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# Masters Dissertation

## PHY5008W

The Application of Machine Learning Techniques towards the Optimization of High Energy Physics Event Simulations in the at

† A Large Ion Collider Experiment

‡ European Organization for Nuclear Research/ Organisation Européenne  
pour la Recherche Nucléaire

͛ Transition Radiation Detector

# Submitted in Fulfilment of the Degree: MSc Data Science



Contents

[Background 3](#_Toc526453772)

[A Large Ion Collider Experiment (ALICE) 3](#_Toc526453773)

[Introduction to the ALICE Experiment 3](#_Toc526453774)

[The ALICE Transition Radiation Detector (TRD) 3](#_Toc526453775)

[Existing Particle Physics Software 6](#_Toc526453776)

[Data Analysis Framework: ROOT 6](#_Toc526453777)

[ALIROOT 6](#_Toc526453778)

[Generative Adversarial Networks 7](#_Toc526453779)

[Introduction to Generative Adversarial Networks 7](#_Toc526453780)

[Mathematical Theory 7](#_Toc526453781)

[Application of GANS to High Energy Physics Problems 14](#_Toc526453782)

[Motivation 14](#_Toc526453783)

[Research Question 14](#_Toc526453784)

[Aims & Objectives 14](#_Toc526453785)

[Methods 14](#_Toc526453786)

[Bibliography 15](#_Toc526453787)

# Abstract

# Background

## A Large Ion Collider Experiment (ALICE)

### Introduction to the ALICE Experiment

A Large Ion Collider Experiment (ALICE) is a large scale collaborative experiment dedicated to studying all collisions involving heavy ions at the Large Hadron Collider (LHC) at CERN (European Organization for Nuclear Research) (1).

In central high energy collisions between heavy ions (i.e. where the centres of colliding nuclei overlap sufficiently), a newly discovered deconfined state of strongly interacting matter, the Quark Gluon Plasma (QGP) can be created in small amounts (1). It is thought that this state of matter was dominant during the first 10-6 s of the Universe’s existence (2). Studying the QGP allows us to explore fundamental research avenues such as Cosmology, the Evolution of our Universe, and one of the fundamental forces in the standard model that is the hardest to probe: the strong nuclear force (2).

ALICE is the first experiment in history capable of producing the QGP in a laboratory setting; and as such, it is equipped to infer a variety of physical variables relating to the QGP, by analysing data from electrons produced during many of the physical processes that occur in the wake of heavy ion collisions, e.g. open heavy-flavour hadron decays, virtual photons, etc (1). Robust electron identification is therefore a crucial part of studying the QGP, and accurately-tuned detector triggers ensure the collection of sufficient amounts of data to guide inferences regarding the statistical distributions of the abovementioned measurables (1).

### The ALICE Transition Radiation Detector (TRD)

#### Introduction to the TRD

The main purpose of the ALICE Transition Radiation Detector (TRD) is the identification of electrons, as well as the operation of event triggers that determine whether data from a specific collision should be kept, based on measurements such as collision centrality, amongst others. As an added benefit, the TRD informs the ALICE central barrel’s calibration, and the data it produces is used extensively during track reconstruction (1).

#### TRD Physical Properties

The TRD is located within the ALICE central barrel, it’s inner boundary sits at a radial distance of 2.90 m from the beam axis. It contains 522 chambers, each of which contains a fiber/ foam radiator, a 3 cm drift region and a multi-wire proportional chamber (MWPC) filled with Xenon-; these chambers are arranged in a six-layer configuration (1). The position of the TRD within the ALICE central barrel is shown in *Figure 1*.

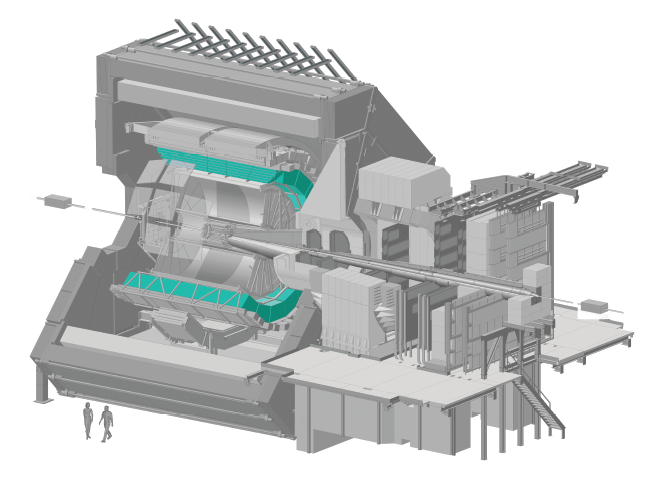


Figure 1: The ALICE TRD, Highlighted in Cyan, within the ALICE main detector (3)

#### TRD Measurement Mechanism

As the name suggests, transition radiation occurs when a particle transits across a dielectric boundary, this radiation is often measured in particle detectors to inform track reconstruction. Multiple boundaries are typically required to increase radiation yield, and since highly relativistic particles emit transition radiation that extends into the X-ray domain, the TRD utilizes gases with high proton-number (Z) to absorb this radiation, resulting in a high yield of energy deposition relative to the energy lost via ionization (1).

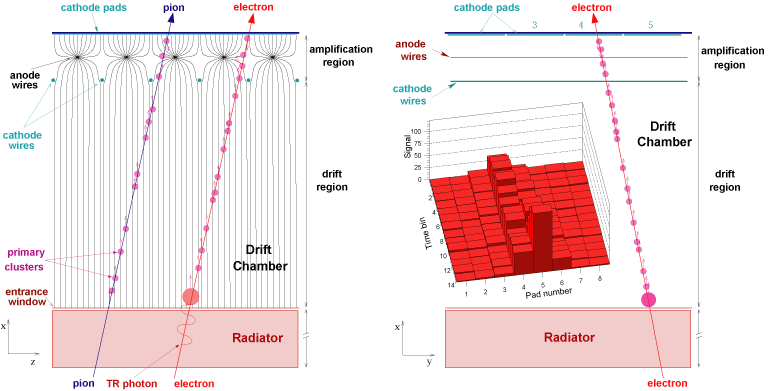


Figure 2: A schematic representation of the components in an MWPC Module (4)

The drift time of gas particles within the MWPC provides fine-grained positional information about where the particle tracklet passed through the radiator. The detected signal takes the form of charged gas molecules, ionized via interaction with transition radiation photons and amplified through a chain of interactions between gas molecules, finally being absorbed by a negatively charged wire (anode) (3), this process is depicted in *Figure 2*.

#### Identifying Electrons

The production of Transition Radiation, as well as a higher specific ionization energy loss , are two features that enable accurate differentiation of electrons from other charged particles; and the temporal data provided by the TRD further enhances the specificity and sensitivity of the electron identification process (1).

#### Current TRD Accuracy

Currently, at a momentum of around 1 GeV/*c*, a pion rejection factor of 410 is achievable in p-Pb (proton-Lead) collisions, with resolution improving by about 40% when TRD data is included in track reconstruction (1).

## Existing Particle Physics Software

### Data Analysis Framework: ROOT

ROOT is an open-source data analysis framework developed by the High Energy Physics (HEP) community; it is an object oriented platform, written in C++ and allows for storage of classes in a compressed binary file format (.root), as well as an object container class (TTree), which facilitates statistical analysis of large datasets via vertical storage methods, and enabling analysis across files on local disks, shared file systems, and the Worldwide LHC Computing Grid (WLCG) (5).

### ALIROOT

AliROOT is an extension of ROOT, used specifically by the ALICE collaboration. It is an integrated ecosystem consisting of event generators (PYTHIA6, HIJING, DPMJET and ISAJET), Virtual Monte Carlo simulators (Geant3, Geant4 and Fluka) and various steering classes for simulation and reconstruction; all of which sits upon the basic ROOT architecture, and which communicates via the ALICE Environment Grid Framework (AliEn) with the WLCG. This architecture is depicted in *Figure3* (6)*.*

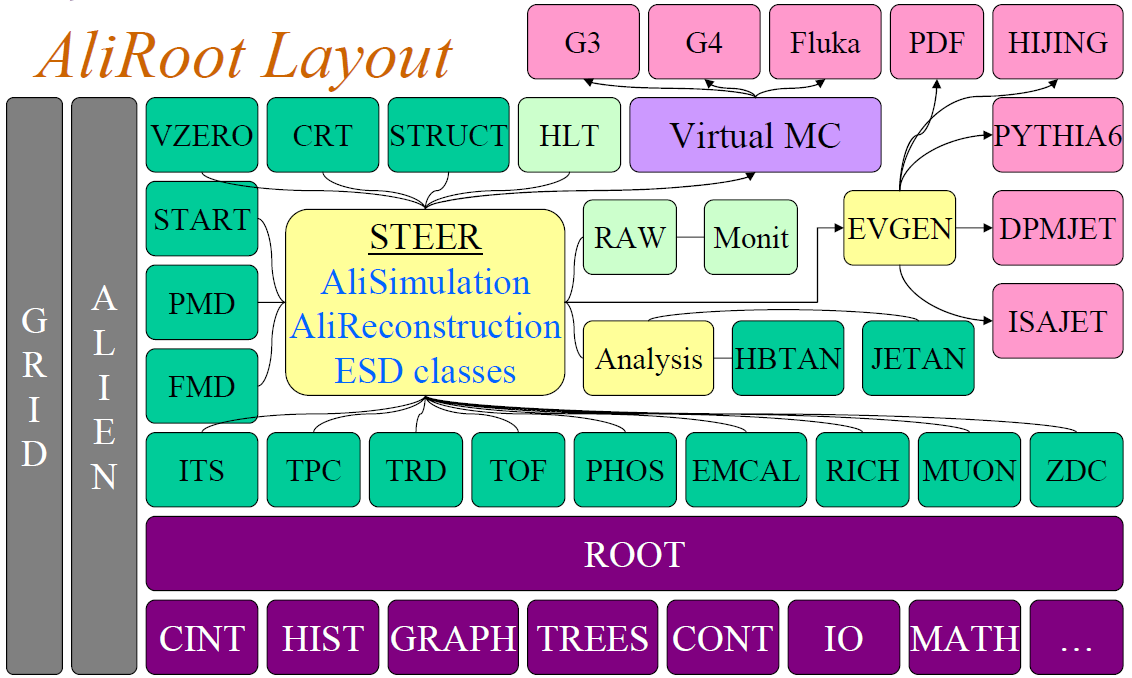


Figure 3: ALIROOT Ecosystem (6).

#### Integration with other Programming Languages

PyROOT and ROOT R are interfaces that allow seamless integration between ROOT and Python as well as R, respectively. Features include calling functions from any Python or R package within ROOT, translating datatypes between languages, as well as access to the R graphical system from within ROOT (7).

## Generative Adversarial Networks

### Introduction to Generative Adversarial Networks

In 2014, Goodfellow et. al. (8) proposed a novel implementation of Deep Learning, involving an adversarial mini-max game between two Artificial Neural Networks (ANNs), which they called Generative Adverserial Nets (GANs). A GAN model consists of two elements: a generative model G, and a discriminative model D. During training, G aims to maximize the loss function of D by accurately capturing the underlying distribution of the training data, and D estimates the probability of whether an observation fed to it is “real”, i.e. it is from the actual data distribution or “fake”, i.e. it was generated by G (8).

If both models are ANNs, they can be trained simultaneously via backpropagation, until a unique solution can theoretically be reached, where G accurately models the data distribution and D outputs 0.5 everywhere (8).

### Mathematical Theory

#### The Perceptron

The field of Deep Learning is based on the original idea of a “perceptron” proposed by Rosenblatt in 1958 (9), originally envisioned as a way to mathematically model neural information processing in the brain, it was not very successful in capturing the complexity inherent in neurobiological information processing, but very useful for learning non-linear patterns in data. ***Figure 4*** informs the mathematical theory that follows.

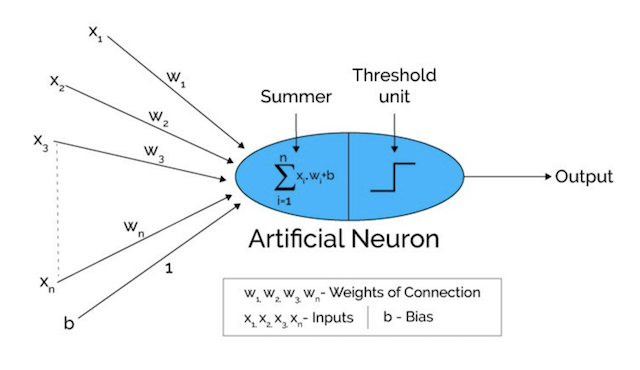


Figure 4: A Schematic Representation of a Single Perceptron (10)

In the figure above an observation , consisting of a vector of input features , … , is mapped to an estimated outcome variable: , by:

1. Multiplying each element of the input vector with the transpose of a corresponding vector of weights, i.e. of the same length as X, i.e. , …,
2. Summing the individual products of all the input features with their corresponding weights, and adding a bias term[[1]](#footnote-1):

Passing the result of step 2 (i.e. Z) through an “Activation Function” , where the function , is typically one of:

* 1. Rectified Linear Unit (ReLU):
  2. Sigmoid function:
  3. Hyperbolic Tangent (Tanh):

The result of is an estimate () for the outcome variable . And a simple cost function, such as the root mean squared error:

RMSE = ,

can be minimized via gradient descent to find the optimal values for and .

The original motivation for the use of the activation function is inspired by the way a biological neuron is triggered: it receives inputs from various other neurons, sums up their inputs and fires once a threshold is reached. Practically, in a deep learning set up non-linearities in the data can be captured by these activation functions, particularly when perceptrons are chained into multiple fully-connected layers, as is the case in Deep Learning, which we’ll discuss next.

#### Deep Learning

Deep Learning extends the concept of a single perceptron, by streaming a matrix of training observations (each of which is a vector of features, e.g. ) through multiple layers of perceptrons stacked together into what is called a hidden layer architecture.

The output of each layer’s activation function becomes the input vector fed to the next layer, i.e. for = hidden layers:

Where is the result of the first activation function, i.e.

##### A Note on Notation:

The initial matrix of inputs can be denoted as , and the output of each subsequent layer’s activation function in the nested equation can also be written in notation.

#### Visual Intuition

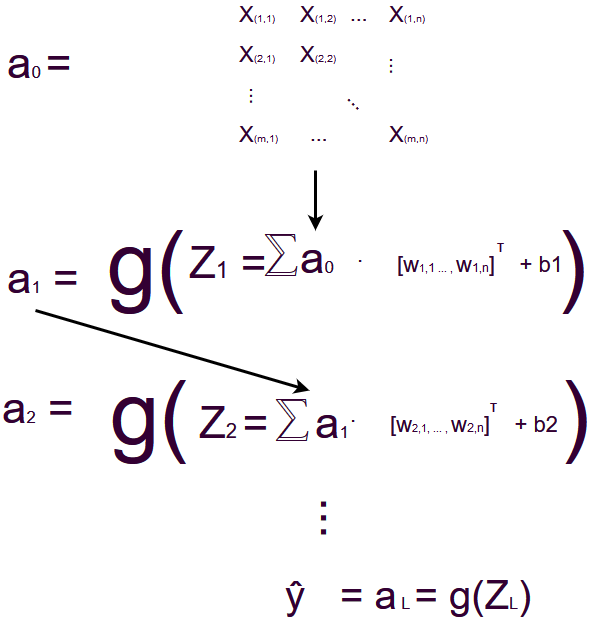


Figure 5: A visual Representation of the mathematics Explained Above (11)

#### Backpropagation

Backpropagation is an iterative process of adjusting weights and biases, by minimizing a cost function , which can be understood as the error in the estimate tied to a specific value of weights and biases.

Each element of the weights and biases are typically updated proportionately to the partial derivative of the cost function with respect to that specific element, multiplied by a learning rate , i.e.

For the element of the weight matrix , is updated as:

Similarly, for the element of the bias vector b, is updated as:

The training dataset is fed through the network multiple times (called epochs), hopefully allowing the cost function to reach a minimum.

#### Hyperparameters

To arrive at an optimal neural network for the defined task, there are multiple hyperparameters that can be optimized. Some of these have already been mentioned in part, i.e. the number of epochs, the choice of activation function, the number of hidden layers and the number of perceptrons within each hidden layer, the distribution of weights to initialize the network with, the learning rate ,etc.; but there are many more, including regularization, dropout, etc., which will be covered in the implementation section of this thesis.

#### Generative Neural Networks Explained at the hand of Pseudocode, based on a minimal example from (12)

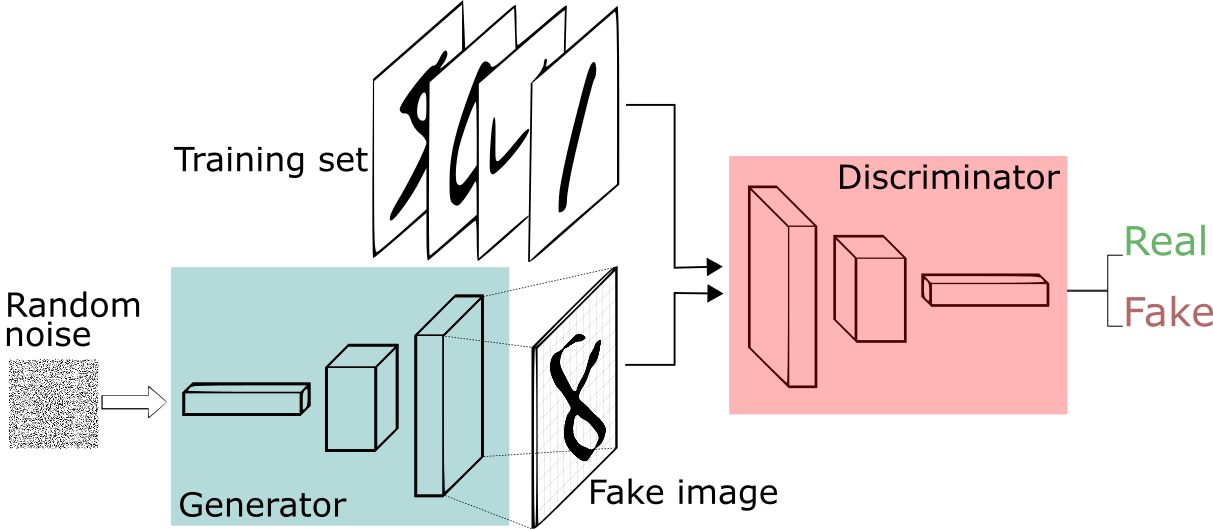


Figure 6: Schematic Representation of a Generative Adverserial Network (12)

Suppose we have a set of training images, each of which consists of 256 pixels, arranged in 28 rows and 28 columns; such as the well-known MNIST database of handwritten images (14), of which a sample is shown in ***Figure 7*** below:

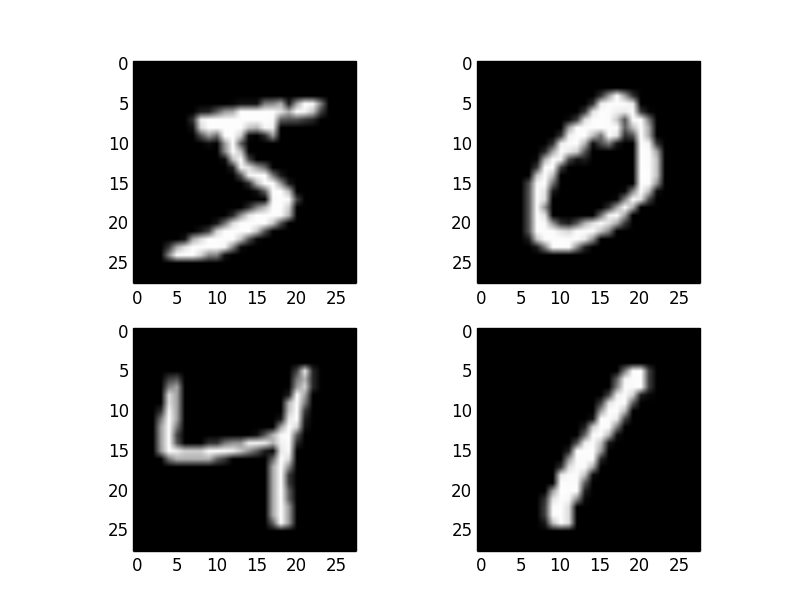


Figure 7: a sample of four handwritten digits from The MNIST Dataset (15)

Our goal is to build a GAN architecture, using these images. GANs is explained in the following lines of pseudocode, with comments indicated in bold text, preceded by a double forward-slash (“//”):

##### Pseudocode

**//DEFINE THE SHAPE OF THE INPUT (AND THEREFORE OUTPUT) IMAGES:**

IMAGE.SHAPE = [ROWS=28,COLUMNS=28]

**//GENERATE A VECTOR RANDOM GAUSSIAN NOISE TO USE AS INPUT TO THE GENERATOR NETWORK:**

A\_0 = RANDOM.NOISE(SIZE=100)

**//DEFINE THE HIDDEN ARCHITECTURE OF THE GENERATOR FUNCTION:**

GENERATOR = SEQUENTIAL\_MODEL[

**//Z\_1 IS THE INPUT LAYER, WITH THE SAME DIMENSIONS AS THE RANDOM NOISE INPUT VECTOR**

Z\_1 = LAYER[NODES=256, INPUT = A\_0]

**//A\_1 IS THE RESULT OF APPLYING A “LEAKY RELU” ACTIVATION FUNCTION TO:**

**//Z\_1 = SUM(W\_T \* A\_0 + BIAS)**

A\_1 = LEAKY\_RELU(ALPHA = 0.2,

**//LEAKY RELU ACTIVATION IS AN INDICATOR FUNCTION,**

**DEFINED AS FOLLOWS:**

FUNCTION = IF Z\_1 > 0 THEN Z\_1 ELSE A\*Z\_1 END,

INPUT = Z\_1)

**//BATCH NORMALIZATION IS A WAY OF SCALING THE TRAINING SAMPLE FEAUTURES, BY REDUCING COVARIANCE SHIFT, AND AS A RESULT,SPEEDING UP LEARNING AND PREVENTING VANISHING OR EXPLODING GRADIENTS DURING BACKPROPAGATION TRAINING**

A\_1 = BATCH\_NORMALIZATION(A\_1)

**//A FURTHER TWO HIDDEN LAYERS ARE ADDED, EACH TIME DOUBLING THE AMOUNT OF PERCEPTRONS PER LAYER, AND APPLYING AN ACTIVATION FUNCTION, AS WELL AS BATCH NORMALIZATION TO EACH LAYER**

Z\_2 = LAYER[NODES=512, INPUT = A\_1]

A\_2 = LEAKY\_RELU(ALPHA = 0.2,

FUNCTION = IF Z\_2 > 0 THEN Z\_2 ELSE ALPHA\*Z\_2 END,

INPUT = Z\_2)

A\_2 = BATCH\_NORMALIZATION(A\_2)

Z\_3 = LAYER[NODES=1024, INPUT = A\_2]

A\_3 = LEAKY\_RELU(ALPHA = 0.2,

FUNCTION = IF Z\_3 > 0 THEN Z\_3 ELSE ALPHA\*Z\_3 END

INPUT = Z\_3)

A\_3 = BATCH\_NORMALIZATION(A\_3)

**//FINALLY, THE SECOND HIDDEN LAYER IS RESHAPED TO THE ORIGINAL DIMENSIONS (28\*28), AND A TANH ACTIVATION FUNCTION (AS DEFINED EARLIER IN THE MATHEMATICAL THEORY SECTION OF THIS THESIS) IS APPLIED TO IT**

Y\_HAT = TANH(A\_3.RESHAPE(IMAGE.SHAPE))

]

DISCRIMINATOR = ANOTHER NEURAL NETWORK OR OTHER FORM OF DISCRIMINATOR

For a defined number of epochs, a sample of both real (training example) and fake (generated by G) images are streamed through the Discriminator Network (D). The loss function of the D informs backpropagation through both networks.

### Application of GANS to High Energy Physics Problems

# Motivation

Detector response simulations is an integral part of all HEP experiments and high accuracy is attainable with first principle methods in current simulation environments such as GEANT, but at a high computational cost (16). This computational cost is particularly relevant to the ALICE experiment, where a much higher charged particle multiplicity is achieved, relative to average transverse momentum . In other words, many more particles are produced in heavy ion collisions () compared to proton-proton ()collisions, which increases simulation time significantly (17) *🡨placeholder reference, since I am just guessing here...*

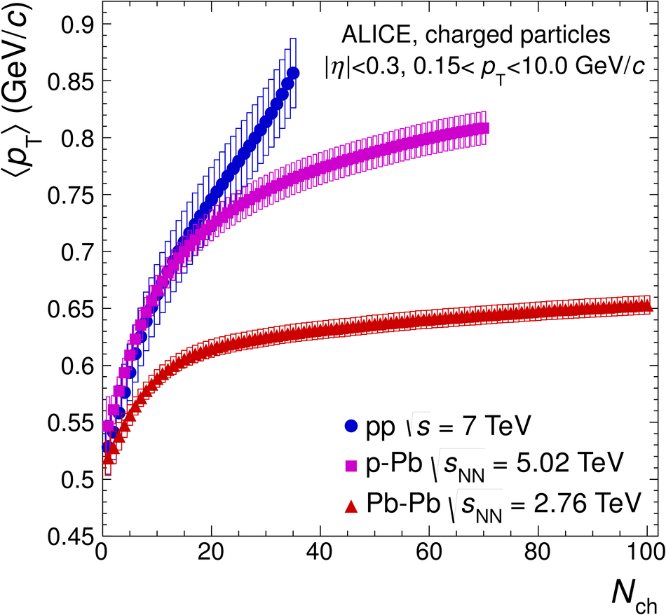


Figure 8: Average Charged Particle Multiplicity vs Average Transverse Momentum in p-p, p-Pb and Pb-Pb collisions at the LHC (18)

# Research Question

# Aims & Objectives

# Methods

# Results

# Discussion

# Conclusion and Future Work

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# Appendix I: ROOT/ AliEn Code

# Appendix II:

1. At this stage, the ReLU model is essentially nothing more than a Multi-variable linear model: [↑](#footnote-ref-1)