

Computer Science NEA Report

An investigation into how Artificial Neural Networks work, the effects of their hyper-parameters and their applications in Image Recognition.

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1 Analysis

1.1 About

Artificial Intelligence mimics human cognition in order to perform tasks and learn from them, Machine Learning is a subfield of Artificial Intelligence that uses algorithms trained on data to produce models (trained programs) and Deep Learning is a subfield of Machine Learning that uses Artificial Neural Networks, a process of learning from data inspired by the human brain. Artificial Neural Networks can be trained to learn a vast number of problems, such as Image Recognition, and have uses across multiple fields, such as medical imaging in hospitals. This project is an investigation into how Artificial Neural Networks work, the effects of changing their hyper-parameters and their applications in Image Recognition. To achieve this, I will derive and research all theory behind the project, using sources such as IBM's online research, and develop Neural Networks from first principles without the use of any third-party Machine Learning libraries. I then will implement the Artificial Neural Networks in Image Recognition, by creating trained models and will allow for experimentation of the hyper-parameters of each model to allow for comparisons between each model's performances, via a Graphical User Interface.

1.2 Interview

In order to gain a better foundation for my investigation, I presented my prototype code and interviewed the head of Artificial Intelligence at Cambridge Consultants for input on what they would like to see in my project, these were their responses:

- Q: "Are there any good resources you would recommend for learning the theory behind how Artificial Neural Networks work?"
A: "There are lots of useful free resources on the internet to use. I particularly like the platform 'Medium' which offers many scientific articles as well as more obvious resources such as IBMs'."
- Q: "What do you think would be a good goal for my project?"
A: "I think it would be great to aim for applying the Neural Networks on Image Recognition for some famous datasets. For you, I would recommend the MNIST dataset as a goal."
- Q: "What features of the Artificial Neural Networks would you like to be able to experiment with?"
A: "I'd like to be able to experiment with the number of layers and the number of neurons in each layer, and then be able to see how these changes effect the performance of the model. I can see that you've utilised the Sigmoid transfer function and I would recommend having the option to test alternatives such as the ReLu transfer function, which will help stop issues such as a vanishing gradient."
- Q: "What are some practical constraints of AI?"

A: "Training AI models can require a large amount of computing power, also large datasets are needed for training models to a high accuracy which can be hard to obtain."

- Q: "What would you say increases the computing power required the most?"

A: "The number of layers and neurons in each layer will have the greatest effect on the computing power required. This is another reason why I recommend adding the ReLu transfer function as it updates the values of the weights and biases faster than the Sigmoid transfer function."

- Q: "Do you think I should explore other computer architectures for training the models?"

A: "Yes, it would be great to add support for using graphics cards for training models, as this would be a vast improvement in training time compared to using just CPU power."

- Q: "I am also creating a user interface for the program, what hyper-parameters would you like to be able to control through this?"

A: "It would be nice to control the transfer functions used, as well as the general hyper-parameters of the model. I also think you could add a progress tracker to be displayed during training for the user."

- Q: "How do you think I should measure the performance of models?"

A: "You should show the accuracy of the model's predictions, as well as example incorrect and correct prediction results for the trained model. Additionally, you could compare how the size of the training dataset effects the performance of the model after training, to see if a larger dataset would seem beneficial."

- Q: "Are there any other features you would like add?"

A: "Yes, it would be nice to be able to save a model after training and have the option to load in a trained model for testing."

1.3 Project Objectives

- Learn how Artificial Neural Networks work and develop them from first principles
- Implement the Artificial Neural Networks by creating trained models on image datasets
 - Allow use of Graphics Cards for faster training
 - Allow for the saving of trained models
- Develop a Graphical User Interface
 - Provide controls for hyper-parameters of models
 - Display and compare the results each model's predictions

1.4 Theory behind Artificial Neural Networks

From an abstract perspective, Artificial Neural Networks are inspired by how the human mind works, by consisting of layers of 'neurons' all interconnected via different links, each with their own strength. By adjusting these links, Artificial Neural Networks can be trained to take in an input and give its best prediction as an output.

1.4.1 Structure

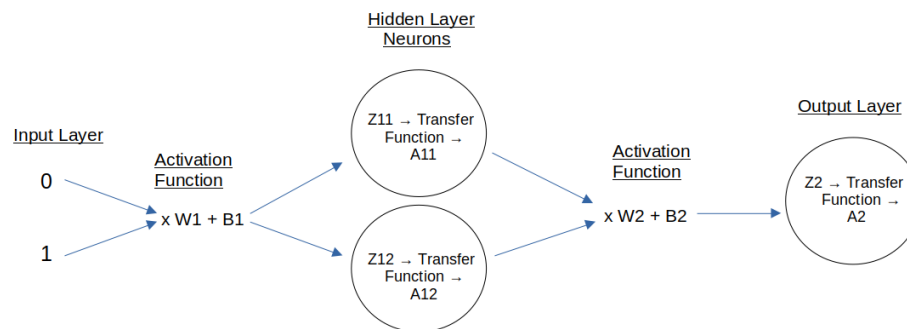


Figure 1: This shows an Artificial Neural Network with one single hidden layer and is known as a Shallow Neural Network.

I have focused on Feed-Forward Artificial Neural Networks, where values are entered to the input layer and passed forwards repetitively to the next layer until reaching the output layer. Within this, I have learnt two types of Feed-Forward Artificial Neural Networks: Perceptron Artificial Neural Networks, that contain no hidden layers and are best at learning more linear patterns and Multi-Layer Perceptron Artificial Neural Networks, that contain at least one hidden layer, as a result increasing the non-linearity in the Artificial Neural Network and allowing it to learn more complex / non-linear problems.

Multi-Layer Perceptron Artificial Neural Networks consist of:

- An input layer of input neurons, where the input values are entered.
- Hidden layers of hidden neurons.
- An output layer of output neurons, which outputs the final prediction.

To implement an Artificial Neural Network, matrices are used to represent the layers, where each layer is a matrix of the layer's neuron's values. In order to use matrices for this, the following basic theory must be known about them:

- When Adding two matrices, both matrices must have the same number of rows and columns.

- When multiplying two matrices, the number of columns of the 1st matrix must equal the number of rows of the 2nd matrix. And the result will have the same number of rows as the 1st matrix, and the same number of columns as the 2nd matrix. This is important, as the output of one layer must be formatted correctly to be used with the next layer.
- In order to multiply matrices, I take the 'dot product' of the matrices, which multiplies the row of one matrix with the column of the other, by multiplying matching members and then summing up.
- Transposing a matrix will turn all rows of the matrix into columns and all columns into rows.
- A matrix of values can be classified as a rank of Tensors, depending on the number of dimensions of the matrix. (Eg: A 2-dimensional matrix is a Tensor of rank 2)

I have focused on just using Fully-Connected layers, that will take in input values and apply the following calculations to produce an output of the layer:

- An Activation function
 - This calculates the dot product of the input matrix with a weight matrix, then sums the result with a bias matrix
- A Transfer function
 - This takes the result of the Activation function and transfers it to a suitable output value as well as adding more non-linearity to the Neural Network.
 - For example, the Sigmoid Transfer function converts the input to a number between zero and one, making it useful for logistic regression where the output value can be considered as closer to zero or one allowing for a binary classification of predicting zero or one.

1.4.2 How Artificial Neural Networks learn

To train an Artificial Neural Network, the following processes will be carried out for each of a number of training epochs:

- Forward Propagation:
 - The process of feeding inputs in and getting a prediction (moving forward through the network)
- Back Propagation:
 - The process of calculating the Loss in the prediction and then adjusting the weights and biases accordingly

- I have used Supervised Learning to train the Artificial Neural Networks, where the output prediction of the Artificial Neural Network is compared to the values it should have predicted. With this, I can calculate the Loss value of the prediction (how wrong the prediction is from the actual value).
- I then move back through the network and update the weights and biases via Gradient Descent:
 - * Gradient Descent aims to reduce the Loss value of the prediction to a minimum, by subtracting the rate of change of Loss with respect to the weights/ biases, multiplied with a learning rate, from the weights/biases.
 - * To calculate the rate of change of Loss with respect to the weights/biases, you must use the following calculus methods:
 - Partial Differentiation, in order to differentiate the multi-variable functions, by taking respect to one variable and treating the rest as constants.
 - The Chain Rule, where for $y = f(u)$ and $u = g(x)$, $\frac{\partial y}{\partial x} = \frac{\partial y}{\partial u} * \frac{\partial u}{\partial x}$
 - For a matrix of $f(x)$ values, the matrix of $\frac{\partial f(x)}{\partial x}$ values is known as the Jacobian matrix
 - * This repetitive process will continue to reduce the Loss to a minimum, if the learning rate is set to an appropriate value

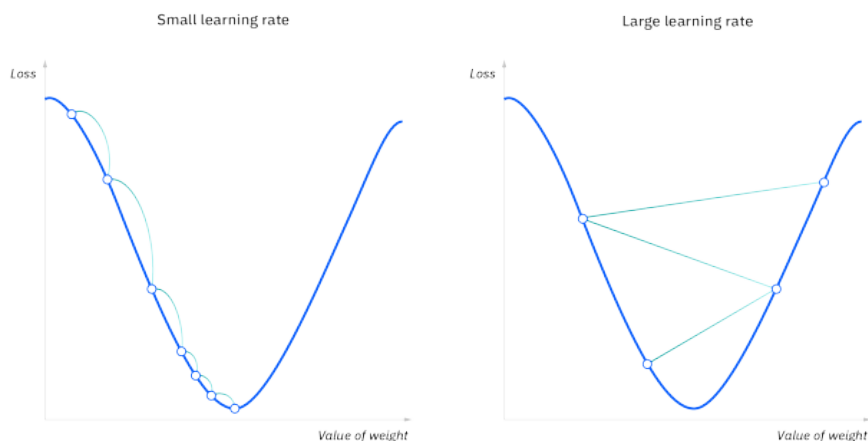


Figure 2: Gradient Descent
sourced from <https://www.ibm.com/topics/gradient-descent>

- * However, during backpropagation some issues can occur, such as the following:
 - Finding a false local minimum rather than the global minimum of the function

- Having an 'Exploding Gradient', where the gradient value grows exponentially to the point of overflow errors
- Having a 'Vanishing Gradient', where the gradient value decreases to a very small value or zero, resulting in a lack of updating values during training.

1.5 Theory Behind Deep Artificial Neural Networks

1.5.1 Setup

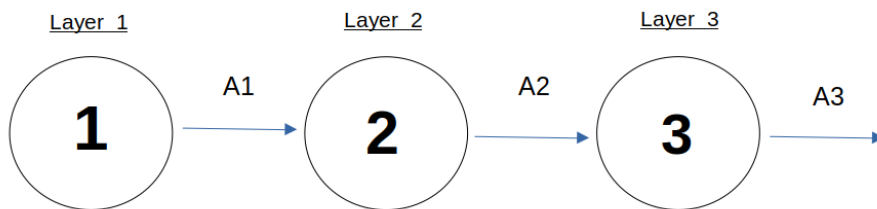


Figure 3: This shows an abstracted view of an Artificial Neural Network with multiple hidden layers and is known as a Deep Neural Network.

- Where a layer takes the previous layer's output as its input X
- Then it applies an Activation function to X to obtain Z , by taking the dot product of X with a weight matrix W , then sums the result with a bias matrix B . At first the weights are initialised to random values and the biases are set to zeros.

$$- Z = W * X + B$$

- Then it applies a Transfer function to Z to obtain the layer's output
 - For the output layer, the sigmoid function (explained previously) must be used for either for binary classification via logistic regression, or for multi- class classification where it predicts the output neuron, and the associated class, that has the highest value between zero and one.

$$* \text{ Where } \text{sigmoid}(Z) = \frac{1}{1+e^{-Z}}$$

- However, for the input layer and the hidden layers, another transfer function known as ReLu (Rectified Linear Unit) can be better suited as it produces largers values of $\frac{\partial L}{\partial W}$ and $\frac{\partial L}{\partial B}$ for Gradient Descent than Sigmoid, so updates at a quicker rate.

$$* \text{ Where } \text{relu}(Z) = \max(0, Z)$$

1.5.2 Forward Propagation:

- For each epoch the input layer is given a matrix of input values, which are fed through the network to obtain a final prediction A from the output layer.

1.5.3 Back Propagation:

- First the Loss value L is calculated using the following Log-Loss function, which calculates the average difference between A and the value it should have predicted Y. Then the average is found by summing the result of the Loss function for each value in the matrix A, then dividing by the number of predictions m, resulting in a Loss value to show how well the network is performing.

– Where $L = -(\frac{1}{m}) * \sum(Y * \log(A) + (1 - Y) * \log(1 - A))$ and "log()" is the natural logarithm

- I then move back through the network, adjusting the weights and biases via Gradient Descent. For each layer, the weights and biases are updated with the following formulae:

– $W = W - learningRate * \frac{\partial L}{\partial W}$

– $B = B - learningRate * \frac{\partial L}{\partial B}$

- The derivation for Layer 2's $\frac{\partial L}{\partial W}$ and $\frac{\partial L}{\partial B}$ can be seen below:

– Functions used so far:

1. $Z = W * X + B$

2. $A_{relu} = \max(0, Z)$

3. $A_{sigmoid} = \frac{1}{1+e^{-Z}}$

4. $L = -(\frac{1}{m}) * \sum(Y * \log(A) + (1 - Y) * \log(1 - A))$

– $\frac{\partial L}{\partial A2} = \frac{\partial L}{\partial A3} * \frac{\partial A3}{\partial Z3} * \frac{\partial Z3}{\partial A2}$

By using function 1, where A2 is X for the 3rd layer, $\frac{\partial Z3}{\partial A2} = W3$

$\Rightarrow \frac{\partial L}{\partial A2} = \frac{\partial L}{\partial A3} * \frac{\partial A3}{\partial Z3} * W3$

– $\frac{\partial L}{\partial W2} = \frac{\partial L}{\partial A2} * \frac{\partial A2}{\partial Z2} * \frac{\partial Z2}{\partial W2}$

By using function 1, where A1 is X for the 2nd layer, $\frac{\partial Z2}{\partial W2} = A1$

$\Rightarrow \frac{\partial L}{\partial W2} = \frac{\partial L}{\partial A2} * \frac{\partial A2}{\partial Z2} * A1$

– $\frac{\partial L}{\partial B2} = \frac{\partial L}{\partial A2} * \frac{\partial A2}{\partial Z2} * \frac{\partial Z2}{\partial B2}$

By using function 1, $\frac{\partial Z2}{\partial B2} = 1$

$\Rightarrow \frac{\partial L}{\partial B2} = \frac{\partial L}{\partial A2} * \frac{\partial A2}{\partial Z2} * 1$

- As you can see, when moving back through the network, the $\frac{\partial L}{\partial W}$ and $\frac{\partial L}{\partial B}$ of the layer can be calculated with the rate of change of loss with respect to its output, which is calculated by the previous layer using the above formula; the derivative of the layer's transfer function, and the layers input (which in this case is A1)

- Where by using function 2, $\frac{\partial A_{relu}}{\partial Z} = 1$ when $Z \geq 0$ otherwise $\frac{\partial A_{relu}}{\partial Z} = 0$
- Where by using function 3, $\frac{\partial A_{sigmoid}}{\partial Z} = A * (1 - A)$
- At the start of backpropagation, the rate of change of loss with respect to the output layer's output has no previous layer's calculations, so instead it can be found with the derivative of the Log-Loss function, as shown in the following:
 - Using function 4, $\frac{\partial L}{\partial A} = (-\frac{1}{m})(\frac{Y-A}{A*(1-A)})$

1.6 Theory behind training the Artificial Neural Networks

Training an Artificial Neural Network's weights and biases to predict on a dataset, will create a trained model for that dataset, so that it can predict on future images inputted. However, training Artificial Neural Networks can involve some problems such as Overfitting, where the trained model learns the patterns of the training dataset too well, causing worse prediction on a different test dataset. This can occur when the training dataset does not cover enough situations of inputs and the desired outputs (by being too small for example), if the model is trained for too many epochs on the poor dataset and having too many layers in the Neural Network. Another problem is Underfitting, where the model has not learnt the patterns of the training dataset well enough, often when it has been trained for too few epochs, or when the Neural Network is too simple (too linear).

1.6.1 Datasets

- MNIST dataset
 - The MNIST dataset is a famous dataset of images of handwritten digits from zero to ten and is commonly used to test the performance of an Artificial Neural Network.
 - The dataset consists of 60,000 input images, made up from 28x28 pixels and each pixel has an RGB value from 0 to 255
 - To format the images into a suitable format to be inputted into the Artificial Neural Networks, each image's matrix of RGB values are 'flattened' into a 1 dimensional matrix of values, where each element is also divided by 255 (the max RGB value) to a number between 0 and 1, to standardize the dataset.
 - The output dataset is also loaded, where each output for each image is an array, where the index represents the number of the image, by having a 1 in the index that matches the number represented and zeros for all other indexes.
 - To create a trained Artificial Neural Network model on this dataset, the model will require 10 output neurons (one for each digit), then by using the Sigmoid Transfer function to output a number between one and zero to each neuron, whichever neuron has the highest value

is predicted. This is multi-class classification, where the model must predict one of 10 classes (in this case, each class is one of the digits from zero to ten).

- Cat dataset
 - I will also use a dataset of images sourced from <https://github.com/marcopeix>, where each image is either a cat or not a cat.
 - The dataset consists of 209 input images, made up from 64x64 pixels and each pixel has an RGB value from 0 to 255
 - To format the images into a suitable format to be inputted into the Artificial Neural Networks, each image's matrix of RGB values are 'flattened' into a 1 dimensional array of values, where each element is also divided by 255 (the max RGB value) to a number between 0 and 1, to standardize the dataset.
 - The output dataset is also loaded, and is reshaped into a 1 dimensional array of 1s and 0s, to store the output of each image (1 for cat, 0 for non cat)
 - To create a trained Artificial Neural Network model on this dataset, the model will require only 1 output neuron, then by using the Sigmoid Transfer function to output a number between one and zero for the neuron, if the neuron's value is closer to 1 it predicts cat, otherwise it predicts not a cat. This is binary classification, where the model must use logistic regression to predict whether it is a cat or not a cat.
- XOR dataset
 - For experimenting with Artificial Neural Networks, I solve the XOR gate problem, where the Neural Network is fed input pairs of zeros and ones and learns to predict the output of a XOR gate used in circuits.
 - This takes much less computation time than image datasets, so is usefull for quickly comparing different hyper-parameters of a Network.

1.6.2 Theory behind using Graphics Cards to train Artificial Neural Networks

Graphics Cards consist of many Tensor cores which are processing units specialised for matrix operations for calculating the co-ordinates of 3D graphics, however they can be used here for operating on the matrices in the network at a much faster speed compared to CPUs. GPUs also include CUDA cores which act as an API to the GPU's computing to be used for any operations (in this case training the Artificial Neural Networks).

2 Design

2.1 Introduction

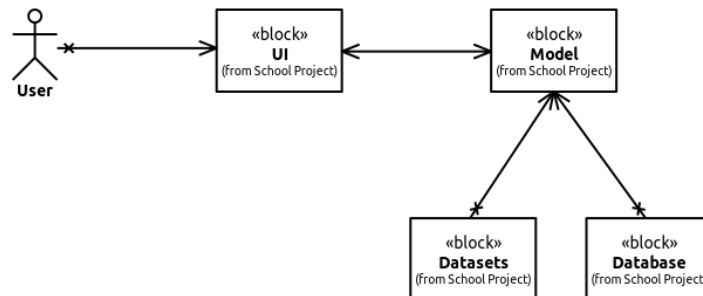
The following design focuses have been made for the project:

- The program will support multiple platforms to run on, including Windows and Linux.
- The program will use python3 as its main programming language.
- I will take an object-orientated approach to the project.
- I will give an option to use either a Graphics Card or a CPU to train the Artificial Neural Networks.

I will also be using SysML for designing the following diagrams.

2.2 System Architecture

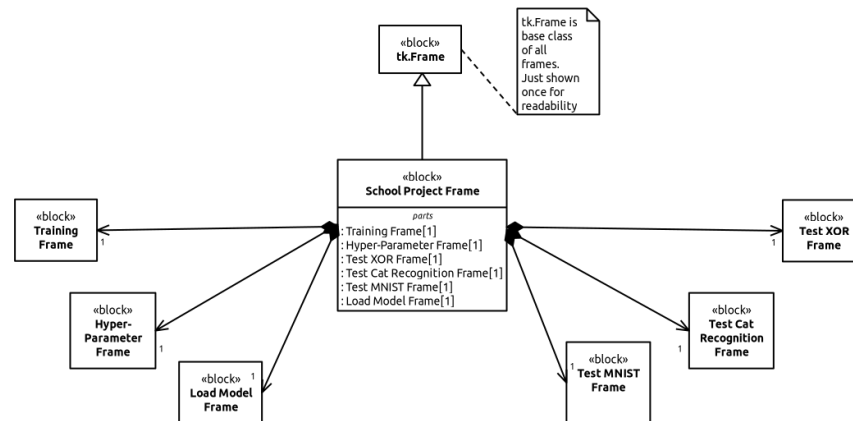
bdd [block] School Project Frame [System Architecture Diagram]



2.3 Class Diagrams

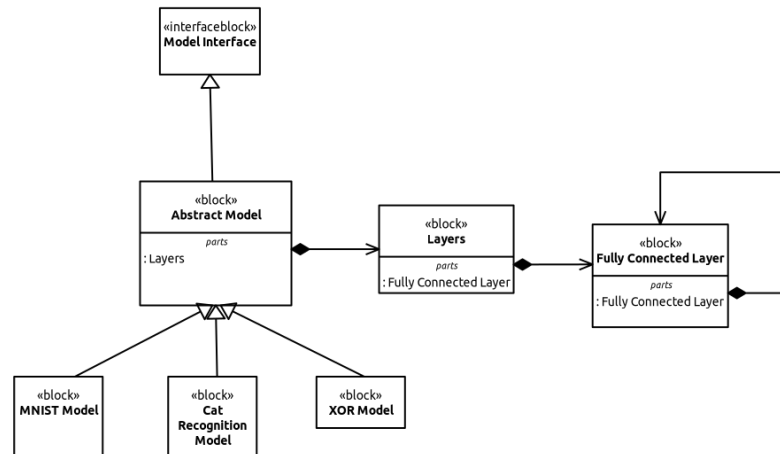
2.3.1 UI Class Diagram

bdd [package] School Project [UI Class Diagram]



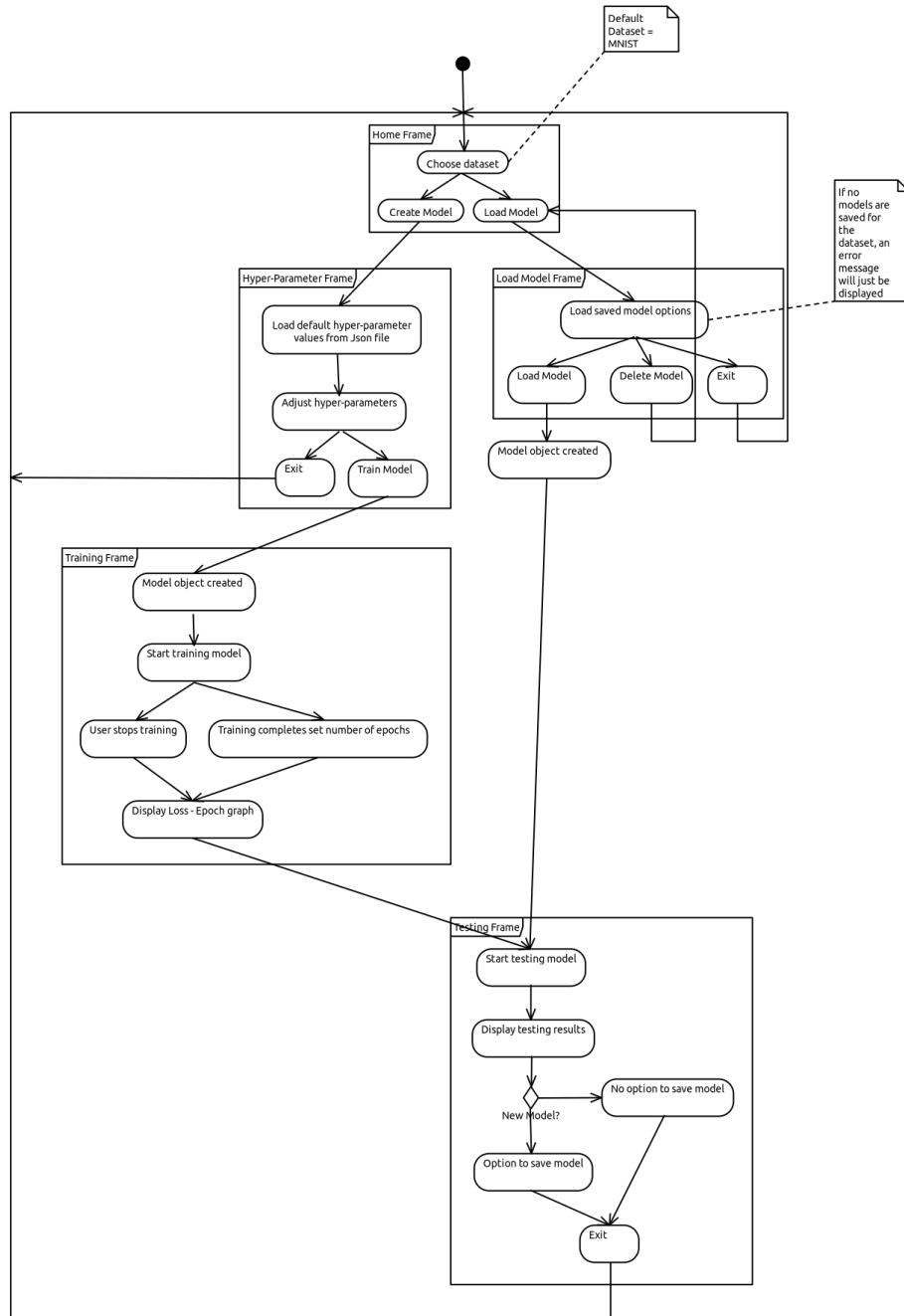
2.3.2 Model Class Diagram

bdd [package] School Project [Model Class Diagram]



2.4 System Flow chart

act [activity] System Flow chart [System Flow chart]



2.5 Algorithms

Refer to Analysis for the algorithms behind the Artificial Neural Networks.

2.6 Data Structures

I will use the following data structures in the program:

- Standard arrays for storing data contiguously, for example storing the shape of the Artificial Neural Network's layers.
- Tuples where tuple unpacking is useful, such as returning multiple values from methods.
- Dictionaries for loading the default hyper-parameter values from a JSON file.
- Matrices to represent the layers and allow for a varied number of neurons in each layer. To represent the Matrices I will use both numpy arrays and cupy arrays.
- A Doubly linked list to represent the Artificial Neural Network, where each node is a layer of the network. This will allow me to traverse both forwards and backwards through the network, as well as storing the first and last layer to start forward and backward propagation respectively.

2.7 File Structure

I will use the following file structures to store necessary data for the program:

- A JSON file for storing the default hyper-parameters for creating a new model for each dataset.
- I will store the image dataset files in a 'datasets' directory. The dataset files will either be a compressed archive file (such as .pkl.gz files) or of the Hierarchical Data Format (such as .h5) for storing large datasets with fast retrieval.
- I will save the weights and biases of saved models as numpy arrays in .npz files (a zipped archive file format) in a 'saved-models' directory, due to their compatibility with the numpy library.

2.8 Database Design

I will use the following Relational database design for saving models, where the dataset, name and features of the saved model (including the location of the saved models' weights and biases and the saved models' hyper-parameters) are saved:

Models	
ID	integer
Dataset	text
File_Location	text
Hidden_Layers_Shape	text
Learning_Rate	float
Name	text
Train_Dataset_Size	integer
Use_ReLu	bool

2.9 Queries

Here are some example queries for interacting with the database:

- I can query the names of all saved models for a dataset with:

```
SELECT Name FROM Models WHERE Dataset=?;
```

- I can query the file location of a saved model with:

```
SELECT File_Location FROM Models WHERE Dataset=? AND Name=?;
```

- I can query the features of a saved model with:

```
SELECT * FROM Models WHERE Dataset=? AND Name=?;
```

2.10 Human-Computer Interaction TODO

- Labeled screenshots of UI

2.11 Hardware Design

To allow for faster training of an Artificial Neural Network, I will give the option to use a Graphics Card to train the Artificial Neural Network if available. I will also give the option to load pretrained weights to run on less computationaly powerfull hardware using just the CPU as standard.

3 Technical Solution TODO

3.1 Test

```
1 import os
2 import sqlite3
3 import threading
4 import tkinter as tk
5 import tkinter.font as tkf
```
