

# Title of the Thesis

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I hereby declare that this thesis was formulated by myself and that no sources or tools other than those cited were used.

Bonn, .....

Date

.....

Signature

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# Contents

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<b>1</b>	<b>Introduction</b>	<b>1</b>
<b>2</b>	<b>The Standard Model of Particle Physics</b>	<b>5</b>
2.1	Interactions . . . . .	5
2.2	Particles . . . . .	5
2.3	Open questions . . . . .	5
<b>3</b>	<b>The LHC and the ATLAS detector</b>	<b>7</b>
3.1	Large Hadron Collider . . . . .	7
3.2	The ATLAS detector . . . . .	8
3.2.1	Tracking detectors . . . . .	9
3.2.2	The ATLAS calorimeter system . . . . .	10
3.2.3	The Muon spectrometer . . . . .	11
3.2.4	The ATLAS coordinate system . . . . .	11
3.2.5	Particle Detection in the ATLAS detector . . . . .	12
3.3	Monte Carlo Simulation . . . . .	12
3.4	tW event topology . . . . .	13
<b>4</b>	<b>The tW Channel</b>	<b>13</b>
<b>5</b>	<b>Machine Learning</b>	<b>15</b>
5.1	The concept of machine learning . . . . .	15
5.2	Neural Networks . . . . .	16
5.3	Regularisation and Optimisation . . . . .	22
5.3.1	Dropout . . . . .	22
5.3.2	Batch normalization . . . . .	22
5.4	Adversarial Neural Networks . . . . .	23
5.4.1	The adversarial neural network . . . . .	24
<b>6</b>	<b>Hyperparameter optimisation of a classifying neural network</b>	<b>27</b>
6.1	The input variables . . . . .	27
6.2	The network architecture . . . . .	27
6.3	Setup of the optimisation . . . . .	28
6.4	Regularisation . . . . .	29

<b>7 Adversarial Neural Network</b>	<b>27</b>
7.1 Setup of the first network . . . . .	27
7.2 Setup of the second network . . . . .	27
<b>8 Conclusions</b>	<b>29</b>
<b>9 Machine Learning Tools</b>	<b>31</b>
9.1 Keras . . . . .	31
9.2 Tensorflow . . . . .	31
<b>Bibliography</b>	<b>33</b>
<b>A Useful information</b>	<b>35</b>
<b>List of Figures</b>	<b>37</b>
<b>List of Tables</b>	<b>39</b>

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# CHAPTER 2

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## The Standard Model of Particle Physics

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Originally in an attempt to unify the electromagnetic, weak and strong force under one theory the standard model of particle physics represents the status quo of particle physics summarizing the elementary particles and their interactions. The model is a gauge quantum field theory and its eternal symmetry is the unitary product group  $SU(3) \times SU(2) \times U(1)$  in which the interactions are represented by particles named gauge bosons.

Although failing to answer open questions like the origin of dark matter or neutrino oscillations the Standard Model is a powerful model and has been successful in providing experimental predictions for decades.

### 2.1 Interactions

### 2.2 Particles

### 2.3 Open questions

three generations of matter (fermions)			interactions / force carriers (bosons)		
	I	II	III		
QUARKS	mass $\approx 2.2 \text{ MeV}/c^2$ charge $\frac{2}{3}$ spin $\frac{1}{2}$	<b>u</b> up	<b>c</b> charm	<b>t</b> top	<b>g</b> gluon
	$\approx 4.7 \text{ MeV}/c^2$ $-\frac{1}{3}$ $\frac{1}{2}$	<b>d</b> down	<b>s</b> strange	<b>b</b> bottom	<b><math>\gamma</math></b> photon
	$\approx 0.511 \text{ MeV}/c^2$ $-1$ $\frac{1}{2}$	<b>e</b> electron	<b><math>\mu</math></b> muon	<b><math>\tau</math></b> tau	<b>Z</b> Z boson
	$< 2.0 \text{ eV}/c^2$ 0 $\frac{1}{2}$	<b><math>\nu_e</math></b> electron neutrino	<b><math>\nu_\mu</math></b> muon neutrino	<b><math>\nu_\tau</math></b> tau neutrino	<b>W</b> W boson
					<b>H</b> higgs
					<b>GAUGE BOSONS</b>
					<b>SCALAR BOSONS</b>
					<b>VECTOR BOSONS</b>

Figure 2.1: Summary table of the Standard Model particles and their properties. The sketch [standard\_model] was updated to PDG 2018 data [PDG]

# CHAPTER 3

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## The LHC and the ATLAS detector

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For most researches in modern particle physics there are two main constraints. The first one arises from the statistical nature of decay and creation processes in particle physics. Many of the most interesting events occur extremely rarely and call for large amount of data, more precisely high luminosity, to achieve significant results. Secondly the energy scale of particle physics is enormously high to allow breaking the structure of particles below the nuclear scale.

This work was carried out using simulations based on the ATLAS [1] detector at the Large Hadron Collider (LHC) [2] which offers both a record energy and luminosity. This chapter gives a summary of both machines and the knowledge necessary to understand the simulations used. First of a summary of the machines' parts and their technical details to are given, followed by a description of how the detector detects particles and how their properties are measured.

### 3.1 Large Hadron Collider

The Large Hadron Collider located at the facilities of the European Organization of Nuclear Research (CERN) close to Geneva was built to extend the frontiers of modern particle physics by delivering high luminosities and reaching unprecedented high energies thereby providing the data for multiple particle physics experiments.

The LHC is a circular particle detector with a circumference of 26.7 km designed to accelerate and collide two counter-rotating beams of protons. The protons are accelerated in bunches of up to  $10^{11}$  protons at energies up to 7 TeV and a luminosity of  $10^{34} \text{ cm}^{-2} \text{ s}^{-1}$  achieving the record center-of-mass energy of up to 14 TeV. The bunches are pre-accelerated by a number of accelerators before being inserted in the last, so called storage ring. An overview of the acceleration system is given in figure 3.1 and for more detailed information see the LHC design report. [2]. The four interaction points, at which the beams are brought to collision, inhabit the main experiments of the LHC. Two of them are general purpose detectors, namely ATLAS [1] and CMS [3], the third is the LHCb [4] focusing on  $b$  physics and lastly ALICE [5] used for investigating heavy ion collisions. Figure 3.2 shows a sketch of the LHC's location and the positions of the four main experiments.

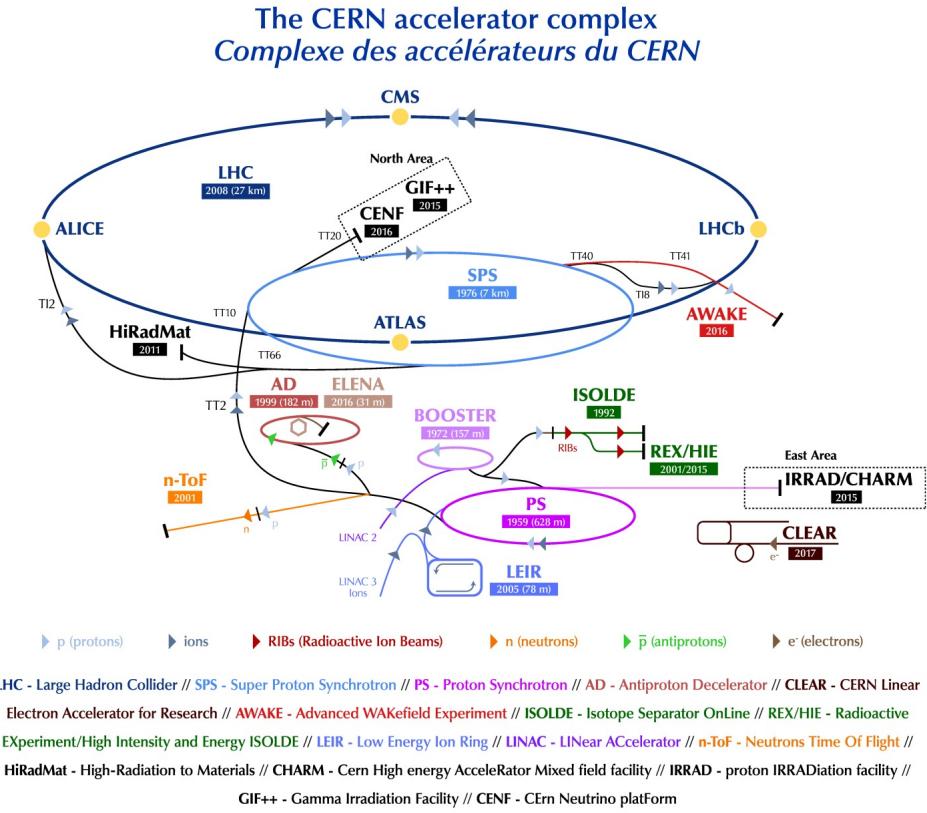


Figure 3.1: Sketch of the accelerator complex of the LHC showing the acceleration systems and the main storage ring with its experiments. [6]

### 3.2 The ATLAS detector

The ATLAS detector is a general purpose detector meaning it aims at covering a maximum number of final states, enabling researchers in many topics of particle physics to use its data.

ATLAS, "A Toroidal LHC Apparatus" has the distinguishing structure of a general purpose detector, its innermost part formed by tracking detectors directly surrounding the interaction point, followed by calorimeters and a further tracking detector for muon detection as the outermost component. All the components are visualized in figure 3.3 including two humans to give an impression of the scale.

The innermost tracking detectors are summarized under the name Inner Detector (ID) and consist of two Silicon detectors namely the Pixel Detector and the Semi Conductor Tracker as well as a straw detector named Transition Radiation Tracker. The Inner Detector allows for precise measurement of not only charged particles' position and thus vertex information, but also for their charge and momentum.

The two calorimeters, being the electromagnetic calorimeter and the hadronic calorimeter, allow to measure the energy of particles by stopping them in the detector material.

The Muon Spectrometer is a further tracking detector identifying particles crossing it as

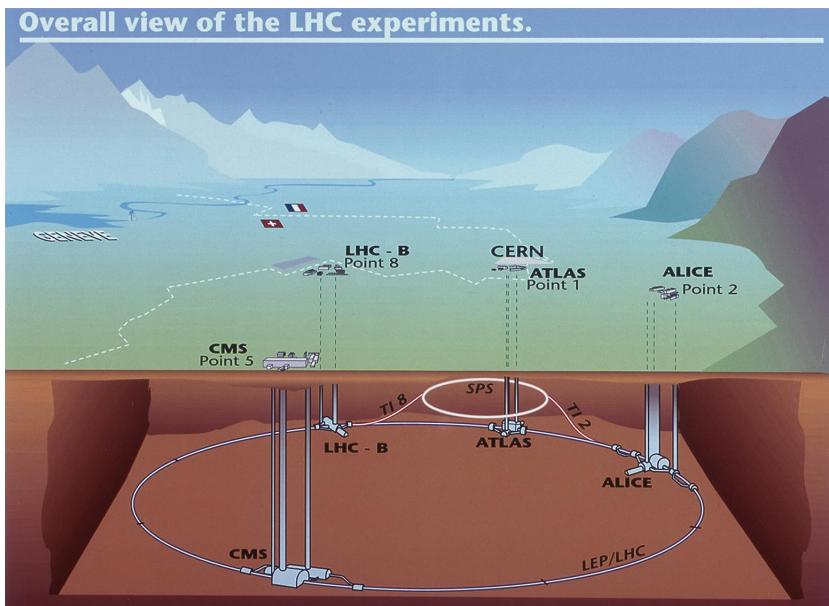


Figure 3.2: Sketch of the LHC ring, the position of the experiments and the surrounding countryside. The four big LHC experiments are indicated (ATLAS, CMS, LHC-B and ALICE) along with their injection lines (Point 1, 2, 4, 8). [7]

muons, as all other charged particles are usually stopped in the other components.

In the following the concept of each detector component is briefly introduced [8] to then summarize how particles can be detected and distinguished.

### 3.2.1 Tracking detectors

Tracking detectors are used to measure a charged particle's trajectory, momentum and charge value, of which two types are used in the ID of the ATLAS detector. The Pixel detector and the Semi Conductor Tracker (SCT) are silicon detectors and the Transition Radiation Tracker (TRT) is a straw-based tracking detector. For all detectors it holds true that they are surrounded by a magnetic field and cover a pseudorapidity range of  $|\eta| < 2.5$ . The magnetic field results in curved trajectories enabling an estimate of momentum and charge.[leo]

Pixel detectors are based on ionisation of charged particles in the semiconductor material. The induced charged is picked up by the detector's pixels providing a position information. To provide a 3-dimensional trajectory the pixel-chips are ordered in 4 layers around the beam pipe where the layer closest to the point of interaction called Insertable B-Layer (IBL) was added in 2015. It is located only 3.3 cm from the beam pipe and allows to detect vertices very close to the interaction point mainly originating from  $b$  quarks giving the layer its name. [10]

The SCT as a silicon microstrip detector is the second silicon-based tracker immediately following on the pixel detector. It consists of modules of four silicon strip sensors organised in four barrel layers and eighteen planar endcap disks.

The TRT is structured in straw tubes each tube being an individual drift chamber with a strong potential difference due to negatively charged walls. The tubes are filled by a gas mixture

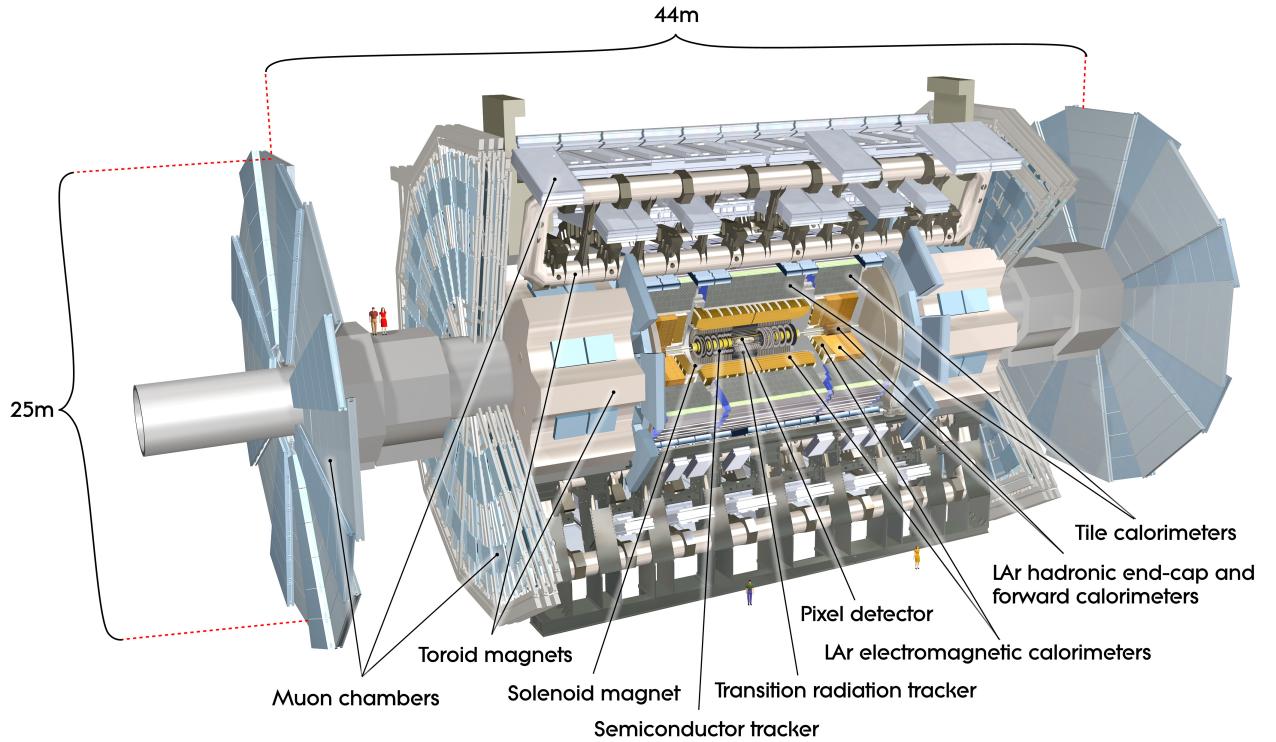


Figure 3.3: Sketch of the ATLAS detector and all its components including two average humans for scale. [9]

(xenon or argon) causing transversing charged particles to ionize and then be accelerated to the walls. A cascade is initiated and a measurable signal in the potential difference is measured. Between the tubes material is inserted resulting in transition radiation. This radiation has a cross section way higher for electrons thus adding particle information to the track information provided by the TRT.

A particle being detected in a layer of the ID is called a hit. The record of hits gives an estimate on the particle's trajectory and can thereby also give information on the vertex the particle originates from. This vertex information is worth mentioning as for an experiment with an event count as large as the ATLAS experiment's events interfere and information from so called pileup events can affect the event's information. As pileup originates from different events it can be separated from the event of interest by separating the vertices.

### 3.2.2 The ATLAS calorimeter system

The ATLAS calorimeter system is divided into three main parts. The electromagnetic (EM) calorimeter, comprising a barrel and two end-caps, and the hadron calorimeter, built by a tile calorimeter, consisting of a barrel and two so called "extended barrels", and the hadron end-caps. The third part is the forward calorimeter which additionally focuses on electromagnetic interaction. The tile calorimeter is scintillator-based apart from that the main part of the

calorimeter system is based on liquid argon. The components cover a pseudorapidity range of  $|\eta| < 4.9$

Calorimeters determine a transversing particle's energy by exploiting the formation of particle showers. [8] Due to inelastic collisions in the detector's material the energy of the original particle is distributed on a cascade of secondary particles finally stopped by ionization. The resulting charge or photons can be picked up as an estimate of the initial energy.

Electromagnetic calorimeters exploit the energy loss of electromagnetic interacting particles in matter. Mainly photons and electrons loose their energy based on pair production and Bremsstarhlung respectively. The energy loss initializes a cascade of particle decays called an electromagnetic shower. The decay stops when the shower particles do not hold sufficient energy for a decay anymore. The energy of the final state shower particles is picked up by the detector representing the initial particle's energy. The ATLAS ECAL is a sampling calorimeter, built of two alternating layers of absorber and detection layer. In the absorber the showers are induced to then be detected in the detection layers. shape, size, precision

As the ECAL uses electromagnetic showers the hadronic calorimeter depends on hadronic shower evolution. Hadronic showers are initialized due to ionisation or strong interaction with the material's nuclei. If the resulting particles still interact with the material a shower evolves.

shape size precision

### 3.2.3 The Muon spectrometer

The second tracking detector of ATLAS is the muon spectrometer which is the outermost part of the detector. The task of the spectrometer is to detect charged particles transversing the calorimeter without being stopped or deploying their complete energy, and to do both collect trigger information and information on trajectory and momentum. Due to these two tasks the spectrometer is bifid with the first part being the trigger chamber covering a range of  $|\eta| < 2.4$ , followed by the high-precision chamber with a range of  $|\eta| < 2.7$ . The main detector's support feet cause a further gap at about  $\phi = 300^\circ$  and  $\phi = 270^\circ$ .

Normally the only charged particles left to be detected in the muon spectrometer are muons giving the component its name and allowing to provide good trigger information for researches interested in muons in the final event topology.

### 3.2.4 The ATLAS coordinate system

The ATLAS coordinate system is a right-handed and right-angled coordinate system with the  $z$ -axis pointing along the LHC's beam pipe. The corresponding transverse plane is defined by the  $x$ -axis pointing towards the ring's centre while the  $y$ -axis points upwards. The origin of the system is defined by the nominal point of interaction. The polar angle  $\theta$ , is the angle between the  $z$ -axis and the  $x$ - $y$ -plane and the azimuthal angle  $\phi$  is the angle between the  $x$ - and the  $y$ -axis.

Alternatively, as in this work, an event's topology is described by the azimuthal angle  $\phi$ , the pseudo-rapidity  $\eta$ , and the transverse momentum  $pT$ . The pseudo-rapidity replaces the polar angle and is defined as

$$\eta = \frac{1}{2} \ln \left[ \tan \left( \frac{\theta}{2} \right) \right]. \quad (3.1)$$

The transverse momentum is defined by

$$pT = \sqrt{p_x^2 + p_y^2} \quad (3.2)$$

where  $p_x$  and  $p_y$  are the momenta along the corresponding axes.

The angular variables are defined within

$$\eta \in [-\infty, \infty], \phi \in [-\pi, \pi]. \quad (3.3)$$

This cylindrical system makes use of the shape of the ATLAS detector and the momentum conversation of the transverse plane due to it being perpendicular to all initial beam momenta.

### 3.2.5 Particle Detection in the ATLAS detector

This section focuses on the detection and distinction of different particle types in the ATLAS detector. The capability and combined information of the detector components is introduced giving an explanation of the general working principle and also of the characteristics defining the events in this work. Figure 3.4 gives an overview of typical particle interactions and detections.

In order to reconstruct the particles in an event low level information is gathered using the direct detector output and then associated to the higher level particle information.

The information from the ID is called a track and contains not only the trajectory but also how consistently a track has hits in every layer. A track offers momentum and charge information and can be associated with a vertex and a possible energy deposition in a calorimeter. The vertex reconstruction arising from the track information allows to define a primary vertex defined by the highest sum of squared transverse momenta while additional vertices are identified as pileup vertices. Secondary vertices originating from tracks connected to the original vertex can be collected to identify short-lived particles.

The calorimeter data is summarised in clusters. Clusters are neighboring calorimeter cells with energy depositions significantly higher than the expected noise. A cluster is formed around a high energy deposition and can be associated to hadrons or jets or even to a corresponding track.

## 3.3 Monte Carlo Simulation

A Monte Carlo simulation is

detector simulation runs on top of Monte Carlo simulation

Simulations are based on cross sections which can be calculated and measured in units of BARN where  $1 \text{ b} = 1 \times 10^{-28} \text{ m}^2$

Simulations heavily rely on quantities than can both be calculated and measured in an experiment thus allowing for predictions and also for controlling the theoretical values. In high energy particle physics there are mainly two such quantities cross section and branching ratio

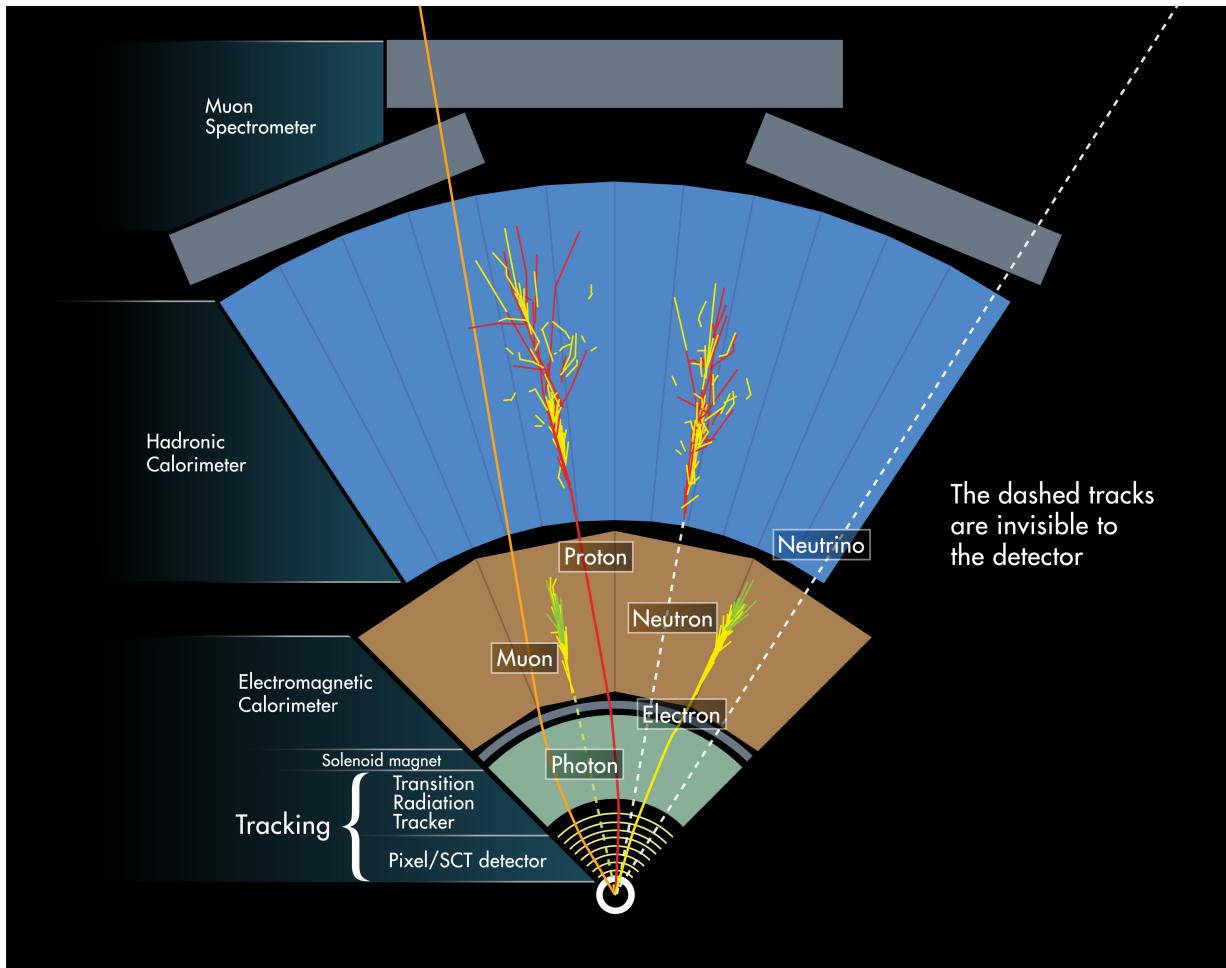


Figure 3.4: Scheme of the ATLAS-detector showing examples of typical particle detections. [9]

In collisions not only the valence quarks but also the sea quarks are relevant which can be explained by the valence quarks radiating gluons and quark antiquark pairs with no net flavour change. also explains the mass

### 3.4 $tW$ event topology



# CHAPTER 5

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## Machine Learning

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### 5.1 The concept of machine learning

For many decades computers have been an integral aspect of science, handling large amounts of data, completing tedious calculations and controlling experiments. For the most part the machines were assigned discrete tasks. They followed step-by-step commands previously designed by human users and had expected outcomes. For particle physics in particular, computers have been used to select and process interesting data from large samples, making the processing of data possible at speeds beyond human capabilities. However the selection rules always had to be generated by the user, therefore requiring an in depth understanding of the underlying system. Machine learning presents a way for a program to establish its own decision rules, improving these over several iterations and thereby learning to solve the problem by itself.

There has been a great effort over the last decades trying to implement a way for machines to learn from known quantities and thereby enable them to analyse complex tasks ranging from voice recognition to object classification. The efficiency and validity of a machine learning model is highly dependent on the human understanding of the problem at hand. The prerequisite to a successful model is the tuning of the degrees of freedom and parameters to the complexity of the assignment. This is called *hyperparameter optimisation*, a task often proportional to the learning process itself.

Machine learning can be exemplified by drawing an analogy to human beings. In order to solve a problem, the machine must understand the system, evaluate a decision step and generate new decision steps. Understanding a system means to be aware of all features and possibilities relevant to the task. Humans have their senses to easily break down their observations into useful features and concepts that can then be processed for decision making. A computer has no senses built in and for most tasks this means that the step of filtering information for a relevant subset of features has still to be done by humans or a good preprocessing algorithm. Once a system has been converted to a subset of features usable by a computer, the step of making its own decisions has to be implemented. This can be done by weighting and interconnecting the information using structures inspired by neurons and synapses in the human brain.

The structure and complexity of the network enables it to learn from data. In addition, a

metric is introduced that measures the quality of the model, called the *cost* or *loss function*. This function allows the network to improve iteratively as a decrease in its value is considered an improvement by the network. Combined with an optimiser which suggests further steps, this function is a basis for a network to independently approach a good decision rule for a somewhat uninvestigated topic.

A very commonly used machine learning technique is the artificial neural network which on its own forms a broad field that builds the base of this work. The most important concepts of machine learning will be explained in the context of neural networks.

## 5.2 Neural Networks

The artificial neural network, or just neural network, is one of the most commonly known approaches to machine learning. Its structure is inspired by the neurons forming the human brain which is also where it gets its name from.

Instead of neurons, a neural network consists of numerous very simple processors, called nodes. These nodes are usually structured into several layers. As presented in fig (todo). In addition to that there are several ways to structure and connect these nodes often times matching a certain problem. In this explanation only the most commonly way is explained. In that case each node of a layer is getting input from each node in the last layer and is outputting to each node of the following layer. Such a network structure is shown in figure 5.1. It describes the step between a node and the previous layer. The underlying math will be explained in detail later. This is called a feed-forward neural network.

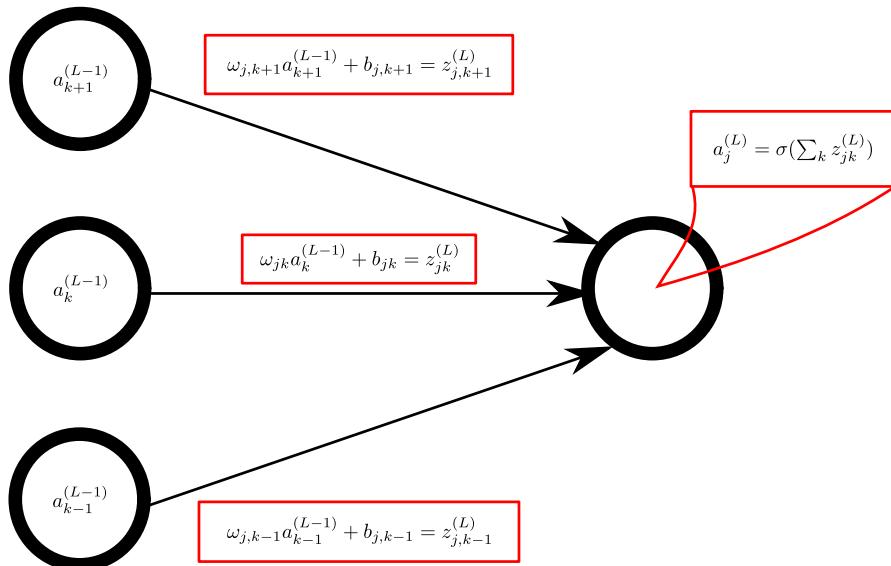


Figure 5.1: Network propagation from layer  $(L - 1)$  to layer  $L$

## The input layer

To understand a task and draw reasonable conclusions first the underlying system has to be understood. Its features need to be found and summarised. The human brain is capable of investigating unknown systems and learn the features that are the most unique or interesting. For that it has its senses to explore the system and process them later. To allow a machine to do something similar the unknown system has to be represented in a way that it is clear for the network what to look out for. This is usually the task that needs the most preprocessing by the user. The simplest case is to submit a list of variables to the network. In particle physics this could be kinematic variables of the final partons in an event. The input to a neural network is just given to the input layer of nodes and then processed through each following layer. For different tasks different layers might deal with different parts of the information but in this work the linear way of giving all information used to an input layer and then processing it is used.

## Decision making process

Computers being not much more than very powerful calculators, excel at performing high numbers of clearly defined calculations. The trick is that the task has to be defined clearly. There usually is no uncertainty.

This is very different for the human brain. We rely on a certain uncertainty when processing information through a net of neurons where the output of every neuron is taken as input for the surrounding neurons. The challenge of machine learning is to represent this fuzziness by many somewhat discrete calculations. In the neural network the neurons and their fuzzy interaction is represented by the nodes which are very simple processors. Like neurons each node can use input from many other nodes to create a new output signal. Thereby the input information can be linked to each other in numerous ways. Combined with a weighting system this allows to create complex models and match a variety of problems.

The input of every node is the weighted output of all previous nodes as shown in equation (5.1).  $z_j^L$  is the input to the  $j$ -th node in the  $L$ -th layer.  $\omega_{jk}^L$  is the weight from the  $k$ -th node in the previous layer to this node,  $a_k^{L-1}$  is that node's output and  $b_k$  the relevant bias, representing a possible intercept of the functionality. The sum indicates that all  $k$  previous nodes contribute to the input to the  $j$ -th node.

$$z_j^L = \sum_{k=0}^N \omega_{jk}^L a_k^{L-1} + b_k \quad (5.1)$$

The weight allows to predict which variables are linked to each other or allow for better decision rules when combined but also easily to weight the importance of features. Furthermore the output of each node is a non-linear combination of the input. This means the output can range from just one and zero to an exponential function and is called the activation function of a node. A common choice is the sigmoid function as presented in equation (5.2). [11]

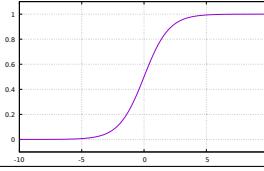
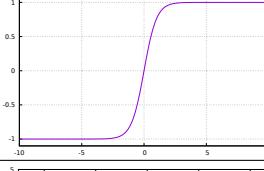
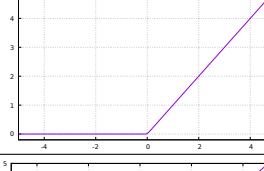
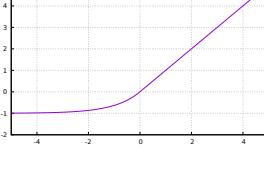
Name	Function	Plot
Sigmoid	$f(x) = \frac{1}{1+e^{-x}}$	
Tangens Hyperbolicus	$f(x) = \frac{2}{1+e^{-2x}} - 1$	
Rectified Linear Unit, RELU	$f(x) = \begin{cases} 0 & \text{if } x < 0 \\ x & \text{if } x \geq 0 \end{cases}$	
Exponential Linear Unit, ELU	$f(x) = \begin{cases} \alpha(e^x - 1) & \text{if } x < 0 \\ x & \text{if } x \geq 0 \end{cases}$	

Table 5.1: Selection of activation functions taken from the Keras documentation. [11]

$$a_j^L = \sigma(z_j^L) = \frac{1}{1 + e^{-z_j^L}} \quad (5.2)$$

The sigmoid function has output between 0 and 1 which is often times what one wants for nodes especially for the final layer as we are looking for predictions of outcome probabilities. A selection of further activation functions is shown in table 5.1.

For this thesis especially the exponential linear unit or *elu* and the rectified linear unit or *relu* were tested. *Elu* is good for converging the cost to zero rather fast and has the possibility of negative output. *relu* allows for the same benefit as sigmoid while requiring less computational power for the simply linear output for positive values.

Of course the network does still not know the task assigned to it but if we add a cost function to estimate the quality of a decision rule created by a certain combination of the input we can easily make the network approach a better decision rule and hopefully the solution of the problem as the cost function just needs to be minimised. In this work the cost function will be called the loss of the model.

In supervised learning the network is trained with a set of known data. Each event of the training set has a label representing the true outcome value referred to as just label or truth label. Comparing this truth information to the network output makes it very easy to calculate the loss as the deviation of the network output from the desired truth output. A possible loss function is the crossentropy or just binary crossentropy for a binary output result. As in this work the

result is binary, signal and background, the binary crossentropy is the natural choice. Equation (5.3) shows the underlying function where  $p$  is the estimated probability for the outcome  $\hat{y}$  and  $y$  is the label for a correct or incorrect guess.

$$C = -(y \log p + (1 - y) \log(1 - p)) \quad (5.3)$$

The loss is the most important observable for the training quality. This quality must not be mixed up with the overall quality of the model as for the loss only the data trained on is taken into account but not a test data set.

### Optimizers - Choosing the next step

The probability interaction of the nodes combined with the loss function enables a network not only to create a model but also to evaluate it. The last missing part is an algorithm that can estimate a step to a model that further minimises the loss. One could certainly do this randomly until the network finds a very low costed decision rule if infinite computational power were provided but that would neither be an efficient nor the desired learning process.

The output of each node in the final layer is defined by the weighted and biased information of the previous nodes and lastly the activation function. For one connection therefore there are three variables that have impact on the loss. Summarising this information for all nodes in a vector defines the loss-vector. The gradient of this vector is an estimator for the impact of each parameter on the overall loss and thereby gives a preferred direction for the model. Updating a network's parameters based on this gradient is called backpropagation. The algorithm works as follows:

1. A certain set of input variables is iterated through all layers of a network resulting in an estimator  $\hat{y}$  at each output node.
2. The sum of deviations from the true value at all output nodes is determined as the loss  $C$  of the setup. The loss just defines how good the model is.
3. The gradient of the loss is calculated as the partial derivative of all network parameters

$$\frac{\partial C}{\partial a_k^{L-1}} = \sum_{j=1}^N \frac{\partial z_j^L}{\partial a_k^{L-1}} \frac{\partial a_j^L}{\partial z_j^L} \frac{\partial C}{\partial a_j^L}$$

4. The parameters are then updated backwards through the layers following the negative loss gradient.

This backpropagation algorithm is the backbone of the neural network's learning process.

The decision step based on the gradient defined above is specified by the networks optimizer and deserves a bit more attention. There are different choices of optimisers trying to accommodate different problems as well as some parameters important to understand and tune for an effective training. The length of a learning step has to match the problem's topology to properly let the

model converge. First we define the gradient  $g$  in a more general way. The batch size is  $m$  and stands for the amount of data processed to evaluate the next step.  $f$  is the network for a current configuration or model  $\theta$  and the output  $\hat{y}$ .  $\theta$  summarises all the parameters optimised by the network during the training. The output target provided by the truth information is  $y$ .

$$g = \frac{1}{m} \nabla_{\theta} \sum_j L(f(\hat{y}^j; \theta), y^j) \quad (5.4)$$

The configuration  $\theta$  is then updated using the gradient and a constant  $\eta$  called the learning rate as it determines the step size for each update.

$$\theta' = \theta - \eta g \quad (5.5)$$

Optimisation processes like this are gradient descent based optimisers and can be considered the basis of all optimisers. Depending on the choice they might be based on the whole training sample or just a mini batch of the sample. The most basic form has the learning rate as its only hyperparameter. A good learning rate should be small enough to avoid oscillations but high enough to approach a minimum efficiently fast. A good estimate is given by the Robbins Monro condition:

$$\sum_k \eta_k = \infty \quad (5.6)$$

$$\sum_k \eta_k^2 < \infty \quad (5.7)$$

As the choice of learning rate will not be perfect for every part of the problem's topology, momentum  $v$  can be introduced as a second parameter to the optimizer. [11] The effect desired is that the stepsize becomes greater when the slope is long and the minimum is still far away and to be shorter when approaching the minimum. Momentum scales each step by how aligned previous steps were. That means it will allow avoiding local minima or moving slowly along a slope by enlarging steps at the beginning of the training but also will slow down at the end of the training when the steps become shorter. It promises to speed up the training with less risk of large oscillations which a large learning rate would probably result in. Momentum also takes a single scaling hyperparameter  $\alpha$  and is updated each step following:

$$v' = \alpha v - \eta \frac{1}{m} \nabla_{\theta} \sum_j L(f(\hat{y}^j; \theta), y^j) \quad (5.8)$$

$$\theta' = \theta + v' \quad (5.9)$$

Alternatively one can use Nesterov momentum [11] which is a more advanced adoption of momentum and updates the step a further time after applying the gradient:

$$\nu' = \alpha\nu - \eta \frac{1}{m} \nabla_{\theta} \sum_j L(f(\hat{y}^j; \theta + \alpha \times \nu), y^j) \quad (5.10)$$

$$\theta' = \theta + \nu' \quad (5.11)$$

Lastly it can be helpful to decrease the learning rate of the network stepwise while approaching a minimum to avoid oscillations or leaving the minimum in general further. This can be accomplished by the hyperparameter of learning rate decay. It just decreases the learning rate in each iteration  $t$  by a small hyperparameter  $\phi$  following the assumption that smaller steps are sufficient close to the minimum. [11]

$$\eta' = \frac{\eta}{1 + \phi t} \quad (5.12)$$

### Adaptive optimisers

In addition to the purely gradient based optimisers there are adaptive optimisers. Learning rate and momentum as previously described are difficult to tune to every part of the training process as the topology of the problem might rapidly change. Therefore adaptive optimisers update their parameters based on the training process. There is a set of adaptive optimisers. [11] Often the adaptive optimiser of choice is ADAM. [12] ADAM updates both, its learning rate and its momentum over the course of the training based on an exponentially decaying average of past gradients and past, squared gradients. The average makes sure that the parameters keep getting updated based on past steps. They should be decaying as otherwise the parameters would rapidly shrink. The decay of the averages is defined by a hyperparameter  $\beta$ .

$$\hat{g}^2 = \frac{\sum g^2}{1 - \beta_1^t} \quad (5.13)$$

$$\hat{g} = \frac{\sum g}{1 - \beta_2^t} \quad (5.14)$$

The model's parameters are then updated according to:

$$\theta' = \theta + \frac{\eta}{\sqrt{\hat{g}^2 + \epsilon}} \hat{g} \quad (5.15)$$

ADAM is often considered a very good algorithm as it contains many corrections to hyperparameters during the training and thereby allows for easier optimisation but it also needs more computational power.

## 5.3 Regularisation and Optimisation

Fluctuations and noise in the training sample can be a big problem for a model trained on the sample as a neural network might pick noise and random fluctuations up as features for the decision rule.

This basically is the process of overfitting. The network observes way more features to work with than those actually present in reality or even in a different test sample. The most extreme scenario is that your network is large and deep enough to pick up every single feature in the training sample. If that happens the training error becomes very low and indicates a very good decision rule. For a different sample this decision rule is at most very unreliable but probably strictly wrong resulting in a high test sample error. The network just picked up and remembered every single feature in the training sample instead of general correlations. It becomes a mask of the sample.

A possible way to solve this issue is to stop the training early or to find a good way when to stop the training. This way noisy features might not yet have been picked up by the training. Then again this might also lead to a suboptimal result of the overall training as one cannot be sure that the correct features always get picked up first.

More sophisticated approaches are called regularisations of a neural network. The most commonly used solution is a so called Dropout layer described in the subsection 5.3.1. Additionally a batch normalisation can have an effect of regularisation and is therefor introduced in this section as well.

### 5.3.1 Dropout

Dropout is attempting to keep the network from relying on subdominant features too much by removing different nodes in each iteration. This forces the network to build models that are not based on strong correlations between nodes. The weights become less interdependent. To simplify it a lot it means training several neural networks depending on which nodes are turned on during a training epoch. It keeps the training in motion for a large number of epochs.

Dropout is added to each layer of a network and can also be restricted to a subset of layers too. It slows down the training as the additional motion slows down the process of finding a minimum but it also accelerates each epoch slightly as it simplifies the network architecture.

### 5.3.2 Batch normalization

In supervised learning the training result is heavily dependent on the set of data the network is trained on. This means that the performance might change a lot when the test data is very different. Imagine a classifier distinguishing between pictures that show cars and pictures that do not show cars. If the training set contains predominantly green cars the colour green might end up as a strong indicator for the classification car. In general the colour green will not be as dominant and the network will perform slightly worse when trying to classify cars of a different colour. Formally such a change of input is called a covariance shift.

A way to reduce the effect of covariance shift is batch normalization. The output of nodes in general and the weight of a connection in a neural network is not necessarily limited allowing

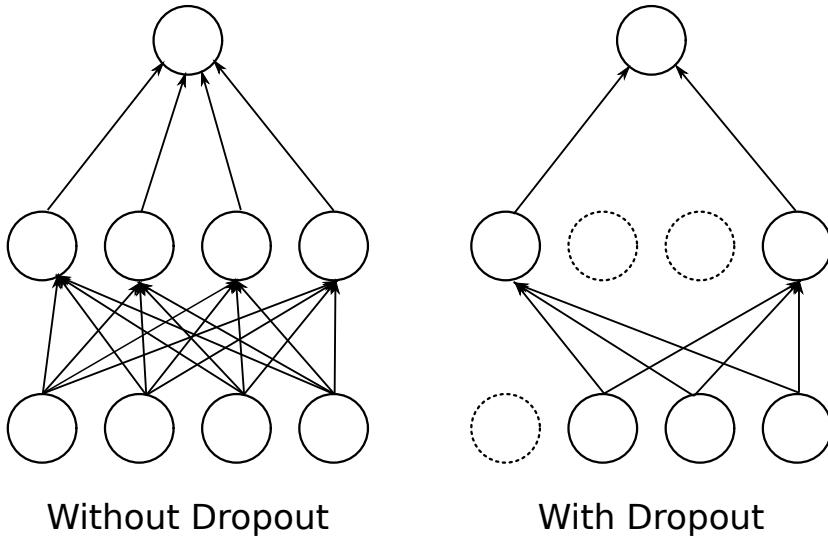


Figure 5.2: Sketch of network before and after the inclusion of dropout. On the left hand side dropout is not applied and all nodes are connected. On the right hand side the dashed circles are nodes excluded by dropout and therefore not connected to the other nodes.

for certain connections to be really dominant and overshadowing less dominant features. We want to avoid this as the dominance of some features might just be present in the training sample. This can be achieved by normalizing the output of each layer in the network to the total output and thereby minimising the effects of strongly overrepresented features. This is done by normalizing each output to the mini-batch mean  $\mu_B$  and the mini-batch standard deviation  $\sigma_B^2$ .

$$\mu_B = \frac{1}{m} \sum_i x_i \quad (5.16)$$

$$\sigma_B^2 = \frac{1}{m} \sum_i (x_i - \mu_B)^2 \quad (5.17)$$

$$x_{i,norm} = \frac{x_i - \mu_B}{\sqrt{\sigma_B^2 + \epsilon}} \quad (5.18)$$

## 5.4 Adversarial Neural Networks

This main part of this work is the examination and training of an adversarial neural network. An adversarial neural network consists of a classifier and a second network that tries to regularise the output of the first classifying network.

In this section the concept of an adversarial neural network is motivated and the underlying mathematics as originally stated in paper [13] are presented. For more information about an approach directly tested on physics see the paper "Learning to Pivot with Adversarial Networks". [14]

### 5.4.1 The adversarial neural network

Neural networks have been very efficient for classifying tasks but less successful for generative tasks. This was the original problem that gave birth to the idea of a generative adversarial network. Generative networks often times have output that is very easy to distinguish from real samples. The solution suggested is adding a classifier that tries to distinguish between generated samples and real samples. As long this adversary is able to accomplish this task the first network fails at its generative task. Training the two networks against each other disincentives the generative network from using the features not dominant in real samples.

In this work the first network is not a generator but a classifier separating signal events from background events in a Monte Carlo simulation. These simulations contain systematic uncertainties and different samples represent a set of plausible data generation processes. The classifier should not be too dependent on variables with high systematic uncertainties as the network cannot account for differences in the training and testing sample or even in rel data. If the classifier has these strong dependencies on systematic uncertainties it might lead to a high co-variance shift.

Instead of a generated sample and a truth sample, a so called nominal sample and systematic samples are used as input for the second network. Systematic samples have slightly different distributions than the original samples because of changes to the variables with the systematic uncertainties. Training the second network on determining whether it is looking at a nominal or a systematic sample allows to estimate how dependent the model is on variables with high systematic uncertainties. Training the classifier against the adversarial network promises to reduce the effect of systematic uncertainties on the model. If the topology of the problem allows for it this should make the model generated by the classifier pivotal. That means it does not depend on the unknown values of the nuisance parameters.

Mathematically this comes down to a minimax decision rule or a competition between two neural networks. Let us call the classifier  $Net1$  and the adversary  $Net2$  then the problem becomes:

$$\min_{Net1} \max_{Net2} V(Net1, Net2) = \mathbb{E}_{x \sim \rho_{data}} [\log Net1(x)] + \mathbb{E}_{z \sim \rho_{sys}} [\log(1 - Net2(z))] \quad (5.19)$$

$V(Net1, Net2)$  is the combined value function for the two adversary networks. The first network is trained to be an optimal classifier represented by  $\log Net1(x)$  while the second network is trained to distinguish between the nominal and systematics distribution  $z \sim \rho_{sys}$  represented by  $\log(1 - Net2(z))$ .

In theory the first classifier should be trained slowly and kept close to its optimum while the second network slowly learns and allows the first network to adapt to it. This is achieved by training the two networks successively over multiple iterations using a combined value function. As this value function a combined loss function is used. It is just the difference between the two separate loss functions with a hyperparameter  $\lambda$  to control the impact of the adversary as shown in equation (5.20).

$$\mathcal{L} = L_{net1} - \lambda L_{net2} \quad (5.20)$$

In the first step of each iteration the first network is trained using the combined loss function  $\mathcal{L}$ . In the second step the second network is trained using its simple loss function  $\lambda L_{net2}$ . Each of the networks has the usual set of hyperparameters to optimise explained in detail in the previous sections missing.

In this work the adversarial network is setup by building a classifying network. The information of the classifier is then fed into both the classifier's output layer and the adversarial network creating a second model based on the first network's model. The networks are then trained successively controlling the combined and separate losses. Figure ?? shows a sketch of the setup.

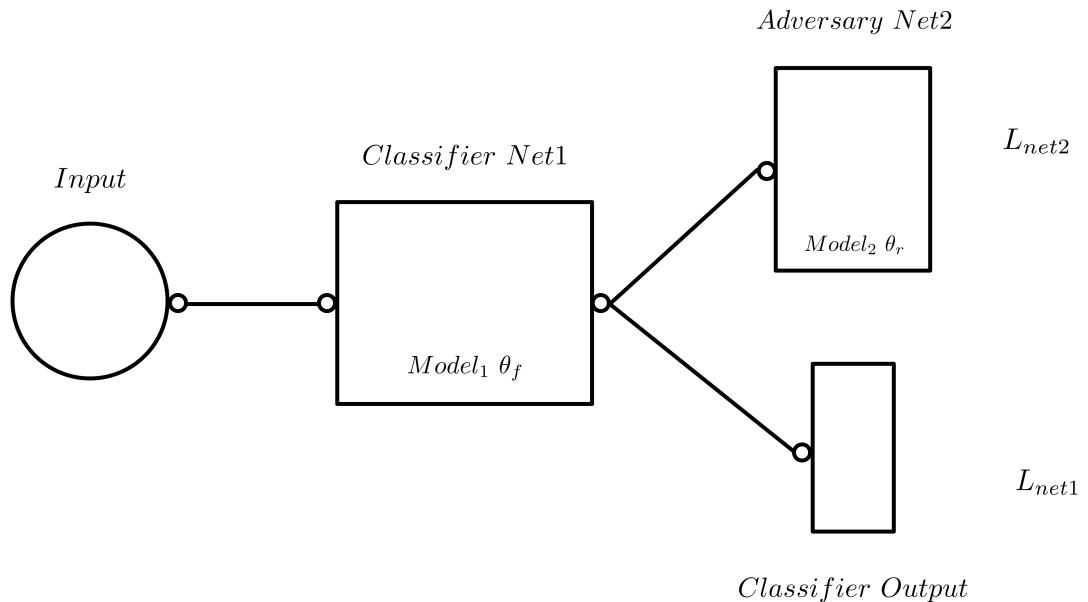


Figure 5.3: Sketch of the network setup. The main part is the classifier. The model generated is fed into both the second network and the classifier's output. This way the two losses  $L_{net1}$  and  $L_{net2}$  are generated. Furthermore the training of the classifier immediately affects both output models.

The hyperparameter  $\lambda$  is set to tune the impact of the second network on the model. A large  $\lambda$  leads to a very pivotal model but can also decrease the overall quality of the classifier.

In order to better understand the figures shown in chapter ?? the three loss values of an adversarial neural network will be introduced as the last part of this chapter. The first loss belongs to the classifier and is expected to first increase as the adversary finds a good model and to decrease once a more pivotal model is found. The second loss displays the adversary's performance ideally decreasing at first to then increase and saturate as a pivotal model renders it impossible to extract any information. Lastly the combined loss is displayed showing the overall performance and decreasing as good models are found for both the classifier and the adversary. Figure 5.4 shows an example for this loss functions taken from the paper "Learning

to Pivot with Adversarial Networks". [14]

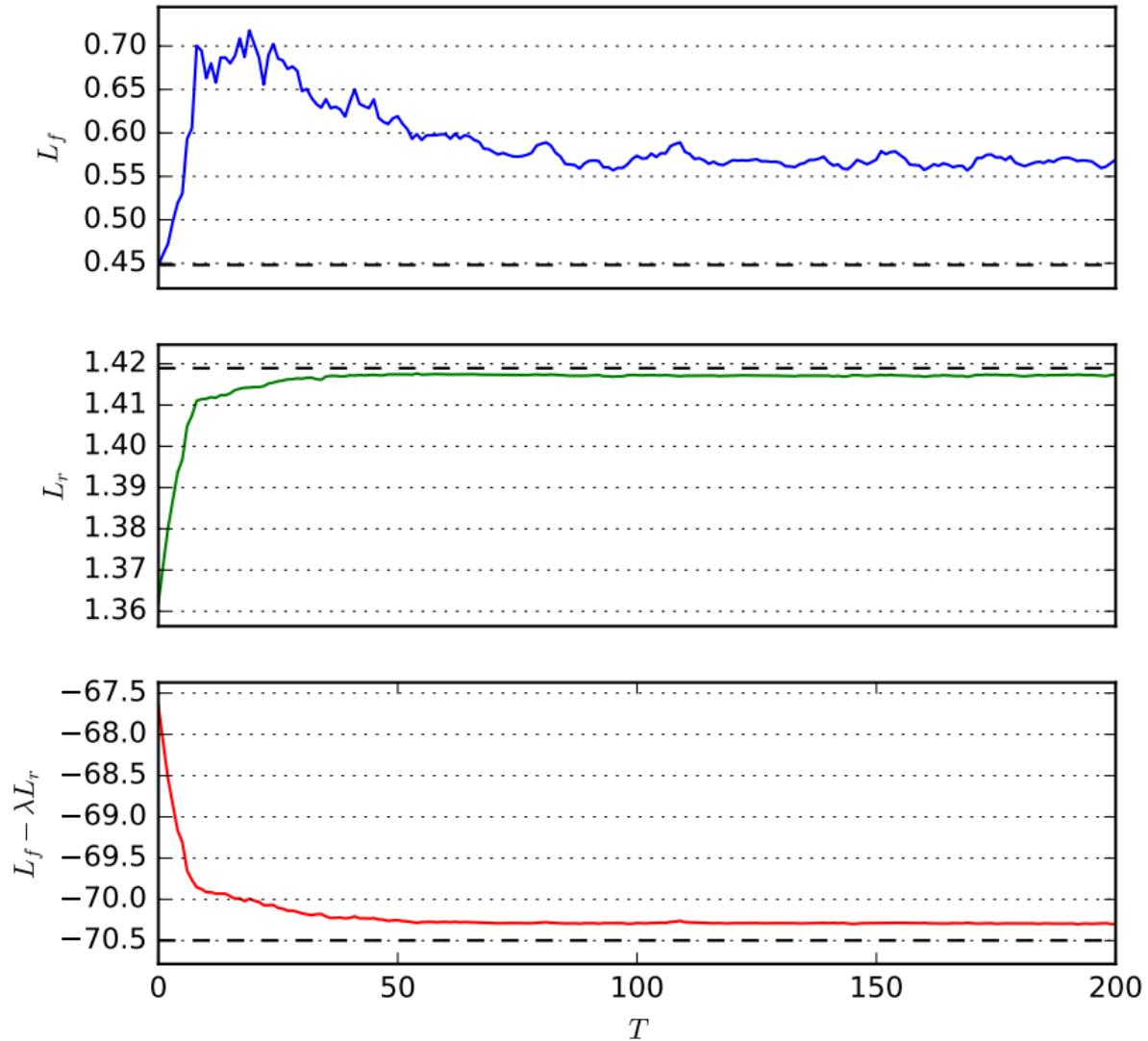


Figure 5.4: Three losses of an adversarial network for  $\lambda = 10$  taken from a toy example. [14] From top to bottom the classifier, adversary and combined loss is presented.  $T$  is the number of training iterations.



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# List of Figures

---

2.1	Standard Model particles . . . . .	6
3.1	Sketch of the LHC accelerator complex . . . . .	8
3.2	Sketch of the LHC ring. . . . .	9
3.3	Sketch of the ATLAS detector . . . . .	10
3.4	Scheme of the ATLAS-detector's detection procedure . . . . .	13
5.1	Network parameter nomenclature . . . . .	16
5.2	Dropout Sketch . . . . .	23
5.3	Adversarial setup sketched . . . . .	25
5.4	Exemplary loss of an adversarial network structure . . . . .	26



# List of Tables

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5.1 Selection of activation functions taken from the Keras documentation. [11] . . .	18
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