Logistic Regression and Data Analysis in Machine Learning

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November 28, 2021

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Introduction

1.1 Motivation

This paper is written for those who want a peek into some of the fundamentals of Machine Learning. More specifically, we will examine Logistic Regression, a very popular and powerful algorithm. The paper can be understood by those who have a basic idea of linear algebra, and the rest of the deeper mathematics required to implement this algorithm will be explained through intuition.

Hopefully, by the end of this paper we can implement this algorithm from scratch, and gain an insight into process behind designing and creating machine learning solutions.

1.2 The Rise of Machine Learning

Machine Learning has existed since the 1950's. However, only until recently have we acquired the resources to store immense amounts of data. With the added benefits of faster computers, Machine Learning has started to flourish from research to business applications.

There are many ways to categorize machine learning: supervised learning, unsupervised learning, reinforcement learning, semi-supervised learning and more. As previously mentioned, we will take a look at one Machine Learning algorithm Logistic Regression, which is a "supervised learning algorithm".

1.3 Expectations

Throughout this paper, we will take a look at many equations that will build the foundations for Logistic Regression. Often, these equations will have summations over many training samples (rows of data from a given dataset). The most basic ways to implement these algorithms would be to use for-loops. However, given the amount of data we operate with we need a faster way to compute many

of these equations. Thus, we will "vectorize" these calculations, or substitute these for-loops with matrix operations, during our implementation. While this is an abstract explanation and we haven't taken a look at any concrete examples yet, the expectation is to have at least basic understanding of linear algebra.

Problem Statement

2.1 Dealing with Classification

A popular goal of Machine Learning is classification, where we create a model that can take data which it hasn't seen before and give it a label. Here are some examples of classification problems -

- Determining whether or not an email is a spam email
- Given data about a cancer patient, determine whether their tumor is malignant or benign
- Given an image, determine whether or not it has a car in it

These are all binary classification problems, where we can for example classify an email as not spam or spam (0 or 1).

2.2 Supervised Learning

Now the inevitable question arises, how do we begin to write a program that can act as a classifier? Before that we must learn about the type of algorithm we are going to be building.

Supervised Learning is when we create a Machine Learning model through labelled data. Data is labelled when the expected data outputs have been provided for every input. Another way of thinking about it is, for every x we have been provided with y. Let's a take a look at some labelled data we could use to train a classifier.

A company want's to create a machine that can figure out whether they want to employee a new person. They look at their past history of employment and collect the following data -

X (Highest Degree)	Y (Employed or not)
High School	0
Undergrad	1
Masters	0
Undergrad	0
PHD	1

Here "1" in the Y column represents whether the person got hired. One of the biggest challenges of Machine Learning is to create optimal dataset we can use for training models from the massive stores of data we possess today.

This dataset is incredibly small to actually train a Machine Learning model. Realistically, the data is more complex and a lot larger. A more realistic example can look like the following -

Highest Degree	Years of Experience	Criminal Record	Y
High School	0	No	0
Undergrad	10	Yes	1
Masters	4	No	0
Undergrad	2	No	0
PHD	4	No	0

Notice, we aren't restrained to having just one X column. We can have many X columns, or "features", which we feed to the model so it can learn to classify better.

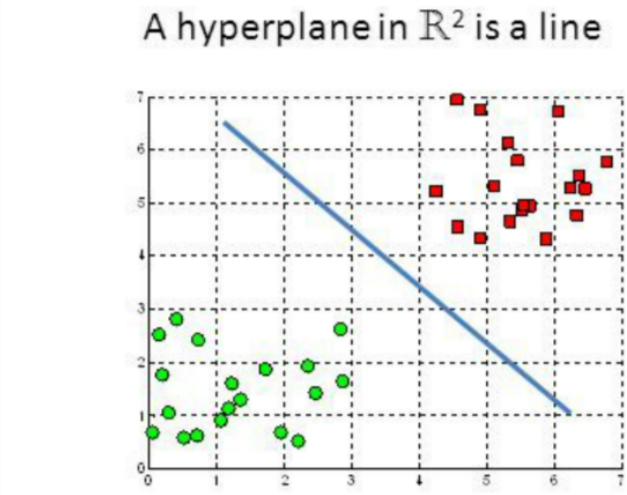
Logistic Regression

Finally, are going to learn the method by which we can classify data.

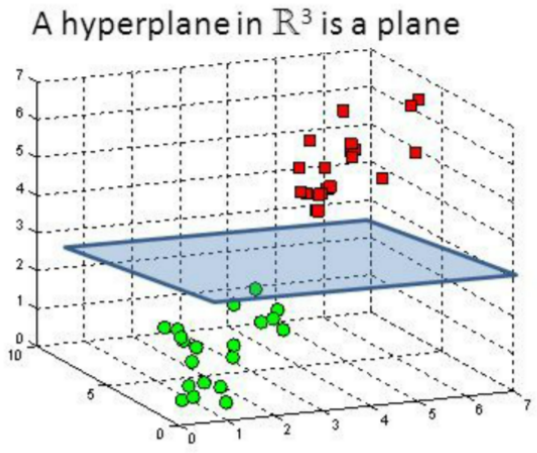
3.1 Fitting the Hyperplane

The goal of logistic regression is to fit a hyperplane through the feature space. This might be a duanting sentence but let's break it up.

Let's first define a hyperplane. Given a $\mathbb{R}^n$ subspace, a hyperplane is a subspace in $\mathbb{R}^{n-1}$. Here is a hyperplane for $\mathbb{R}^2$, which is a line



Similarly, a hyperplane for $\mathbb{R}^3$ would be a plane



Notice, in these pictures we have two clusters of data. The axis are our features, and the hyperplane is dividing these clusters. This is the goal of logistic regression - to know which hyperplane will optimally help us differentiate these clusters.

3.2 Defining the Model

Now that we understand the goal of logistic regression, let's dive deeper into how we can build our desired hyperplane.

Let's consider the equation of a line: $y = \theta_1 x + \theta_0$
Here is a vectorized implementation for the equation of a line:
Let $\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \end{bmatrix}$ and $X = \begin{bmatrix} 1 \\ x \end{bmatrix}$

Then $y = \theta^T X = \begin{bmatrix} \theta_0 & \theta_1 \end{bmatrix} \begin{bmatrix} 1 \\ x \end{bmatrix} = \theta_0 + \theta_1 x$

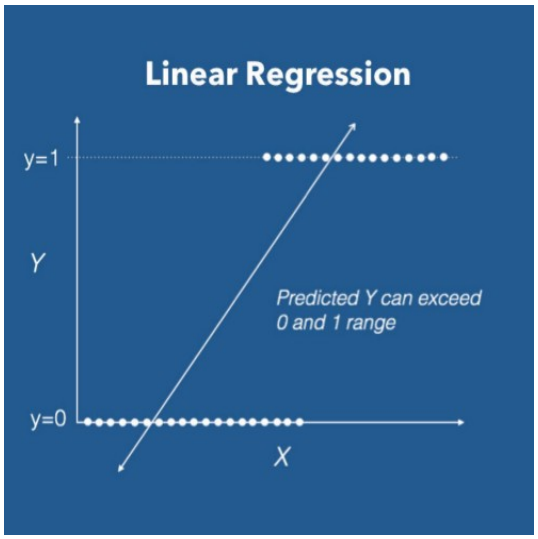
This can be generalized for all linear equations: $y = \theta_0 + \theta_1 x_1 + \cdots + \theta_n x_n$

Let $\theta = \begin{bmatrix} \theta_0 \\ \theta_1 \\ \vdots \\ \theta_n \end{bmatrix}$ and $X = \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_n \end{bmatrix}$

Then $y = \theta^T X = \begin{bmatrix} \theta_0 & \theta_1 & \cdots & \theta_n \end{bmatrix} \begin{bmatrix} 1 \\ x_1 \\ \vdots \\ x_n \end{bmatrix} = \theta_0 + \theta_1 x_1 + \cdots + \theta_n x_n$

Notice that X is a row of a given dataset, so every "feature" or column of the data has a value of theta value associated with it. This gives us multidimensional linear models.

Now that we know what a linear model looks like, let's take a look at a whether we can use it to build a classifier. We want the model to give us the probability of whether a given data is either 0 or 1.

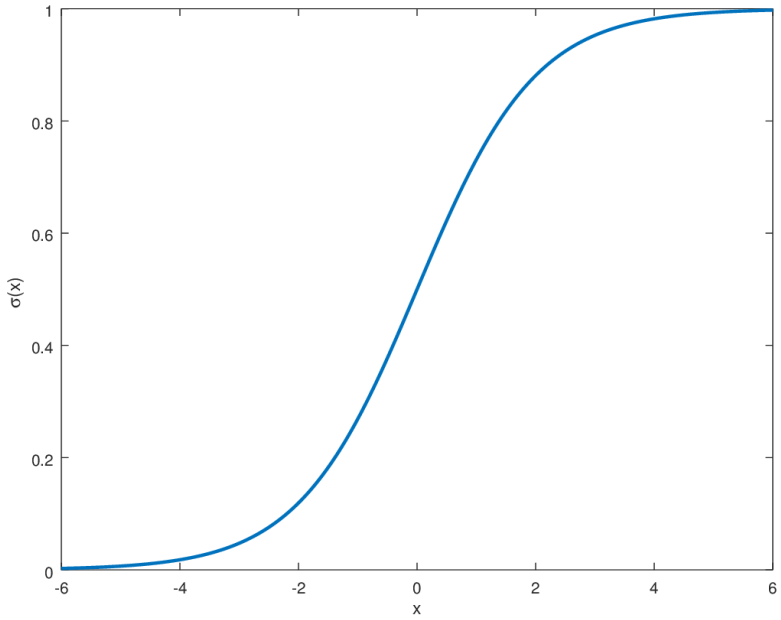


This model isn't very helpful. Notice that to classify whether something is 0 or 1, we need a probability. If it's 50% or less, we'll classify it as 0, and more than 50% becomes 1. However, using a line overshoots this (for example you can't have negative probabilities), making it impractical for our use.

Thus, we can utilize a function known as the sigmoid function. It is defined as the following function

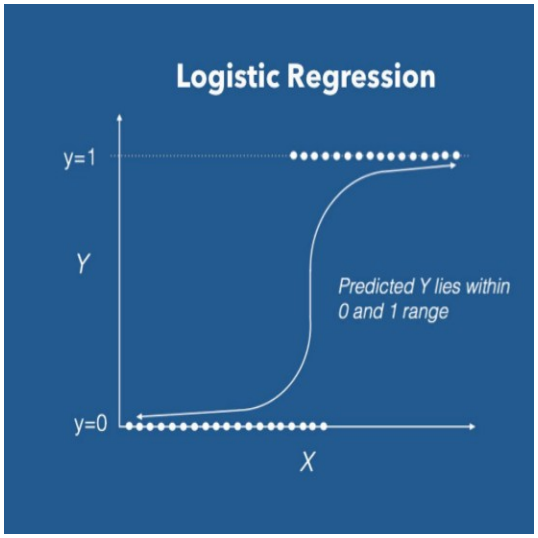
$$\sigma(x) = \frac{1}{1 + e^{-x}}$$

and looks like the following graph.

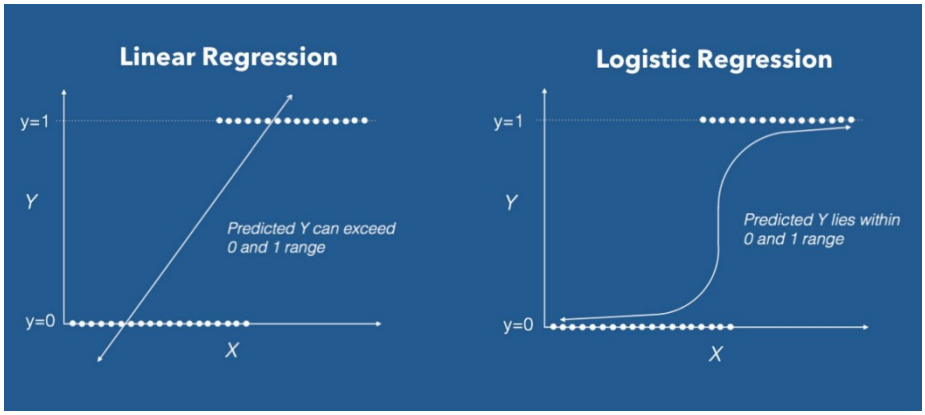


This function always returns a value between 0 and 1, which can be interpreted as a probability. For logistic regression, we can take a linear model and put it through the sigmoid function, giving us the following equation.

$$h_\theta(X) = \frac{1}{1 + e^{-\theta^T X}}$$



Thus, we get the following summary. Our logistic regression model is defined by $h_\theta(X)$, which now returns us a probability between 0 and 1.



https://miro.medium.com/max/1050/1*dm6ZaX5fuSmuVvM4Ds-vcg.jpeg

3.3 Idea of Cost

The idea of cost is to create a metric by which we can measure how "error prone" our model is. Notice, this is not the same as measuring the accuracy of our model. Although they are somewhat correlated and similar, we do both in Machine Learning.

In Machine Learning, finding the cost of model is standard practice. Given one data sample, in logistic regression we can calculate the cost through the following equation -

$$Cost(x) = -y \log h_\theta(X) + (1-y)(1-h_\theta(X))$$

Now that we have found a way to evaluate the cost of one data sample, we want find the average cost over our entire dataset, which gives us a more general understanding for how error prone the model is. We do this by the following equation

$$\text{Cost: } J(\theta) = -\frac{1}{m}\sum_{i=1}^{m} y^{(i)} \log h_\theta(x^{(i)}) + (1-y^{(i)}) \log 1 - h_\theta(x^{(i)})$$

The goal is minimize this cost, $J(\theta)$

3.4 Gradient Descent

We know know the definition of Logistic Regression model, and how to evaluate the model. However, we haven't yet learned how to find the parameters θ which lower our cost.

We do this through "training" our model, or a process by which we find the optimal theta values for our model.

There are many ways to do this, but we will take a look at a popular algorithm gradient descent. In this algorithm, we are looking to find the global minumum of cost given some theta parameters.

Finally, for those who are experienced with calculus, one way to converge to the global minimum is to take the partial derivative with respect to theta. Then, we add this gradient to theta, which will optimize it closer towards the global minimum. This gives us the following equations

$$\theta_j := \theta_j - \alpha \frac{\partial}{\partial \theta_j} J(\theta)$$

After evaluating the partial derivative we get -

$$\theta_j := \theta_j - \frac{\alpha}{m} \sum_{i=1}^{m} (h_\theta(x^(i)) - y^{(i)}) x_j^i$$

where $1 \leq j \leq n$ and n is the number of features and α is the learning rate (a predetermined constant value).

A Practical Look

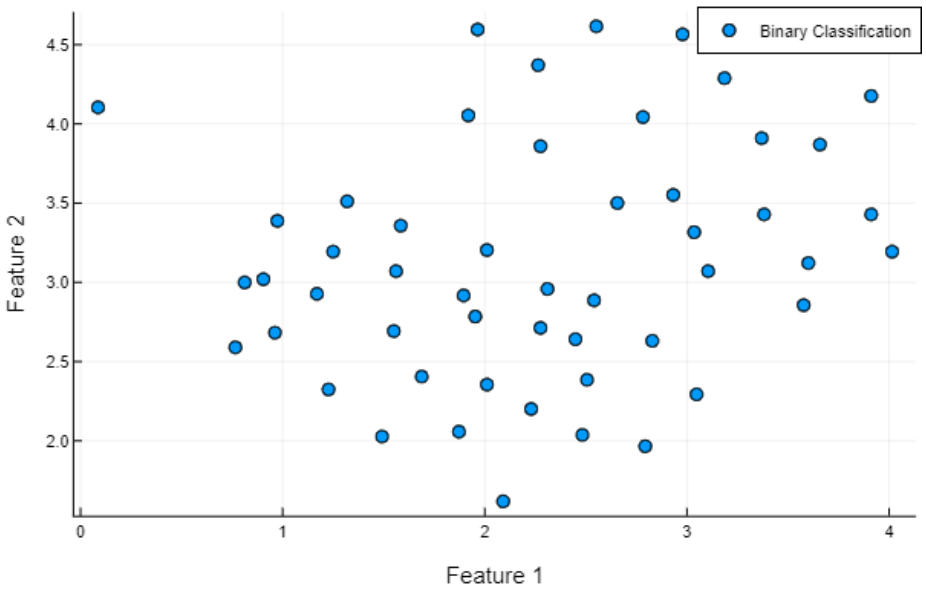
The links to the data and code used to implement this will be provided in the appendix.

4.1 Examining Data

Let's load the binary classification dataset into Julia. Here's a small sample from the dataset. We do this through the following code -

Feature 1	Feature 2	Classification
1.9643	4.5957	1
2.2753	3.8589	0
2.9781	4.5651	0
2.932	3.5519	1
3.5772	2.856	1
4.015	3.1937	1
3.3814	3.4291	0

Graphing feature 1 and feature 2 gives us the following graph.



From just the graph it is apparent that there seems to be two distinct clusters. The goal will be to fit a hyperplane in this feature space such that we can divide the two clusters.

4.2 Training vs Testing Split

A practical idea in Machine Learning is taking a dataset and splitting it two datasets, one specifically for training and the other for testing. Imagine that you are learning how to drive by practicing in your neighborhood. You might learn to recognized certain sharp turns or stop signs, making you a good driver. However, this does not mean you can drive everywhere in the world. To check whether you are a good driver, we expect you drive well in places you haven't seen before.

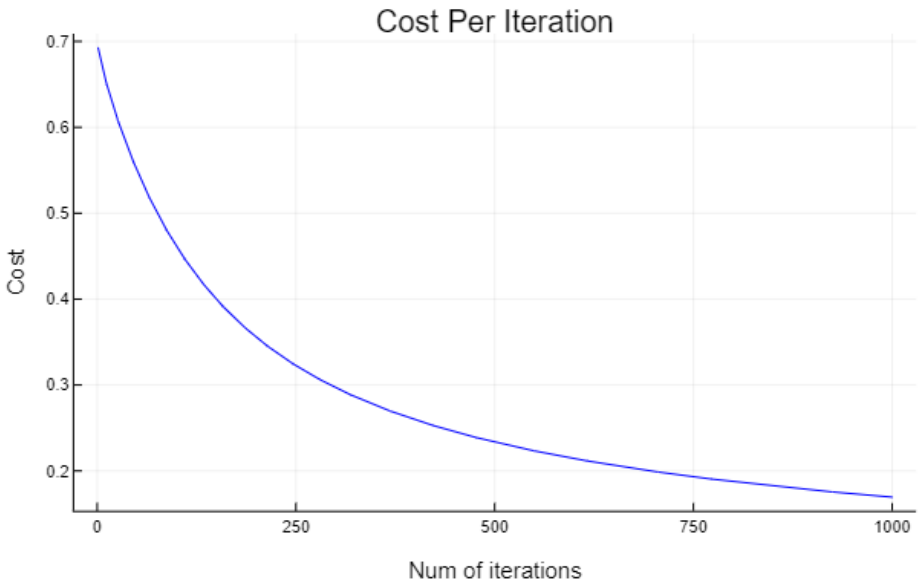
Similarly, the model is trained using a training dataset. The testing dataset is some small amount of data the model has never seen before. We can judge its accuracy over this dataset to determine whether our model is generalized and accurate.

For this data, we will use 80% of the data for training and %20 for testing.

4.3 Training a model

Using what we have learned so far, we can successfully train a model. At every step of gradient descent (which we perform many, many times), we can keep

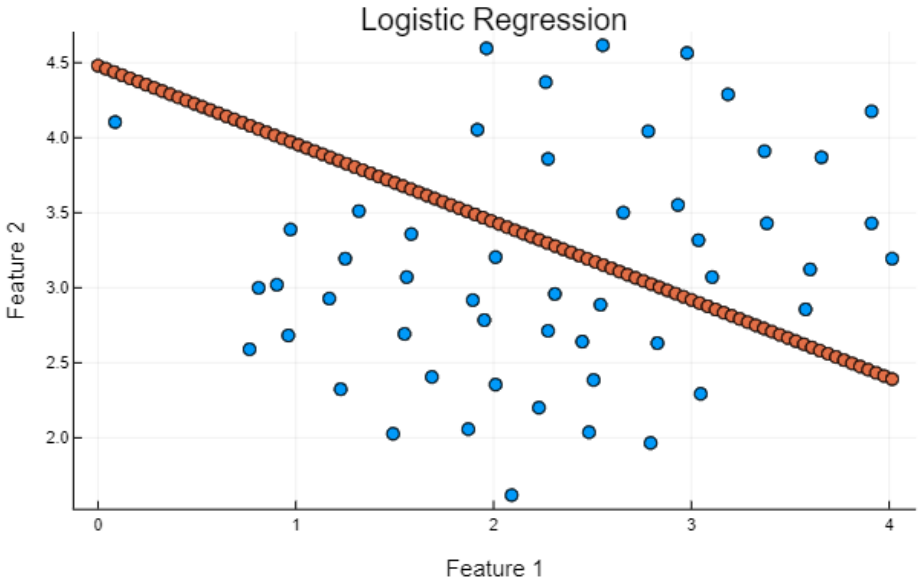
track of our cost. Here is the history of my cost as I trained my model -



Visually speaking the model looks promising based on the overall cost decreasing at every iteration. However, if the cost becomes too low then it might suggest that we have successfully learned everything about the training dataset, but it's performance on the testing dataset might be worse.

4.4 Evaluating Accuracy

Informally, we can test whether our model did well by visualizing the hyperplane it created.



The model learned which line would best divide the clusters. This type of accuracy evaluation only works with two dimensional features. For a more concrete metric, we will evaluate the accuracy of our model over our testing data.
We can do this using the following steps -

- Train our model
- Run the model over the data in the testing dataset (predictions)
- Find the percentage of predictions that were accurate with the label

Thus, the total accuracy we got was -

Multiclass Classification

5.1 One VS All Classification

We have looked at creating a binary classification model. However, what if we have more than just two clusters or labels?

Here we use one versus all classification. The idea is to choose one label, make it 1 and set all the other labels to 0. Then we train a binary classification logistic regression model. Similarly, we repeat this process for all the labels, making our desired label 1 and the rest 0. This will result in the same number of binary classification models as the number of labels.

The idea is to differentiate just one label from all the other labels, hence the name one versus all.

5.2 One VS All Prediction

Now that we have many binary classification models, how do we predict a data sample's label?

The answer is to run the data sample through all of the models. The model which returns the highest probability, or degree of confidence, is the model we choose as the most accurate. This label that is associated with this model becomes the same label predicted for the data sample.

Another Practical Look

This time we will be classifying handwritten digits.

6.1 Examining Data

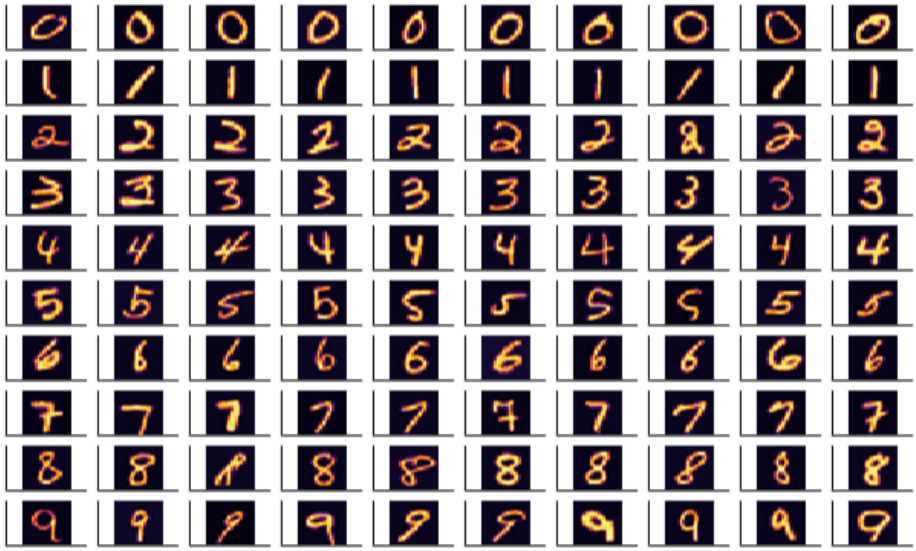
Taking a look at just one data sample is going to be tough since it is an image. The dataset has 5000 samples and 400 features.

$$\underbrace{\overset{5000}{\left\{\begin{bmatrix} Image_1 \\ Image_2 \\ \vdots \\ Image_{5000} \end{bmatrix}\right.}}_{400}$$

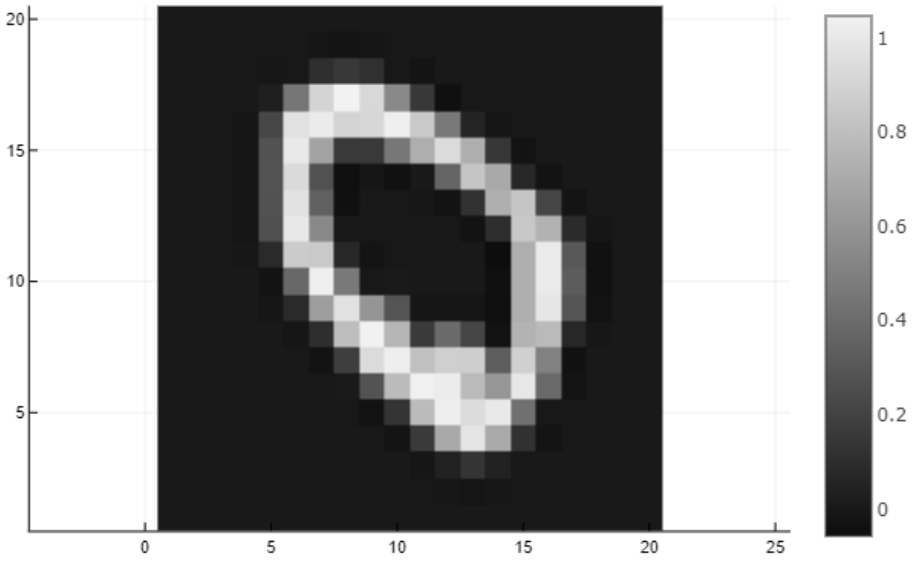
Here every feature is a pixel. An arbitrary data sample is just a flattened 400 pixel image and looks like the following -

$$Image_i = \underbrace{\begin{bmatrix} pixel_1 & pixel_2 & \cdots & pixel_{400} \end{bmatrix}}_{400 \text{ pixels}}$$

So can take a 400 pixel flattened image, and reshape it into a 20×20, which will help us visualize the image. Taking a few random samples we get the following images -



Taking a look at just one of the images we get the following picture -



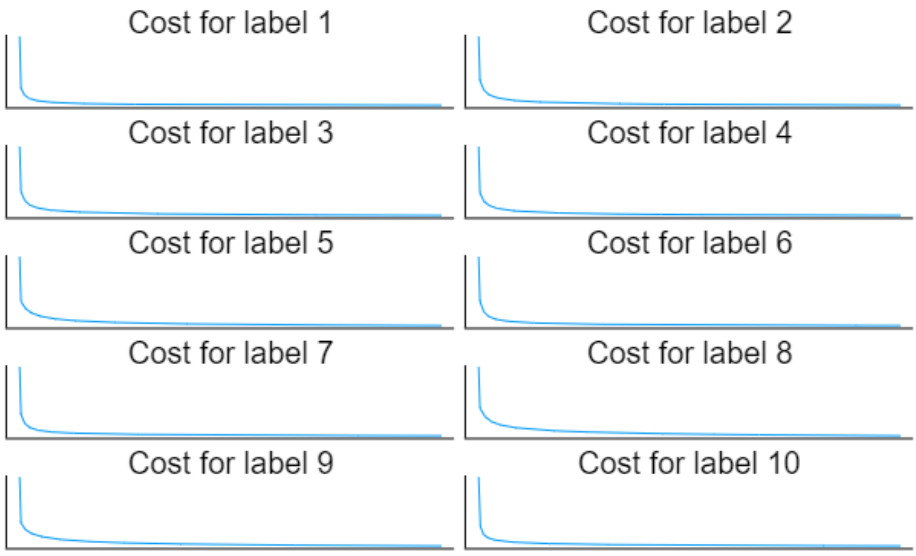
Notice, both the x and y axis go from 0 to 20, which means the image is in fact a $20 \times 20 = 400$ pixel image

6.2 Training vs Testing Split

Similar to the first practical example, we will create a 80/20 split. 80% of the data will be used for training the other 20% will be used to evaluate the accuracy of our model.

6.3 Training a Model

This time we train a model for every digit. During this training process, the one label will be set to 1 and the rest will be set to 0. Doing this for every label will give us 10 different models. Here are the graphs for the history their cost while training -



Here label 1 represents the digit 0, label 2 is the digit 1, and so on. All of the ten binary classification models seem to be fairly optimized since their cost has decreased.

6.4 Evaluating Accuracy

We will perform predictions over our testing dataset. The accuracy of the models trained resulted in the overall accuracy of

Visualizing Data: PCA

7.1 Motivation

As we have seen, the data that we could potentially use for training logistic regression models can be incredibility complex and high dimensional. Not all data can be modelled using logistic regression. Even though it worked for hand written digits, often in Machine Learning we aren't entirely sure.

Something that always helps is visualizing the data. Besides the pros of dimensional reduction we have learned in class, this is another motivational aspect of it.

7.2 PCA Analysis

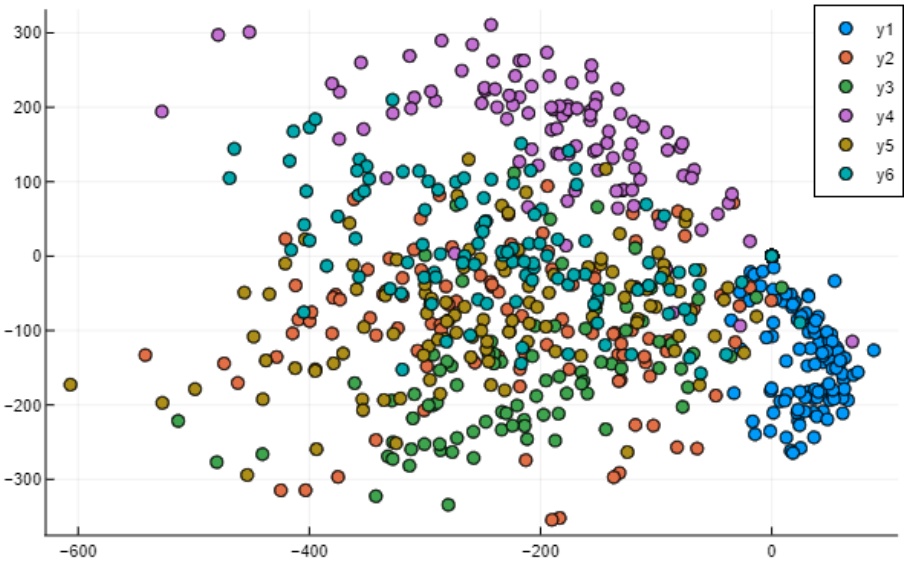
To perform PCA Analysis we perform the following steps -

- We first find the center for the data. This means we average every column in the matrix D to find the mean value for every feature
- We find the covariance matrix (more on this later)
- We calculate the eigenvalues and their eigenvectors for the covariance matrix
- We choose the eigenvectors that have the largest eigenvalues to form the matrix W
- Then we calculate to $W^T D^T$ to reduce the dimensions of the data

Here is an example for the following dataset -

7.3 Visualizing Handwritten Digits

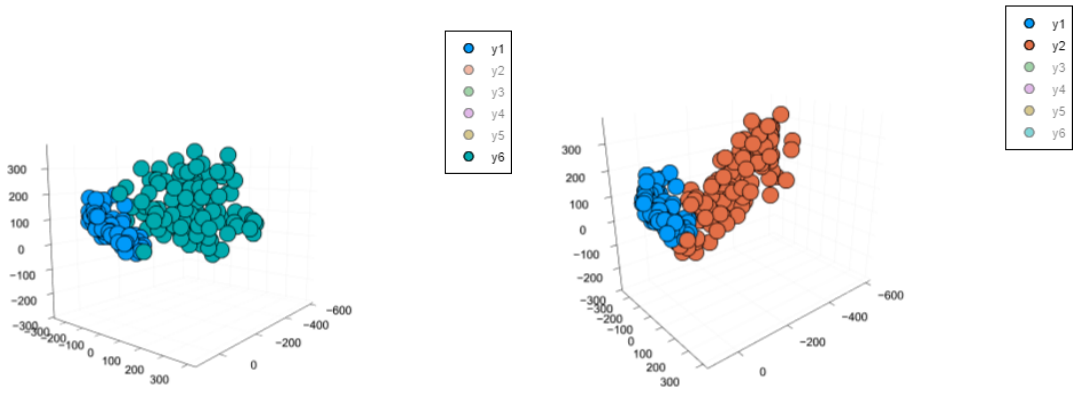
After performing PCA Anlaysis here are some results -



Here is a 2D reduction of some random samples from our dataset. This random sample has the digits from 0 to 5. Just looking visually, we can see there are some clusters for each digit.

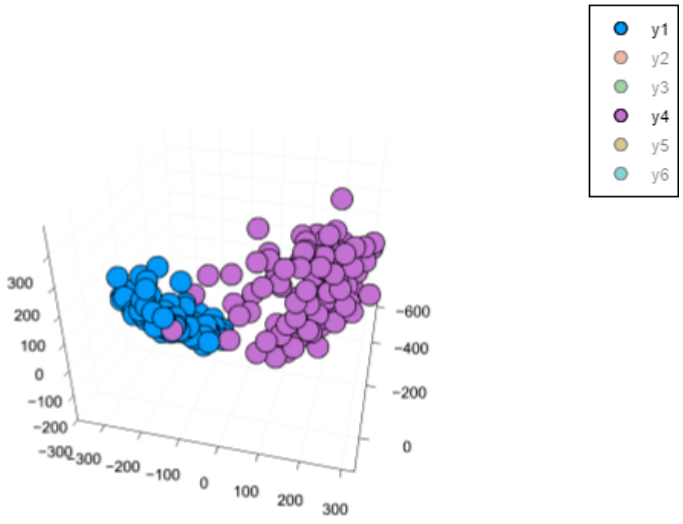
However, they seem to overlap a lot. This is expected since we lost a lot of data from reducing the dimensions of the data. However, the most important aspects of the dataset were retained, giving us a 2 pixel representation of an image.

Similarly, if we reduce the same data to 3D we get some of the following graphs



Here we are comparing a three pixel representation between the 0/5 digits, and

the 0/1 digits.



For this example, there seems to be two distinct clusters between the 0 digit and the 3 digit. This concludes the paper.

Appendix

Link to code/data

1. Supervised Learning: A process by which labelled data is used to train a Machine Learning model. Data is labelled when expected data outputs have been provided every data inputs.