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MÁSTER UNIVERSITARIO EN CIENCIA DE DATOS (*Data Science*)

## TRABAJO FINAL DE MÁSTER

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Autor: Miguel Tablado

Tutor: Baris Kanber

Profesor: Nombre del profesor responsable del área de TF

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# Contents

<b>Abstract</b>	<b>4</b>
<b>1 Introduction</b>	<b>6</b>
1.1 Context and project justification . . . . .	6
1.2 Aim of the project . . . . .	8
1.3 Project Plan . . . . .	8
1.3.1 Resources . . . . .	8
1.3.2 High Level Plan . . . . .	9
1.3.3 Tasks . . . . .	10
<b>2 State of the art: related works</b>	<b>12</b>
2.1 Overview . . . . .	12
2.2 Variational Autoencoders . . . . .	12
2.3 MR Images and datasets . . . . .	15
2.4 Related Works . . . . .	17
<b>3 Design and Implementation</b>	<b>20</b>
3.1 Analysis of MRI images dataset . . . . .	20
<b>Acronyms</b>	<b>25</b>
<b>Glossary</b>	<b>26</b>

# FICHA DEL TRABAJO FINAL

Título del trabajo:	Artificial MRI brain images creation with Variational Autoencoders
Nombre del autor:	Miguel Tablado León
Nombre del Tutor/a de TF:	Baris Kanber
Nombre del/de la PRA:	Baris Kanber
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# Abstract

Artificial Intelligence is set to be key technology at medicine projects in where models will help doctors at diagnostics with image processing. Magnetic Resonance Images allow doctors to scan brains and create a images that can be used for training models. However, it is too expensive and slow to be able to create large dataset required for models to work at highest accuracy and this project aims to create artificial brain MR images that would enlarge the base dataset combining with real images.

A potential use case in where AI-generated images could be used are anomaly detection by comparing an input image with healthy images to detect if it presents any anomaly to be analyzed by a doctor.

During this project Variational Autoencoders will be used in order to create new images where different existing network architectures will be analyzed before working on the performance tuning with the one which brings better results at initial analysis.

The duration of the project implementation will start on October 24th and will end up by December 25th with one Data Scientist working on the project with a budget of 300 hours that will be distributed during that frame and that will require GPU compu-

tation for processing the different training and testing networks.

This project aims to be a Proof of Concept and the resulting images will be visually analyzed and compared to real images to check if the network is able to generate images that could be used as valid images.

# Chapter 1

## Introduction

### 1.1 Context and project justification

Artificial Intelligence has arrived to change the world in almost (if not all) any field. Today, we are surrounded by (and we are using many) AI products like smartphones' face recognition capabilities, home cleaning robots or cars with autopilot options.

From the different AI fields, computer vision is maybe the most popular one and the one which is usually used for explaining AI capabilities to general public. Identifying a cat in a picture could perfectly be the example used in every AI presentation to welcome people to AI.

Image processing is intuitively matched with medical diagnosis by anyone having or not any expertise on the field. Every single citizen will have heard of magnetic resonance imaging, and anyone easily transposes 'cat detection' to 'anomaly detection', being the anomaly a tumor or anything else.

There are different techniques to scan people and create images for clinical diagnosis like X-Ray or Magnetic Resonance Imaging. In this project, we will work with Magnetic Resonance Images (MRI) which are images created by a machine with a large bore that scans people lying inside it. The MR technique is non-invasive, it produces no radiation, and is used to scan

almost any part of the body from which we will focus on brain images.

Combining AI diagnosis capabilities on image processing and MRI images, we can think of helping doctors to identify the presence of anomalies or looking for concrete diagnosis for a specific disease.

Obviously, these projects are not easy at all and they face a lot of challenges. One of the first challenges that such AI project faces is the difficulty to obtain a large set of brain images that are needed to train an accurate AI model. Scanning people is too costly and requires a lot of time. and the challenge of having a large dataset gets harder once we understand that brain images may differ depending on age or gender.

Today, there is a clear limitation on how to reproduce or obtain healthy brain images for AI-based diagnosis projects while the appearance of new AI techniques known as Autoencoders and Variational Autoencoders introduces a new area of investigation to mitigate the gap.

This project aims to be a proof of concept to create AI-created images with new variational autoencoders that would serve to augment any existing MRI dataset and that will help to improve the accuracy of brain anomaly detection projects, including those which could be used for overall anomaly detection to others more specific which would help on concrete disease diagnosis.

Personal motivation comes from various angles:

- One is to prove myself that I can work with new AI architectures demonstrating that I have acquired the knowledge needed (deep enough) to be productive and to be able to innovate in the health sector.
- Deep Learning has been the subject which I enjoyed the most, hence continuing with Autoencoders seems natural to me as the next step on AI adoption

- At no doubts, if I can contribute to help on brain issue detection or diagnosis, I will feel my life been completely fulfilled

## 1.2 Aim of the project

The aim of this project is to serve as a Proof of Concept on how MRI brain images can be artificially generated with Variational Autoencoders which ultimately would serve to enhance existing or new datasets to improve model accuracy by having bigger samples of data

Foreseen projects objectives are:

- Obtain basic knowledge about MRI images and the NIFTI file format
- Obtain and visualise 2-D images from 3-D images in the dataset
- Select what range of slices (2-D images) from brain to be created
- Test different existing networks and choose the one to be used
- Tune network parameters
- Compare generated brain images against real ones, qualitatively

## 1.3 Project Plan

### 1.3.1 Resources

1. 1 Data Scientist: Miguel Tablado will be playing this role and will dedicate 300h
2. 1 Coach/Tutor: Baris Kanber will be assisting Miguel Tablado during the project
3. MRI images and demographic information from IXI Dataset
4. GPU resources are needed to train and test the network



### 1.3.2 High Level Plan

The plan will be executed in 3 different phases with the listed tasks:

1. Phase 1: Analysis
  - (a) Gain knowledge on MRI and NIFTI protocol
  - (b) Describe images and dataset
  - (c) Extract 2D images
  - (d) Pre-processing images
2. Phase 2: MR Images creation
  - (a) Test different Network architectures
  - (b) Tune-up architectural network
3. Phase 3: Project documentation
  - (a) Write conclusions
  - (b) Create project documentation
  - (c) Create project presentation

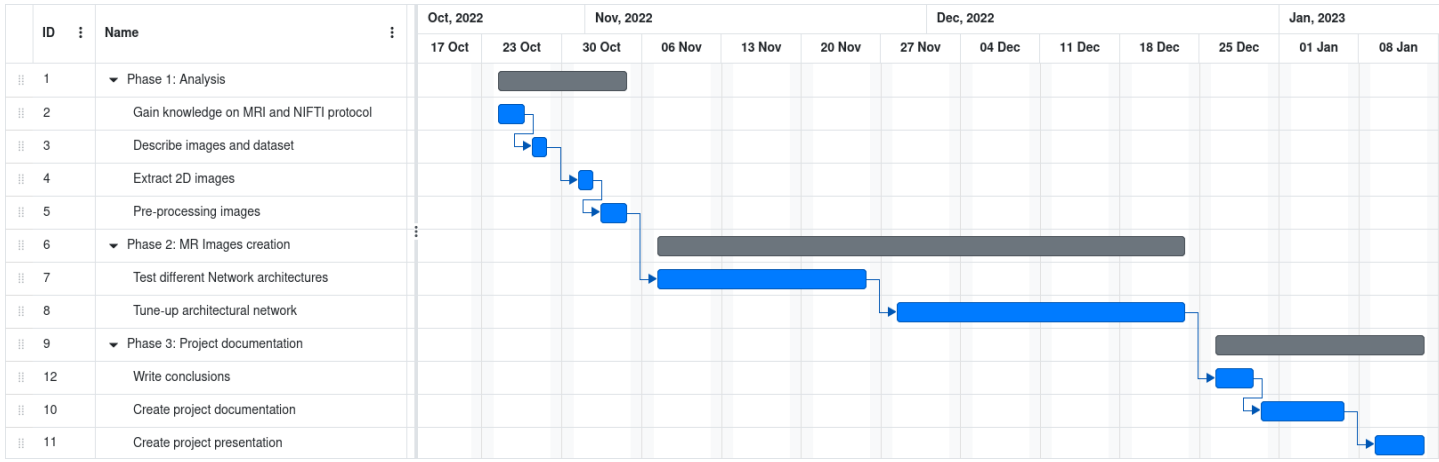


Figure 1.1: Project Plan. source: <https://www.onlineantt.com>

### 1.3.3 Tasks

#### Phase 1: Analysis

During this face the different tasks will be executed to prepare the work and includes:

1. Gain knowledge on MRI and the NIFTI file format: This activity consists of reading papers and documents to gain sufficient knowledge to execute the project. There is no need to become an expert on the matter but understanding how those files are and how to process them.
2. Describe images and dataset: During this activity, a description of the dataset will be generated with a view of the quality of the dataset for the aim of the project and any findings which could result.
3. Extract 2D images: Load 3D images and extract 2D slices from the original dataset, which will be depicted with code.
4. Pre-processing images: Decide which transformations on the 2D images would help the project like pixel changes or applying gray-scale transformations.

**Phase 2: MR Images creation**

1. Test different Network architectures: This task will take few existing network architectures and be tested with the dataset so that one of them will be selected to be improved and used as the project architecture.
2. Tune-up architectural network: Tune the selected architecture with useful techniques like changing network layers

## Chapter 2

# State of the art: related works

### 2.1 Overview

Since our project is based on brain anomaly detection with variational autoencoders (VAEs), in this section, the state of the art will be described with focus on previous existing anomaly detection projects and variational autoencoders.

Anomaly detection with VAEs has been used in several areas such as fraud detection, KPIs in web applications and, of course, MRI-based brain diagnosis.

In this section, the state of the art is covered by describing VAEs and MRI datasets first, and describing the related works later.

### 2.2 Variational Autoencoders

The history of Variational Autoencoders could be summarised by sequentially looking into the following papers:

- An and Cho, 2015. Variational autoencoder based anomaly detection using reconstruction probability. [1]

- Xu et al., 2018. Unsupervised anomaly detection via variational autoencoder for seasonal KPIs in web applications [8]
- Zimmerer et al., 2019. Unsupervised anomaly localization using variational auto-encoders. [9]

The first paper must be used to understand the differences between Autoencoders and Variational Autoencoders. This is important since VAE can be interpreted as a new technique with origin on Autoencoders, thus, sharing fundamentals and architectures.

An and Cho [1], described a VAE as "a probabilistic graphical model that combines variational inference with deep learning". Because VAE reduces dimensions in a probabilistically sound way, theoretical foundations are firm. The advantage of a VAE over an autoencoder and a PCA is that it provides a probability measure rather than a reconstruction error as an anomaly score, which we will call the reconstruction probability. Probabilities are more principled and objective than reconstruction errors and does not require model specific thresholds for judging anomalies."

In other words, Jeremy Jordan [6] describes the same in simpler words "A variational autoencoder provides a probabilistic manner for describing an observation in latent space. Thus, rather than building an encoder which outputs a single value to describe each latent state attribute, we'll formulate our encoder to describe a probability distribution for each latent attribute."

An and Cho [1] conclude "To summarize, it is the distribution parameters that are being modeled in the VAE, not the value itself."

To understand the differences between Autoencoders and VAEs, An and Cho [1] listed 3 differences:

1. VAE latent space are stochastic variables, not deterministic ones

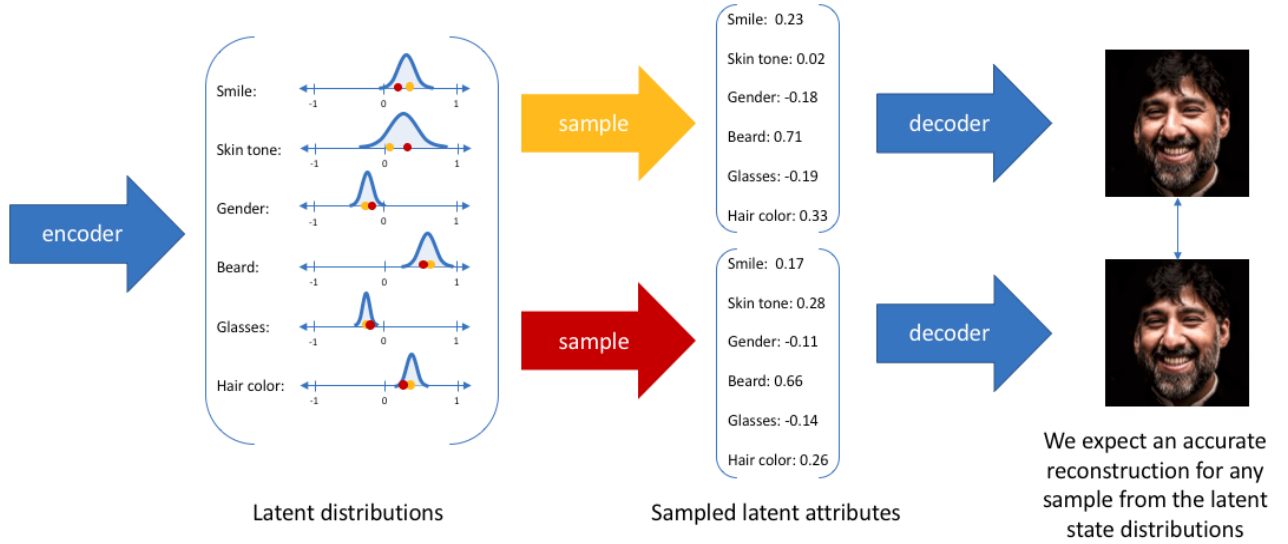


Figure 2.1: Variational Autoencoders by Jerermy Jordan [6]

2. Reconstruction in VAE adds the variability of the reconstruction by considering the variance parameter of the distribution function.
3. Autoencoders use reconstruction errors as anomaly score, while VAE reconstructions are probability measures which work best for heterogeneous data and deciding the reconstruction probability threshold is easier and more objective than deciding for reconstruction error.

Finally, An and Cho [1] proved that VAE outperformed autoencoders and PCA based methods on 2 different popular datasets, MNIST [7] and KDD [5].

Xu et al. later proved the same on a large internet company dataset that shows a combination of seasonal patterns with local variations and the statistics of the Gaussian noises.

The project consisted of detecting anomalies on KPIs on a website; KPIs are time series data measuring metrics such as number of connected users,

transactions or orders. Websites for retail industry follow a seasonal distribution and a local variation that explains the increasing trend over days.

Finally, Zimmerer et al. [9], 2018 proved that VAEs could keep the assumption-free principle by improving the used network architecture with a combination of the reconstruction term with the density-based anomaly scoring. Before, the VAEs had shown great potential on unsupervised learning of data distributions but required modifications on the model architecture to perform well for the problem seen during the evaluation, which breaks the assumption-free principle.

In detail, VAE can approximate data distributions by optimizing a lower bound, often termed evidence lower bound (ELBO) which is usually employed as a proxy to compare the likelihood. ELBO is a combination of the reconstruction error and the Kullback-Leibler (KL)-divergence, a backpropagation mechanism. This combination is called a context-encoder VAE or *ceVAE*.

## 2.3 MR Images and datasets

The IXI dataset is published at [brain-development.org](http://brain-development.org) website from Imperial College London and it is the chosen dataset for this project. IXI dataset is a collection of 600 Brain MR Images, in 3-D, collected from 3 different hospitals in London. The images are scanned in 1.5 and 3 Tesla which is the range of the quality that we could usually find in hospitals around the world. Scanners with higher quality (7T) are very rare in the world and so working with this dataset makes sense if you plan to export your work to real production environments.

The images are stored as volumes or 3-D images which require an intense computational effort to process, in this project we will work with 2-D images,

or brain slices, which will allow us to scale the number of samples that our model will work with.

Other datasets exist on the internet which can be used for this project, and of course, much more private ones are expected to exist. We will cover a few of them to show the state of the art in this area.

The one sponsored by Facebook AI and hosted at NYU Langone Health is called fastMRI and includes knees and brain MRIs. Nothing better than its overview to describe the aim of this dataset “fastMRI is a collaborative research project from Facebook AI Research (FAIR) and NYU Langone Health to investigate the use of AI to make MRI scans faster”.

The dataset consists of 6.970 fully sampled MRI brain images obtained in 3 and 1.5 Tesla magnets like the IXI dataset and includes T1, T2 and FLAIR images.

We can also find Brain Tumor Segmentation (BraTS) challenge [4] which encloses two different tasks of brain tumor detection and classification. The challenge is 10+ years old and as of 2021 provided 2.000 cases with 8.000 MRI scans. Like fastMRI, BraTS provides T1, T2 and FLAIR images in NIFTI files.

BraTS dataset has been pre-processed prior to its release, i.e., co-registered to the same anatomical template, interpolated to the same resolution and skull-stripped.

In conclusion, IXI dataset, which includes a spreadsheet of democratization of the dataset, could be enlarged with BraTS or fastMRI for further research (with the corresponding pre-process alignment).

Since the project aims to create artificial images that could be used with real images to train specific models, using them with different datasets would be interesting for validating the portability of the created images to different



hospitals.

## 2.4 Related Works

In July 2021, Jorge Cardoso published an article [2] describing how 3-D MRI images were created using AI models for diagnosis and prediction of diseases on brains by using a supercomputer called Cambridge-1 and Vector-Quantized Variational Autoencoder (VQ-VAE)

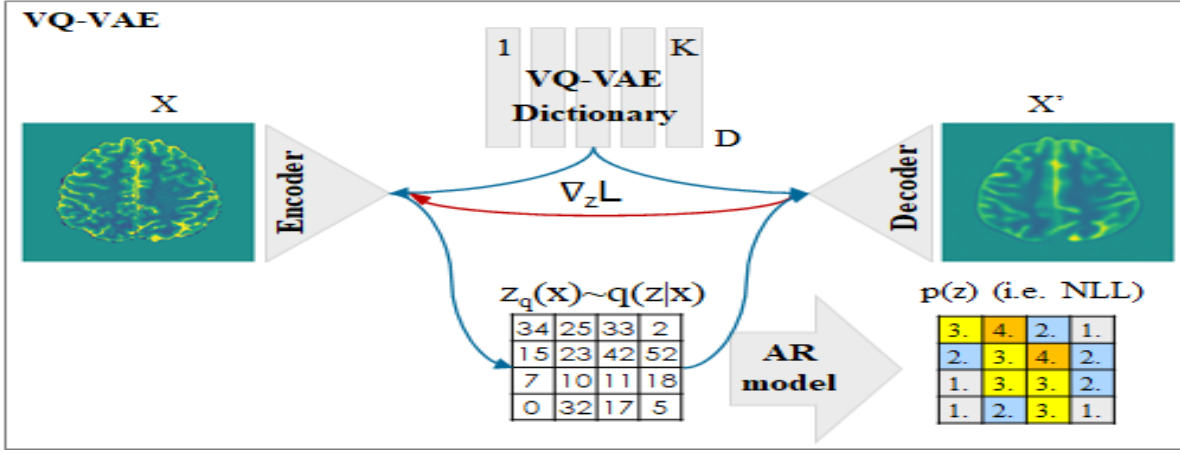


Figure 2.2: VQ-VAE Proposed Approach by Marimont and Tarroni

More recently, In September 2022, Soumick et al. [3] published a paper on how a pipeline (called StRegA) with specific pre-processing and post-processing functions outperformed the Context-Encoder Variational Autoencoder (ceVAE) architectures on unsupervised anomaly detection in brain MRIs.

While Cardoso describes how a supercomputer with 100 GPUs (and other high-quality features) was employed to create MRI brain images across ages, genders and diseases which allows to not only diagnose but to predict diseases, StRegA describes how adding pre and post processing steps to the network architecture on regular computers improves results compared to

bare VAE network architectures.

Soumick et al. [3] explains in detail why the unsupervised learning is needed in the field by mainly comparing with supervised learning and by emphasizing its properties. The paper highlights the following list of reasons to justify the usage unsupervised learning:

- Supervised learning relies on the quality and quantity of data, ranging from thousands to millions of labeled data which is a laborious manual annotation work.
- Supervised learning is often focused on one type of pathology
- Supervised learning has demonstrated to work well on concrete anomalies detection with simulated data but many perform poorly with clinical data
- Supervised learning solutions are challenging to develop on some abnormalities such as small vessel disease since the damage is complex on lesion size, contrast, or morphology
- A wide variety of abnormalities can be present in human brain MRI (even simultaneously) which renders a representation of all possible anomalies very challenging (including labeling)
- Anomaly detection is an approach that distinguishes anomalies completely based on characteristics that describe regular data.
- Unsupervised Anomaly Detection is useful for anomalies detection when their manifestation is not known or are very rare; making it difficult to create a large dataset for supervised learning

The StRegA pipeline used for unsupervised anomaly detection used a compact version of the ceVAE (cceVAE) combined with pre and post processors (creating a pipeline) which outperformed VAEs working alone. However, those achievements are only relevant to this project since they have been worked with the same MRI brain images (on a different dataset, BraTS vs IXI), hence it demonstrates that VAEs are optimal for MRI Brain images processing.

In conclusion, the state-of-the-art shows that VAEs have been implemented in combination with supercomputers to create models for diagnosis and prediction of brain diseases using 3-D MRI datasets and that the AI community is looking for cheaper and affordable implementations by innovating new VAE architectures or combining VAEs with pre and post processing actions.

## Chapter 3

# Design and Implementation

### 3.1 Analysis of MRI images dataset

#### MRI and the NIFTI file format

#### MRI and the NIFTI file format

Describe images and dataset: During this activity, a description of the dataset will be generated with a view of the quality of the dataset for the aim of the project and any findings which could result.

#### Loading images

Extract 2D images: Load 3D images and extract 2D slices from the original dataset, which will be depicted with code.

The NIFTI protocol stores the 3D

After loading NIFTI images with the nibabel library ...

Images are loaded in the following shape:

- 256 Coronal or trasversal plane
- 256 Axial or horizontal plane
- 130 Sagittal

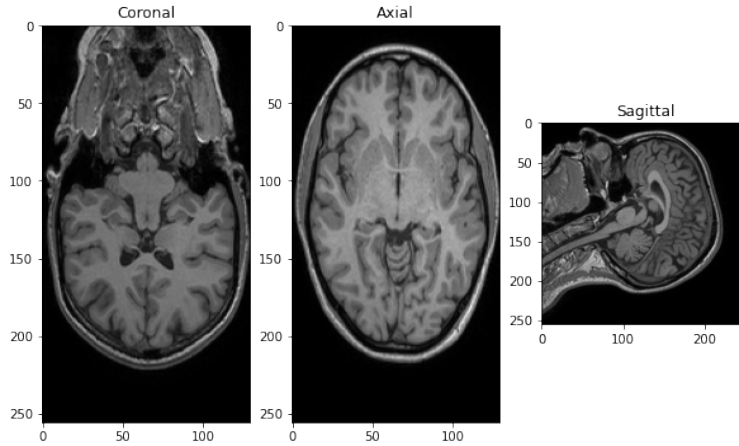


Figure 3.1: Coronal, Axial and Sagittal images

### Deciding what slices to use

Looking at the three different slices in Figure 3.1, it is obvious that images have not been processed to show only the brain. The aim of the project is to create artificial brain images, not head images. A model that would learn head images would require much more time and resources than for learning just the brain (which is not a an easy task at all either).

While observing the BraTS [4] challenge dataset and project description, the skull stripping concept arise. Before publishing the dataset, slices are processed to remove anything that does not pertain to brain.

This project cannot afford such implementation within the project scope. So, when deciding what slices to use, it became the only decision factor. It happened to be that the rest of considerations where just debatable.

In conclusion, the noise that bones, eyes and the rest of the items visible in coronal and sagittal axis look very high compared to the axial slices in where, properly selected, slices will only show a surrounding skull bone.

Once that the axial slices were chosen, a sample of brain scans were visually analyzed to find a range of slices that could be used.

The range must exclude as much non-brain pixels as possible while and that happens using the range that goes from above eyes to the top.

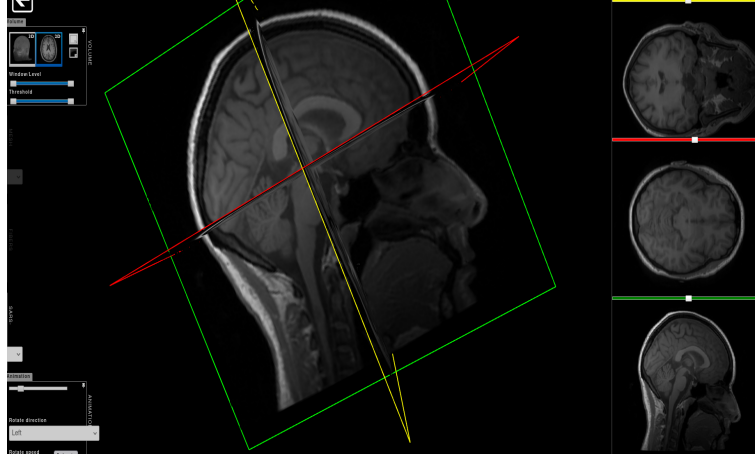


Figure 3.2: In red, slice 160 as bottom delimiter

Also, the slices closer to the top were also discarded to avoid higher heterogeneity on brain images and sizes.

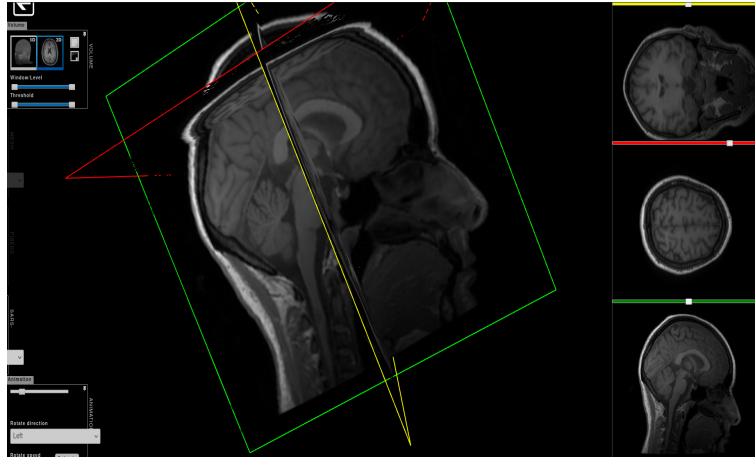


Figure 3.3: In red, slice 190 as top delimiter

It can be interpreted that 3D images are in use since 30 slices of each brain are used which constitute a 3D section of a brain. But, similarly, it could be interpreted that each and every slice of those 30 could happen to

Technique	Decision	Justification
Gray scale	Approved	Applying gray scale to scans seems a natural choice and is usually applied on image processing
Rescaling	Approved	Rescaling RGB values from 0-256 to 0-1 that can be better handled by the model
Pixel	Approved	Down-pixeling images from 256 to 128 which requires much less resources and wouldn't lose much quality
Shear Intensity	Declined	Slanting images would distort the latent space leading to create distorted artificial images
Shifts and Rotation	Declined	Similar to shear intensity shifting images is seen as a method not accurate for MRI processing as NIFT images will not appear shifted in any prediction phase
Add Noise	Declined	Adding noise is interesting for improving results and key to allow model transferring to other datasets obtained with different scanners and their settings or image quality. It was declined due to time constraints.

be data augmentation or different people with very similar brains.

### Data Pre-processing and Data Augmentation

Different pre-processing and data augmentation techniques were briefly evaluated to decide wheter they would improve the model's results. The following table shows the decisions made on each evaluated technique:

#### Storing data

In order to isolate image loading from model training into different steps, selected 2D images are stored in PNG format after being pre-processed.

The images are stored in 2 different directories splitting the dataset into

90% for training and 10% for test subsets resulting in 16.268 and 1.162 images respectively.

It was concluded that some of them could badly interfere into the latent space representation. For example, Due to time constraint other data augmentation techniques were not implemented.

1. Gain knowledge on MRI and the NIFTI file format: This activity consists of reading papers and documents to gain sufficient knowledge to execute the project. There is no need to become an expert on the matter but understanding how those files are and how to process them.
- 2.
- 3.
4. Pre-processing images: Decide which transformations on the 2D images would help the project like pixel changes or applying gray-scale transformations.



# Acronyms

**ceVAE** Context-Encoder Variational Autoencoder. 17, 19

**PCA** Principal Component Analysis. 13, 14

**PNG** Portable Network Graphics. 23

**RGB** Red Green Blue. 23

**StRegA** Segmentation Regularised Anomaly. 17, 19

**VQ-VAE** Vector-Quantized Variational Autoencoder. 17

# Glossary

**IXI** IXI dataset is a collection of 600 Brain MR Images, in 3-D, collected from 3 different hospitals in London. The images are scanned in 1.5 and 3 Tesla which is the range of the quality that we could usually find in hospitals around the world. 15

**KDD** KDD cup 1999 network intrusion dataset. 14

**KPI** Key Performance Indicator. 12, 14

**MNIST** The MNIST database of handwritten digits used for training models. 14

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