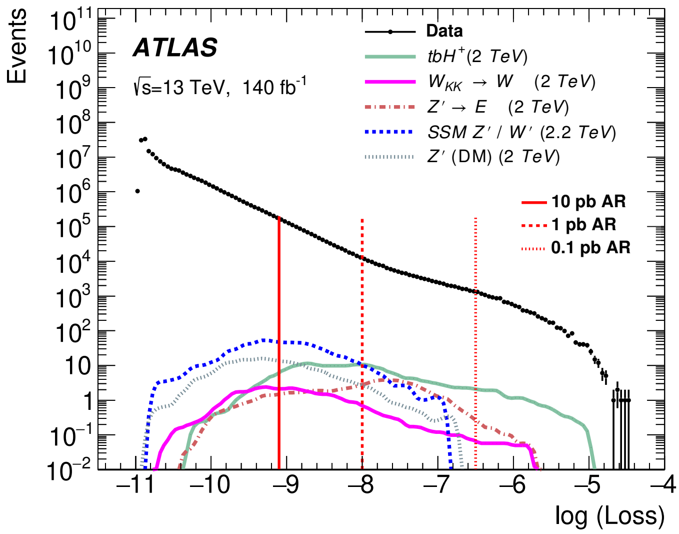

Figure 1: Distributions of the anomaly score from the AE for data and five benchmark BSM models.

3. Results

3.1 Background modeling

The nine invariant mass spectra in each AR are examined for localized excesses above the background hypothesis using a nonparametric kernel density estimation method. The SM background is estimated directly from data, avoiding potential biases introduced by MC-based background models. The method utilizes a kernel density estimator to model the background, employing a Gaussian kernel to smooth the invariant mass distribution in each AR. The background is normalized to the data in each invariant mass distribution, with uncertainties derived from the statistical fluctuations of the data.

3.2 Search for Localized Excesses

The search for localized excesses is conducted across the nine invariant mass distributions in each AR using the BumpHunter algorithm [21] , seeking any significant deviations from the SM background hypothesis. No significant excess is observed in any of the distributions, and the largest local significance across all distributions is found to be 2.9σ in the $m_{j\mu}$ spectrum near 4.8 TeV in the 10 pb AR.

3.3 Limits on Gaussian Signals

In the absence of any significant resonant signals, upper limits at 95% confidence level (CL) on the cross section times acceptance, efficiency, and branching ratio are set for Gaussian-shaped signals with an intrinsic width of 0 % or 15 % and masses ranging from 0.3 TeV to 7 TeV. The limits in the 10 pb AR are shown in Figure 2.

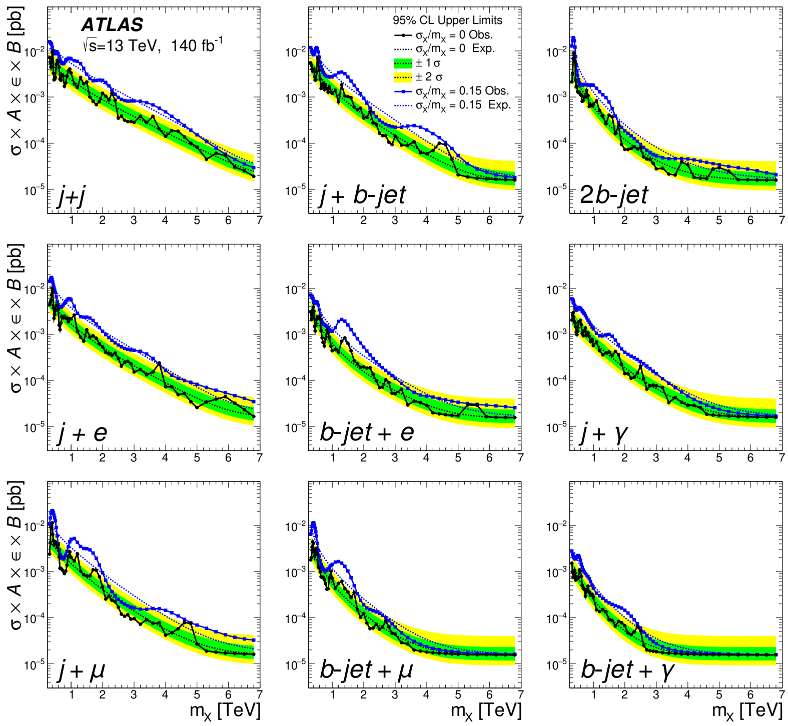

Figure 2: The 95% CL upper limits on the cross section times acceptance (A), efficiency (ϵ), and branching ratio (B) for Gaussian-shaped signals with different signal widths.

4. Conclusion

This paper presents a search for new resonances in nine two-body invariant mass distributions using an unsupervised ML anomaly detection technique applied to 140 fb^{-1} of pp collision data at $\sqrt{s}$ = 13 TeV recorded by the ATLAS detector at the LHC. The AE is trained with a randomly selected 1 % sample of the preselected collision events. Three anomaly regions are defined using the reconstruction loss of the AE and are subsequently analyzed for deviations from the SM predictions. No significant excess is observed and upper limits are set on the production cross section times branching ratio for generic Gaussian signals. The obtained limits demonstrate the potential of unsupervised ML in searches for new physics, providing a foundation for future studies in this domain.

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