

Master's thesis

Deployment of semi-unsupervised learning in the search for new physics at the LHC with the ATLAS detector

Benchmarking autoencoders for anomaly detection at the LHC with the ATLAS detector

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**Deployment of semi-unsupervised learning
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Professor Farid Ould-Saada
Dr. James Catmore

Abstract

This master thesis investigates the performance and usage of autoencoders in Beyond Standard Model (BSM) searches, using n-tuples from ATLAS that are converted to python dataframe structures. The Rapidity-Mass matrix is proposed as the input data features, with 6 b-jets and 6 l-jets, and 5 of each lepton. The goal was to test and understand the performance in the 3 lepton + e_T^{miss} final state, but due to poor results, the 2 lepton + e_T^{miss} dataset was used instead. To deal with the large dataset size, megasets were used to conserve the overall distribution in smaller batches. The autoencoders were benchmarked by creating anomalous events by altering the p_T of standard model events and testing on two supersymmetric signal models. The performance was measured in three categories: reconstruction error, background and signal reduction, and significance when performing cuts. The regular autoencoder performed better in the first and second categories, while the variational autoencoder performed slightly better in the third. Increasing the training data improved the performance in all categories. A blind test with ATLAS data and BSM signals showed that the autoencoder, when trained on the 2 lepton + e_T^{miss} dataset, managed to separate out some signals from the ATLAS data, indicating its potential use in more rigorous analyses. The thesis also discusses future work and challenges, such as computational bottlenecks, further investigation of the RMM, and better feature engineering.

Acknowledgments

To be blunt, this exercise is the equivalent of fishing in the dark, with a blindfold on, with a net of an arbitrary size, in an ocean trying to not catch fish, but something else that may or may not look like fish that might or might not be in the ocean.

Sakarias Frette / Spring 2023

This thesis has been a rollercoaster of a project, with its ups and downs, periods of joy and of mild clinical depression. Nevertheless, it is finally done, my master project. It, like so much in my life could not have been done without help. First, thanks to the No Carbs Company for creating the most delicious and addictive energy drink, the NOCCO. They have served my limbic system well and kept my need for caffeine somewhat at bay. I would also thank Bunnpris at Frederikkes plass for selling them for as long as you did, although I have to pick a bone with you guys about the somewhat axiomatically wrong choice to stop selling them. On the other hand, I enjoyed your warm burgers as well, I guess that makes a bit up for it.

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Introduction

Not only is the Universe stranger than we think, it is stranger than we can think.

Werner Heisenberg[4]

So goes the quote by Werner Heisenberg, acclaimed for his work in quantum physics in the early to mid 20th century. The quote is a reminder and a statement of the fact that the world we live in is immensely strange, beautiful, complex and interesting. From the fundamental particles to the largest galaxy clusters, the universe is a place of wonder and mystery. It is perhaps easy to forget what science tries to do when studying nature. Its fundamental duty is to model the universe as well as possible given the tools available. These models get better over time, but unlike what scientific absolutists might think and argue for, we will never know the whole truth. One should always remember Heisenberg's quote, for it illustrates the very point that nature is indeed stranger than we can think. Science with its predictive power is only an approximation, one can never truly know if the model we have of nature is a hyperfitted model or the actual instruction manual for nature itself.

As physicists, we develop and extend, replace and debunk models at the most fundamental level of nature, one of which is the Standard Model (SM). At higher energies, it is the most accurate, experimentally tested model to date, only rivalled by general relativity. From the 1930s to around 1973, there were huge leaps within the field of particle physics. Even then, the SM leaves several important questions unaddressed. Dark matter, dark energy and the energy density are phenomena that we observe around us but cannot be answered by the SM. Attempts have been made to create theoretical frameworks that could extend the SM with the strange behavior, but all have yet to be experimentally verified. One could ask oneself why this is the case. Why is this New Physics, what ever it may look like, so difficult to find? Is the framework wrong? Are the theories not well enough understood or wrong? Or it could be that the New Physics is hiding within the data already collected, in some set of features, too subtle for traditional analysis techniques, but available through advanced data analysis tools? The answer is, perhaps not to anyone's shock, we have no idea. In fact, they may all be true or false.

This story does not end here, as there are countless departments all over the world searching for this New Physics. The ATLAS experiment at CERN is one organization that has taken upon itself this task, including my supervisors Professor Farid Ould-Saada and Dr. James Catmore working on searches for New Physics at the University of Oslo. This thesis will take a somewhat different search approach than conventional analyses done at ATLAS. In a humble attempt, the assumption is made that if the New Physics exist, it is too subtle for existing analysis techniques, and that it is hiding in the data in some set of features. Further, it is assumed that by focusing on data we can label and that we know from experiment to exist, deviations from this would be of interest for more narrow searches. The hope is to filter out the events of interest, that with some certainty differs from the established theory, and then try to understand them better.

In the last decade, data analysis tools such as neural networks have become more and more available to the public, getting optimized, upgraded and extended more computationally powerful every day. Google's Tensorflow[5] and Facebook's PyTorch[6] are two increasingly popular frameworks that are used within industry, academia, and even within the particle physics community. Tensorflow was chosen for this thesis, and all the neural networks are using this framework, together with several other third party pieces of software.

Outline of the Thesis

The master thesis is outlined in the following way. The first two chapters are dedicated to machine learning and SM physics background required to understand the analysis done and tools used in the thesis. The third chapter goes through the implementation of the project, the input dataset, the ATLAS architecture, the programming libraries and feature choice. Chapter four goes through the results from the implementation as

well as discussion and interpretation of the results, the pros and cons of the implementation, aspects for future improvement, and other thoughts around the process. The final chapter is dedicated to the conclusion, where the results are summarized.

Chapter 1

Data Analysis

1.1 Anomaly detection

Anomaly detection is a versatile tool that finds application in a diverse range of scenarios, including fraud detection, anomalous sensor data analysis and time series data. The primary objective of this tool is to identify data that deviates from a predetermined standard of normal behavior. The definition of this standard can vary from situation to situation, based on the context and the expected anomalous behavior. According to Chandola, Banerjee, and Kumar [7], anomalies can be classified into three categories: *point anomalies*, *contextual anomalies*, and *collective anomalies*. *Point anomalies* represent singular or few outliers from a larger group or context and can occur in various situations. A notable example of a point anomaly is Michael Phelps, who is able to swim intensively for longer periods due to his body producing less lactic acid. *Contextual anomalies*, on the other hand, are determined based on the context of the anomaly and data, rather than as a whole. For instance, in the case of continuous gas flow data, a sudden change in flow on a Saturday, despite being within the range of Friday's flow, could be categorized as a contextual anomaly. The third type, *collective anomalies*, represents a group of anomalies that deviate from the expected behavior of the dataset. In particle physics experiments, collective anomalies are of particular interest as there are many sources of anomalous behavior where only collective anomalies are worth investigating. A single anomalous event in the detector could be explained by electronic noise, a cosmic ray or radioactive decay. Additionally, the noise generated by numerous components in such experiments makes it essential to consider collective anomalies.

1.2 Neural Networks

In the field of machine learning, statistical algorithms are commonly used for data analysis. Neural networks, a specific category of such algorithms, have experienced growth in usage in both industry and academia over the past decade. Although most of the theory behind it was developed as far back as the 1980s, the technology has only now in the last 10 to 15 years become good enough. These statistical models are of extensive use in a variety of applications, ranging from image analysis to weather prediction.

The fundamental principle behind feed forward neural networks (FFNN) involves the data being fed forward through the network, with the end output evaluated and corrections then back propagated through the network to update the weights and biases. This training process is repeated until a certain threshold is met. Figure 1.1 shows a general layout of a neural network, wherein the input layer consists of one node per feature in the dataset. The number of hidden layers and nodes per layer can be fine-tuned, with the last hidden layer connected to the output layer. The latter is determined by the problem being addressed, and in the case of the binary classification problem shown in figure 1.1, the nodes interact via tunable weights w and biases b that must be trained on the dataset prior to making predictions. The neural network, especially deep¹ ones become black boxes, meaning that once the training data or the test data is fed in through the input layer it is hard to know exactly what happens with the data until it comes out as a prediction. It is because of this that some² have shown some hesitancy with using neural networks for problems of high importance. Nonetheless, they can be very effective if used correctly.

¹Deep here refers to a neural network with more than one hidden layer, and often also a network where the layers have many neurons. One example would be a network with say a 200 - 500 - 500 - 700 - 500 - 200 - 1 network where the numbers correspond to number of nodes in their layers.

²In cases where a lot of money is at stake or lives are dependent on the output and performance of the neural network, it is reasonable to expect some explainability from the engineers if something goes wrong. There are other algorithms that are less

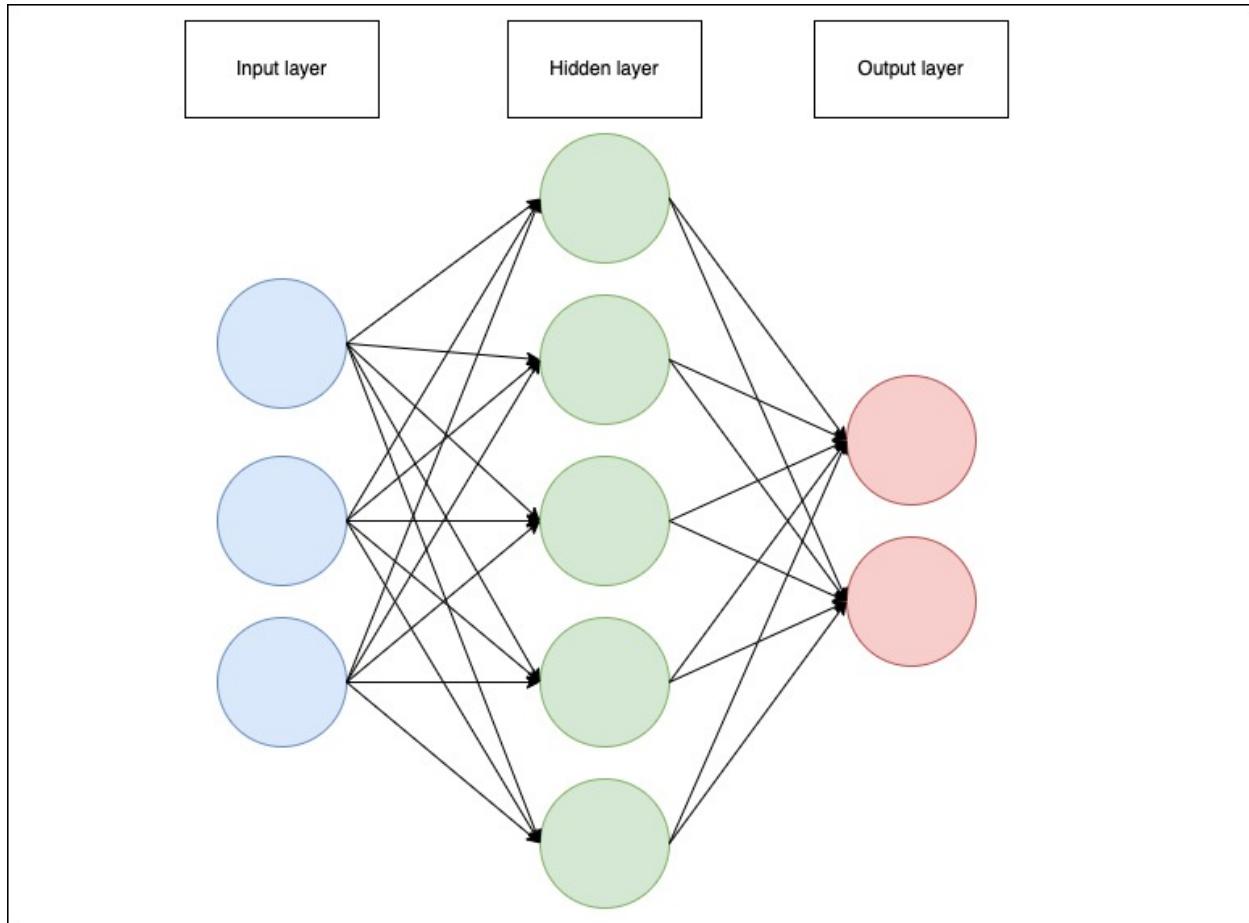


Figure 1.1: Simple neural network diagram drawn using Draw.io. Here the blue dots constitute the input layer, the green dots constitute the hidden layer, and the red dots constitute the output layer. The arrows show the connections between the nodes.

In order to avoid confusion, we will adhere to table 1.1 for the notation used in the following sections. Some of the following subsections contain work previously done by myself and two co-students, and can be found here[10].

"black box" machines, such as decision trees[8] or support vector machines[9], both of which have their pros and cons compared to neural networks.

Matrices and vectors		
Notation	Description	Type
X	Design Matrix (input data).	$\mathbb{R}^{N \times \# \text{features}}$
t	Target values.	$\mathbb{R}^{N \times \# \text{categories}}$
y	Model output, the prediction from our network.	$\mathbb{R}^{N \times \# \text{categories}}$
W^l	The weight matrix associated with layer l which handles the connections between layer $l - 1$ and l .	$\mathbb{R}^{n_{l-1} \times n_l}$
B^l	The bias vector associated with layer l which handles the biases for all nodes in layer l .	$\mathbb{R}^{n_l \times 1}$
Elements		
w_{ij}^l	The weight connecting node i in layer $l - 1$ to node j in layer l .	\mathbb{R}
b_j^l	Bias acting on node j in layer l .	\mathbb{R}
z_j^l	Node output before activation on node j on layer l .	\mathbb{R}
a_j^l	Activated node output on node j on layer l .	\mathbb{R}
Functions		
C	Cost function.	
σ^l	Activation function associated with layer l .	
Quantities		
n_l	The number of nodes in layer l .	
L	Number of layers in total with $L - 2$ hidden layers.	
N	Total number of data points.	
All indexing starts from 1: $i, j, k, l = 1, 2, \dots$		

Table 1.1: Table containing notation used for deriving the mathematical formulas for the neural network found in previous work[10]. The # here refers to number of.

Gradient descent

Let us now consider a general n-dimensional problem, with parameters $\theta = \{\theta_1, \theta_2, \dots, \theta_n\}$. Our objective is to find the set of θ that minimize a cost function with respect to the data and target. One way to solve this problem is using ordinary least squares. For this approach, the optimal paramters θ_{opt} are derived from minimizing the cost function, as shown here:

$$\theta_{opt} = (\mathbf{X}^T \mathbf{X})^{-1} \mathbf{X}^T \mathbf{t},$$

where \mathbf{X} is the design matrix containing the data, and \mathbf{t} is the target vector. This could however lead to a problem. Suppose the design matrix is sufficiently large, then the matrix inversion will get computationally expensive, or it might not even exist for a given \mathbf{X} . Thus, an alternative approch is to iteratively approximate the ideal parameters θ_{opt} .

Suppose we have a cost function $C(\theta)$ for a given problem. We can approximate the minimum of the cost function by calculating the gradient $\nabla_{\theta}C$ with respect to θ . The negative of this gradient indicates the direction for the minimum of C when evaluating it in a specific point θ_i in the parameter space [10]. This is expressed as follows

$$\theta_{i+1} = \theta_i - \eta \nabla_{\theta}C(\theta_i), \quad (1.1)$$

where η is a step size, also called the learning rate. The choice of η is not a trivial case. It is one of several hyperparameters[11] that can be altered, and that highly depend on the given problem. With regard to the learning rate, there are only three situations to consider, shown in figure 1.2.

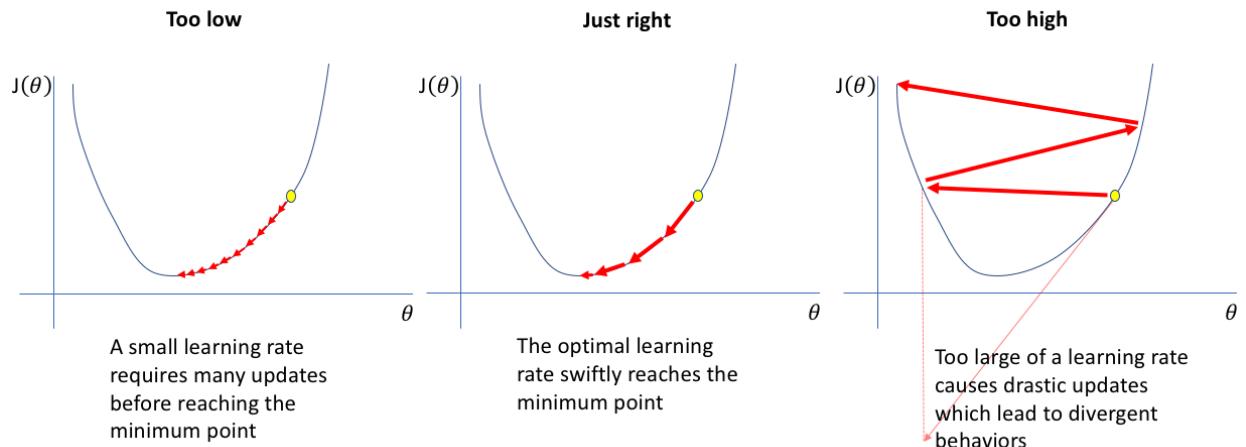


Figure 1.2: Figures showing different choices of learning rate for a given cost function, with respect to the tunable parameters. Source: [Jeremy Jordan](#), accessed 03.10.22.

Figure 1.2 visualizes the relation between the learning rate and the cost function. In the left most figure we note that the learning rate is too small. This leads to many iterations before you reach a minimum. In the rightmost figure we note that the learning rate is too high, and the result is that we get divergent behavior. Thus, the goal is to find the optimal learning rate, shown in the middle figure. There are several algorithms that try to do what is shown in the middle figure above, one of which is ADAM[12]

A modified and preferred version of gradient descent is the so-called stochastic gradient descent. Regular gradient descent can, for large datasets be quite slow, and is prone to getting stuck in a local minimum. To circumvent this issue, mini batches are introduced. For each epoch (training step) the input data is divided into M mini batches of size m . For each batch we compute the gradient and update the unknown parameter according to equation 1.1. The parameter θ_{i+1} is then updated M times for each epoch. This will reduce computation time as well as reduce the risk of getting stuck in local minima. [10].

Feed forwarding

Inference (prediction) and training both use the same feed-forward algorithm. Let's then assume that we have generated a network. The network initializes the weights and biases usually with normal or uniformly distributed values, that can later be adjusted. The procedure is to send the data through the network, weighting each connection according to the neural network's architecture, and produce an output. The procedure can be summarized in the following steps[10]:

- The data is received by the input nodes in the network for each feature.
- Each input node weights the data value according to the connection of each node in the next layer.
- Every node in the hidden layers sums the weighted data values and adds the bias associated to the given node. The resulting number is denoted as z .
- This value z is then sent through an activation function σ , which produces the output of the node, denoted as $a = \sigma(z)$.
- This process is repeated for each hidden layer, and it is important to note that the number of nodes in the hidden layers is not dependent on the number of features in the original dataset.

- The last hidden layer then sends the activated values to the output layer, where the number of nodes and choice of activation function depends on the problem to solve.

Mathematically this is expressed as follows:

$$z_j^l = \sum_{i=1}^{n_{l-1}} w_{ij}^l a_i^{l-1} + b_j^l, \quad a_j^l = \sigma^l(z_j^l), \quad (1.2)$$

where l is the layer index, j is the node index, and i is the index of the node in the previous layer, and $l \neq 1$, as it is not used on the input layer.

Backpropagation

The way neural networks learn is conventionally by the use of the backpropagation algorithm, first proposed by Rumelhart et al[13]. This is a bit misleading, as the backpropagation algorithm actually only refers to how to compute the gradient with respect to the weights at each unit[11]. The algorithm allows us to alter the weights and biases such that we get an ideal output. Assuming a cost function C , we can calculate the gradient $\nabla_{w,b}C$, and use this to back propagate the error correction from the last to the first layer. The gradient $\nabla_{w,b}C$ comprises two derivatives.

$$\nabla_{w,b}C = \left(\frac{\partial C}{\partial w_{i,j}^l}, \frac{\partial C}{\partial b_j^l} \right).$$

We have to use the chain rule to calculate the derivatives, and using that the last layer is $l = L$, we get the derivative with respect to the weights as

$$\frac{\partial C}{\partial w_{i,j}^L} = \frac{\partial C}{\partial a_j^L} \frac{\partial a_j^L}{\partial z_j^L} \frac{\partial z_j^L}{\partial w_{i,j}^L},$$

where

$$a_j^L = \sigma(z_j^L), \quad z_j^L = \sum_{i=1}^{n_L-1} w_{i,j}^L a_i^{L-1} + b_j^L.$$

This then gives us

$$\frac{\partial C}{\partial w_{i,j}^L} = \frac{\partial C}{\partial a_j^L} \sigma'(z_j^L) a_i^{L-1},$$

where we defined that

$$\sigma'(z_j^L) = \frac{\partial a_j^L}{\partial z_j^L}. \quad (1.3)$$

This derivative is very easy to calculate given a specific cost function and activation function. The derivative with respect to the bias is given as follows:

$$\frac{\partial C}{\partial b_j^L} = \frac{\partial C}{\partial a_j^L} \frac{\partial a_j^L}{\partial z_j^L} \frac{\partial z_j^L}{\partial b_j^L},$$

which gives us the final expression as

$$\frac{\partial C}{\partial b_j^L} = \frac{\partial C}{\partial a_j^L} \sigma'(z_j^L).$$

We will now introduce a new notation, a local gradient commonly called the "error". It reflects how the rate of change of the cost function depends on the j 'th node in the l 'th layer.

$$\delta_j^l \equiv \frac{\partial C}{\partial z_j^l}.$$

Using this we get the following expression:

$$\delta_j^L = \frac{\partial C}{\partial z_j^L} = \frac{\partial C}{\partial a_j^L} \frac{\partial a_j^L}{\partial z_j^L} = \frac{\partial C}{\partial a_j^L} \sigma'(z_j^L),$$

giving us the more compact forms of the derivatives with respect to the weights and biases:

$$\frac{\partial C}{\partial w_{i,j}^L} = \delta_j^L a_i^{L-1}, \quad \frac{\partial C}{\partial b_j^L} = \delta_j^L.$$

We can now let $\boldsymbol{\delta}^l$ be the vector of all the errors in the l 'th layer, and $\boldsymbol{\delta}^L$ be the vector of all the errors in the last layer. The error in the l 'th layer can then be expressed as a matrix equation for the last layer as follows:

$$\boldsymbol{\delta}^l = \nabla_a C \odot \frac{\partial \sigma}{\partial z^L}, \quad \nabla_a C = \left[\frac{\partial C}{\partial a_1^L}, \frac{\partial C}{\partial a_2^L}, \dots, \frac{\partial C}{\partial a_{n_L}^L} \right]^T.$$

Here \odot is the Hadamard product (element wise product). This local gradient can now be defined recursively for the j 'th node in a layer l as a function of the local error in the next layer:

$$\delta_j^l \equiv \frac{\partial C}{\partial z_j^l} = \sum_k \frac{\partial C}{\partial z_k^{l+1}} \frac{\partial z_k^{l+1}}{\partial z_j^l} = \sum_k \frac{\partial z_k^{l+1}}{\partial z_j^l} \delta_k^{l+1}. \quad (1.4)$$

We also note that

$$z_k^{l+1} = \sum_{j=1}^{n_l} w_{j,k}^{l+1} a_j^l + b_k^{l+1} = \sum_{j=1}^{n_l} w_{j,k}^{l+1} \sigma(z_j^l) + b_k^{l+1},$$

thus the partial derivative is given as

$$\frac{\partial z_k^{l+1}}{\partial z_j^l} = w_{j,k}^{l+1} \sigma'(z_j^l), \quad (1.5)$$

using the substitution from equation 1.3. This allows us to substitute equation 1.5 into equation 1.4 to get the following expression:

$$\delta_j^l = \sum_k w_{j,k}^{l+1} \sigma'(z_j^l) \delta_k^{l+1}. \quad (1.6)$$

Using this, we can derive a three-step formula for the backpropagation algorithm:

- Compute the local gradient for the last layer, $\boldsymbol{\delta}^L$.
- Recursively compute the local gradient for the remaining layers, $\boldsymbol{\delta}^l$ for $l = L-1, L-2, \dots, 1$.
- Update the weights and biases via gradient descent³ for all layers, $l = 1, 2, \dots, L$, given the learning rate η as shown below:

$$\begin{aligned} w_{i,j}^l &\leftarrow w_{i,j}^l - \eta \delta_j^l a_i^{l-1}, \\ b_j^l &\leftarrow b_j^l - \eta \delta_j^l. \end{aligned}$$

1.3 Autoencoders

Autoencoders are a subset of neural networks. Whereas a general neural network in principle can take any shape, autoencoders are more restrictive. This restrictiveness can in its most general sense be condensed into the following points:

- Same number of output categories as input categories
- A latent space with smaller dimensionality than the input/output layer
- They are trained on their own input, using reconstruction as metric

What we end up with are two funnel shaped parts linked together. The two funnels are called the encoder (left funnel) and decoder (right funnel) respectively. This architecture is not accidental, but rather designed with a very specific solution of problems in mind, namely reconstruction. A good example to illustrate this is image reconstruction, illustrated in figure 1.3. Suppose you have an image, and want to reconstruct it. By feeding the encoder an image, and comparing the decoder output to the actual image, the autoencoder can tune itself to recreate the image it trained on.

³In practice one would use gradient descent with an optimizer, such as ADAGrad or ADAM as mentioned in section 1.4

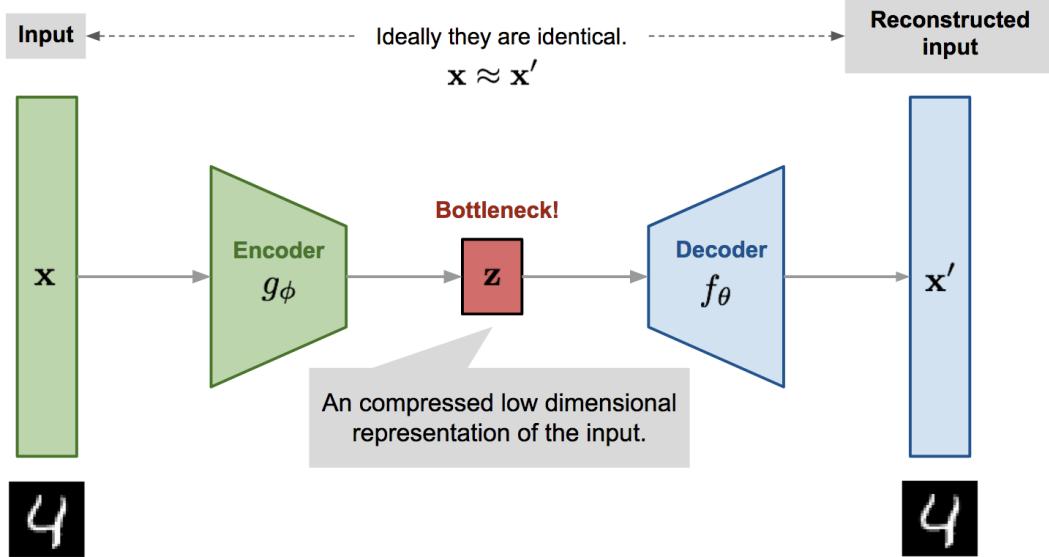


Figure 1.3: Figure depicting a model for an autoencoder. Here the input \mathbf{x} is the original image, \mathbf{x}' is a reconstructed version of \mathbf{x} , g_ϕ is the encoder, f_θ is the decoder, and \mathbf{z} is the latent space. Found 14.01.23 at lilianweng.github.io [1].

1.3.1 Regular autoencoder

Mathematically the regular autoencoder is represented as follows[1]. Using the annotations of each component in figure 1.3 the decoded information is defined as follows

$$\mathbf{z} = \mathbf{g}_\phi(\mathbf{x}),$$

and the reconstruction given as

$$\mathbf{x}' = \mathbf{f}_\theta(\mathbf{g}_\phi(\mathbf{x})).$$

The parameters (ϕ, θ) are the tuneable parameters adjusted according to the loss function. In our case, the goal is reconstruction without copying⁴, thus we can use mean squared error, given as

$$L_{AE}(\phi, \theta) = \frac{1}{N} \sum_{i=0}^{N-1} (\mathbf{x}^i - \mathbf{f}_\theta(\mathbf{g}_\phi(\mathbf{x}^i)))^2. \quad (1.7)$$

1.3.2 Variational autoencoders

Another popular method for reconstruction is the so-called variational autoencoder. The work by Kingman and Welling [14] showed how one can use the variational bayesian approach for efficient approximate posterior inference, leading to the use of variational autoencoders. Here, contrary to regular autoencoders, the latent space is a distribution that can be sampled from. In the context of reconstruction, this means that we want to create a latent space distribution based on the true distribution in the data, and use this latent space distribution to then generate data given that latent space.

The variational autoencoder contains two neural networks. The generative model $p_\theta(x|z)$ is the decoder of the network and $q_\phi(z|x)$ is the encoder. Under certain conditions[14] the KL divergence⁵ can be computed analytically, and it can then be showed[14] that the variational approximate posterior is:

$$\mathcal{L}(\theta, \phi; x^{(i)}) \simeq \frac{1}{2} \sum_{j=1}^J (1 + \log((\sigma_j^{(i)})^2) - (\mu_j^{(i)})^2 - (\sigma_j^{(i)})^2) + \frac{1}{L} \sum_{l=1}^L \log p_\theta(x^{(i)}|z^{(i,l)}), \quad (1.8)$$

where $z^{(i,l)} = \mu^{(i)} + \sigma^{(i)} \odot \epsilon^{(l)}$ and $\epsilon^{(l)} \sim \mathcal{N}(0, I)$. This is the cost function for the variational autoencoder.

⁴In some cases the autoencoder can train itself to learn the identity matrix, which leads to reconstruction by copying, not training.

⁵The KL divergence is a measure of how one probability distribution is different from a second reference probability distribution, and is related to the cost function via the marginal likelihood $\log p_\theta(x^{(i)}) = D_{KL}(q_\phi(z|x^{(i)})||p_\theta(z|x^{(i)})) + \mathcal{L}(\theta, \phi; x^{(i)})$

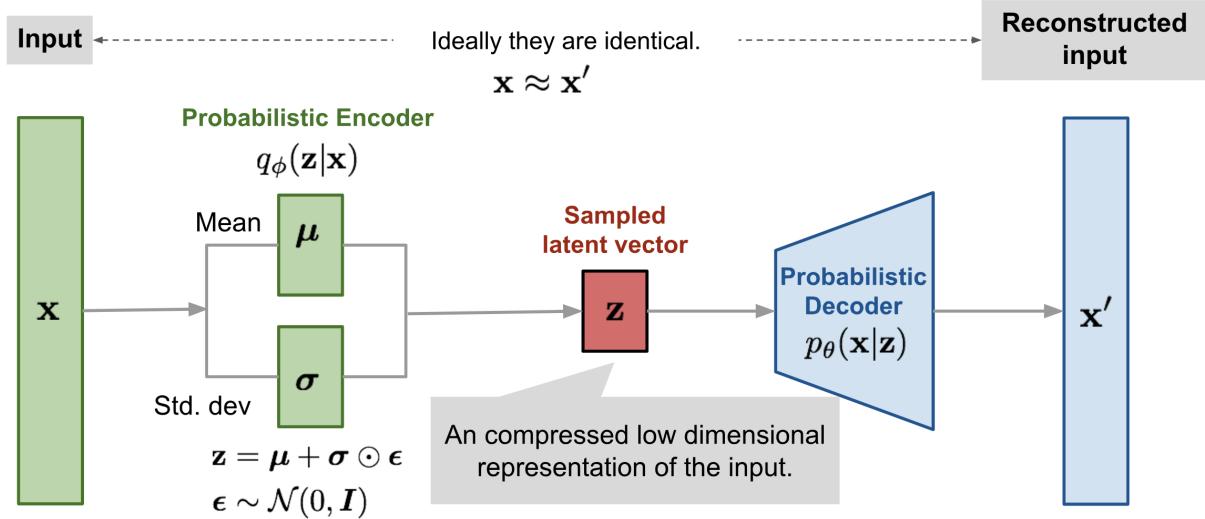


Figure 1.4: Figure depicting a model for a variational autoencoder. Found 14.01.23 [here](#) [1].

Figure 1.4 is a graphical representation of a variational autoencoder. The encoder produces a mean and a standard deviation based on the input data, which then produce a latent space distribution from which the decoder can sample and produce an output.

1.3.3 Inference

As with the cost function for the autoencoder, the inference evaluation is also done by reconstruction. To look for anomalies in the data, the reconstruction error will span a range of values, where the lower end represents events that the autoencoder reconstructed well. The reconstruction error used in the analyses is defined below.

$$err = \log_{10} \left[\sum_i (x_i - \tilde{x}_i)^2 \right], \quad (1.9)$$

where x is the input data and \tilde{x} is the output from inference. The background and signal distributions made from the reconstruction error is key to analyse the performance of the autoencoders.

1.4 Other tools and algorithms

Adaptable moment estimation (ADAM) Optimizer

Stochastic gradient descent, though very useful, lack the ability to adapt to the feature space. One algorithm that address this issue is the ADAM optimizer [12]. The Adaptable Moment Estimation (ADAM) algorithm uses stochastic gradient descent, but with an adaptive learning rate. This learning rate is adjusted by calculating estimates for the first and second moment⁶. Thus, a large gradient would indicate proximity to a minimum in feature space, thus a lower learning rate would yield a more accurate result, where as a small gradient would suggest far proximity to a local minimum, and thus a larger learning rate would increase the chance of approaching a minimum.

Activation functions

Several activation functions are used in neural networks, and how one chooses the best combination for a given problem is not trivial. This often leads to the use of tuning. Below are a list of the activation functions used in this thesis, and their mathematical definitions.

1. $\text{sigmoid}(x) = \frac{1}{1+e^{-x}}$

⁶In statistics the first moment is the expectation value for a distribution, $E[X - \mu]$. The second moment is the expectation value of the distribution squared, i.e the variance, $E[(X - \mu)^2]$

2. $\tanh(x) = \frac{e^x - e^{-x}}{e^x + e^{-x}}$
3. $\text{ReLU}(x) = \max(0, x)$
4. $\text{LeakyReLU}(x) = \max(\alpha x, x)$
5. $\text{Softmax}(x) = \frac{e^x}{\sum_{i=1}^n e^x}$
6. $\text{Linear}(x) = x$

Statistical significance

In the frequentist statistics, the Poisson distribution can be approximated with a Gaussian distribution in the limit of large number of events[15]. The expression for the significance is given then as

$$Z = \frac{s}{\sqrt{b}}, \quad (1.10)$$

where s is the amount of signal, and b is the amount of background. For low statistics we have that the significance is given as

$$Z = \sqrt{2 \left[(s+b) \ln \left(1 + \frac{s}{b} \right) - s \right]}. \quad (1.11)$$

It can be shown that in the limit where $s \ll b$, the two expressions are approximately the same[15].

Chapter 2

The Standard Model and Beyond Standard Model physics

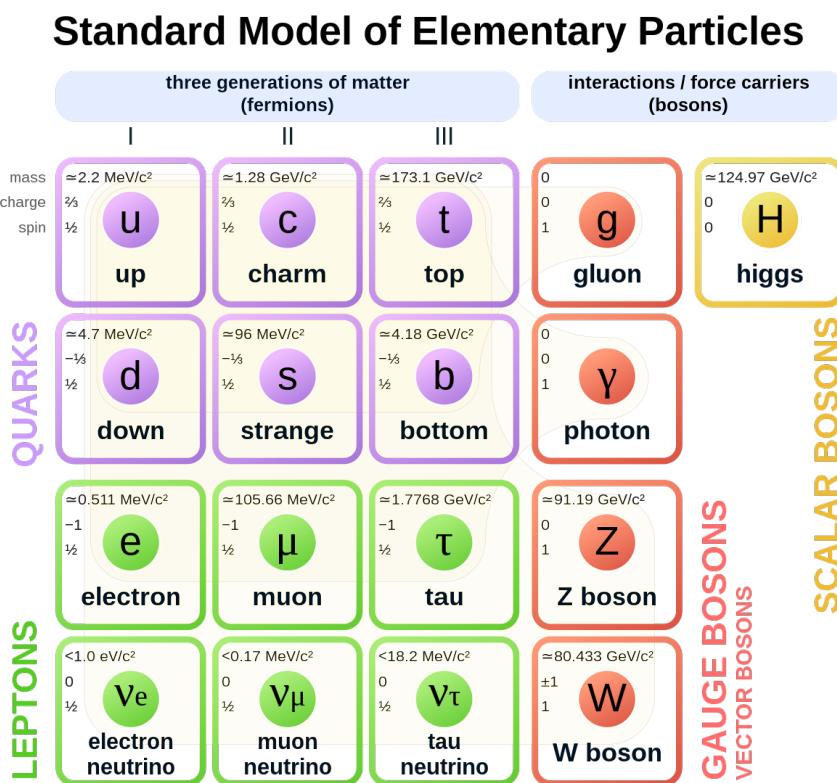


Figure 2.1: The SM of elementary particles. Source [here](#). Accessed 07.10.22

2.1 Structure and composition of the Standard Model

This section will describe the SM in a phenomenological way, as the mathematics and physical reasoning behind the theory is not of great importance to understand the work, results or discussion in this thesis. For a more technical explanation, see (Pich, 2008)[16] for a well written paper containing some more SM fundamentals as well as summarizing the experimental status regarding the SM. For more mathematical understanding of the SM, Peskin and Schroeder's "An introduction to Quantum Field theory" (Peskin and Schroeder, 1995)[17] is highly recommended. Finally, see Thomson's "Modern Particle physics" (Thomson, 2013) [18] for a very comprehensive and up-to-date book that is easy to read and understand.

The SM is to physicists what the periodic table is to chemists, and is to this day the most fundamental description of matter as we know it at the subatomic scale. It comprises two parent class particles, fermions with half integer spin and bosons with full integer spin. The model contains 6 leptons, 6 quarks, coming in 3

colors each, 4 gauge bosons mediating the electroweak interactions (γ, W^\pm, Z^0), 8 gluons behind the strong interaction and one scalar Higgs explaining particle masses, all of which are shown in figure 2.1.

Fermions

The fermions are the building blocks of matter, and contain two types of particles, leptons and quarks. The up and down quarks form protons and neutrons, which together with electrons form the atoms. Fermions, unlike bosons, are spin half particles. The fermions are grouped into three so-called families:

$$\begin{bmatrix} \nu_e & u \\ e^- & d' \end{bmatrix}, \quad \begin{bmatrix} \nu_\mu & c \\ \mu^- & s' \end{bmatrix}, \quad \begin{bmatrix} \nu_\tau & t \\ \tau^- & b' \end{bmatrix}$$

The left column contains the leptons whilst the right column contains the quarks. Within the left column, the subscripted ν denotes what kind of neutrino that corresponds to the given lepton. Here, the first family consists of the electron, the electron neutrino, the up and down quarks. The second family consists of the muon and the muon neutrino, the charm and strange quarks. The third family consists of the tau and the tau neutrino, the top and bottom quarks. The masses of these particles increases for each particle in the matrix as the family number increases, i.e. the muon is heavier than the electron, and the tau is heavier than the muon, and so on for the other charged fermions. It is not known whether or not the neutrinos follow this pattern as well due to their very low mass. Below is a table with specific properties of the fermions.

Generation	Name	Symbol	Antiparticle	Spin	Charge	Mass (MeV/c ²)
Quarks						
1	up	u	\bar{u}	1/2	2/3	$2.2^{+0.6}_{-0.4}$
	down	d	\bar{d}	1/2	-1/3	$4.6^{+0.5}_{-0.4}$
2	charm	c	\bar{c}	1/2	2/3	1280 ± 30
	strange	s	\bar{s}	1/2	-1/3	96^{+8}_{-4}
3	top	t	\bar{t}	1/2	2/3	172100 ± 600
	bottom	b	\bar{b}	1/2	-1/3	4180^{+40}_{-30}
Leptons						
1	electron	e^-	\bar{e}^-	1/2	-1	0.511
	electron neutrino	ν_e	$\bar{\nu}_e$	1/2	0	$< 9 \cdot 10^{-7}$
2	muon	μ^-	$\bar{\mu}^-$	1/2	-1	105.7
	muon neutrino	ν_μ	$\bar{\nu}_\mu$	1/2	0	< 0.170
3	tau	τ^-	$\bar{\tau}^-$	1/2	-1	1776.86 ± 0.12
	tau neutrino	ν_τ	$\bar{\nu}_\tau$	1/2	0	< 15.5

Table 2.1: Table showing properties of all the fermions, including name, symbol, antiparticle, spin, charge, generation and mass. The masses were found here [2] and [3].

Another mystery regarding the neutrinos is the relation to antiparticles. To each particle corresponds an antiparticle, i.e. for $l^- \rightarrow l^+, q \rightarrow \bar{q}$, where the antiparticle and particle are different. With neutrinos however it is not known whether the neutrinos and antineutrinos are the same particle $\nu = \bar{\nu}$ (Majorana neutrino), or if they are different $\nu \neq \bar{\nu}$ (Dirac neutrino).

Quarks are fractional charge particles, with defined charge of either 2/3 or -1/3, as shown in table 2.1. They are the main building blocks of protons and neutrons, and are bound by the strong force, the strongest of the four fundamental forces. The force mediator is the gluon. The other half of fermions are the leptons. They are split into the charged leptons (electrons, muons and taus), and the uncharged leptons (neutrinos). The charged leptons can interact via the electroweak force, where the Z, W bosons as well as the photon can be a mediator. Note that the neutrinos can only interact through the weak force.

Bosons

Bosons are integer number spin particles, with spin 0, 1, 2, Within bosons there are so-called elementary bosons, some of which are force carriers or mediators such as the W^\pm , Z and the photon. The Higgs boson is

the only elementary scalar boson, but it is not a force carrier. It is the excitation of the Higgs field which is responsible for providing masses to the fermions via a process called spontaneous symmetry breaking[16]. Other bosons are so-called composite bosons, mesons ($q\bar{q}$) and baryons (qqq) which are particles constructed by even or half integer spin. Bosons also have antiparticles, where (γ, g, H^0, Z^0) are equal to their respective antiparticle, and the $W^- \rightarrow W^+$ are not equal.

Feynman diagrams

A graphical way to understand particle interactions are through Feynman diagrams. Feynman diagrams are drawn based on the Feynman rules for a given Lagrangian[16][19], and each component can be linked to a part in the Lagrangian for the system.

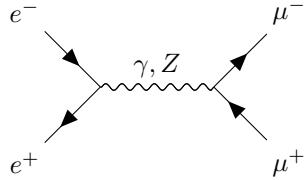


Figure 2.2: Feynman diagram of muon pair production from electron annihilation. Here, both Z and γ can work as the propagator.

In figure 2.2 we have a Feynman diagram describing electron-positron annihilation into muon-antimuon pairs. In this thesis, all diagrams will be interpreted from left to right, i.e. figure 2.2. The diagram contains all the components in the Lagrangian, and arrows, curly lines and so on all have its own meaning. A straight line with an arrow usually means a fermion, where the direction of the arrow tells if the particle is a particle (arrow towards the vertex) or an antiparticle (arrow away from the vertex). There is often also a propagator between the left and right side of the Feynman diagram, and they depend on the processes we want to study. In the diagram above we have lepton annihilation, thus we can both have the photon and the Z-boson as a propagator. This process is called a neutral current[16], as the total charge coming out of the interaction is 0. There are also so-called charged currents, where the sum of charge is not 0. Note that we only require charge conservation, thus there is nothing wrong with either having a neutral or a charged current, as long as charge conservation is preserved.

Feynman diagrams are used for both visualizing scatterings, annihilations and decays. An example is provided in figure 2.3.

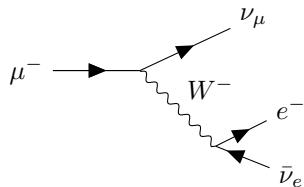


Figure 2.3: Muon decay into an electron, an electron neutrino and a muon neutrino via the W^- boson. Read the graph from left to right.

In figure 2.3 we have a decay of a muon into an electron and two neutrinos through a charged current. The examples above in figure 2.2 and 2.3 show interactions with the electroweak force, but along with the electroweak interactions, are also the quantum chromodynamics (QCD), responsible for interactions between quarks and gluons. A strange property of QCD, is that the coupling constant α_S , unlike the α_{EM} for electromagnetism, gets stronger as the energy decreases. This is because QCD (and weak interactions) are based on non-abelian groups[17], thus to study such interactions, one needs to create collisions at very high energies.

Proton-proton collisions

During an interaction between the protons in proton-proton collisions both the quarks and gluons can interact as shown below:

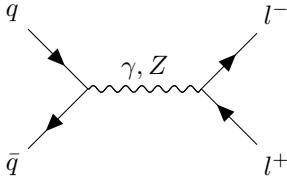


Figure 2.4: Proton-proton collision with lepton pair production via the Z boson or photon. Read from left to right.

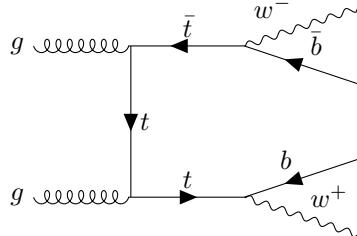


Figure 2.5: Proton-proton collision showing the $t\bar{t}$ channel. Read from left to right.

In figure 2.4 and figure 2.5 we have two examples of Feynman diagrams of possible interactions in proton-proton collisions. Figure 2.4 displays a lepton pair production via the Z boson or photon from quark-antiquark annihilation, and figure 2.5 displays the $t\bar{t}$ production via gluon-gluon fusion.

Some limitations

Although the SM has had great success comparing predictions with experiments, there are still several problems not addressed by it. Gravity is one example. The SM as described above cannot incorporate gravity in a quantized way. There are models that try, without success so far, to address this problem. They supplement the SM, and do not derive from it. Another problem with the SM is a curious property of the weak interaction, namely that parity is broken. Parity as a mathematical operation is equivalent to the spatial inversion through the origin[18]:

$$x \rightarrow -x. \quad (2.1)$$

In other words, parity can be thought of as left-right symmetry, or mirror symmetry. Breaking of parity is observed in weak currents, where the mediator of the charged currents W^\pm , only interacts with left-handed fermions and right-handed antifermions. In the SM, neutrinos are assumed to be massless, and the righthanded neutrinos are sterile, i.e. they do not interact in the SM.

This asymmetry is strange, and hints towards new physics that perhaps can restore the parity breaking at much higher energies. Another note to make is that it has been experimentally verified through observation of neutrino oscillations that the neutrinos are massive[20], with an upper limit on the mass for the anti electron neutrino of $m_\nu < 0.8\text{eV}c^2$ at 90% confidence level. This is direct experimental evidence that the SM is wrong, as the tiny masses of the neutrinos are not predicted by the SM.

2.2 Beyond Standard Model (BSM) physics

The approach of using an autoencoder is an attempt to try and detect NP in an as model agnostic way as possible. This is because there are numerous amounts of possible BSM physics signals that could exist in nature. To test the autoencoder two signals from supersymmetry were used. The testing was done only after having trained on SM background only.

Supersymmetry

Supersymmetry is a BSM theory that attempts to solve two problems that the SM has. First we have the hierarchy problem. As the SM is a perturbative theory, the Higgs mass increases at higher energies. The problem is that when you approach higher and higher energies, the Higgs mass goes to infinity, which is not physical. Supersymmetry solves this problem by introducing a supersymmetric partner to each particle in the SM. The result is that the contributions to the Higgs mass from fermions and bosons mainly cancel each other out, thus fixing the hierarchy problem. Another problem we have with the SM is that is does not

have a candidate for dark matter, whereas some supersymmetry models have a dark matter candidate. As supersymmetry in theory could solve some problems with the SM it is a topic of great interest with both theoretical and experimental physicists. Still, after two LHC runs supersymmetry has not been observed[21].

To test the autoencoders, two signal models from SUSY were picked. The chosen signal samples have a final state with 3 leptons + e_T^{miss} , as the background does. The signal final state is shown below in figure 2.6.

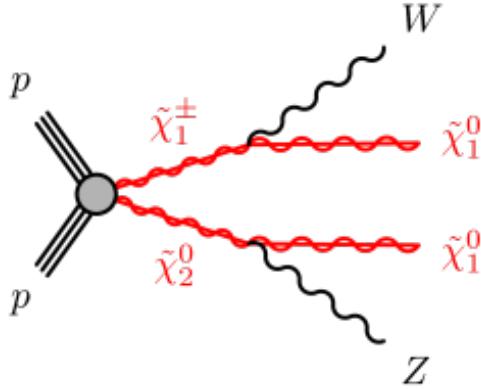


Figure 2.6: SUSY diagram showing chargino-neutralino production in proton-proton collision. The test samples we look for with this signal is where the W and Z boson decay leptonically.

Figure 2.6 shows chargino($\tilde{\chi}_2^{\pm}$)-neutralino($\tilde{\chi}_1^0$) production via proton-proton collisions. The chargino is the supersymmetric partner to the charged bosons and the neutralino is the supersymmetric partner of the neutral bosons. The neutralino is the lightest and stable supersymmetric particle, and is therefore a good candidate for dark matter. The search for these particles was similarly done by ATLAS in 2021[21].

Chapter 3

Implementation

3.1 The ATLAS detector

The ATLAS detector comprises several main components for recording proton-proton collisions. Amongst them are the muon detectors, the electromagnetic calorimeters, the hadronic calorimeters and the inner detector. The kinematics and geometry describing the collisions are written below.

Kinematics and detector geometry

Before the data can be analysed, it has to be collected and processed in a detector. The data used in the work of this thesis are generated from proton-proton collisions in the ATLAS detector at the Large Hadron Collider (LHC). The ATLAS inner detector itself is contained in a solenoid field, and the kinematic variables are measured based on the following coordinate system. The z-axis is defined to go along the center axis of the solenoid, whereas the y-axis points upwards in the detector and the x-axis radially outwards from the center axis. This allows for all transverse variables to be defined in the x-y plane^[22]. From this we construct the azimuthal and polar angles ϕ and θ , where the azimuthal angle ϕ is the angle around the z-axis, and the polar angle θ is the angle from the z-axis, as shown in figure 3.1.

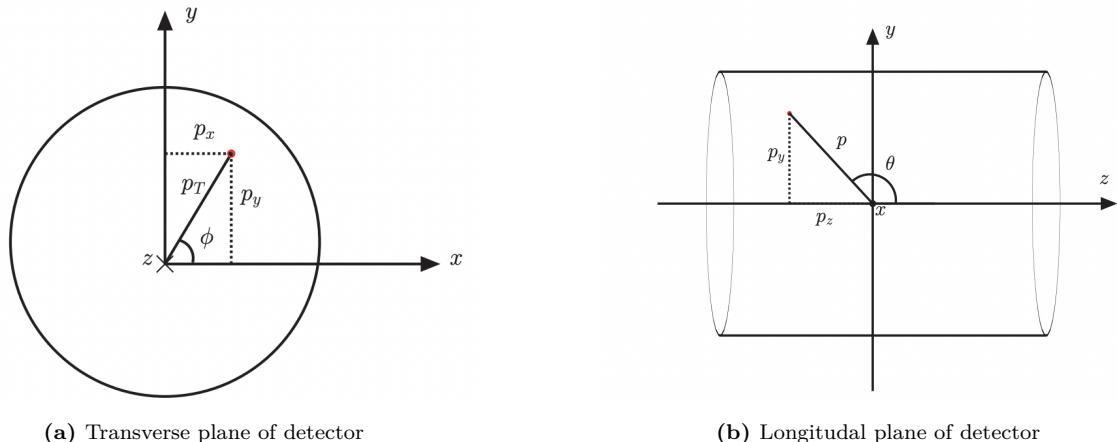


Figure 3.1: Spherical coordinate definitions with the azimuthal and polar angles ϕ and θ . Here figure 3.1a of the transverse plane shows the z-axis into the paper, whereas figure 3.1b of the longitudinal plane shows the positive x-axis going out of the paper. Figure taken from [22].

In figure 3.1 the kinematic variables for proton-proton collisions are described by the energy, rest mass and momentum, given as E , m , and $\mathbf{p} = (p_x, p_y, p_z)$ respectively. As the particles move with very high energy, we will use the relativistic four momentum⁷, given as $\mathbf{P} = (E, \mathbf{p})$. We also have that

$$\gamma = \frac{1}{\sqrt{1 - \beta^2}},$$

⁷In special relativity, four momentum is used as both energy and momentum are conserved, and thus by creating the four momentum, you achieve a Lorentz invariant quantity[18].

where γ is the Lorentz factor, and $\beta = \frac{v}{c}$, which gives us the following definitions for energy $E = \gamma m$ and momentum $\mathbf{p} = \beta \gamma m$ [22]. From this we can derive the energy momentum formula:

$$\begin{aligned}\mathbf{p}^2 &= \beta^2 \gamma^2 m^2 \\ \mathbf{p}^2 + m^2 &= m^2 (\beta^2 \gamma^2 + 1) \\ \mathbf{p}^2 + m^2 &= m^2 \gamma^2 \\ \mathbf{p}^2 + m^2 &= E^2\end{aligned}$$

$$E = \sqrt{p^2 + m^2}. \quad (3.1)$$

It can be shown that the phase space of a particle is given by[23]:

$$d\mathbf{p} = dp_x dp_y dp_z = p^2 dp d\Omega = dp_z p_T dp_T d\phi, \quad (3.2)$$

where p_z is the momentum along the beam direction, p_T is the projected momentum on the transverse plane, and Ω is the solid angle. An analog to the relativistic longitudinal velocity is the rapidity y . To define this we have that the relativistic generalization of equation 3.2 is given by:

$$d^4 p \delta(E^2 - p^2 - m^2) = d\mathbf{p} \frac{1}{E} = p_T dp_T d\phi dy, \quad dy = \frac{dp_z}{E}.$$

Using the fact that $p = \sqrt{p_T^2 + p_z^2}$ and equation 3.1 we can integrate dy to get the rapidity:

$$\begin{aligned}\int dy &= \int \frac{dp_z}{\sqrt{p_T^2 + p_z^2 + m^2}} \\ y &= \cosh^{-1} \left(\frac{E}{\sqrt{p_T^2 + m^2}} \right)\end{aligned} \quad (3.3)$$

For particles with little to no mass relative to the transverse momentum, we have that $p_T^2 + m^2 \approx p_T^2$ where $p_T = E \sin(\theta)$, which gives us the following relations:

$$\begin{aligned}\cosh(y) &= \frac{1}{\sin(\theta)}, \\ \sinh(y) &= \frac{1}{\tan(\theta)}, \\ \tanh(y) &= \cos(\theta).\end{aligned}$$

which can be used to show that $e^{-y} = \tan \frac{\theta}{2}$. From this we define the pseudorapidity η as:

$$\eta = -\ln \left(\tan \frac{\theta}{2} \right), \quad (3.4)$$

which is, in the relativistic limit, the same as the rapidity y . A useful property of the pseudorapidity is that the phase space of a single particle is uniformly distributed for both η and ϕ , making them good features for controls and verification of SM MC.

Data collection



Figure 3.2: Figure describing how particles are detected at ATLAS, fetched from [ATLAS detector slice \(and particle visualisations\)](#), by Sascha Mehlhase [24].

The features in the dataset used in this analysis are computed with or fetched from the quantities measured from the detector itself. Such measured properties include the momentum, energy, angles etc., all of which are either measured or computed based on the measurements in the detector. In figure 3.2 a visualization shows how different particles move through the detector and how they are detected. For example, energy deposits are measured using electromagnetic and hadronic calorimeters, specifically designed to efficiently measure the energy of all particles interacting through the electromagnetic and strong interactions, respectively. Charged particles leave tracks in the inner tracking device. Thus, electrons leaves tracks in the inner tracker and deposit energy in the electromagnetic calorimeter, muons pass through the muon spectrometer leaving electrical signal and momentum and energy of a muon is then based on the curvature of the track of the muon in the muon detector. Between the calorimeters and the muon detector there is another magnetic field to help on the measure of the muons. Photons only deposit energy in the electromagnetic calorimeter. Hadrons such as protons and neutrons deposit energy in the hadronic calorimeters, and charged hadrons also leaves tracks in the inner tracker. This is shown in figure 3.2.

The ATLAS detector has a few selection stages before the data is stored. In order to reach the highest intensity of collisions, the LHC accelerates packets of around 10^{11} protons, and collides each batch every 25 nanoseconds, yielding a collision rate of 40 MHz[25].

Data preparation

During data recording at the ATLAS detector, triggers on the hardware and software level select out the events⁸ that are of most interest. Most of the initial collisions are discarded with about 1 in 40000 events being accepted. This is because the amount of recorded events simply are too high to realistically analyse and store. Also, most of the events are of no interest for BSM analysis anyway as they do not yield massive particles. There are therefore no large deposits of energy or tracks with high transverse momentum. Instead, these collision fragments leave the interaction region with very small angles between their trajectory and the beam pipe.

Once the trigger selection is done, the data is reconstructed. This means that the objects in the recorded events are being reconstructed into particles like jets and photons using advanced software algorithms. The reconstruction is done based on the tracks and measurements in the detector, but it is not perfect, and can lead to fake leptons or jets. By fake, it is meant that an object might look like a lepton but is in reality a jet

⁸An event here is defined as a collision recorded and reconstructed.

or vice versa[26]. Once the reconstruction is done, further slimming of the data is done. Derivations are slimmings of the data where the selection of events are further reduced to match the needs of the different analysis groups.

The simulated data go through parts of the same process as the recorded data from ATLAS. These events are first generated by software that simulates the initial interaction and then run through the detector to simulate the interaction of the particles with the detector and the resulting production of digital signals. Since these signals mimic the real detector signals, the events can be reconstructed and go through derivations just like the proton-proton collision data, and then be used in analysis.

Steps from Data Collection to Physics Results

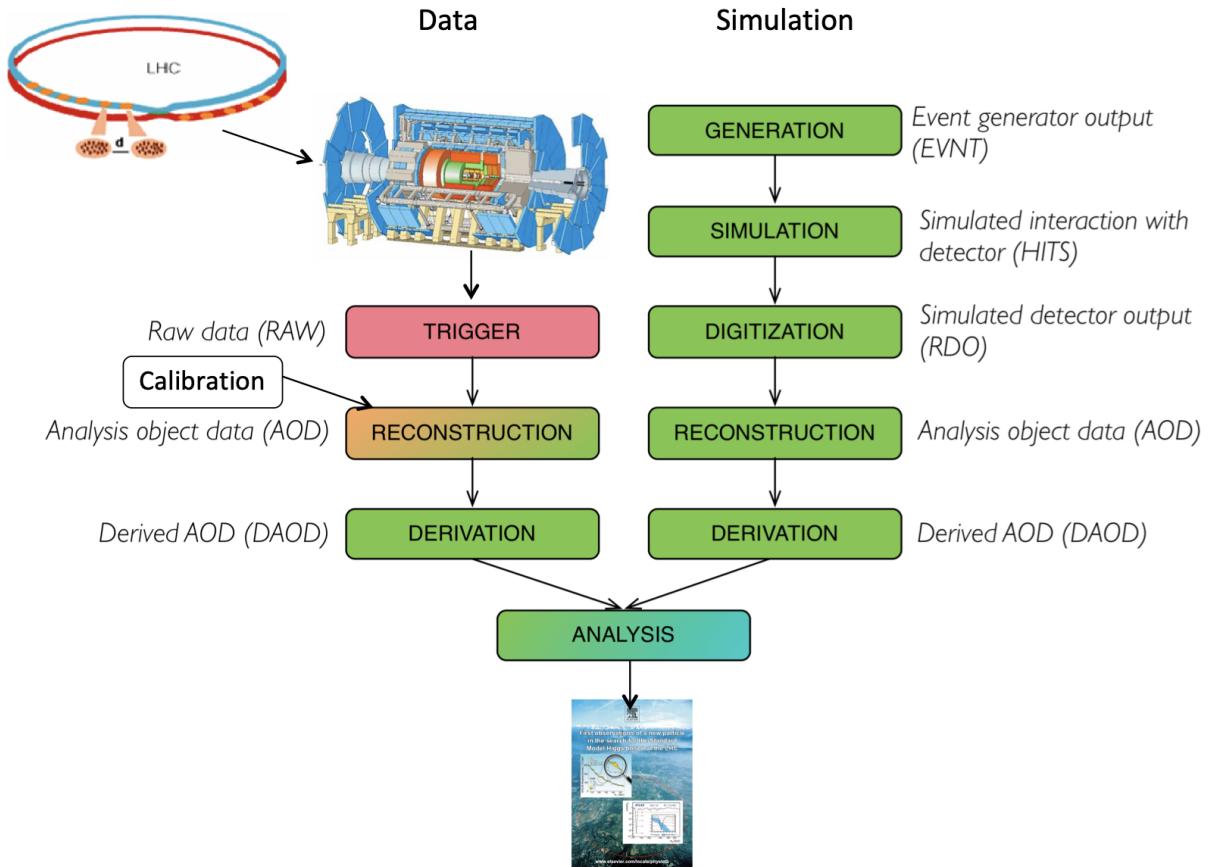


Figure 3.3: Figure describing the steps to take for data collection at ATLAS, fetched from [Hybrid ATLAS Induction Day + Software Tutorial workshop](#), part [Computing and Data preparation](#), initially drawn by Dr. James Catmore, later held by S.M Wang [25].

Jets

Photons and electrons are detected in the electromagnetic calorimeter, and are easy to track and detect as they separate easily. Quarks, however, are bound by QCD and thus cannot be separated as individual particles. An illustration of how quarks and gluons materialise as jets during a proton-proton collision is shown below in figure 3.4.

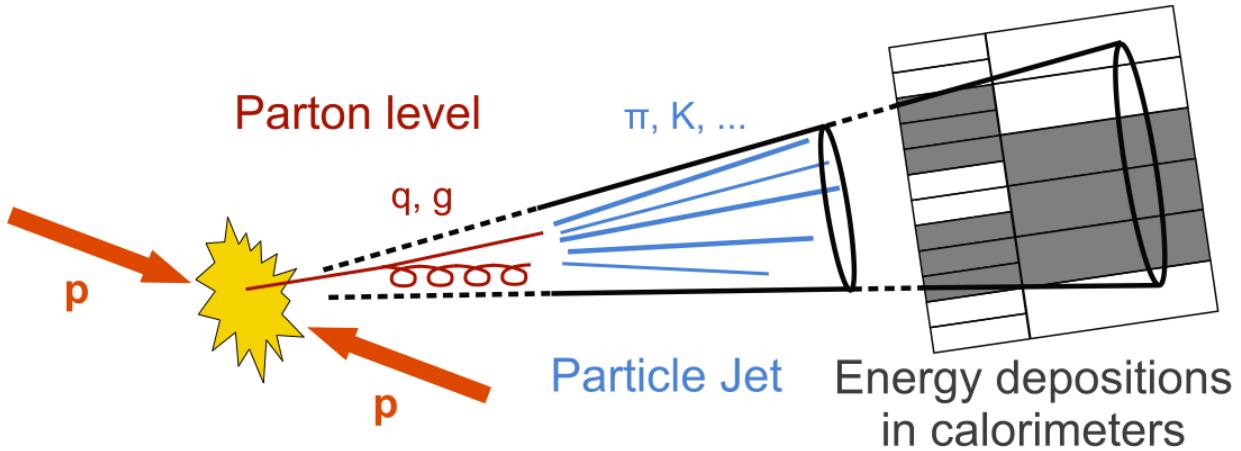


Figure 3.4: Figure describing how quarks and gluons are treated in the detector, and thus why we name them jets, fetched from [the CMS webpage](#).

In a proton-proton collision, the quarks and gluons form stable or unstable hadrons such that the color confinement^[27] is upheld. These particles then decay to other stable hadrons that can be tracked, and these collimated tracks are called jets. To determine which hadrons came from which decays can be particularly difficult because different definitions with different performance working points exist. Another point to make is that some quarks yield more information than others. Using the properties of heavy quarks such as the b- and c-quarks and their non-negligible lifetime allows us to differentiate jets containing these quarks from jets only consisting of light quarks. The b-jet coming from a b quark are particularly interesting as they are produced in the decay of top quarks. The Higgs can be produced from, and in association with, top-quarks. The behavior of hadrons containing b-quarks may be indirectly sensitive to BSM physics as well.

3.2 ROOT

ROOT is an open-source data analysis framework used by high energy physics. It can do fast data manipulation, save and access data, create graphics for publication, and even combine with high level languages such as R and Python.

RDataFrame

RDataFrame's main purpose is to make reading and handling of ROOT files easier, especially in relation to modern machine learning tools and their respective frameworks and environments. This is done by creating a dataframe type of structure of the ROOT n-tuples, and then lazily⁹ apply constraints to the data. Using PyROOT¹⁰, RDataFrame can be accessed in Python, as the functionality is wrapped around a C++ class. Below is a code example of how to create a RDataFrame object, apply a cut and then create a column for later use. Here, good leptons are defined first, denoted as "ele_SG" and "muo_SG". A cut is then applied where we require that the number of good leptons is always 3. Finally, a column is created where the combination of type of leptons in the 3 lepton system is stored, as well as creating a histogram containing the results for that given channel¹¹ k. Notice here that if the variable already exists as a column in the dataframe, arithmetic and logic can be applied directly using those columns to create new one. More complicated variables, such as the flavor combination for the leptons, or the invariant mass of two particles must be found or calculated using C++ functions. An example of such a C++ function is shown below the python code example.

⁹In this context lazily means that the functions and or cuts are done first after all have been registered, see [ROOT guidelines](#) for more.

¹⁰[PyROOT website](#)

¹¹A channel here refers to a certain decay channel. The simulations of the SM is divided into several channels, and some look more alike than others. One example is the Higgs decay channel, with possible decays such as two photons, W bosons or Z bosons. This pertains to simulated events only, as we cannot control what decay channels we get in the data recorded at ATLAS

```

1 import ROOT as R
2
3 R.EnableImplicitMT(200) # Enable multithreading, sets number of threads to 200 or the highest
4 # number possible if the number of threads is less than 200
5 R.gROOT.ProcessLine(".L helperFunctions.cxx+") # Load the C++ helper functions in ROOT
6 # interpreter
7 R.gSystem.AddDynamicPath(str(dynamic_path)) # Add the path to the library with the helper
8 # functions to the ROOT interpreter
9 R.gInterpreter.Declare(
10 '#include "helperFunctions.h"'
11 ) # Header with all helper functions
12 R.gSystem.Load("helperFunctions_cxx.so") # Library with the myFilter function
13
14 df_mc = getDataFrames(mypath_mc) # Function to create a dictionary of RDataFrames for each
15 # channel in the SM MC and possible signal samples
16 df_data = getDataFrames(mypath_data) # Function to create a dictionary of RDataFrames for ATLAS
17 df = {**df_mc, **df_data} # Combine the two dictionaries
18
19
20
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```

Figure 3.5: Example of event selection done using RDataFrame. Four example features are created here, the "good electrons", "good muons", "good leptons" and flavor combination of leptons. Then a filter is applied to the RDataFrame structure, and finally a histogram is created. In section B.1 it is shown how to implement the Rapidity-Mass matrix from section 3.4 in event selection.

In the code example above we see how RDataFrame can be used for event selection. Line 1-9 are settings for ROOT, number of threads to use in the parallelization, extra helper functions written in C++ with .h and .so files and the path to the folder. Lines 11-13 create a dictionary containing the ROOT RDataFrames used for event selection. These are categorized by channel name. The loop on line 15 does event selection for each channel sample, defining new variables in the RDataFrame, applying filters and creating histograms.

Some variables are constructed using variables already in the ROOT files such as energy and mass. Through custom C++ functions these properties can be added to the RDataFrames. The example below shows a custom C++ function which is used in work of this thesis.

```

1 double getM(VecF_t &pt_i, VecF_t &eta_i, VecF_t &phi_i, VecF_t &e_i,
2             VecF_t &pt_j, VecF_t &eta_j, VecF_t &phi_j, VecF_t &e_j,
3             int i, int j)
4 {
5     /*
6      * Calculates the invariant mass between two particles.
7      * If the particles are not found, or the index is out of range,
8      * function returns zero, else returns the invariant mass.
9      */
10
11    const auto size_i = int(pt_i.size());
12    const auto size_j = int(pt_j.size());
13
14    if (size_i == 0 || size_j == 0){return 0.;}
15    if (i > size_i-1){return 0.;}
16    if (j > size_j-1){return 0.;}
17
18    TLorentzVector p1;
19    TLorentzVector p2;
20
21    p1.SetPtEtaPhiM(pt_i[i], eta_i[i], phi_i[i], e_i[i]);
22    p2.SetPtEtaPhiM(pt_j[j], eta_j[j], phi_j[j], e_j[j]);
23
24    double inv_mass = (p1 + p2).M();
25
26    return inv_mass;
27 }
```

Figure 3.6: Example of a C++ function used in event selection. This function is used to calculate the invariant mass between two particles. It takes the kinetic parameters for both particles and the index for which of the leptons available to compute for. If the particles do not exist for that event, it returns zero.

This C++ function creates Lorentz vectors for two particles, and then returns the invariant mass based on the parameters sent in. This function will be used on all the leptons in a given event. If one particle or both do not exist, the C++ function will return zero as the invariant mass.

```

1 import pandas as pd
2
3 def Convert_RDF_to_numpy(df, PATH_TO_STORE):
4
5
6     cols = df.keys()
7
8     for k in cols:
9
10         print(f"Transforming {k}.ROOT to numpy")
11         numpy = df[k].AsNumpy(DATAFRAME_COLS) #* DATAFRAME_COLS is a list of columns to be
12         converted to a numpy array
13         print(f"Numpy conversion done for {k}.ROOT")
14         df1 = pd.DataFrame(data=numpy) #* Convert to pandas dataframe
15         print(f"Transformation done")
16
17         #* Convert to HDF5
18         df1.to_hdf(
19             PATH_TO_STORE + f"/{k}_3lep_df_forML_bkg_signal_fromRDF.hdf5", "mini"
20         )
21
22         #* Flush memory for new dataframe
23         df1 = pd.DataFrame()
```

Figure 3.7: Loop converting RDataFrames to NumPy structures, before being stored as HDF5 files. Her $df[k]$ is a dictionary containing each channel, with channel name as key.

Once event selection is done, the features have been chosen and histograms have been drawn, the RdataFrame can be converted to a Pandas dataframe. This is a very popular choice for data structure when

doing data analysis in python. This is done through an intermediary step of converting the RDataframe to a numpy filestructure, which then can be converted to a Pandas[28] dataframe or some other framework. The new Pandas dataframes are stored as HDF5[29] files to be used later. This is because the HDF5 format has a very good compression ratio, and is very fast to read and write.

3.3 Background samples

To look for anomalies in the 2 or 3 lepton final states we need to train on background Monte Carlo samples with that specific final state. This means in a sense that we want the autoencoder to learn what is expected from the SM in terms of this final state. The 2 and 3 lepton + e_T^{miss} background Monte Carlo contains the following channels:

3 lepton + e_T^{miss}	2 lepton + e_T^{miss}
Channel names:	
Wjets	Wjets
ttbar	ttbar
Singletop	Singletop
ZeeJets	ZeeJets
ZmmJets	ZmmJets
ZttJets	ZttJets
Higgs	Diboson
Triboson	
TopOther	
Diboson2L	
Diboson3L	
Diboson4L	

Table 3.1: SM MC channels for both the 2 and 3 lepton + e_T^{miss} final state background.

Below are three Feynmann diagrams, two of which are both represented in the 2 and 3 lepton + e_T^{miss} background MonteCarlo shown in table 3.1. The selected ones are likely Feynman diagrams for $t\bar{t}$, Higgs and Zeejets channels.

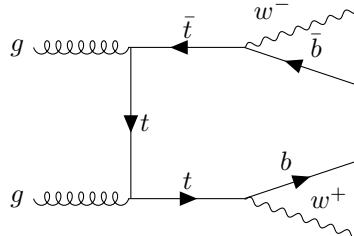


Figure 3.8: Proton-proton collision showing the $t\bar{t}$ channel. Here the w bosons decay leptonically and one or more jets can be misreconstructed as fake leptons by the detector.

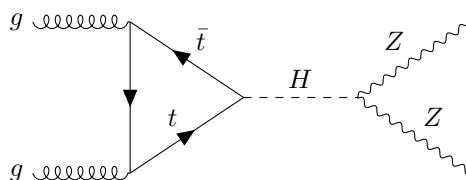


Figure 3.9: Proton-proton collision showing the Higgs channel. Here the Z bosons decay leptonically.

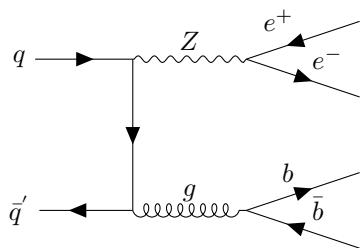


Figure 3.10: Proton-proton collision showing the Zeejets channel. Here one of the Z bosons decay leptonically and the gluon decays hadronically.

3.4 The dataset features

The Rapidity-Mass matrix (RMM)

Most of the features in the analysis are elements in the Rapidity-Mass matrix (RMM) inspired by the work of Chekanov [30]. The RMM is a convenient structure to create a feature space for the dataset. It contains information of various reconstructed objects and their combinations about mass, rapidity, momenta and missing transverse energy, all of which are useful in searches for new physics in HEP[31]. One example of an analysis that has used some features from the RMM is demonstrated in [32]. The main reason however for using this structure is the systematic layout and automated featurespace, that maintains low to no correlation between the cells in the matrix, which is optimal when using neural networks.

The RMM is determined as a square matrix of $1 + \sum_{i=1}^T N_i$ columns and rows, where T is the total number of objects (i.e. jets, electrons etc.), and N_i is the multiplicity of a given object. In the case where the multiplicity of a particle is equal to the number of different particles, we can denote the RMM matrix as a $TmNn$ matrix, where m is the number of objects, and n is the multiplicity of each object. One should already here choose appropriately the number of objects and the multiplicity of each, as the computation time increases significantly when expanding the RMM. Each cell in the matrix contains information about either single or two particle properties. It is also important to remember that each event gets its own RMM, therefor each event creates its own signature that the autoencoder hopefully can learn trends from. An example of a small RMM is shown in matrix 3.5.

$$\begin{pmatrix} \mathbf{e}_T^{miss} & m_T(j_1) & m_T(j_2) & m_T(e_1) & m_T(e_2) \\ h_L(j_1) & \mathbf{e}_T(j_1) & m(j_1, j_2) & m(j_1, e_1) & m(j_1, e_2) \\ h_L(j_2) & h(j_2, j_1) & \delta\mathbf{e}_T(j_2) & m(j_2, e_1) & m(j_2, e_2) \\ h_L(e_1) & h(e_1, j_1) & h(e_1, j_2) & \mathbf{e}_T(e_1) & m(e_1, e_2) \\ h_L(e_2) & h(e_2, j_1) & h(e_2, j_2) & h(e_2, e_1) & \delta\mathbf{e}_T(e_2) \end{pmatrix} \quad (3.5)$$

In matrix 3.5 we have the RMM matrix for a T2N2 system, in other words we have two types of objects, jets ¹² and electrons, and for ach ogjct we consider a multiplicity of two. The matrix itself is partitioned into three parts. The diagonal represents energy properties, the upper triangle represents mass properties and the lower triangle represents longitudinal properties related to rapidity. The diagonal has three different properties, \mathbf{e}_T^{miss} , \mathbf{e}_T and $\delta\mathbf{e}_T$. \mathbf{e}_T^{miss} is placed in the (0,0) position in the matrix. It accounts for the missing transverse energy of the system, which is of high interest for analyses in searches for BSM physics such as heavy neutrinos. \mathbf{e}_T is the transverse energy defined as

$$\mathbf{e}_T = \sqrt{m^2 + p_T^2} \quad (3.6)$$

but for light particles such as electrons, this can be approximated to $\mathbf{e}_T \approx p_T$. $\delta\mathbf{e}_T$ is the transverse energy imbalance. It is defined as

$$\delta\mathbf{e}_T = \frac{E_T(i_{n-1}) - E_T(i_n)}{E_T(i_{n-1}) + E_T(i_n)}, \quad n = 2, \dots, N, \quad (3.7)$$

where i_n is the nth entry of object i. The first column in the RMM matrix, except the first element, is related to the longitudinal property of the given particle. It is defined as

$$h_L(i_n) = C(\cosh(y(i_n)) - 1).$$

C is a constant to ensure that the average $h_L(i_n)$ values do not deviate too much from the ranges of the invariant masses or the transverse masses, found to be 0.15, as it ensures that rapidity ranges in the range $[-2.5, 2.5]$ produces $h_L(i_n)$ values in the $[0, 1]$ interval[30]. $y(i_n)$ is the rapidity of the particle, and i_n is the particle number. In the lower triangle we have the longitudinal properties of the combinations of particles. Similar to $h_L(i_n)$, this property is defined as

$$h(i_n, j_k) = C(\cosh(\Delta y) - 1),$$

where $\Delta y = y_{i_n} - y_{j_k}$ is the rapidity difference between particle i_n and j_k .

¹²Jets here can both be b- or l-jets. Ljet is defined as jets with $\text{jetdl1r} < 0.665$, whereas bjet77 is defined as jets with $\text{jetdl1r} >= 2.195$. jetdl1r is a machine learning output from a network trained to distinguish b- and ljets.

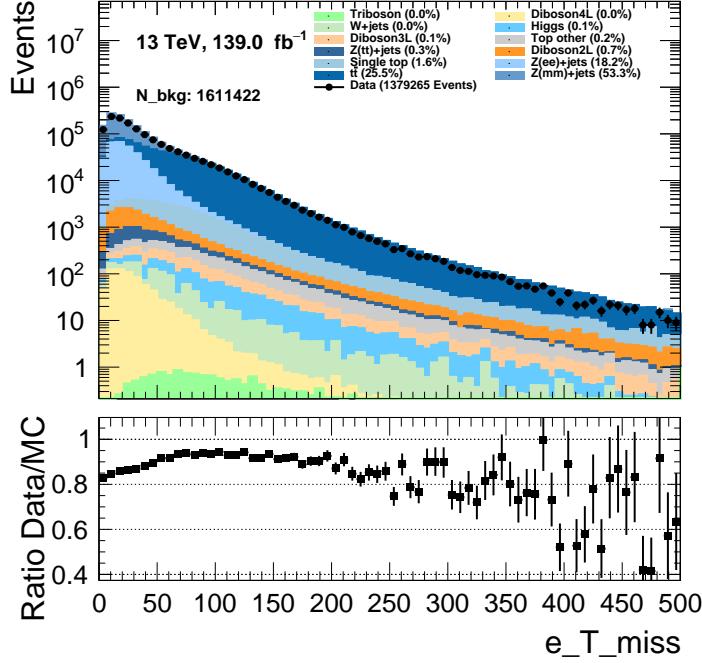
Tabular and sparse data

A consequence of using the RMM structure is that the RMM for the data and SM MC can be sparse for some events. This is due to the fact that the RMM allows for the variety of final states of the reconstructed events, i.e. that one event has two ljets, zero bjets, one electron and two muons, whereas another event can have four ljets, three bjets and three electrons. This means that the non-zero elements of the RMM will vary from event to event, and for neural networks this is a problem. To solve this problem, Chekanov simply pads the missing values with zeros[30].

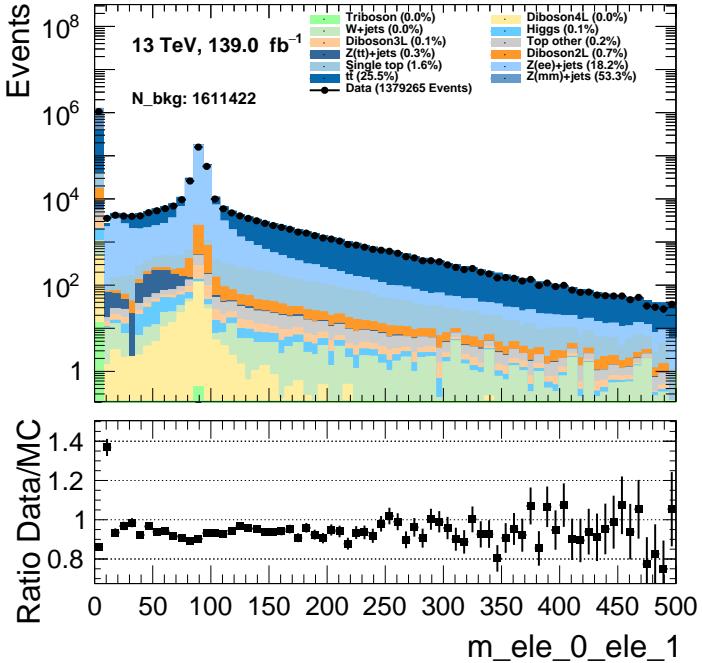
Standard Model Monte Carlo and data comparison

Before we can start the analysis, we need to compare the SM MC and data. This is done to ensure that the measured features used are well modelled by the SM MC training samples we use. As described by R. Stuart Geiger et al. [33], the concept of "Garbage in, garbage out" is of key importance in computer science, and is indeed important in high energy physics. To ensure that the models we train actually learn physical processes, the training set must closely resemble the data. The SM MC simulations are indeed very good, but they are numerical approximations and can sometimes be off. Thus, every feature that will be used for training must be checked before being used. This is done by comparing the distributions of the features in the SM MC and ATLAS data. Monte Carlo simulations are based on the actual theory itself, and comparisons with data taken from ATLAS and other detectors alike are necessary to ensure that the SM background events look like data. This is done by creating control regions where there with high confidence is no signatures of New Physics. This of course becomes problematic if the New Physics are embedded in the background.

Now, if we compare all SM MC and ATLAS data, we would usually expect there to be a good agreement. To ensure that the SM MC actually represents the physics, we create signal and background regions to optimize for amount of signal and amount of background. If we can create a background region where we believe with very high certainty that only SM processes can occur, and we get a good match, we usually conclude that the SM MC is good enough. Since the data from ATLAS used in the work for this thesis has been thoroughly analysed for New Physics without finding any, it is not needed here to create these control regions. Traditional searches using rectangular cuts have only excluded some models, which is why machine learning is getting more popular. The hope is that the signal, whatever it might be, can be revealed with more clever feature engineering and smart machine learning algorithms. Particle physics differs here from more day-to-day machine learning as the recorded data from ATLAS, the true data, is completely unlabeled.



(a) Missing transverse energy for the three lepton final state in GeV. The histogram contains the entire Run 2 dataset.

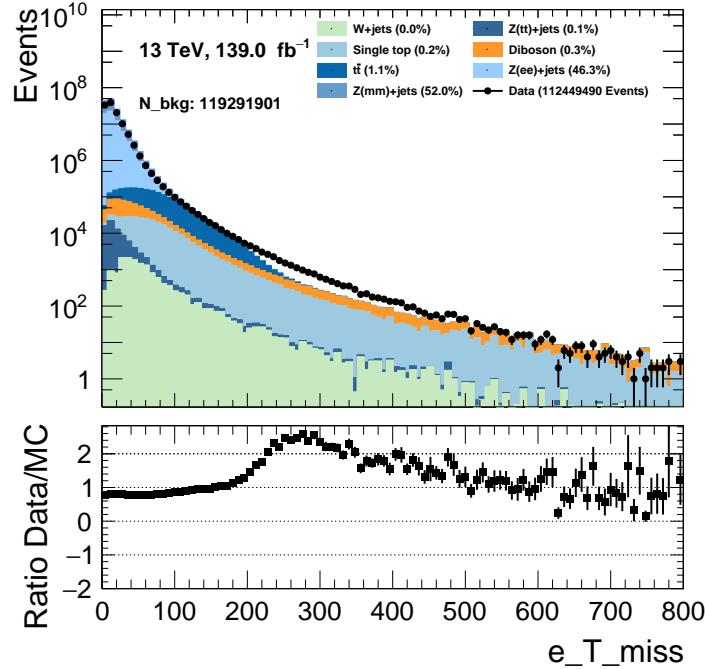


(b) Invariant mass for the first and second electron in GeV. The histogram contains the entire Run 2 dataset.

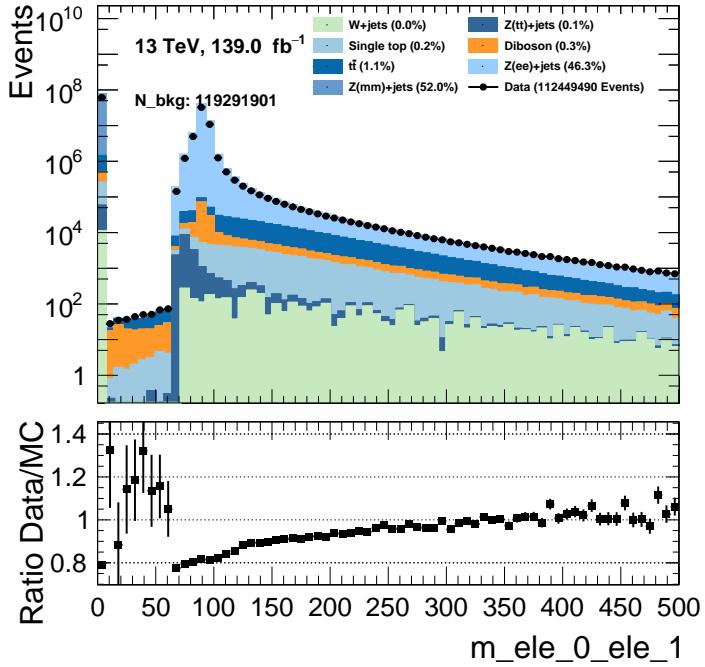
Figure 3.11: Comparison of the Monte Carlo and data for the three lepton + e_T^{miss} final state with the features e_T^{miss} and flavor composition.

In figure 3.11 two features have been selected to visualize the comparison between SM MC and ATLAS data, e_T^{miss} and $m(\text{ele}_0, \text{ele}_1)$ in the 3 lepton + e_T^{miss} dataset. The e_T^{miss} and $m(\text{ele}_0, \text{ele}_1)$ shows a ratio between SM MC and ATLAS data reasonably close to 1, thus we can safely move forward with the analysis. All

features were checked, and can be found in the GitHub repository for this thesis at [Figures/Histo_var_check¹³](https://github.com/Gadangadang/MasterThesis/tree/main/FIGURES/histo_var_check) under the 3lep folder.



(a) Missing transverse energy for the three lepton final state in GeV. The histogram contains the entire Run 2 dataset.



(b) Invariant mass for the first and second electron in GeV. The histogram contains the entire Run 2 dataset. Note the sharp reduction of events from 10-70 GeV.

Figure 3.12: Comparison of the SM MC and data for the 2 lepton + e_T^{miss} final state with the features e_T^{miss} and flavor composition. In figure 3.12b a cut on the invariant mass above 70 GeV of the leading lepton pair. In some cases the first and second electron are not the leading pair, thus there will be some events in this histogram below 70 GeV.

¹³Full link: https://github.com/Gadangadang/MasterThesis/tree/main/FIGURES/histo_var_check

Similar checks were done for the 2 lepton + e_T^{miss} dataset. In figure 3.12 the features e_T^{miss} and $m(e_{l0}, e_{l1})$ do not satisfy the same ratio between SM MC and ATLAS data, as with the 3 lepton + e_T^{miss} case. It appears that RDataframe struggles with some diboson events, leading to a discrepancy. This could be a trigger matching issue or an issue with RDataFrame. The samples were run using both C++ ROOT event selection and RDataFrame by one of the supervisors, and the issue seems to only occur with RDataFrame. Therefore all results regarding the 2 lepton + e_T^{miss} dataset should be interpreted with this in mind. One attempt can be shown in figure 3.12b where a cut on the invariant mass above 70 GeV of at least the two leptons with the highest energy was done to try to accommodate the trigger issue. It did not seem to work, and we proceeded with the dataset. All features were checked, and can be found in the GitHub repository for this thesis at [Figures/Histo_var_check¹⁴](#) under the 2lep folder.

Triggers

The triggers used in the 2 lepton + e_T^{miss} and 3 lepton + e_T^{miss} dataset are shown in Table 3.2, 3.3, 3.4 and 3.5 for the 2015, 2016, 2017 and 2018 data taking periods.

	Name
2015	<i>HLT_2e15_lhvloose_nod0_L12EM13VH</i>
	<i>HLT_2e12_lhloose_L12EM10VH</i>
	<i>HLT_2mu10</i>
	<i>HLT_mu18_mu8noL1</i>
	<i>HLT_e17_lhloose_mu14</i>
	<i>HLT_e7_lhmedium_mu24</i>

Table 3.2: Triggers used in the 2015 SM MC and ATLAS data samples for the 2 lepton 0 e_T^{miss} dataset.

	Name
2016	<i>HLT_2e15_lhvloose_nod0_L12EM13VH</i>
	<i>HLT_2e17_lhvloose_nod0</i>
	<i>HLT_2mu10</i>
	<i>HLT_2mu14</i>
	<i>HLT_mu20_mu8noL1</i>
	<i>HLT_mu22_mu8noL1</i>
	<i>HLT_e17_lhloose_nod0_mu14</i>
	<i>HLT_e24_lhmedium_nod0_L1EM20VHI_mu8noL1</i>
	<i>HLT_e7_lhmedium_nod0_mu24</i>

Table 3.3: Triggers used in the 2016 SM MC and ATLAS data samples for the 2 lepton 0 e_T^{miss} dataset.

	Name
2017	<i>HLT_2e17_lhvloose_nod0_L12EM15VHI</i>
	<i>HLT_2e24_lhvloose_nod0</i>
	<i>HLT_2mu14</i>
	<i>HLT_mu22_mu8noL1</i>
	<i>HLT_e17_lhloose_nod0_mu14</i>
	<i>HLT_e26_lhmedium_nod0_mu8noL1</i>
	<i>HLT_e7_lhmedium_nod0_mu24</i>

Table 3.4: Triggers used in the 2017 SM MC and ATLAS data samples for the 2 lepton 0 e_T^{miss} dataset.

¹⁴Full link: https://github.com/Gadangadang/MasterThesis/tree/main/Figures/histo_var_check/LEP2

	Name
2018	<i>HLT_2e17_lhvloose_nod0_L12EM15VHI</i>
	<i>HLT_2e24_lhvloose_nod0</i>
	<i>HLT_2mu14</i>
	<i>HLT_mu22_mu8noL1</i>
	<i>HLT_e17_lhloose_nod0_mu14</i>
	<i>HLT_e26_lhmedium_nod0_mu8noL1</i>
	<i>HLT_e7_lhmedium_nod0_mu24</i>

Table 3.5: Triggers used in the 2018 SM MC and ATLAS data samples for the 2 lepton $0 e_T^{miss}$ dataset.

Each trigger is designed to detect certain base expectations in the detector, for example reconstructed leptons. In the tables above, the triggers are laid out, showing which were used for a given data taking year. For a more in-depth understanding of trigger, it is recommended to look at the "Performance of the ATLAS Trigger System in 2015" paper[34], as well as the paper for the electron and photon triggers paper[35] and the muon trigger paper[36]. The most important thing to note about these triggers is that the second argument in the trigger, in other words the component after "HLT_" indicates the leptons and their transverse momentum criteria. The trigger "HLT_2mu14" requires two reconstructed muons with a transverse momentum of at least 14 GeV to be triggered for a given event. The other components in some other triggers are more complicated, and describe reconstruction quality working points and more.

For the 3 lepton + e_T^{miss} final state, applying the trigger system on the data did not work as expected, thus a simple cut of requiring at least two leptons with a p_T above 20 GeV was implemented. Note that further triggers would refine the dataset even more.

3.5 Code implementation

Machine learning implementation

The machine learning analysis was written with Keras[37] using the Tensorflow api[5]. The machine learning structure was written using a functional structure¹⁵. In practice, this model could just as well have been written as a Sequential model¹⁶, but at a cost of flexibility and lack of the possibility for creating non-linear structure in the architecture. The code consists of one general class for the autoencoder, where the different testing cases are different classes inheriting from the parent class.

Construction of a neural network in Tensorflow

Using the functional structure, a general neural network in the Tensorflow API can be constructed as shown in the python code below.

¹⁵Functional structure uses a function call for layers, i.e. for layers a, b, then b(a) will connect the two layers, and equals a sequential link a → b. This allows for more flexible structures. More on the functional api can be found [here](#).

¹⁶Sequential structure adds layers in sequence, i.e. for layers a, b, c we have that a → b → c, with a strict structure. This allows for more organized code. More on sequential models can be found [here](#).

```

1 import tensorflow as tf
2
3
4 inputs = tf.keras.layers.Input(shape=data_shape, name="input")
5
6 # First hidden layer
7 First_layer = tf.keras.layers.Dense(
8     units=30,
9     activation="relu"
10 )(inputs)
11
12 # Second hidden layer
13 Second_layer = tf.keras.layers.Dense(
14     units=45,
15     activation="relu"
16 )(First_layer)
17
18 # Second hidden layer
19 output_layer = tf.keras.layers.Dense(
20     units=1,
21     activation="sigmoid"
22 )(Second_layer)
23
24
25 # Model definition
26 nn_model = tf.keras.Model(inputs, output_layer, name="nn_model")
27
28 hp_learning_rate = 0.0015
29 optimizer = tf.keras.optimizers.Adam(hp_learning_rate)
30 nn_model.compile(loss="mse", optimizer=optimizer, metrics=["mse"])

```

Figure 3.13: Functional structure for Tensorflow neural network.

The neural network in the code above contains one input layer, one hidden layer and an output layer. The choice of nodes and activation functions are arbitrary here as the use case has not been defined. Note that code example 3.14 is exactly the same as code example 3.13, but using the sequential structure.

```

1 import tensorflow as tf
2
3 nn_model = tf.keras.Sequential(
4     [
5         tf.keras.layers.Dense(30, activation="relu", input_shape=data_shape),
6         tf.keras.layers.Dense(45, activation="relu"),
7         tf.keras.layers.Dense(1, activation="sigmoid"),
8     ]
9 )
10
11 hp_learning_rate = 0.0015
12 optimizer = tf.keras.optimizers.Adam(hp_learning_rate)
13 nn_model.compile(loss="mse", optimizer=optimizer, metrics=["mse"])

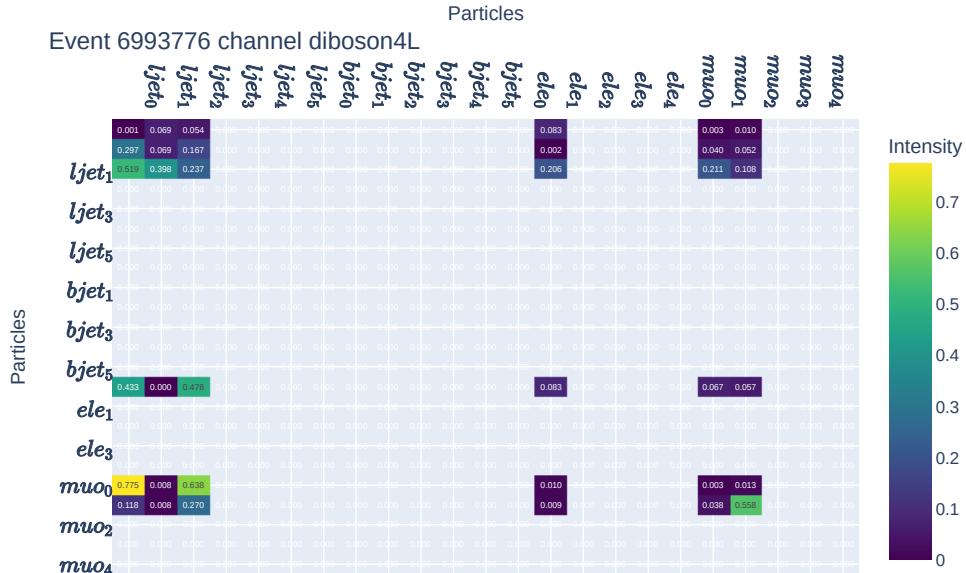
```

Figure 3.14: Sequential structure for Tensorflow neural network.

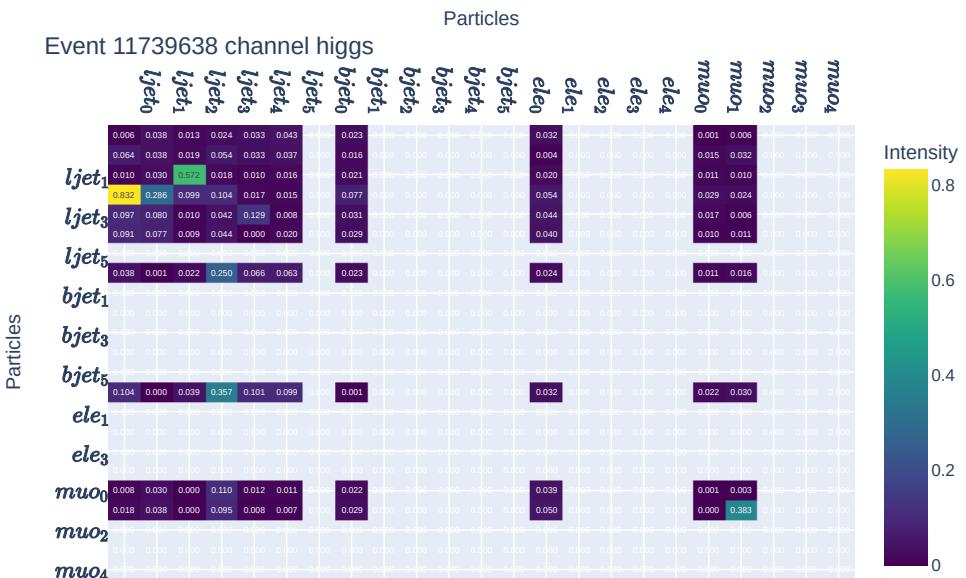
Data handling python side

Implementation of the RMM matrix

Examples of RMM matrices used in this thesis is shown are figure 3.15.



(a) RMM matrix for event number 6993776 from the Monte Carlo diboson4L event. Each feature is scaled based on a fit for that feature for all events in the training set ($\approx 80\%$ of total MC). This event contains two ljets, one electron and two muons.



(b) RMM matrix for event number 11739638 from the Monte Carlo Higgs event. Each feature is scaled based on a fit for that feature for all events in the training set ($\approx 80\%$ of total MC). This event contains five ljets, one bjet, one electron and two muons.

Figure 3.15: Two RMM matrices for one diboson4L (3.15a) event and one Higgs (3.15b) event.

The two RMM matrices are created from two different channels in the MC samples. This RMM is of type T4N5¹⁷. For easier interpretability, the gray area corresponds to a missing value, leading to so-called "islands" in the RMM matrix. Note here that the y-axis for the RMM's lack every other label, due to lack of space in the y-axis of the plot. If looked more closely upon, one can see that each figure have all RMM cells,

¹⁷T4 → 4 particle types: bjets, ljets, electrons and muons. N5 → 5 particles per particle type. Note here that we have 5 particles only for the leptons, and 6 particles for each of the types of jets, so it is not technically a T4N5 matrix.

just that the labels, which are identical to the x-axis label, only show every other. The RMM plots were created using Plotly[38].

Setup for 3 lepton dataset

The 3 lepton dataset is about 96 GB of data or circa 381873 events when implementing the RMM structure for 6 b- and ljets, 5 electrons and 5 muons. The dataset is converted from a ROOT N-tuple using RDataframe to a Pandas dataframe[28] for further preprocessing. Having added the channel name column¹⁸, weights, trilepton mass¹⁹ as well as the RMM structure, the datasets are divided into a training and a validation/test set in an 80-20 split. The split was done using the `train_test_split()` function from the Scikit-learn library[39]. Then the data and SM MC was scaled using the MinMax scaler via the `".fit_transform()"` and `".transform()` functions from the Scikit-learn library. The training and validation/test set are then converted to numpy arrays[40] for faster loading and easier indexing, and saved as `".npy"` files. This allows for faster reuse of the arrays.

Setup via iterative training for 2 lepton dataset

The two lepton dataset contains about 1.5 - 2 TB of data or about 119291900 events when implementing the RMM structure for 6 b- and ljets, 5 electrons and 5 muons, as for the 3 lepton dataset. This is too much to hold in memory at the same time, thus it had to be split into several smaller datasets, called megasets. Figure 3.16 visualize the structure used.

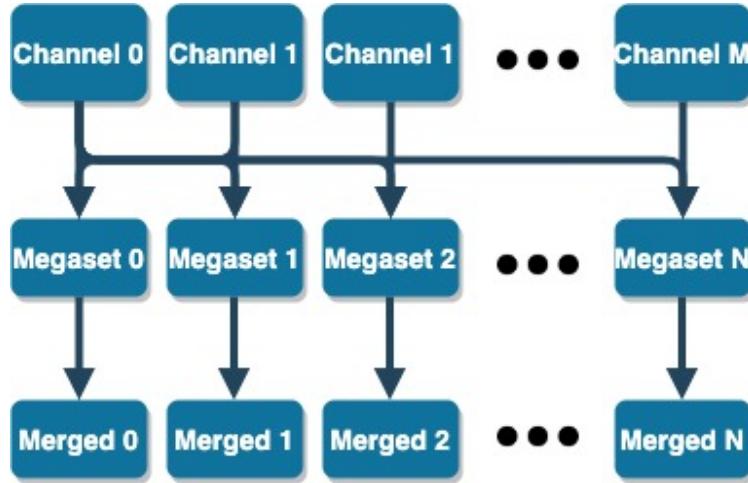


Figure 3.16: Megaset structure for the 2lep dataset. This figure generalises to M channels, and N megasets, where M and N does not have to be equal. The more you increase the number of megasets, the smaller each megaset will be in bytesize, but in order to keep the SM MC distribution, it is not recommended to make too small sets. In this thesis 10 megasets were created where the simulated data contained 7 channels.

Pandas is not built for very large datasets since it is not running in a parallelized way. To handle this, the library Polars²⁰ [41] was used instead. When all channels were split, a merging was done combining all the channels in a given megaset to a separate dataset. The selection of events from each channel was done randomly, which is important, as we want to the best of our ability keep the distribution signature of the entire dataset in each megaset. If not, the model will be biased towards those datasets with the most events. Once each of the megasets were merged, the training could begin in an iterative fashion. Because Tensorflow is statically compiled, one cannot call the fit function over and over again. Instead, the weights trained based on one megaset is stored and reloaded into a new model, thus the weights are still trained on the entire set, but in a batch like manner. The implementation used in this thesis is shown in code example 3.17.

¹⁸This column would in a fully supervised setting be used as a target vector, but in this thesis it will only be used for legends in histograms and to index out certain channels in the validation and training set.

¹⁹Invariant mass of three leptons. This is assured to exist from event selection in the 3 lepton dataset.

²⁰Polars uses all available cores on the system and has excellent memory handling capability, see [Polars User Guide](#)

```

1 for megaset in range(totmegasets):
2
3     #* Load model
4
5     autoencoder = getModel()
6
7     if megaset != 0:
8         autoencoder.load_weights('./checkpoints/Megabatch_checkpoint')
9
10
11    #* Run Training
12    with tf.device("/GPU:0"):
13
14        tf.config.optimizer.set_jit("autoclustering")
15
16        autoencoder.fit(
17            xtrain,
18            xtrain,
19            epochs=epochs,
20            batch_size=b_size,
21            validation_data=(xval, xval),
22            sample_weight=x_train_weights,
23        )
24
25
26    AE_model.save_weights('./checkpoints/Megabatch_checkpoint')

```

Figure 3.17: Example code for training a neural network on megasets with Tensorflow.

3.6 The chosen neural network architectures

The regular Autoencoder

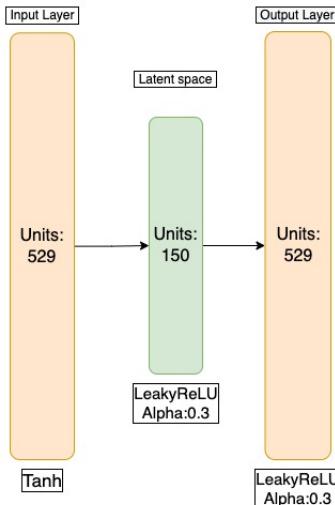


Figure 3.18: Small autoencoder architecture.

Figure 3.18 shows the small autoencoder. It consists of an input and output layer of 529 nodes, with one latent space layer of 150 nodes. The activation functions for the input us Tanh while the latent space and the output layer use LeakyReLU with $\alpha = 0.3$ respectively.

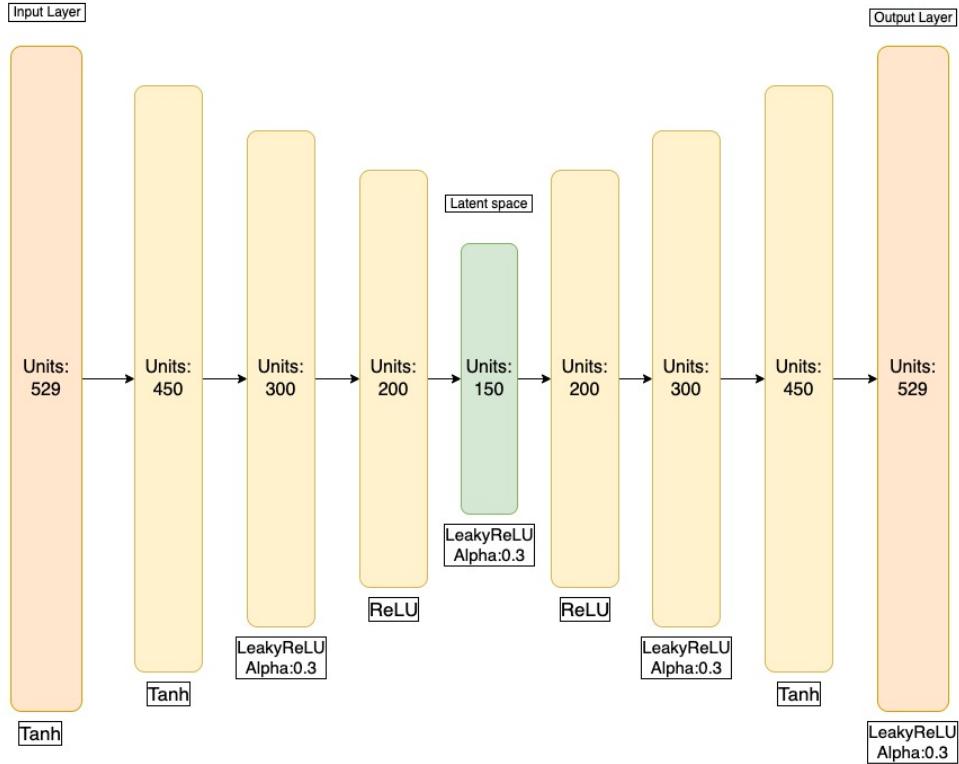


Figure 3.19: Large autoencoder architecture.

Figure 3.19 shows the large regular autoencoder. It consists of an input and output layer of 529 nodes, with three hidden layers of 450, 300 and 200 nodes respectively in the encoder and three hidden layers of 200, 300 and 450 in the decoder respectively. The activation functions for the input and output layers are the Tanh and LeakyReLU with $\alpha = 0.3$. The encoder layers have the activation functions Tanh, LeakyReLU with $\alpha = 0.3$ and ReLU. The decoder layers have the activation functions ReLU, LeakyReLU with $\alpha = 0.3$ and Tanh. The latent space has 150 nodes, with the LeakyReLU activation function with $\alpha = 0.3$. The activation functions as well as the number of nodes per layer were chosen based on earlier work done on the ATLAS open data[42], as well as some light hyperparameter testing using Keras-Tuner[43].

The variational Autoencoder

Figure 3.20 and 3.21 two models used for the variational autoencoder.

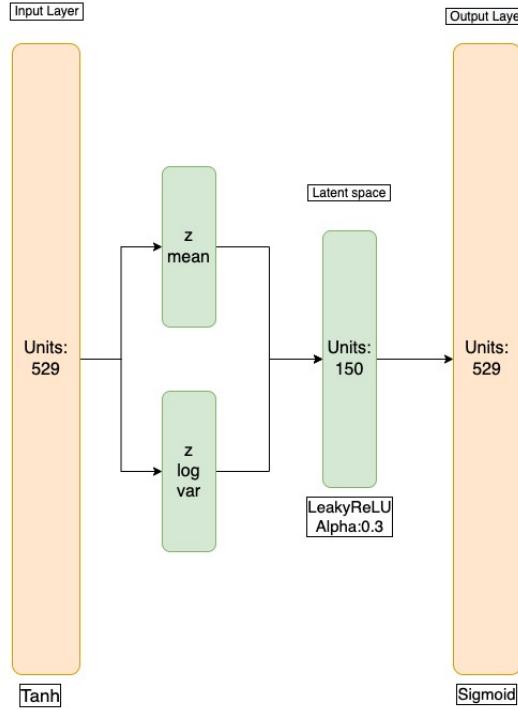


Figure 3.20: Small variational autoencoder architecture.

In figure 3.20 we have the small variational autoencoder. It consists of an input and output layer of 529 nodes, with one latent space layer of 150 nodes sampling from a mean and variance layer of same size. The activation functions for the input, latent space and output are the Tanh, LeakyReLU with $\alpha = 0.3$ and Sigmoid.

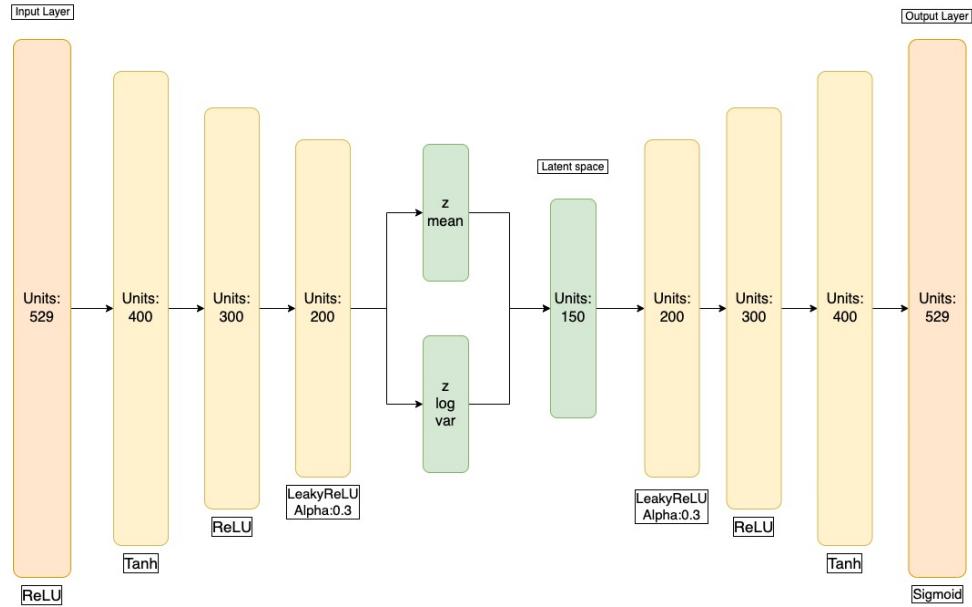


Figure 3.21: Large variational autoencoder architecture.

It consists of an input and output layer of 529 nodes, with three hidden layers of 400, 300 and 200 nodes respectively in the encoder and three hidden layers of 200, 300 and 400 in the decoder. The activation functions for the input and output layers are the ReLU and Sigmoid respectively. The hidden layers in the encoder have the activation functions Tanh, ReLU, LeakyReLU with $\alpha = 0.3$ respectively. The hidden layers in the decoder have the activation functions LeakyReLU with $\alpha = 0.3$, ReLU and Tanh respectively. The

activation functions as well as the number of nodes per layer were chosen based on earlier work done on the ATLAS open data[42], as well as some light hyperparameter testing using Keras-Tuner[43].

3.7 The search strategy

The strategy used to look for anomalies in the 3 lepton + missing energy final state is presented as follows. First, the SM MC and ATLAS data for training and inference are constructed with the RMM from section 3.4 as features. After scaling and splitting, 80% of the MC will be used for training the neural network, and the remaining 20% will be used for inference. The reconstruction error from inference will then be used to separate the anomalies from background. The hope is that the anomalous events will be skewed towards higher reconstruction errors.

Standard analyses rely on what is called a signal region. The signal region is a region in the feature space in which the signal is expected to be enriched. These are often not inspected until all analysis selections are fixed ("blind" analysis). We use this region to calculate the significance of a result in the search, which is really the only metric that is of use. The statistical uncertainty and noise is proportional to the amount of SM MC, thus with lower amounts of SM MC, the better the significance will be. This is *a*) given that the signal does not reduce in the same (or more extreme) manner and *b*) that one does not run out of SM MC statistics. Because then one does not have any predictive power anymore. Using the reconstruction error, the autoencoder can create its own signal region, more specifically the areas of high reconstruction error. By placing a cut at "high" reconstruction error one can look at e.g. the missing transverse energy or other features of interest to see if the AE has managed to select events which have anomalous behavior (wrt. the SM) in these distributions. I.e. the cut on the reconstruction error from the AE replaces the pre-selection cuts one typically design in an ordinary cut-and-count analysis using traditional kinematic variables.

The signal region for the regular autoencoder models were created by calculating the median m_{err} of the reconstruction error. Then, 3 cuts were made, starting at $m_{err} + im_{err}/5$ for $i = 1, 2, 3$. This was a direct result of the shape of the background reconstruction error being a hill-like shape. The median then became a good place to start to remove much of the SM MC. This is however just a guess for an optimal signal region, as the true signal is unknown, and the method has to be as unbiased as possible. There is however an issue to keep in mind here. The method to find the cut is in some sense based on the slope shape of the SM MC reconstruction error distribution, thus three cuts based on the median seems like a good choice. However, if one then uses all the events in the signal region, it might be that one misses the ideal amount of background and signal to create the significance. Thus, for each reconstruction error cut, there is an associated plot showing the significance as a function of e_T^{miss} for the events passing a given cut on the AE reconstruction error. The e_T^{miss} would be the final discriminating variable for where we look for deviations from the expected SM background. Thus, you can find the ideal cut, within the signal region, for where to choose the amount of background and signal to get a better significance.

Since the analysis is based on semi supervised learning, one should avoid tuning on specific signal models. Therefor one should also prepare a blind test.

Testing strategy

Before testing the AE and VAE on signal samples, it is interesting to test the sensitivity of both the regular and variational autoencoders on anomalous SM MC events. This can be thought of as initial testing.

Channel removing

One idea was to test the anomaly detection capability by removing one of the channels in the SM. The idea was that some of the channels differ enough in the final states and thus in their RMM signature that they might be treated like anomalous data by the autoencoders. All channels were tested on as signal.

Altering transverse momentum

Another idea for anomaly detection testing with the SM MC was to alter the transverse momentum of some particles. Random events were selected, and their transverse energy was changed by scaling it with a factor. The hope is that especially events with atleast a scaling of 5 in transverse momentum should be picked up. Note that by changing the transverse momentum, the elements in the RMM related to the difference in transverse energy between the objects change. From equation 3.7 we have that a scale change k in p_T yields the following new relation:

$$\delta e_T^k = \frac{kE_T(i_n - 1) - E_T(i_n)}{kE_T(i_n - 1) + E_T(i_n)}, \quad n = 2, \dots, N. \quad (3.8)$$

Thus, both the transverse energy and the difference in transverse energy between the various objects are changed for this test.

Signal testing

It is not correct to refer to the machine learning algorithm used in this thesis as unsupervised learning. This is mostly due to the fact that we show it labeled MonteCarlo to train on, and thus essentially gives the models a target to aim for. But, since we do not show the autoencoders any signals in training, it can be allowed to name the learning strategy as semi-supervised learning. Because of this, one does not bias oneself too much if the algorithm is tested on one or more signal samples. This type of testing can be separated into two different categories, the open signal testing and the blind signal testing.

The open signal testing first takes a trained model that has only seen SM MC and then runs inference on both SM MC and the given signal. Then the search strategy mentioned in the previous section is done on those collected reconstruction error distributions. The blind signal testing is the final test, where a dataset is prepared encapsulating SM MC or ATLAS data, and one or multiple signals. The labels are kept, for verification. That way, if one were to do open signal testing on many signal samples from many theories, one could in principle bias oneself too much. This way one can get an unbiased measurement of the performance.

Chapter 4

Results and Discussion

4.1 Non signal testing of the regular and variational autoencoder

Channel removing

Results following removal of specific channels are shown in figures 4.1 - 4.6. The left plots in the figures show the results from the small AE while the right plots show the corresponding result using the large AE. Figure 4.1 - 4.3 show the results where the Higgs, single top and ttbar channel, respectively, has been removed in the training of the AE. The inference of the AE is applied on the removed process (shown as markers in the distributions). Figure 4.4 - 4.6 show the corresponding results using a variational autoencoder. These three channels were chosen since they are the most unlike the rest of the background channels.

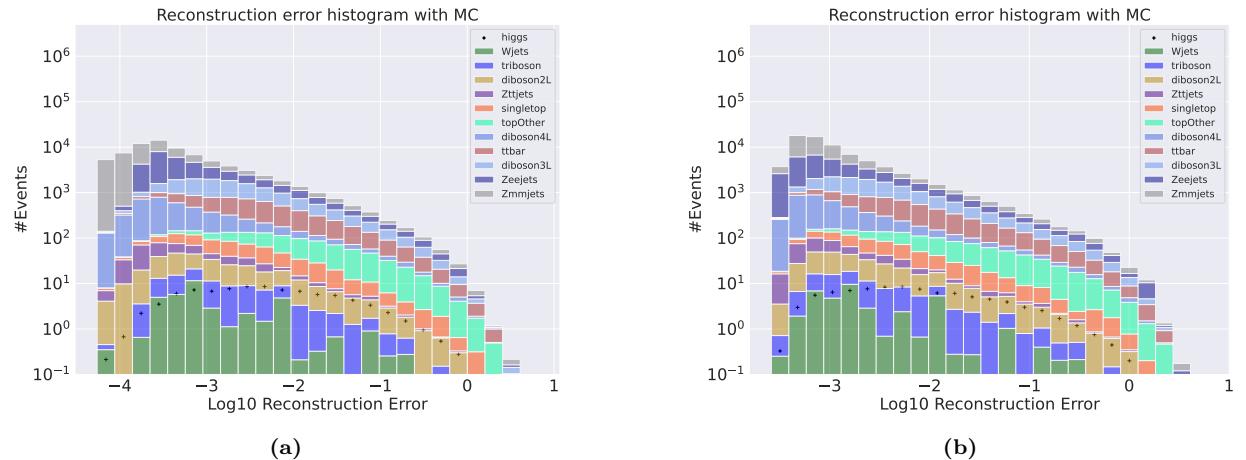


Figure 4.1: Reconstruction error on validation SM MC from the small (a) and large (b) autoencoders. The Higgs channel has been removed from training and is used as signal. No significant difference in distributions is found.

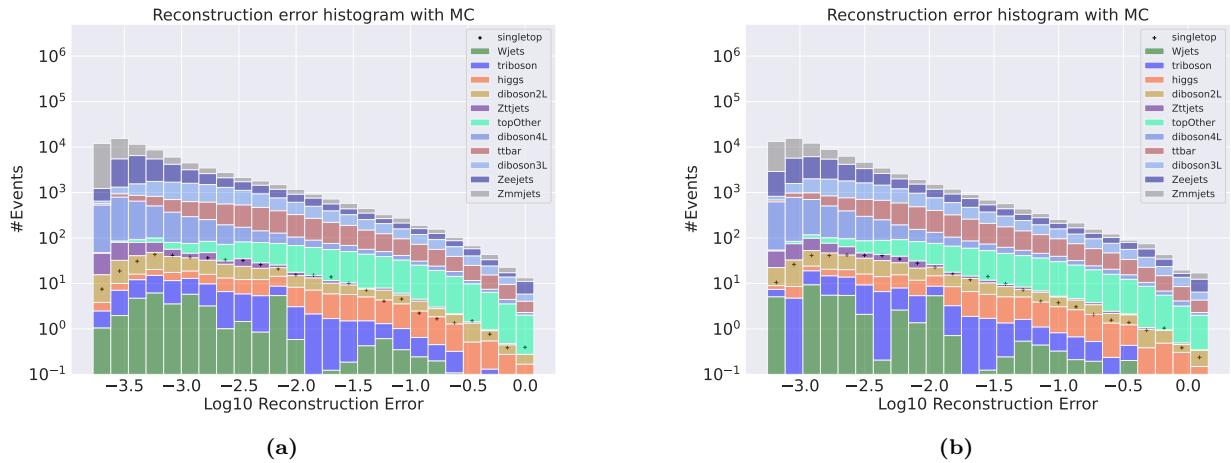


Figure 4.2: Reconstruction error on validation SM MC from the small (a) and large (b) autoencoders. The single top channel has been removed from training and is used as signal. No significant difference in distributions is found.

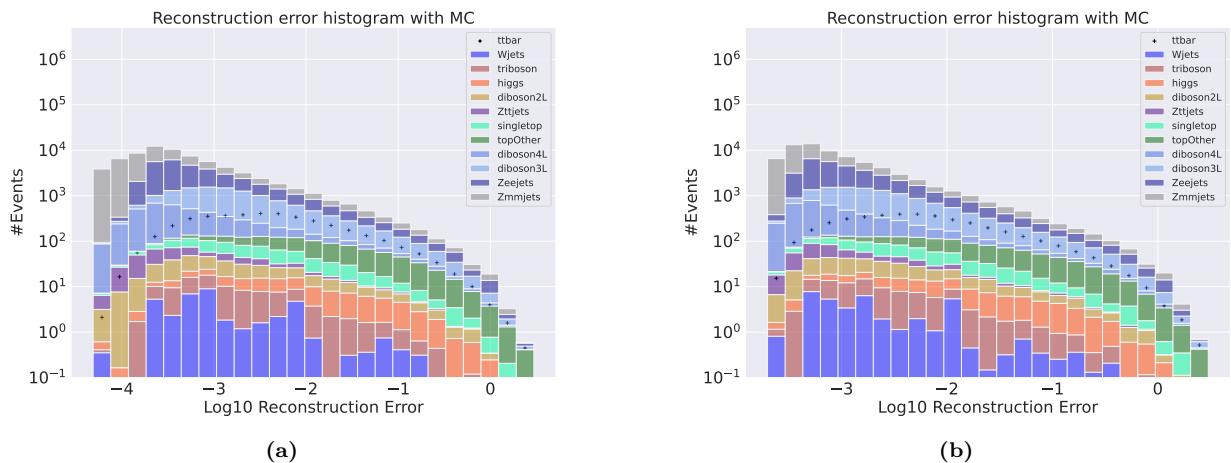


Figure 4.3: Reconstruction error on validation SM MC from the small (a) and large (b) autoencoder. The ttbar channel has been removed from training and is used as signal. No significant difference in distributions is found.

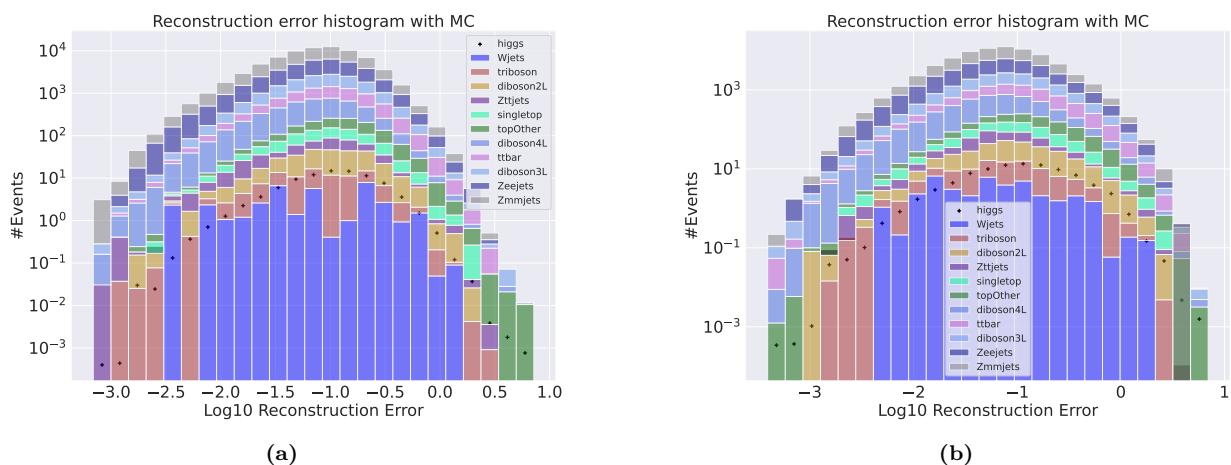


Figure 4.4: Reconstruction error on validation SM MC from the small (a) and large (b) variational autoencoder. The Higgs channel has been removed from training and is used as signal. No significant difference in distributions is found.

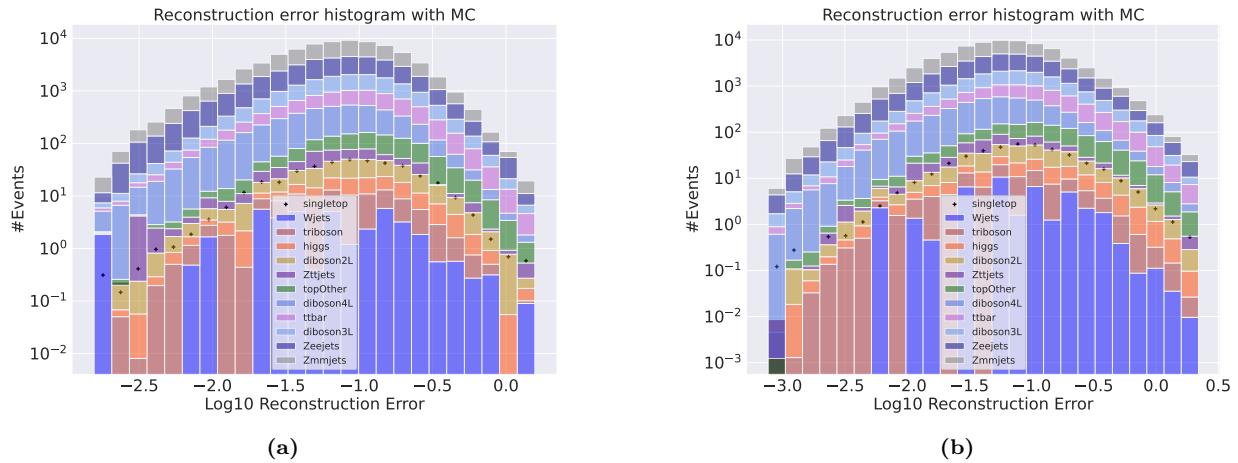


Figure 4.5: Reconstruction error on validation SM MC from the small (a) and large (b) variational autoencoder. The single top channel has been removed from training and is used as signal. No significant difference in distributions is found.

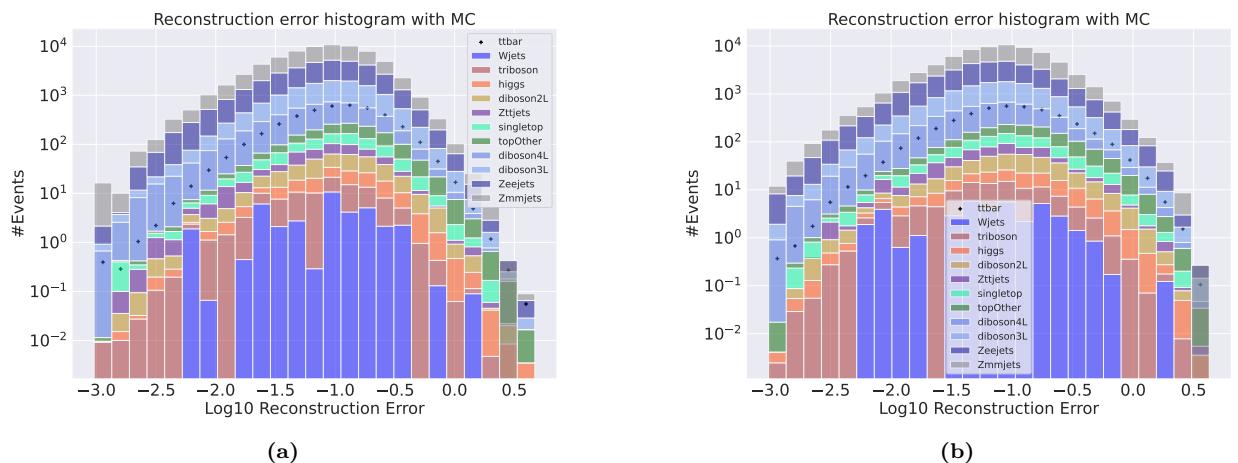


Figure 4.6: Reconstruction error on validation SM MC from the small (a) and large (b) variational autoencoder. The ttbar channel has been removed from training and is used as signal. No significant difference in distributions is found.

It is clear from figures that the reconstruction error distributions for the removed SM channel and the remaining SM MC are very similar. The same behavior is also shown for the other channels, which can be found in section A.1 in the appendix. Although the two models did not demonstrate much separation of reconstruction error distributions, the regular autoencoder seems to have a more shifted pattern of reconstruction to lower values than the variational autoencoder. In fact, the regular autoencoder's reconstruction error distribution peak is about 3 order of magnitude lower than the variational autoencoder's error distribution peak along the x-axis. There could be several reasons for this, one of which could be that the variational autoencoder might require more input data to approximate the distribution, as well as the fact that the balance between the KL divergence and MSE loss can be difficult to handle[44]. The variational autoencoder is a larger and more complex model. Given that the natural distributions in the data are quite complex, learning the natural distribution might require more data. This can lead to comparably poorer performance of the neural network compared to the regular autoencoder. It should be noted that although the three channels selected here, as well as the rest in section A.1 in the appendix, do not differ that much from one another, and it was not expected that the networks would be able to separate the two distributions created. However, it does provide us with a baseline, as well as insight for what to expect if we were to test on signals that look a lot like some background channels.

Altering of transverse momentum

Altering the transverse momentum of some particles would in the extreme be anomalous, and the hypothesis was that some of those trends would be picked up by the autoencoder. Scaling of $k \in [1.5, 3, 5, 7, 10]$ for the

transverse momentum were used according to equation 3.8. A scaling of p_T for the regular and variational autoencoder are shown in figures 4.7 and 4.8, respectively. The other scaling plots can be found in section A.2 in the appendix.

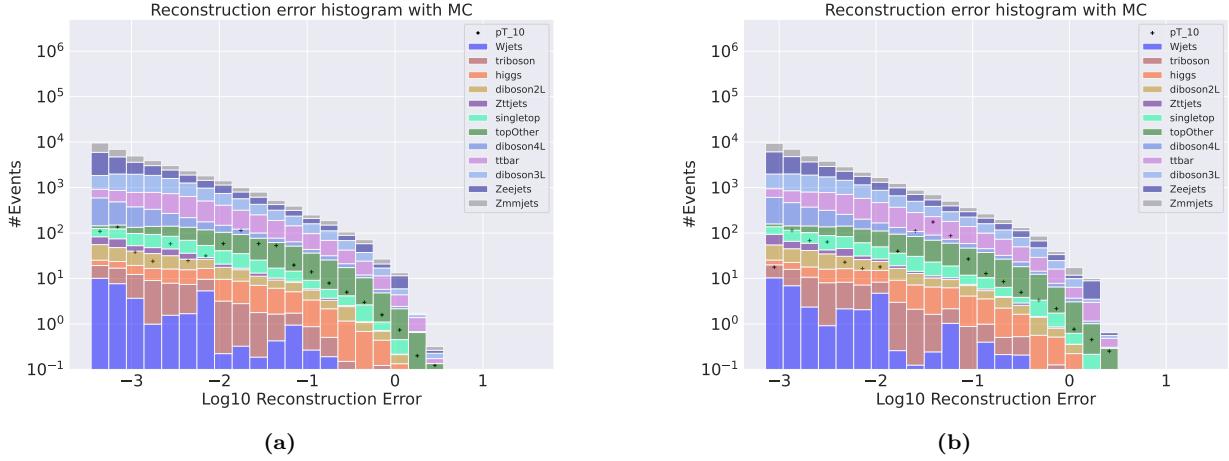


Figure 4.7: Reconstruction error on validation SM MC from the small (a) and large (b) regular autoencoder. The signal is a subsample of the validation set where the transverse momentum of the first electron and the first muon has been increased with a scale of 10. The difference in transverse energy between the objects has also been changed according to the scaling of transverse momentum. A peak is found around $10^{-1.6}$.

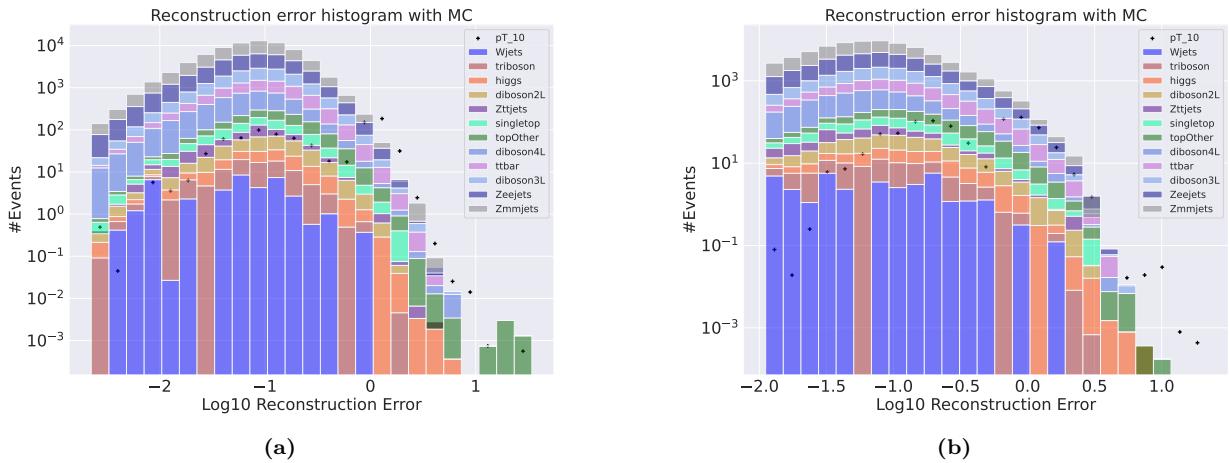


Figure 4.8: Reconstruction error on validation SM MC from the small (a) and large (b) variational autoencoder. The signal is a subsample of the validation set where the transverse momentum of the first electron and the first muon has been increased with a scale of 10. The difference in transverse energy between the objects has also been changed according to the scaling of transverse momentum. A peak is found around $10^{-1.6}$.

The first thing to notice here is that, as with the channel removal, the distribution shape of the output from the regular autoencoder compared to the variational autoencoder is different. The shape from the regular autoencoder is clearly shifted to the left end, with low reconstruction error compared to the shape from the variational autoencoder, where the peak of the distribution is around -1. From the p_T altering test we also see here that the variational autoencoder falls short to the regular one. It is also interesting to observe here that the high p_T events are picked up as anomalous from both autoencoders, with both shallow and deep structure. In the regular autoencoder it is arguably even separated distributions. This is also a good sign as it indicates that the network has learned which ranges the p_T should be in for the 3 lepton plus missing energy final state. The most extreme case is, as expected, in the case where the p_T is multiplied by 10. There is a clear separation in reconstruction error distributions for the signal and background for the deep regular autoencoder, and a slightly more subtle separation of reconstruction error distributions for the shallow regular autoencoder. For the variational autoencoder, the separation in figure 4.8 is not as clear, but the signal is still picked up as anomalous. The peaks are separated, but not to the same degree.

4.2 3 lepton training for bump search testing

To better ascertain and map the usefulness of the regular and variational autoencoder in the search for new physics, two MonteCarlo signals were used as test cases. They both are 3 lep + e_T^{miss} final state SUSY signals, and thus are fit to use for testing. The two autoencoders will be tested on four metrics.

- Low reconstruction error on SM MC
- Background to signal ratio in e_T^{miss} signal region
- Possible resonance in trilepton signal region
- Significance search in e_T^{miss} signal region

Regular autoencoder output

Below are the reconstruction error distributions for the two signals for both the shallow and deep regular autoencoder.

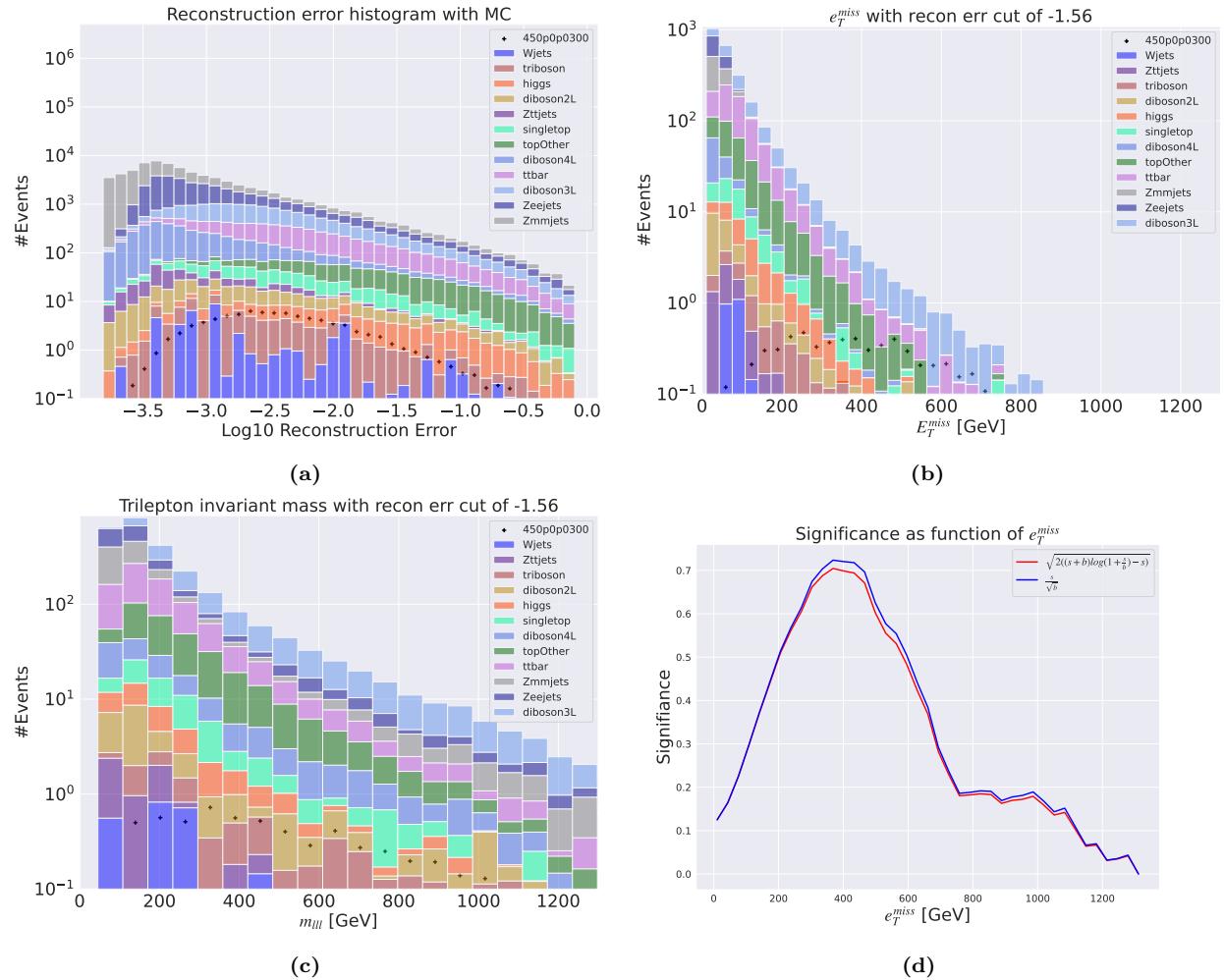


Figure 4.9: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the deep regular autoencoder using the SUSY 450p300.

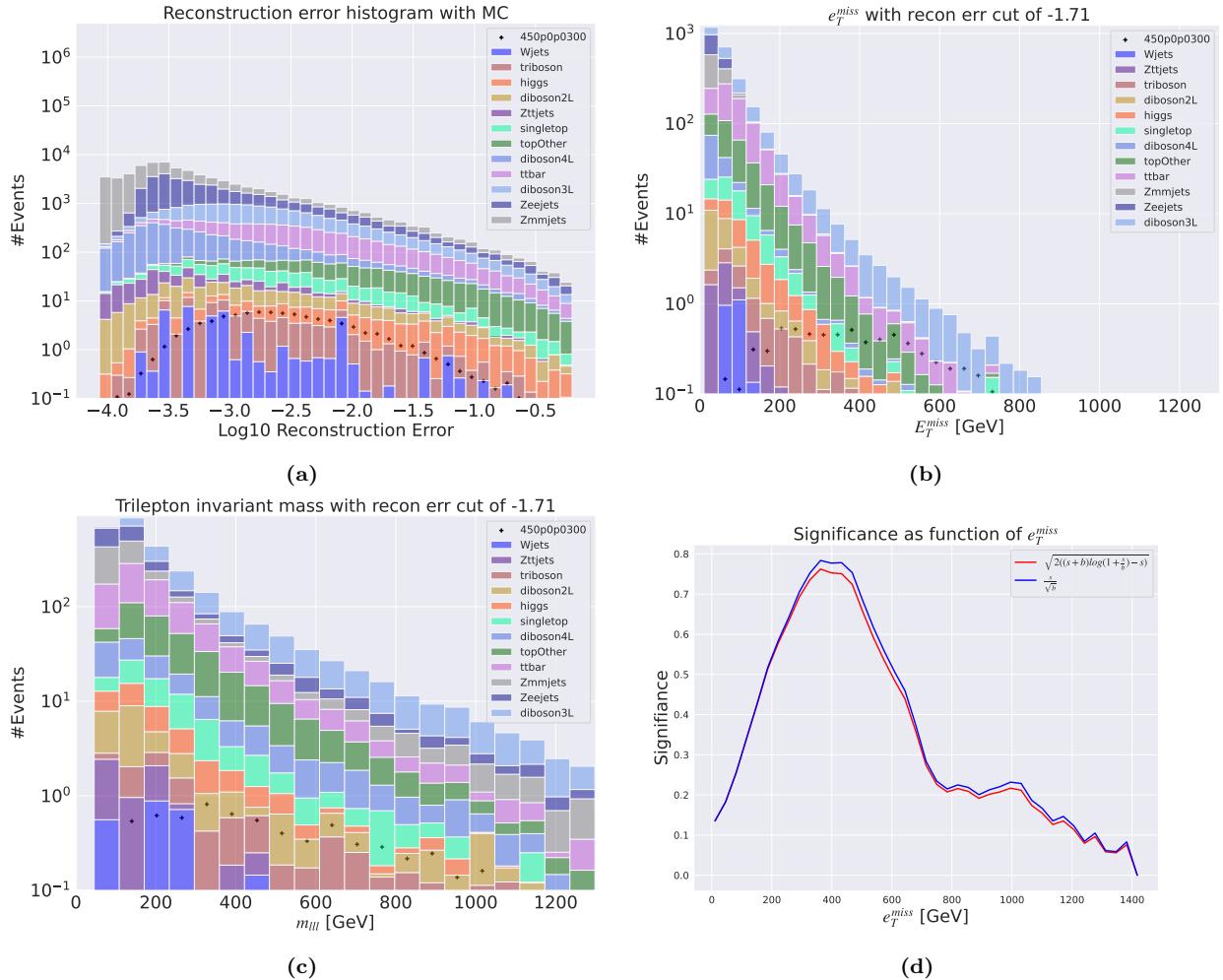


Figure 4.10: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the shallow regular autoencoder using the SUSY 450p300 model.

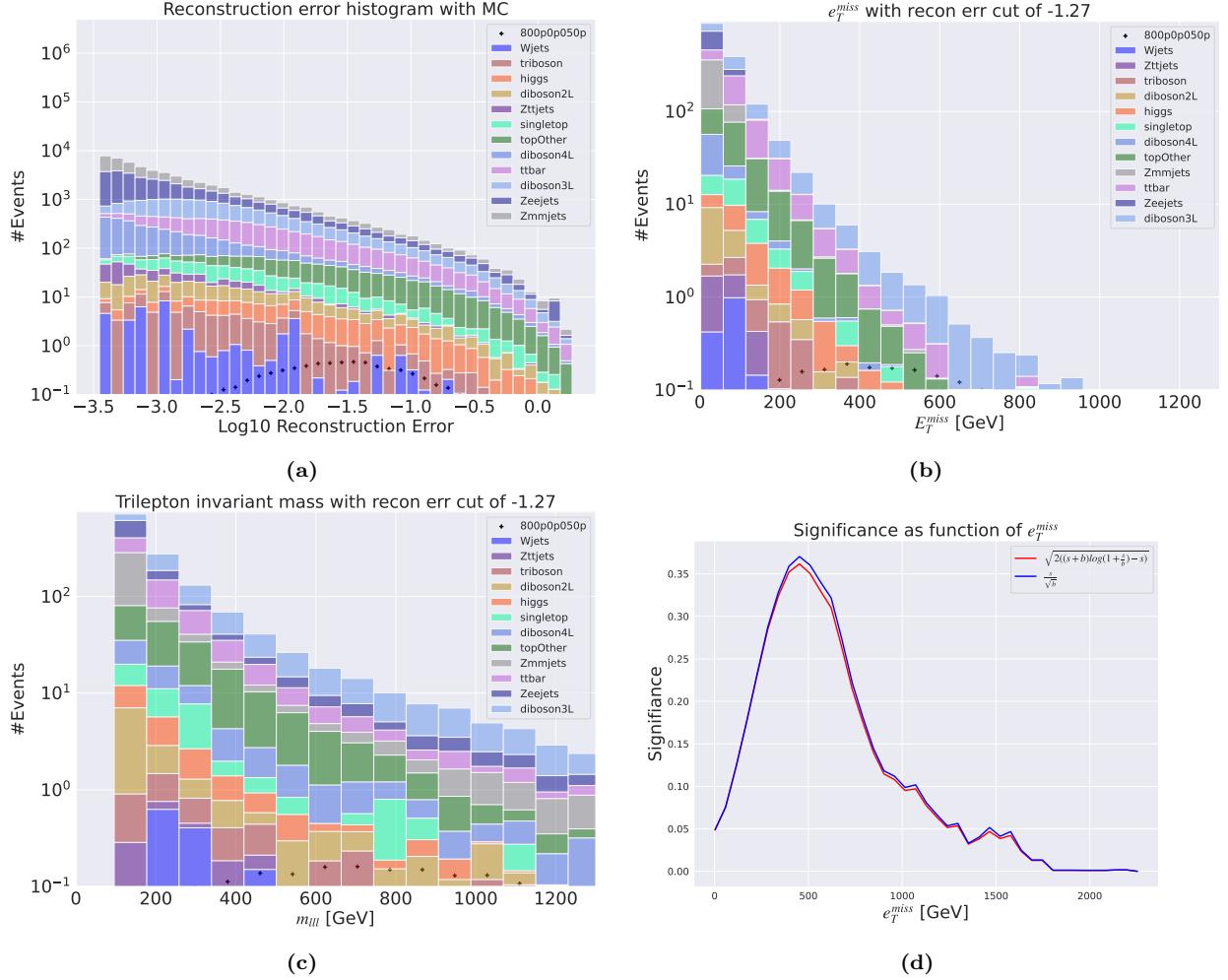


Figure 4.11: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the deep regular autoencoder using the SUSY 800p50.

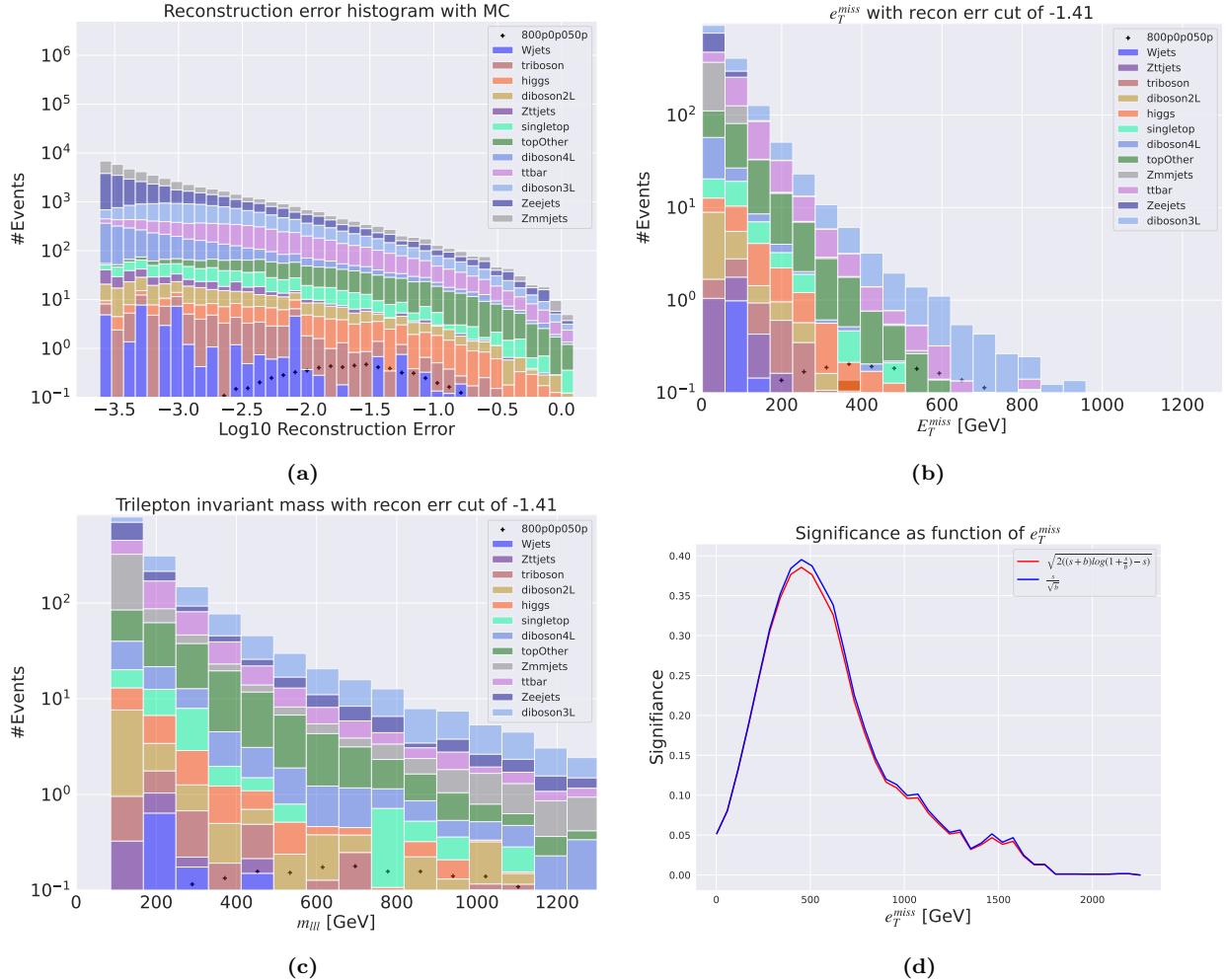


Figure 4.12: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the shallow regular autoencoder using the SUSY 800p50.

In figures 4.9, 4.10, 4.11 and 4.12 we have four subplots containing the total reconstruction error distributions, the e_T^{miss} signal region, the m_{lll} signal region and the significance as function of e_T^{miss} curve respectively for the shallow and deep regular autoencoder. From figures 4.9a, 4.10a, 4.11a, 4.12a it is clear here that the autoencoder manages to somewhat separate the peaks of the signal and background distributions. Still, the distributions themselves are not separated. The SUSY 800p50 signals has the best separation of peaks, which is expected considering its rather extreme tail in the e_T^{miss} distribution of the signal. It is also interesting to observe the slope trend in the SM MC reconstruction error distribution. The steepness of the slope seems to be somewhat similar for both the shallow and deep regular autoencoder, indicating at least that the difference in these two models does not differ much when it comes to performance. The bulk of the events are below 10^{-2} reconstruction error, indicating that the autoencoder has learned a lot of the internal RMM structures for the 3 lepton + e_T^{miss} final state MC.

In figures 4.9b, 4.10b, 4.11b and 4.12b we have a signal region created for each of the SUSY models from both the shallow and deep regular autoencoder. The cuts were created using the median and then iteratively increasing the error requirement, as explained in section 3.7. Only one of the three cuts done are shown here, the rest can be found in the appendix. The histograms in figures 4.9b, 4.10b, 4.11b and 4.12b displays the e_T^{miss} distribution in the signal region for the SM MC and the SUSY signals. They represent the signal region with the most relaxed cut, in other words, the least strict and thus the signal region with the most amount of total events, both SM MC and signal. This is to illustrate the difficulty of this method since we only have the reconstruction error to go on. Thus, too strict a cut will most likely eliminate all possible signal events in the signal region, whereas too loose a cut and the SM MC background will dominate completely. In figures 4.9c, 4.10c, 4.11c and 4.12c we have the m_{lll} distributions in the signal regions from both the shallow and deep regular autoencoder for both SUSY signals. As with the e_T^{miss} distributions, the m_{lll} distributions with the least strict cut in the signal region are shown here, with the rest shown in the appendix. From these figures it is not easy to see any resonances in the distributions. There is also little separation between signal

and background distributions in the m_{lll} feature, although there is some for the SUSY 800 p_{T} 50 model. It is also shown that the difference between the shallow and deep neural network architecture has little to no effect here or in the e_T^{miss} distributions in terms of separation.

In figures 4.9d, 4.10d, 4.11d and 4.12d we have the significance as a function of the e_T^{miss} . It displays that a further cut on the e_T^{miss} will get an even better significance, the best case provided from the SUSY 450 p_{T} 300 signal with the deep autoencoder, using a cut on the e_T^{miss} around 400 GeV.

Variational autoencoder output

In the Variational autoencoder case, we have the same distributions as above. Below we have the full reconstruction error distributions for both signals from the shallow and deep variational autoencoder.

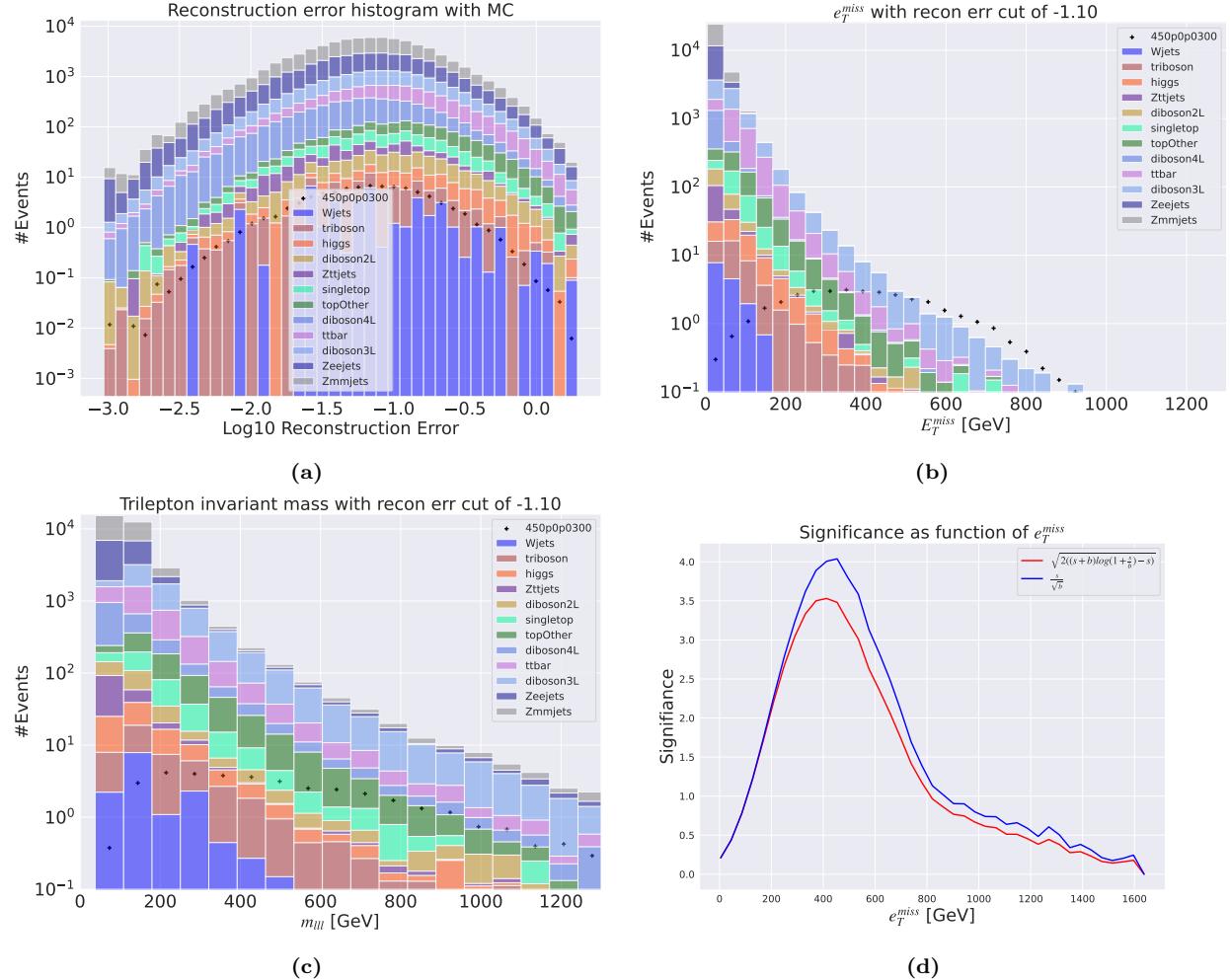


Figure 4.13: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the deep variational autoencoder using the SUSY 450p300.

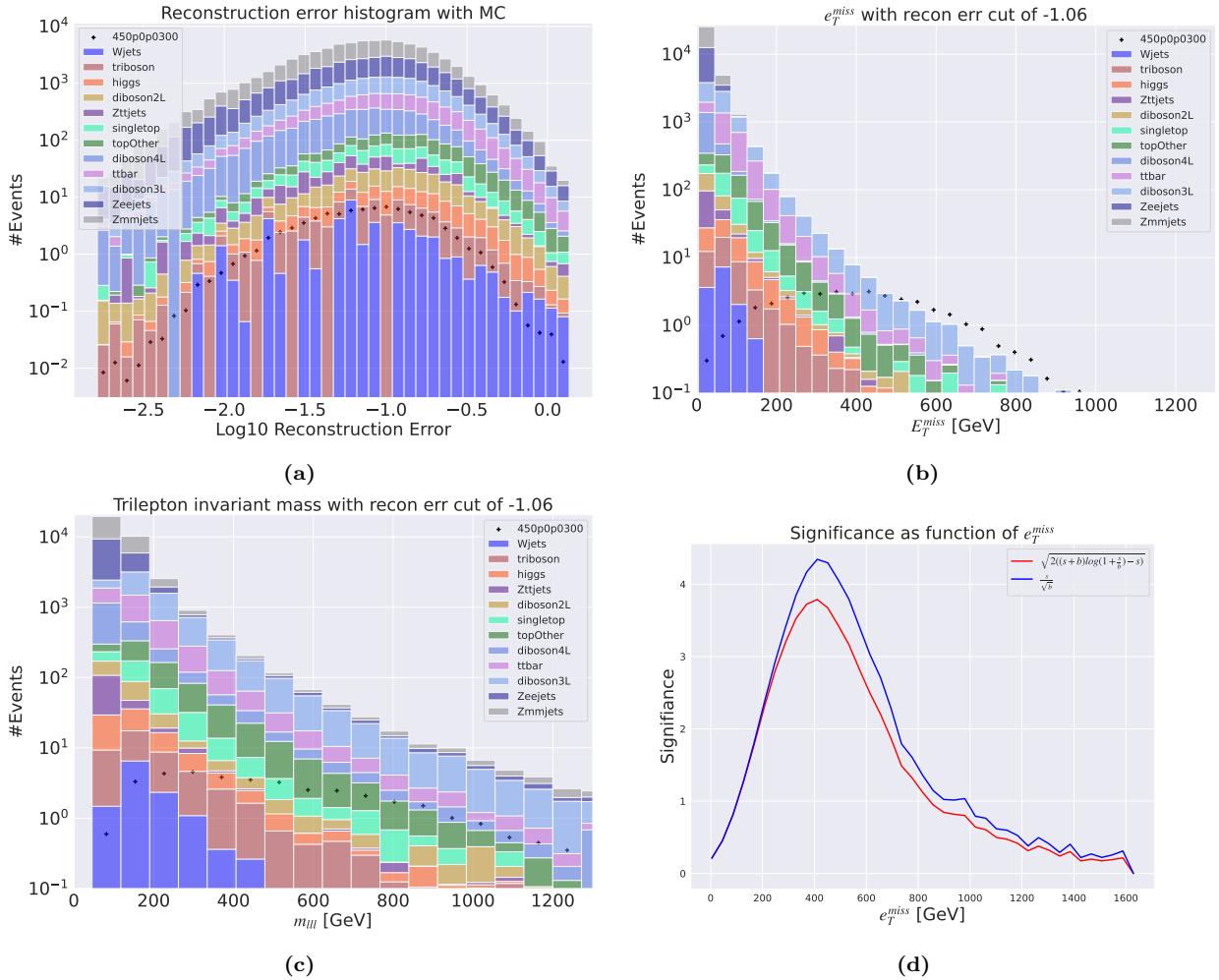


Figure 4.14: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the shallow variational autoencoder using the SUSY 450p0300.

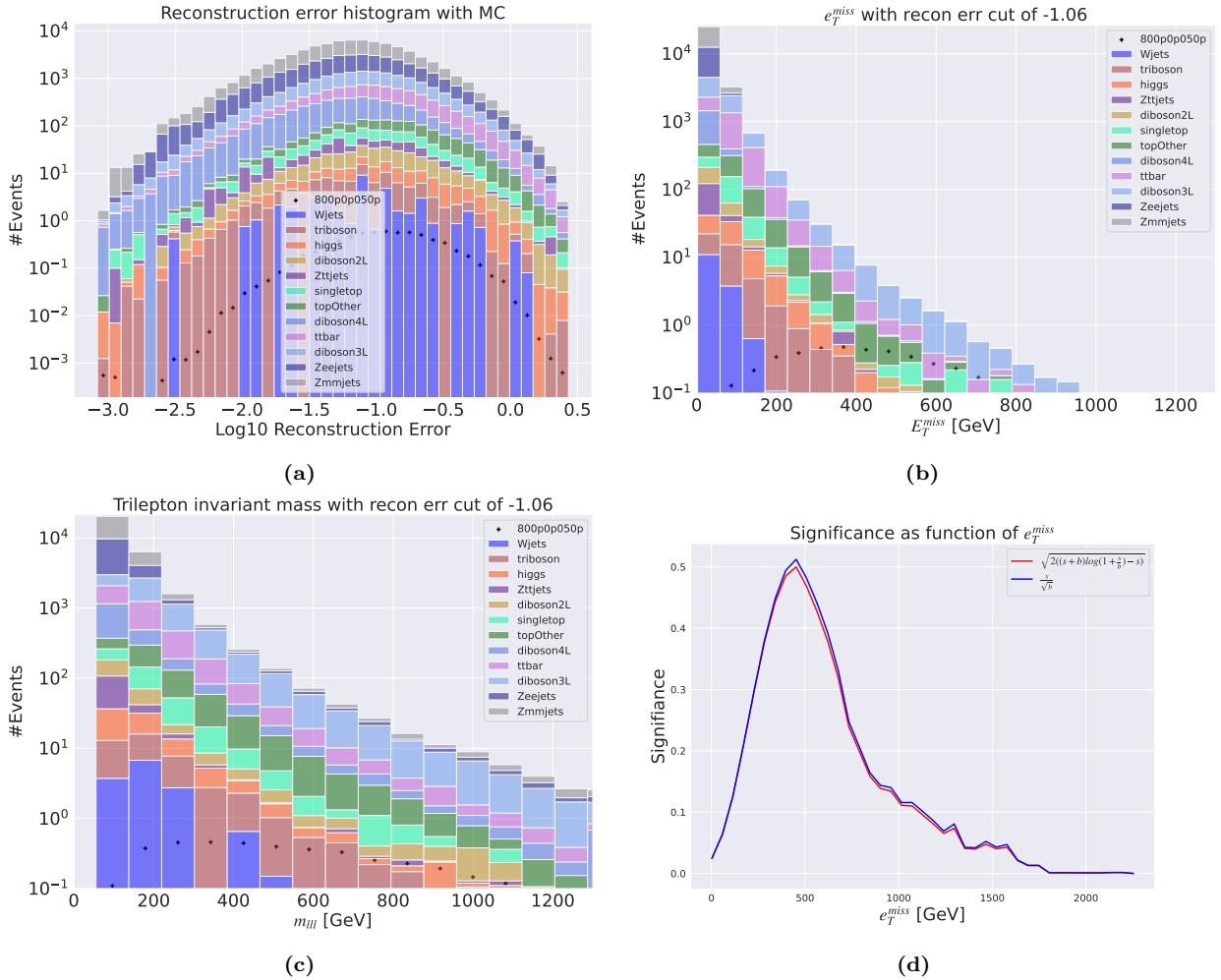


Figure 4.15: Reconstruction error, e_T^{miss} signal region, m_{ll} signal region and significance as function of e_T^{miss} for the deep variational autoencoder using the SUSY 800p50.

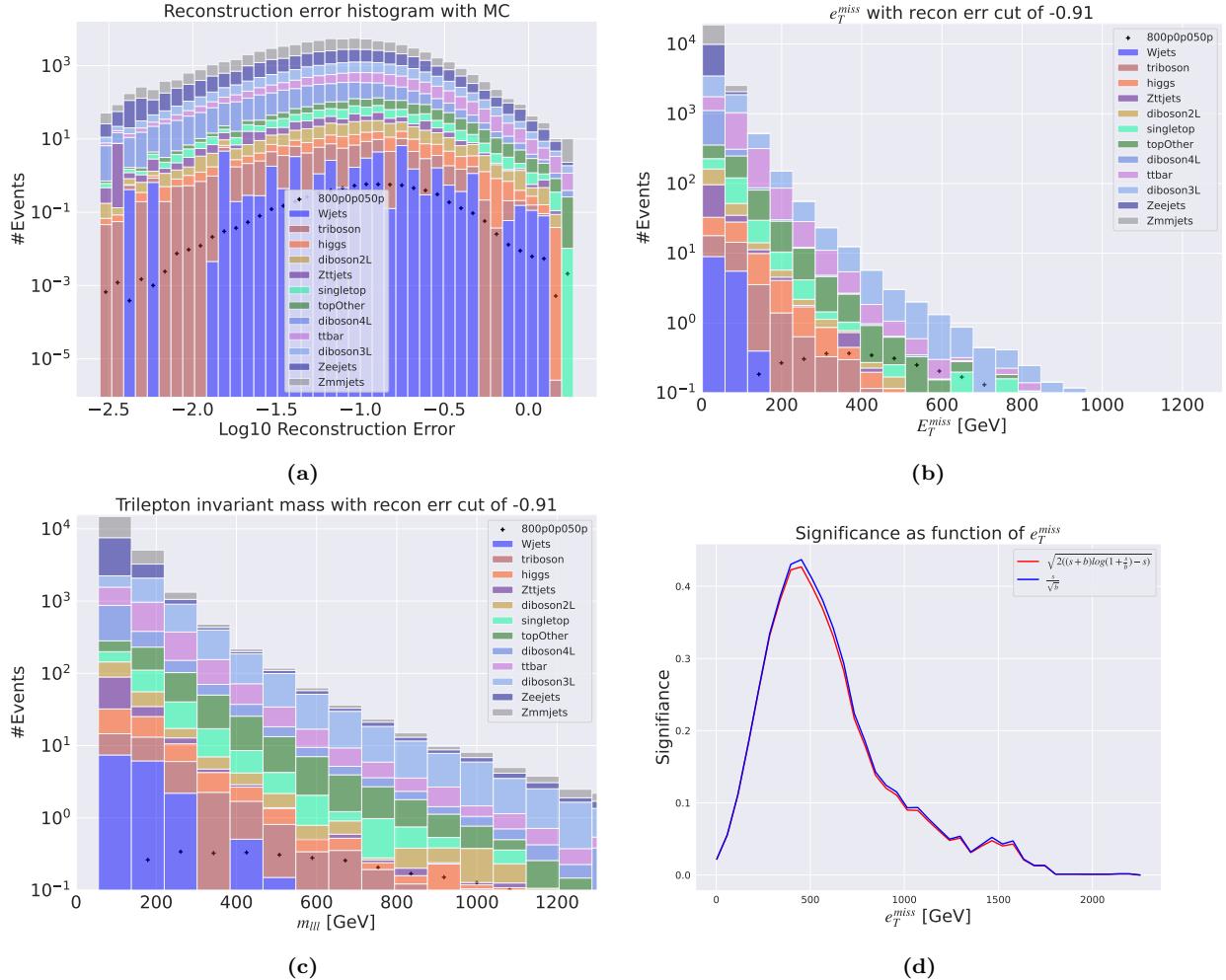


Figure 4.16: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the shallow variational autoencoder using the SUSY 800p50.

In figures 4.13, 4.14, 4.15 and 4.16 we have four subplots containing the total reconstruction error distributions, the e_T^{miss} signal region, the m_{lll} signal region and the significance as function of e_T^{miss} curve respectively for the shallow and deep variational autoencoder. From figures 4.13a, 4.14a, 4.15a, 4.16a we observe that the variational autoencoder seems to struggle with differentiating between background and signal, having the two distributions laying on top of each other. There is however a slight difference in the shape of the distributions from the shallow and deep network. The shallow has a more narrow and slightly more left leaning shape, whereas the deep network has a slightly more broad distribution shifted a bit to the right. The bulk of the events are between 10^{-2} and $10^{-0.5}$ reconstruction error, indicating that the autoencoder struggles to learn the internal RMM structures for the 3 lepton + e_T^{miss} final state MC. The somewhat Gaussian distribution differs between the two SUSY samples. As the networks were retrained each time, it could indicate that the distribution in part is due to the sampling in the latent space.

In figures 4.13b, 4.14b, 4.15b and 4.16b we have the reconstruction error cut imposed on the SM MC and the signal samples. Interestingly, one should note that although the total reconstruction error distributions are not well separated, the signal regions show a separation in distribution peaks. Now, unlike in the regular autoencoder case, the variational autoencoder allows for almost two orders of magnitude more background events in the signal region. This is because of the algorithm used to determine the reconstruction error cut by means of finding the median and iteratively increasing the criterion. Because the two distributions are on top of each other, we get a lot of background events, but we also get the peak of the signal distributions, which is why we see the clear separation in the figures 4.13b, 4.14b, 4.15b and 4.16b.

In figures 4.13c, 4.14c, 4.15c and 4.16c we have the signal region in the m_{lll} feature. Here, as with the e_T^{miss} distribution, the least strict reconstruction error cut has been imposed on the region. There are little to no separation between the peaks to observe.

In figures 4.13d, 4.14d, 4.15d and 4.16d we have the significance as a function of the e_T^{miss} . Interestingly, for the SUSY 450p300 case, we have that both the deep and shallow autoencoder manages to get a significance

of around 4, which is much better than the regular autoencoder which got around 0.7. Likewise for the other SUSY signal, but here the difference was small. From these figures a further cut on the e_T^{miss} on around 400 GeV provides the best significance. Also note the tails of the significance figures, as they all contain little background and or signal and are thus not of interest.

4.3 2 lepton training for bump search testing

The 3 lepton + e_T^{miss} dataset has fewer events, and thus allows for less training of the neural networks. Thus, the 2 lepton + e_T^{miss} dataset was tried as well. The event selection was done choosing at least 2 leptons, meaning that the RMM signatures of some events will look similar to the RMM signatures of the 3 lepton + e_T^{miss} dataset. A consequence of this is that the signal samples for the 3 lepton case will be a good start point for testing. The two autoencoders will be tested on three of the four metrics used for the 3 lepton + e_T^{miss} case.

- Low reconstruction error on SM MC
- Background to signal ratio in e_T^{miss} signal region
- Significance search in e_T^{miss} signal region

Regular autoencoder performance

Below are some results from training on the 2 lepton case with the regular autoencoder, using the same two SUSY signals as test cases.

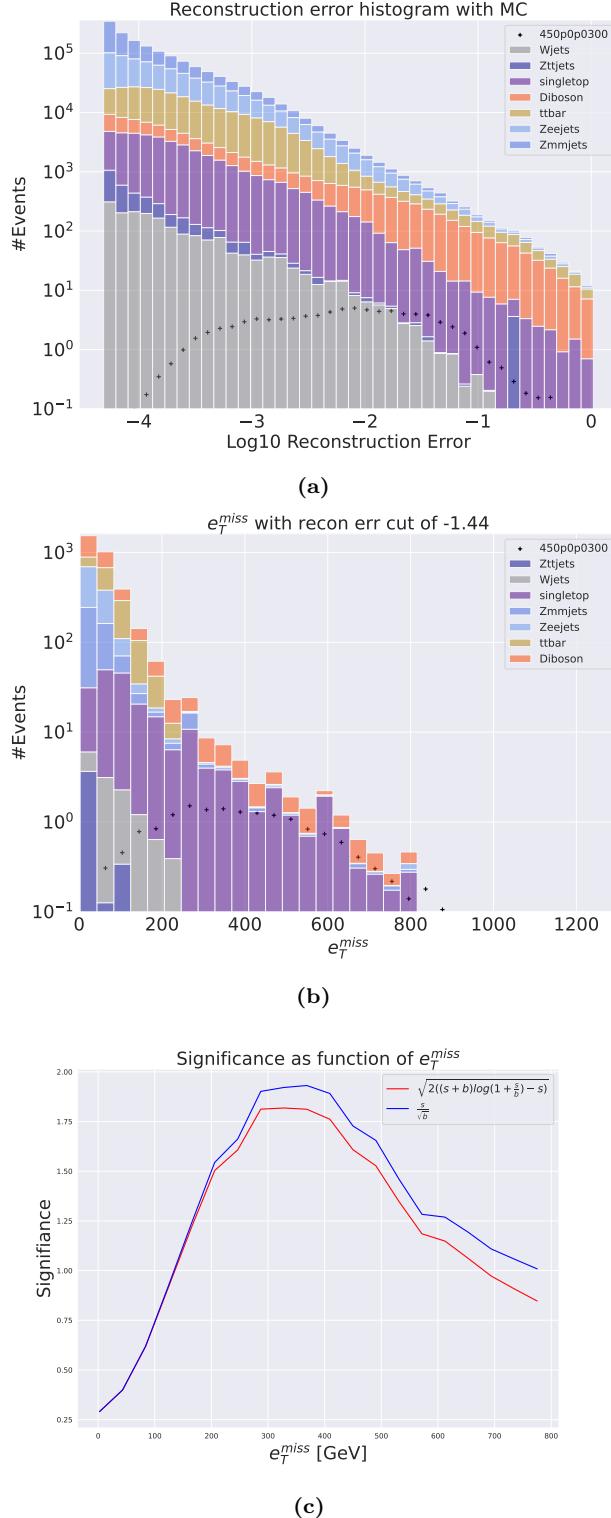


Figure 4.17: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the deep regular autoencoder using SUSY 450p300. In figure 4.17a the background distribution is highly shifted to the lower end of the reconstruction error range. In figure 4.17b there is a small separation between the peaks of the background and the signal. There is still mostly overlap between the two distributions. From figures 4.17c we have the significance as a function of e_T^{miss} . The shallow autoencoder gets a significance of almost 1.9 when imposing a cut on around 350 GeV.

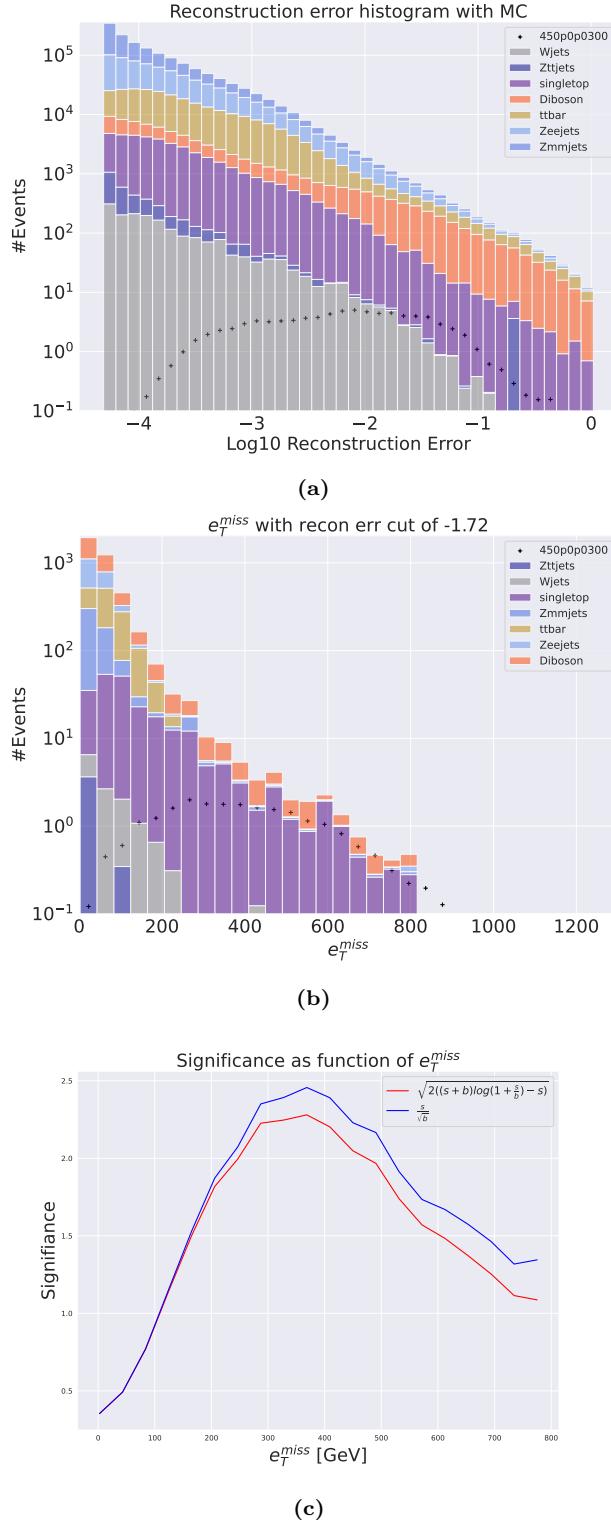


Figure 4.18: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the deep regular autoencoder using SUSY 450p300. In figure 4.18a the background distribution is highly shifted to the lower end of the reconstruction error range. In figure 4.18b there is a small separation between the peaks of the background and the signal. There is still mostly overlap between the two distributions. From figures 4.18c we have the significance as a function of e_T^{miss} . The shallow autoencoder gets a significance of almost 2.5 when imposing a cut on around 380 GeV.

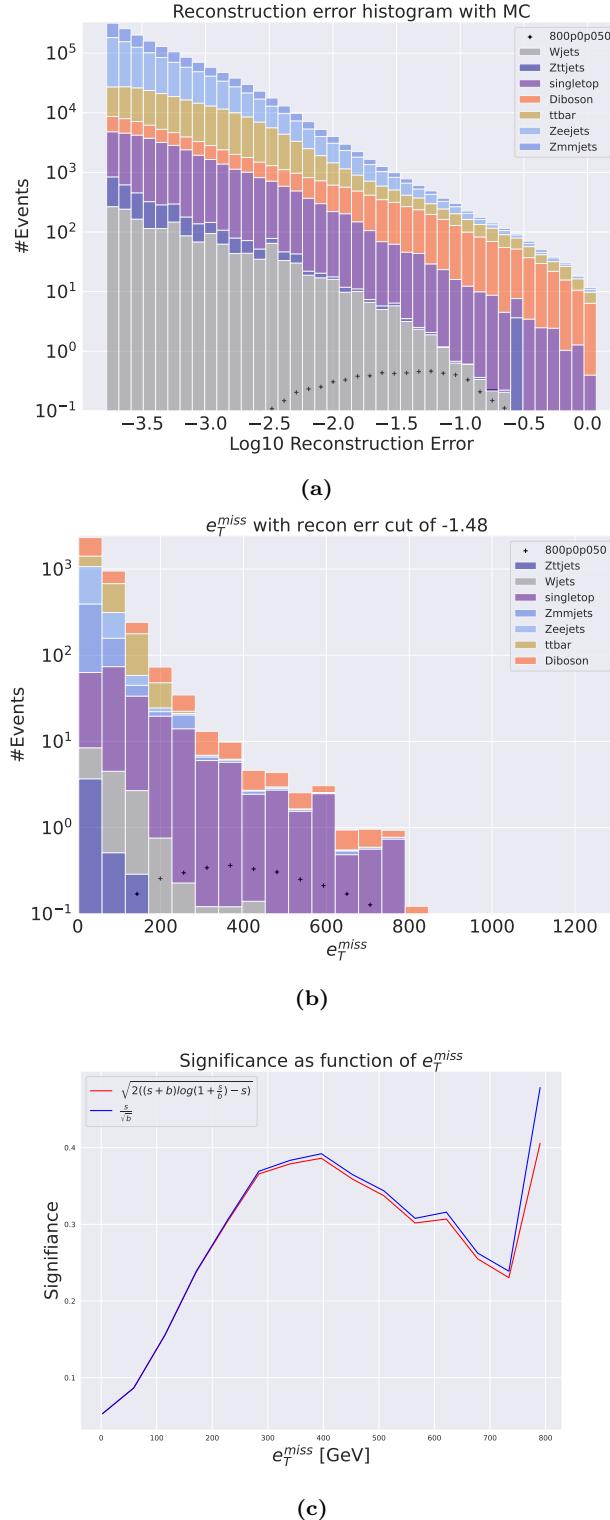


Figure 4.19: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the deep regular autoencoder using SUSY 800p50. In figures 4.19a the background distribution is highly shifted to the lower end of the reconstruction error range. In figure 4.19b there is a small separation between the peaks of the background and the signal. There is still mostly overlap between the two distributions. From figures 4.19c we have the significance as a function of e_T^{miss} . The deep autoencoder gets a significance of about 0.39 when imposing a cut on around 400 GeV.

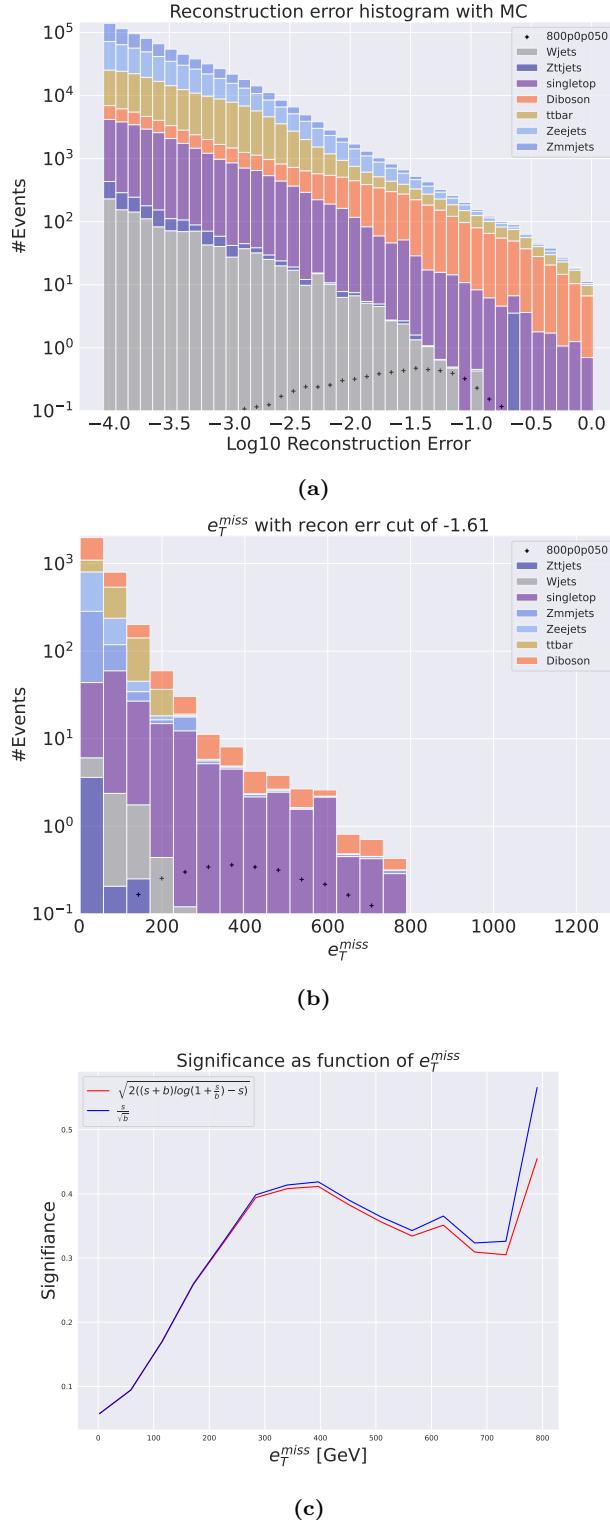


Figure 4.20: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the shallow regular autoencoder using SUSY 800p50. In figure 4.20a the background distribution is highly shifted to the lower end of the reconstruction error range. In figure 4.20b there is a small separation between the peaks of the background and the signal. There is still mostly overlap between the two distributions. From figures 4.20c we have the significance as a function of e_T^{miss} . The shallow autoencoder gets a significance of about 0.41 when imposing a cut on around 400 GeV.

In figures 4.17, 4.18, 4.19 and 4.20 we have three subplots containing the total reconstruction error distributions, the e_T^{miss} signal region, and the significance as function of e_T^{miss} curve respectively. They were created using the shallow and deep regular autoencoder with the 2 lepton + e_T^{miss} dataset. In figures 4.17a, 4.18a, 4.19a, 4.20a there is a continuing trend following the 3 lepton + e_T^{miss} case shown in figures 4.9a, 4.10a,

[4.11a](#), [4.12a](#). This indicates that as we increase the statistics, in other words the amount of background events used for training, the ability of the autoencoder to learn the internal structure increases. As expected, Zmmjets and Zeejets along with ttbar are the channels with the highest statistics in the 2 lepton + e_T^{miss} dataset, thus it should be easier to learn to better reconstruct those events. However, note the amount of diboson in the higher end of the reconstruction error histograms, as well as in the e_T^{miss} post reconstruction error cut distributions.

In figures [4.17b](#), [4.18b](#), [4.19b](#) and [4.20b](#) we have the e_T^{miss} distributions for the least strict cuts for the regular autoencoder models. One indication that the search strategy used in this thesis could work is if the models can improve the significance from just looking at the e_T^{miss} distributions of the background and the signal in mind. Thus, we want to compare the pre reconstruction error significance with the signal region based on the autoencoder output. The significance in the pre reconstruction error case were for the SUSY 450p300 signal 0.017 using both the small and large statistics formula, and 0.0014 for the SUSY 800p50 signal. Note here that for e_T^{miss} , no physics informed cuts have been used, but there are certain cuts that can increase the significance, so the significance in should be considered to possibly be somewhat higher.

In figures [4.17c](#), [4.18c](#), [4.19c](#) and [4.20c](#) we have the significance as function of e_T^{miss} . This plot shows how implementing another cut in the signal region, namely from which bin in the e_T^{miss} distribution to select events, allows for higher significance. The highest significance was found with the shallow autoencoder with the SUSY 450p300 signal model. It should be noted that the significance for the 800p50 signal model is a lot smaller than for the 450p300 signal model, even though the separation shown in figures [4.17a](#), [4.18a](#), [4.19a](#), [4.20a](#) would suggest otherwise. Although the peak in both signal models are fairly separated from the peak of the SM MC, the SUSY 800p50 signal model is shifted a lot more. This is consistent with expectation, for the same reason that the significance tails are the way they are. The reason for the low significance is most likely the fact that the signal sample contains low statistics, in other words, the weights are just a lot lower, compared to the other signal sample.

Variational autoencoder performance

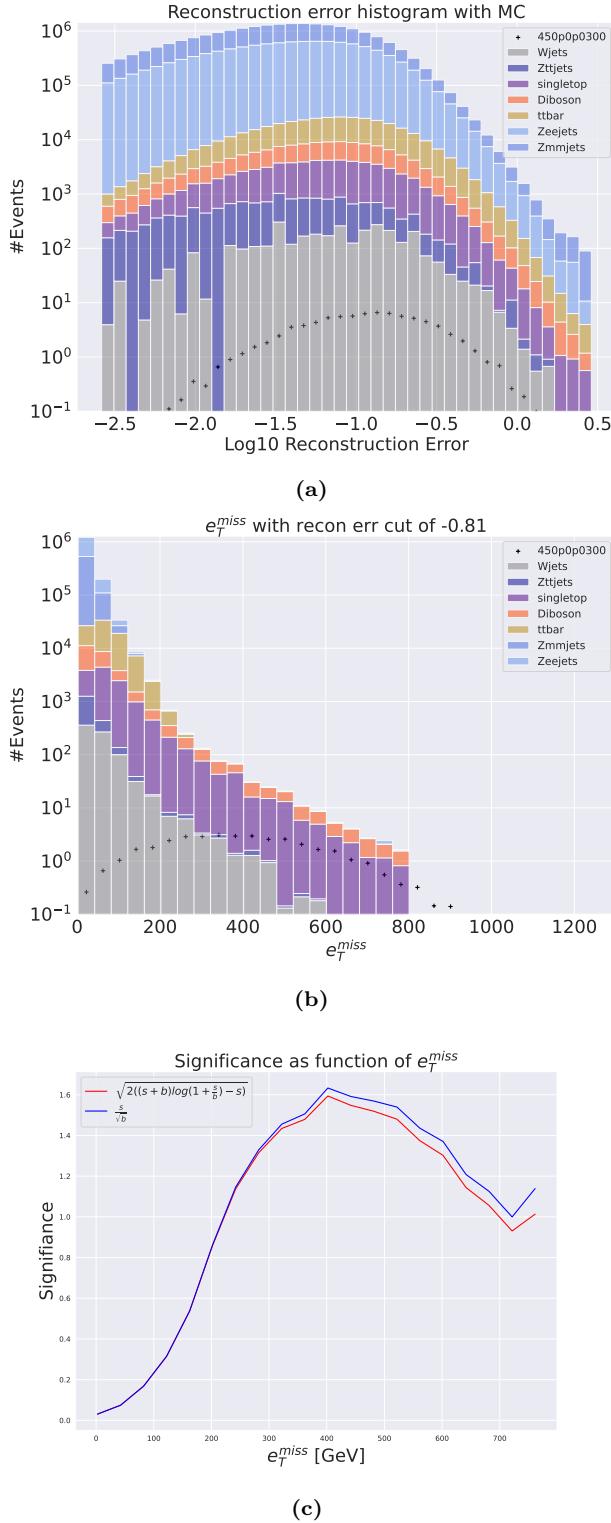


Figure 4.21: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the deep regular autoencoder using SUSY 450p300. In figure 4.21a the peak of the distribution is somewhat centered in the middle of the reconstruction error range forming a bell-like shape. The peaks of the background and signal distributions are not well separated, with almost identical trends. Figure 4.21b, shows a signal region with large background distribution. The peaks in the signal region are also somewhat separated, but the overall distributions are overlapping still. Figure 4.21 shows the significance as function of e_T^{miss} . The peak significance is around 1.61 at around 400 GeV.

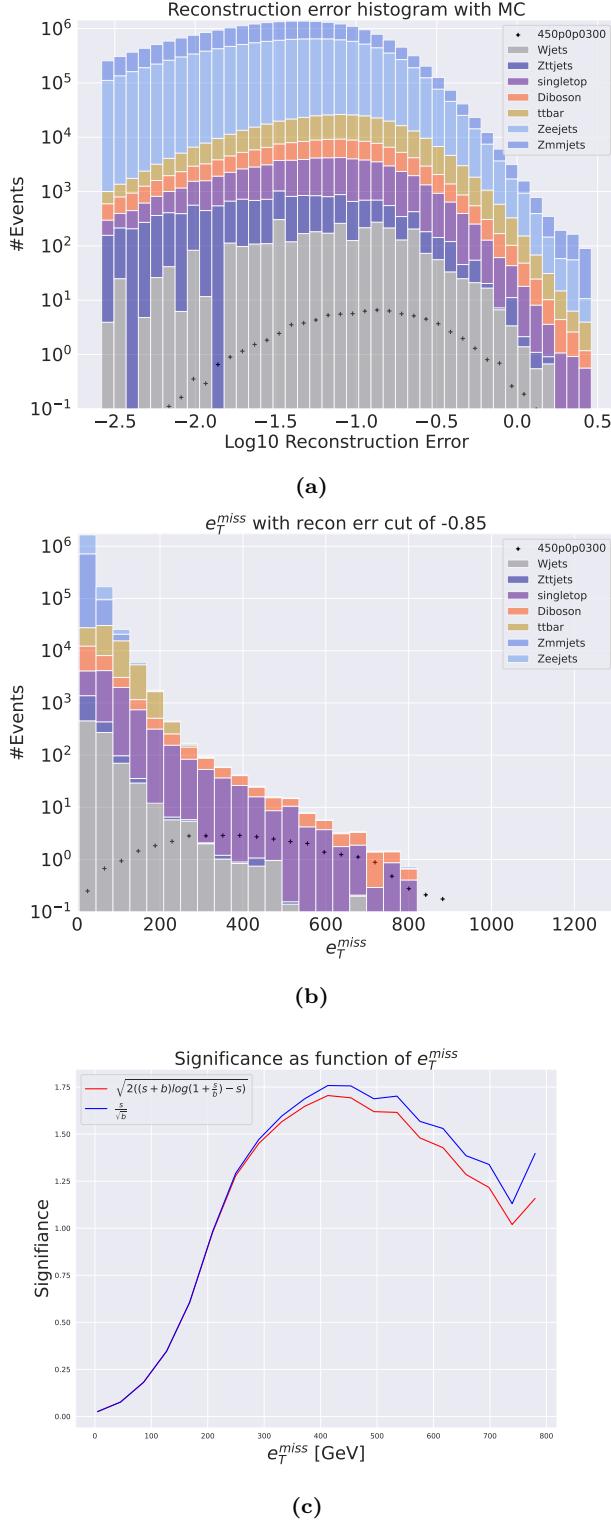


Figure 4.22: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the shallow regular autoencoder using SUSY 450p300. In figure 4.22a, the peak of the distribution is somewhat centered in the middle of the reconstruction error range forming a bell-like shape. The peaks of the background and signal distributions are not well separated, with almost identical trends. Figure 4.22b shows a signal region with large background distribution. The peaks in the signal region are also somewhat separated, but the overall distributions are overlapping still. Figure 4.22 shows the significance as function of e_T^{miss} . The peak significance is around 1.75 at around 420-450 GeV.

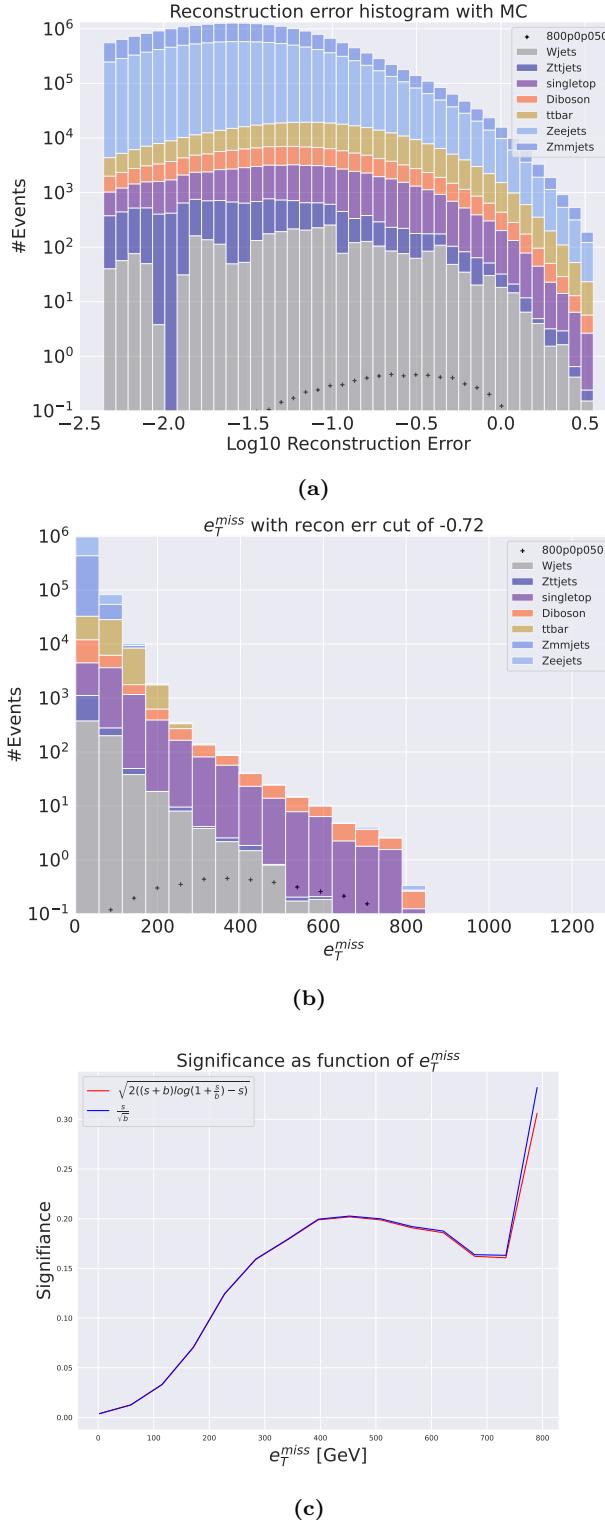


Figure 4.23: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the deep variational autoencoder using SUSY 800p50. In figure 4.23a, the peak of the distribution is somewhat centered in the middle of the reconstruction error range forming a bell-like shape. The peaks of the background and signal distributions are not well separated, with almost identical trends. Figure 4.23b shows a signal region with large background distribution. The peaks in the signal region are also somewhat separated, but the overall distributions are overlapping still. Figure 4.21, 4.22, 4.23 and 4.24 shows the significance as function of e_T^{miss} . The peak significance is around 0.20 at around 450 GeV.

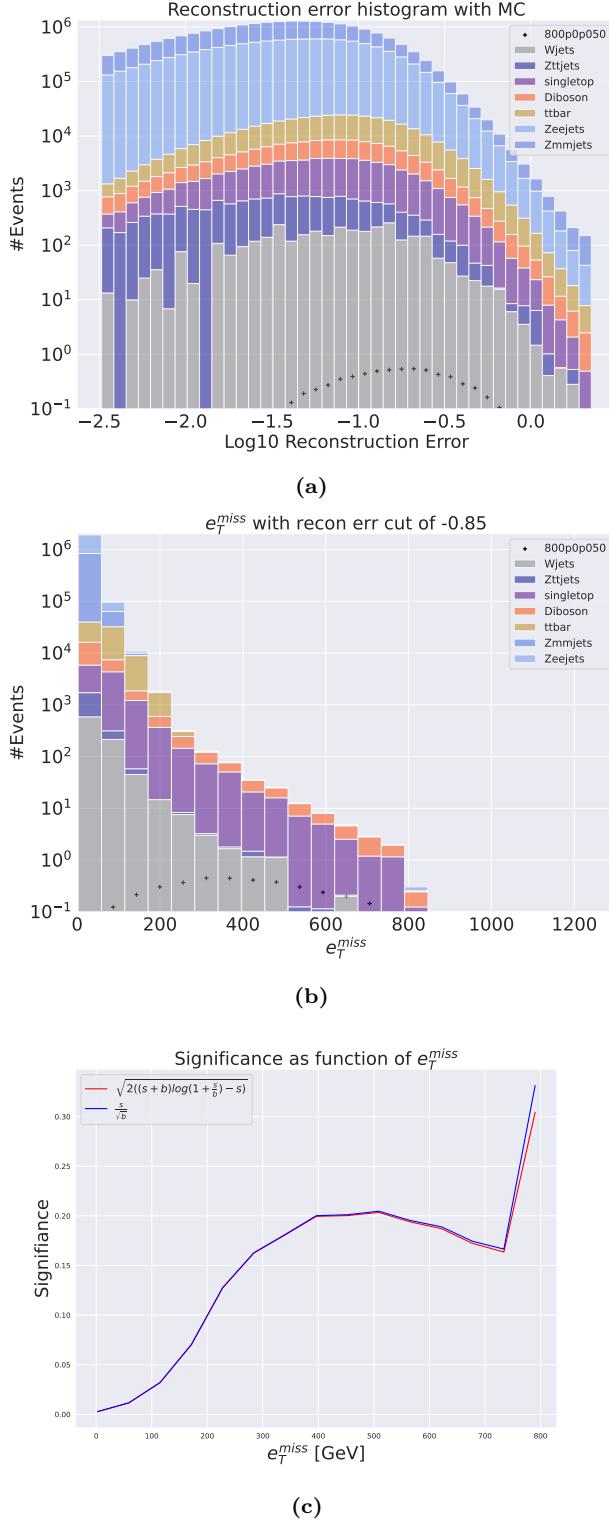


Figure 4.24: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the shallow variational autoencoder using SUSY 800p50. In figure 4.24a the peak of the distribution is somewhat centered in the middle of the reconstruction error range forming a bell-like shape. The peaks of the background and signal distributions are not well separated, with almost identical trends. Figure 4.24b shows a signal region with large background distribution. The peaks in the signal region are also somewhat separated, but the overall distributions are overlapping still. Figure 4.24 shows the significance as function of e_T^{miss} . The peak significance is around 0.21 at around 500 GeV.

In figures 4.21, 4.22, 4.23 and 4.24 we have three subplots containing the total reconstruction error distributions, the e_T^{miss} signal region, and the significance as function of e_T^{miss} curve respectively. They were created using the shallow and deep regular autoencoder with the 2 lepton + e_T^{miss} dataset.

In figures 4.21a, 4.22a, 4.23a, 4.24a we have the reconstruction error distributions for both SUSY signals for the small and large variational autoencoder. The steepness here differs from the steep slope in figures 4.17a, 4.18a, 4.19a, 4.20a. Interestingly, we see here that the deepness of the neural network here plays a role, which is different from the regular autoencoder output, where both the small and large autoencoder made a steep slope shape of the SM MC reconstruction error distribution. The peak of the distribution here is slightly shifted to the left for the shallow autoencoder model, and slightly shifted to the right of the center with the deep autoencoder model. One possible reason for this somewhat bell-like distribution could be that the variational autoencoder samples from a Gaussian distribution that has yet to be trained on enough data to produce a good enough error distribution. This is also supported with the fact that the shape is even more bell-like like in the 3 lepton + e_T^{miss} case shown in figures 4.13a, 4.14a, 4.15a, 4.16a. It could also be that the batch size is too large, and that the model has to train on smaller batches to get a better result.

In figures 4.21b, 4.22b, 4.23b and 4.24b we have the e_T^{miss} distribution for the least strict cut for each signal. We see that the cuts are somewhat similar to the regular autoencoder, but with two key differences. First, because the peaks of the distributions from figures 4.21a, 4.22a, 4.23a, 4.24a are so close, the cuts allowed for more background events in the signal region. Here, as with the regular autoencoder output, m_{err} was used to create the signal region, but was not a good discriminator for the background events. One could perhaps make a new strategy for setting the cuts in the event one has a bell-like shape. Still, because we set cuts based on reconstruction error to minimize the background in the signal region, if one does not have a slope like shape, the results will be poor in comparison.

Secondly, the background that remains are slightly different from the signal region from the regular autoencoder. In the lower energy range there is a large excess of Zeejets, Zmmjets and ttbar events that have a high reconstruction error, which is not the case for the variational autoencoder, dominated by diboson events in all bins. In the higher energy range, diboson are largest contributer to the background, but the number of bins are exceptionally smaller than the Zmmjets/Zeejets/ttbar events, by a magnitude of 3 at the most.

4.4 Blind ATLAS data sample testing

The final test to run on the autoencoder is a blind test. The blind test will compare the reconstruction error from the autoencoder on an ATLAS dataset with the reconstruction error on the same ATLAS dataset where about 1.6 million events have been randomly removed and switched with samples from many BSM samples. The signal samples have been given the same weight as the ATLAS data. Therefor the total amount of events before eventselection are the same in both datasets. The dataset was prepared by one of the supervisors of this thesis, and not shown to the author. The ATLAS data contains events from the data collection from 2015 and 2016, and the signal samples are created according to those runs. The ATLAS data will therefor be referred to as ATLAS data 15 and data 16 for the ATLAS events, and the mix set will be referred to data1516 mix.

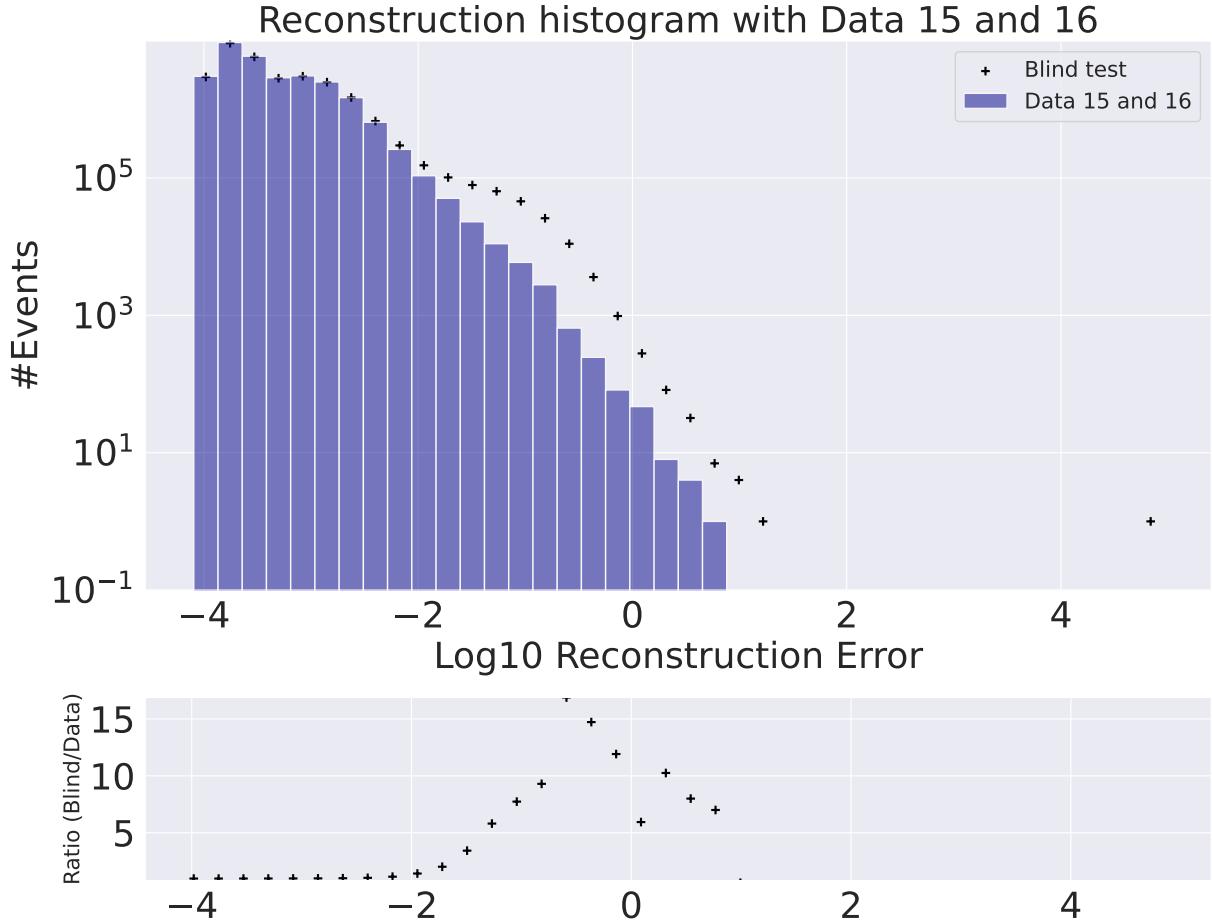


Figure 4.25: Reconstruction error for the blind test. The blue histogram is the ATLAS data 15 and data 16 sample and the black crosses are the ATLAS data mixed with BSM samples. Between a reconstruction error of 10^{-2} and $10^{0.5}$ there is a separation of the peaks of the two distributions. The biggest difference is a ratio difference of around 15.

In figure 4.25 the reconstruction error for the blind test is shown. The ratio subplot beneath the histogram shows the reconstruction error discrepancy. This indicates that the autoencoder is able to distinguish between the ATLAS data 15 and data 16, and BSM samples. The highest ratio difference is around 15 between the two datasets. The ratio discrepancy is also due to event selection. The mix set contains the same events as the ATLAS data 15 and data 16 sample set, but has around 1.6 million ATLAS events removed and replaced with BSM events. It appears that a higher number of BSM signal samples than the events that were removed passed the cuts in event selection.

The model has not been changed after running inference on the blind test, and we can therefore unblind the test, and see how well the autoencoder actually did in separating out the BSM events.

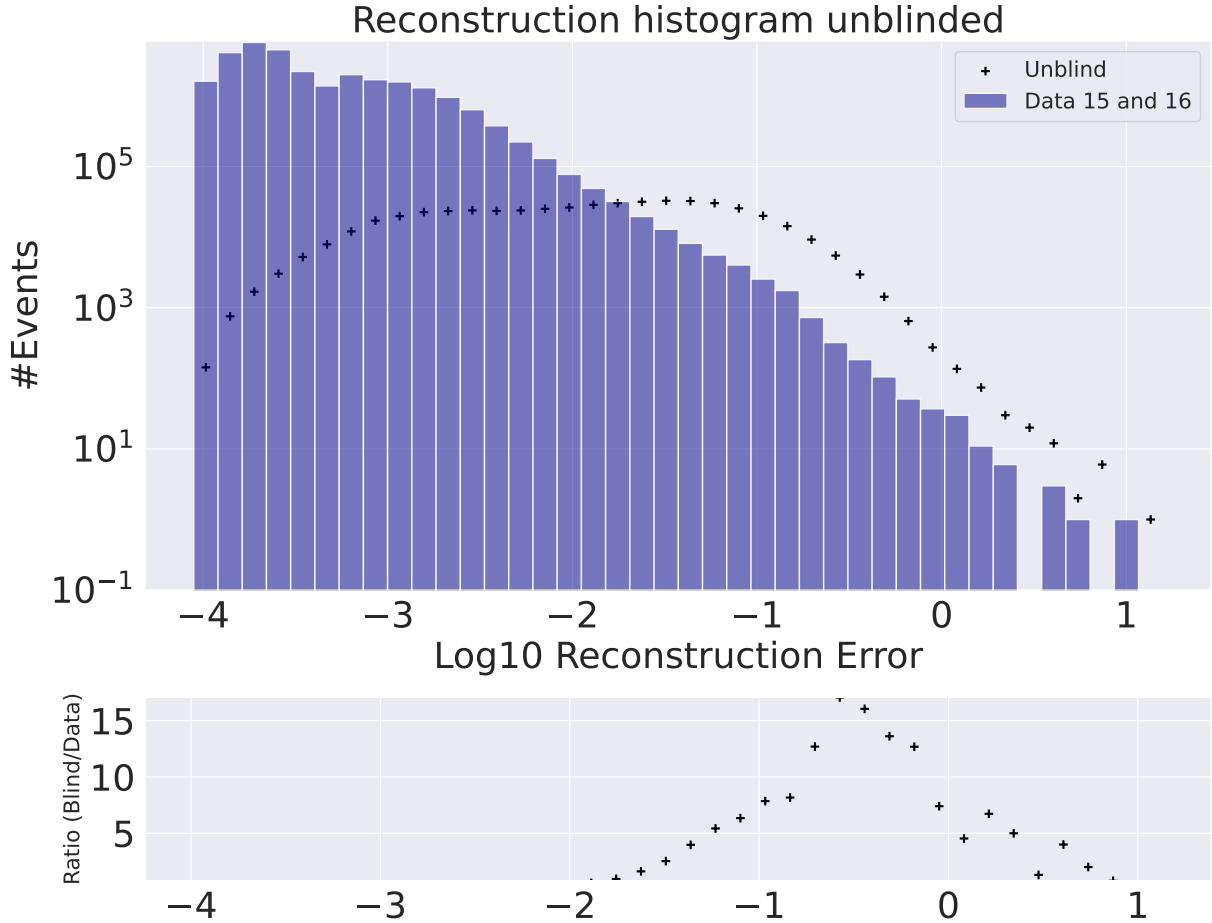


Figure 4.26: Reconstruction error for the unblind test. In the histogram the blue bins are the ATLAS data 15 and data 16 samples from the mix dataset and the black crosses are the BSM samples with the legend "Unblind". Between a reconstruction error of 10^{-2} and $10^{0.5}$ there is a separation of peaks of the two distributions. The biggest difference is a ratio difference of around 15.

In figure 4.26 the reconstruction error distributions for both ATLAS data 15 and data 16 samples, and BSM signals samples are shown. Although some samples have low reconstruction error, the peak is between 10^{-2} and $10^{0.5}$ reconstruction error. The hishget ratio discrepancy is around 15 between the two distributions, and it is shown to be in the same area of the peak.

4.5 Final remarks on the results

In sections 4.1, 4.2, 4.3 and 4.4 the performance of the regular and variational autoencoder with respect to usage in BSM searches has been shown through various tests. The final remarks can be summed up in five points:

- Shape of SM MC reconstruction error distribution
- Dataset altering testing
- Megaset changes
- Network architecture
- Blind tests

First, it appears that the shape of the reconstruction error is more sensitive to the choice between variational and regular autoencoder than it is to the number of training samples it uses. However, the steepness of the shape in the case of the regular autoencoder increases with the increase of training data. From this obervation it is reasonable to assume that to increase the ability of the autoencoder to perform, one needs large amounts of training samples. This is also shown in the case of the variational autoencoder, where if one

increases the amount of training data by going from the 3 lepton + e_T^{miss} case to the 2 lepton + e_T^{miss} case we observe the peak to move more to the left end of the reconstruction error distribution. It was not well investigated why the outputs of the two models are so different, but one reason could be that the decoder that samples from the latent space distribution in the variational autoencoder needs even more training data to get good separation.

Secondly, with the increase in training data it would be interesting to do the "altering p_T " test, as well as some other SM MC altering tests with especially the regular autoencoder. Based on the signal tests and the "altering p_T " test done with the 3 lepton + e_T^{miss} trained regular autoencoder, it is reasonable that the autoencoder would perform even better. Other tests could for example be to swap certain features in the RMM in order to create unphysical events, or swap events from one decay channel with another in order to create unphysical events. Essentially, by making these anomalous events and testing the autoencoder, one would get a better picture on the reach and ability of the autoencoder. This is of importance given the fact that the target signal or signals could in theory look very strange or perhaps in some feature space very similar to the SM MC.

A third point to note is in regard to the megaset training done in the 2 lepton + e_T^{miss} case. An arbitrary choice of 10 megasets were chosen, but it might be better to choose a larger or smaller number of megasets²¹, and that might have an impact on how well the autoencoders learn the SM signatures. A key criterion to uphold when doing that training is to ensure that the megasets, when sampled, all maintain the natural distribution of the entire training set and thus the SM. If not, the algorithm will learn with a bias that is not constructive.

The fourth point to draw from the results are that it appears that the results are not too sensitive to the architecture of the networks. The two different architectures chosen were one model with only a latent space layer between the input and output layer, and a model with three layers on each side of the latent space. The choice of layers and nodes per layer was somewhat arbitrary, and after inference it was also clear that really only the latent space was sensitive to change with respect to performance in reconstruction error. This is though more related to the size of the input layer and the complexity of the data, more than the number of events in the training and test set.

The fifth point is in regard to the blind test done with the 2 lepton + e_T^{miss} trained deep autoencoder. This test was done in order to see if the autoencoder could pick up on signals mixed with SM events in ATLAS data. From the results in section ?? it appears that the autoencoder is able to some extent separate out BSM signals. This indicates that there might be use for this search method and therefore more to learn about the autoencoders. Further in-depth research into the method should be done to figure out its usefulness in high energy physics research.

4.6 Challenges with the search method and tools

In the previous sections, the output and results of using the autoencoder for anomaly detection have been shown. The method and results, as produced and shown in this thesis, have yielded some promising results given the nature of the search method. However, it should be known what the challenges of the task actually are to truly understand why the results are only promising, and not great compared to other search methods. The challenges can be divided into three main points, all of which are entangled together. The three challenges are listed below.

- Model independence
- Reconstruction error minimization
- Feature engineering

Model independence is the first challenge. By model, it is here referring to signal models.

As mentioned in the theory section for the SM, the SM, although very successful in certain predictions, lack the ability to explain a whole number of behavior around us, and so there have been made many suggested solutions to the issues. These new models are often called extensions to the SM, and although mathematically consistent, not necessarily physically possible. And even if they are physically possible, in other words, they adhere to certain fundamental physical principles, they still might not exist, as several searches at ATLAS have excluded but never found any new physics.

²¹As the total amount of events would be the same, the difference with using say 20 megasets would be faster loading and writing time. The batchsize for a given training session with a batch would still be the same.

The search method is inherently biased as one assumes that the new physics looks like the signal, and thus do analysis, data preparation etc. with that signal in mind. But we do not know, at all, what the new physics looks like, even the assumption that we are looking for particles are implying a bias that might not be true. From the collisions in the detector to the analysis, there are biased decisions, we cannot avoid them, but we can minimize them as much as possible, which is a goal with the search strategy in this thesis.

This leads us to the second challenge, which is reconstruction error minimization. The proposed method in this thesis is to learn the signature of the SM so well, that even subtle anomalous behavior will be picked up by the analysis tool. The autoencoder learns the signature of the SM via reconstruction error minimization, and then hopefully the anomalous data will be picked up in a signal region. One problem with this is that one first blinds oneself to signals that might be very, very similar to the SM in some feature space, but with very low statistics. These events will for a given set of features, never be found.

The third challenge is the choice of features. This thesis utilized the RMM structure by Chekanov et al., as it maximizes the amount of information in the input data by using almost completely uncorrelated features. However, as we do not know the signals we are looking for, there is no way to know if this choice is the optimal choice for new physics. In fact, even if we found an ideal set of features, based on some physical principles or something else, it is not trivial that the reconstruction error calculation should weight the error of each feature equally. It might very well be that some features are less important than others. Essentially, the goal is to optimize for a signal we do not know, using features we don't know are optimal, and weighting them as "unbiased" as possible, simply taking the average, to dictate how the autoencoder learns and updates its internal weights and biases.

4.7 Future work

Autoencoders and their applications to anomaly detection in high energy physics are not well understood, and this thesis has scraped on some issues and attempts that needs to be done. It is a recent topic in within the HEP community, and consequently much work is needed to reach a better understanding of how autoencoders behave with HEP data. The work done in this thesis has led to three areas of focus that should be explored more, listed below.

- Computational bottlenecks
- Data and feature engineering
- Network and architecture engineering

Computational bottlenecks

From sections 4.2 and 4.3 there seems to be a positive trend in increasing the amount of training data for the autoencoders, both regular and variational. With a continual increase in data from Run3 and onward [45], so will the loading and storing time used for doing analyses increase.

Figure 4.27: LHC nominal luminosity projections for the next 2 decades

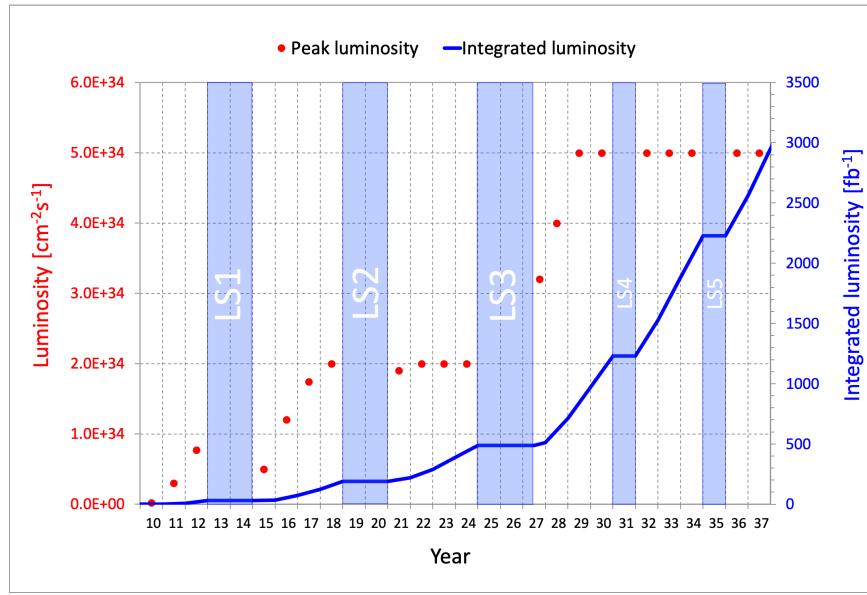


Figure 4.27 shows the expected time periods for data collection and the amount of data expected for the next two decades.

One bottleneck²² that was discovered during the work in this thesis was the use of Pandas pre the 2.0 version release, which is written on top of NumPy. Although Pandas has many very useful features and is the industry standard for data analysis and feature engineering, it is somewhat slow. NumPy is not parallelized, thus all operations are done in serial. Polars has proven useful as a replacement. Though in its early stages still, it unlike Pandas has a Rust backend, which natively parallelizes. Thus, if one works with rather large datasets one should use Polars, or some other parallelized tool. Another tool used for training and inference was to store training and test data post-processing in numpy arrays such that one can just load them up. NumPy makes this very simple, but as mentioned above it is serial in its execution and thus takes long time for large arrays. In the 2 lepton case the clear bottleneck both in processing of the training and testing data, as well as inference and training of the models, was the loading and storing time using NumPy's load and save functions. Sadly there is not much one can do per now as NumPy's load and save functions are the fastest, provided one has a lot of storage available. This can also be generalised to number of conversion steps from ROOT files to an useable python format. In the future this might be better incorporated in ROOT such that many conversion steps are not needed.

Another bottleneck is computation time of training and inference. There is a continuing battle between speed and accuracy in terms of choosing an appropriate batchsize. The choice of batchsize for this thesis is 8192. It is common to choose a batchsize that is a multiple of two, as this is most optimized for GPU's. 8192 is 2^{13} , and it a rather large batchsize. Although this allows for epoch training time to be as low as less than 2 minutes for 2 lepton case and less than 1 minute for 3 lepton case, it does decrease the model's ability to learn more about the dataset[11]. With better and faster equipment this could be improved whilst decreasing the batchsize.

Data and feature engineering

Scaling

One aspect that was not explored in this thesis is the choice of scaling for the data. The choice used for this thesis was the MinMax scaling algorithm from Sci-kit learn. From previous work done on the ATLAS Open data [46] it appeared that MinMax was better for overall accuracy than Standard scaling. Still, it should be looked at and more understood why this is or is not the case for the Run2 dataset used in this thesis.

Interpretation and possible feature changes

This thesis used the Rapidity-Mass matrix described by Chekanov[30] as features in the dataset. Whilst containing features that are very uncorrelated it creates a feature signature that could be used by the

²²The bottleneck problem explained here is not in regard to the recording of the events. It is rather in the amount of data the analysis tools have to ingest. Figure 4.27 is used as a tool to illustrate the amount that will have to be ingested.

autoencoder to learn underlying structures in the SM. There are however some aspects to discuss. First, every nonexisting entry in the RMM for a given event is replaced with a zero value. This creates "islands" in the RMM structure which contributes to create the signatures for the events. It is however not clear how these zero values propagate through the network, and how they affect the performance and really the autoencoder's ability to learn the underlying structures in the SM. In cases where one uses tools like decision trees, this is not an issue, as they can just remove the feature if it holds a certain value, but as we need a tabular and rectangular shape to do the matrix multiplication that is neural network feed forwarding and backpropagation, a value has to be put in the missing entries, and it is not obvious or known what the choice of using zeros does.

Another choice to consider is the amount of particles in the RMM. This thesis tried allowing for 5 electrons and 5 muons, and 6 b- and ljets, yeilding a total of 529 elements in the RMM. This choice was an arbitrary one, but it is not unreasonable to think that an even larger RMM would be more beneficial, as it contains more information. Some events might have even more jets in them, or leptons. But with a larger RMM comes a larger amount of zero valued features as well. And also, with a larger RMM, the memory needed for a given array increases, which in the case of the 2 lepton case, would mean more megasets of smaller size. The computation time, from event selection and conversion from Rdataframe to Numpy, and training and inference, would increase a lot. A third point to make is that the RMM alone might not be the ideal set of features. It would be interesting to test a combination of RMM and some other features, were we remove some of the features that are on average are zero and replace them with other useful information. If the goal is to learn the autoencoders the signature of the SM, then it is not unreasonable to assume that more specific information would be better. It should be better understood what it means to learn the signature of a channel, and of the SM as a whole.

Architecture engineering

The regular autoencoder appears to provide a better anomaly detection performance than the variational autoencoder. The architecture is somewhat simple, given the hard task it is meant to perform. It might be possible to add some more complex layer structures like CNN autoencoders or PCA to make a more complicated and better performing network architecture. This is of course only speculation, and was not investigated much in depth. General trends were found to vary depending on the size of the dataset, and it is not trivial that for example a deep neural network is beneficial as the training sample increases. What was important though was to ensure that the latent space was large enough to store enough information for the decoder. In the early attempts the latent space were set between 10 and 50 nodes, which was too little for the encoded information to be useful. As there is no clear way to find the optimal architecture, an educated guess on the number of nodes were done. In theory, one can create a tunable network where the number of layers and nodes in each layer are hyperparameters, but the sheer number of combinations would lead to much longer computation time than what was available during this thesis. Tools like Keras-Tuner could facilitate this search, but if this were a PhD thesis or a long term research project it would be benefitial with more significant hardware or a more rigorous way to set an optimal architecture.

Another point to think about is how the autoencoder is trained. As explained in section 1.3 the autoencoder is trained by how well it manages to reconstruct the input data. This is done by calculating the error of each feature for a given event, and averaging the error for all features. This has its pros and cons, and should be investigated further. Suppose one has an RMM which is very sparse, with 10 bjets, 10 ljets, 10 electrons, 10 muons, and 10 photons, i.e a T5N10 matrix of 2601 colums and rows. In this case, one can easily assume that the RMM would be very sparse, as few if any SM events produced at the current energy level as the LHC contains that many particles. Thus, one could argue that some features are more important to learn correctly than others, and thus should be weighted more. It is however difficult to know which features that should be in focus, as the signatures for each event's might differ, and some might look completely different from one another. One way to deal with this issue is to calculate the average RMM for a given channel, and then see if there are general trends in the RMM for those channels. Then one could perhaps weigh the most used features more than the more sparse areas.

Chapter 5

Conclusion

The main goal of this thesis was to benchmark and investigate the performance and usage of autoencoders in BSM searches. The analysis and testing were done using n-tuples from ATLAS that was converted to python dataframe structures. We argued for using the Rapidity-Mass matrix as features in our input data, with 6 bjets and 6 ljets, and 6 of each lepton. The original goal was to test and understand the performance in the case where we have a 3 lepton + e_T^{miss} final state. In testing, it was shown that the performance was not too impressive, thus the choice was made to use the 2 lepton + e_T^{miss} dataset which contains much more data. Due to the large size of the total dataset, we proposed a solution where the overall distribution in the total set was conserved in smaller batches, called megasets. Several tests were devised to benchmark the autoencoders, making anomalous events by altering the p_T of standard model events and testing on two supersymmetric signal models. We showed that the autoencoders performance increased with larger training samples, but argue for more testing as these methods are not well understood yet. The performance was measured in three categories: how well it reconstructs the test dataset; how much background and signal is left in the signal region; and the significance it achieves when performing cuts in the signal region. It was shown that for the first category, the regular autoencoder is much better than the variational autoencoder, creating a reconstruction error distribution with slope like shape pushed to the lower end. In the second category the regular autoencoder is much better at reducing the background, but not that much better at increasing the amount of signal. In the third category the regular autoencoder performs better than the variational autoencoder. It was also shown that with an increase in training data, the first category was improved for both the regular autoencoder and the variational autoencoder. The final test of the autoencoder was a blind test with ATLAS data and BSM signals. It showed that the autoencoder, when trained on the 2 lepton + e_T^{miss} dataset, managed to separate out some signals from the ATLAS data. This indicates that there might be a usecase for it in more rigorous analyses at ATLAS, and should be better understood.

We also argue for future work and challenges with the method. Amongst other issues where computational bottlenecks related to writing and loading of data from training and inference. It is recommended to further investigate the RMM, as well as alter the training process by physics informed or machine learning informed choices, such as a weighted MSE. The autoencoder might perform even better with better feature engineering, and this should be of focus for futher research as well.

Appendices

Appendix A

A.1 Channel removal testing

In this section the remaining histograms for the channel removal test are shown. Each figure contains the same subfigure structure as shown in the results and discussion section.

Regular autoencoder

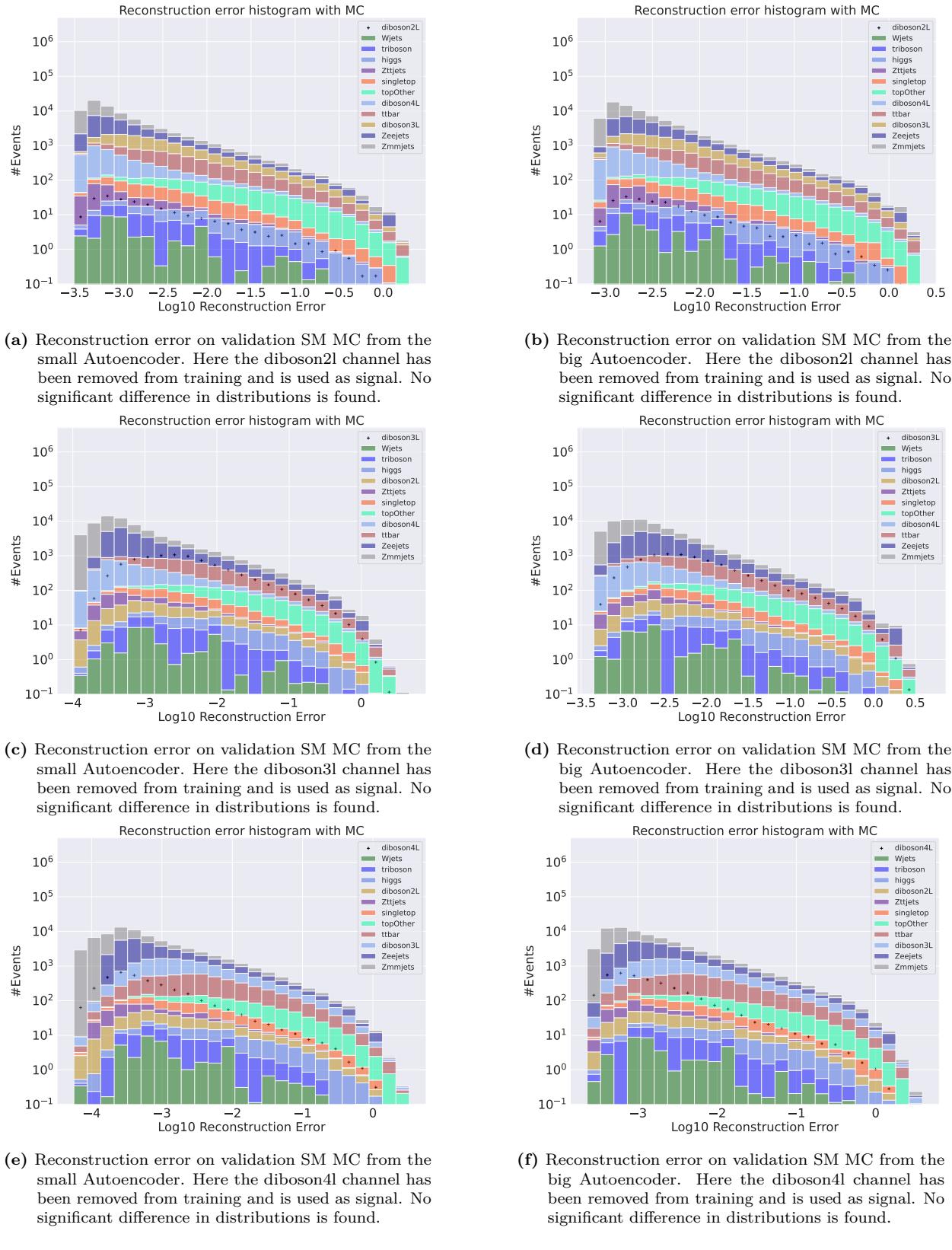


Figure 1: Reconstruction error on validation SM MC from the small and big Autoencoder. Here the diboson2L, diboson3L and diboson4L have been used for the small (left) and large (right) regular autoencoder

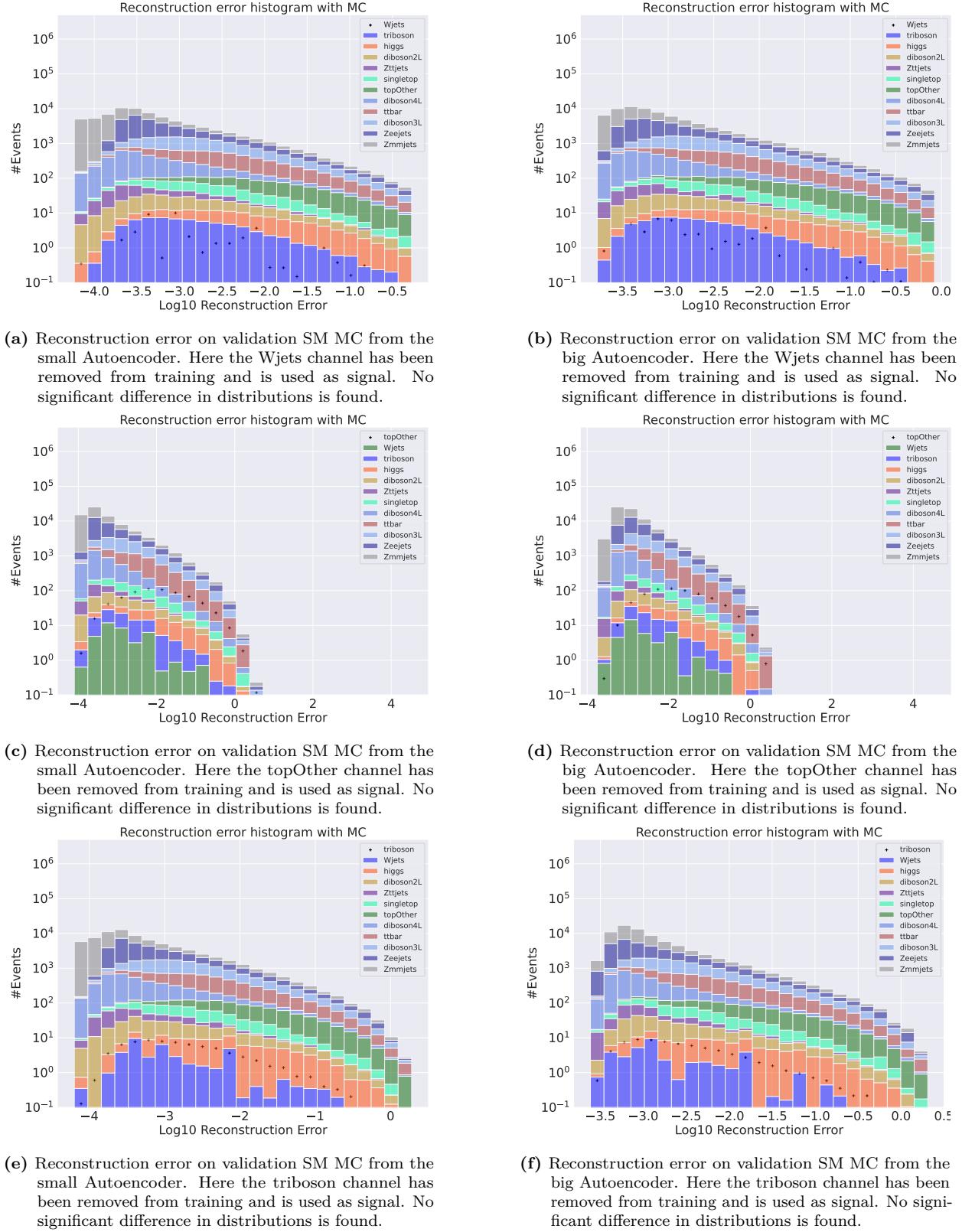


Figure 2: Reconstruction error on validation SM MC from the small and big Autoencoder. Here the Wjets, topOther and triboson have been used for the small (left) and large (right) regular autoencoder

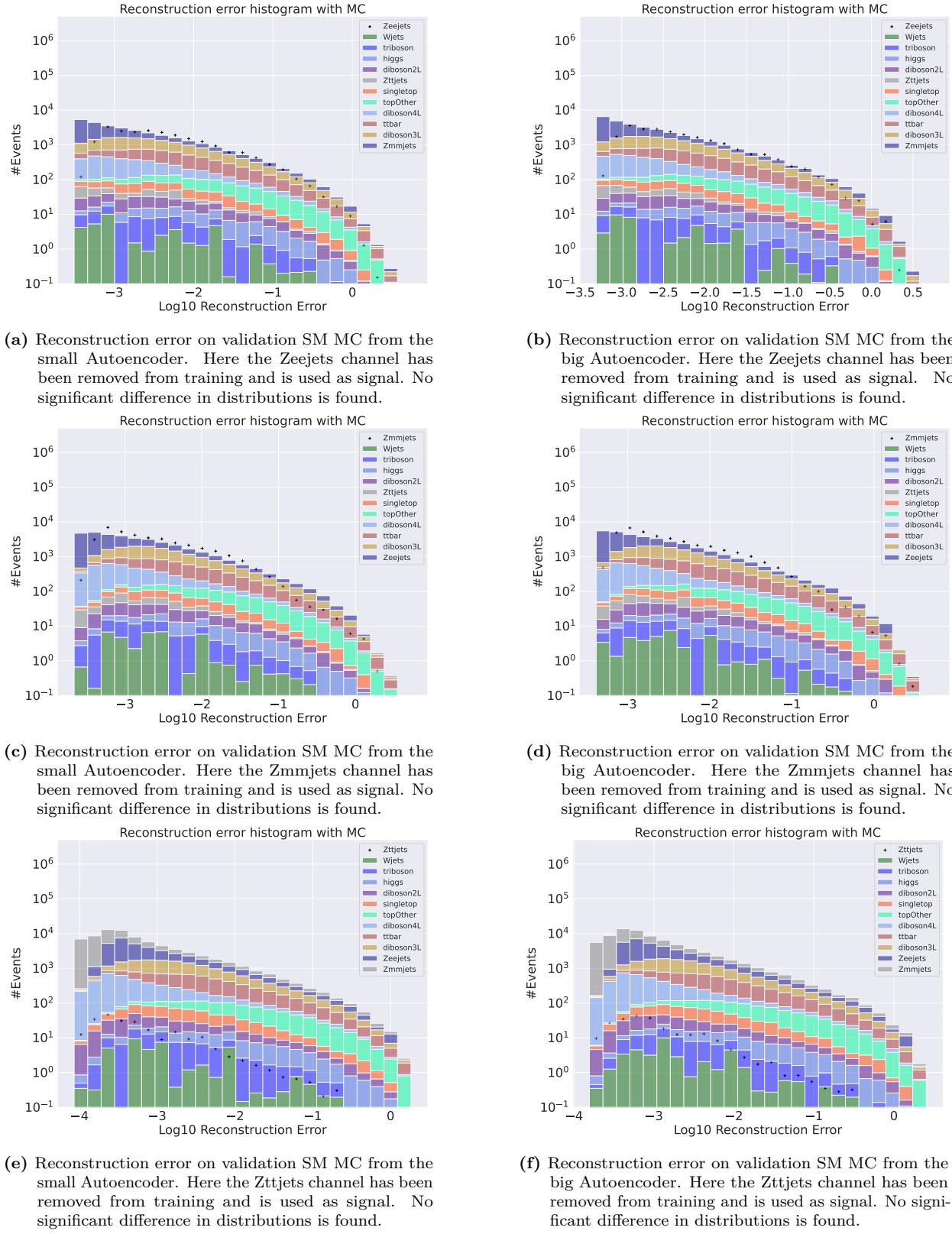


Figure 3: Reconstruction error on validation SM MC from the small and big Autoencoder. Here the Zeejets, Zmmjets and Zttjets have been used for the small (left) and large (right) regular autoencoder

Variational autoencoder

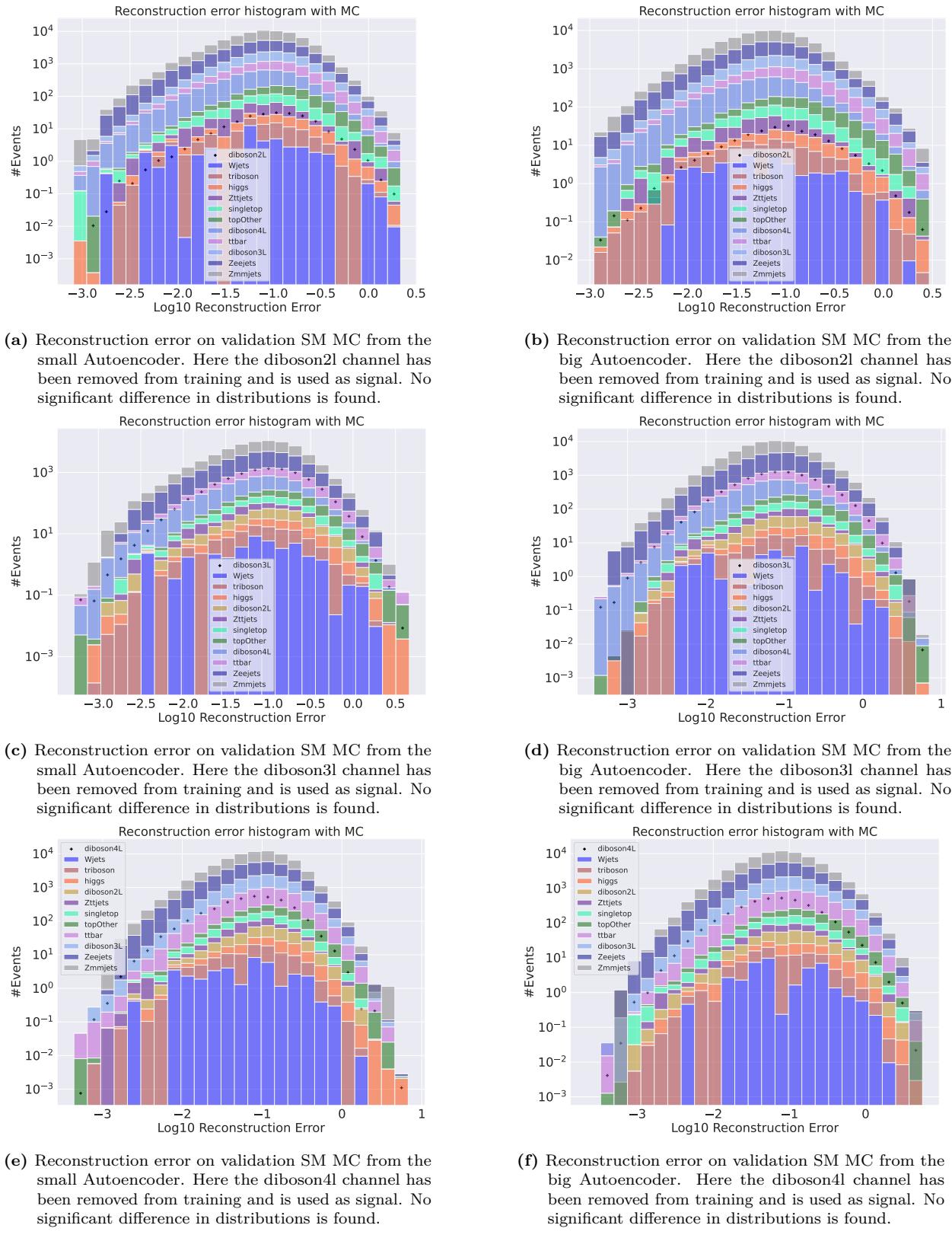


Figure 4: Reconstruction error on validation SM MC from the small and big Autoencoder. Here the diboson2l, diboson3l and diboson4l have been used for the small (left) and large (right) variational autoencoder

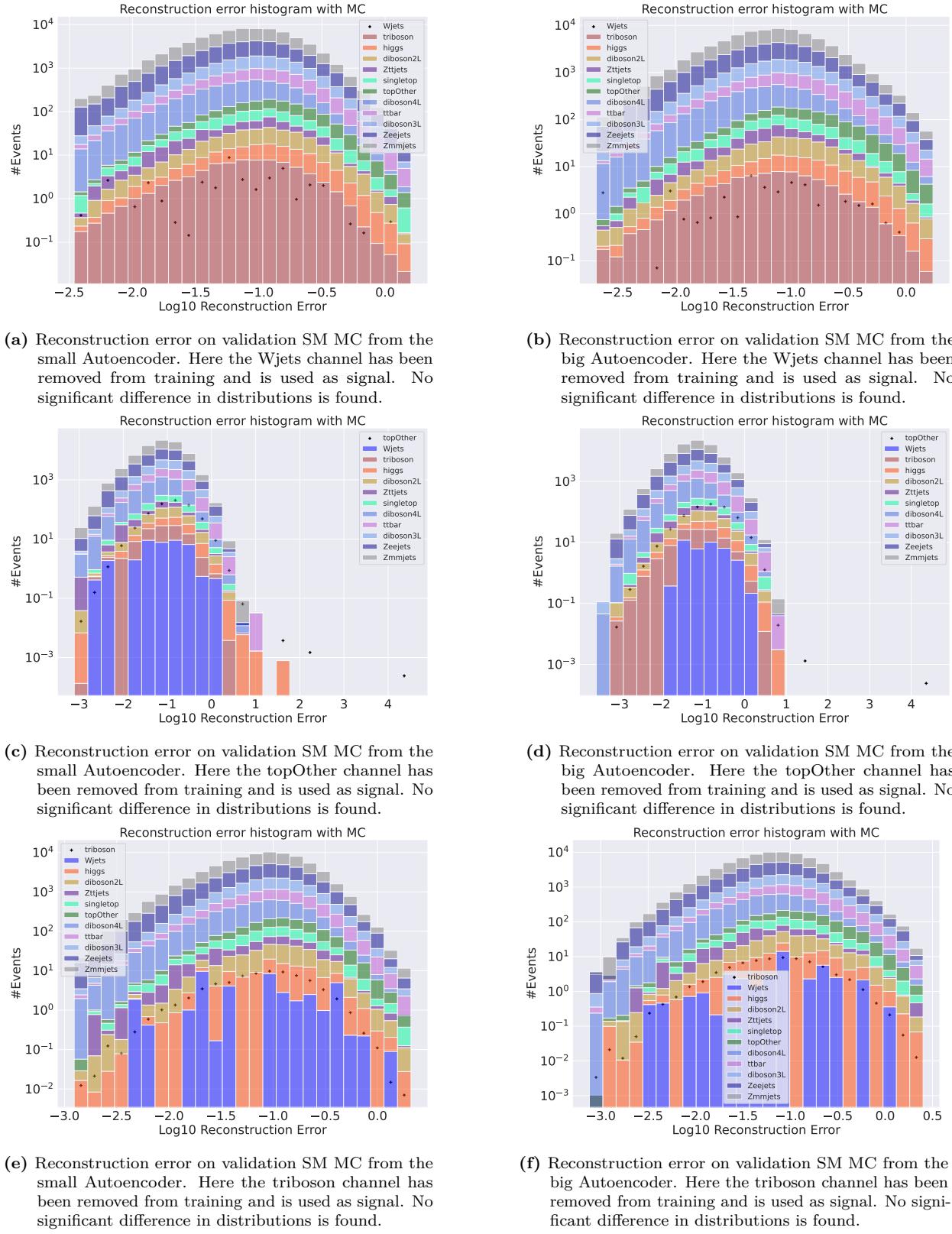


Figure 5: Reconstruction error on validation SM MC from the small and big Autoencoder. Here the Wjets, topOther and triboson have been used for the small (left) and large (right) variational autoencoder

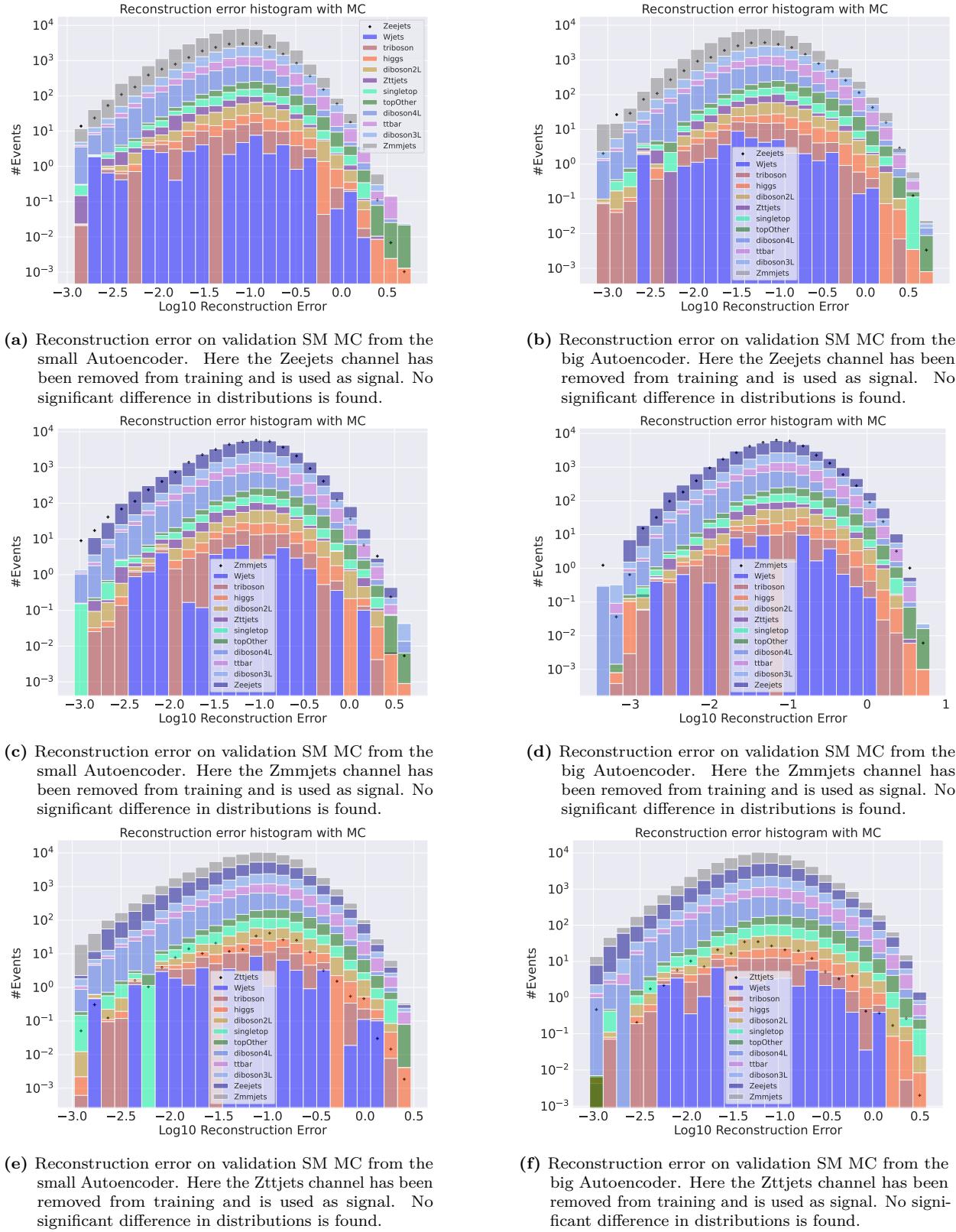


Figure 6: Reconstruction error on validation SM MC from the small and big Autoencoder. Here the Zeejets, Zmmjets and Zttjets have been used for the small (left) and large (right) variational autoencoder

A.2 Transverse momentum altering

Regular autoencoder output

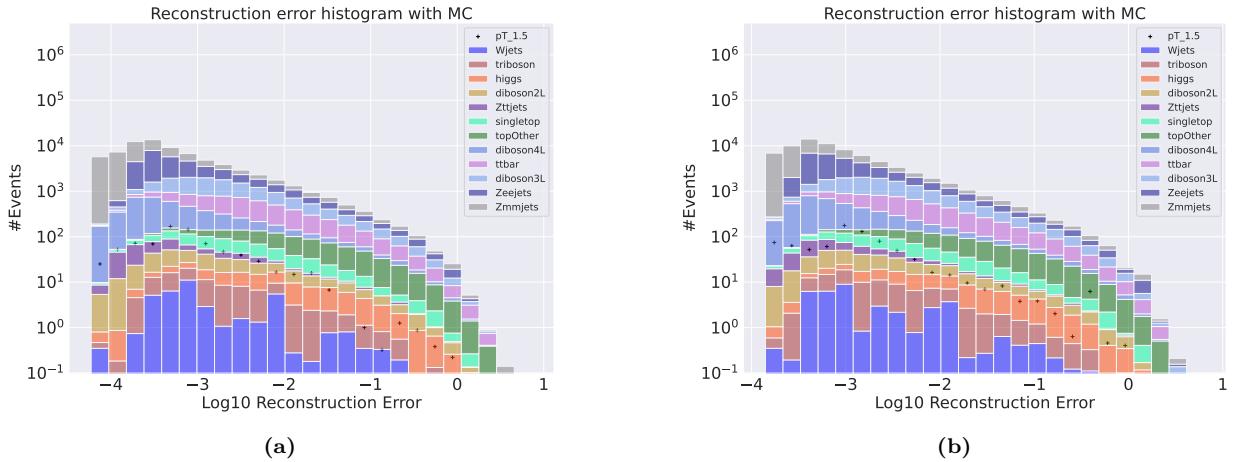


Figure 7: Reconstruction error on validation SM MC from the small (a) and large (b) regular autoencoder. The signal is a subsample of the validation set where the transverse momentum of the first electron and the first muon has been increased with a scale of 1.5. The change of transverse energy has also been changed according to the scaling of transverse momentum. A small peak is found around $10^{-3.3}$.

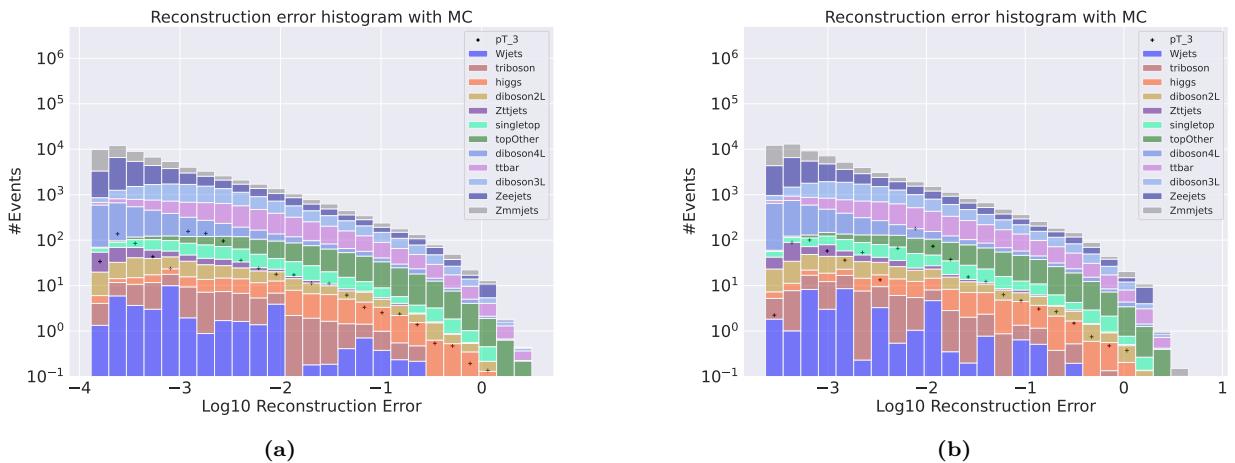


Figure 8: Reconstruction error on validation SM MC from the small (a) and large (b) regular autoencoder. The signal is a subsample of the validation set where the transverse momentum of the first electron and the first muon has been increased with a scale of 3. The change of transverse energy has also been changed according to the scaling of transverse momentum. A small peak is found around $10^{-2.8}$.

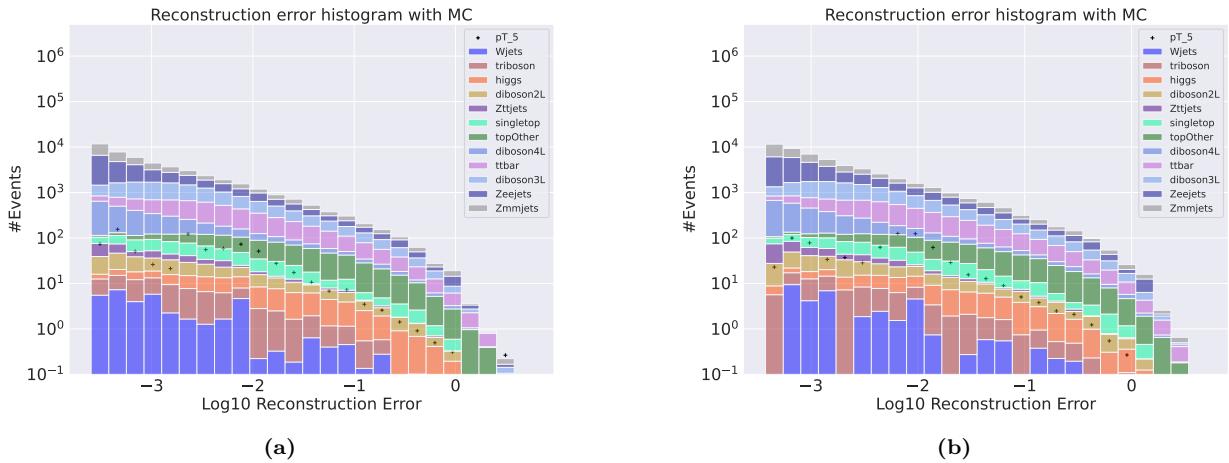


Figure 9: Reconstruction error on validation SM MC from the small (a) and large (b) regular autoencoder. The signal is a subsample of the validation set where the transverse momentum of the first electron and the first muon has been increased with a scale of 5. The change of transverse energy has also been changed according to the scaling of transverse momentum. A small peak is found around 10^{-2} .

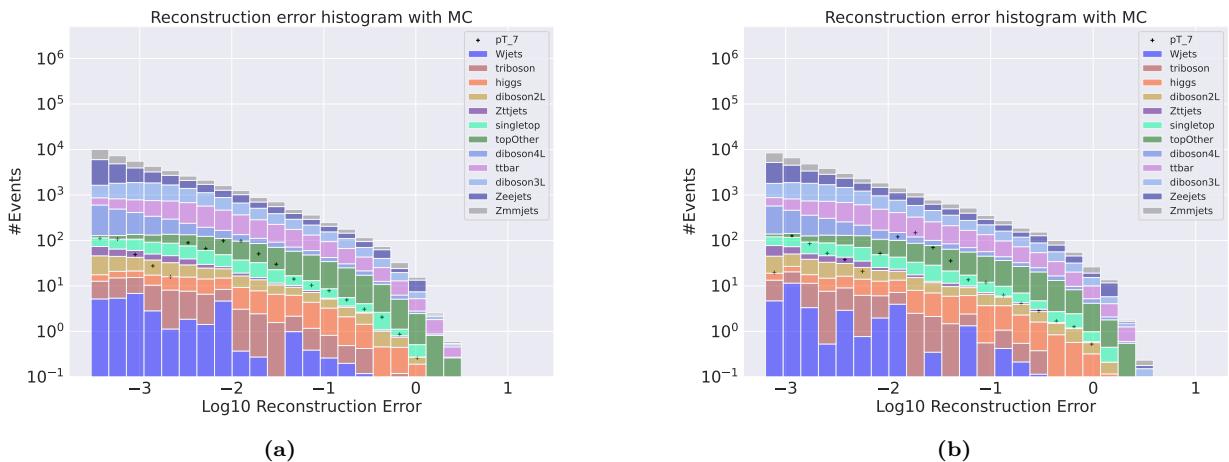


Figure 10: Reconstruction error on validation SM MC from the small (a) and large (b) regular autoencoder. The signal is a subsample of the validation set where the transverse momentum of the first electron and the first muon has been increased with a scale of 7. The change of transverse energy has also been changed according to the scaling of transverse momentum. A small peak is found around 10^{-2} .

Variational autoencoder output

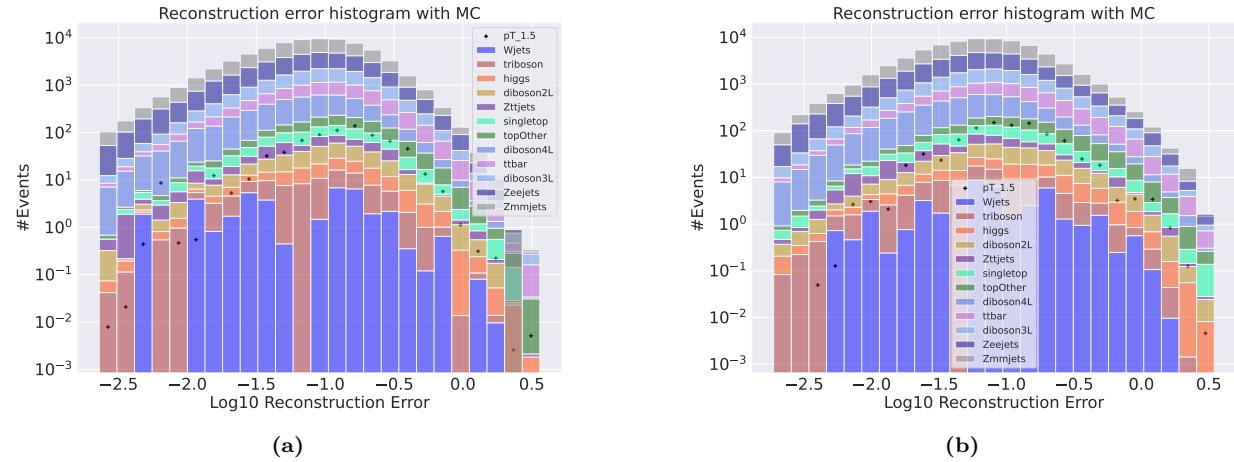


Figure 11: Reconstruction error on validation SM MC from the small (a) and large (b) variational autoencoder. The signal is a subsample of the validation set where the transverse momentum of the first electron and the first muon has been increased with a scale of 1.5. The change of transverse energy has also been changed according to the scaling of transverse momentum. A small peak is found around $10^{-0.8}$.

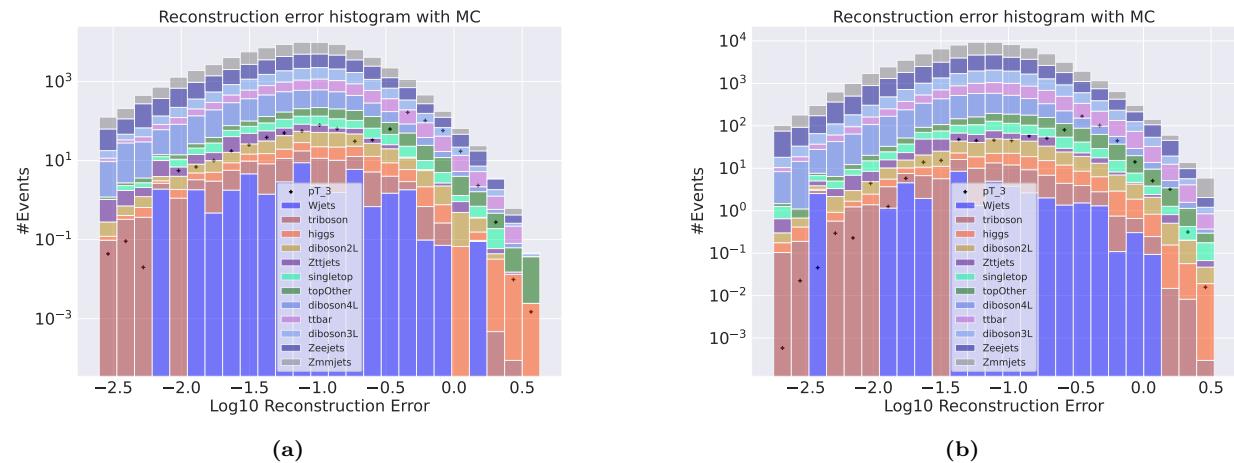


Figure 12: Reconstruction error on validation SM MC from the small (a) and large (b) variational autoencoder. The signal is a subsample of the validation set where the transverse momentum of the first electron and the first muon has been increased with a scale of 3. The change of transverse energy has also been changed according to the scaling of transverse momentum. A small peak is found around $10^{-0.5}$.

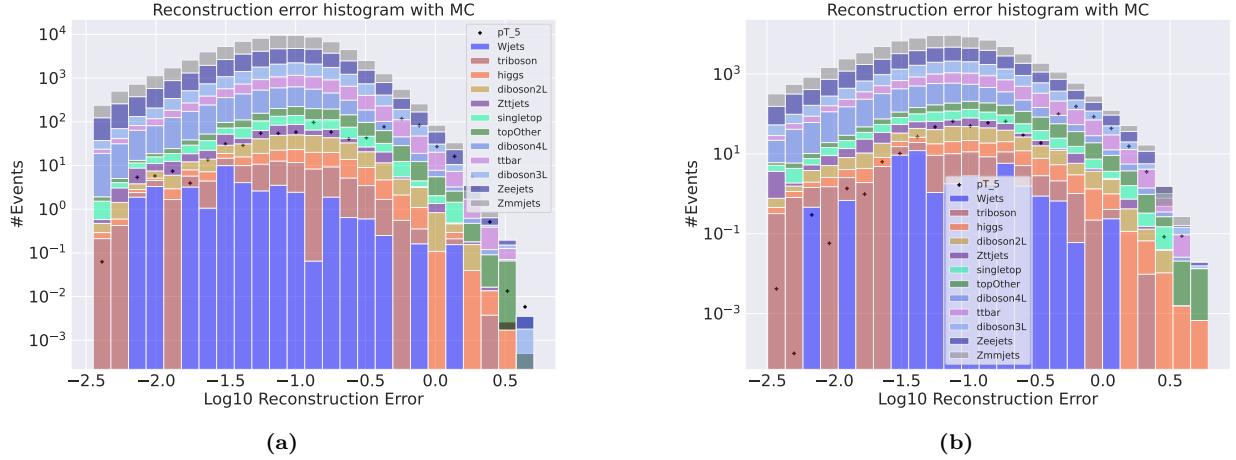


Figure 13: Reconstruction error on validation SM MC from the small (a) and large (b) variational autoencoder. The signal is a subsample of the validation set where the transverse momentum of the first electron and the first muon has been increased with a scale of 5. The change of transverse energy has also been changed according to the scaling of transverse momentum. A small peak is found around $10^{-0.3}$.

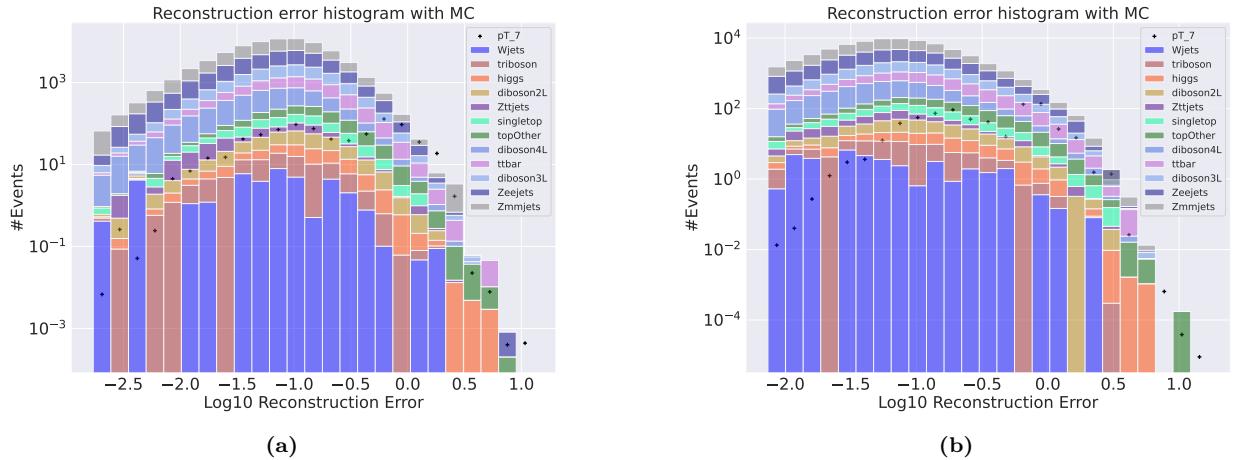


Figure 14: Reconstruction error on validation SM MC from the small (a) and large (b) variational autoencoder. The signal is a subsample of the validation set where the transverse momentum of the first electron and the first muon has been increased with a scale of 7. The change of transverse energy has also been changed according to the scaling of transverse momentum. A small peak is found around $10^{-0.3}$.

A.3 Reconstruction error cuts for 3 leptons + e_T^{miss}

In this section the remaining two reconstruction error cuts in the 3 lepton + e_T^{miss} are shown. The figures here are shaped with the same subfigure structure as the figures in the results and discussion section.

Regular autoencoder output

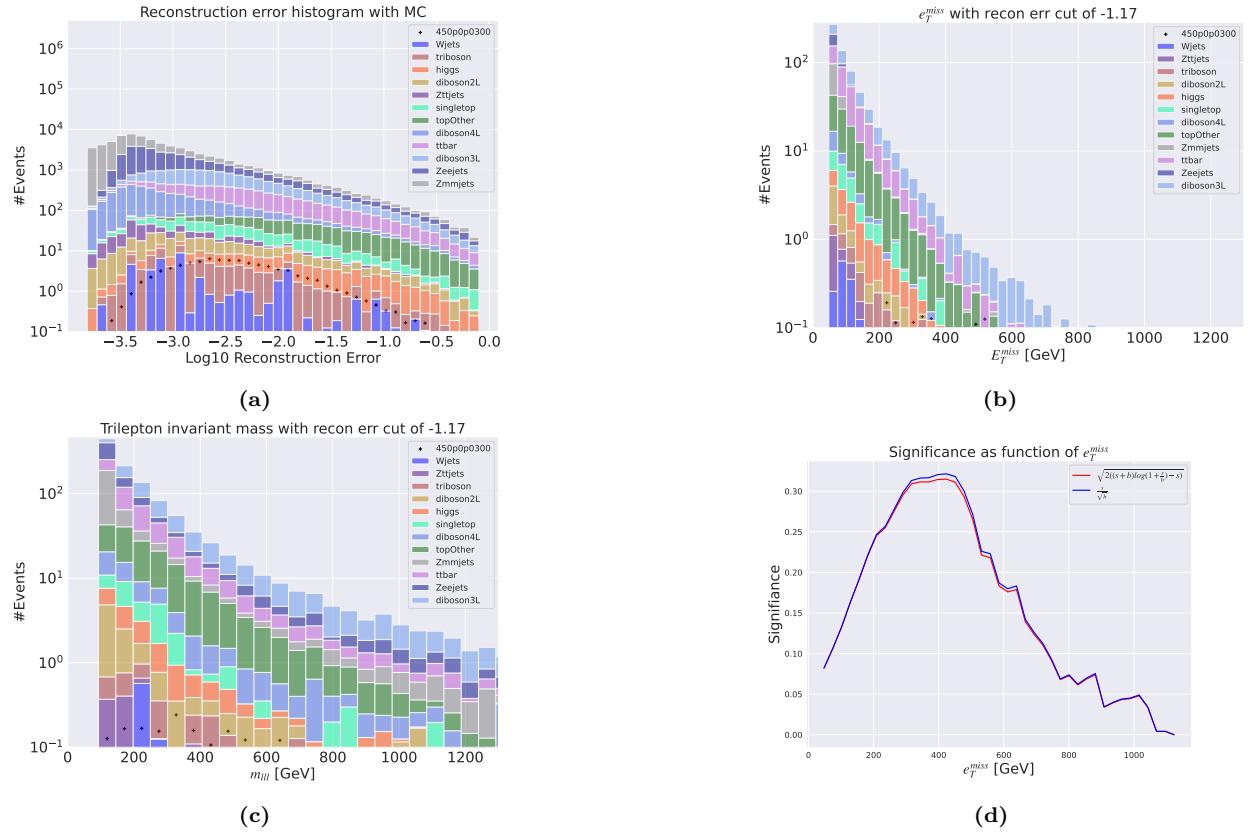


Figure 15: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the deep regular autoencoder. Here the SUSY 450p300 model is used.

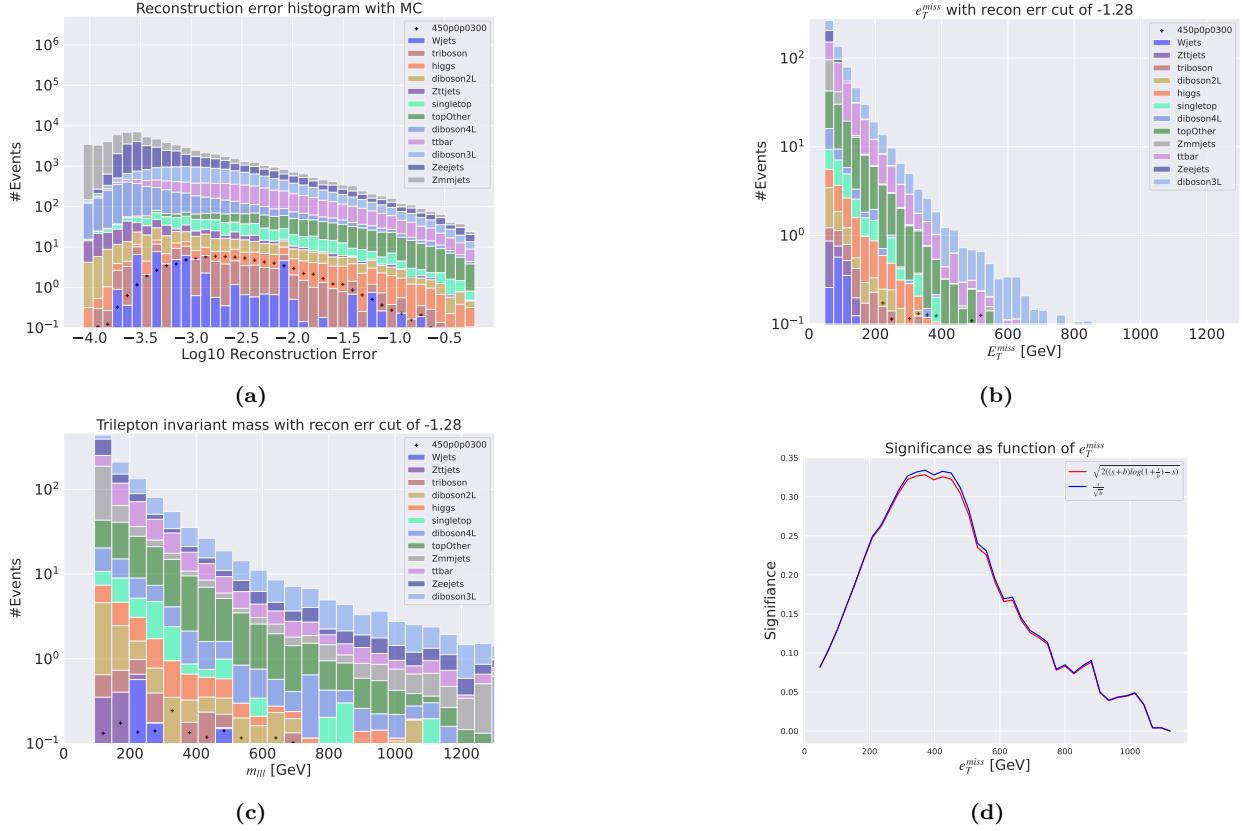


Figure 16: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the shallow regular autoencoder. Here the SUSY 450p300 model is used.

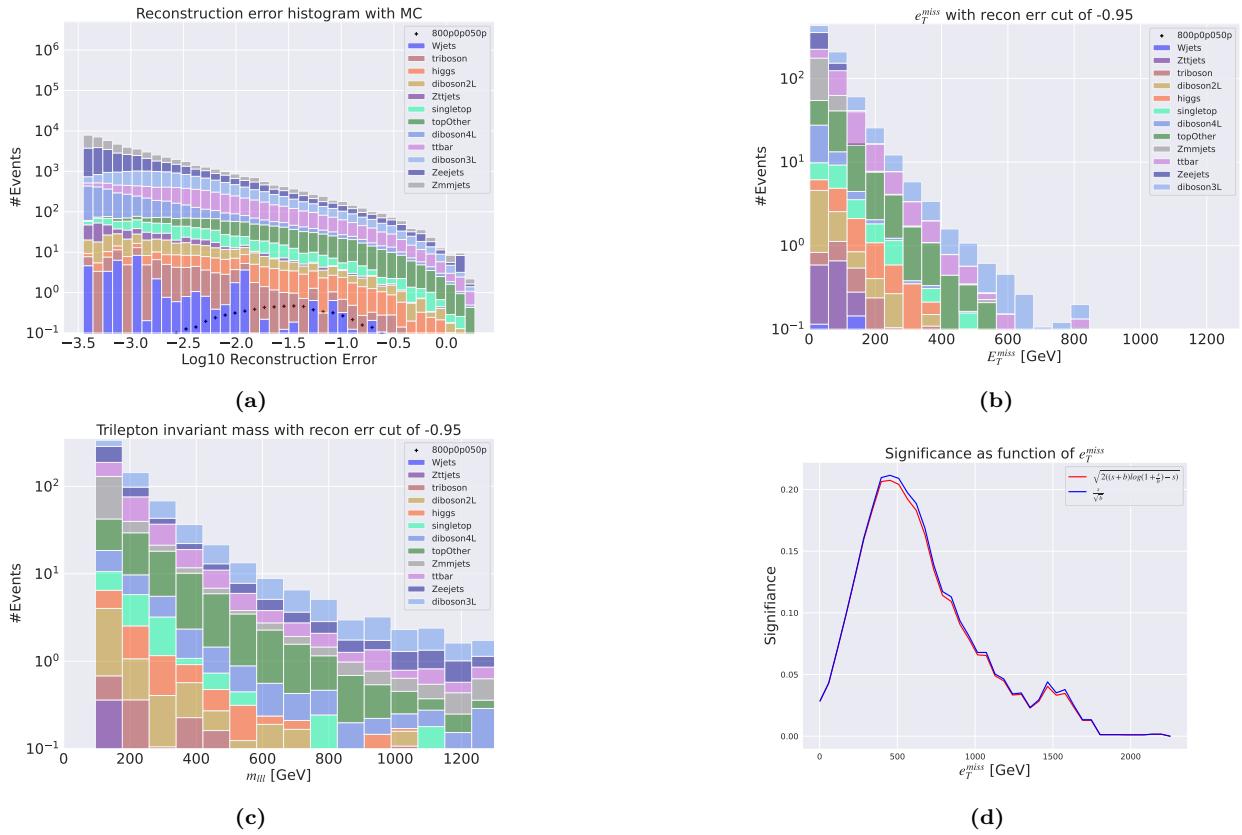


Figure 17: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the deep regular autoencoder. Here the SUSY 450p300 model is used.

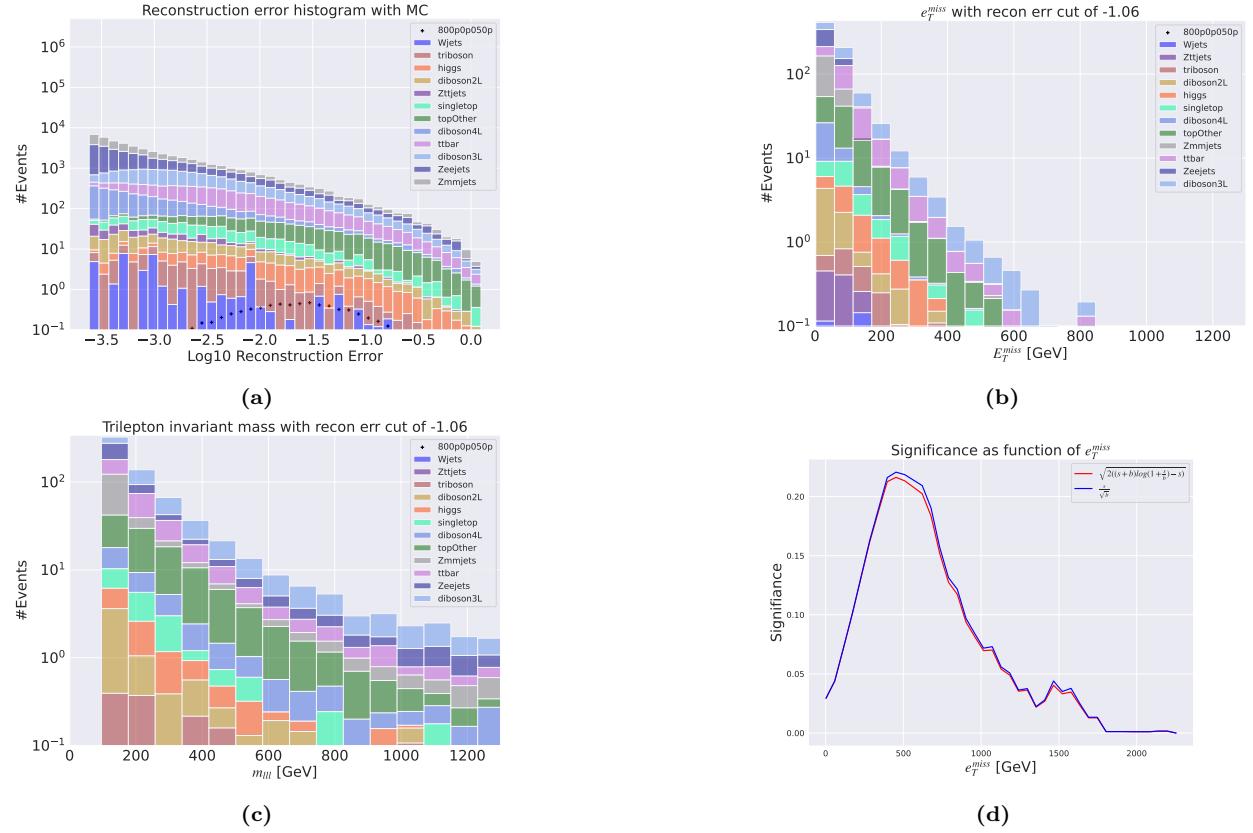


Figure 18: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the shallow regular autoencoder. Here the SUSY 450p300 model is used.

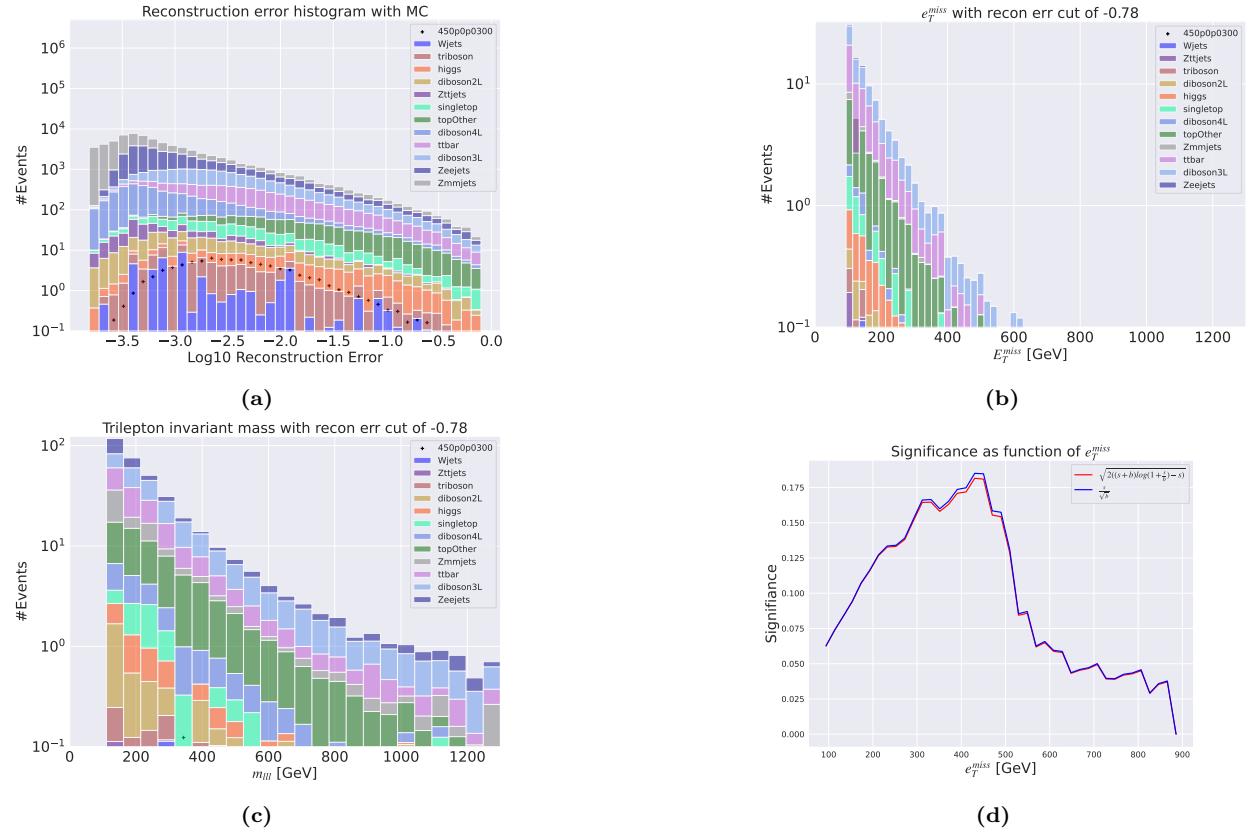


Figure 19: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the deep regular autoencoder. Here the SUSY 450p300 model is used.

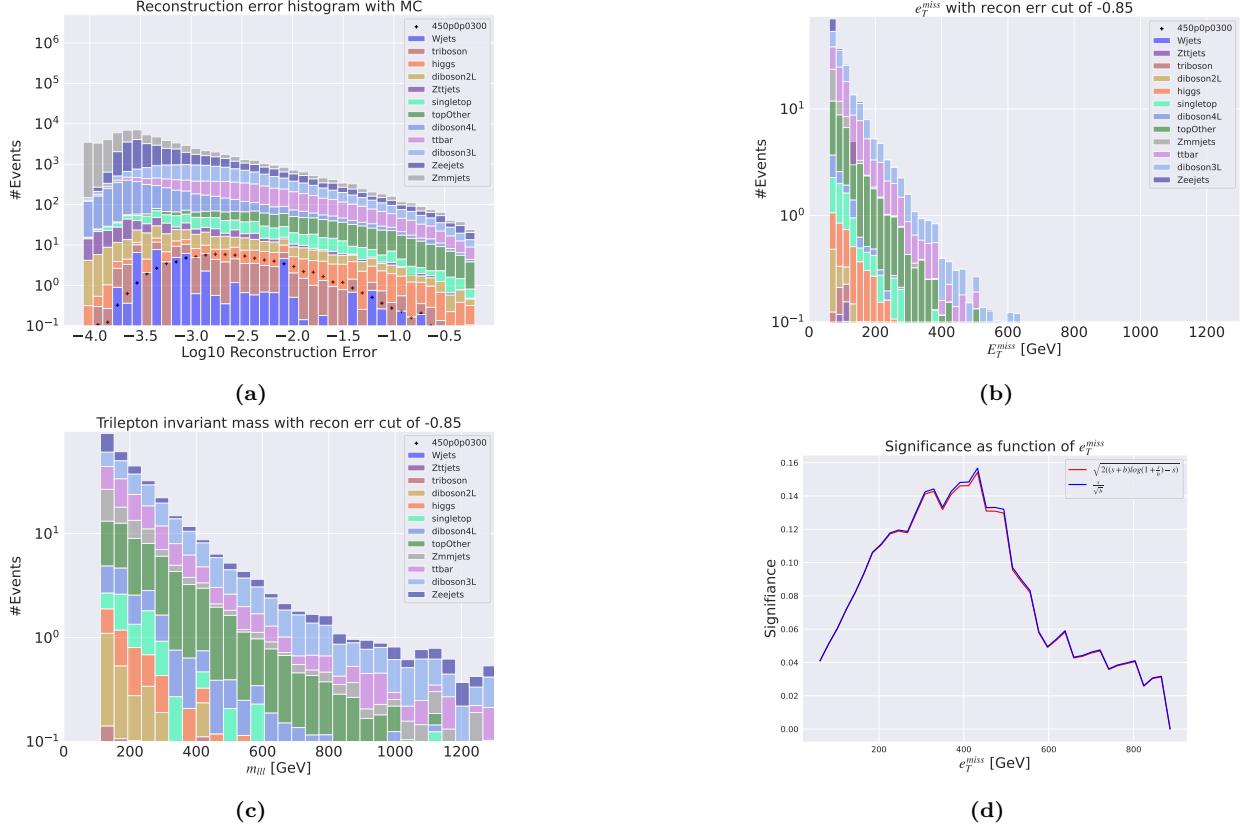


Figure 20: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the shallow regular autoencoder. Here the SUSY 450p300 model is used.

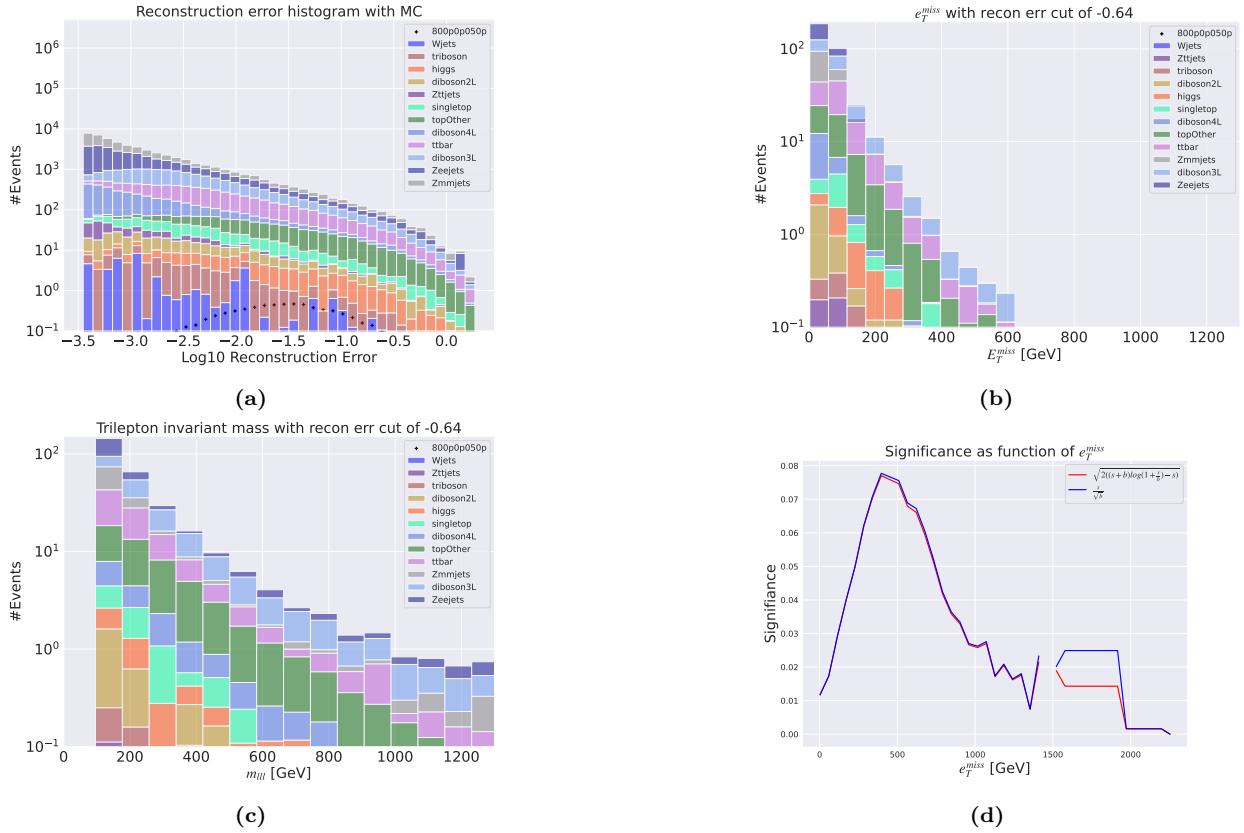


Figure 21: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the deep regular autoencoder. Here the SUSY 450p300 model is used.

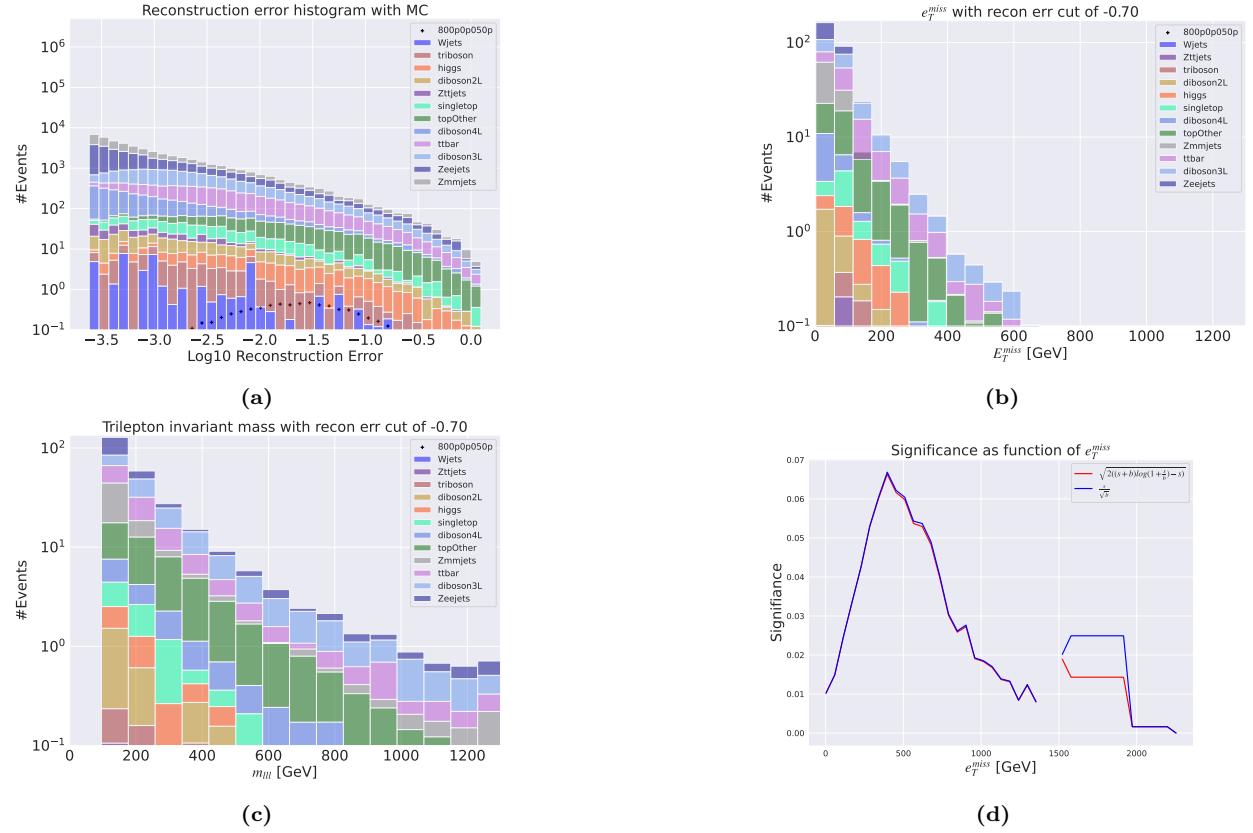


Figure 22: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the shallow regular autoencoder. Here the SUSY 450p300 model is used.

Variational autoencoder output

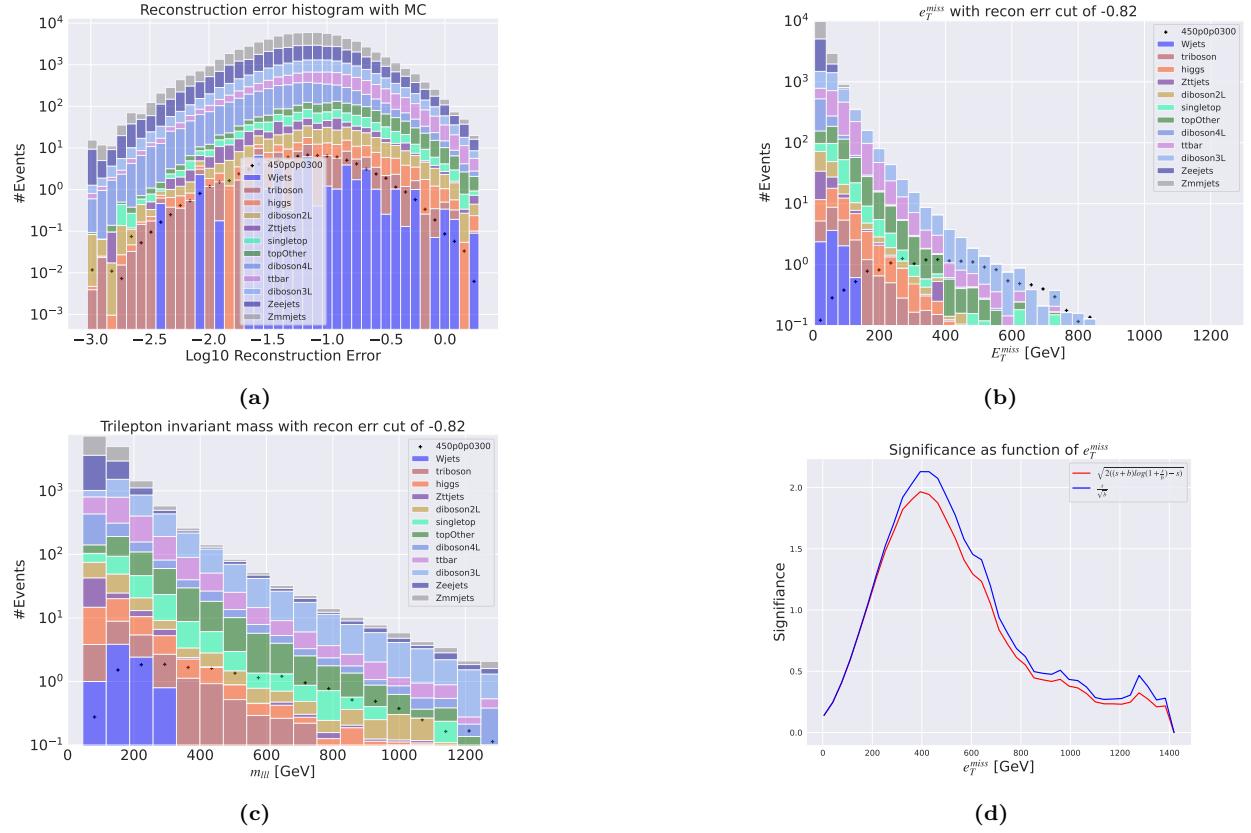


Figure 23: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the deep variational autoencoder. Here the SUSY 450p300 model is used.

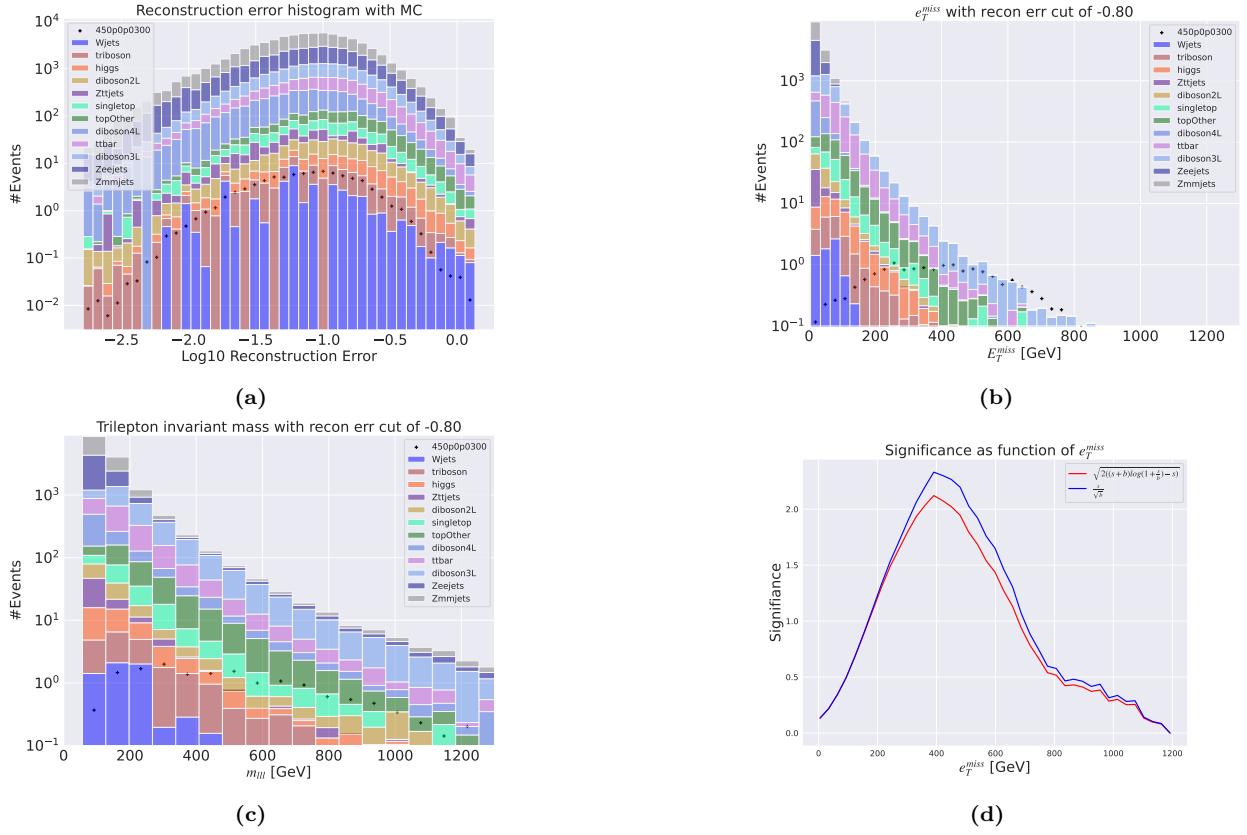


Figure 24: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the shallow variational autoencoder. Here the SUSY 450p300 model is used.

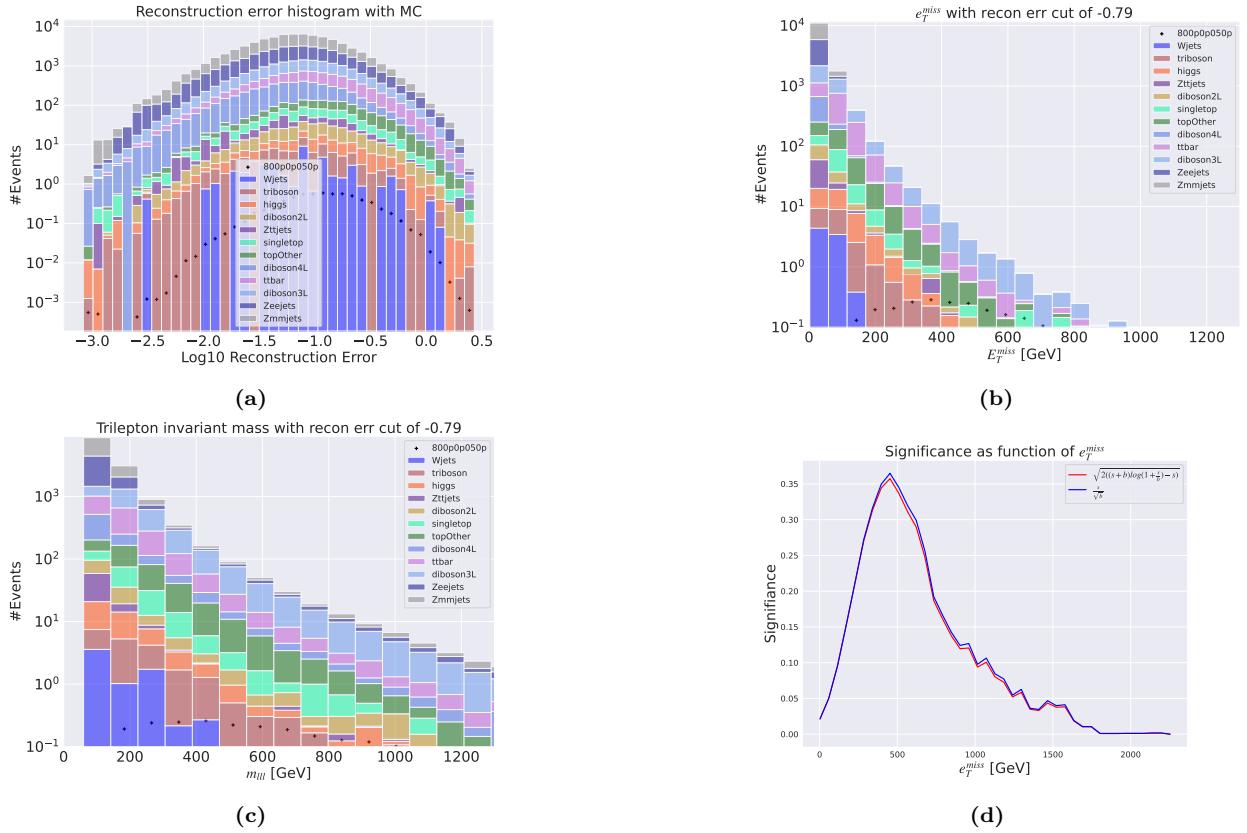


Figure 25: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the deep variational autoencoder. Here the SUSY 450p300 model is used.

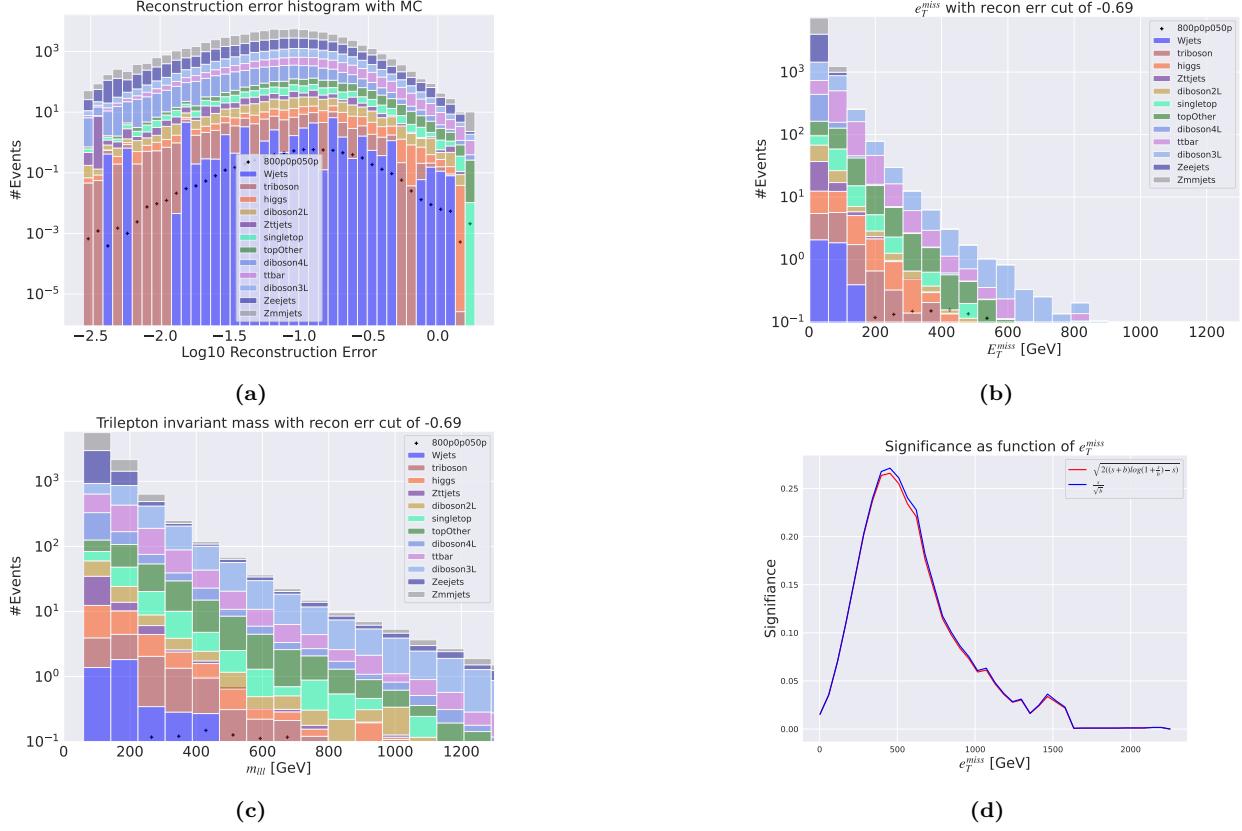


Figure 26: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the shallow variational autoencoder. Here the SUSY 450p300 model is used.

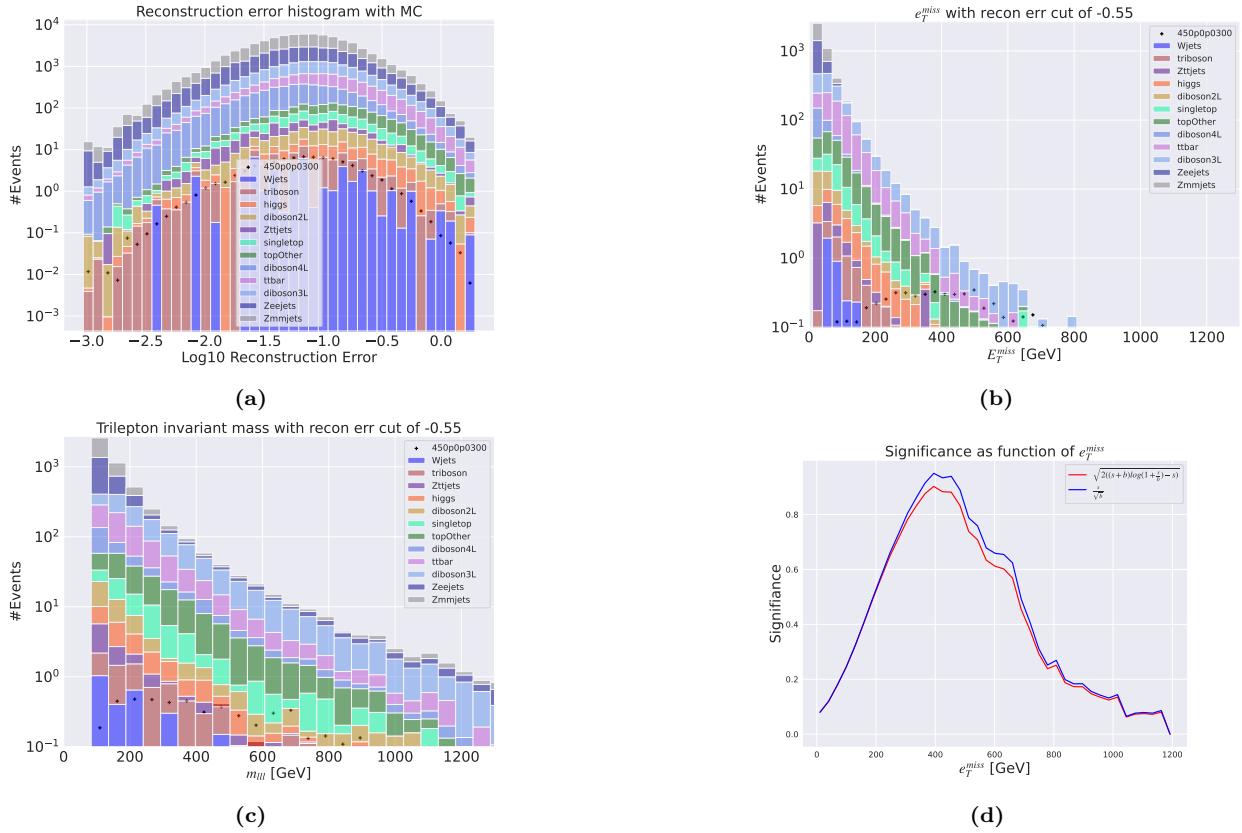


Figure 27: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the deep variational autoencoder. Here the SUSY 450p300 model is used.

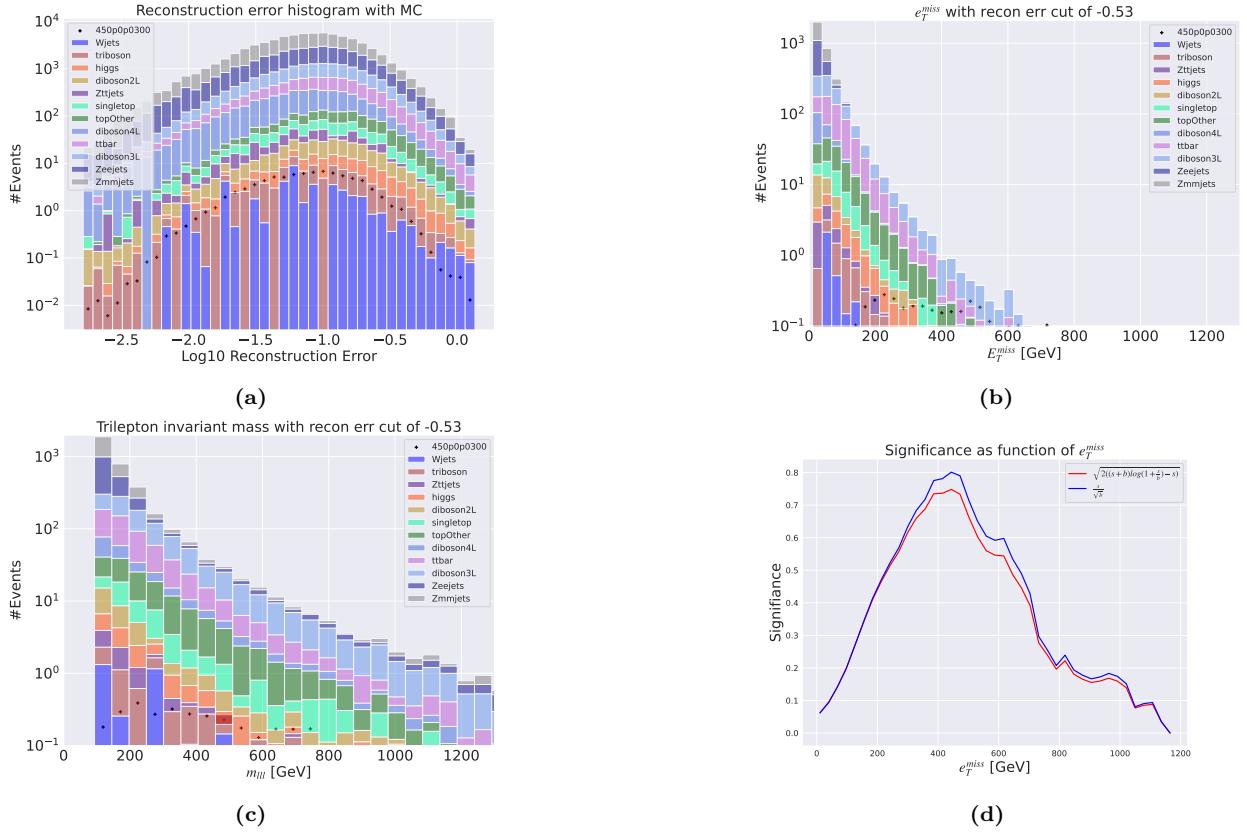


Figure 28: Reconstruction error, e_T^{miss} signal region, $m_{\ell\ell\ell}$ signal region and significance as function of e_T^{miss} for the shallow variational autoencoder. Here the SUSY 450p300 model is used.

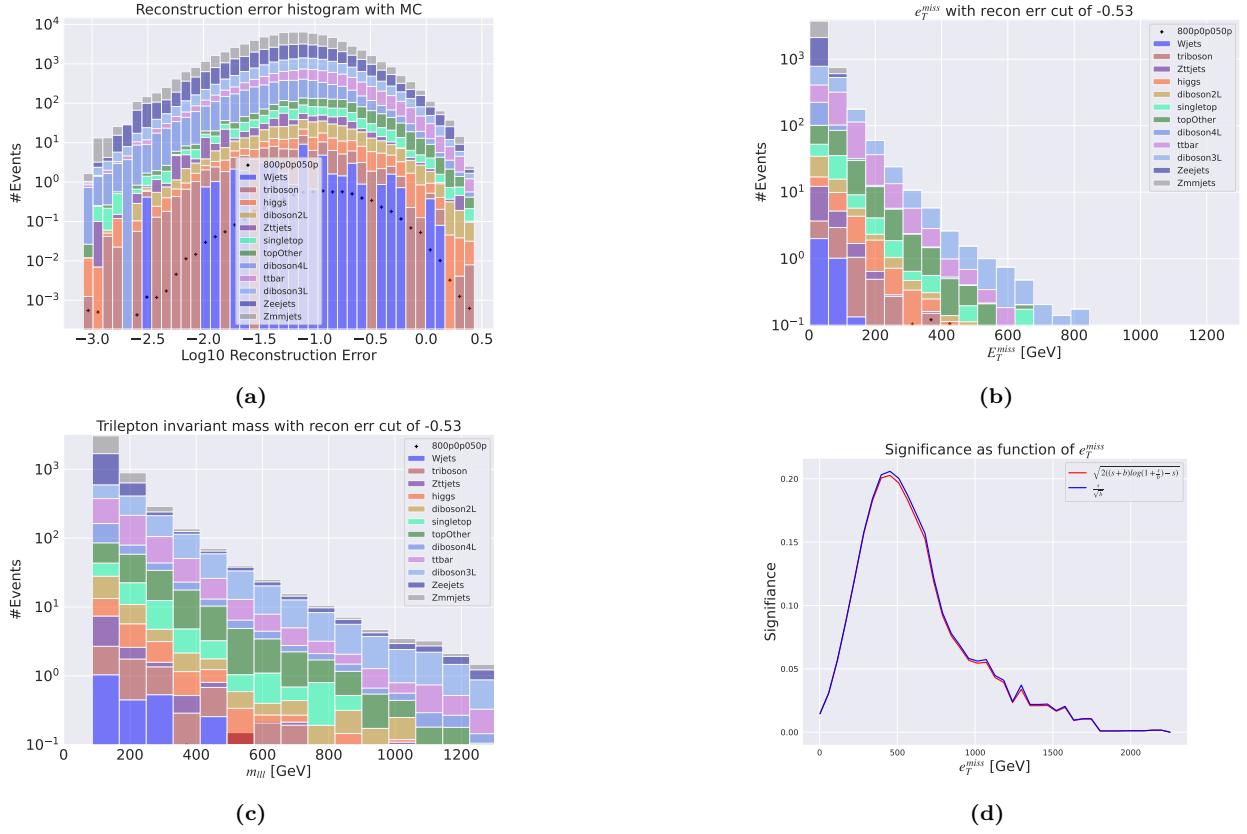


Figure 29: Reconstruction error, e_T^{miss} signal region, $m_{\ell\ell\ell}$ signal region and significance as function of e_T^{miss} for the deep variational autoencoder. Here the SUSY 450p300 model is used.

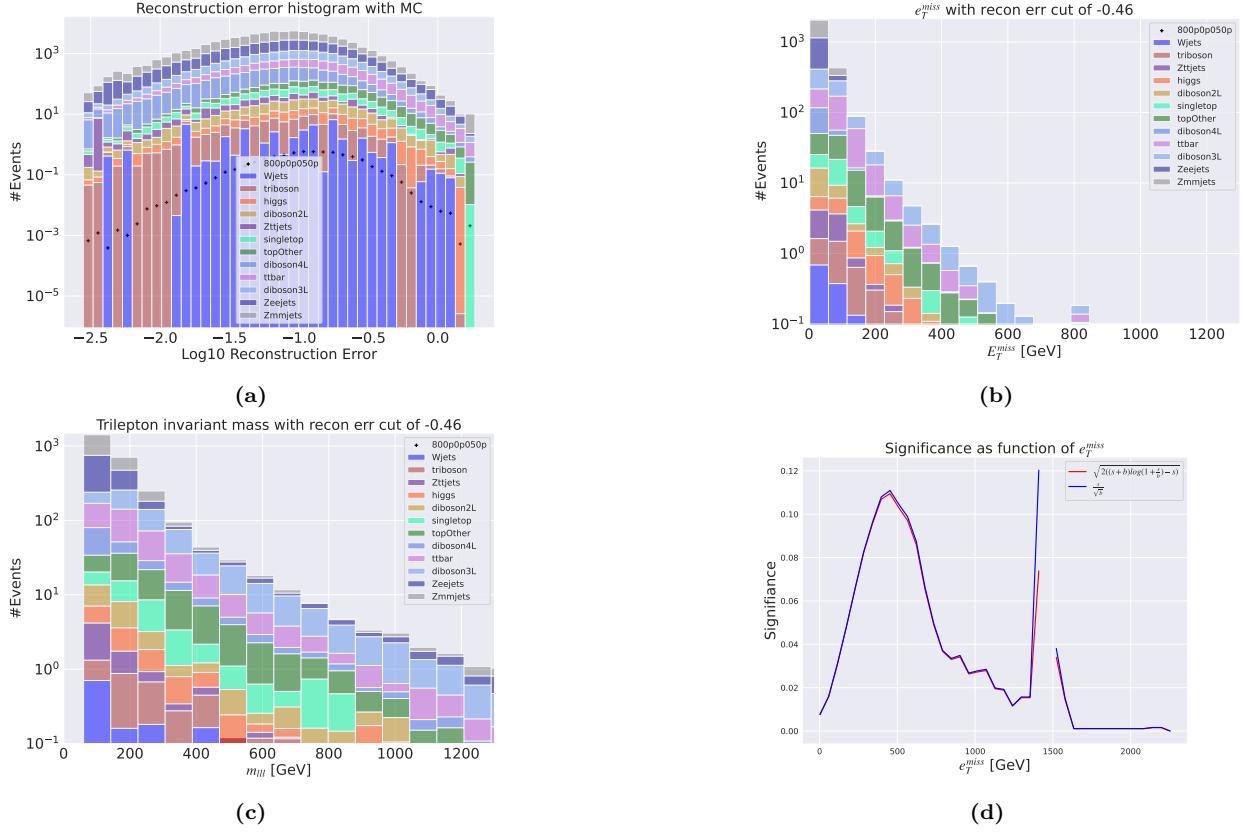


Figure 30: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the shallow variational autoencoder. Here the SUSY 450p300 model is used.

A.4 Reconstruction error cuts for 2 leptons + e_T^{miss}

In this section the remaining two reconstruction error cuts in the 2 lepton + e_T^{miss} are shown. The figures here are shaped with the same subfigure structure as the figures in the results and discussion section.

Regular autoencoder output

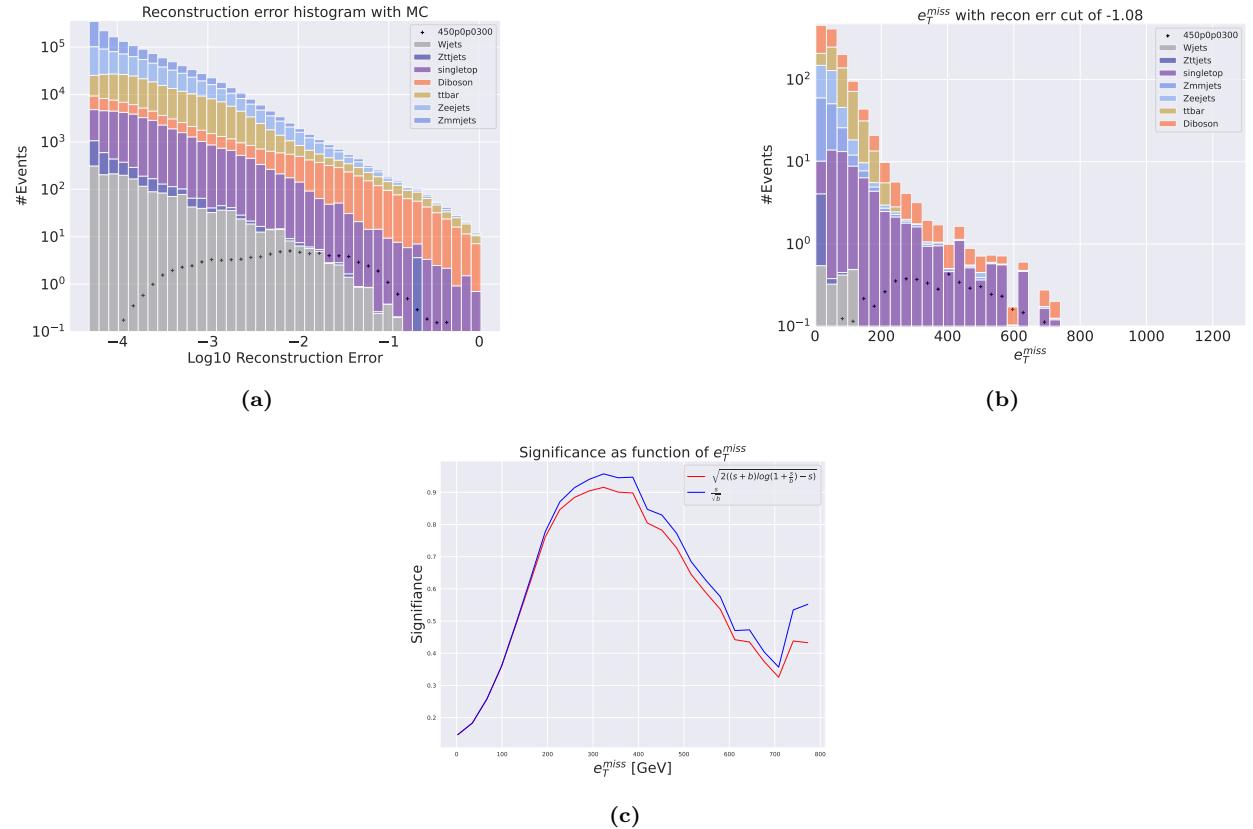


Figure 31: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the deep regular autoencoder. Here the SUSY 450p300 model is used.

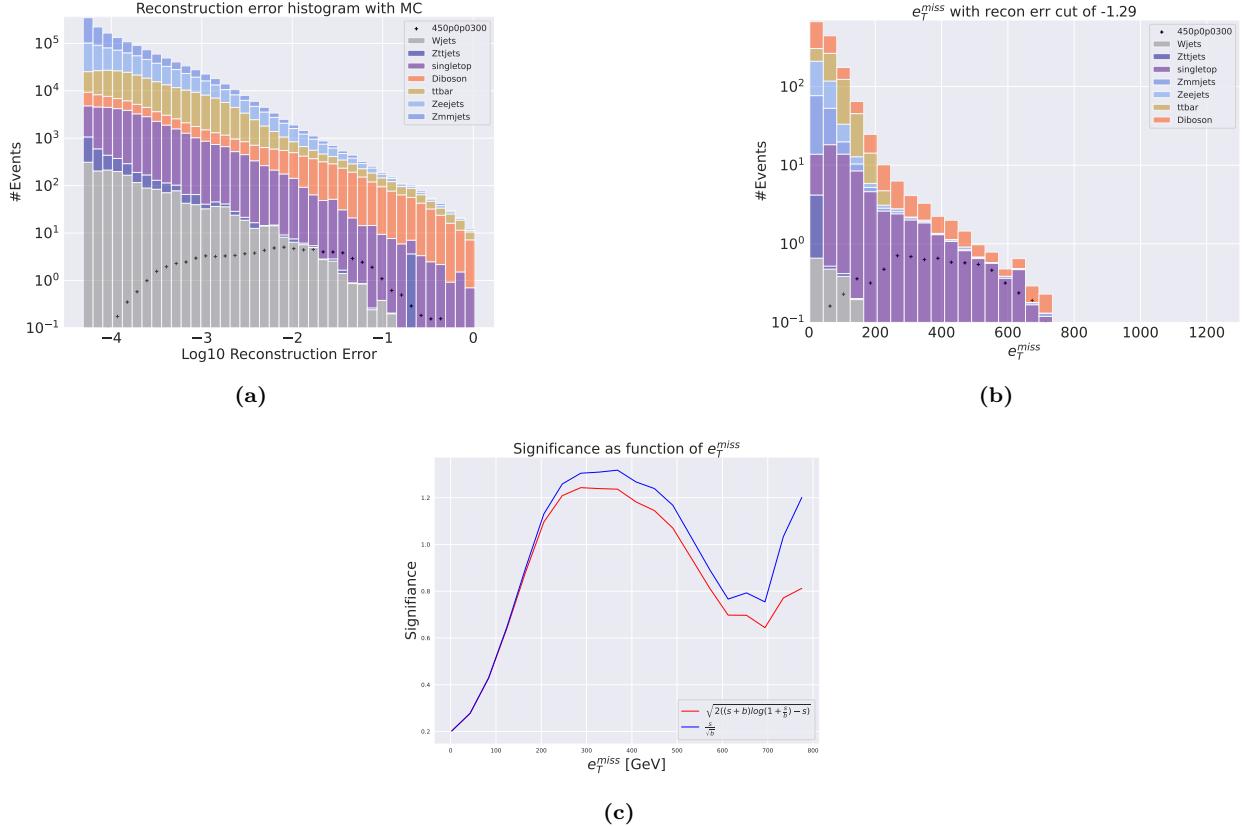


Figure 32: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the deep regular autoencoder. Here the SUSY 450p300 model is used.

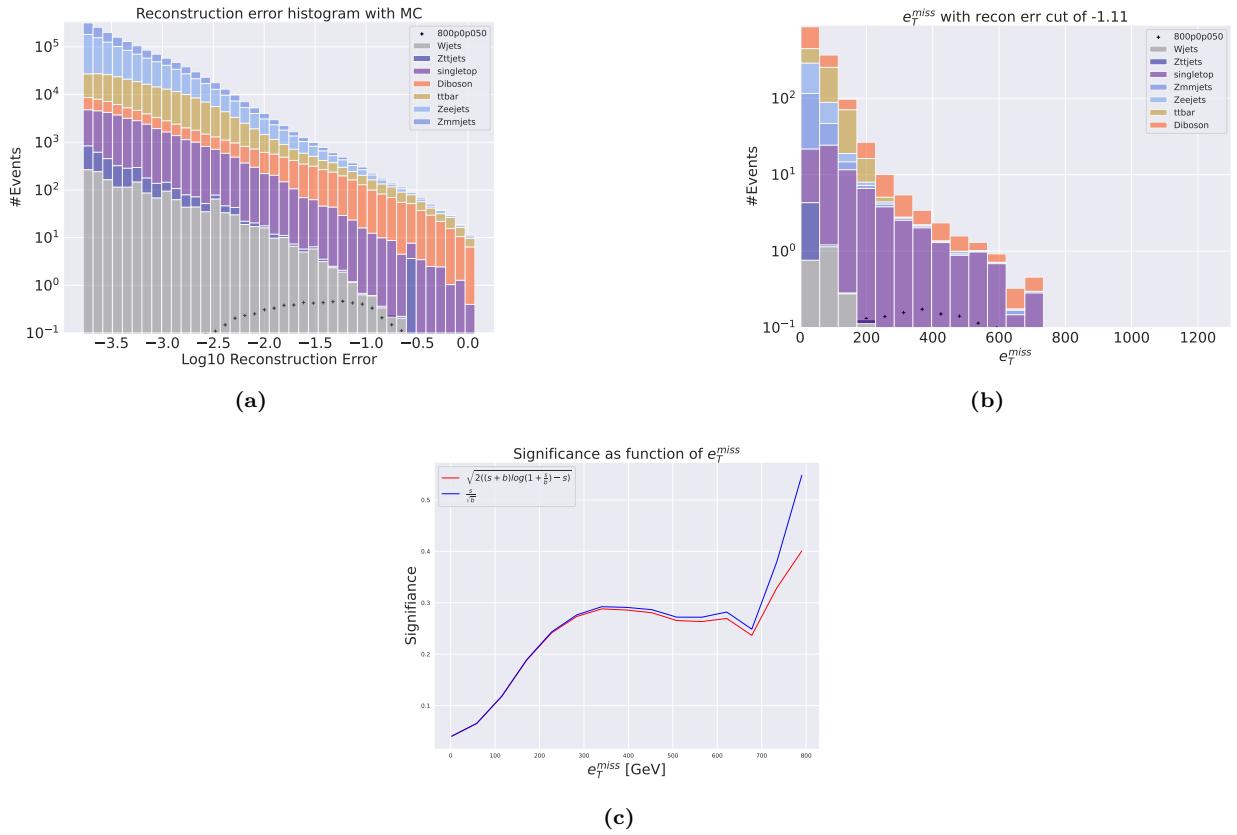


Figure 33: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the deep regular autoencoder. Here the SUSY 800p50 model is used.

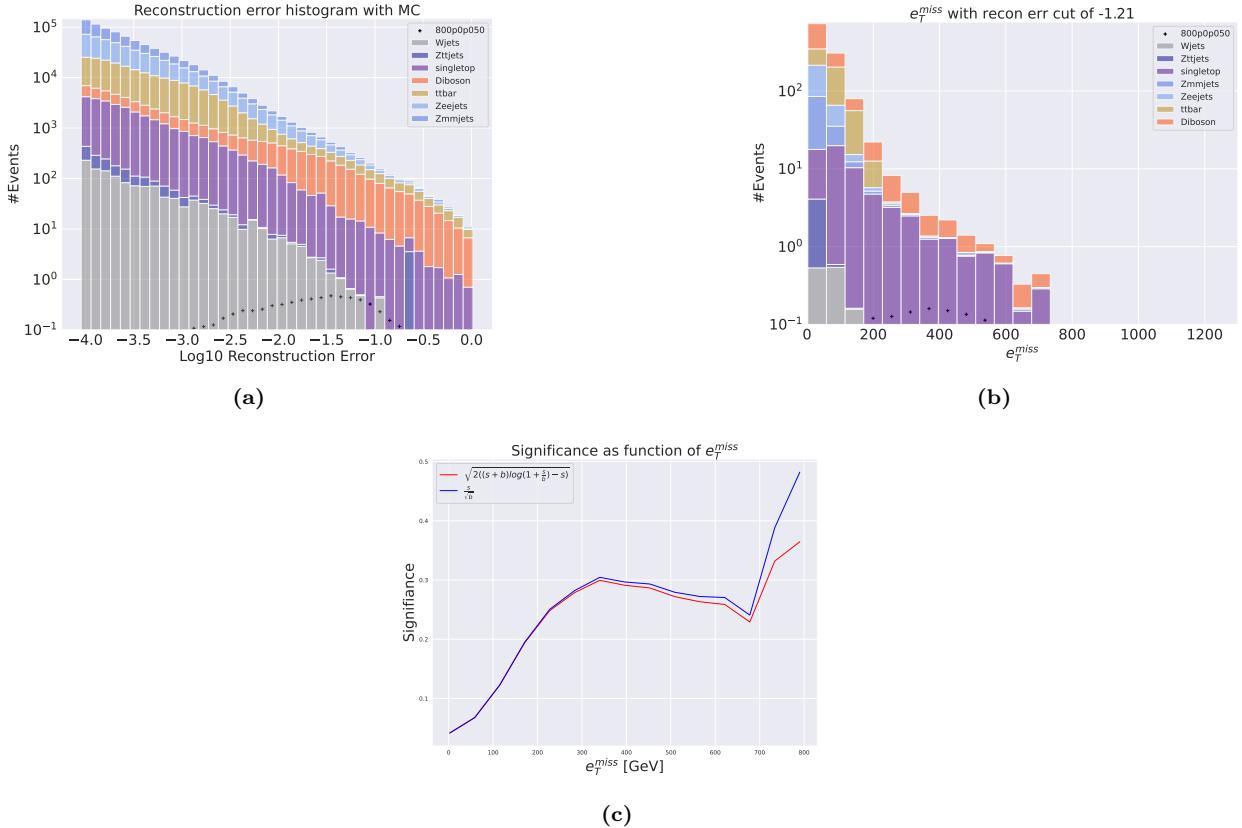


Figure 34: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the shallow regular autoencoder. Here the SUSY 800p50 model is used.

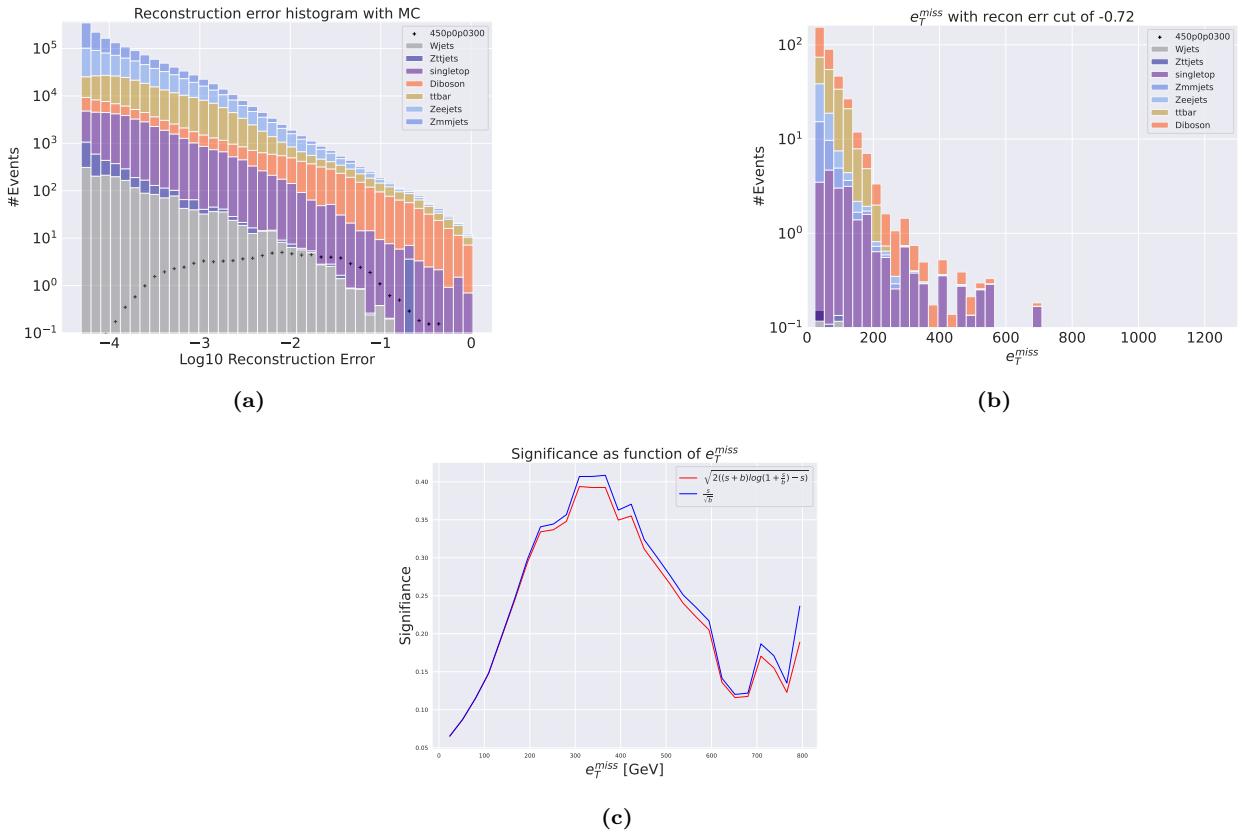


Figure 35: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the deep regular autoencoder. Here the SUSY 450p300 model is used.

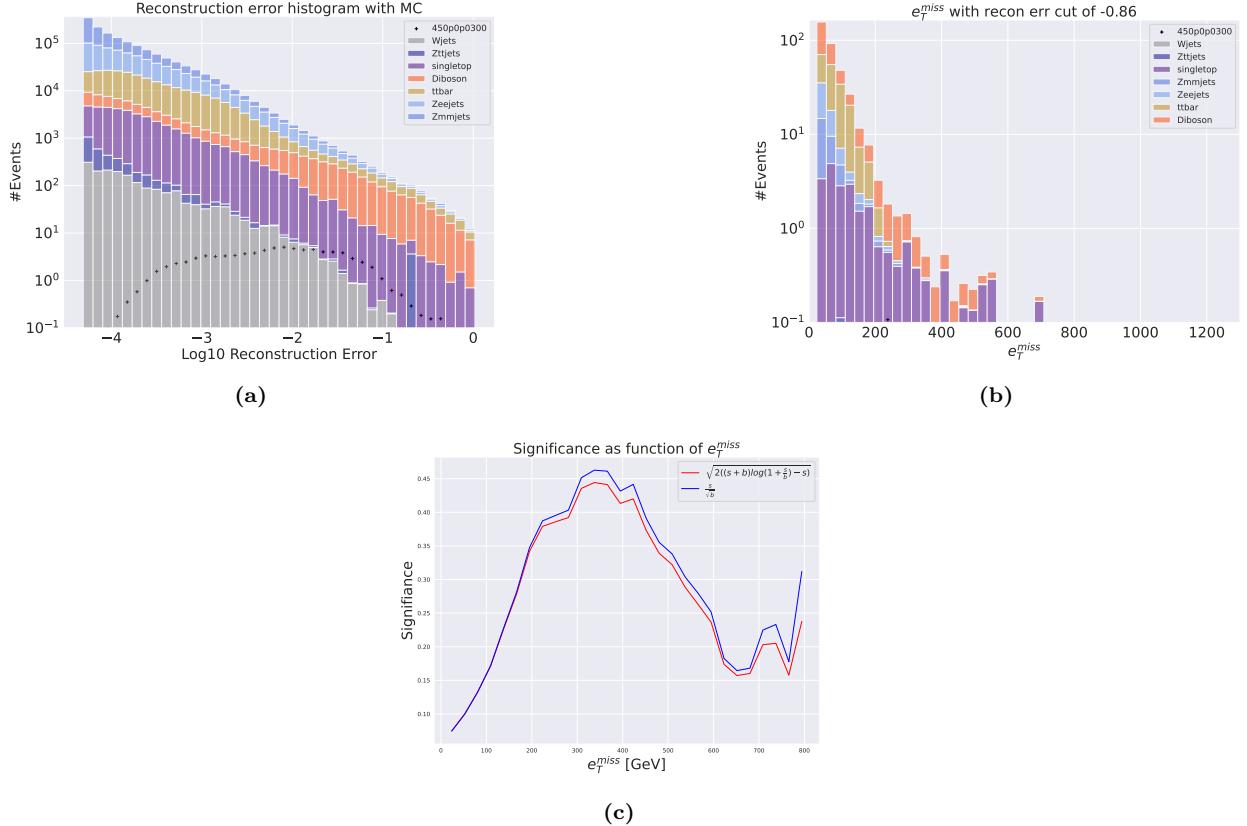


Figure 36: Reconstruction error, e_T^{miss} signal region, m_{ll} signal region and significance as function of e_T^{miss} for the deep regular autoencoder. Here the SUSY 450p300 model is used.

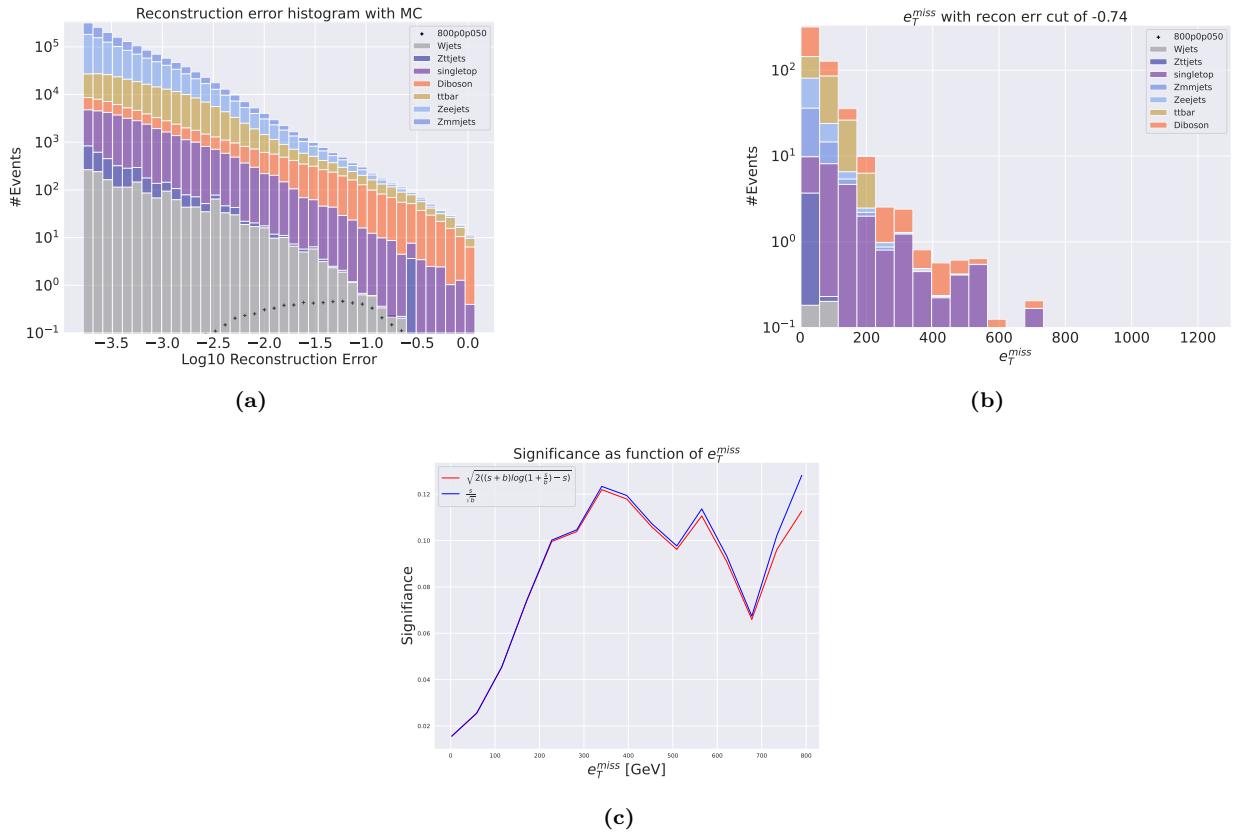


Figure 37: Reconstruction error, e_T^{miss} signal region, m_{ll} signal region and significance as function of e_T^{miss} for the deep regular autoencoder. Here the SUSY 800p50 model is used.

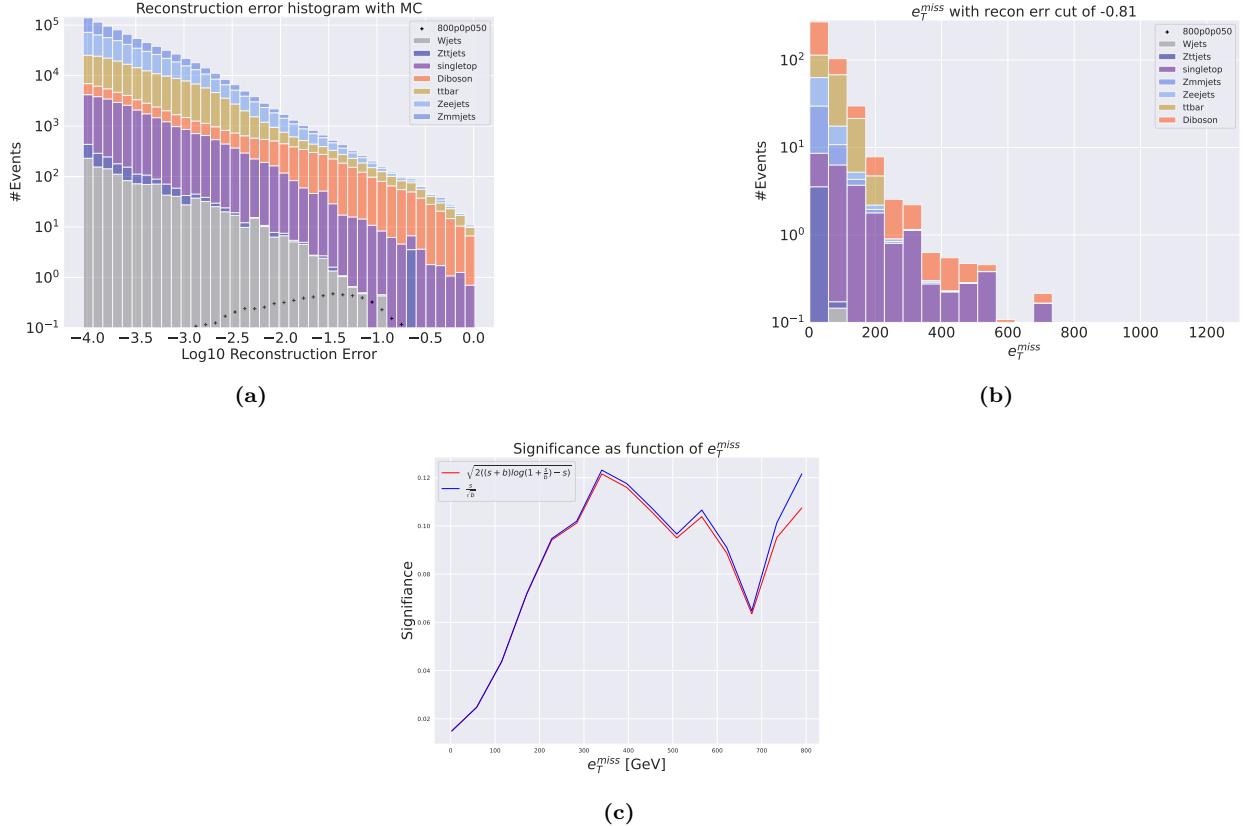


Figure 38: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the shallow regular autoencoder. Here the SUSY 800p50 model is used.

Variational autoencoder output

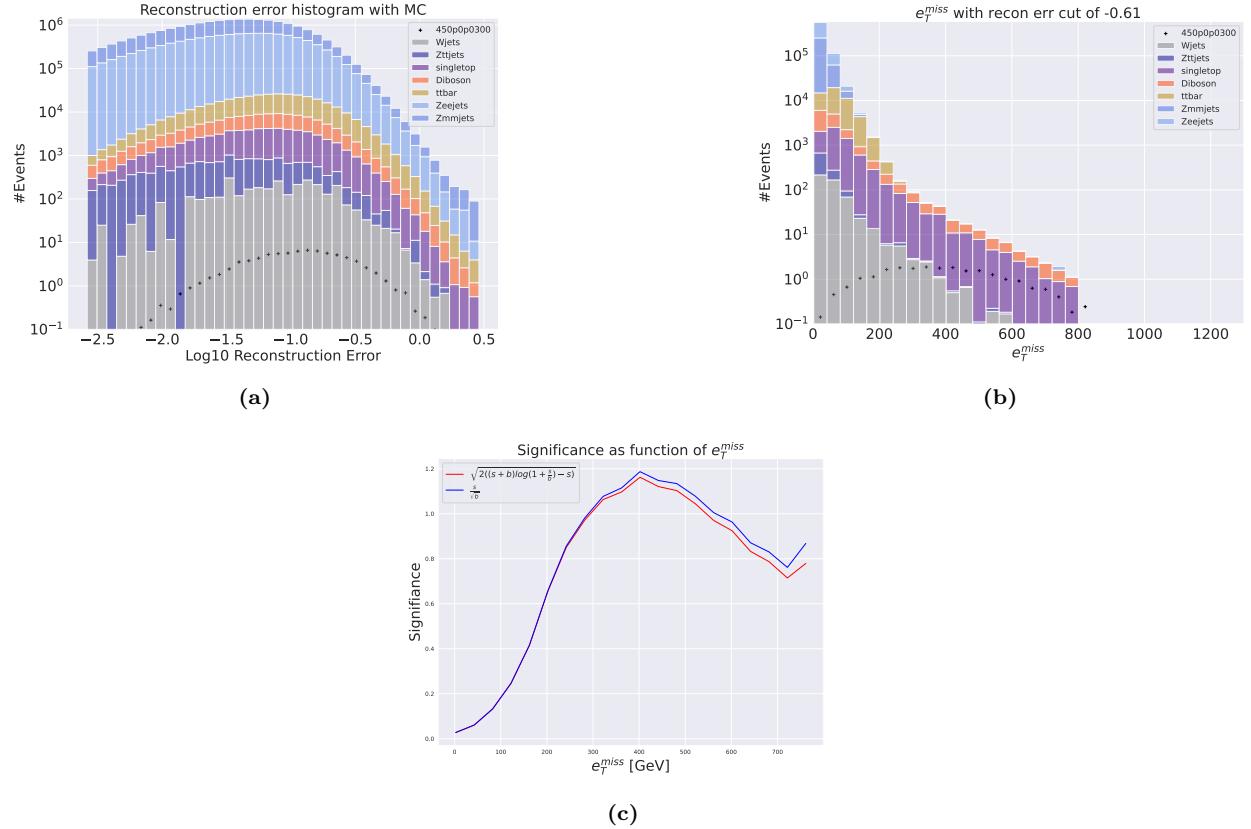


Figure 39: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the deep regular autoencoder. Here the SUSY 450p300 model is used.

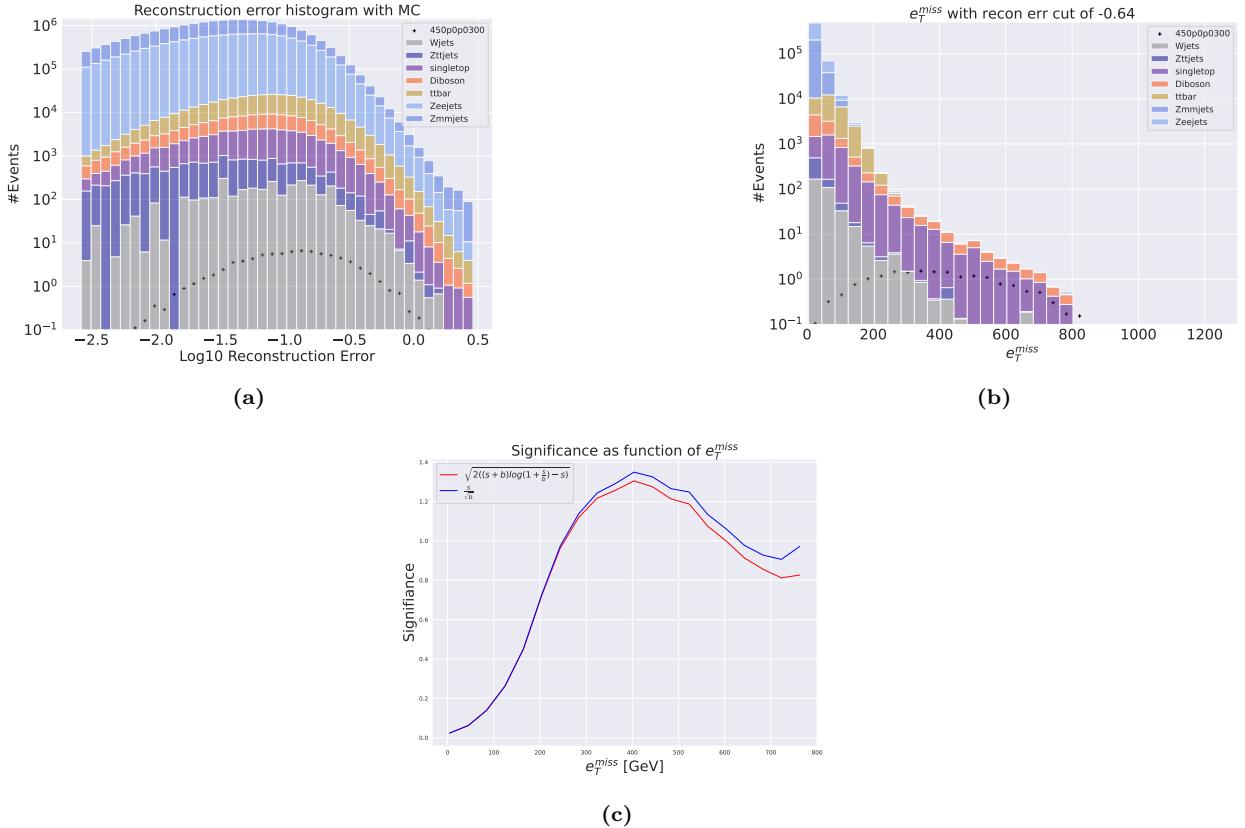


Figure 40: Reconstruction error, e_T^{miss} signal region, m_{ll} signal region and significance as function of e_T^{miss} for the deep regular autoencoder. Here the SUSY 450p0300 model is used.

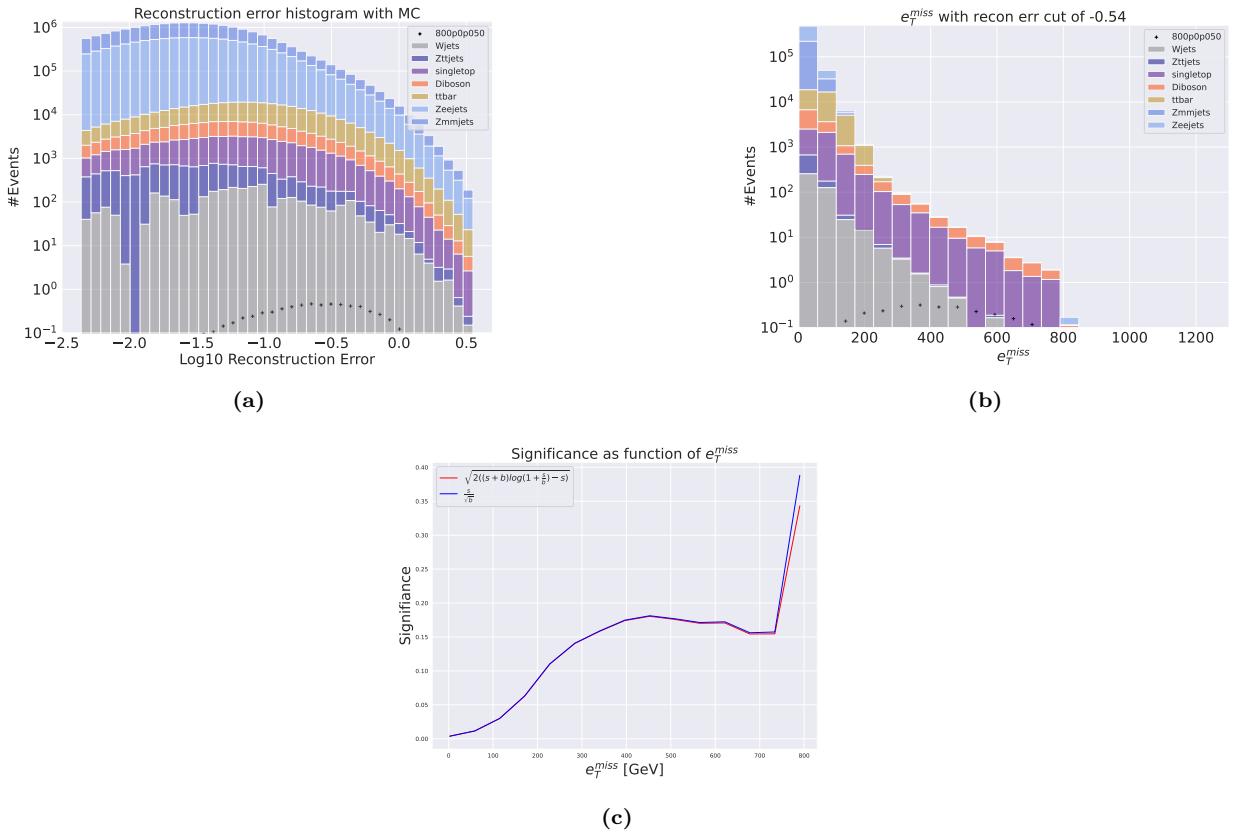


Figure 41: Reconstruction error, e_T^{miss} signal region, m_{ll} signal region and significance as function of e_T^{miss} for the deep regular autoencoder. Here the SUSY 800p050 model is used.

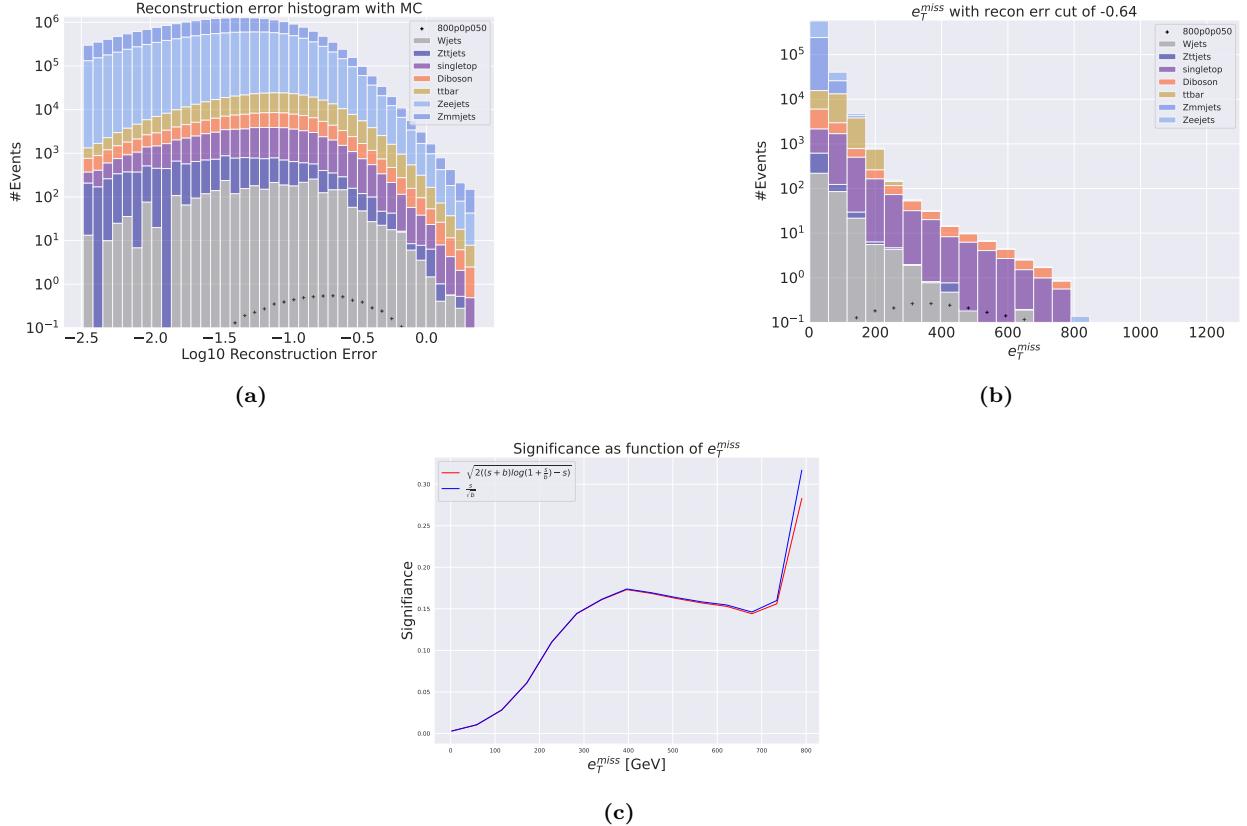


Figure 42: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the shallow regular autoencoder. Here the SUSY 800p50 model is used.

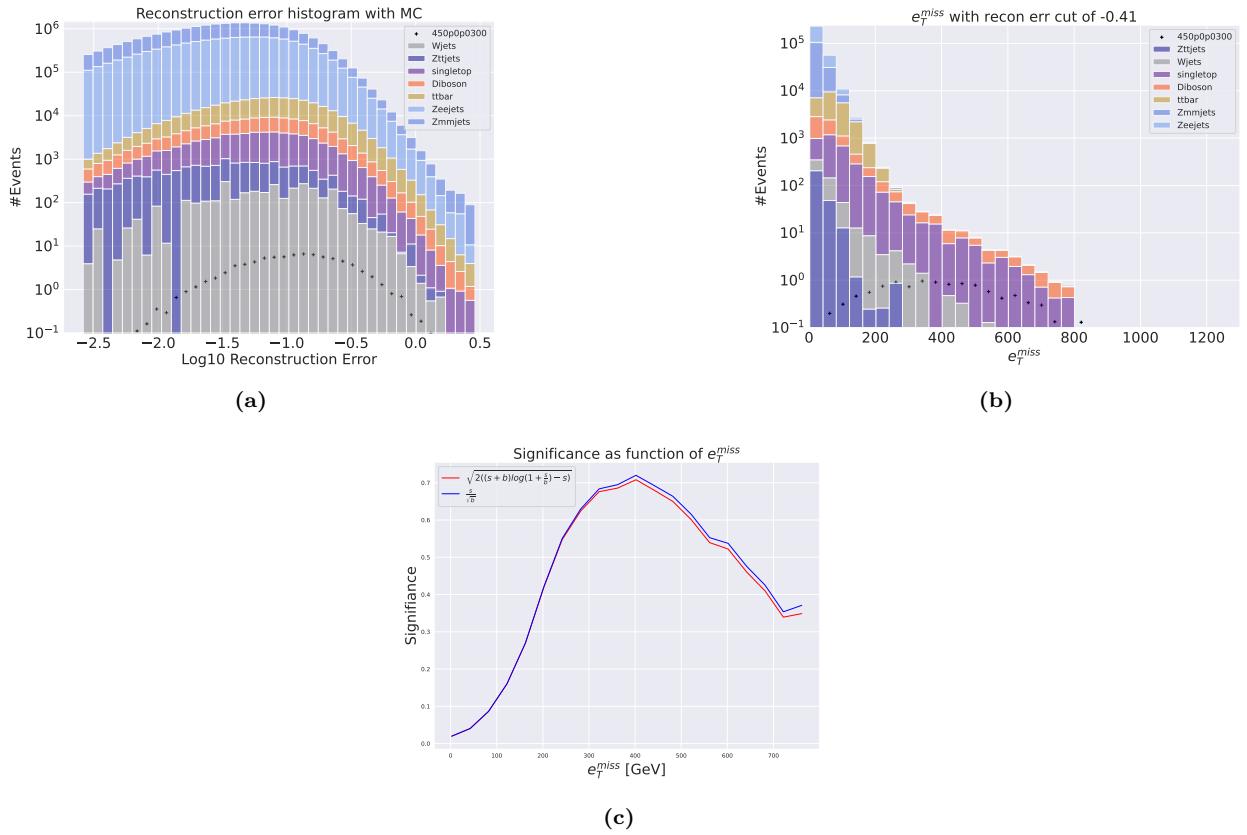


Figure 43: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the deep regular autoencoder. Here the SUSY 450p300 model is used.

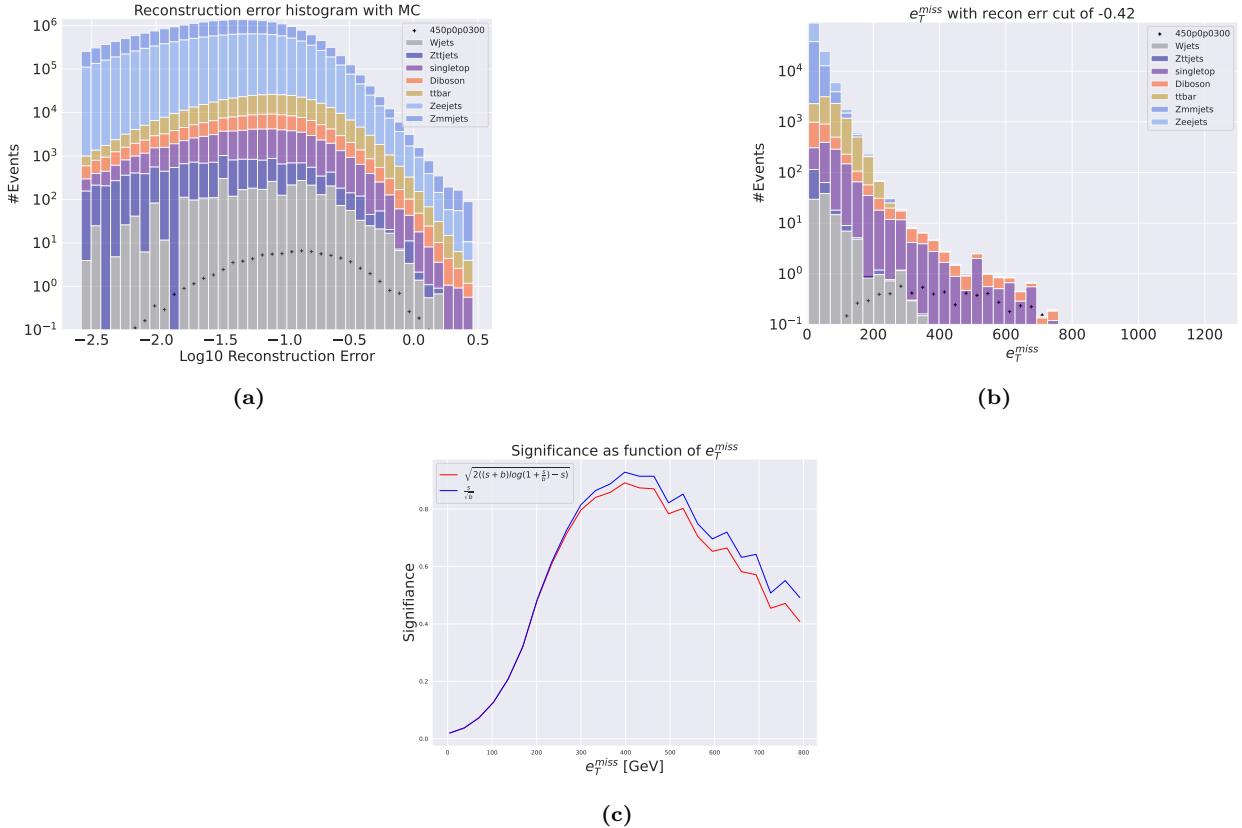


Figure 44: Reconstruction error, e_T^{miss} signal region, m_{ll} signal region and significance as function of e_T^{miss} for the deep regular autoencoder. Here the SUSY 450p300 model is used.

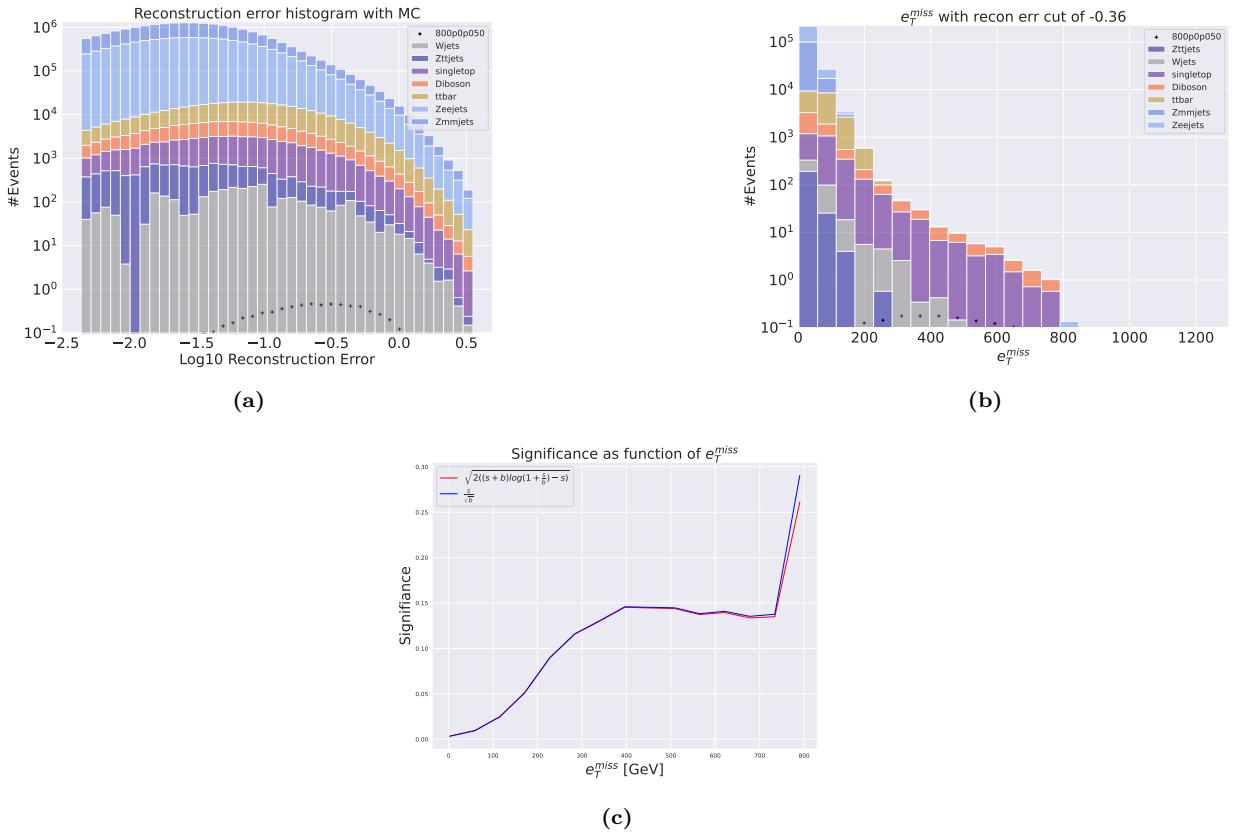


Figure 45: Reconstruction error, e_T^{miss} signal region, m_{ll} signal region and significance as function of e_T^{miss} for the deep regular autoencoder. Here the SUSY 800p50 model is used.

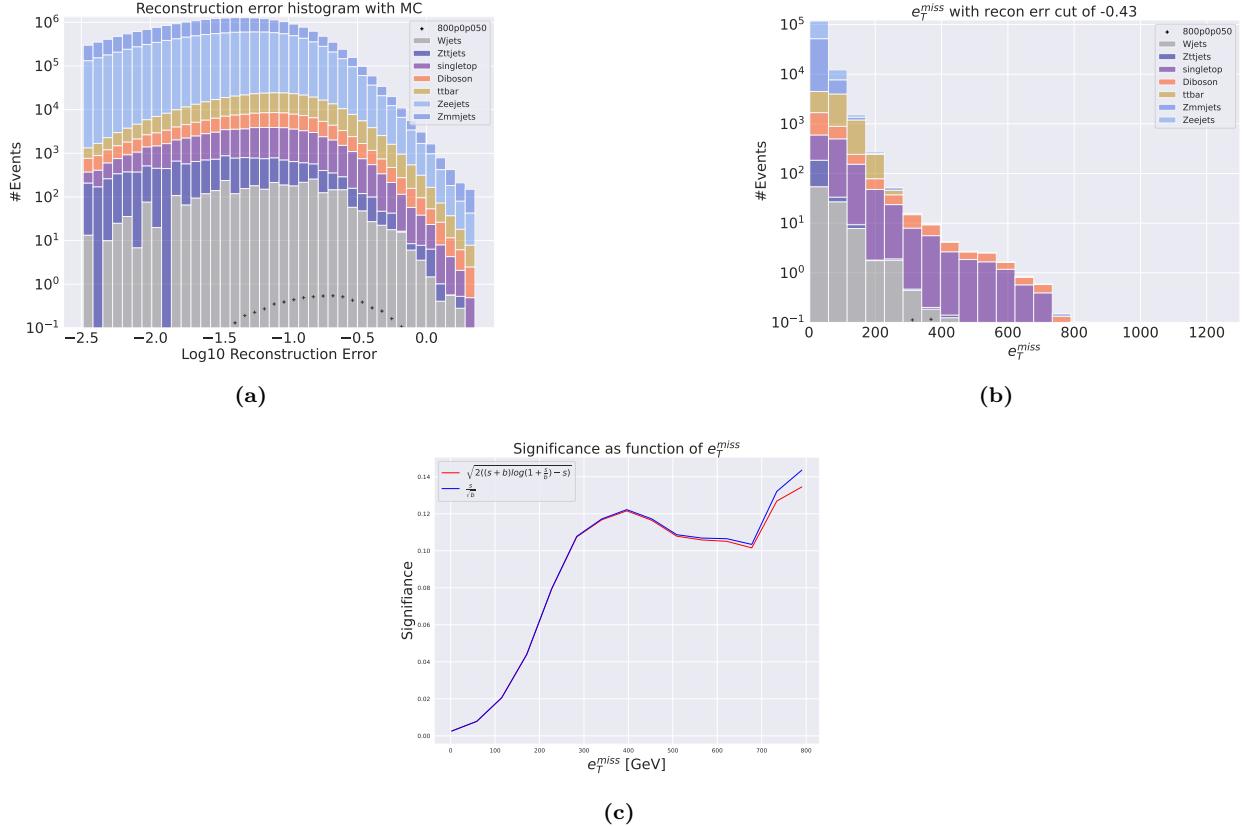


Figure 46: Reconstruction error, e_T^{miss} signal region, m_{lll} signal region and significance as function of e_T^{miss} for the shallow regular autoencoder. Here the SUSY 800p50 model is used.

Appendix B

B.1 Algorithmic implementation

The RMM as a set of features were a bit tricky to implement, and one way to implement it was to use a dictionary containing the names of features already in the RDataFrame set. RDataFrame allows for custom c++ functions to be run on the entire dataframe, and because almost all the features in the RMM use the kinematical variables for each particle they were needed to be accessed. Each element in the dictionary contains a number ID corresponding to the column it belongs to, a name, the 4 kinematic variables pt , η , ϕ and E , and the rank within its particle type. Thus, ele_0 is the first electron, and its rank is 0.

```

1 rmm_structure = {
2     1: ["ljet_0", "jetPt[ljet]", "jetEta[ljet]", "jetPhi[ljet]", "jetM[ljet]", 0,],
3     2: [ "ljet_1", "jetPt[ljet]", "jetEta[ljet]", "jetPhi[ljet]", "jetM[ljet]", 1,],
4     3: [ "ljet_2", "jetPt[ljet]", "jetEta[ljet]", "jetPhi[ljet]", "jetM[ljet]", 2,],
5     4: [ "ljet_3", "jetPt[ljet]", "jetEta[ljet]", "jetPhi[ljet]", "jetM[ljet]", 3,],
6     5: [ "ljet_4", "jetPt[ljet]", "jetEta[ljet]", "jetPhi[ljet]", "jetM[ljet]", 4,],
7     6: [ "ljet_5", "jetPt[ljet]", "jetEta[ljet]", "jetPhi[ljet]", "jetM[ljet]", 5,],
8     7: [ "bjet_0", "jetPt[bjet77]", "jetEta[bjet77]", "jetPhi[bjet77]", "jetM[bjet77]", 0,],
9     8: [ "bjet_1", "jetPt[bjet77]", "jetEta[bjet77]", "jetPhi[bjet77]", "jetM[bjet77]", 1,],
10    9: [ "bjet_2", "jetPt[bjet77]", "jetEta[bjet77]", "jetPhi[bjet77]", "jetM[bjet77]", 2,],
11   10: [ "bjet_3", "jetPt[bjet77]", "jetEta[bjet77]", "jetPhi[bjet77]", "jetM[bjet77]", 3,],
12   11: [ "bjet_4", "jetPt[bjet77]", "jetEta[bjet77]", "jetPhi[bjet77]", "jetM[bjet77]", 4,],
13   12: [ "bjet_5", "jetPt[bjet77]", "jetEta[bjet77]", "jetPhi[bjet77]", "jetM[bjet77]", 5,],
14   13: [ "ele_0", "lepPt[ele_SG]", "lepEta[ele_SG]", "lepPhi[ele_SG]", "lepM[ele_SG]", 0,],
15   14: [ "ele_1", "lepPt[ele_SG]", "lepEta[ele_SG]", "lepPhi[ele_SG]", "lepM[ele_SG]", 1,],
16   15: [ "ele_2", "lepPt[ele_SG]", "lepEta[ele_SG]", "lepPhi[ele_SG]", "lepM[ele_SG]", 2,],
17   16: [ "ele_3", "lepPt[ele_SG]", "lepEta[ele_SG]", "lepPhi[ele_SG]", "lepM[ele_SG]", 3,],
18   17: [ "ele_4", "lepPt[ele_SG]", "lepEta[ele_SG]", "lepPhi[ele_SG]", "lepM[ele_SG]", 4,],
19   18: [ "muo_0", "lepPt[muo_SG]", "lepEta[muo_SG]", "lepPhi[muo_SG]", "lepM[muo_SG]", 0,],
20   19: [ "muo_1", "lepPt[muo_SG]", "lepEta[muo_SG]", "lepPhi[muo_SG]", "lepM[muo_SG]", 1,],
21   20: [ "muo_2", "lepPt[muo_SG]", "lepEta[muo_SG]", "lepPhi[muo_SG]", "lepM[muo_SG]", 2,],
22   21: [ "muo_3", "lepPt[muo_SG]", "lepEta[muo_SG]", "lepPhi[muo_SG]", "lepM[muo_SG]", 3,],
23   22: [ "muo_4", "lepPt[muo_SG]", "lepEta[muo_SG]", "lepPhi[muo_SG]", "lepM[muo_SG]", 4,],
24 }
```

The dictionary is then used in the nested for loop below. The loop is partitioned into several scenarios. Firstly, the first element in the matrix is the e_T^{miss} . Once that is set, the loop has three cases to check, the upper triangle, the lower triangle and the diagonal. The upper triangle is related to masses, and the lower triangle is related to longitudinal properties. Using this, the number ID helps ID which particle(s) to use and where to put the properties calculated based on them.

```

1 for row in range(N_row):
2     if row == 0:
3         # Calculate e_T^miss and m_T for all objects
4         for column in range(N_col):
5             if column == 0:
6                 # Set e_T_miss
7                 df[k] = df[k].Define("e_T_miss", "met_Et")
8             else:
9                 # Set m_T for all particles
10                name, pt, eta, phi, m, index = rmm_structure[column]
11                df[k] = df[k].Define(
12                    f"m_T_{name}", f"getM_T({pt},{eta},{phi},{m},{index})"
13                )
14
15     else:
16         # Calculate rest of matrix
17         for column in range(N_col):
18             if column == 0:
19                 # Set h_L for all particles
20                 name, pt, eta, phi, m, index = rmm_structure[row]
21
22                 df[k] = df[k].Define(
23                     f"h_L_{name}", f"geth_L({pt},{eta},{phi},{m},{index})"
24                 )
25             elif column == row:
26                 name, pt, eta, phi, m, index = rmm_structure[column]
27                 if index == 0:
28                     # If particle is the first of its type, calculate e_T of particle
29                     df[k] = df[k].Define(
30                         f"e_T_{name}", f"getET_part({pt},{m},{index})"
31                     )
32                 else:
33                     # If particle is not the first of its type, calculate the difference in e_T
34                     df[k] = df[k].Define(
35                         f"delta_e_t_{name}", f"delta_e_T({pt},{m},{index})"
36                     )
37
38             elif column > row:
39                 # For invariant mass
40                 # Particle 1
41                 name1, pt1, eta1, phi1, m1, index1 = rmm_structure[row]
42
43                 # Particle 2
44                 name2, pt2, eta2, phi2, m2, index2 = rmm_structure[column]
45
46                 histo_name = f"m_{name1}_{name2}"
47                 df[k] = df[k].Define(
48                     histo_name,
49                     f"getM({pt1},{eta1}, {phi1}, {m1}, {pt2}, {eta2}, {phi2}, {m2}, {index1}, {index2})",
50                 )
51             elif row > column:
52                 # For h longitudinal stuff
53                 # Particle 1
54                 name1, pt1, eta1, phi1, m1, index1 = rmm_structure[row]
55
56                 # Particle 2
57                 name2, pt2, eta2, phi2, m2, index2 = rmm_structure[column]
58
59                 histo_name = f"h_{name1}_{name2}"
60                 df[k] = df[k].Define(
61                     f"{histo_name}",
62                     f"geth({pt1},{eta1}, {phi1}, {m1}, {pt2}, {eta2}, {phi2}, {m2}, {index1}, {index2})",
63                 )

```

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