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# **Project 2: Classification and Regression, from Linear and Logistic Regression to Neural Networks**

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## **Abstract**

## **Reproducibility**

The code used for this report can be accessed at:

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## Introduction

Supervised machine learning problems can broadly be divided into the domains of regression and classification. Regression involves developing models that can predict continuous function values, such as a salary, velocity, or temperature. On the other hand, classification involves developing models that can predict labels (or classifications) of data, for instance whether a tumor is malignant or benign, or whether an image contains a cat or a dog.

The focus of Project 1 was on simple regression methods: ordinary least squares, ridge, and lasso regression. These methods demonstrate great performance and explainability on problems with a lower degree of complexity, namely problems with (at least roughly) linear dependence between the input and output. The analogue to these simple regression methods in the domain of classification is logistic regression. Logistic regression models can be trained to output the probability that a datapoint belongs to a given class, and works best when the data's classes are easily delineated.

However, many machine learning problems have a higher degree of complexity, due to nonlinear relationships between variables and/or nonlinear separations between data classes. This motivates the need for more sophisticated models that can handle nonlinearities, such as neural networks. Neural networks are based on the perceptron model of how neurons work in the brain, where a neuron's activation is dependent on input features and weights (Rosenblatt, 1958). By combining multiple neurons in multiple layers, in what are called "deep" neural networks, increasingly complex problems can be solved. The development and use of neural networks actually stagnated for many decades until the early 2010s, when computational power had increased enough for them to be implementable. Now there is a revolution in which neural networks are used commonly and to great success on a variety of problems. While the advantage and power of neural networks is most apparent when moving to highly complex data, they can sometimes outperform traditional methods on simple data as well.

Part of the beauty and effectiveness of neural networks is how they can be applied to both regression and classification problems. This is done by 1) changing the cost function used in its training, which can then be optimized with a variety of methods such as gradient descent. And 2) by changing the output layer of neurons, to either output a continuous value (for regression), or a set of probabilities for the various labels (for classification). Furthermore, neural networks can utilize different activation functions to determine how easily and in what manner neurons will activate.

In this project, we develop our own neural network code to perform both regression and classification tasks. Our goal is to show that neural networks can do as well as, and perhaps outperform, traditional regression and classification methods on simple datasets. We start with explaining the theory behind gradient descent, gradient descent with momentum, stochastic gradient descent, and learning rate tuning methods that are used in the optimization of training cost functions. Then we explain the theory of logistic regression and neural networks. In our tests, we first compare the performance of the various optimization methods for regression on a simple quadratic function. We then demonstrate our neural network for

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regression, again on the quadratic function, but also with comparison to a neural network developed in Tensorflow. Finally, we demonstrate our neural network applied towards a classification task - the classification of tumors as malignant or benign from the Wisconsin Breast Cancer Dataset - and compare its performance to logistic regression, and a classification neural network built in Tensorflow.

## Theory

### Optimization Methods

In supervised machine learning problems, one of the most important concepts is optimizing - or finding the minimum of - a cost function that measures how well your model is performing. There exist a number of methods to iteratively solve for the minima of cost functions, as well as algorithms to tune the "learning rate" at which these methods progress. We will explore those here.

#### *Gradient Descent*

Gradient descent is an optimization method that is used to iteratively solve for minima or maxima in differentiable functions. It is used commonly in machine learning in order to solve for the minima of a cost function that measures the performance of a model in training. Gradient descent iteratively solves for points  $x$  that approach the minima by going in the direction of steepest descent, which is the direction of the negative gradient (Boyd and Vandenberghe, 2004).

$$x^{(k+1)} = x^{(k)} - (J(f(x^{(k)})))^{-1} f(x^{(k)}) \quad (1)$$

In the above equation  $x^{(k)}$  is an initial guess for the  $x$  point corresponding to the minima,  $J$  is the Jacobian matrix (which is a matrix of first-order partial derivatives, where the  $i$ th row is the gradient of the  $i$ th component of the function  $f(x)$ ,  $f(x^{(k)})$  is the function we want to minimize evaluated at  $x^{(k)}$ , and  $x^{(k+1)}$  is the updated value of  $x$  which is closer to the minima point. This process then repeats itself in the next iteration with the old value of  $x^{(k+1)}$  set to  $x^{(k)}$ , and so on until the minima is reached. This equation can be written in terms of the Hessian matrix  $H$  (the matrix of second order partial derivatives) and the gradient of the function  $f$ :

$$x^{(k+1)} = x^{(k)} - (H(x^{(k)}))^{-1} \nabla f(x^{(k)}) \quad (2)$$

Because calculating the Hessian is often very computationally expensive, one of the most common methods is to set it to a scalar value, which is referred to as the learning rate. This learning rate can also be thought of as the step size of this iterative solver.

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$$x^{(k+1)} = x^{(k)} - \eta \nabla f(x^{(k)}) \quad (3)$$

If the learning rate is too large, the gradient descent method might miss the local function's extrema. On the other hand, if the learning rate is too small, it might take a lot of time before it reaches the extrema, and thus be computationally inefficient. One issue often arises in the case of complex functions with several extrema - the solver can get stuck in a local extrema instead of reaching the global minima (which is the intention). Thus gradient descent is very sensitive to the type of function it is applied on, with convex functions being preferable, and is also sensitive to the setting of its learning rate.

### *Gradient Descent with Momentum*

One improvement to gradient descent is including a momentum parameter. This parameter is analogous to momentum or inertia in an equation of motion, which represents some memory of the speed and direction being travelled in. In gradient descent, this can be thought of as memory of the direction and magnitude one is travelling in parameter space in order to find the function's minima. The implementation in equation form looks like:

$$v^{(k+1)} = \gamma v^{(k)} - \eta \nabla_{\theta} f(\theta_k) \quad (4)$$

where  $\theta_{k+1} = \theta_k - v_k$ , and  $\gamma$  is the momentum parameter which should take values between 0 and 1. The updates  $v^{(k+1)}$  can then be interpreted as a running average of the gradients.

### *Stochastic Gradient Descent*

Stochastic gradient descent (or SGD) is another improvement to gradient descent that works by randomly sampling smaller portions of the data. The process involves first dividing the dataset randomly into portions called "minibatches", and then calculating the gradients and updating for each minibatch (Goodfellow et al., 2016). After completing this process for every minibatch, the entire dataset has been seen, and it is said that one "epoch" or "iteration" has been completed. The relation between the number of datapoints  $n$  and the minibatch size  $M$  is such that there are  $n/M$  minibatches. If we define a cost function that we want to minimize,  $C(\beta)$ , then the iterative gradient descent equation then becomes the following for stochastic gradient descent:

$$\beta^{(k+1)} = \beta^{(k)} - \eta_k \sum_{i \in B_k}^n \nabla_{\beta} c_i(x_i, \beta) \quad (5)$$

where  $B_k$  is the  $k$ th minibatch of the data. The main advantage of stochastic gradient descent is how it reduces the computational demands of calculating gradients, as it does this on smaller minibatches of the data. This leads to a lower computational time for each iteration compared to regular gradient descent. While estimations of the gradients may not always be as accurate

as for regular gradient descent (which is looking at the whole data), the methods are usually very close in their results, and the much faster convergence makes SGD often preferred.

### *Learning Rate Tuning Methods*

In the section on gradient descent we described a simple procedure of setting the learning rate to a constant value. However, there exist many methods to iteratively tune the learning rate. These methods can lead to better convergence to the minima.

One of these methods is AdaGrad, which means Adaptive Gradient Algorithm. This algorithm works by scaling the learning rate of the different model parameters by the root mean squared of all the previous gradient values (Goodfellow et al., 2016). In this way, parameters that have larger gradients experience a larger decrease in their learning rates, and parameters with smaller gradients experience a smaller decrease in their learning rates. This leads to an adaptive shift of the learning rate in order to make more progress in the parameter directions that have lower gradients. The update rule for AdaGrad is given by the equation, where  $g$  represents the gradient, and  $\delta$  is a very small value (usually on the order of  $1e-8$ ) used to avoid potential division by 0:

$$x_i^{(k+1)} = x_i^{(k)} - \frac{\eta}{\sqrt{\sum_{\tau=1}^k g_{\tau,i}^2 + \delta}} g_{k,i} \quad (6)$$

The next learning rate tuning method is RMSprop, which means Root Mean Squared Propagation. RMSprop is an extension of AdaGrad which instead of using the regular RMS average of the gradients, uses a decaying moving average of the gradients (Goodfellow et al., 2016; Hinton, 2012). The potential advantage of RMSprop in comparison to AdaGrad is that by using the moving average, it can focus less on the early values of the gradient, and instead focus more on more recent values of the gradient that are more relevant to the current status of the search for the minima. The update equation is as follows:

$$x_i^{(k+1)} = x_i^{(k)} - \frac{\eta}{\sqrt{\mathbb{E}[g^2]_k + \delta}} g_k \quad (7)$$

Where  $\mathbb{E}[g^2]_k$  is a moving average of the expectation values of the squared gradients, given by:

$$\mathbb{E}[g^2]_k = \gamma \mathbb{E}[g^2]_{k-1} + (1 - \gamma) g_k^2 \quad (8)$$

A good value for  $\gamma$  is typically on the order of 0.9 (Hinton, 2012).

The final learning rate tuning algorithm that we will implement is called Adam, whose name derives from adaptive moment estimation. The key concept of the Adam algorithm is that it keeps track of a running average of the squared gradients, as well as a running average of the unsquared gradients (Kingma and Ba, 2014; Goodfellow et al., 2016). In this way it

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is like a combination of RMSprop and momentum gradient descent. The running average of the gradients is referred to as the first moment  $m$ , and the running average of the squared gradients is referred to as the second moment  $v$ , which are given iteratively by:

$$m_{k+1} = \beta_1 m_k + (1 - \beta_1) g_k \quad (9)$$

$$v_{k+1} = \beta_2 v_k + (1 - \beta_2) g_k^2 \quad (10)$$

However, these moments tend to be stuck around zero when initialized as such, and thus need to be corrected with bias terms:

$$\hat{m}_k = \frac{m_k}{1 - \beta_1^k} \quad (11)$$

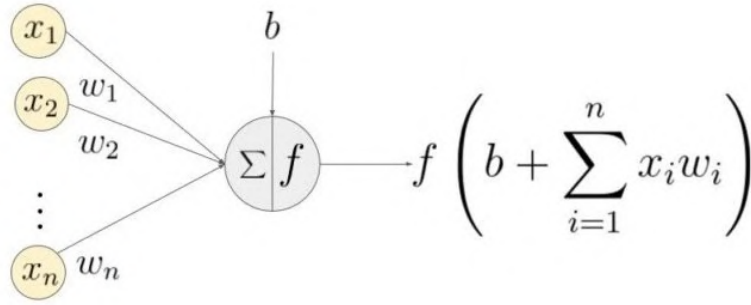
$$\hat{v}_k = \frac{v_k}{1 - \beta_2^k} \quad (12)$$

Putting this all together in terms of the bias-corrected moments, the update rule for Adam becomes:

$$x_{k+1} = x_k - \frac{\eta}{\sqrt{\hat{v}_k} + \delta} \hat{m}_k \quad (13)$$

## Feed Forward Neural Networks

Feed Forward Neural Networks (FFNNs) are the simplest type of artificial neural networks. They are made up of multiple nodes (also called neurons or perceptrons) in multiple layers, forming a network. Each node can be thought of as a decision-maker that takes in multiple inputs and produces a single output. The way that a node makes a decision is by applying weights and biases to the input values, and determining if the resulting output meets some threshold criterion (Nielsen, 2015). Weights are values that scale the inputs according to their relative importance, and biases are static shifts that are applied that affect how easy it is for the node to activate. This process can be visualized and mathematically represented as seen in Figure 1:



**Figure 1:** Diagram showing the process of input, weighting, and activation occurring at a neural network node. From Sharma, 2017.

The inputs are the values  $x_i$ , and the weights  $w_i$ . Within the node, the sum of the bias and the weighted sum of the inputs,  $b + \sum_{i=1}^n x_i w_i$ , is evaluated with what is called an activation function  $f$ . There exist several activation functions that can be used - we will implement three simple ones in this project: the sigmoid, ReLU, and leaky relu.

The sigmoid function is designed so as to take an input value, and yield an output between 0 and 1. It is defined by the following equation:

$$\sigma(z) = \frac{1}{1 + e^{-z}} \quad (14)$$

The sigmoid function is also known as the logistic activation function, because it is used in logistic regression as we will explore later. It is especially appropriate for classification problems, because it yields values between 0 and 1, which can represent probabilities that a datapoint belongs to a given class. However, one of the disadvantages of sigmoid activation functions is that they can lead to so-called vanishing gradients (Mehta et al., 2019). This occurs when a large change in the input to a sigmoid function produces a small change in the output (because the output is squashed from 0 to 1), yielding a very small derivative or vanishing gradient. For this reason, the hyperbolic tangent function is commonly used in place of the sigmoid, as it has a similar curve but with larger derivatives (though we do not implement tanh in this project for the sake of brevity).

The next activation function we will implement is the ReLU, or Rectified Linear Unit. The ReLU is a piecewise function defined as:

$$\sigma(z) = \begin{cases} z & \text{if } z \geq 0 \\ 0 & \text{if } z < 0 \end{cases} \quad (15)$$

The main advantages of ReLU over sigmoid are twofold. 1) It is less computationally expensive because it simply involves an if statement instead of the calculation of an exponential as in the

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sigmoid. And 2) it does not as easily experience the problem of vanishing gradients because its derivative is usually 1. These advantages make ReLU more commonly used, and able to be implemented in deep neural networks (Mehta et al., 2019).

A modified version of the ReLU that further remediates the problem of vanishing gradients is called the Leaky ReLU. This function takes the portion of the ReLU function less than 0, and multiplies it by a (small, usually about 0.01) constant so that the derivative is not zero. It is defined as such:

$$\sigma(z) = \begin{cases} z & \text{if } z \geq 0 \\ cz & \text{if } z < 0 \end{cases} \quad (16)$$

With this understanding of a node and its activation developed, we can explain the overall construction and training of a feed forward neural network. The key aspect of a neural network is that the weights and biases at each node are trainable - they are adjusted during the learning process until a given cost function is minimized (Nielsen, 2015). In general, the more complex a problem is, the more nodes and layers of nodes are required in order to yield a good result.

The simplest FFNN consists of an input layer and an output layer. The input layer consists of a set of nodes, each of which is connected to one of the input values. The output layer consists of a set of output nodes, each of which is connected to one of the output values. In between the input and output layers, there may be one or more hidden layers. A hidden layer is simply a layer of nodes that is not directly connected to the input or output. Hidden layers allow the network to learn more complex patterns. The nodes in each layer are fully connected to the nodes in the adjacent layer. That is, each node in the input layer is connected to every node in the hidden layer (if any), and each node in the hidden layer is connected to every node in the output layer.

The training process for an FFNN involves presenting the network with a set of training data. The training data consists of a set of input values and the corresponding output values. The network adjusts the weights of the nodes based on the error between the actual output values and the predicted output values. The error is calculated using a cost function that measures how well the network is performing. After the weights have been updated, the training data is presented to the network again, and the process is repeated. This process is continued until the error is minimized. Once the training process is complete, the network can be used to predict the output for unseen testing data.

In the training of a neural network, the cost function can be optimized with a method such as SGD. However, the calculation of the gradients of the cost function requires a more sophisticated method, because simple calculation of all the gradients with respect to all the weights and biases in the network would be far too computationally complex. This is where the backpropagation algorithm comes in.

The backpropagation algorithm is a feedback-based method, meaning that it uses feedback



from the network itself to adjust the weights of the connections between the neurons. The method propagates the error in the output of a neural network back through the network, and the weights of the connections being adjusted accordingly (Nielsen, 2015). The backpropagation algorithm is composed of two parts: the forward propagation phase and the backward propagation phase. In the forward phase, the inputs to the network are fed forward through the network, and the output of the network is computed. In the backward phase, the error in the output is propagated back through the network, and the weights of the connections are adjusted accordingly. The backpropagation algorithm is able to learn the weights of the connections between the neurons in a neural network by iteratively adjusting the weights in accordance with the error in the output of the network. The backpropagation algorithm is highly efficient, and allows the gradients to be calculated in a reasonable amount of time.

Mathematically, the backpropagation algorithm can be described in four steps (Nielsen, 2015):

- 1) Input: Set the corresponding activation  $a^1$  for the input layer.
- 2) Feedforward: For each layer  $l$ , compute  $z^l = w^l a^{l-1} + b^l$  and  $a^l = \sigma(z^l)$
- 3) Output Error: Compute the output error  $\delta^{(L)} = \nabla_a C \odot \sigma'(z^{(L)})$ , where  $\odot$  is the hammond product
- 4) Backpropagate the Error: For each layer  $l$ , compute  $\delta^{(l)} = ((w^{l+1})^T \delta^{(l+1)}) \odot \sigma'(z^{(l)})$
- 5) Output: Return the gradient of the cost function with respect to the weights as  $\frac{\partial C}{\partial w_{jk}^{(l)}} = a_k^{(l-1)} \delta_j^{(l)}$ , and with respect to the biases as  $\frac{\partial C}{\partial b_j^{(l)}} = \delta_j^{(l)}$

By using an optimization method like SGD in combination with gradient calculation via backpropagation, a neural network can be trained to perform a variety of tasks. Two main tasks we will describe in this project are classification and regression, which a neural network can be designed for by changing its cost function and input/output layers. In the case of regression tasks, the cost function used is usually that of the Mean Squared Error (MSE) or the Mean Absolute Error (MAE), which we have described in Project 1 on regression. In the case of classification, the cost function is usually that of cross-entropy, which we will describe in the next section on logistic regression.

## Logistic Regression

Logistic regression is a type of model that can be trained to predict classifications of data. It heavily relies on the sigmoid function described earlier, and is essentially the most simple version of a neural network with only one layer. Consider that we have an input observation  $x$  with  $n$  features:  $x = [x_1, x_2, \dots, x_n]$ . In this project we will consider the case of binary classification, so we want to predict whether the observation belongs to class 0 or class 1. The output of the classifier, which we will call  $y$ , can then be 0 or 1. Our goal in logistic regression

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is to have this classifier output the probability  $P(y = 1|x)$  that the observation is part of class 1 (Jurafsky and Martin, 2021).

The sigmoid function is the perfect choice for this task, as it outputs a value between 0 and 1. Thus we can input the value  $x$  into the sigmoid function with trainable weights  $w$  and biases  $b$ , similar to a neural network approach:

$$P(y = 1) = \sigma(wx + b) = \frac{1}{1 + e^{-(wx+b)}} \quad (17)$$

We then need to set a threshold for the output in order to determine how the sigmoid will make the classification. Traditionally this value is set at 0.5, with values at or above 0.5 corresponding to a majority-probability that the data belongs to class 1. Thus we convert the output from the sigmoid using the following rule:

$$Decision(x) = \begin{cases} 1 & \text{if } P(y = 1|x) \geq 0.5 \\ 0 & \text{if } P(y = 1|x) < 0.5 \end{cases} \quad (18)$$

In order to train a logistic regression model, we need a cost function that represents the difference between the correct output  $y$  (which is 0 or 1) and the sigmoid output  $\hat{y} = \sigma(wx + b)$ . This cost function can be derived by first noting that the probability of a correct label given  $x$ ,  $p(y|x)$  follows a Bernoulli distribution because there are only two outcomes (Jurafsky and Martin, 2021). It is this quantity that we desire to maximize:

$$P(y|x) = \hat{y}^y (1 - \hat{y})^{1-y} \quad (19)$$

By taking the logarithm of both sides, and then taking the negative of the quantity (because we want a cost function to minimize), we obtain our cost function, which is called the cross-entropy loss:

$$C = -P(y|x) = -(y \log(\hat{y}) + (1 - y) \log(1 - \hat{y})) \quad (20)$$

From here, optimization methods like SGD can be applied to train the weights and biases of the model until the cost function is minimized. While it is beyond the scope of this report, it is important to note that there also exist modifications to logistic regression that can be made to perform multi-class (3+ classes) classification. The main modification is changing the activation function from a sigmoid to softmax, which can output probabilities corresponding to multiple classes. Models designed as such are commonly called multinomial logistic regression models (Jurafsky and Martin, 2021).

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## Implementation Details

### *Data*

In our regression tests using gradient descent, OLS, and a feed forward neural network, we use a simple quadratic function of the form:

$$y = 4 + 3x + 2x^2 + \sigma(0, 0.1) \quad (21)$$

where  $\sigma(0, 0.1)$  is Gaussian noise with mean 0 and standard deviation 1. We sample 100 random points in the range [0,3] in our implementation, and use 80 for the training dataset and 20 for the testing dataset.

In our classification tests using a feed forward neural network and logistic regression, we use the Wisconsin Breast Cancer Dataset. This dataset is openly available through the scikit-learn Python package, in `sklearn.datasets`. This data has 569 datapoints and 30 features, with the features consisting of observations like tumor radius, perimeter, and area. The diagnosis column is the output classification, and consists of 212 malignant tumors and 357 benign tumors. We apply a standard scalar (subtraction of the mean and division by the standard deviation) to the data in order to compensate for the effect of radically different feature units and values (for instance radius vs concavity). There is no missing data or large outliers, and thus no interpolation or data editing other than the scaling was applied.

### *Cost Functions and Metrics*

In our regression tests we use a cost function of mean squared error (MSE) in order to measure the error between our predicted values and the true values. The MSE is also used as a metric in testing.

In our classification tests we use a cost function of binary cross-entropy, as defined in the theory section on logistic regression. For our testing metric, we use the accuracy, which is defined as (James et al., 2013):

$$Accuracy = \frac{TP + TN}{TP + FP + TN + FN} \quad (22)$$

where TP is the number of true positives (correct predictions of malignant), FP is the number of false positives (incorrect predictions of malignant), TN is the number of true negatives (correct predictions of benign), and FN is the number of false negatives (incorrect predictions of benign). It is the number of correct predictions over the number of incorrect predictions. While there exist more sophisticated metrics like the F1-score, that are used commonly on imbalanced and/or multi-class datasets, we have a very simple binary classification dataset that is relatively balanced. Therefore we use only the accuracy.

# Results

## Optimization Methods

### Gradient Descent

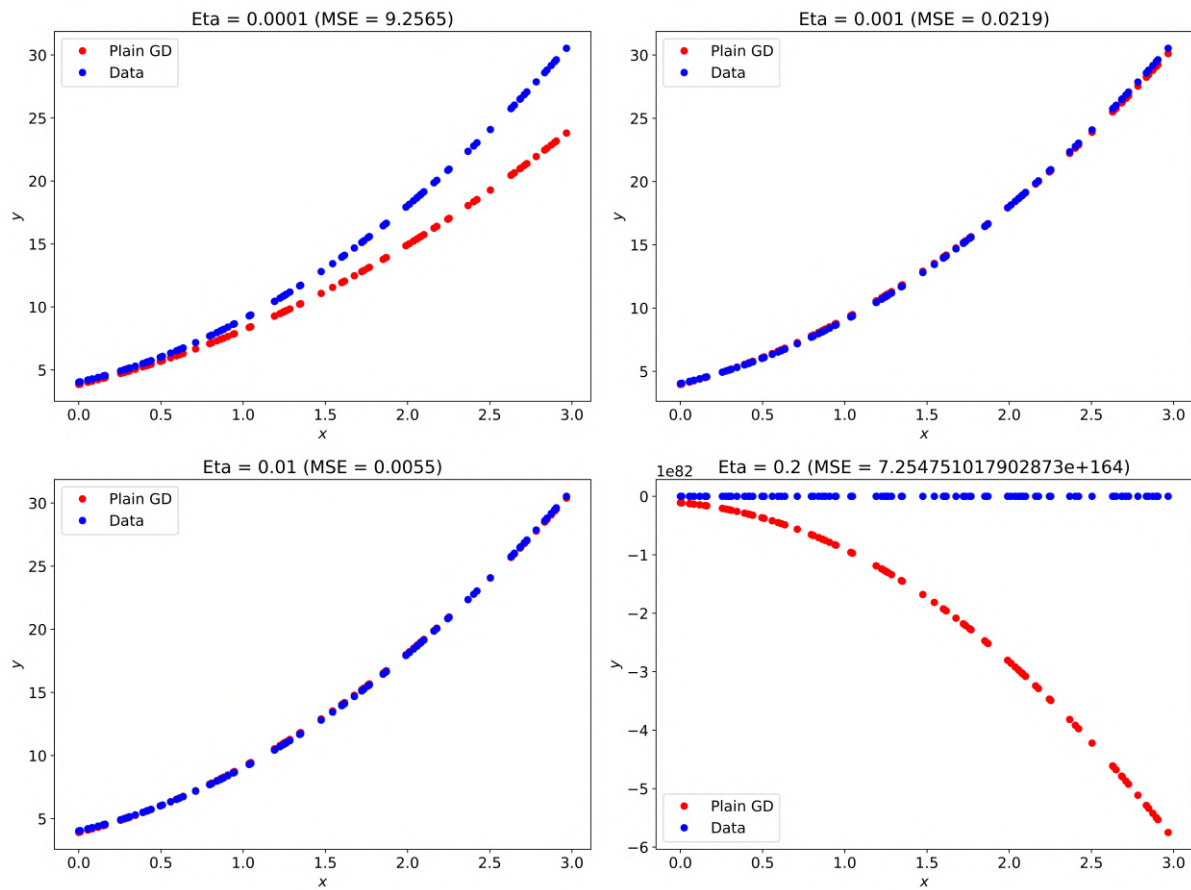


Figure 2

### Momentum Gradient Descent

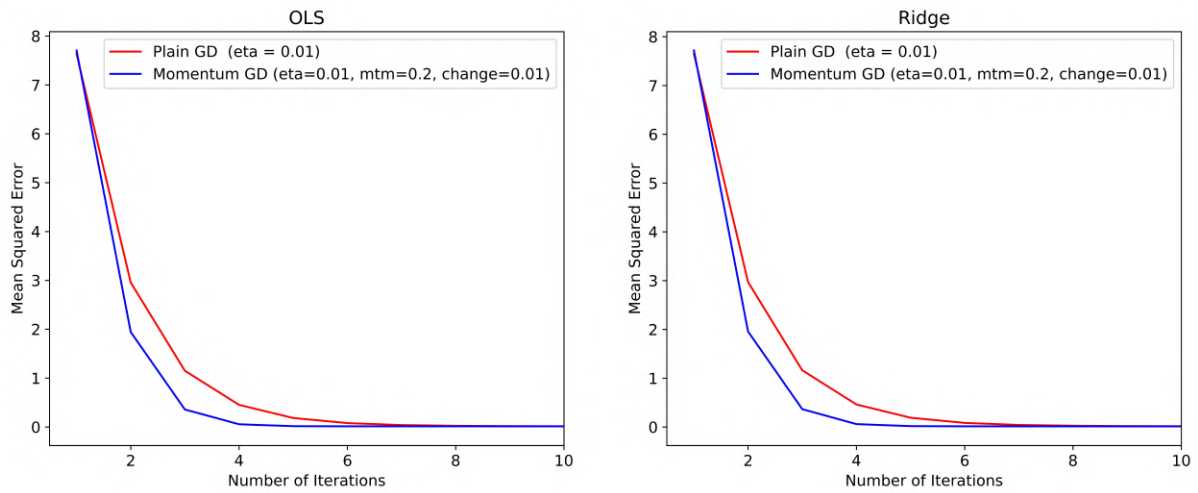


Figure 3

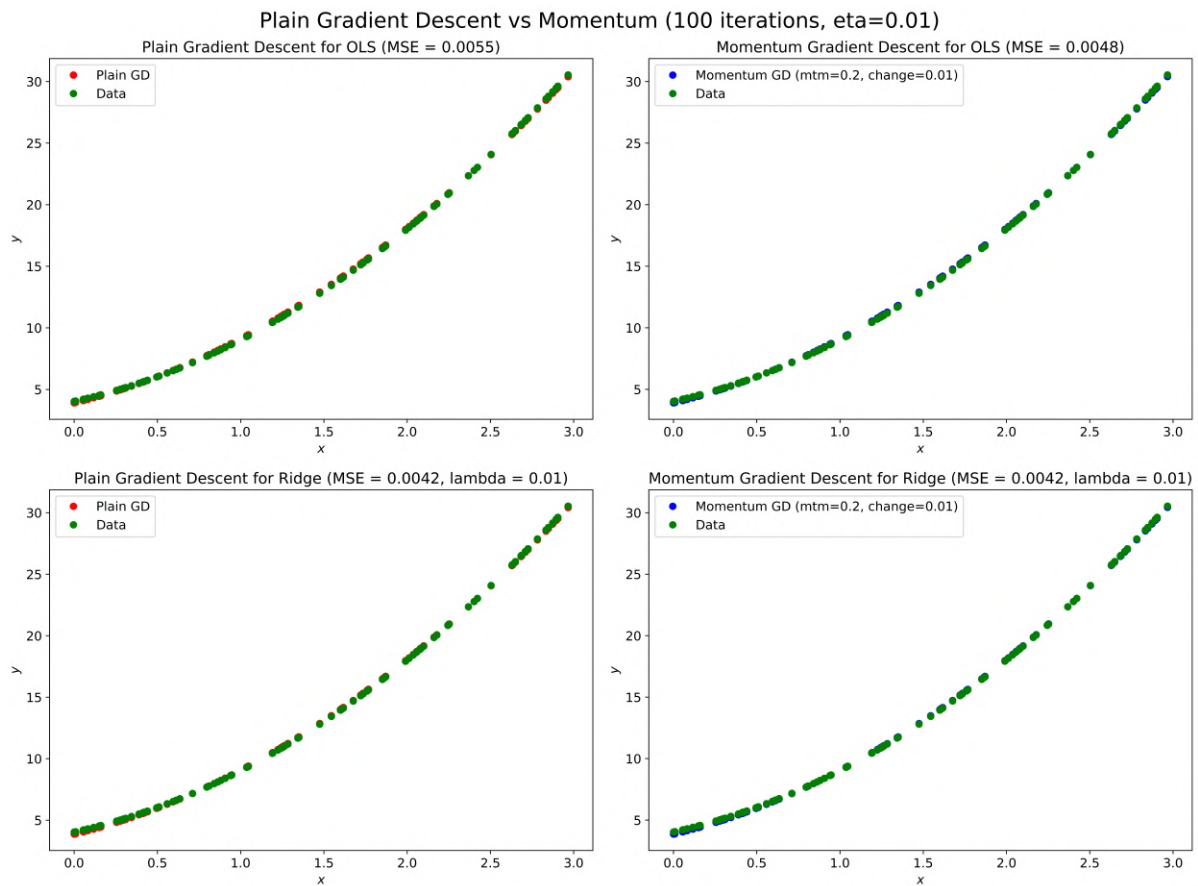
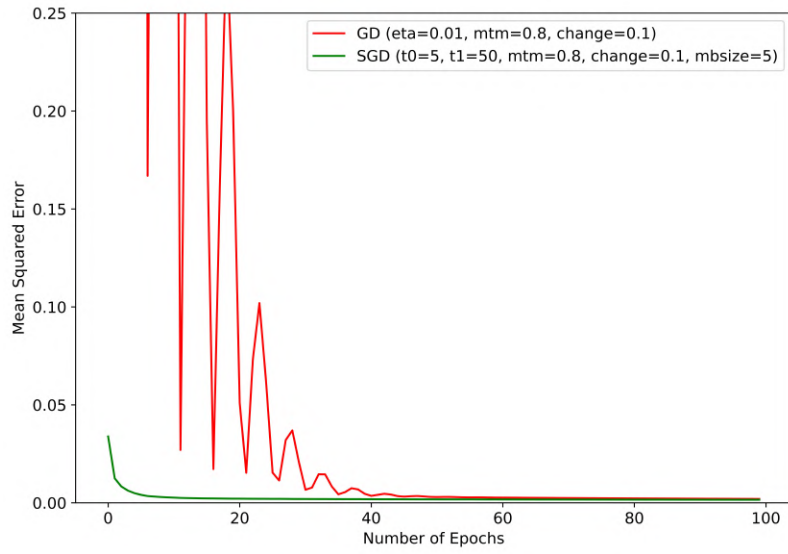
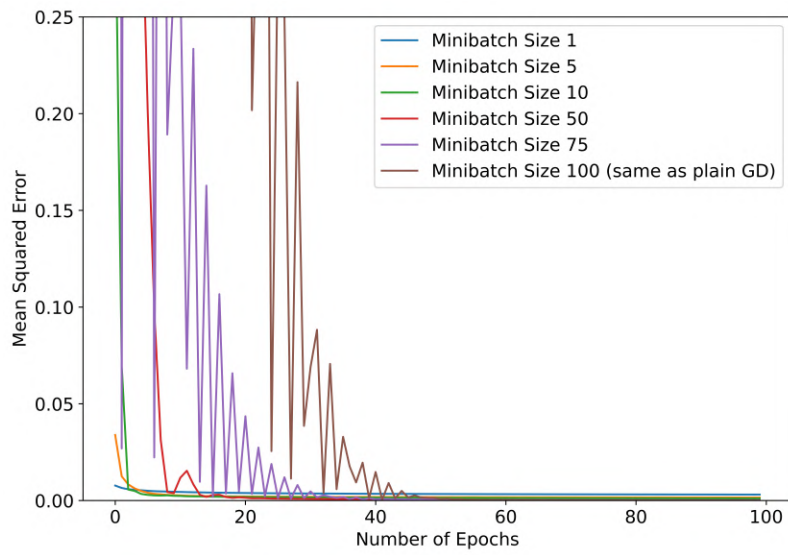


Figure 4

## Stochastic Gradient Descent

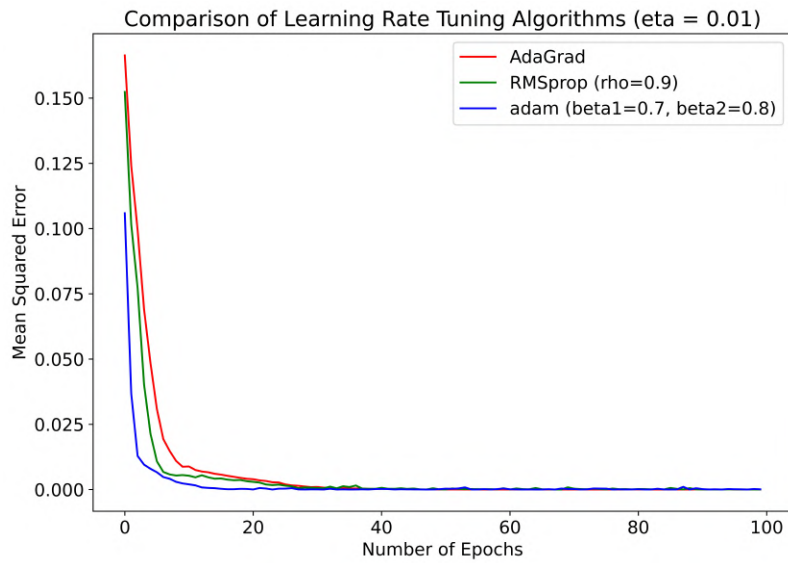


**Figure 5**



**Figure 6**

## Learning Rate Tuning Methods



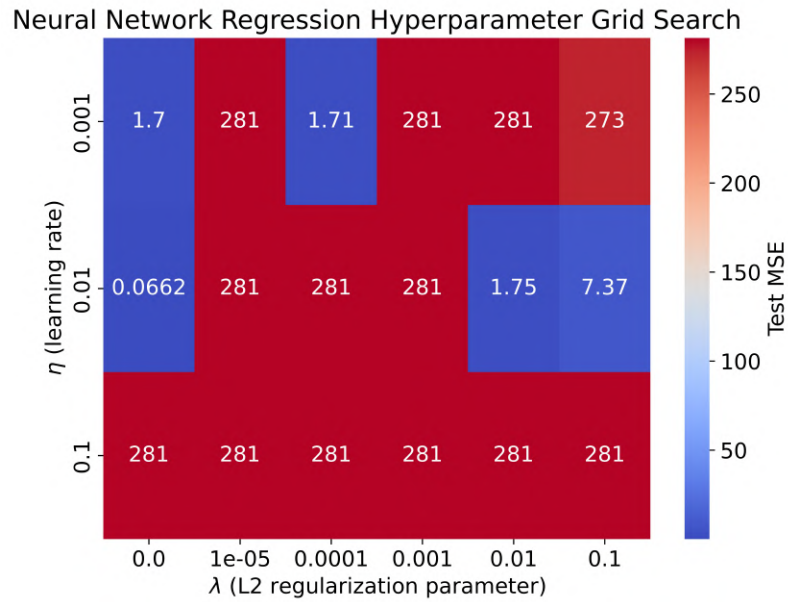
**Figure 7**

## Regression on a Quadratic Function

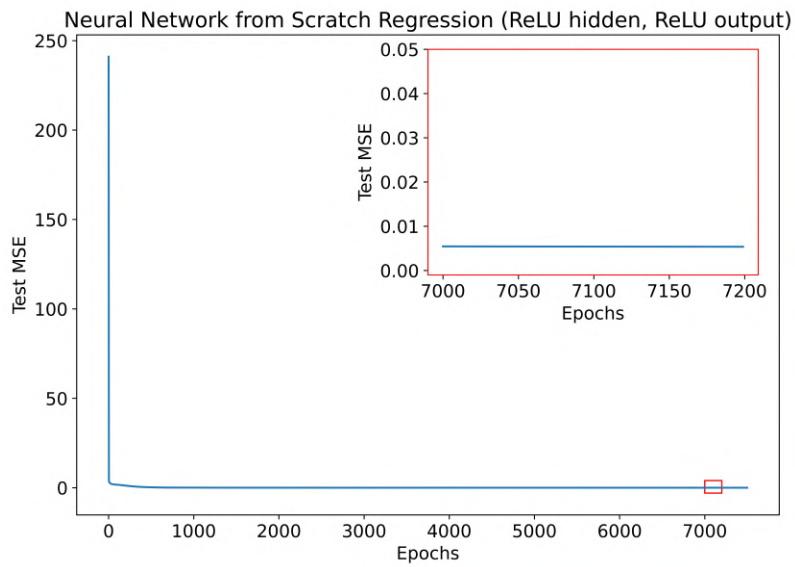
### *Feed Forward Neural Network Regression*

	ReLU hidden, 50 nodes	sigmoid hidden, 50 nodes	leaky ReLU hidden, 5 nodes	two ReLU hidden, 50 nodes each	ReLU hidden, 100 nodes
Minimum Test MSE	0.078	0.71	1.85	0.517	281.44

**Figure 8**



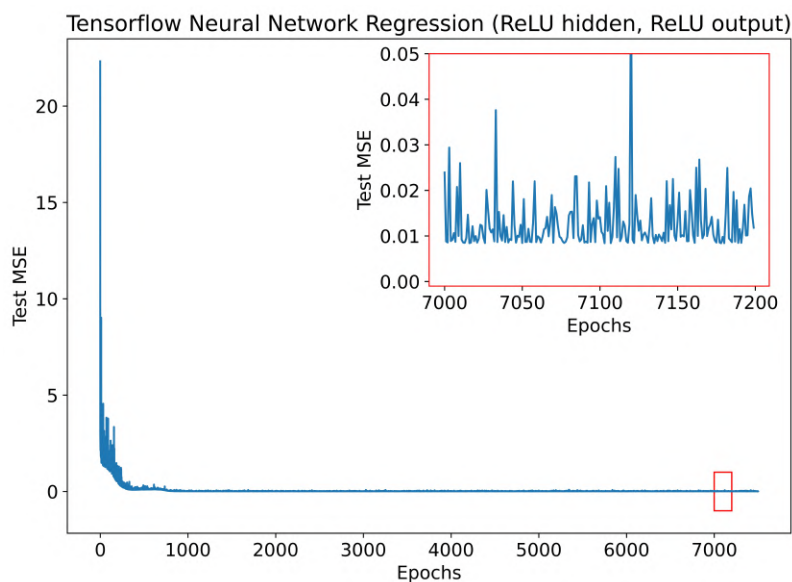
**Figure 9**



**Figure 10**

*Tensorflow Feed Forward Neural Network Regression*

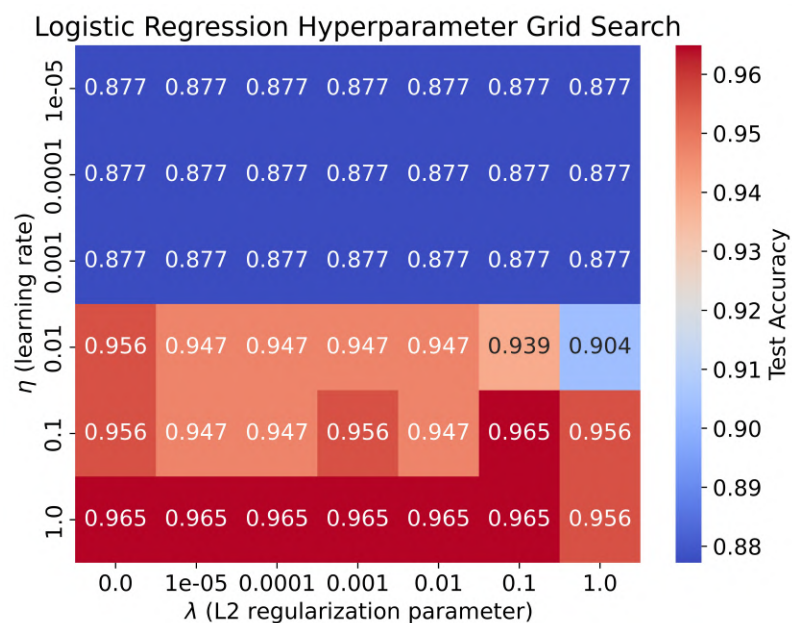




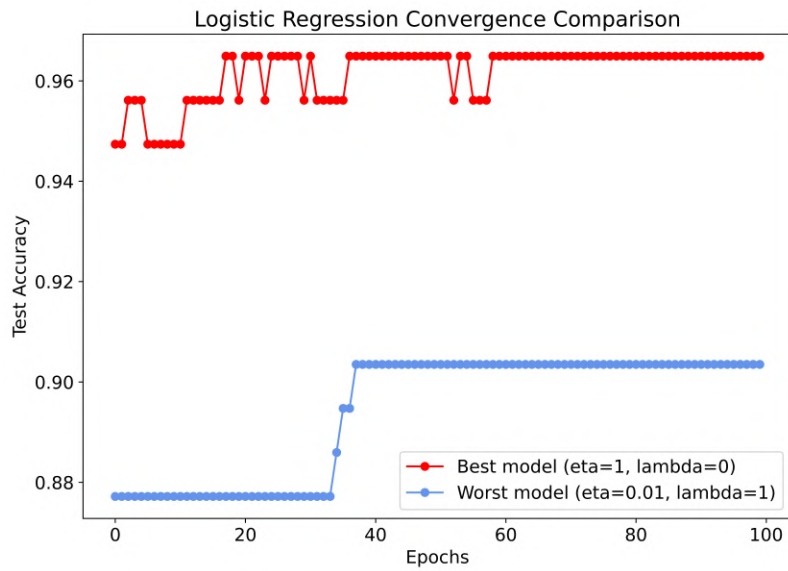
**Figure 11**

## Classification on Breast Cancer Data

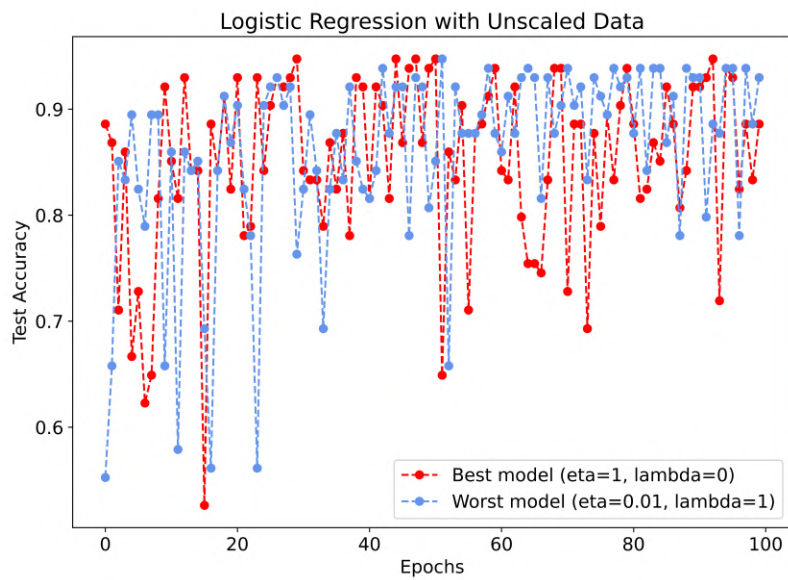
### *Logistic Regression*



**Figure 12**



**Figure 13**



**Figure 14**

### Feed Forward Neural Network Classification

	ReLU hidden, 5 nodes	sigmoid hidden, 5 nodes	leaky ReLU hidden, 5 nodes	two sigmoid hidden, 5 nodes each	sigmoid hidden, 20 nodes
Max Test Accuracy	0.939	0.947	0.921	0.921	0.956

**Figure 15**

Neural Network Classification Hyperparameter Grid Search

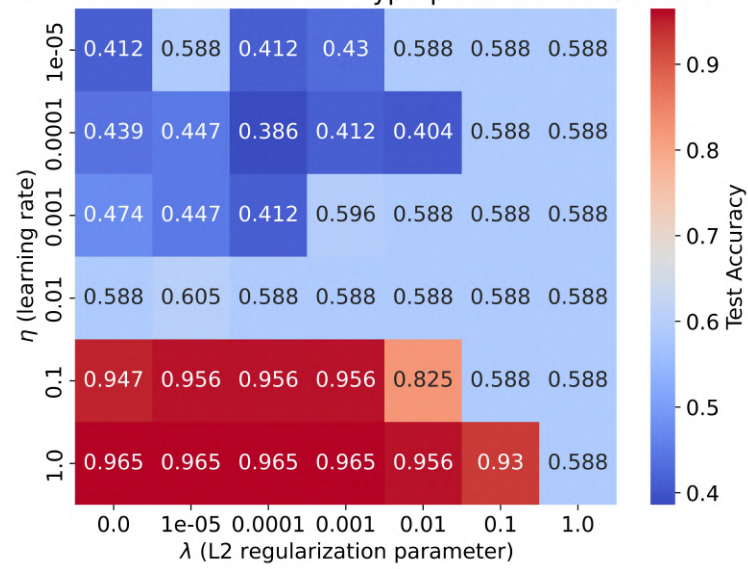


Figure 16

Neural Network Classification from Scratch (1 hidden layer, 20 nodes, sigmoid)

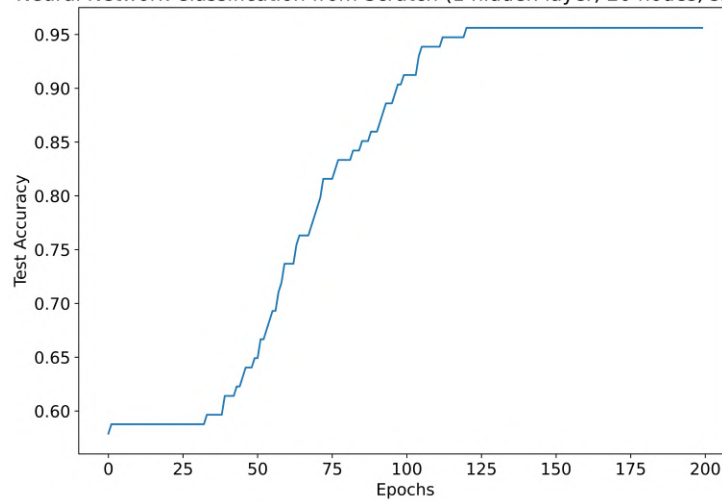
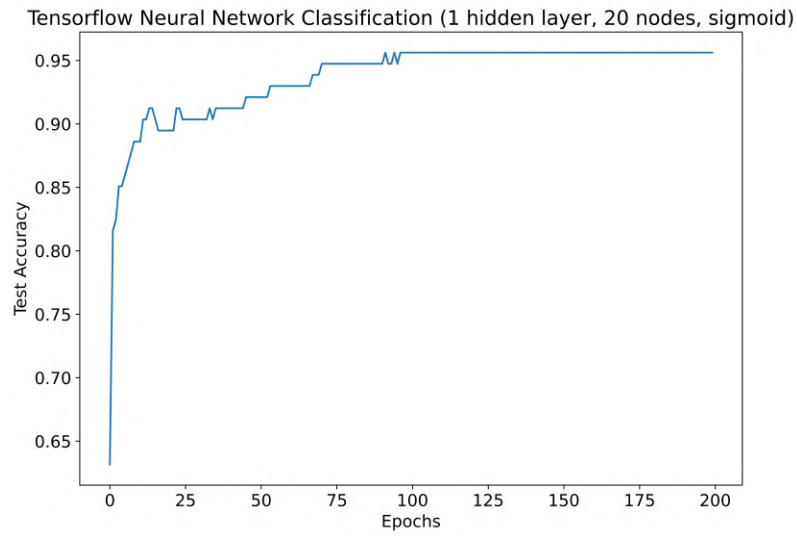


Figure 17

## Tensorflow Feed Forward Neural Network Classification



**Figure 18**

## Discussion

Regression				Classification			
	Best NN from Scratch	Tensorflow NN	OLS		Best NN from Scratch	Tensorflow NN	Best Logistic Regression
Lowest Test MSE	0.0052	0.008	~ 0	Highest Test Accuracy	0.956	0.956	0.965

**Figure 19**

## Conclusions

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