

Implementation of ANN

The ANN is designed with a flexible number of inputs and hidden nodes in mind but assumes there is only one output node.

It is developed using Spyder IDE (Python), which includes additional libraries that are installed by default. The only additional library used is pandas, which allows it to read excel spreadsheets

The code was developed with guidance from <https://machinelearningmastery.com/implement-backpropagation-algorithm-scratch-python/>

The code is also provided in a separate text file.

The program generates a network as a twice nested list of weights. For example:

[[[weights:x,y,z],[weights:x,y,z],[weights:x,y,z]]. Where the first nested list is the hidden layer and the second is the output layer.

The data is also read as a nested list.

When the algorithm calculates the outputs it initially uses the data entry as an input. It then iterates through each node in a layer and appends the output (activation function) to the node. It then moves to the next layer, using the outputs of the previous nodes as inputs.

[[[weights:x,y,z output: a],[weights:x,y,z output: a]],[weights:x,y,z output:a]].

The algorithm then works backwards through the network, calculating the value of delta for a node and appending it to the list.

[[[weights:x,y,z output: a delta :b],[weights:x,y,z output: a delta: b]],[weights:x,y,z output:a delta: b]]

The weights are then updated for each node in the network and the algorithm iterates through the next data entry. After each data entry the error squared of that iteration is calculated and added to a total. At the end of each epoch the Root Mean Squared Error is calculated to use as a performance indicator.

The ANN is designed so that it can train, validate and test the ANN.

It can also train the network using momentum , bold driver and simulated annealing, although I think there is an error in the bold driver code.

There are two sections highlighted by a string of #:

The backpropagation algorithm, split into forward pass, backwards pass and updating the weight

The improvements to the algorithm

Code

```
1. """
2.
3. @author: Alex Vong B827861
4.
5. Developed using spyder IDE
6. some guidance from https://machinelearningmastery.com/implement-backpropagation-algorithm-scratch-
  python/
7. """
8.
9.
10. '''imports'''
11. import math
12. import random
```

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13. #reads from excel
14. import pandas as pd
15.
16. '''initialise the network'''
17. def initialise(inputn,hidden,outputn): #takes number of inputs, hidden nodes (assuming 1 hidden 1
    ayer) and outputs as parameters
18.     network = list() #nested list of weights/biases for each node in the network
19.     #generate weights and bias for each node in the hidden layer
20.     hiddenlayer = [{"weights":[random.random() for i in range(inputn+1)]}for j in range(hidden)]
    #{"n": splits the list into sections
21.     network.append(hiddenlayer)
22.     #generate weights and bias for output layer
23.     outputlayer = [{"weights":[random.random() for i in range(hidden+1)]}]
24.     network.append(outputlayer)
25.     return network
26.     #print(network)
27.
28. '''calculates weighted sum'''
29. def weightedsum(weights, inputs):
30.     wsum = weights[-1] #assume bias to be last value in list
31.     for i in range(len(weights)-1): #for each weight (-1 to exclude bias)
32.         wsum += weights[i] * inputs[i] #sum of weight x input
33.     return wsum
34.
35. '''activation/transfer function'''
36. def activationf(wsum):
37.     activation = 1 / (1 + math.exp(-wsum))
38.     return activation
39.
40.
41. '''derivative of the transfer function'''
42. def transferderiv(output):
43.     return output * (1.0 - output)
44.
45. '''
46. Backpropagation algorithm
47. #####
    #####
48. '''
49.
50. '''does the forward propagation'''
51. def forwardprop(network, inputv): #takes the network and input values as parameters
52.     inputs = inputv
53.     for layer in network: #for each layer in the network
54.         newinputs = [] #inputs for next layer
55.         for node in layer: #for each node in the layer
56.             s = weightedsum(node["weights"],inputs) #find weighted sum at node
57.             node["output"] = activationf(s) #return transfer function of node
58.             newinputs.append(node["output"])
59.         inputs = newinputs
60.     return inputs #returns the outputs for each node
61.
62.
63. '''does the backpropagation'''
64. def backprop(network,expected):
65.     for i in reversed(range(len(network))): #work backwards through the network
66.         layer = network[i] #current layer
67.         #if not at output layer (at hidden layer)
68.         if i != len(network)-1:
69.             for j in range(len(layer)):
70.                 nodeh = layer[j] #get node at layer
71.                 #get weight and delta of output layer
72.                 for node in network[i+1]: #for loop seems to be the only way to get the values
73.                     outweight = node['weights'][j]
74.                     outdelta = node["delta"]
75.                     #calculate delta at node (weight of node to output x delta at output x (output * (
    1 - output)))
76.                     nodeh["delta"] = (outweight* outdelta * transferderiv(node["output"]))
77.
78.             #at output layer
79.             else:
80.                 #find delta of output node
81.                 node = layer[0] #only 1 output node so will be the first node in the layer

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82.         #get error (expected output - actual output)
83.         errorout = expected - node["output"]
84.         outdelta = errorout * transferderiv(node["output"]) #get delta
85.         node["delta"] = outdelta #set delta for node
86.
87.
88.     '''update weight of nodes'''
89.     def updateweights(network, data, lr):
90.         for i in range (len(network)): #for each layer in the network
91.             inputs = data[:-1] #all data except for the last
92.             if i !=0: #if the output layer
93.                 inputs = [node["output"]for node in network[i - 1]] #inputs are the outputs of previous
layer
94.
95.                 for node in network[i]: #for each node in the layer
96.                     for j in range(len(inputs)): #for each weight
97.                         node['weights'][j] += lr * node['delta'] * inputs[j] #add learning rate x delta x
output
98.                         node['weights'][-1] += lr * node['delta'] #for bias output is always 1
99.
100.
101.
102.
103.
104.         '''
105.         #####
106.         '''
107.
108.
109.     '''train the network'''
110.     def trainnetwork(network, data, lr, epochs, outputs,):
111.         for epoch in range(epochs): #iterate through epochs
112.             sumerror = 0
113.             for row in data: #for each data entry
114.                 outputs = forwardprop(network,row) #forward pass
115.                 expected = row[-1]
116.                 sumerror += (expected-outputs[0])**2 #sum of the errors squared
117.                 backprop(network,expected) #backwards pass
118.                 updateweights(network,row,lr) #update the weights
119.                 rmse = math.sqrt(sumerror/len(data)) #calculate root mean squared error for epo
ch
120.                 #print('>epoch=%d, lrate=%.3f, RMSE=%.3f' % (epoch+1, lr, rmse)) #print the epo
ch number, learning rate and RMSE for that epoch
121.                 print("RMSE=%.3f" % (rmse))
122.
123.
124.
125.         '''
126.         Improvements
127.         #####
128.         '''
129.
130.
131.     '''updates weights with momentum added'''
132.     def updatewithmomentum(network, data, lr, mfunction):
133.         for i in range (len(network)): #for each layer in the network
134.             inputs = data[:-1] #all data except for the last
135.             if i !=0: #if the output layer
136.                 inputs = [node["output"]for node in network[i - 1]] #inputs are the outputs of
previous layer
137.
138.                 for node in network[i]: #for each node in the layer
139.                     for j in range(len(inputs)): #for each weight
140.                         wchange =lr * node['delta'] * inputs[j] #calculate change in weight
141.                         node['weights'][j] += wchange + (mfunction * wchange) #add weight + moment
um
142.                         wchange = lr * node['delta'] #for bias output is always 1
143.                         node['weights'][-1] += wchange + (mfunction * wchange)
144.
145.
146.     '''train the network with momentum'''

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147.     def trainwithmomentum(network, data, lr, epochs, outputs,):
148.         for epoch in range(epochs): #iterate through epochs
149.             sumerror = 0
150.             for row in data: #for each data entry
151.                 outputs = forwardprop(network,row) #forward pass
152.                 expected = row[-1]
153.                 sumerror += (expected-outputs[0])**2
154.                 backprop(network,expected) #backwards pass
155.                 updatewithmomentum(network,row,lr,0.9) #update the weights
156.                 rmse = math.sqrt(sumerror/len(data)) #calculate root mean squared error for epo
ch
157.                 #print('>epoch=%d, lrate=%.3f, RMSE=%.3f' % (epoch+1, lr, rmse)) #print the epo
ch number, learning rate and RMSE for that epoch
158.                 print("RMSE=%.3f" % (rmse))
159.
160.         '''train the network with bold driver'''
161.         def trainwithbdriver(network, data, lr, epochs, outputs,):
162.             rmse = 0
163.             learning_rate = lr
164.             for epoch in range(epochs): #iterate through epochs
165.                 errorincrease = True
166.                 preverror = rmse
167.                 networkcopy = network #make a backup of the network
168.                 if (epoch+1) % 1000 == 0: #every 1000 epochs try bold driver
169.                     print("implementing bold driver")
170.                     while errorincrease == True:
171.                         sumerror = 0
172.                         for row in data: #for each data entry
173.                             outputs = forwardprop(network,row) #forward pass
174.                             expected = row[-1]
175.                             sumerror += (expected-outputs[0])**2
176.                             backprop(network,expected) #backwards pass
177.                             updateweights(network,row,learning_rate) #update the weights
178.                             rmse = math.sqrt(sumerror/len(data)) #calculate root mean squared error for
epoch
179.                             if rmse - preverror > 0: #if the error function increased and it isnt the f
irst epoch
180.                                 print("error increased")
181.                                 network = networkcopy #restore network to previous iteration
182.                                 if learning_rate * 0.5 >= 0.01: #keep within the boundary
183.                                     print("learning rate decreased")
184.                                     learning_rate = learning_rate * 0.5 #half the learning rate
185.                                 else:
186.                                     print("learning rate unchanged")
187.                                     errorincrease = False
188.                             else:
189.                                 print("error decreased")
190.                                 if learning_rate * 1.1 <= 0.5 :
191.                                     print("learning rate increased")
192.                                     learning_rate = learning_rate * 1.1
193.                                     errorincrease = False
194.
195.                                 print("learning rate: "+str(learning_rate))
196.                             else:
197.                                 sumerror = 0
198.                                 for row in data: #for each data entry
199.                                     outputs = forwardprop(network,row) #forward pass
200.                                     expected = row[2]
201.                                     sumerror += (expected-outputs[0])**2
202.                                     backprop(network,expected) #backwards pass
203.                                     updateweights(network,row,learning_rate) #update the weights
204.                                     rmse = math.sqrt(sumerror/len(data)) #calculate root mean squared error for epo
ch
205.                                     #print('>epoch=%d, lrate=%.3f, RMSE=%.3f' % (epoch+1, lr, rmse)) #print the epoch n
umber, learning rate and RMSE for that epoch
206.                                     print("RMSE=%.3f" % (rmse))
207.
208.         '''calculate learning rate through annealing'''
209.         def calculatelr(epochn,maxepoch, startlr, endlr):
210.             lr = endlr + ((startlr - endlr)*(1 - (1/ (1+ math.exp(10 - ((20 * epochn)/maxepoch))))))
211.         return lr
212.

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213.         '''train the network with annealing'''
214.     def trainwithanneal(network, data, lr, epochs, outputs):
215.         for epoch in range(epochs): #iterate through epochs
216.             learning_rate = calculatelr(epoch, epochs, 0.1, 0.01) #calculate leraning rate for
this epoch
217.             sumerror = 0
218.             for row in data: #for each data entry
219.                 outputs = forwardprop(network,row) #forward pass
220.                 expected = row[-1]
221.                 sumerror += (expected-outputs[0])**2 #sum of the errors squared
222.                 backprop(network,expected) #backwards pass
223.                 updateweights(network,row,learning_rate) #update the weights
224.                 rmse = math.sqrt(sumerror/len(data)) #calculate root mean squared error for epoch
225.                 #print('>epoch=%d, lrate=%.3f, RMSE=%.3f' % (epoch+1, lr, rmse)) #print the epoch n
umber, learning rate and RMSE for that epoch
226.                 print("RMSE=%.3f" % (rmse))
227.
228.
229.         '''
230.         #####
231.         '''
232.
233.         '''validate the network'''
234.     def validatenetwork(network, data, lr, epochs, outputs):
235.         preverror = 0
236.         rmse = 10 # set the initial rmse to a high value so that it doesnt stop early
237.         stop = False
238.         for epoch in range(epochs): #iterate through epochs
239.             sumerror = 0
240.             preverror = rmse #get error of previous epoch
241.             if stop == False: #as long as error isnt increasing
242.                 for row in data: #for each data entry
243.                     outputs = forwardprop(network,row) #forward pass
244.                     expected = row[-1]
245.                     sumerror += (expected-outputs[0])**2
246.                     backprop(network,expected) #backwards pass
247.                     updateweights(network,row,lr) #update the weights
248.                     rmse = math.sqrt(sumerror/len(data)) #calculate root mean squared error for epo
ch
249.                     #print('>epoch=%d, lrate=%.3f, RMSE=%.3f' % (epoch+1, lr, rmse)) #print the epo
ch number, learning rate and RMSE for that epoch
250.                     if preverror - rmse < 0: #if error increases
251.                         print("STOPPED EARLY") #notify if stopped early
252.                         stop = True
253.                         break
254.                     else:
255.                         break
256.                 print("RMSE=%.3f" % (rmse))
257.                 return epoch
258.
259.         '''calculate outputs using the network and find average error'''
260.         '''doesn't backpropagate'''
261.     def testnetwork(network, data):
262.         sumerror = 0
263.         for row in data: #for each data entry
264.             outputs = forwardprop(network,row) #forward pass
265.             expected = row[-1]
266.             sumerror += (expected-outputs[0])**2 #sum of the errors squared
267.             rmse = math.sqrt(sumerror/len(data)) #calculate root mean squared error for epoch
268.             print('RMSE=%.3f' % (rmse)) #print the epoch number, learning rate and RMSE for that ep
och
269.
270.
271.
272.         '''create training dataset from excel'''
273.     def createtrainingdata():
274.         #read excel spreadsheet
275.         print("function started")
276.         df = pd.read_excel('TestData.xlsx',sheet_name="Training")
277.         print("Spreadsheet opened")
278.         #get inputs and output from fields in spreadsheet
279.         input1 = df['ST'].tolist() #input 1

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280.         input2 = df['sW'].tolist() #input 2
281.         input3 = df['sSr'].tolist() #input 3
282.         input4 = df['sDSP'].tolist() #input 4
283.         input5 = df['sDRH'].tolist() #input 5
284.         output = df['sPanE'].tolist() #predictand
285.         print("Pulled data")
286.         dataset = [[input1[i],input2[i],input3[i],input4[i],input5[i],output[i]] for i in range
(len(input1))] #form data entries as nested list
287.         print("data formed into list")
288.         return dataset
289.
290.     '''create validation dataset from excel'''
291.     def createvalidationdata():
292.         #read excel spreadsheet
293.         print("function started")
294.         df = pd.read_excel('TestData.xlsx',sheet_name="Validation")
295.         print("Spreadsheet opened")
296.         #get inputs and output from fields in spreadsheet
297.         input1 = df['sT'].tolist() #input 1
298.         input2 = df['sW'].tolist() #input 2
299.         input3 = df['sSr'].tolist() #input 3
300.         input4 = df['sDSP'].tolist() #input 4
301.         input5 = df['sDRH'].tolist() #input 5
302.         output = df['sPanE'].tolist() #predictand
303.         print("Pulled data")
304.         dataset = [[input1[i],input2[i],input3[i],input4[i],input5[i],output[i]] for i in range
(len(input1))] #form data entries as nested list
305.         print("data formed into list")
306.         return dataset
307.
308.
309.     '''create test dataset from excel'''
310.     def createtestdata():
311.         #read excel spreadsheet
312.         print("function started")
313.         df = pd.read_excel('TestData.xlsx',sheet_name="Testing")
314.         print("Spreadsheet opened")
315.         #get inputs and output from fields in spreadsheet
316.         input1 = df['sT'].tolist() #input 1
317.         input2 = df['sW'].tolist() #input 2
318.         input3 = df['sSr'].tolist() #input 3
319.         input4 = df['sDSP'].tolist() #input 4
320.         input5 = df['sDRH'].tolist() #input 5
321.         output = df['sPanE'].tolist() #predictand
322.         print("Pulled data")
323.         dataset = [[input1[i],input2[i],input3[i],input4[i],input5[i],output[i]] for i in range
(len(input1))] #form data entries as nested list
324.         print("data formed into list")
325.         return dataset
326.
327.     '''test code'''
328.     def test():
329.         print("PROGRAM START")
330.         trainingdata = createtrainingdata()
331.         validationdata = createvalidationdata()
332.         testdata = createtestdata()
333.         #sample data for quick testing
334.         sampledata = [[0.32,0.36,0.19,0.68,0.71,0.14],[0.38,0.64,0.22,0.35,0.69,0.18],[0.36,0.5
1,0.19,0.51,0.72,0.17]]
335.         sampledata2 = [[0.3,0.7,0],[0.7,0.3,0],[0.7,0.2,1.0],[0.8,0.3,1.0],[0.6,0.3,1.0],[0.7,0
.4,1.0],[0.3,0.6,1.0]]
336.         #initialise network
337.         print("DATA PROCESSED")
338.         #set number of inputs and hidden nodes here
339.         network = initialise(5, 2, 1)
340.         print("NETWORK INITIALISED")
341.         #train network
342.         trainwithanneal(network, trainingdata, 0.1, 1000, 1)
343.         print("NETWORK TRAINED")
344.         #validate network
345.         validatenetwork(network, validationdata, 0.1, 1000, 1)
346.         print("NETWORK VALIDATED")
347.         #test the network

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348.         testnetwork(network, testdata)
349.         print("NETWORK TESTED")
350.         #end of program
351.         print("PROGRAM COMPLETE")
352.
353.     test()

```

Data Pre-Processing

To remove extreme values the interquartile range of each predictor was calculated and upper and lower bounds set using:

Lower bound = 1st quartile – 1.5 * interquartile range

Upper bound = 3rd quartile + 1.5* interquartile range

The data was then filtered and any entries that exceeded the limits were removed

For some predictors a value below 0 would also be invalid (such as humidity in %) so entries where those predictors were below 0 were also removed.

The data was then standardised into values between 0.1 and 0.9

To split the data into subsets a random value between 0 and 1 was generated for each entry and the data split where the values ranged from 0 – 0.6, 0.61 – 0.8, 0.81 – 1. This meant that the data should be split into 60%, 20% and 20% of the total data.

The data set used in this ANN is also available in a separate file.

Training the ANN

The performance of the ANN is measured using the Root Mean Squared Error (RMSE) returned after the network has performed a given number of epochs. A lower RMSE would suggest that the ANN is more accurate.

Using the basic backpropagation algorithm, the number of epochs was first decided.

Using the training and validation data, 2 hidden nodes and a learning rate of 0.1:

Hidden Nodes = 2	Learning Rate = 0.1	
Epochs	Training RMSE	Validation RMSE
1000	0.02	0.019
2000	0.013	0.012
3000	0.013	0.013
5000	0.014	0.013
10000	Returned math range error	

There is a substantial improvement between 1000 and 2000 epochs but afterwards the change in error becomes quite small and increases at 5000, which shows that the ANN may be over trained at that point.

At 10000 epochs the algorithm stops working, not sure whether there is a coding error or if the numbers are too extreme at that point.

I will go with 2000 epochs from this point as it seems to be the point where the performance starts to stabilise.

Now the number of hidden nodes will be decided. As there are 5 inputs 2-10 hidden nodes should be tested.

Using the same data and learning rate and 2000 epochs:

Epochs = 2000	Learning rate = 0.1	
Hidden Nodes	Training RMSE	Validation RMSE
2	0.013	0.012
4	0.014	0.013

5	0.013	0.013
6	0.018	0.016
8	0.014	0.013
10	0.012	0.012

From the results it appears that the ANN performs best with 10 hidden nodes, but the error does increase around 6-8 nodes. I will go with 5 hidden nodes as it seems to be a stable number to go with.

These are the weights on each node of a network with 5 hidden nodes after 2000 epochs:

RMSE: 0.014

Hidden nodes:

[weight, weight, weight, weight, weight, bias]

[0.33377520635076835, -0.3204135151685644, 0.11547621750966765, 0.7844796875635062, 0.21683714969746468, 0.2579279923298947]

[-1.4820388140101834, -0.09758342367361017, -1.5811144016053778, 1.6344336460103595, 3.524542352716634, 6.914915089333097]

[0.5811922788585482, -0.1789040505145315, 0.2368482662292241, -0.021010791527175002, -0.13555971985423085, -0.8750008127892623]

[1.533083810726213, 1.079226842042484, 1.197231280924445, -0.46145901416188456, -1.3293110088183417, -2.457424844909402]

[0.17801120537111279, 0.25649785177962997, 0.22926397493096665, 0.7260662866789053, 0.23399925842776875, -1.5284544558286868]

Output node:

[0.5595430909635305, -5.126740337702883, 3.984951225966446, 6.150019474751223, 2.347237087712582, 0.530169532365318]

Evaluation of final model

A new network will be initialised and its performance tested on the test data. It will also be trained using the improvements on the backpropagation algorithm and their performance compared as well.

Epochs = 2000	Learning Rate = 0.1	Hidden Nodes = 5	
Algorithm	Training RMSE	Validation RMSE	Test RMSE
Basic Backpropagation	0.014	0.013	0.016
With momentum	0.014	0.014	0.016
With bold driver	0.09	0.014	0.016
With annealing	0.013	0.013	0.014

The error for bold driver is a lot higher than expected, which I think may be due to an error in the code, so the results won't be look at.

The errors from the training set and the validation set are almost the same with each test, which shows that the ANN is performing as it should.

The basic backpropagation algorithm and the algorithm with momentum added seem to have a similar performance, although the difference in error may be very small given the size of the numbers, which cannot be seen due to the rounding of the numbers.

Adding annealing into the algorithm improved performance to a measurable extent, which may be due to the learning rate decreasing every epoch, which reduces the likelihood of overtraining the ANN.

Comparison with another data model

Using LINEST in excel I generated weights for each predictor and the bias of the equation. I then formed it into a single layer network and found the RMSE of the data model.

Weights: T, W, Sr, DSP, DRH, bias

0.53864, 0.247723, 0.393995, 0.033318, -0.15136, -0.16677

When comparing it with a newly generated ANN:

Model	Test RMSE
ANN	0.015
LINEST	0.256

From the results the ANN is far more accurate than the LINEST model.