

# ME 793 Assignment 5

19D100011

## Neural Network from Scratch

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Reference: Online blogs, [towardsdatascience.com](https://towardsdatascience.com)

Consider  $Y, X_1, X_2, X_3$

$A_1$  i.e. value to input at the first neuron on in the network is

$$f(X_1, X_2, X_3) = W_{11}X_1 + W_{12}X_2 + W_{13}X_3 + b_{11}$$

This is further activated by

$$A_1 = g(f(X_1, X_2, X_3)) = g(W_{11}X_1 + W_{12}X_2 + W_{13}X_3 + b_{11})$$

Similarly

$$A_2 = g(f(X_1, X_2, X_3)) = g(W_{21}X_1 + W_{22}X_2 + W_{23}X_3 + b_{21})$$

$$A_3 = g(f(X_1, X_2, X_3)) = g(W_{31}X_1 + W_{32}X_2 + W_{33}X_3 + b_{31})$$

$g$  is an activation function. Here are a few examples of activation functions

If there are two hidden layers, activated values on the hidden layers are given by  $A$  and  $B$ .

$$A = W_1 X + b_1$$

$$B = W_2 A + b_2$$

$Y_{\text{pred}} = W_3 B + b_3$

$W_1, W_2, W_3$  will be matrices of appropriate sizes.

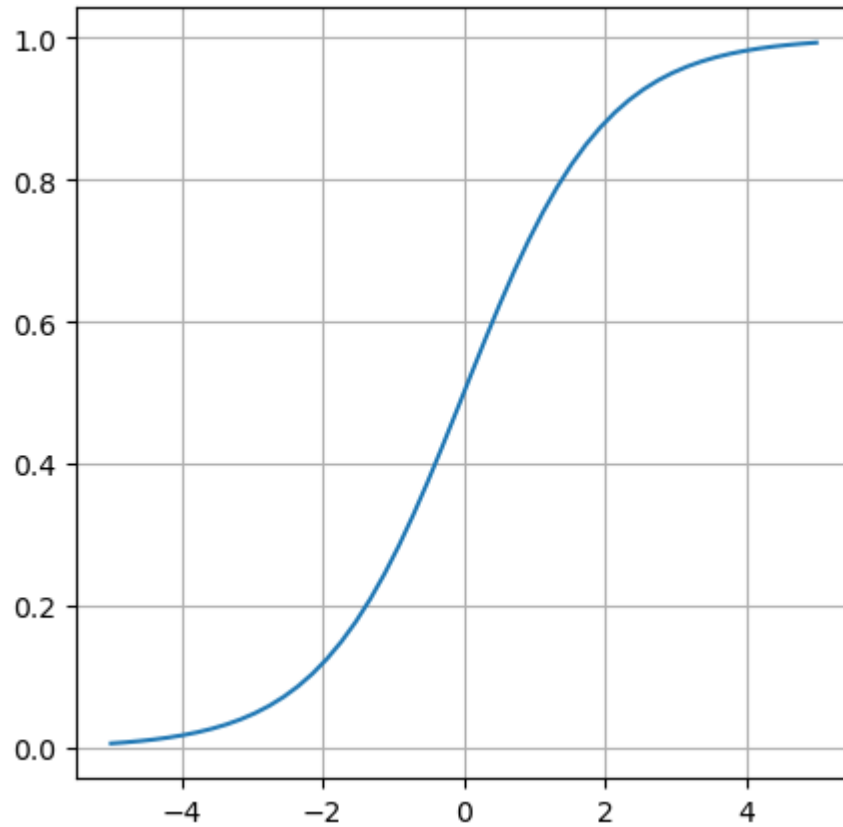
```
In [48]: import pandas as pd
import numpy as np
import matplotlib.pyplot as plt

from sklearn.model_selection import train_test_split
from sklearn.metrics import mean_squared_error
from sklearn.preprocessing import StandardScaler
```

## Sigmoid function in Python

```
In [49]: x = np.linspace(-5, 5, 50)
z = 1/(1 + np.exp(-x))

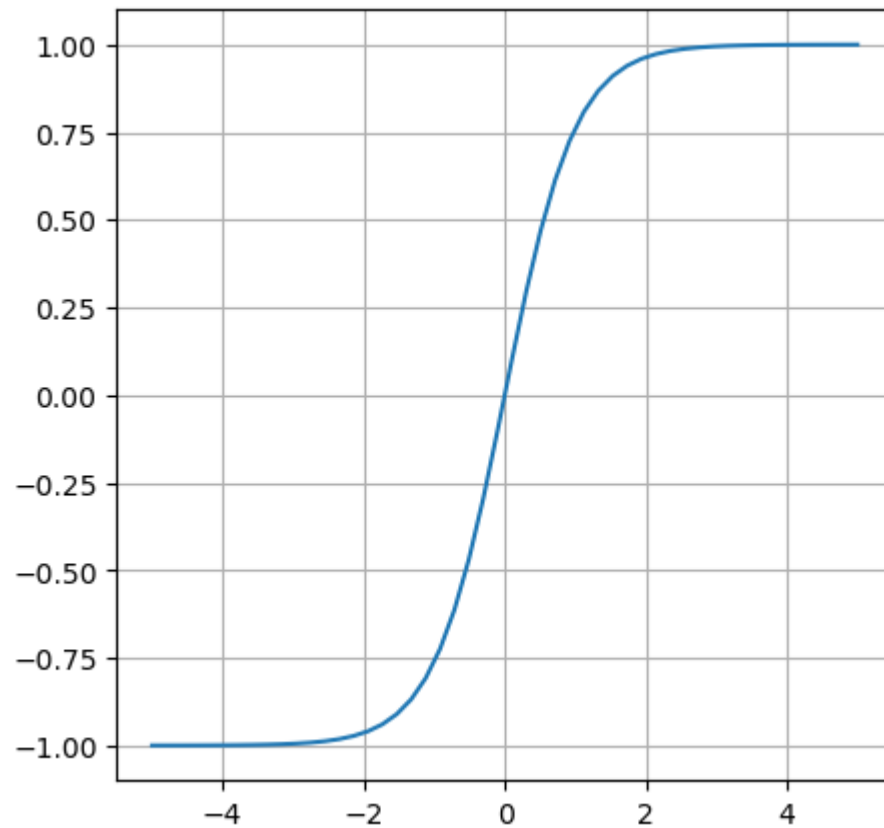
plt.subplots(figsize=(5, 5))
plt.plot(x, z)
plt.grid()
plt.show()
```



## tanh function in Python

```
In [50]: # tanh function in Python
x = np.linspace(-5, 5, 50)
z = np.tanh(x)

plt.subplots(figsize=(5, 5))
plt.plot(x, z)
plt.grid()
plt.show()
```



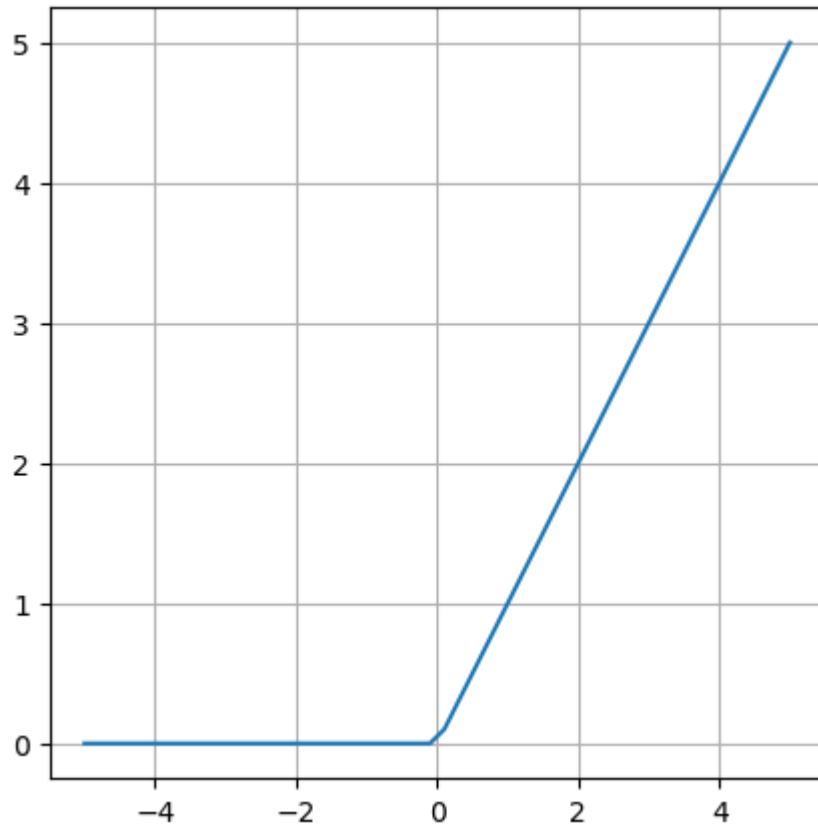
## Softmax function in Python

Softmax is a generalization sigmoid i.e. Softmax is used in multiple dimensions. And is generally used as an activation function in the output layer.

## Rectified Linear Unit (ReLU)

```
In [51]: # ReLU in Python
x = np.linspace(-5, 5, 50)
z = [max(0, i) for i in x]

plt.subplots(figsize=(5, 5))
plt.plot(x, z)
plt.grid()
plt.show()
```



## Define ReLU function

```
In [52]: def relu(z): # takes a numpy array as input and returns activated array
         a = np.maximum(0,z)
         return a
```

## Initialize parameters

```
In [53]: def initialize_params(layer_sizes): #takes a list of the layer sizes as input and returns initialized parameters
         params = {}
         for i in range(1, len(layer_sizes)):
             params['W' + str(i)] = np.random.randn(layer_sizes[i], layer_sizes[i-1])*0.01
             # rand(d0,d1) will return an array of size d0 x d1.
```

```

    params['B' + str(i)] = np.random.randn(layer_sizes[i],1)*0.01
    return params

```

Loss or cost is defined as  $J(W, B) = \frac{1}{2m} * \sum (Y_{pred} - Y_{true})^2$

W and B represent weight and bias matrices. m is the number of observation i.e. data points.

```

In [54]: def compute_cost(values, Y_train): #takes true values and dictionary having activations of
# all layers as input and returns cost
    layers = len(values)//2
    Y_pred = values['A' + str(layers)]
    cost = 1/(2*len(Y_train)) * np.sum(np.square(Y_pred - Y_train))
    return cost

```

## Define forward propagation

```

In [55]: def forward_propagation(X_train, params):
#takes input training features and parameters as input and returns a dictionary
# containinng the numpy arrays of activations of all layers
    layers = len(params)//2
    values = {}
    for i in range(1, layers+1):
        if i==1: # transformation from input layer
            values['Z' + str(i)] = np.dot(params['W' + str(i)], X_train) + params['B' + str(i)]
            values['A' + str(i)] = relu(values['Z' + str(i)])
        else: # transformation from non-input layer
            values['Z' + str(i)] = np.dot(params['W' + str(i)], values['A' + str(i-1)]) + params['B' + str(i)]
            if i==layers: # Do not use activation function in the output layer
                values['A' + str(i)] = values['Z' + str(i)]
            else: # use activation function for non-output layers
                values['A' + str(i)] = relu(values['Z' + str(i)])
    return values

```

## Define function for backward propagation

```

In [56]: def backward_propagation(params, values, X_train, Y_train):
#takes parameters, activations, training set as input and returns gradients wrt parameters
    layers = len(params)//2

```

```

m = len(Y_train)
grads = {}
for i in range(layers,0,-1):
    if i==layers:
        dA = 1/m * (values['A' + str(i)] - Y_train)
        dZ = dA
    else:
        dA = np.dot(params['W' + str(i+1)].T, dZ)
        dZ = np.multiply(dA, np.where(values['A' + str(i)]>=0, 1, 0))
    if i==1:
        grads['W' + str(i)] = 1/m * np.dot(dZ, X_train.T)
        grads['B' + str(i)] = 1/m * np.sum(dZ, axis=1, keepdims=True)
    else:
        grads['W' + str(i)] = 1/m * np.dot(dZ, values['A' + str(i-1)].T)
        grads['B' + str(i)] = 1/m * np.sum(dZ, axis=1, keepdims=True)
return grads

```

## Function for updating paramters (this is done after backpropagation)

```

In [57]: def update_params(params, grads, learning_rate):
    #takes parameters, gradients and learning rate as input and returns updated parameters
    layers = len(params)//2
    params_updated = {}
    for i in range(1,layers+1):
        params_updated['W' + str(i)] = params['W' + str(i)] - learning_rate * grads['W' + str(i)]
        params_updated['B' + str(i)] = params['B' + str(i)] - learning_rate * grads['B' + str(i)]
    return params_updated

```

## Define function for accuracy

```

In [58]: def compute_accuracy(X_train, X_test, Y_train, Y_test, params, layer_sizes): #compute accuracy on test and training data given le
    values_train = forward_propagation(X_train.T, params)
    values_test = forward_propagation(X_test.T, params)
    train_acc = np.sqrt(mean_squared_error(Y_train, values_train['A' + str(len(layer_sizes)-1)].T))
    test_acc = np.sqrt(mean_squared_error(Y_test, values_test['A' + str(len(layer_sizes)-1)].T))
    return train_acc, test_acc

```

## Define function for predicting

```
In [59]: def predict(X, params): #predict on new array X given Learnt parameters
          values = forward_propagation(X.T, params)
          predictions = values['A' + str(len(values)//2)].T
          return predictions
```

## Assemble the model i.e. create the model i.e. setup the model

```
In [60]: def model(X_train, Y_train, layer_sizes, num_iters, learning_rate): #trains the model
          params = initialize_params(layer_sizes)
          cost_values = []
          for i in range(num_iters):
              values = forward_propagation(X_train.T, params)
              cost = compute_cost(values, Y_train.T)
              cost_values.append(cost)
              print(f'cost of {i+1}th iteration: {cost}')
              grads = backward_propagation(params, values, X_train.T, Y_train.T)
              params = update_params(params, grads, learning_rate)
              #print('Cost at iteration ' + str(i+1) + ' = ' + str(cost) + '\n')
          return params, cost_values
```

## Load Data

```
In [61]: df = pd.read_csv('material_data.csv')
          df.head()
```

```
Out[61]:
```

	Elements	Atomic_Number	Electronegativity	Atomic_Radius	Thermal_Conductivity	Density	Crystal_System
0	H	1	2.20	0.25	0.1805	0.09	HEX
1	He	2	0.00	1.20	0.1513	0.18	HCP
2	Li	3	0.98	1.45	85.0000	530.00	BCC
3	Be	4	1.57	1.05	190.0000	1850.00	HCP
4	B	5	2.04	0.85	27.0000	2340.00	RHO

```
In [62]: df.columns
```



```
Out[62]: Index(['Elements', 'Atomic_Number', 'Electronegativity', 'Atomic_Radius',
        'Thermal_Conductivity', 'Density', 'Crystal_System'],
        dtype='object')
```

## Scale the numerical features

This will improve convergence of model

```
In [63]: # Scaling numerical features
cols_to_scale = ['Electronegativity', 'Atomic_Radius', 'Density']

scaler = StandardScaler()
X_scaled = pd.DataFrame(scaler.fit_transform(df[cols_to_scale]), columns=cols_to_scale)
df[cols_to_scale] = X_scaled

df.head()
```

```
Out[63]:
```

	Elements	Atomic_Number	Electronegativity	Atomic_Radius	Thermal_Conductivity	Density	Crystal_System
0	H	1	0.729657	-3.102623	0.1805	-1.289589	HEX
1	He	2	-2.346765	-0.715481	0.1513	-1.289574	HCP
2	Li	3	-0.976359	-0.087286	85.0000	-1.199138	BCC
3	Be	4	-0.151319	-1.092398	190.0000	-0.973824	HCP
4	B	5	0.505917	-1.594955	27.0000	-0.890185	RHO

```
In [64]: # Separate features (X) and target variable (y)
X, Y = df[['Electronegativity', 'Atomic_Radius', 'Density']].values, df['Thermal_Conductivity'].values

print(X.shape)
print(Y.shape)

(95, 3)
(95,)
```

## Split data into train set and test set

```
In [65]: # Split the data into training and testing sets
X_train, X_test, Y_train, Y_test = train_test_split(X, Y, test_size=0.2, random_state=42)
```

```
X_test.shape
```

```
Out[65]: (19, 3)
```

## Run the model

```
In [66]: # Iteration= 1000
# Learning Rate= 0.01
#layer_sizes = [3, 50, 100, 100, 1]

layer_sizes = [3, 50, 100, 100, 1]
num_iters = 1000
learning_rate = 0.01

m1, c = model(X_train, Y_train, layer_sizes, num_iters, learning_rate)
```

cost of 1th iteration: 4011.112090069308  
cost of 2th iteration: 4010.771384414561  
cost of 3th iteration: 4010.4306853189696  
cost of 4th iteration: 4010.09001032972  
cost of 5th iteration: 4009.7494121193295  
cost of 6th iteration: 4009.408902845375  
cost of 7th iteration: 4009.0685945271616  
cost of 8th iteration: 4008.728563597549  
cost of 9th iteration: 4008.388618639769  
cost of 10th iteration: 4008.0487591366436  
cost of 11th iteration: 4007.709028604979  
cost of 12th iteration: 4007.369413817398  
cost of 13th iteration: 4007.0298825354207  
cost of 14th iteration: 4006.6904333579705  
cost of 15th iteration: 4006.351065341124  
cost of 16th iteration: 4006.0117784465706  
cost of 17th iteration: 4005.6725719613673  
cost of 18th iteration: 4005.3334452780023  
cost of 19th iteration: 4004.9943978479496  
cost of 20th iteration: 4004.6554291287416  
cost of 21th iteration: 4004.3165384485665  
cost of 22th iteration: 4003.977725156755  
cost of 23th iteration: 4003.638988617376  
cost of 24th iteration: 4003.300328168746  
cost of 25th iteration: 4002.9617431476117  
cost of 26th iteration: 4002.6232336380863  
cost of 27th iteration: 4002.284811307589  
cost of 28th iteration: 4001.946504324572  
cost of 29th iteration: 4001.608335539054  
cost of 30th iteration: 4001.270250261352  
cost of 31th iteration: 4000.9322363860883  
cost of 32th iteration: 4000.5942919926997  
cost of 33th iteration: 4000.2564121555606  
cost of 34th iteration: 3999.9185943824664  
cost of 35th iteration: 3999.5808439657967  
cost of 36th iteration: 3999.243161163741  
cost of 37th iteration: 3998.905545816868  
cost of 38th iteration: 3998.567997255159  
cost of 39th iteration: 3998.230514804769  
cost of 40th iteration: 3997.893097781497  
cost of 41th iteration: 3997.5557497062046  
cost of 42th iteration: 3997.218504323882  
cost of 43th iteration: 3996.8813534734904  
cost of 44th iteration: 3996.544250483036

cost of 45th iteration: 3996.2071968957152  
cost of 46th iteration: 3995.870195083589  
cost of 47th iteration: 3995.5332505441397  
cost of 48th iteration: 3995.1963648218543  
cost of 49th iteration: 3994.859456699866  
cost of 50th iteration: 3994.5225576814323  
cost of 51th iteration: 3994.1857099455747  
cost of 52th iteration: 3993.8489183019897  
cost of 53th iteration: 3993.5121830227363  
cost of 54th iteration: 3993.1755036036943  
cost of 55th iteration: 3992.8388814156187  
cost of 56th iteration: 3992.5023329233095  
cost of 57th iteration: 3992.165879076186  
cost of 58th iteration: 3991.8294895795743  
cost of 59th iteration: 3991.493153711781  
cost of 60th iteration: 3991.156868832547  
cost of 61th iteration: 3990.8206341735677  
cost of 62th iteration: 3990.484448955033  
cost of 63th iteration: 3990.1483122263053  
cost of 64th iteration: 3989.812208762911  
cost of 65th iteration: 3989.4761344718786  
cost of 66th iteration: 3989.140103960691  
cost of 67th iteration: 3988.8041192602423  
cost of 68th iteration: 3988.468141683298  
cost of 69th iteration: 3988.1321744100446  
cost of 70th iteration: 3987.796249900474  
cost of 71th iteration: 3987.460367513194  
cost of 72th iteration: 3987.124526397284  
cost of 73th iteration: 3986.7887256833706  
cost of 74th iteration: 3986.452964494226  
cost of 75th iteration: 3986.117241883497  
cost of 76th iteration: 3985.781556666887  
cost of 77th iteration: 3985.445908070549  
cost of 78th iteration: 3985.1102953777504  
cost of 79th iteration: 3984.7747174153887  
cost of 80th iteration: 3984.439172935318  
cost of 81th iteration: 3984.1036612416474  
cost of 82th iteration: 3983.7681813021172  
cost of 83th iteration: 3983.432732265011  
cost of 84th iteration: 3983.09731333428  
cost of 85th iteration: 3982.7619232889615  
cost of 86th iteration: 3982.4265587156624  
cost of 87th iteration: 3982.0912140530777  
cost of 88th iteration: 3981.7558947718535

cost of 89th iteration: 3981.4206008848405  
cost of 90th iteration: 3981.085331378188  
cost of 91th iteration: 3980.7500846406083  
cost of 92th iteration: 3980.4148589031415  
cost of 93th iteration: 3980.0796490668918  
cost of 94th iteration: 3979.7444451115393  
cost of 95th iteration: 3979.4092489133745  
cost of 96th iteration: 3979.0740670902755  
cost of 97th iteration: 3978.738902105461  
cost of 98th iteration: 3978.4037530024407  
cost of 99th iteration: 3978.0686186646494  
cost of 100th iteration: 3977.7334979650054  
cost of 101th iteration: 3977.398389763366  
cost of 102th iteration: 3977.063292906571  
cost of 103th iteration: 3976.728206234211  
cost of 104th iteration: 3976.3931306240065  
cost of 105th iteration: 3976.0580696490374  
cost of 106th iteration: 3975.7230307889013  
cost of 107th iteration: 3975.38801047623  
cost of 108th iteration: 3975.0530089332765  
cost of 109th iteration: 3974.7180184993767  
cost of 110th iteration: 3974.3830303638147  
cost of 111th iteration: 3974.048042793069  
cost of 112th iteration: 3973.713054392849  
cost of 113th iteration: 3973.3780638822013  
cost of 114th iteration: 3973.0430699537665  
cost of 115th iteration: 3972.708071303599  
cost of 116th iteration: 3972.37306661517  
cost of 117th iteration: 3972.038054291577  
cost of 118th iteration: 3971.703032781918  
cost of 119th iteration: 3971.3679975108753  
cost of 120th iteration: 3971.0329441913404  
cost of 121th iteration: 3970.6978712536884  
cost of 122th iteration: 3970.362783777479  
cost of 123th iteration: 3970.02768284794  
cost of 124th iteration: 3969.6925725543088  
cost of 125th iteration: 3969.3574502070846  
cost of 126th iteration: 3969.0223092392353  
cost of 127th iteration: 3968.6871468035056  
cost of 128th iteration: 3968.3519612410605  
cost of 129th iteration: 3968.016751027738  
cost of 130th iteration: 3967.681514612994  
cost of 131th iteration: 3967.3462504327954  
cost of 132th iteration: 3967.0109569070282

cost of 133th iteration: 3966.6756324324315  
cost of 134th iteration: 3966.340275390308  
cost of 135th iteration: 3966.0048841429766  
cost of 136th iteration: 3965.669457033988  
cost of 137th iteration: 3965.3339923969324  
cost of 138th iteration: 3964.9984728825125  
cost of 139th iteration: 3964.66286148631  
cost of 140th iteration: 3964.3272069658174  
cost of 141th iteration: 3963.9915080988308  
cost of 142th iteration: 3963.6557631213186  
cost of 143th iteration: 3963.3199704242134  
cost of 144th iteration: 3962.9841291512275  
cost of 145th iteration: 3962.6482374406714  
cost of 146th iteration: 3962.3122935202996  
cost of 147th iteration: 3961.9762963182775  
cost of 148th iteration: 3961.6402435219884  
cost of 149th iteration: 3961.304133491066  
cost of 150th iteration: 3960.9679647546195  
cost of 151th iteration: 3960.631733543297  
cost of 152th iteration: 3960.2954370268217  
cost of 153th iteration: 3959.959071862888  
cost of 154th iteration: 3959.622636344837  
cost of 155th iteration: 3959.2861264517574  
cost of 156th iteration: 3958.949539137062  
cost of 157th iteration: 3958.612873605004  
cost of 158th iteration: 3958.2761297844086  
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cost of 160th iteration: 3957.6024000883863  
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cost of 163th iteration: 3956.5911669156467  
cost of 164th iteration: 3956.253909783459  
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cost of 166th iteration: 3955.579112483462  
cost of 167th iteration: 3955.2415675431134  
cost of 168th iteration: 3954.9039218622765  
cost of 169th iteration: 3954.566176074234  
cost of 170th iteration: 3954.228346132161  
cost of 171th iteration: 3953.8904138454463  
cost of 172th iteration: 3953.552371105385  
cost of 173th iteration: 3953.214215045146  
cost of 174th iteration: 3952.8759430667146  
cost of 175th iteration: 3952.5375525412137  
cost of 176th iteration: 3952.1990408141037

cost of 177th iteration: 3951.860405191642  
cost of 178th iteration: 3951.5216429465627  
cost of 179th iteration: 3951.1827513181197  
cost of 180th iteration: 3950.8437275398087  
cost of 181th iteration: 3950.5045687802535  
cost of 182th iteration: 3950.1652721713463  
cost of 183th iteration: 3949.8258348433283  
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cost of 185th iteration: 3949.1465262617858  
cost of 186th iteration: 3948.8066490663446  
cost of 187th iteration: 3948.466619191958  
cost of 188th iteration: 3948.1264335843134  
cost of 189th iteration: 3947.7860892131343  
cost of 190th iteration: 3947.4455828378486  
cost of 191th iteration: 3947.1049112938917  
cost of 192th iteration: 3946.764071333244  
cost of 193th iteration: 3946.42305968763  
cost of 194th iteration: 3946.0818730521887  
cost of 195th iteration: 3945.740508082839  
cost of 196th iteration: 3945.3989614308043  
cost of 197th iteration: 3945.057229652096  
cost of 198th iteration: 3944.715309260343  
cost of 199th iteration: 3944.3731966308114  
cost of 200th iteration: 3944.030888251391  
cost of 201th iteration: 3943.6883805908396  
cost of 202th iteration: 3943.3456699935823  
cost of 203th iteration: 3943.002752680483  
cost of 204th iteration: 3942.6596248350174  
cost of 205th iteration: 3942.3162829140483  
cost of 206th iteration: 3941.972723108505  
cost of 207th iteration: 3941.6289415837787  
cost of 208th iteration: 3941.2849344515316  
cost of 209th iteration: 3940.940697704955  
cost of 210th iteration: 3940.596227329509  
cost of 211th iteration: 3940.2515193609893  
cost of 212th iteration: 3939.9065696489843  
cost of 213th iteration: 3939.5613739376636  
cost of 214th iteration: 3939.215928018351  
cost of 215th iteration: 3938.8702275682663  
cost of 216th iteration: 3938.524268314049  
cost of 217th iteration: 3938.1780458646626  
cost of 218th iteration: 3937.831555886629  
cost of 219th iteration: 3937.4847941334942  
cost of 220th iteration: 3937.137755970585

cost of 221th iteration: 3936.790436544485  
cost of 222th iteration: 3936.442830755425  
cost of 223th iteration: 3936.0949345544846  
cost of 224th iteration: 3935.746743131025  
cost of 225th iteration: 3935.398251819062  
cost of 226th iteration: 3935.049456312206  
cost of 227th iteration: 3934.7003512383126  
cost of 228th iteration: 3934.3509317006956  
cost of 229th iteration: 3934.001192726616  
cost of 230th iteration: 3933.6511295481228  
cost of 231th iteration: 3933.3007366840266  
cost of 232th iteration: 3932.9500091022483  
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cost of 237th iteration: 3931.1911533720304  
cost of 238th iteration: 3930.838299780455  
cost of 239th iteration: 3930.4850720218765  
cost of 240th iteration: 3930.13146464284  
cost of 241th iteration: 3929.777472022893  
cost of 242th iteration: 3929.4230880770174  
cost of 243th iteration: 3929.0683069011566  
cost of 244th iteration: 3928.713122284461  
cost of 245th iteration: 3928.357528103018  
cost of 246th iteration: 3928.00151823166  
cost of 247th iteration: 3927.6450863283962  
cost of 248th iteration: 3927.288226281227  
cost of 249th iteration: 3926.9309315319333  
cost of 250th iteration: 3926.5731952772644  
cost of 251th iteration: 3926.2150110981897  
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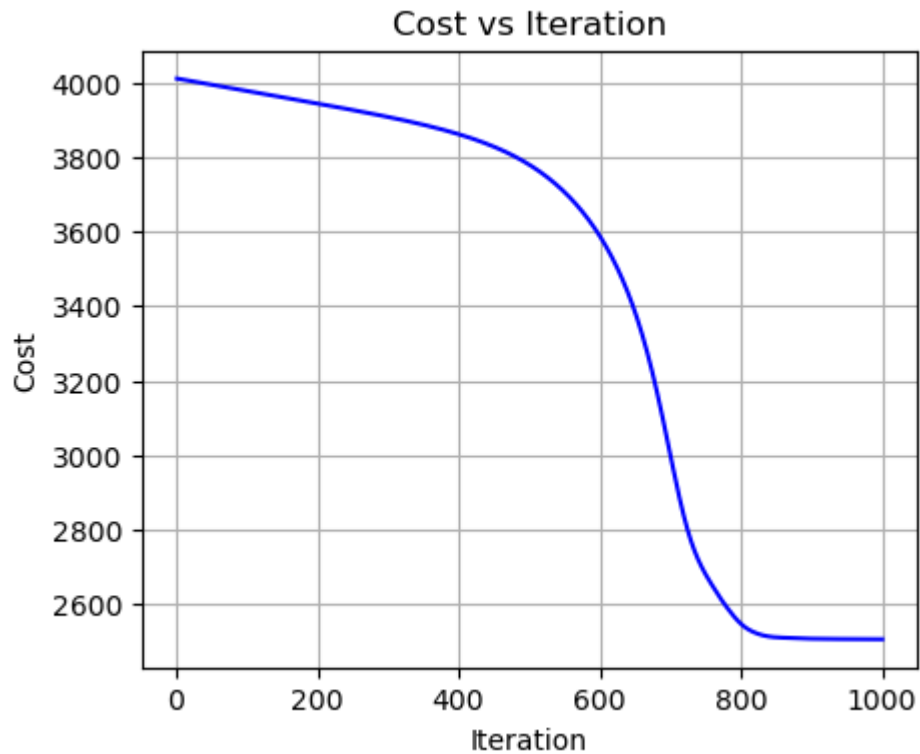
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cost of 999th iteration: 2504.902979031398
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```

```
In [67]: plt.figure(figsize=(5, 4))
plt.plot(np.arange(1, num_iters+1), c, color='blue')
plt.title('Cost vs Iteration')
plt.xlabel('Iteration')
plt.ylabel('Cost')
plt.grid(True)
plt.show()
```



## Calculate train and test accuracy

```
In [68]: train_acc, test_acc = compute_accuracy(X_train, X_test, Y_train, Y_test, m1, layer_sizes)
print(f"Train Accuracy: {train_acc:.4f}, Test Accuracy: {test_acc:.4f}")
```

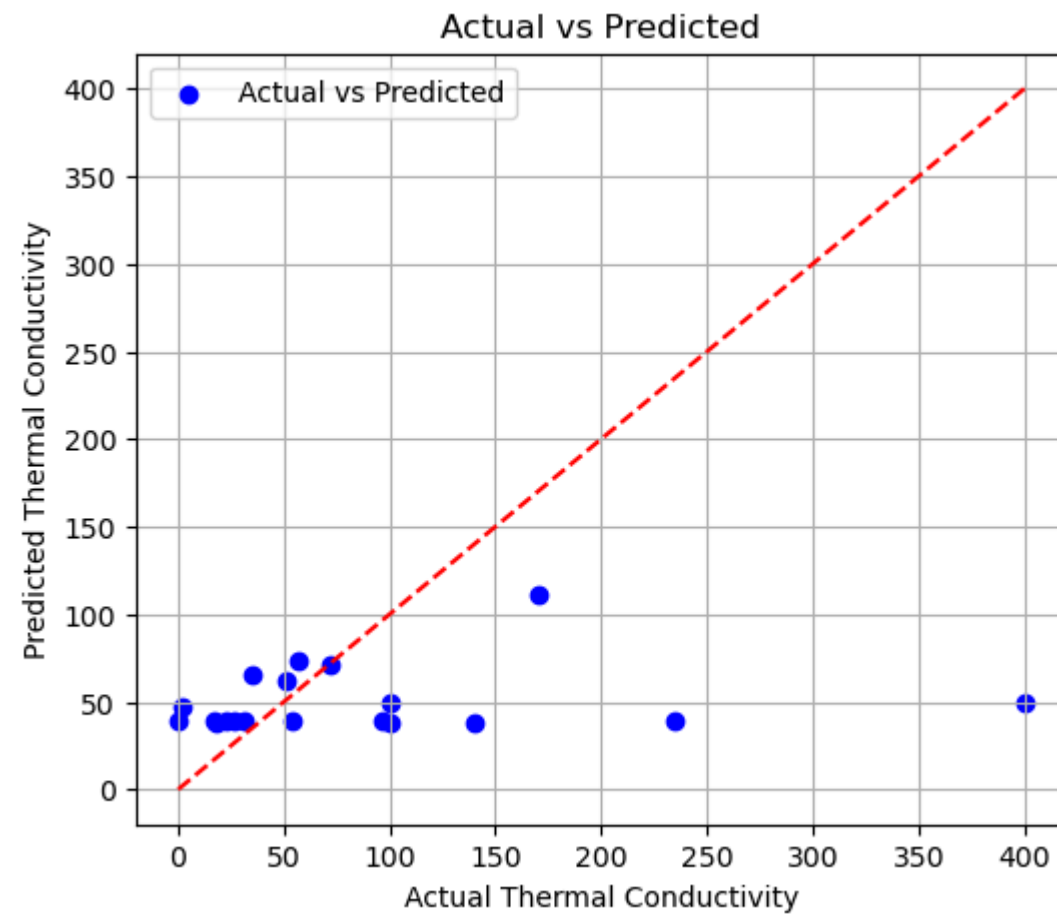
Train Accuracy: 70.7797, Test Accuracy: 100.2068

## Prediction of Thermal Conductivity

```
In [69]: Y_pred = predict(X_test, m1)

# Plot th predicted thermal conductivity
plt.figure(figsize=(6, 5))
plt.scatter(Y_test, Y_pred, color='blue', label='Actual vs Predicted')
plt.plot([min(Y_test), max(Y_test)], [min(Y_test), max(Y_test)], color='red', linestyle='--')
plt.title('Actual vs Predicted')
plt.xlabel('Actual Thermal Conductivity')
```

```
plt.ylabel('Predicted Thermal Conductivity')  
plt.legend()  
plt.grid(True)  
plt.show()
```



In [ ]: