Introduction

The idea of this notebook is to explore a step-by-step approach to create a **single layer neural network** without the help of any third party library. In practice, this neural network should be useful enough to generate a simple non-linear regression model, though it's final goal is to help us understand the inner workings of one.

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1. Working Data

First we will create a **secret function** that will generate a test score based on students hours of sleep and study. Note that in real life scenarios not only these secret functions will be unknown but in practice they usually dont exist, meaning, underlying relations between variables such as a Sleep and Study is far more complex and cannot be defined by a simple continuous function.

Additionally, as we will later observe, we expect that our neural network should provide us good approximations or predictors of the score but the actual secret function will remain unknown. In other works, we will only have a different, complex continuous function in which its output should be enough to approximate the original one.

In [1]:

```
# Our secret function
secretFunction <- function(x) {
  y <- (x[,1]^2 + x[,2]^2)
  return(t(t(y)))
}
print("Secret Function loaded")
```

```
[1] "Secret Function loaded"
```

Let's assume a sample of 9 students, where each one had 3 days (72 hours) prior to the test and they either slept or studied.

In [2]:

```
# Our train (X) and test (xTest) data
Study <- round(runif(9,1,24))
Sleep <- 72 - Study
X <- data.frame(Study=Study,Sleep=Sleep)
xTest = rbind(c(3,7),c(2,8))

# We generate our Y train (y)
y <- secretFunction(X)
```

In [3]:

```
# This is our Study, Sleep and Score table
cbind(X,Score=y)
```

A data.frame: 9 × 3

Study	Sleep	Score
<dbl>	<dbl>	<dbl>
12	60	3744
13	59	3650
12	60	3744
20	52	3104
17	55	3314
9	63	4050
13	59	3650
21	51	3042
8	64	4160

2. Generating the model

2.1 Functions

First, we need some functions to be defined:

- **Rand**: Generate random numbers
- **Sigmoid**: Our non-linear activation function to be executed by our Sigmoid neuron.
- **Forward**: Our forward propagation function.
- **Sigmoid Prime**: Gradient of our Sigmoid function for Backward Propagation.
- **Cost**: Cost calculation funtion (sum of squared errors)

In [4]:

```
# Random Function
rand <- function(x) {
  return(runif(1, 5, 100)/100)
}

# Sigmoid Function
sigmoid <- function(x) {
  return(1/(1+exp(1)^-x))
}

# Forward Propagation Function
Forward <- function(X,w1,w2) {
  X <- cbind(X[,1],X[,1])
  z2 <- X %*% w1
  a2 <- sigmoid(z2)
  z3 <- a2 %*% w2
  yHat <- sigmoid(z3)
  return(yHat)
}

# Sigmoid Gradient Function
sigmoidPrime <- function(x) {
  return((exp(1)^-x)/(1+(exp(1)^-x))^2)
}

# Cost Function
cost <- function(y,yHat) {
  sum(((yHat-y)^2)/2)
}
print("Functions loaded")
```

```
[1] "Functions loaded"
```

2.2 Parameter Initialization

Next, we need to define our parameters. We have two sets of parameters:

- **Hyperparameters:** Parameters that the network cannot learn and are pre-defined.
  - **Number of hidden layers:** In this case we have 1, since it's a simple single layered neural network.
  - **Number of Neurons of hidden layers:** We will use 6.
  - **Learning Rate:** We will use 2.
- **Learning Parameters:** Parameters that our network will **learn**.
  - **Weights:** We will use 2 weights since by design we will need at leas N+1 weights where N is equivalent to the number of Hidden Layers.

In [5]:

```
# Hyperparameters
inputLayerSize = ncol(X)
outputLayerSize = 1 # Dimension of outputs (1 since it's only score)
hiddenLayerSize = 6 # Number of neurons
```

```
LearningRate <- 2

# Weights
w1 <- matrix(runif(inputLayerSize*hiddenLayerSize), nrow = inputLayerSize, ncol = hiddenLayerSize )
w2 <- matrix(runif(hiddenLayerSize*outputLayerSize), nrow = hiddenLayerSize, ncol =
outputLayerSize )
print("Parameter initialization completed")
```

```
[1] "Parameter initialization completed"
```

2.3 Data Normalization

In [6]:

```
# We normalize train data
X = X/max(X)
y = y/max(y)

# We normnalize test data
xTest <- xTest/max(X)
yTest <- secretFunction(xTest)/max(y)
print("Data normalization completed")
```

```
[1] "Data normalization completed"
```

3. Propagation

3.1 Forward Propagation

In [7]:

```
# We propagate
yHat <- Forward(X,w1,w2)
print("Forward propagation completed")
```

```
[1] "Forward propagation completed"
```

3.1.1 Cost Calculation

In [8]:

```
# We calculate cost
J <- sum(((yHat-y)^2)/2)
J
```

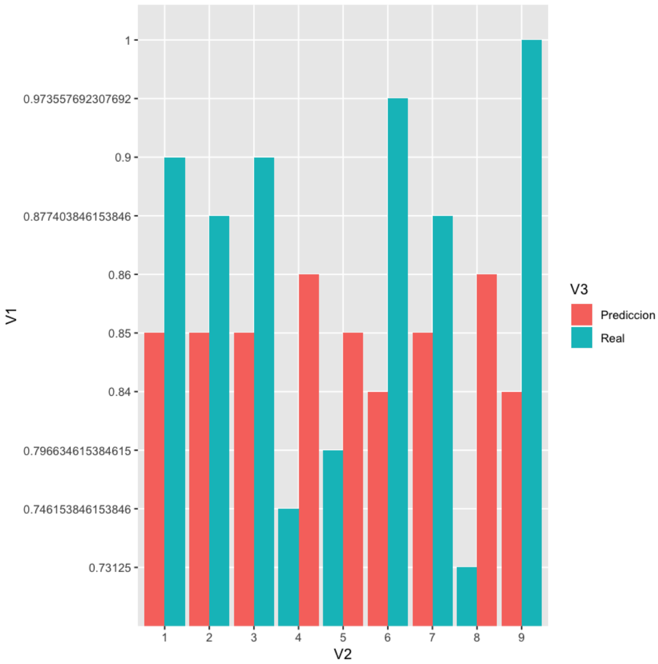
0.0406940979768502

3.1.2 We evaluate the results

In [9]:

```
library(ggplot2)
resultPlot <- as.data.frame(rbind(cbind(y,1:nrow(y),"Real"),cbind(round(yHat,2),1:nrow(yHat),"Predi
ccion")))
ggplot(resultPlot, aes(x=V2, y=V1, fill=V3)) + geom_bar(stat="identity", position="dodge")
```

```
Registered S3 methods overwritten by 'ggplot2':
  method         from
  [.quosures     rlang
  c.quosures     rlang
  print.quosures rlang
```



3.2 Back propagation

In [10]:

```
# We derivate W2 in respect to the cost
dJdW2 <- function(X,w1,w2) {
  X <- cbind(X[,1],X[,1])
  z2 <- X %*% w1
  a2 <- sigmoid(z2)
  z3 <- a2 %*% w2
  yHat <- sigmoid(z3)
  delta3 <- -(y-yHat)*sigmoidPrime(z3)
  cost <- t(a2) %*% delta3
  return(cost)
}

# We adjust W2
w2 <- w2 - (LearningRate * dJdW2(X,w1,w2))

# We derivate W1 in respect to the cost
dJdW1 <- function(X,w1,w2) {
  X <- cbind(X[,1],X[,1])
  z2 <- X %*% w1
  a2 <- sigmoid(z2)
  z3 <- a2 %*% w2
  yHat <- sigmoid(z3)
  delta3 <- -(y-yHat)*sigmoidPrime(z3)
  delta2 <- (delta3 %*% t(w2)) * sigmoidPrime(z2)
  cost <- t(X) %*% delta2
  return(cost)
}
w1 <- w1 - (LearningRate * dJdW1(X,w1,w2))
print("Back propagation completed")
```

```
[1] "Back propagation completed"
```

3.3 We forward propagate again

In [11]:

```
# We propagate Again!
yHat <- Forward(X,w1,w2)
print("Forward propagation completed")
```

```
[1] "Forward propagation completed"
```

3.3.1 New Cost Calculation

In [12]:

```
# We calculate cost
J <- sum(((yHat-y)^2)/2)
J
```

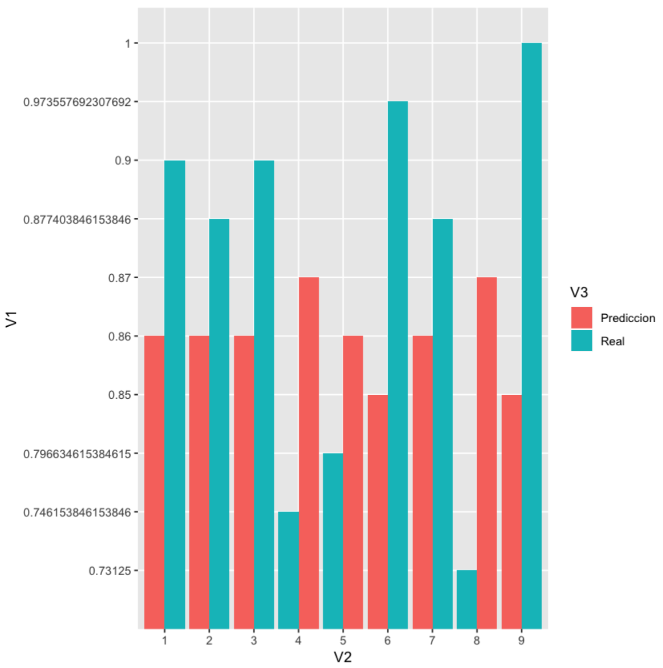
0.0394141923624708

Note: We should observe a small improvement in cost due to the new parameters.

3.3.2 We evaluate again

In [13]:

```
library(ggplot2)
resultPlot <- as.data.frame(rbind(cbind(y,1:nrow(y),"Real"),cbind(round(yHat,2),1:nrow(yHat),"Predi
ccion")))
ggplot(resultPlot, aes(x=V2, y=V1, fill=V3)) + geom_bar(stat="identity", position="dodge")
```



4. Backpropagate, Forwardpropagate and repeat

We will now repeat the previous process until we cannot minimize our cost any more. When this happens, it means we have found a **local minima**. We will stop when we observe that error calculated at **step n+1** is equal or superior than the one found in **step n**, meaning we cannot improve any more with out jumping around the local minima.

In [14]:

```
costTrain <- data.frame(Training=NA,Cost=NA)
costTest <- data.frame(Training=NA,Cost=NA)
InitialError <- sum((y-yHat)^2)
FinalError <- 0
i <- 1

while(round(FinalError,5) <= round(InitialError,5)) {
  w1 <- w1 - (LearningRate * dJdW1(X,w1,w2))
  w2 <- w2 - (LearningRate * dJdW2(X,w1,w2))
  yHat = Forward(X,w1,w2)
```

```
  costo <- cost(y,yHat)

  costTrain[i,]$Training <- i
  costTrain[i,]$Cost <- costo

  FinalError <- sum((y-yHat)^2)

  i <- i + 1
  if(i %% 1000==0) {
    # Print on the screen some message
    cat(paste0("Iteration ", i,": ",FinalError,"\n"))
  }
  if(i == 30000) {
      break()
  }
}
```

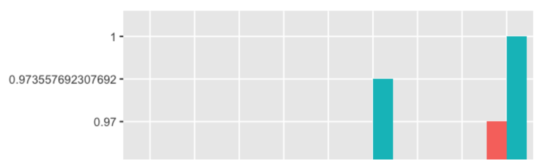
```
Iteration 1000: 0.00481584089668459
Iteration 2000: 0.0041359734308611
Iteration 3000: 0.00393871947102891
Iteration 4000: 0.00372143672994218
Iteration 5000: 0.0034924806052441З
Iteration 6000: 0.00326134930936602
Iteration 7000: 0.00303633770539048
Iteration 8000: 0.0028234085677745
Iteration 9000: 0.00262605678298945
Iteration 10000: 0.00244575603038661
Iteration 11000: 0.00228257085383198
Iteration 12000: 0.00213570371719112
Iteration 13000: 0.00200390180557296
Iteration 14000: 0.00188572744690734
Iteration 15000: 0.00177972281833611
Iteration 16000: 0.00168450161210436
Iteration 17000: 0.00159879386769361
Iteration 18000: 0.00152146252140866
Iteration 19000: 0.00145150388690322
Iteration 20000: 0.00138803971122357
Iteration 21000: 0.00133030539309178
Iteration 22000: 0.00127763699851438
Iteration 23000: 0.00122945850621331
Iteration 24000: 0.00118526999666641
Iteration 25000: 0.00114463708252138
Iteration 26000: 0.00110718164679011
Iteration 27000: 0.00107257383403121
Iteration 28000: 0.00104052518267471
Iteration 29000: 0.00101078276584012
Iteration 30000: 0.000983124206808979
```

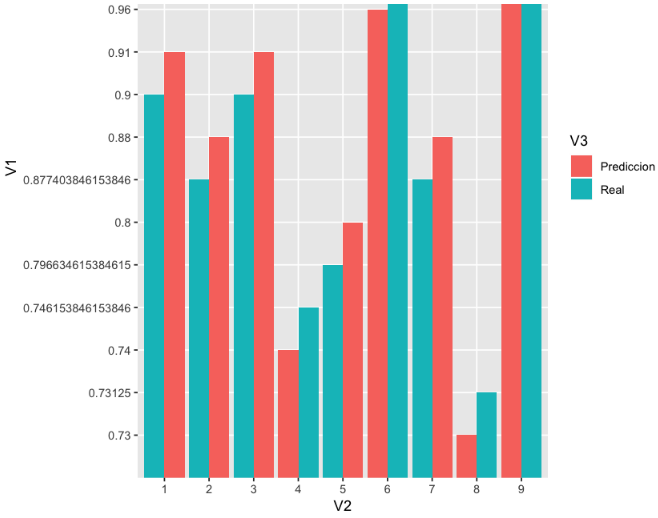
4.1 We evaluate again

In [15]:

```
library(ggplot2)
resultPlot <- as.data.frame(rbind(cbind(y,1:nrow(y),"Real"),cbind(round(yHat,2),1:nrow(yHat),"Predi
ccion")))
ggplot(resultPlot, aes(x=V2, y=V1, fill=V3)) + geom_bar(stat="identity", position="dodge")
Improvement <- (InitialError-FinalError)/InitialError
cat(paste("Initial Error: ",InitialError,"
Final Error: ",FinalError,"
Improvement: ",round(Improvement,2)*100,"%
Took ",i," Iterations",sep=""))
```

```
Initial Error: 0.0788283847249415
Final Error: 0.000983124206808979
Improvement: 99%
Took 30000 Iterations
```



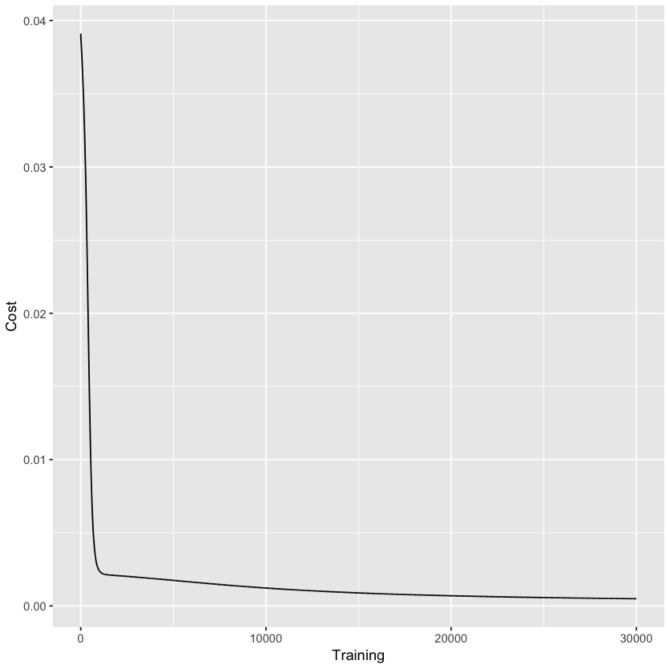


As seen in the results above it seems our model was able to predict very similar scores to our "Secret Function", even though the actual model is a mix of a more complex combination of vector products and non-linear functions. This means our new model approximates quite well our actual "Secret Function Model".

5. How our training improved our model?

In [16]:

```
costTrain$Data <- "Train"
ggplot(costTrain, aes(x=Training, y=Cost)) + geom_line()
```



As seen above it seems that there was little cost improvement after 1k iterations.

6. Evaluation on known (in sample) Data

In [17]:

```
Train <- X
```

In [18]:

```
# Note: this output represents a normalized representation of Study and Sleep
cbind(Train,RealScore=secretFunction(Train),PredictedScore=Forward(Train,w1,w2))
```

A data.frame: 9 × 4

Study	Sleep	RealScore	PredictedScore
<dbl>	<dbl>	<dbl>	<dbl>
0.187500	0.937500	0.9140625	0.9051446
0.203125	0.921875	0.8911133	0.8827864
0.187500	0.937500	0.9140625	0.9051446
0.312500	0.812500	0.7578125	0.7440203
0.265625	0.859375	0.8090820	0.7953386
0.140625	0.984375	0.9887695	0.9608078
0.203125	0.921875	0.8911133	0.8827864
0.328125	0.796875	0.7426758	0.7301721
0.125000	1.000000	1.0156250	0.9734991

Lets translate this to our original scale

In [19]:

```
X <- data.frame(Study=Study,Sleep=Sleep)
y <- secretFunction(X)
cbind(X,Score=secretFunction(X),Prediction=round(Forward(Train,w1,w2)*max(y)))
```

A data.frame: 9 × 4

Study	Sleep	Score	Prediction
<dbl>	<dbl>	<dbl>	<dbl>
12	60	3744	3765
13	59	3650	3672
12	60	3744	3765
20	52	3104	3095
17	55	3314	3309
9	63	4050	3997
13	59	3650	3672
21	51	3042	3038
8	64	4160	4050

As expected, it seems our model provide us very good approximations to actual test scores.

7. Evaluation on unknown (out of sample) data

Let's evaluate which test score we should expect from a student who **studied 16 hours and slept 56**

In [30]:

```
xTrain <- data.frame(Study=16,Sleep=56)
yTrain <- secretFunction(xTrain)
cbind(xTrain,Score=yTrain)
```

A data.frame: 1 × 3

Study	Sleep	Score
<dbl>	<dbl>	<dbl>
16	56	3392

What is our predicted score?

In [31]:

```
as.integer(round(Forward(xTrain/max(X),w1,w2)*max(y)))
```

3393

Seems pretty close to the real expected score (3292)

Simulation: How our model predicts new data

Lets simulate 72 students, starting from a student who studied 0 hours and slept 72, up to the opposite scenario.

In [84]:

```
Test <- data.frame(Study=seq(0,72))
Test$Sleep <- 72-Test$Study
Test$Score <- secretFunction(Test)
Test$Prediction <- as.integer(round(Forward(Test/max(X),w1,w2)*max(y)))
Test$SquaredError <- (Test$Score - Test$Prediction)^2
Test
```

A data.frame: 73 × 5

Study	Sleep	Score	Prediction	SquaredError
<int>	<dbl>	<dbl[,1]>	<int>	<dbl[,1]>
0	72	5184	4159	1050625
1	71	5042	4158	781456
2	70	4904	4156	559504
3	69	4770	4153	380689
4	68	4640	4146	244036
5	67	4514	4135	143641
6	66	4392	4117	75625
7	65	4274	4089	34225
8	64	4160	4050	12100
9	63	4050	3997	2809
10	62	3944	3931	169
11	61	3842	3853	121
12	60	3744	3765	441
13	59	3650	3672	484
14	58	3560	3577	289
15	57	3474	3483	81
16	56	3392	3393	1
17	55	3314	3309	25
18	54	3240	3230	100
19	53	3170	3159	121
20	52	3104	3095	81
21	51	3042	3038	16
22	50	2984	2986	4
23	49	2930	2940	100
24	48	2880	2899	361
25	47	2834	2862	784
26	46	2792	2829	1369
27	45	2754	2800	2116

Study	Sleep	Score	Prediction	SquaredError
<int>	<dbl>	<dbl[,1]>	<int>	<dbl[,1]>
28	44	2720	2773	2809
29	43	2690	2748	3364
⋮	⋮	⋮	⋮	⋮
43	29	2690	2535	24025
44	28	2720	2524	38416
45	27	2754	2514	57600
46	26	2792	2504	82944
47	25	2834	2494	115600
48	24	2880	2485	156025
49	23	2930	2476	206116
50	22	2984	2467	267289
51	21	3042	2458	341056
52	20	3104	2449	429025
53	19	3170	2441	531441
54	18	3240	2433	651249
55	17	3314	2425	790321
56	16	3392	2417	950625
57	15	3474	2410	1132096
58	14	3560	2403	1338649
59	13	3650	2396	1572516
60	12	3744	2389	1836025
61	11	3842	2382	2131600
62	10	3944	2375	2461761
63	9	4050	2369	2825761
64	8	4160	2363	3229209
65	7	4274	2357	3674889
66	6	4392	2351	4165681
67	5	4514	2345	4704561
68	4	4640	2339	5294601
69	3	4770	2334	5934096
70	2	4904	2328	6635776
71	1	5042	2323	7392961
72	0	5184	2318	8213956

8. Final Thoughts

Let's see how well our model predicts outside our training space.

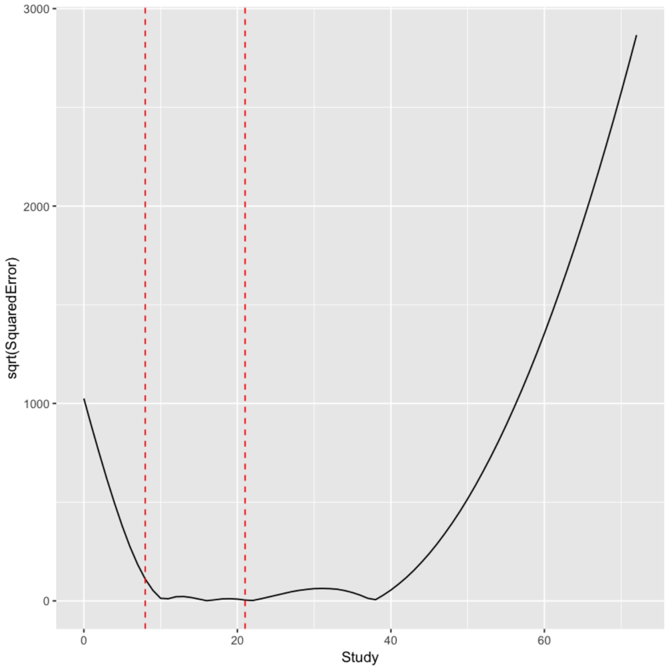
In [100]:

```
ggplot(Test, aes(x=Study, y=sqrt(SquaredError))) +
    geom_line() +
    geom_vline(xintercept=min(X$Study), linetype="dashed", color = "red") +
    geom_vline(xintercept=max(X$Study), linetype="dashed", color = "red")
cat(paste("Training Space Known by model:\n   Min Study Hours:",min(X$Study)),"\n   Max Study Hours
:",max(X$Study))
RMSEWithin <- round(sqrt(mean(Test$SquaredError[which(Test$Study >= min(X$Study) & Test$Study <=max
(X$Study))])))
RMSEBelow <- round(sqrt(mean(Test$SquaredError[which(Test$Study < min(X$Study))])))
RMSEAbove <- round(sqrt(mean(Test$SquaredError[which(Test$Study > max(X$Study))])))
cat(paste("\n\nAverage Root Mean Squared Error:\n   Below Known Range:",RMSEBelow, "\n   Within
Known Range:",RMSEWithin,"\n   Above Known Range:",RMSEAbove))
```

```
Training Space Known by model:
   Min Study Hours: 8
```

```
   Max Study Hours: 21

Average Root Mean Squared Error:
   Below Known Range: 639
   Within Known Range: 35
   Above Known Range: 1148
```



As observed by the errors from the table and the plot above, it seems that our new function had somewhat better prediction capabilities within the training space which is represented by our vertical lines. As expected, our new model is not able to predict out-of-sample data that falls outside of our training space.

In other words, our model is able to interpolate quite well the approximation of Students score by providing their time of Study and Sleep, in contrast, is not able to extrapolate very well outliers or data outside its training space.