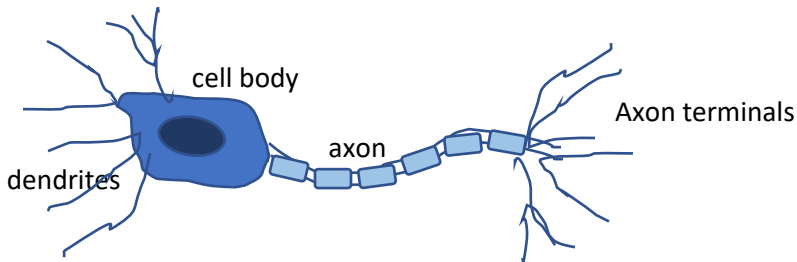# 7   ARTIFICIAL NEURAL NETWORK I

Neurons are nerve cells in the brain. They use electrical impulses and chemical signals to transmit information to other nerve cells, and between the brain and the rest of the nervous system. Neurons are composed of dendrites (signal inputs), cell body (processing), and axon with terminals (outputs). Neurons can connect with other neurons to form a chain of complex input and output responses. Signals pass from one neuron to another via synapses connecting axon terminals with dendrites of the next neuron. Refer to the diagram above.

Artificial intelligence (AI) fundamentally is about harnessing computer programming to mimic human behavior such as choice and recognition using large data inputs. Machine learning (ML) may be viewed as a specific AI domain to perform specific tasks such as prediction and classification. One major area of ML in this context is neural network (NN) that builds an architecture or structure of input-processing-output nodes mimicking the structure of human brain neurons. The processing of input information and the eventual output of prediction and classification is contained in the algorithm of the ML. Deep AI in such areas refers to more complex algorithms.

In this chapter, we study a basic NN called Multi-Layer Perceptron (MLP). This is sometimes referred to as Artificial Neural Network (ANN). In the next chapter we will study some other more complex NNs.

Understanding Neural Networks mainly includes two aspects, one is the structure of neural networks, and the other is the training and learning of neural networks. It is just like how our brain structure is composed, and how we learn and recognize different things based on this composition.

A single layer perceptron may be characterized as follows in the simple architecture with inputs, the computation process node in the middle, and output(s).
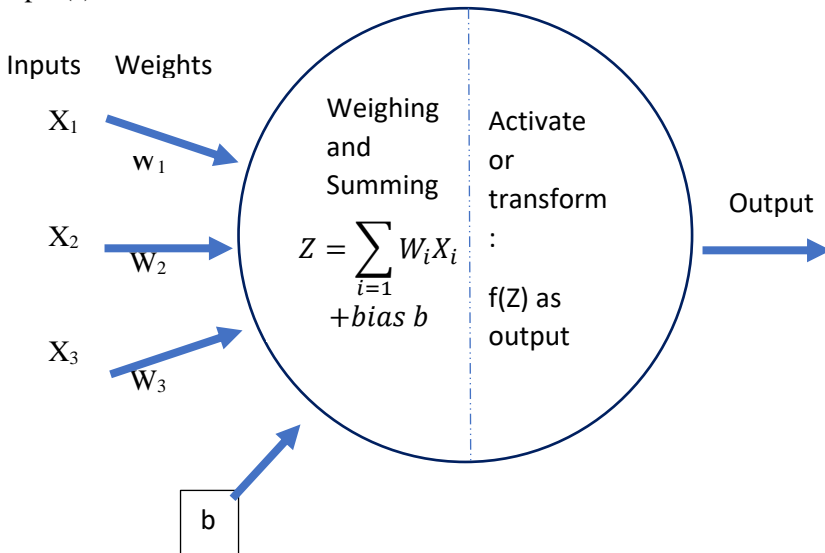
Inputs   Weights

X_1

w_1

X_2

W_2

X_3

W_3

b

Weighing and Summing

$$Z = \sum_{i=1} W_i X_i + bias\ b$$

Activate or transform :

f(Z) as output

Output

Figure 7.1

This embryonic version of today's NN essentially takes inputs or features of a subject or case, $\{X_1, X_2. X_3\}$, aggregates it with corresponding weights $\{W_1, W_2, W_3\}$, adds a bias term b, then computes the output

$$f\left(\sum_{i=1}^{3} W_i X_i + b\right)$$

where the bias (or adjustment of mean) can be treated like an input of 1 with weight b. The weights W_j's in a NN are initiated typically randomly as small positive or negative numbers, e.g., between (-1,+1). f(.) is an activation or transformation function.

An example is f (Z) = 1 if Z ≥ θ , and 0 otherwise. This could be an effective one in classifying cases that can be represented as binary 1 or 0 and where the 1 or 0 cases are largely separated by a linear plane. See Figure 7.2.
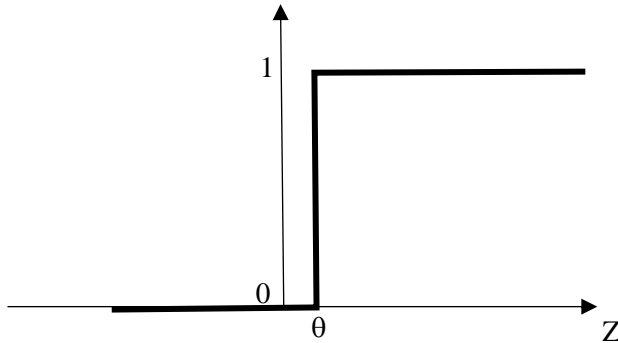
Figure 7.2

If cases with 1 typically have higher positive value in feature of value x_1, then optimal selection of the weights could be to put adequately high positive weight on the feature x_1 for a fixed threshold $\theta > 0$. See in Figure 7.3 such a separation of cases with high positive x_1 versus cases with low positive x_1.

Input x_2

$f(w_1x_1+w_2x_2+b) = 1$
for high $w_1 > 0$
as $w_1x_1+w_2x_2+b > \theta$

$f(w_1x_1+w_2x_2+b) = 0$
for high $w_1 > 0$
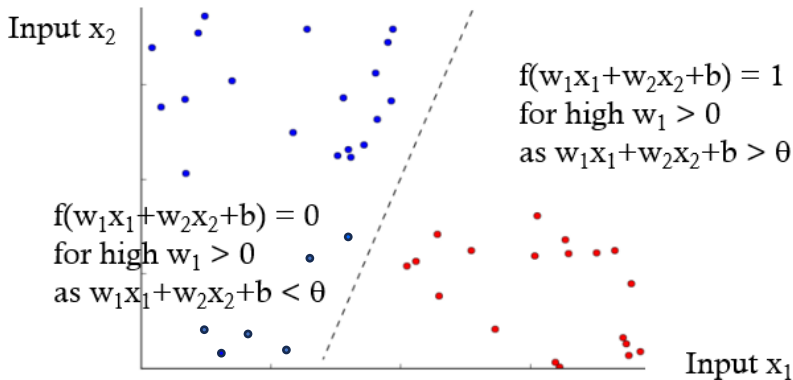as $w_1x_1+w_2x_2+b < \theta$

Input x_1

Figure 7.3

In network language, the inputs are like nodes and the weights are edges.[1] (Sometimes the latter are referred to as the synapses.) The computation node may be called a neuron.

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[1] In mathematics and computer science, networks are structures that are represented by nodes, edges, and other abstract connections – they form a part of graph theory.

Suppose we use two layers of computations as follows. We call such NN multi-layer perceptron (MLP) when there is more than 1 layer. Some authors prefer to call the following a single layer perceptron (not including the output layer as the second layer).

The same inputs or features are now fed to not one, but three different nodes or neurons #1[1], #2[1], #3[1] in the first layer. Notationally, superscript [j] denotes the jth computational layer. The first layer neurons each has output just like in a single layer perceptron and these outputs become inputs (with no change of values) to the next (output) layer of neuron. In the latter it is neuron #1[2]. Neuron #1[2] then produces one output.

Inputs

#1[1]

X_1

Output

X_2

#2[1]

#1[2]

X_3

#3[1]

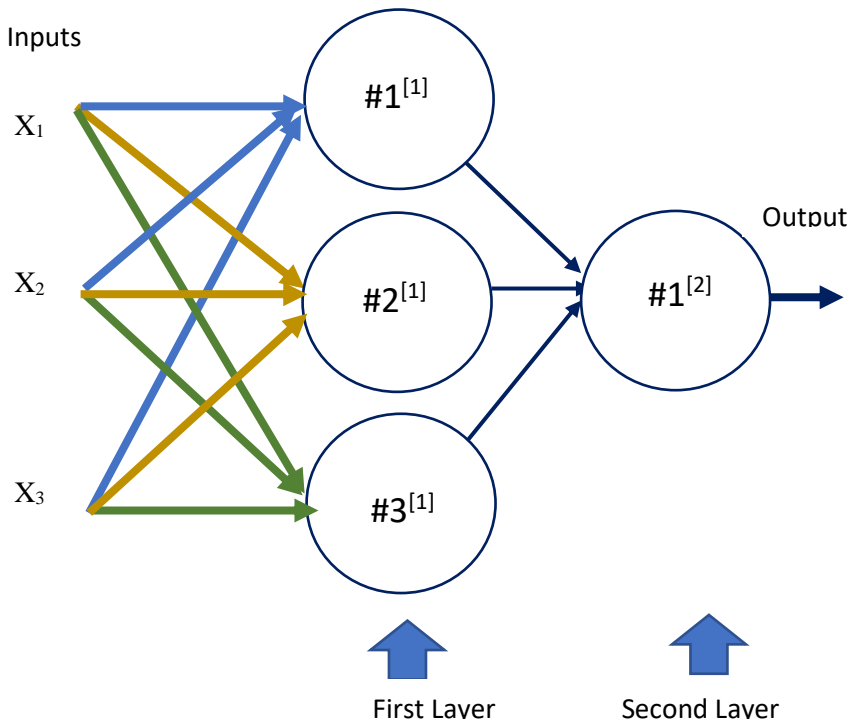First Layer   Second Layer

Figure 7.4

The above is a Many-to-One (many inputs toward one output) ANN. For a different problem, the structure could also be a Many-to-Many ANN (see

below) where there are now two nodes or neurons in the second (output) layer and then two outputs accordingly from neurons #1[2] and #2[2].

Inputs

#1[1]

Outputs

X_1

#2[1]

#1[2]

X_2

#3[1]

#2[2]
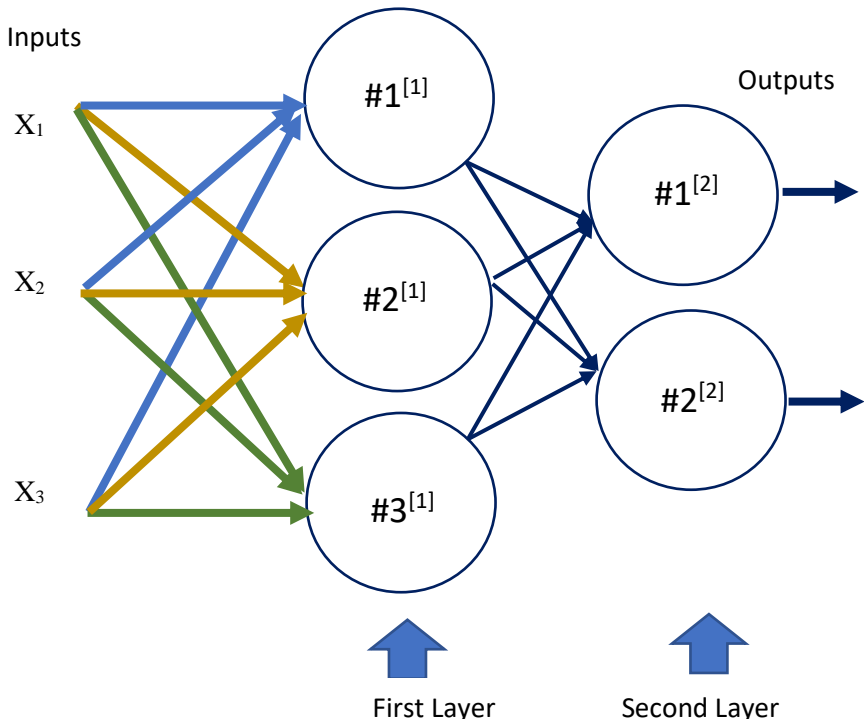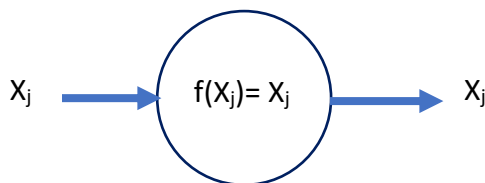
X_3

First Layer   Second Layer

Figure 7.5

Note that we have not yet shown the weights and the bias in the diagram. In the following diagram, if we consider an input X_j producing identical output X_i (with a trivial identity activation function), then we can treat an input as a neuron.

X_j ⟶ $f(X_j) = X_j$ ⟶ X_j

Then all the inputs can be represented as input nodes or neurons – now drawn similarly as circles. Moreover, we envelope neurons together that belong to the same forward step.
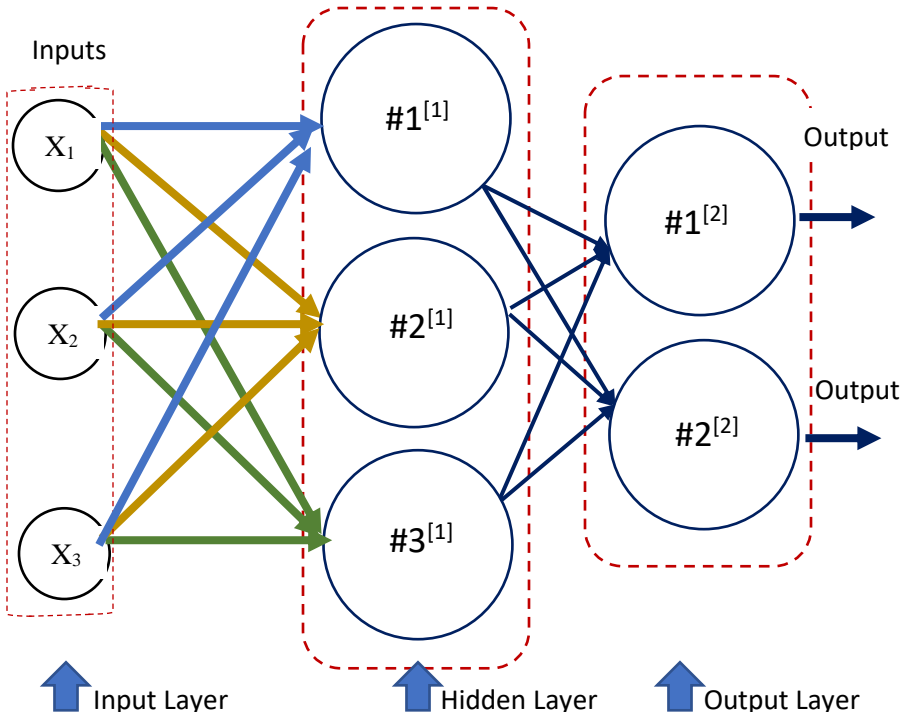
Figure 7.6

Thus, there is an input layer of input nodes or neurons, an output layer of outputs or neurons, and a middle layer called "hidden layer" as the computed outputs from the nodes in this layer are not explicitly observed, unlike those in the input and output layer nodes. For the same prediction or classification problem, an ANN can be made wider (larger number of input nodes or neurons in the same layer) and/or deeper (higher number of hidden layers). These affect the size (total number of neurons in the NN). A deeper NN can increasingly learn more nonlinear patterns. In this standard structure, each neuron will connect with all neurons in the forward pass process.

The rule of thumb is that the number of nodes in the hidden layer could be about 2/3 those of in the input layer and the output layer, and less than twice the number in the input layer.

Pruning removes nodes where input weights are close to zero – pruning occurs during training of model. Normalizing features also avoids some weights being close to 0 as out-scale feature sizes are standardized.

Suppose an ANN has two hidden layers and a similar input layer of 3 nodes (besides bias) and one output node. It can be represented diagrammatically as follows.
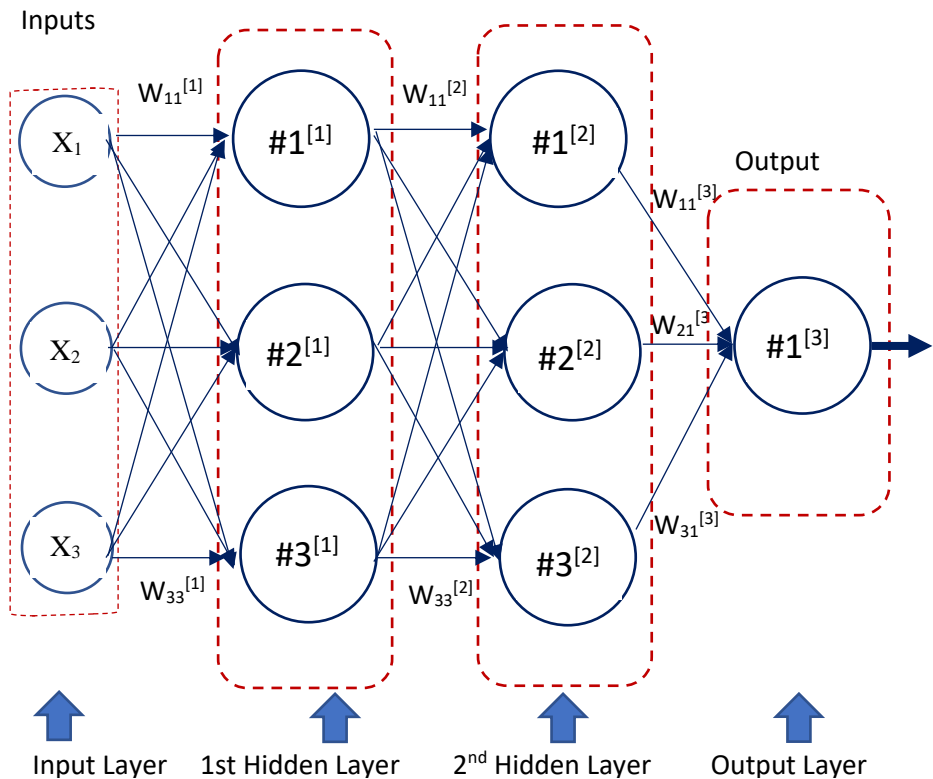

Figure 7.7

The edges or synapses connecting different neurons in different layers continue to represent weights. We depict some weights in the diagram above

(not all – so as not to clutter up the diagram). The weights of input X_1 on neurons #1[1], #2[1], #3[1] are respectively $W_{11}^{[1]}$, $W_{12}^{[1]}$, and $W_{13}^{[1]}$. The weights of input X_2 on neurons #1[1], #2[1], #3[1] are respectively $W_{21}^{[1]}$, $W_{22}^{[1]}$, and $W_{23}^{[1]}$. The weights of input X_3 on neurons #1[1], #2[1], #3[1] are respectively $W_{31}^{[1]}$, $W_{32}^{[1]}$, and $W_{33}^{[1]}$.

The weights of output from neuron #1[1] on neurons #1[2], #2[2], #3[2] are respectively $W_{11}^{[2]}$, $W_{12}^{[2]}$, and $W_{13}^{[2]}$. The weights of output from neuron #2[1] on neurons #1[2], #2[2], #3[2] are respectively $W_{21}^{[2]}$, $W_{22}^{[2]}$, and $W_{23}^{[2]}$. The weights of output from neuron #3[1] on neurons #1[2], #2[2], #3[2] are respectively $W_{31}^{[2]}$, $W_{32}^{[2]}$, and $W_{33}^{[2]}$.

The weights of outputs from neurons #1[2], #2[2], #3[2] on neuron #1[3] are respectively $W_{11}^{[3]}$, $W_{21}^{[3]}$, and $W_{31}^{[3]}$. The weights are connections from one neuron to another in the next forward layer. There is no connection between neurons in the same layer. In general, the weight from nth hidden layer #j[n] neuron to the next layer #k[n+1] neuron is $w_{jk}^{[n+1]}$.

The purpose of the ANN is to perform prediction or classification on a set of data containing subjects or cases with associated features or characteristics. Examples are predictions of likely default (target status) given cases of borrowers with different background features/characteristics, of treatment success (target status) given patients (subjects) with different medical background features/conditions, of correctly identifying criminals (target status) given subjects' profile and history, of click-through rate (CTR) in a digital marketing campaign with different campaign resources, of next stock price or corporate earnings given latest corporate financial and other information, of identifying an object whether it belongs to a particular classification given features/characteristics of the object, and so on.

To prepare a model for prediction with new data, the model must be trained using many known cases/subjects with their known target statuses and with associated features/characteristics or conditions in the training data set. Once the model is adequately trained, the weights are determined optimally by this stage, and the ANN can perform the necessary computations based on these optimal weights (including optimal biases) and the fresh inputs to find the predicted output(s) or target value(s) in the test data set.

The ANN computes the output(s) in the output layer in a forward pass process called Forward Propagation – this is discussed as follows. At the end of the pass, the errors of the fittings of all training data points are measured by a loss function to be minimized. The reduction in fitting errors requires the revision of the weights and biases – this uses a process called Backward Propagation which will also be discussed later. One forward propagation together with one backward propagation of the entire training data set is called an epoch. Sometimes the training data set (whole batch) is broken down into (mini-) batches that are smaller subsets in a random partitioning. If the size of each mini batch is fixed at n, then the number of mini batches in an epoch is total training sample size divided by the mini batch size. The forward and backward propagations are then done one mini-batch after another until the whole training data set has gone through one epoch. The number of mini batches implies the number of iterations in updating or revising the weights and biases.

Many epochs can be performed, which means a new epoch will require a new re-sampled training set. Each forward propagation on a new mini batch of same epoch or next epoch uses the updated weights and biases from the previous backward propagation. The total number of iterations is equal to the number of epochs multiplied by the number of mini batches in each epoch. Sometimes it may not be necessary to increase the number of epochs or mini batches per epoch when the fitting/prediction error in the training data set is sufficiently small.

7.1 Forward Propagation

We use a single hidden layer MLP to illustrate the forward propagation computation of a single output. The bias inputs are depicted as originating from the unfilled circles – we use a more general structure whereby the bias can be different for each of hidden and output layer neuron – shown as $b_j^{[n]}$ – corresponding to the $\#j^{[n]}$ neuron. (Another approach is to use the same bias for all neurons in the next forward layer.) The different biases are reflected as different weights with the input as 1.
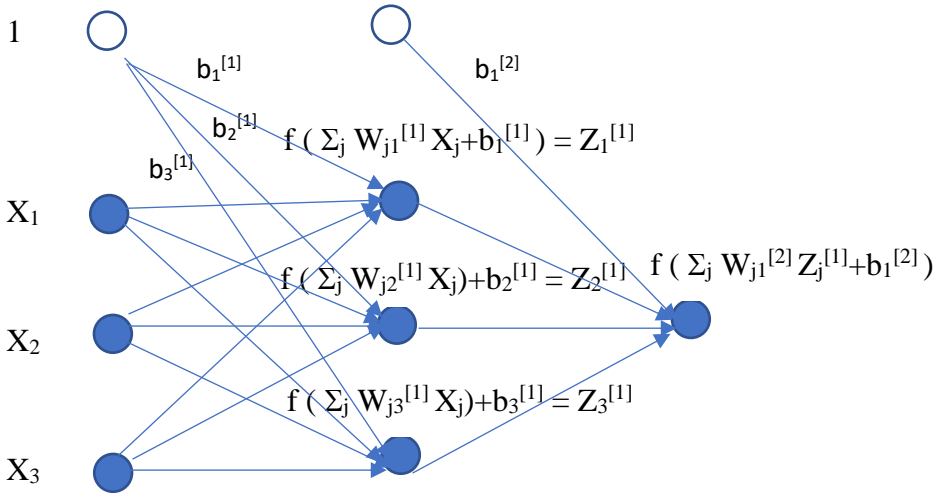
Figure 7.8

Given the various weights, biases, and inputs, the final output is

$$f \left(\Sigma_j W_{j1}^{[2]} Z_j^{[1]} + b_1^{[2]} \right) = \hat{Y}$$

for a particular case or training sample point with associated features (X_1, X_2, X_3) where superscript [1] to output Z_j denotes output is at hidden layer 1. In a standard ANN structure, the activation function f(.) remains the same for every layer.

Activation Function f (.)

The weighted inputs and biases are passed through activation function f(Z). The latter is typically a nonlinear function with an S-curve such as the Sigmoid function (logistic function) $f(Z) = 1/(1 + e^{-Z})$, the Hyperbolic Tangent function $f(Z) = (e^Z - e^{-Z})/(e^Z + e^{-Z})$, or the Rectifier Linear Unit function (ReLU) that is $f(Z) = \max(Z, 0)$.[2] The nonlinear functions are depicted graphically as

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[2] An alternative version, the Leaky ReLu is sometimes used. Unlike ReLu, Leaky ReLu has a small positive slope instead of zero slope for negative Z values. This slope is pre-fixed before training. Using Leaky ReLu appears to help in reaching convergence faster than the standard ReLu.

follows. In the standard ANN, the activation function remains the same for each neuron in the same layer and remains the same also for different layers.
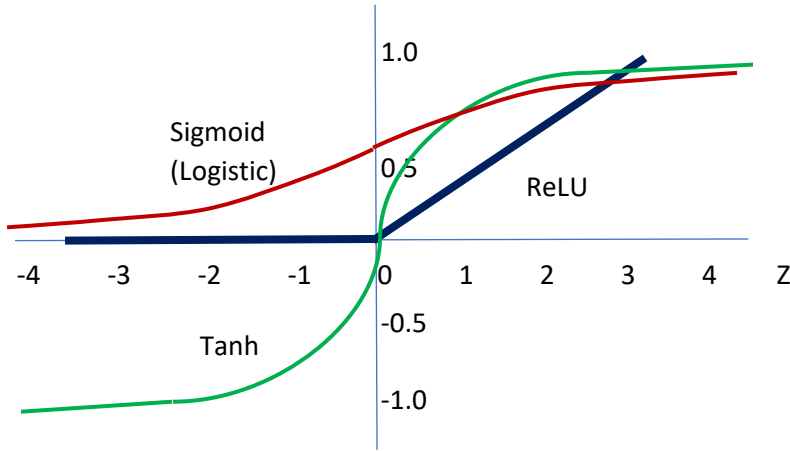
Figure 7.9

Suppose we have N number of data points (sample points or cases) in our training data set. Each case/subject k has an actual output Y_k and associated features $(X_{1,k}, X_{2,k}, X_{3,k})$. The forward propagation computations after optimal revisions of weights and biases end up with a target prediction of

$$\hat{Y}_k = f\left(\Sigma_j\, W_{j1}^{[2]}\, Z_{j,k}^{[1]} + b_1^{[2]}\right)$$

where $Z_{m,k}^{[1]} = f\left(\Sigma_j\, W_{jm}^{[1]}\, X_{j,k} + b_1^{[1]}\right)$ denotes the kth case output at m^{th} neuron of hidden layer. $\hat{Y}_k$ is notationally also the same as $Z_{1,k}^{[2]}$ in the ANN here with one output. As the final output or target prediction is computed in a forward pass manner, this ANN is also called a feedforward NN due to this simple architecture. We consider NNs with more complicated architecture in a later chapter – those are sometimes referred to as deep learning NNs.

Error or Loss Functions

The training fitting/prediction error is an error or loss function based on the training data set of all training sample points and measures 'deviations' of NN outputs (target predictions) of all cases with the actual outputs of the associated

cases. The idea in training the model is to find optimal weights and biases so that the training set error or loss function is minimized or reduced toward zero. A commonly used error/loss function for continuous variable targets is the average least squares of deviations (or mean square error, MSE):

$$L(Y, \hat{Y}) \equiv \frac{1}{N} \sum_{k=1}^{N} L(Y_k, \hat{Y}_k) = \frac{1}{N} \sum_{k=1}^{N} (Y_k - \hat{Y}_k)^2. \qquad (7.1)$$

where $Y = (Y_1, Y_2, Y_3, \dots, Y_N)$ and $\hat{Y} = (\hat{Y}_1, \hat{Y}_2, \hat{Y}_3, \dots, \hat{Y}_N)$. This is also called L^2 loss function and is common for target variables that are continuous variables and not categorical or binary numbers. Sometimes its square root, the root mean square error (RMSE) is used. An alternative is the mean absolute loss or L^1 loss function

$$L(Y, \hat{Y}) = \frac{1}{N} \sum_{k=1}^{N} |Y_k - \hat{Y}_k|.$$

In scenarios where there are outliers, MSE will usually be much larger than MAE because the difference between estimated target values and actual target values will be amplified after squaring. MAE is thus more robust in the presence of some outliers, i.e., producing more stable results. However, MSE has better convergence properties when it comes to finding optimal weights.

The Huber loss function $L_\delta(Y, \hat{Y})$ is a combination of MSE and MAE, including a hyperparameter δ: $\frac{1}{N} \sum_{k=1}^{N} L_\delta(Y_k, \hat{Y}_k)$ where :

$$L_\delta(Y_k, \hat{Y}_k) = \begin{cases} \frac{1}{2}(Y_k - \hat{Y}_k)^2, & \text{if } |Y_k - \hat{Y}_k| < \delta \\ \delta |Y_k - \hat{Y}_k| - \frac{1}{2}\delta^2, & \text{otherwise} \end{cases}$$

When $|Y_k - \hat{Y}_k| < \delta$, L_δ becomes MSE. When $|Y_k - \hat{Y}_k| \geq \delta$, it functions like MAE. Huber loss function overcomes the shortcoming of MSE when the deviation becomes larger perhaps due to an outlier.

When the actual target or output is categorical, different types of error/loss functions may be more practicable. In a binary classification where the target is either 1 or 0, e.g., it rains or it does not in weather prediction, or it is a bird or it is not based on picture pixels, or the firm has earnings increase or not, then error function could be 1 minus the accuracy where accuracy is the

fraction of correct prediction. However, this function may not be easily differentiable which makes it harder to use for finding optimal weights.

Typically, a binary classification prediction using features would provide a probability estimate $\hat{P}$ of the target status whether it is 1. Otherwise, $1-\hat{P}$ would be estimate of the probability the target status is 0. A useful error/loss function for the binary classification is binary cross-entropy that employs estimate $\hat{P}_k$ for each case k: $L(Y, \hat{P}) = \frac{1}{N} \sum_{k=1}^{N} L(Y_k, \hat{P}_k)$ where

$$L(Y_k, \hat{P}_k) = -[\, Y_k \ln \hat{P}_k + (1-Y_k) \ln (1 - \hat{P}_k) \,].$$

This is also the log loss function for binary classification. $\hat{P}_k$ is the predicted probability that $Y_k = 1$, and $1 - \hat{P}_k$ is the predicted probability that $Y_k = 0$. Note that here when $Y_k = 1$, the loss function is reduced when $\hat{p}_k \in (0,1)$ is higher. When $Y_k = 0$, the loss function is reduced when $\hat{p}_k \in (0,1)$ is lower. This loss function therefore captures the idea of ensuring the estimated or predicted probability of $(Y_k = 1)$, $\hat{P}_k$, is high when $Y_k = 1$, and that the predicted probability of $(Y_k = 1)$, $\hat{P}_k$, is low when $Y_k = 0$. The log loss function above is positive. The smaller is the log loss function or the smaller the binary cross-entropy measure toward zero, the less is the uncertainty and hence better prediction.

Recall that we may deem $\hat{Y}_k = 1$ or 0 if $\hat{P}_k > 0.5$ or else ≤ 0.5. Note that unlike the MSE error/loss function where the predictor $\hat{Y}_k$ enters intuitively in the loss function $L(Y_k, \hat{Y}_k)$, the loss function in the categorical output cases is $L(Y_k, \hat{P}_k)$ where the predicted classification is not exactly the predicted output $\hat{P}_k$ but a function of it, $\hat{Y}_k(\hat{P}_k)$.

When there is more than one output, e.g., Q outputs for Q number of categories, then the (categorical) cross-entropy loss function for each case k is

$$L(Y_{k,c}, \hat{P}_{k,c}) = -\sum_{c=1}^{Q} Y_{k,c} \ln \hat{P}_{k,c}$$

where $Y_{k,c}$ is 1 (otherwise 0) if case Y_k belongs to class c, and $\hat{P}_{k,c}$ is the predicted probability of case k belonging to class c. We may in general use the notation of error/loss function as $L(Y_k, \hat{Z}_k)$ where $\hat{Z}_k \equiv \hat{Y}_k$ in the continuous variable case and $\hat{Z}_k \equiv \hat{P}_k$ in the categorical case.

7.2 Backward Propagation

In each epoch or training of the entire training data set from inputs to final output(s) in the output layer, the predicted outputs are compared with the actual (target) outputs and the loss function $L(Y, \hat{Z})$ is computed. Thus, the epoch involves passing the entire training set of points forward, then backward with revision of weights and biases before final passing forward to obtain the output and loss function. The second epoch will involve a resampled training data set, continued updating with a second backward propagation and then forward pass to obtain the updated loss function. This may continue for many epochs where necessary to obtain satisfactory convergence in the loss function.

When the loss function or binary cross entropy measure is too high, the model needs further improvement – we need to train the NN further, by updating/revising/fine-tuning the weights and biases and then run a second epoch and so on, and hopefully end with an acceptable loss function outcome.

The Backward Propagation is the mechanism of training the NN toward an acceptable loss before proceeding for application to the test data set. While forward propagation performs computations by moving forward in the process from inputs to the final output, backward propagation involves backwards pass that performs computations by moving backward from the loss function at the final output to the weight or bias inputs.

The weights and biases feeding into each layer forward are initially obtained by random draws from usually a small range (-1,+1). In the single hidden layer MLP, the weights are { $W_{11}^{[1]}$, $W_{21}^{[1]}$, $W_{31}^{[1]}$, $b_1^{[1]}$ } (including the bias) for neuron #1[1] with output $Z_{1,k}^{[1]}$. The weights are { $W_{12}^{[1]}$, $W_{22}^{[1]}$, $W_{32}^{[1]}$, $b_2^{[1]}$ } (including the bias) for neuron #2[1] with output $Z_{2,k}^{[1]}$, and { $W_{13}^{[1]}$, $W_{23}^{[1]}$, $W_{33}^{[1]}$, $b_3^{[1]}$ } (including the bias) for neuron #3[1] with output $Z_{3,k}^{[1]}$. In the output layer, the weights are { $W_{11}^{[2]}$, $W_{21}^{[2]}$, $W_{31}^{[2]}$, $b_1^{[2]}$ } (including the bias) for neuron #1[2] with output $Z_{1,k}^{[2]} \equiv f\left(\Sigma_j W_{j1}^{[2]} Z_{j,k}^{[1]} + b_1^{[2]}\right)$ $= \hat{Y}_k$. Hence in this structure there are altogether 16 parameters of weights and biases to update/revise/fine-tune: { $W_{11}^{[1]}$, $W_{21}^{[1]}$, $W_{31}^{[1]}$, $b_1^{[1]}$, $W_{12}^{[1]}$, $W_{22}^{[1]}$, $W_{32}^{[1]}$, $b_2^{[1]}$, $W_{13}^{[1]}$, $W_{23}^{[1]}$, $W_{33}^{[1]}$, $b_3^{[1]}$, $W_{11}^{[2]}$, $W_{21}^{[2]}$, $W_{31}^{[2]}$, $b_1^{[2]}$ }.

To update $W_{11}^{[1]}$ toward minimizing the error/loss objective function, a standard approach is to use the gradient descent method/algorithm or its variants. The gradient descent method requires the computation of the partial slope of the objective function with respect to each of the weights and biases.

The estimation uses the chain rule. In the single layer MLP, the diagram below shows how

$$\frac{\partial L(Y,\hat{Z})}{\partial W_{11}^{[1]}} = \frac{\partial \sum_{k=1}^{N} \frac{1}{N} L(Y_k,\hat{Z}_k)}{\partial W_{11}^{[1]}}$$

is computed. For each case k,
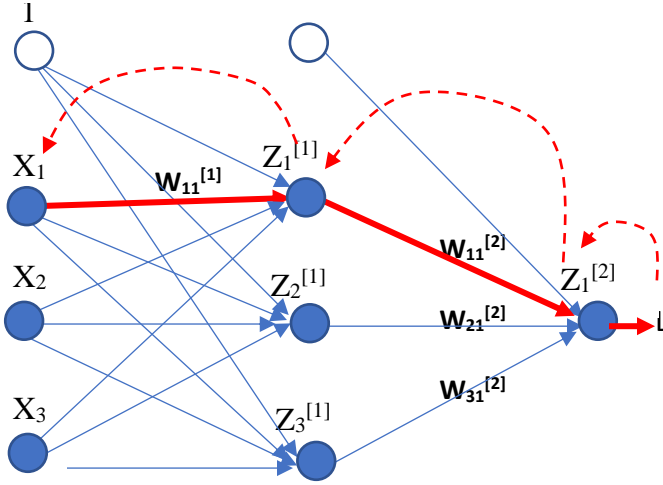
Figure 7.10

$$\frac{\partial L(Y_k,\hat{Z}_k)}{\partial W_{m1}^{[1]}} = \left(\frac{\partial L(Y_k,\hat{Z}_k)}{\partial Z_{1,k}^{[2]}} \times \frac{\partial Z_{1,k}^{[2]}}{\partial \Sigma j \, (W_{j1}^{[2]} Z_{j,k}^{[1]} + b_1^{[2]})} \right)$$

$$\times \left(\frac{\partial \Sigma j \, (W_{j1}^{[2]} Z_{j,k}^{[1]} + b_1^{[2]})}{\partial Z_{1,k}^{[1]}} \times \frac{\partial Z_{1,k}^{[1]}}{\partial \Sigma j \, (W_{j1}^{[1]} X_j + b_1^{[1]})} \right)$$

$$\times \frac{\partial \Sigma j \, (W_{j1}^{[1]} X_j + b_1^{[1]})}{\partial W_{m1}^{[1]}} \qquad (7.2)$$

for m=1,2,3. In the case m=1, Figure 7.10 shows the backwards pass along the path of the forward pass process starting at X_1 with edge or synapse weight

$W_{11}{}^{[1]}$ (see bold line). The partial derivatives components follow the dotted lines.

Similarly,

$$\frac{\partial L\left(Y_k, \widehat{Z}_k\right)}{\partial W_{m2}^{[1]}} = \frac{\partial L\left(Y_k, \widehat{Z}_k\right)}{\partial Z_{1,k}^{[2]}} \times \frac{\partial Z_{1,k}^{[2]}}{\partial \Sigma j\ (W_{j1}^{[2]} Z_{j,k}^{[1]} + b_1^{[2]})} \times \frac{\partial \Sigma j\ (W_{j1}^{[2]} Z_{j,k}^{[1]} + b_1^{[2]})}{\partial Z_{2,k}^{[1]}}$$

$$\times \frac{\partial Z_{2,k}^{[1]}}{\partial \Sigma j\ (W_{j2}^{[1]} X_j + b_2^{[1]})} \times \frac{\partial \Sigma j\ (W_{j2}^{[1]} X_j + b_2^{[1]})}{\partial W_{m2}^{[1]}}$$

for m = 1,2,3.

$$\frac{\partial L\left(Y_k, \widehat{Z}_k\right)}{\partial W_{m3}^{[1]}} = \frac{\partial L\left(Y_k, \widehat{Z}_k\right)}{\partial Z_{1,k}^{[2]}} \times \frac{\partial Z_{1,k}^{[2]}}{\partial \Sigma j\ (W_{j1}^{[2]} Z_{j,k}^{[1]} + b_1^{[2]})} \times \frac{\partial \Sigma j\ (W_{j1}^{[2]} Z_{j,k}^{[1]} + b_1^{[2]})}{\partial Z_{3,k}^{[1]}}$$

$$\times \frac{\partial Z_{3,k}^{[1]}}{\partial \Sigma j\ (W_{j3}^{[1]} X_j + b_3^{[1]})} \times \frac{\partial \Sigma j\ (W_{j3}^{[1]} X_j + b_3^{[1]})}{\partial W_{m3}^{[1]}}$$

for m = 1,2,3.

And

$$\frac{\partial L\left(Y_k, \widehat{Z}_k\right)}{\partial b_1^{[1]}} = \frac{\partial L\left(Y_k, \widehat{Z}_k\right)}{\partial Z_{1,k}^{[2]}} \times \frac{\partial Z_{1,k}^{[2]}}{\partial \Sigma j\ (W_{j1}^{[2]} Z_{j,k}^{[1]} + b_1^{[2]})} \times \frac{\partial \Sigma j\ (W_{j1}^{[2]} Z_{j,k}^{[1]} + b_1^{[2]})}{\partial Z_{1,k}^{[1]}}$$

$$\times \frac{\partial Z_{1,k}^{[1]}}{\partial \Sigma j\ (W_{j1}^{[1]} X_j + b_1^{[1]})} \times \frac{\partial \Sigma j\ (W_{j1}^{[1]} X_j + b_1^{[1]})}{\partial b_1^{[1]}}$$

$$\frac{\partial L\left(Y_k, \widehat{Z}_k\right)}{\partial b_2^{[1]}} = \frac{\partial L\left(Y_k, \widehat{Z}_k\right)}{\partial Z_{1,k}^{[2]}} \times \frac{\partial Z_{1,k}^{[2]}}{\partial \Sigma j\ (W_{j1}^{[2]} Z_{j,k}^{[1]} + b_1^{[2]})} \times \frac{\partial \Sigma j\ (W_{j1}^{[2]} Z_{j,k}^{[1]} + b_1^{[2]})}{\partial Z_{2,k}^{[1]}}$$

$$\times \frac{\partial Z_{2,k}^{[1]}}{\partial \Sigma j\ (W_{j2}^{[1]} X_j + b_2^{[1]})} \times \frac{\partial \Sigma j\ (W_{j2}^{[1]} X_j + b_2^{[1]})}{\partial b_2^{[1]}}$$

$$\frac{\partial L(Y_k, \hat{Z}_k)}{\partial b_3^{[1]}} = \frac{\partial L(Y_k, \hat{Z}_k)}{\partial Z_{1,k}^{[2]}} \times \frac{\partial Z_{1,k}^{[2]}}{\partial \Sigma j \ (W_{j1}^{[2]} Z_{j,k}^{[1]} + b_1^{[2]})} \times \frac{\partial \Sigma j \ (W_{j1}^{[2]} Z_{j,k}^{[1]} + b_1^{[2]})}{\partial Z_{3,k}^{[1]}}$$

$$\times \frac{\partial Z_{3,k}^{[1]}}{\partial \Sigma j \ (W_{j3}^{[1]} X_j + b_3^{[1]})} \times \frac{\partial \Sigma j \ (W_{j3}^{[1]} X_j + b_3^{[1]})}{\partial b_3^{[1]}}$$

and so on.

For example, if $L(Y, \hat{Y}) = \frac{1}{N} \Sigma_{k=1}^{N} (Y_k - \hat{Y}_k)^2$, then

$$\frac{\partial L(Y_k, \hat{Y}_k)}{\partial Z_{1,k}^{[2]}} = -2(Y_k - \hat{Y}_k) .$$

Note that if f(X) = 1/(1 + e^{-X}), df(X)/dX = e^{-X}/(1 + e^{-X})^2 = (1-f(X)) f(X). Note that $Z_{1,k}^{[2]} = f(\ \Sigma j \ (W_{j1}^{[2]} Z_{j,k}^{[1]} + b_1^{[2]}), \ Z_{1,k}^{[2]} \equiv \hat{Y}_k$. Then,

$$\frac{\partial Z_{1,k}^{[2]}}{\partial \ \Sigma j \ (W_{j1}^{[2]} Z_{j,k}^{[1]} + b_1^{[2]})} = (1 - \hat{Y}_k) \ \hat{Y}_k.$$

$$\frac{\partial \Sigma j \ (W_{j1}^{[2]} Z_{j,k}^{[1]} + b_1^{[2]})}{\partial Z_{1,k}^{[1]}} = W_{11}^{[2]}$$

$$\frac{\partial Z_{1,k}^{[1]}}{\partial \Sigma j \ (W_{j1}^{[1]} X_j + b_1^{[1]})} = (1 - Z_{1,k}^{[1]}) \ Z_{1,k}^{[1]}.$$

and $\frac{\partial \Sigma j \ (W_{j1}^{[1]} X_j + b_1^{[1]})}{\partial W_{11}^{[1]}} = X_1.$

Hence,

$$\frac{\partial L(Y_k, \hat{Y}_k)}{\partial W_{11}^{[1]}} = -2(Y_k - \hat{Y}_k) \times (1 - \hat{Y}_k) \ \hat{Y}_k \times W_{11}^{[2]} \times (1 - Z_{1,k}^{[1]}) \ Z_{1,k}^{[1]} \times X_1$$

and

$$\frac{\partial L(Y,\hat{Y})}{\partial W_{11}^{[1]}} = -\frac{1}{N}\sum_{k=1}^{N} 2(Y_k - \hat{Y}_k) \times (1 - \hat{Y}_k)\,\hat{Y}_k \times W_{11}^{[2]} \times (1 - Z_{1,k}^{[1]})\,Z_{1,k}^{[1]} \times X_1 \,.$$

For a shorter forward pass from $Z_1^{[1]}$ to L, the partial derivative of

$$\frac{\partial L(Y_k,\hat{Y}_k)}{\partial W_{11}^{[2]}} = \left(\frac{\partial L(Y_k,\hat{Y}_k)}{\partial Z_{1,k}^{[2]}} \times \frac{\partial Z_{1,k}^{[2]}}{\partial \Sigma j\,(W_{j1}^{[2]} Z_{j,k}^{[1]} + b_1^{[2]})}\right)$$

$$\times \frac{\partial \Sigma j\,(W_{j1}^{[2]} Z_{j,k}^{[1]} + b_1^{[2]})}{\partial W_{11}^{[2]}} \qquad (7.3)$$

which is just part of (7.2). For longer forward pass involving a deeper NN such as the following with 3 hidden layers and two final outputs, the partial derivative of error/loss function (possibly weighted linear combination of the loss functions L_1 and L_2 of the two final outputs) with respect to $W_{11}^{[1]}$ (the first edge or weight from input X_1) is the sum of each of $3^3 \times 2$ backward derivative chain computations – one such backward pass is shown in bold below.
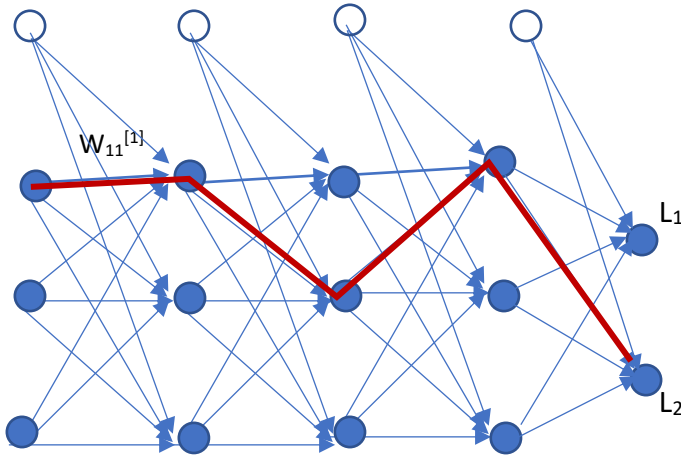

Figure 7.11

The purpose of finding all derivatives of loss function with respect to all the weights and biases in the ANN is as follows. Suppose for a particular weight (or bias) W, $\partial L/\partial W > (<) \; 0$, then we could try to attain a lower loss

by decreasing (increasing) the weight (or bias). To do so, we could find a revised weight (or bias) by adjusting it lower (higher) from the previous one. Hence the adjustment for each iteration (over mini batches and over epochs) updating of all weights at the same time is as follows.

$$W_{ij}^{*[r]} = W_{ij}^{[r]} - \alpha \frac{\partial L}{\partial W_{ij}^{[r]}}$$

where updated weight is $W_{ij}^{*[r]}$, and $\alpha > 0$ is a learning rate that determines how fast is the descent toward the minimum. α is a hyperparameter in this algorithm. These adjustments toward a small loss function form the gradient descent approach in the loss function minimization.

In Eqs. (7.1) and (7.2), we see that one backward propagation computation (and the initial forward pass) in one epoch (across all data points N in the training set) involves at least N times the number of computations of the partial derivatives for one case/subject k such as in (7.2). The computing memory resource may be overstretched with the large number of sample point derivatives. With E epochs, there would only be E number of iterations or updates on the parameters (and this may not be adequate if the NN is highly nonlinear, and E is not grossly large).

To attain a (reasonably) minimum error/loss function with not a massive number of epochs, a variant of the (batch) gradient descent, is to perform the backpropagation using not the entire training sample of size N in one epoch, but smaller (mini) batches of size n < N. In this way, the computational memory burden for each iteration involving only n sample points and correspondingly fewer partial derivatives is lesser.

The number of mini batches in an epoch is then N/n. There are then N/n number of iterations in each epoch, i.e., all the data need to pass through before one epoch is counted. If E number of epochs is run, then in total there will be E × N/n number of iterations in updating the parameters in the training. This is called the 'mini-batch' gradient descent approach.

Another popular variant is the stochastic gradient descent (SGD) that randomly (by default random generator in the algorithm) sequentially computes the gradients and update for each sample point within the batch – it is like the mini-batch with a batch size of 1. The updating of the stochastic gradient descent partial derivatives for each sample point can cause the convergence to the minimum error/loss function to be more volatile than when using the (full) batch or mini-batch training data set. However, there are far more iterations. Different platforms such as TensorFlow may, however, have

related SGD algorithms that are built a bit differently with momentum factor to adjust the learning rate.

Besides batch size strategy in achieving computationally efficient convergence, another related algorithm is in adjusting the learning rate with each parameter/weights update/iteration instead of keeping it constant throughout the training. One popular algorithm is Adam (adaptive moment estimation). The algorithm computes the exponentially decaying (moving) averages of past gradients and past squared gradients, viz.

$$M_t = \beta_1 M_{t-1} + (1 - \beta_1)G_t$$

and

$$V_t = \beta_2 V_{t-1} + (1 - \beta_2)G_t^2$$

where t is each iteration step forward, G_t and G_t^2 are the computed gradient and squared gradient at t. M_0 and V_0 are typically initialized at 0. M_t and V_t are moving averages of G_t and G_t^2 respectively.

Now,

$M_1 = (1 - \beta_1)G_1$, $M_2 = \beta_1(1 - \beta_1)G_1 + (1 - \beta_1)G_2$, $M_3 = \beta_1^2(1 - \beta_1)G_1 + \beta_1(1 - \beta_1)G_2 + (1 - \beta_1)G_3$,..., $M_t = (1 - \beta_1) \sum_{i=1}^{t} \beta_1^{t-i} G_i$. Taking unconditional expectation,

$E(M_t) = (1 - \beta_1) \sum_{i=1}^{t} \beta_1^{t-i} E(G_i)$.

Assuming $E(G_i)$ for every i is approximately constant, then

$E(M_t) \approx E(G_t) (1 - \beta_1) \sum_{i=1}^{t} \beta_1^{t-i} = E(G_t) (1 - \beta_1^t)$.

The approximate mean of G_t, $E(G_t) \approx E(M_t) / (1 - \beta_1^t)$. It is said that the M_t process supposedly converging over long-term to some exponentially (decreasing) weighted averages of past and current G_t is biased away from $E(G_t)$ and M_t needs to be adjusted to $\widehat{M}_t = M_t/(1 - \beta_1^t)$ so that $E(\widehat{M}_t) = E(M_t)/(1 - \beta_1^t) \approx E(G_t)$. Now $\widehat{M}_t$ is (approximately) unbiased so that its long-term weighted averaging of past and current G_t should lead to $E(G_t)$.

In a similar analysis,

$V_1 = (1 - \beta_2)G_1^2$, $V_2 = \beta_2(1 - \beta_2)G_1^2 + (1 - \beta_2)G_2^2$, $V_3 = \beta_2^2(1 - \beta_2)G_1^2 + \beta_2(1 - \beta_2)G_2^2 + (1 - \beta_2)G_3^2$,..., $V_t = (1 - \beta_2) \sum_{i=1}^{t} \beta_2^{t-i} G_i^2$. Taking unconditional expectation,

$E(V_t) = (1 - \beta_2) \sum_{i=1}^{t} \beta_2^{t-i} E(G_i^2)$.

Assuming $E(G_i^2)$ for every i is approximately constant, then

$E(V_t) \approx E(G_i^2) (1 - \beta_2) \sum_{i=1}^{t} \beta_2^{t-i} = E(G_i^2) (1 - \beta_2^t)$.

The approximate "uncentered variance" (second moment) of G_t, $E(G_i^2) \approx E(V_t) / (1 - \beta_2^t)$. It is said that the V_t process supposedly converging over

long-term to some exponentially (decreasing) weighted averages of past and current G_t^2 is biased away from $E(G_t^2)$ and V_t needs to be adjusted to $\hat{V}_t = V_t/(1 - \beta_2^t)$ so that $E(\hat{V}_t) = E(V_t)/(1 - \beta_2^t) \approx E(G_t^2)$. Now $\hat{V}_t$ is (approximately) unbiased so that its long-term weighted averaging of past and current G_t^2 should lead to $E(G_t^2)$.

The Adam update rule for gradient descent in the weight adjustment during backward propagation is:

$$W_{ij,t}^{[r]} = W_{ij,t-1}^{[r]} - \theta\, \frac{\hat{M}_t}{\sqrt{\hat{V}_t} + \varepsilon}$$

where given a step size θ (hyperparameter to be tuned – it is typically a small positive number), adjustment or descent is faster with higher $\hat{M}_t$ and lower $\hat{V}_t$ (more persistent gradient in one direction with less variability). In most implementations, default values for β_1 and β_2 are 0.9 and 0.999. ε is included to prevent G_t (hence also G_t^2) disappearing to 0 when division becomes not possible in the second term. Typical value for ε is 10^{-8}. A comparison with the gradient descent shows the learning rate in Adam may be construed as changing according to $\alpha_t = \theta\, \hat{M}_t / G_t(\sqrt{\hat{S}_t} + \epsilon)$.

Any algorithm can also set a limit time to the iterations or stop the iterations when the loss function is close to minimum and not reducing anymore with iterations.

7.3 Worked Example – Data

The data set -- "Churn_Modelling.csv" – is found in public resource: https://www.kaggle.com/datasets/. The data set contains a bank's 10,000 customers' details, viz., nationality, gender, credit score (higher score means more credit-worthy), age, tenure (years with the bank), USD bank balance in the period of the data, the number of bank products used by the customer, whether the customer has the bank credit card, is active customer, and estimated USD salary of the customer. These serve as features of each customer that could explain the target variable – which is whether the customer exited or left the bank. In the latter the customer had closed his bank account during the data period and the classification of exit is "1". Otherwise, the customer continues with the bank and the classification of exit is "0". For ease of interpretation, assume the exit prediction is for a year forward.

The ability to predict if an existing customer is likely to exit the bank (or analogously to exit as customer of a store or as employee of a company) is

important as customer exit or attrition or loss of company clients could be highly damaging to the bottom line or even reputation of a company. If a customer is predicted to be likely to exist, or certain types or characteristics of customers are likely to exit, then the bank or company can step up certain strategies to try to retain such customers and promote customer loyalty.

The following code lines [1] to [3] in demonstration file Chapter7-1.ipynb show the data set. Note that TensorFlow (incorporating Keras) is the key platform and API/algorithms used for the building the MLP neural networks here.

```
In [1]: #Importing necessary Libraries
        import numpy as np
        import pandas as pd
        import tensorflow as tf
```

```
In [2]: #Loading Dataset
        data = pd.read_csv("Churn_Modelling.csv")
```

```
In [3]: #Generating Dependent Variable Vectors
        Y = data.iloc[:,-1].values
        X = data.iloc[:,3:13]
        X.head()
```

Out[3]:

	CreditScore	Geography	Gender	Age	Tenure	Balance	NumOfProducts	HasCrCard	IsActiveMember	Estimated Salary
0	619	France	Female	42	2	0.00	1	1	1	101348.88
1	608	Spain	Female	41	1	83807.86	1	0	1	112542.58
2	502	France	Female	42	8	159660.80	3	1	0	113931.57
3	699	France	Female	39	1	0.00	2	0	0	93826.63
4	850	Spain	Female	43	2	125510.82	1	1	1	79084.10

In code lines [4] and [5], the Gender variable and the Geography variable are transformed to dummy or 1, 0 variables.

```
In [4]: #Generating Dependent Variable Vectors
        Y = data.iloc[:,-1].values
        X = data.iloc[:,3:13]
        X['Gender']=X['Gender'].map({'Female':0,'Male':1})
        ### above is used instead of a more complicated package involving -- from sklearn.preprocessing import LabelEncoder
        ### converts Female -- 0, Male -- 1, i.e. hot-encoding categorical variables
        print (X['Gender'])

        0       0
        1       0
        2       0
        3       0
        4       0
               ..
        9995    1
        9996    1
        9997    0
        9998    1
        9999    0
        Name: Gender, Length: 10000, dtype: int64
```

```
In [5]: #Encoding Categorical variable Geography
        from sklearn.compose import ColumnTransformer
        from sklearn.preprocessing import OneHotEncoder
        ct =ColumnTransformer(transformers=[('encoder',OneHotEncoder(),[1])],remainder="passthrough")
        X = np.array(ct.fit_transform(X))
        ### Geography is transformed into France -- 1,0,0; Spain -- 0,0,1; Germany -- 0,1,0.
        ### Moreover -- this encoded vector of ones-zeros is now put in first 3 cols. Credit Score pushed to 4th col.
```

Code lines [6], [7] split the dataset into training and test data sets. Note that validation set is bypassed here as the model is predetermined to be a MLP and the training set itself is used to try out different hyperparameters to select the good performing hyperparameter values. The hyperparameters are the number of hidden layers (depth) and the number of neurons in each layer (width).

```
In [6]: ### convert X to dataframe X1
        X1 = pd.DataFrame(X)
        X1.head()
        ### Note there are 12 features including onehotencoder for the Geography feature--
        ### The features are encoded using a one-hot (aka 'one-of-K' or 'dummy') encoding scheme
```

```
In [7]: #Splitting dataset into training and testing dataset
        from sklearn.model_selection import train_test_split
        X_train,X_test,Y_train,Y_test = train_test_split(X,Y,test_size=0.2,random_state=1)
```

Next comes the scaling of the data (both features and target variable) which is useful if the features are data with different orders of magnitudes.

```
In [8]: #Performing Feature Scaling
        from sklearn.preprocessing import StandardScaler
        sc = StandardScaler()
        X_train = sc.fit_transform(X_train)
        X_test = sc.transform(X_test)
```

We call fit_transform() method on our training data and transform() method on our test data. Each feature in the training set is scaled to mean 0, variance 1. In sklearn.preprocessing.StandardScaler(), centering and scaling happens independently on each feature. The fit method is calculating the mean and variance of each of the features present in the data. The transform method is transforming all the features (and target variable) using the respective features' (target)'s mean and variance. Note that normalizing the features avoids some weights being close to 0 as out-scale feature sizes are standardized.

Code lines [9] to [12] use the tf.keras.models.Sequential() API to build the MLP neural network model.

```
In [9]: ### This is the very first step while creating NNmodel -- you can rename this model. Here we are going to create NNmodel object
        ### by using a certain class of Keras named Sequential. As a part of tensorflow 2.0, Keras is now integrated with
        ### tensorflow and is now considered as a sub-library of tensorflow. The Sequential class is a part of the models module
        ### of Keras library which is a part of the tensorflow library now.
        ### It used to be "import tensorflow as tf; from tensorflow import keras; from tensorflow.keras import layers"
        ### See documentation at https://keras.io/guides/sequential_model/

        #Initialising the NN model name -- NNmodel
        NNmodel = tf.keras.models.Sequential()
        ### Sequential specifies to keras that the model NNmodel is created sequentially and the output of each layer added
        ### is input to the next specified layer. Note that keras Sequential is not appropriate when the model has multiple outputs
```

```
In [10]: ### Creating a network that has 1 hidden layer together with 1 input layer and 1 output layer.
         #Adding First Hidden Layer
         NNmodel.add(tf.keras.layers.Dense(units=2,activation="sigmoid"))
         ### units = 2 refer to 2 neurons in hidden layer
         ### modelname.add is used to add a layer to the neural network -- need to specify as an argument what type of layer --
         ### Dense is used to specify the fully connected layer - i.e. all neurons are forward connect to all forward layer nodes
```

In the above, first hidden layer is created using the Dense class which is part of the 'layers' module. This class accepts 2 inputs -- (1) units: number of neurons that will be present in the respective layer (2) activation: specifying

which activation function to be used. This example uses first input as 2. There is no correct answer which is the right number of neurons in the layer – trial and error. Not too large to be computationally impractical or redundant; not too small to be ineffective. For the second input, we try the sigmoid or logistic function as an activation function for hidden layers. We can also try "relu" [rectified linear unit].

```
In [11]: ### now we create the output Layer
         #Adding Output Layer
         NNmodel.add(tf.keras.layers.Dense(units=1,activation="sigmoid"))
         ### Only 1 output neuron
```

For a binary classification problem as above, actual case output is 1 or 0. Hence we require only one neuron to output layer - output could be estimated probability of case's actual output = 1. For multiclass classification problem, if the output contains m categories, then we need to create m different neurons, one for each category. In the binary output case, the suitable activation function is the sigmoid function. For multiclass classification problem, the activation function is typically 'softmax'. The 'softmax' function predicts a multinomial probability distribution.

```
In [12]: ### After creating the Layers -- require compiling the NNmodel. Compiling allows the computer to run and understand the program
         ### without the need of more fundamental steps in the programming. Compiling adds other elements or linking other libraries, and
         ### such that after compiling the results are readily computed e.g. in a binary executable program as an output.
         #Compiling NNmodel
         NNmodel.compile(optimizer="adam",loss="binary_crossentropy",metrics=['accuracy'])
         ### Note optimizer here is a more sophisticated version of the Mean Square loss
```

Compile method above accepts inputs -- (1) optimizer: specifies which optimizer to be used in order to perform gradient descent (2) error/loss function, e.g., 'binary_crossentropy' here. For multiclass classification, it should be categorical_crossentropy, (3) metrics is the performance metrics to use in order to compute performance. 'accuracy' is one such performance metric.

Next, we check the dimension of X_train.

```
In [13]: X_train.shape
Out[13]: (8000, 12)
```

In code line [14], we run the training of the NN on the training data set. This uses the '.fit' in TensorFlow-Keras.

```
In [14]: #### Last step in creation of NNmodel NNmodel is trained on the training set here with Tensor-Keras .fit based on Compiler
         #Fitting NNmodel
         history=NNmodel.fit(X_train,Y_train,batch_size=8000,epochs = 100)
         ### Note that tf.keras.models.Sequential() by default uses glorot initializer -- drawing intial weights from a uniform
         ### distribution -- see other possibilities in https://keras.io/api/layers/initializers/
         ### Or you could try own customized wts inputs using
         ### for layer in model.layers:
         ###     init_layer_weight = [] # the weights yourself in this layer
         ###     layer.set_weights(init_layer_weight)
```

We show the last part of the output as follows. Since we specify in [14] batch size of 8000 on a 8000 sample point training set, the entire training set is run in one iteration to update the parameters. This constitutes one epoch. Then the

next epoch is run. The outputs show the updated loss and accuracy after 1 batch run 1/1 92/100 and then into the next epoch 93/100 where there is a total of 100 epochs to run.

```
1/1 [==============================] - 0s 0s/step - loss: 0.6139 - accuracy: 0.7111
Epoch 92/100
1/1 [==============================] - 0s 2ms/step - loss: 0.6133 - accuracy: 0.7121
Epoch 93/100
1/1 [==============================] - 0s 0s/step - loss: 0.6127 - accuracy: 0.7132
Epoch 94/100
1/1 [==============================] - 0s 0s/step - loss: 0.6121 - accuracy: 0.7139
Epoch 95/100
1/1 [==============================] - 0s 0s/step - loss: 0.6114 - accuracy: 0.7150
Epoch 96/100
1/1 [==============================] - 0s 0s/step - loss: 0.6108 - accuracy: 0.7163
Epoch 97/100
1/1 [==============================] - 0s 0s/step - loss: 0.6102 - accuracy: 0.7176
Epoch 98/100
1/1 [==============================] - 0s 2ms/step - loss: 0.6097 - accuracy: 0.7195
Epoch 99/100
1/1 [==============================] - 0s 0s/step - loss: 0.6091 - accuracy: 0.7201
Epoch 100/100
1/1 [==============================] - 0s 0s/step - loss: 0.6085 - accuracy: 0.7211
```

It is noted that after 100 epochs, the loss is 0.6085 and accuracy (% of correct predictions of exit or retention) is 0.7211 (72.11%). The updated weights after this epoch is typically used in the .evaluate computation of the prediction – see below.

Code line [15] provides a summary of the architecture/structure of this NN.

```
In [15]: NNmodel.summary()

         Model: "sequential"
         _____
         Layer (type)                Output Shape              Param #
         =================================================================
         dense (Dense)               (8000, 2)                 26

         dense_1 (Dense)             (8000, 1)                 3

         =================================================================
         Total params: 29
         Trainable params: 29
         Non-trainable params: 0
         _____
```

As there are 12 features as inputs, and one bias as input to each of the two neurons in the first hidden layer, there are $(12+1) \times 2 = 26$ weight parameters in the first dense (fully connected) hidden layer. In the 2 outputs of the first hidden layer, adding the next bias, there are $2+1 = 3$ weight parameters in the next dense layer which is also the output layer.

The outputs of losses and accuracies in code line [14] can be captured in the 'history' output of the NNmodel. They are plotted as shown in [16].

```
In [16]: import matplotlib.pyplot as plt
         print(history.history['accuracy'])
         print(history.history['loss'])
         plt.plot(history.history['accuracy'])
         plt.plot(history.history['loss'])
         plt.title('model accuracy')
         plt.ylabel('accuracy and loss')
         plt.xlabel('epoch')
         plt.legend(['accuracy', 'loss'], loc='upper left')
         plt.show()
```
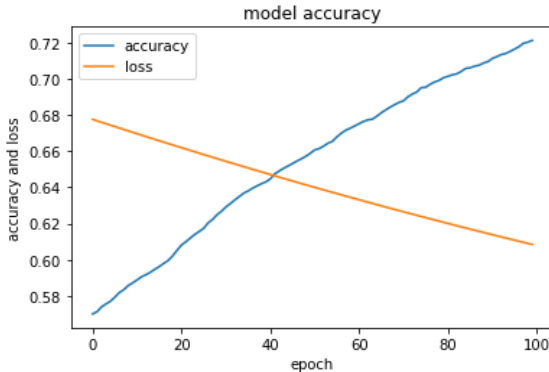

The plot shows that as the number of training iterations (epochs) increases, the loss decreases, and the accuracy increases to about 72%.

We can obtain the final iteration weights and biases of the trained NN and use these to compute any predicted output (which is a probability of exit) given the features' values. This is shown in code lines [17] to [28]. Specifically the new case is shown in [22] and predicted using '.predict' in the algorithm as 0.493171 in [23]. [24] through [28] then go through the forward pass computation process to calculate and verify the .predict number as 0.493171 in [28]. Note the logistic function in [28].

```
In [17]: ### Below are the weights in the final iteration
         first_layer_weights = NNmodel.layers[0].get_weights()[0]
         first_layer_biases  = NNmodel.layers[0].get_weights()[1]
         second_layer_weights = NNmodel.layers[1].get_weights()[0]
         second_layer_biases  = NNmodel.layers[1].get_weights()[1]
```

```
In [18]: print(first_layer_weights)
         first_layer_weights.shape
```

```
[[ 0.2901938   0.25264168]
 [-0.7470228  -0.40918842]
 [ 0.02371722 -0.52462083]
 [ 0.4342153  -0.34347007]
 [ 0.7357036   0.3798818 ]
 [-0.48699933  0.7370789 ]
 [ 0.01408681  0.020531  ]
 [-0.18185025 -0.23582737]
 [ 0.13013802  0.0582539 ]
 [-0.41049713  0.5149377 ]
 [-0.5165592   0.313679  ]
 [ 0.31938234 -0.3098878 ]]
```

```
Out[18]: (12, 2)
```

```
In [19]: print(first_layer_biases)
         first_layer_biases.shape  ### (2,) here basically means 2 elements in a 1-dim array. .T has no effect on 1d array
```

```
[ 0.09777266 -0.09516037]
```

```
Out[19]: (2,)
```

166

```
In [20]: print(second_layer_weights)
         second_layer_weights.shape

         [[-0.9391421 ]
          [ 0.62109536]]
Out[20]: (2, 1)
```

```
In [21]: print(second_layer_biases)
         second_layer_biases.shape

         [-0.09638941]
Out[21]: (1,)
```

```
In [22]: ### Now we use the trained weights and biases to try to predict based on a new case
         tr=sc.transform([[1, 0, 0, 500, 1, 40, 3, 60000, 2, 1, 1, 100000]])
         print(tr)   ### tr.shape is (1,12)

         [[ 1.00150113 -0.58312392 -0.57273139 -1.55489968  0.91509065  0.10629772
           -0.70174202 -0.26396987  0.80225696  0.64376017  0.97725852 -0.00249134]]
```

```
In [23]: ### Example
         ### Predicting result for Single Observation
         print(NNmodel.predict(tr))
         ### note in each recompute -- this no. will change slightly because of the random initiation of the weights

         1/1 [==============================] - 0s 64ms/step
         [[0.49317122]]
```

```
In [24]: ### now we compute the predicted prob of 1, manually
         tr.dot(first_layer_weights)  ### gives a 1 x 2 matrix
Out[24]: array([[0.03161255, 2.48552524]])
```

```
In [25]: Flayerneurons_sum=tr.dot(first_layer_weights) + first_layer_biases
         print(Flayerneurons_sum)  ### 1 x 2 matrix

         [[0.12938521 2.39036488]]
```

```
In [26]: Flayerneurons_act=1/(1+np.exp(-Flayerneurons_sum))
         print(Flayerneurons_act)  ### 1 x 2 matrix -- output of neurons in hidden layer

         [[0.53230125 0.91608962]]
```

```
In [27]: Slayerneurons_sum=Flayerneurons_act.dot (second_layer_weights)+second_layer_biases
         print(Slayerneurons_sum)

         [[-0.02731692]]
```

```
In [28]: predprob=1/(1+np.exp(-Slayerneurons_sum))
         print(predprob) ### Note this is the same output as NNmodel.predict(tr)
         ### This manual computation of the forward pass should have output same as in NNmodel.predict(tr)

         [[0.49317119]]
```

In code line [29], we use '.evaluate' (based on the trained NN in [14]) to predict outputs for X_train and then compare with the actual outputs in Y_train. This returns a loss of 0.6079 and accuracy of 0.7229. Thus '.evaluate' performs one step beyond just '.predict' in [23].

```
In [29]: ### Now we use the trained NNmodel to predict output in X_train sample
         NNmodel.evaluate(X_train,Y_train)  ### evaluates the loss and accuracy as specified in the Compiler

         250/250 [==============================] - 0s 520us/step - loss: 0.6079 - accuracy: 0.7229
Out[29]: [0.6078730225563049, 0.7228749990463257]
```

We check that this is based on the final weights after the 100 epochs and should be consistent with '.predict'. Code lines [30] to [39] check the predicted outputs and compare with the actual outputs and returns also an accuracy of 0.7229 in [39].

```
In [30]: ### Now we use the trained NNmodel to predict output in X_train sample -- computing manually via .predict
         TE=NNmodel.predict(X_train)  ### note X_train has 8000 data points
```

```
In [31]: TE.shape
Out[31]: (8000, 1)
```

```
In [32]: h=(TE > 0.5).astype(int) ### Convert TE>0.5 == true ==> 1, False to 0
```

```
In [33]: print(h)
         h.shape
```

```
In [34]: ### replace all elements in numpy array of value 0 with value -1
         h[h==0]=-1
```

```
In [35]: print(h)
         h.shape
```

```
In [36]: ### replace all elements in numpy array of value 0 with value -1
         Y_train1=Y_train
         Y_train1[Y_train1==0]=-1
```

```
In [37]: print(Y_train1)
```

```
         [-1 -1  1 ...  1 -1  1]
```

```
In [38]: Y_train1.shape
```

```
Out[38]: (8000,)
```

```
In [39]: J=np.multiply(Y_train1.T,h.T)  ### element by element multiplication
         c=np.count_nonzero(J > 0)
         print(c,c/8000)
```

```
         5783 0.722875
```

In code line [40], we finally use the trained NN to perform prediction of exits in the test sample (of 2000 points). This is verified in [41], [42] as 72.50%. Note the '.evaluate' here used the trained weights in [14] '.fit'. It should be noted that as the weights and biases feeding into each layer forward are initially obtained by random draws from usually a small range (-1,+1), a MLP will produce slightly different predictive results for each new run unless we fix the random seed.[3]

```
In [40]: ### Now we use the trained NNmodel to predict output in X_test sample
         NNmodel.evaluate(X_test,Y_test)  ### evaluates the loss and accuracy as specified in the Compiler
```

```
         63/63 [==============================] - 0s 521us/step - loss: 0.6028 - accuracy: 0.7250
```

```
Out[40]: [0.6028271913528442, 0.7250000238418579]
```

```
In [41]: ### Now we use the trained NNmodel to predict output in X_test sample -- computing manually via .predict
         TE1=NNmodel.predict(X_test)  ### note X_test has 2000 data points
```

```
In [42]: h1=(TE1 > 0.5).astype(int) ### Convert TE1>0.5 == true ==> 1, False to 0
         h1[h1==0]=-1
         Y_test1=Y_test
         Y_test1[Y_test1==0]=-1
         J1=np.multiply(Y_test1.T,h1.T)  ### element by element multiplication
         c1=np.count_nonzero(J1 > 0)
         print(c1,c1/2000)
```

```
         1450 0.725
```

---

[3] This can be done by putting in the first code line of the notebook the following. import json \ import numpy as np \ import tensorflow as tf \ import keras \ from keras import layers \ from keras import initializers\ keras.utils.set_random_seed(5) ## set a seed number 5 or something else \ tf.config.experimental.enable_op_determinism()

The TE1 in code line [41] of keras provides the vector of predicted probabilities in the context of binary cross entropy loss in predicting the binary class of "1" or "0". The vector also translates into a vector of predicted 1's or 0's depending on whether the predicted probability (of "1") is > 0.5 or not. These vectors can be used to compute the confusion matrix, the classification table, and the ROC AUC using sklearn.metrics.

## 7.4 Improving the NN and Understanding the Results

Although the accuracy of the prediction of bank customer exit in the single hidden layer (2 neurons) MLP shown in the last section is 72.5%, which is reasonably good, it can perhaps be improved. Also, sometimes a single batch may not yield robust or stable results. A telltale sign of the possibility of improvement is indicated in [16] where the training performance graph shows the loss is still decreasing and accuracy still climbing at the end of the training iterations. We increase the number of backward passes and iterations, hence parameter revisions, by using "mini-batches" of batch size = 100 (instead of the entire batch size of 8000), and still using 100 epochs. See demonstration file Chapter7-2.ipynb. This yields the following loss and accuracy graph.
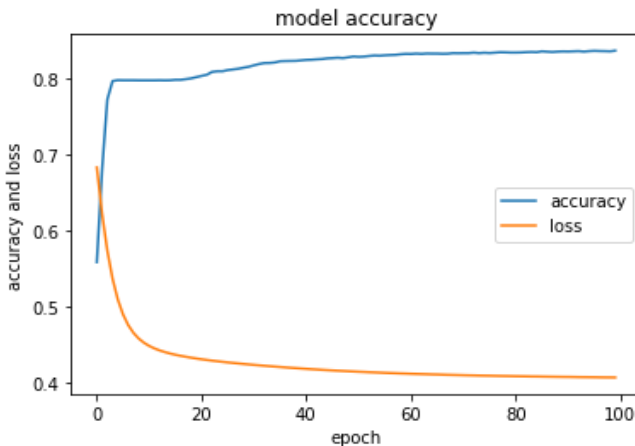
It is seen that after 3 epochs or 240 iterations (each epoch has 80 mini-batch iterations; 80 = 8000/100), the accuracy had already climbed to over 77%. The loss and accuracy stabilize at higher epochs, ending with training accuracy of about 83.6% (see output last line to code line [14]). The test accuracy is 83.35%

(see output last line to code line [42]). Both accuracies are better than those of 72.29% and 72.50% in the previous case of batch size = 8000 and 100 epochs. Hence higher number of iterations, such as in stochastic descent, is useful to improve accuracy.

We also document the case of keeping batch size = 100 but using to 500 epochs. This created a total of $80 \times 500 = 40{,}000$ iterations. See demonstration file Chapter7-3.ipynb. This yields the following loss and accuracy graph.
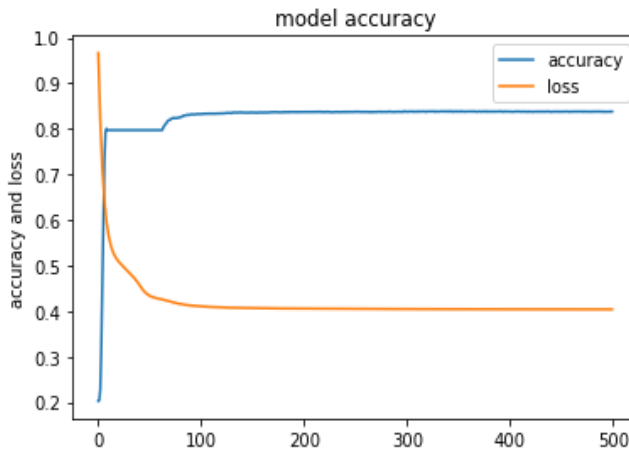
The loss and accuracy stabilize after about 10 epochs, ending with training accuracy of 83.80%. The test accuracy is 83.30%. Both accuracies are about similar to the case of batch size = 100 and 100 epochs. The initial few epochs saw a sharp hike in accuracy from a starting low of about 20%. The latter is possible as the initiating weights are random draws and could start off with first several iterates of large error/loss. Overall, it is seen that having 100 epochs in this case and a batch size of 100 may already clock in a sufficient number of iterations to adequately train the NN.

We employ the same batch size = 100 and 500 epochs, but attempt 3 different models (1), (2), and (3). In (1) (see demonstration file Chapter7-4.ipynb), we adjust the optimizer to SGD instead of Adam. In (2) (see demonstration file Chapter7-5.ipynb), we add a second hidden layer with now 4 neurons in both the first and second hidden layers. We create an even deeper NN in (3) (see demonstration file Chapter7-6.ipynb) where the number of neurons in the first and the second hidden layers are increased from 4 to 8. In (3) there is therefore a total of $(12+1) \times 8 = 104$ neurons in the first hidden

layer, $(8+1) \times 8 = 72$ neurons in the second hidden layer, and $8 + 1 = 9$ neurons in the output layer.

For (3), the code lines for building the NN are shown as follows. Note how the second hidden layer is built in the Keras-Sequential algorithm.

```
### This is the very first step while creating NNmodel. Here we are going to create our ann object by using a certain class
### of Keras named Sequential. As a part of tensorflow 2.0, Keras is now integrated with tensorflow and is now considered as a
### sub-library of tensorflow. The Sequential class is a part of the models module of Keras library which is a part of the
### tensorflow library now.
### It used to be "import tensorflow as tf; from tensorflow import keras; from tensorflow.keras import layers"
### See documentation at https://keras.io/guides/sequential_model/

#Initialising the NN model name -- NNmodel
NNmodel = tf.keras.models.Sequential()
```

```
### Creating a network that has 2 hidden layers together with 1 input layer and 1 output layer.
#Adding First Hidden Layer
NNmodel.add(tf.keras.layers.Dense(units=8,activation="sigmoid"))
### units = 8 refer to 8 neurons in hidden layer
```

```
### Creating 2nd hidden layer
#Adding Second Hidden Layer -- note this is added sequentially to the first hidden layer
NNmodel.add(tf.keras.layers.Dense(units=8,activation="sigmoid"))
### units = 8 refer to 8 neurons in hidden layer
```

```
### now we create the output layer -- this is added sequentially
#Adding Output Layer
NNmodel.add(tf.keras.layers.Dense(units=1,activation="sigmoid"))
### Only 1 output neuron
```

```
### After creating the layers -- require compiling the NNmodel. Compiling allows the computer to run and understand the program
### without the need of more fundamental steps in the programming. Compiling adds other elements or linking other libraries, and
### such that after compiling the results are readily computed e.g. in a binary executable program as an output.
#Compiling NNmodel
NNmodel.compile(optimizer="adam",loss="binary_crossentropy",metrics=['accuracy'])
### Note optimizer here is a more sophisticated version of the Mean Square Loss
```

```
#### Last step in creation of NNmodel. NNmodel is trained on the training set here with Tensor-Keras .fit based on Compiler
#Fitting NNmodel
NNmodel.fit(X_train,Y_train,batch_size=100,epochs = 500)
```

The minimized (after the specified number of iterations) loss value and the accuracy of the predictions for the different models of (1), (2), (3) are reported below. Note the results may change a little for any new run since the initialization of the parameters is random.

Metrics:	(1)	(2)	(3)
Training Set			
Loss	0.4193	0.3424	0.3230
Accuracy (%)	81.69%	86.11%	86.80%
Test Set			
Loss	0.4130	0.3359	0.3319
Accuracy (%)	82.35%	86.25%	86.25%

In (1), it is seen that the SGD optimizer performs a little worse than Adam with the same number of iterations in batch size = 100, epochs = 500, one

hidden layer and 2 neurons in the layer. Model (2) with 2 hidden layers of 4 neurons each improves accuracy by about 3% compared to the case of only 1 hidden layer. The deeper NN with 8 neurons in each hidden layer in (3) improves a little on the training accuracy, though the test accuracy is the same as that in case (2) with 4 neurons in each hidden layer.

During the training, pruning or reducing the number of total number of neurons or nodes could occur to improve the performances.

We also tap on the Scikit-learn (Sklearn) python library to use the LogisticRegression codes to perform classification test on the training data set. The code lines are shown as follows.

```
from sklearn.linear_model import LogisticRegression
LogReg=LogisticRegression()
```

```
Lresult = LogReg.fit(X_train, Y_train)
print(Lresult.coef_, Lresult.intercept_)
### SKLearn LogisticRegression adds regularization so the results are a bit different from the statsmodel package above

[[-0.1231805   0.21764563 -0.07679625 -0.05350094 -0.26540571  0.74686475
  -0.02786673  0.16927536 -0.04035424 -0.03663908 -0.54912598  0.01607395]] [-1.6543875]
```

```
Lpredict=LogReg.predict(X_test)
```

```
### Using Score method to obtain accuracy (% correct prediction) of model
score = LogReg.score(X_test,Y_test)
print(score)
```
```
0.8125
```

The prediction accuracy using the estimated logit regression coefficients (where estimated probability > 0.5 is designated as predicting 1, otherwise 0) shows 81.25%. This is better than the base case in the last section with 1 hidden layer but batch gradient descent and epoch = 100. It is just slight below case (1) with 1 hidden neural network layer but batch size = 100 and epoch = 500. The better trained and deeper NNs in (2) and (3) appear to perform better than logistic regression prediction.

We also perform a logit regression of the exit variable (1 or 0) on the feature variables using package 'statsmodel' in python. The regression outputs are summarized as follows. See demonstration file Chapter7-7.ipynb.

The estimated coefficients and their statistical significance provide some observations to help understand how the NN outputs indicate regarding the influence of the features on the prediction of 'exit'.

```
Optimization terminated successfully.
         Current function value: 0.429076
         Iterations 8
                      Logit Regression Results
==============================================================================
Dep. Variable:                     y   No. Observations:                 8000
Model:                         Logit   Df Residuals:                     7988
Method:                          MLE   Df Model:                           11
Date:               Fri, 21 Oct 2022   Pseudo R-squ.:                  0.1490
Time:                       10:57:49   Log-Likelihood:                -3432.6
converged:                      True   LL-Null:                       -4033.5
Covariance Type:           nonrobust   LLR p-value:                6.481e-251
==============================================================================
                  coef    std err          z      P>|z|      [0.025      0.975]
------------------------------------------------------------------------------
Constant       -1.6549      0.035    -47.918      0.000      -1.723      -1.587
France         -0.1232   1.73e+06  -7.12e-08      1.000   -3.39e+06    3.39e+06
Spain           0.2178   1.51e+06   1.44e-07      1.000   -2.95e+06    2.95e+06
Germany        -0.0768   1.49e+06  -5.14e-08      1.000   -2.93e+06    2.93e+06
CrScore        -0.0535      0.030     -1.771      0.077      -0.113       0.006
Gender         -0.2657      0.030     -8.768      0.000      -0.325      -0.206
Age             0.7477      0.030     24.800      0.000       0.689       0.807
Tenure         -0.0279      0.030     -0.924      0.355      -0.087       0.031
Balance         0.1694      0.036      4.715      0.000       0.099       0.240
Products       -0.0403      0.031     -1.319      0.187      -0.100       0.020
CrCard         -0.0367      0.030     -1.220      0.222      -0.096       0.022
Active         -0.5499      0.032    -16.996      0.000      -0.613      -0.486
Salary          0.0161      0.030      0.530      0.596      -0.043       0.076
==============================================================================
```

It is seen that (at 10% 2-tailed significance level or a p-value of < 0.10), lower credit score (CrScore), Gender (Male $= 1$, Female $= 0$), higher Age, higher Balance, and low activity (Active) increases exit probability, and vice-versa.

We can use the trained NN in (3) to check on the effect of changing the feature input levels on predicted probability of exit. For example, in checking the effect of credit score levels, the following outputs show that the output of NNmodel.predict(tr1) is decreasing as the credit score increases. See demonstration file Chapter7-8.ipynb code line [18].

```
### Now we use the trained weights and biases to try to predict based on new cases
### Increasing credit score here
tr1=sc.transform([ [1,  0, 0, 400, 1, 40, 3, 60000, 2, 1, 1, 100000],
                   [1,  0, 0, 500, 1, 40, 3, 60000, 2, 1, 1, 100000],
                   [1,  0, 0, 600, 1, 40, 3, 60000, 2, 1, 1, 100000],
                   [1,  0, 0, 700, 1, 40, 3, 60000, 2, 1, 1, 100000],
                   [1,  0, 0, 800, 1, 40, 3, 60000, 2, 1, 1, 100000]])
print(tr1)   ### tr.shape is (5,12)
### Predicting result for 5 cases/subjects
print(NNmodel.predict(tr1))
### note in each recompute -- this no. will change slightly because of the random initiation of the weights
```

```
[[0.03330604]
 [0.02859351]
 [0.0247239 ]
 [0.02155222]
 [0.01895096]]
```

This is consistent with the negative coefficient of CrScore in the logit regression. Increasing credit score, increasing tenure, lesser balance produce a lower probability of exit. The other features show some mixed results.

7.5 Summary

One major application of ML is the use of neural network (NN) that processes input information and produces output(s) of prediction and classification. The Multi-Layer Perceptron (MLP) or Artificial Neural Network (ANN) is seen to be able to predict up to over 86% accuracy in the bank customer exit data set when the NN is adequately structured with sufficiently deep number of hidden layers and adequate training iterations. When the training accuracies are high, it is more likely that the testing accuracies are also high. The trained NN can also help to provide understanding of how the various features affect the final output such as the predicted probability in the case of classification.

7.6 Other References

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