Weight evolution and mass shuffling in a shallow NN

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1 Introduction

This is a little notebook that has a single initial intention: that of showing the process of optimization in a Neural Network (NN) from the perspective of mass shuffling. In the future I will investigate other scenarios too.

First we import some libraries

```
[1]: import numpy as np
import tensorflow as tf
#from tensorflow.python.framework import ops
%matplotlib inline
import matplotlib.pyplot as plt
import matplotlib.animation as animation
from mpl_toolkits import mplot3d
import seaborn as sns
sns.set(style="darkgrid")
```

1.1 Creating some data

The problem lies in the category of supervised learning: we have a sample of elements of type (X_i, Y_i) , for $1 \le i \le N$, all independent and identically distributed, and we would like to train a predictor.

Let's start by generating a sample X_i , which will be normally distributed.

$$[2]: N = 1000$$

X = 10*np.random.randn(2,N)

With regards to the label Y, we are going to use the following classifier:

Y=1 whenever $x_1 \ge 0$, Y=0 otherwise.

[3]: Y = np.array((X[0,:]>=0),np.int32)

Let's count how many of each we have:

[4]: print(np.sum(Y), Y.shape)

467 (1000,)

which is more or less half of the sample.

```
[5]: colors =['red','blue']
vec_color = [colors[i] for i in Y[:]]
plt.figure(figsize=(10,8))
plt.scatter(X[0,:100],X[1,:100],color=vec_color[:100])
```

[5]: <matplotlib.collections.PathCollection at 0x133236048>



1.2 Augmenting the dimension

I would like to make the dimension of this problem a bit higher. The ith element in our sample has coordinates X[i,:], and so far it is in \mathbb{R}^2 ; we shall consider this as a set of points lying on an embedded, 2 dimensional, manifold in a higher dimensional space.

[6]: additional_dimension = 13
Additional_dimension_coordinates = np.zeros([additional_dimension,N])

[7]: X = np.concatenate((X,Additional_dimension_coordinates),axis=0)

Just to check the dimensions, X should now have dimension $(2 + 13) \times N$

[8]: X.shape

[8]: (15, 1000)

which is indeed the case. In these "extra dimensions" we would like to add some small noise. The idea is that, as we collect data, these entries play the role of irrelevant features (but we didn't know that at the time of data gathering! How could we?!).

```
[9]: X[2:,:] = .01*np.random.randn(additional_dimension,N)
```

For instance, if we plot the first 3 dimensions, we will see that most of the points are clustered around the plane (x_1, x_2) defined by the first two coordinates

```
[10]: fig = plt.figure()
```

```
plt.figure(figsize=(10,8))
ax = plt.axes(projection='3d')
ax.scatter3D(X[0,:1000],X[1,:1000],X[2,:1000],color=vec_color[:1000]);
ax.view_init(20, 30)
```

<Figure size 432x288 with 0 Axes>



Note the difference in magnitude of all the x,y axis to the z axis. We can make this difference visualy more pronounced if we plot everythin with the same scale:

```
[11]: fig = plt.figure()
plt.figure(figsize=(10,8))
ax = plt.axes(projection='3d')
ax.scatter3D(X[0,:1000],X[1,:1000],X[2,:1000],color=vec_color[:1000]);
ax.set_xlim3d(-30, 30)
ax.set_ylim3d(-30, 30)
ax.set_zlim3d(-30, 30)
ax.view_init(40, 60)  # This sets the angle by which we rotate the axis
```

<Figure size 432x288 with 0 Axes>



1.3 Constructing a training and a test set

We would like to set part of the sample apart so that it can be used for testing the model. However, we would like to have a stratified sample: both training, test, and CV set should have more or less the same proportion of Y = 1 and Y = 0

[12]: from sklearn.model_selection import StratifiedShuffleSplit

Just a quick remark on the above computation: note that we are using a strange "transpose" on X and Y to do the "split_sample.split(,). That's the case because the arguments for this function are of type Х : array-like, shape (n_samples, n_features) (see https://scikitlearn.org/stable/modules/generated/sklearn.model_selection.StratifiedShuffleSplit.html) That's not a big deal though: as the output is an array of integers, we can use i in the columns. That's why we don't use the transpose when we assign X_train, Y_train and so.

Let's count the proportion in each group:

Proportion of elements in whole sample is: 0.467

Proportion of elements in train set is: 0.4675

Proportion of elements in test set is: 0.465

1.4 Visualizing mass shuffle

One thing that we would like to do is vizualizing entries in a matrix as colors. Higher values will be redded, lower, more negative values, will have a colder value.

```
[14]: M = np.random.rand(5,5)
print(M)
fig, ax = plt.subplots(figsize=(2,2))
ax.imshow(M,cmap='hot')
```

```
[[0.48476252 0.34550478 0.54460021 0.2460338 0.66292761]
[0.53447239 0.86646543 0.76368555 0.00767189 0.42999264]
[0.98304474 0.45872573 0.91924365 0.35856625 0.43997758]
[0.71775006 0.68744951 0.06954802 0.45188963 0.87539893]
[0.22460292 0.70602693 0.03025972 0.75933301 0.46396242]]
```

[14]: <matplotlib.image.AxesImage at 0x135623b38>



2 Training a simple logit regression (a shallow NN)

In the process of training a log regression I would like to see how the mass gets reshuffled in the weigh matrix. The model goes like this: denote the sigmoid function by $\sigma(\cdot)$, which we write as

$$\sigma(z) = \frac{1}{1 + \exp(z)}, \quad z \in \mathbb{R}.$$

In our case we are going to use the following: we are interested in finding a vector $W \in \mathbb{R}^k$ and a quantity $b \in \mathbb{R}$ that will be used in our predictor. To be more precise, we will have

$$\hat{Y} = \begin{cases} 1, & if \\ 0, & if \end{cases} \qquad \begin{array}{c} \sigma(W \cdot X + b) \ge \eta \\ \sigma(W \cdot X + b) < \eta \end{cases}$$

In fact, we know that $W = e_1 = (1, 0, 0, ..., 0)$ is the predictor that we are looking for. So, as we train our model we would like to see the entries W_i (weights) in the matrix W to decay to 0 for $i \ge 2$ and converge to a positive number for W_1 .

It is not hard to do this training using scilearn-kit, but this is not what we want: we want to go old school on this, so we are going to design the method by ourselves.

Let's first create some auxiliary functions.

Remark: in the code you will see no η . That's because the tensorflow.round automatically sets $\eta = .5$. This function was used as a matter of convenience, and it is not hard to change it to the general case, that includes η as parameter.

2.1 Auxiliary functions

First we design a weigh initializer. Afterwards we design a forward propagation.

Note that we will keep k as a variable, for we want to study the effect of dimensionality in the model. So, to begin with we get a numpy vector with the number of nodes in each layer. This is going to be the vector "nodes_per_layer". Note that the number of nodes in the ith column will be given by "nodes_per_layer[i]"

```
[15]: k = 2 + additional_dimension
nodes_per_layer = np.array([k,1],ndmin=1)
```

Now we can initialize the weights that will connect the layers. Note that, from the perspective we want to study here, the "mass" will flow throught "pipes" that have weights given by the matrices W

```
[16]: def weight_initializer(nodes_per_layer):
```

```
///
Initialize the matrix W with dimensions 1xk and the 1x1 parameter b
///
L = len(nodes_per_layer)
W, b = {},{}
for i in range(1,L):
    W[str(i)] = tf.
-get_variable("W"+str(i),[nodes_per_layer[i],nodes_per_layer[i-1]],initializer=tf.
-contrib.layers.xavier_initializer())
    b[str(i)] = tf.
-get_variable("b"+str(i),[nodes_per_layer[i],1],initializer=tf.
-zeros_initializer())
parameters = (W,b)
return parameters
```

Let's test it

```
[17]: tf.reset_default_graph()
    W,b = weight_initializer(nodes_per_layer)
    print(W)
```

```
WARNING: The TensorFlow contrib module will not be included in TensorFlow 2.0. For more information, please see:
```

* https://github.com/tensorflow/community/blob/master/rfcs/20180907-contribsunset.md

```
* https://github.com/tensorflow/addons
```

If you depend on functionality not listed there, please file an issue.

```
WARNING:tensorflow:From /miniconda3/lib/python3.7/site-
packages/tensorflow/python/framework/op_def_library.py:263: colocate_with (from
tensorflow.python.framework.ops) is deprecated and will be removed in a future
version.
Instructions for updating:
Colocations handled automatically by placer.
{'1': <tf.Variable 'W1:0' shape=(1, 15) dtype=float32_ref>}
```

The next thing that we need to do is a propagator. For tris we will receive a tuple with strings, whose entries describe the activation function in that layer. What we have is the following:

```
Z[i] = W[i] \cdot A[i-1] + b[i]
```

where A[i-1] denotes the output of the previous layer. Note that the dimensions math: A[i-1] has dimension $n_{i-1} \times 1$, while W[i] has dimensions $n_i \times n_{i-1}$, hence Z[i] is a vector of dimensions $n_i \times 1$.

Before we write the propagation function, we are going to set the activation function vector:

```
[18]: type_activation = ['sigmoid']
```

```
[19]: def propagator(parameters,type_activation,X_tensor):
  L = len(type_activation)
  W, b = parameters
  A = X_tensor
  for i in range(L):
      if type_activation[i]=='relu':
        Z = tf.add(tf.matmul(W[str(i+1)],A),b[str(i+1)])
        if i !=L-1:
            Z = tf.nn.relu(Z)
      elif type_activation[i]=='sigmoid':
        Z = tf.add(tf.matmul(W[str(i+1)],A),b[str(i+1)])
        if i !=L-1:
            Z = tf.nn.sigmoid(Z)
    return Z
```

Do you see the big difference in the last propagation? That happens because in the last layer we don't need an activation function. This is due to the structure of the cross entropy function as implemented in tensorflow. In this link they say that: [https://www.tensorflow.org/api_docs/python/tf/nn/sigmoid_cross_entropy_with_logits]

```
Well... so let's compute the loss function:
```

```
[21]: tf.reset_default_graph()
```

```
with tf.Session() as sess:
```

```
X_tensor = tf.placeholder(shape =[k,None],name='X',dtype=tf.float32)
Y = tf.placeholder(shape=[1,None],name='Y',dtype=tf.float32)
parameters =weight_initializer(nodes_per_layer)
Z = propagator(parameters,type_activation,X_tensor)
```

```
print(cost_function(Z,Y))
```

```
Tensor("Mean:0", shape=(), dtype=float32)
```

Now we run the model. Let's first set some parameters for the search:

```
[22]: optimization_parameters={
    'learning_rate':0.0001,
```

```
'epochs':30000,
 'printing':True
}
ntwk_settings={
    'number_nodes':nodes_per_layer,
    'activation_type':type_activation
}
```

And now we draw the model and run the data through it

```
[23]: def

→full_model(optimization_parameters,ntwk_settings,X_train,Y_train,X_test,Y_test):
         ## Unpacking
         nodes_per_layer = ntwk_settings['number_nodes'] ## Recall, this is au
      \rightarrow dimension k x 1 matrix
         type_activation = ntwk_settings['activation_type']
         learning_rate = optimization_parameters['learning_rate']
         epochs = optimization_parameters['epochs']
         printing = optimization_parameters['printing']
         tf.reset_default_graph()
         # first we create placeholders: they are the ones that will get the data
         k = nodes_per_layer[0]
         X_tensor= tf.placeholder(dtype=tf.float32,shape=[k,None])
         Y_tensor= tf.placeholder(dtype=tf.float32,shape=[1,None])
         # Now we define the weights
         parameters = weight_initializer(nodes_per_layer)
         W,b = parameters
         Z = propagator(parameters,type_activation,X_tensor)
         # And we finally compute the cost. This is the function that will be
      →minimized
         cost= cost_function(Z,Y_tensor)
         ## Now we set up an optimizer
         optimizer_type = tf.train.AdamOptimizer(learning_rate=learning_rate)
         objective_function= optimizer_type.minimize(cost)
         ...
         Ok, so the above part only set up the graph over which we will compute \Box
      \leftrightarrow things. You can see the graph as a
         pipeline, that tells you where things are put in, combined, and where we get d
      \rightarrowoutputs
```

```
(that is, where we open the "faucet")
   ...
   # Below, we start running data throw these pipes! Let's do it.
   #For bookkeeping purposes, let's define two auxiliary quantities
   total_cost = [] #array that will save the cost values
   W_movie = []
                   #array that will save the weights for a movie
   initialize= tf.global_variables_initializer()
   with tf.Session() as sess:
       ## Initialize the nodes
       sess.run(initialize)
       for i in range(epochs):
           _,cost_now = sess.run([objective_function,cost],feed_dict={X_tensor:
→X_train[:k,:],Y_tensor:Y_train})
           if i\%1000 == 0 and printing:
               print("\n Cost at "+str(i)+"th iterate: "+str(cost_now))
           if i%40 == 0:
               total_cost.append(cost_now)
               W_movie.append(sess.run(W["1"]))
       # Now we stack the matrices with respect to last coordinate in order tou
\rightarrow create a video with them later on
       Movie = np.stack(W_movie,2)
       if printing:
           plt.figure(figsize=(15,7))
           plt.plot(total_cost)
           plt.xlabel('Number of iterations',size=22)
           plt.ylabel('Cost',size=22)
           plt.title('Cost decay per iteration')
           plt.grid(True)
           plt.show()
       ### At this point we get the value of the optimized parameter and use it_{\sqcup}
\rightarrow to make a prediction
       param = sess.run(parameters)
       # Prediction
       predicted_classification = tf.round(tf.sigmoid(Z))
       accuracy_of_prediction= tf.reduce_mean(tf.cast(tf.
→equal(predicted_classification,Y_tensor),"float"))
       ## Now we do some statistics:
```

accuracy_train = sess.run(accuracy_of_prediction,feed_dict={X_tensor: →X_train[:k,:],Y_tensor:Y_train}) if printing: print("Accuracy of training:", accuracy_train) accuracy_test = sess.run(accuracy_of_prediction,feed_dict={X_tensor: →X_test[:k,:],Y_tensor:Y_test}) if printing: print("Accuracy of test/validation:", accuracy_test) return (total_cost, accuracy_train,accuracy_test, Movie)

[24]: _,_,_,Movie=

→full_model(optimization_parameters,ntwk_settings,X_train,Y_train,X_test,Y_test)

Cost at 0th iterate: 4.3329387 Cost at 1000th iterate: 3,4253223 Cost at 2000th iterate: 2.5442781 Cost at 3000th iterate: 1.718967 Cost at 4000th iterate: 1.024744 Cost at 5000th iterate: 0.5893747 Cost at 6000th iterate: 0.40491867 Cost at 7000th iterate: 0.31554875 Cost at 8000th iterate: 0.25768864 Cost at 9000th iterate: 0.21581575 Cost at 10000th iterate: 0.18390281 Cost at 11000th iterate: 0.15878399 Cost at 12000th iterate: 0.13858381 Cost at 13000th iterate: 0.12209348 Cost at 14000th iterate: 0.108478755 Cost at 15000th iterate: 0.09713336 Cost at 16000th iterate: 0.0876004 Cost at 17000th iterate: 0.0795272

```
Cost at 18000th iterate: 0.0726378

Cost at 19000th iterate: 0.06671402

Cost at 20000th iterate: 0.061582662

Cost at 21000th iterate: 0.057105456

Cost at 22000th iterate: 0.05317184

Cost at 23000th iterate: 0.049692594

Cost at 24000th iterate: 0.046595518

Cost at 25000th iterate: 0.043822154

Cost at 26000th iterate: 0.041324873

Cost at 27000th iterate: 0.039064627

Cost at 28000th iterate: 0.037009157

Cost at 29000th iterate: 0.035131622
```



Accuracy of training: 1.0 Accuracy of test/validation: 0.995

2.2 Visualizing mass shuffle and dynamic behavior of weights

Let's create a video with the weights in order to see how they evolve through time, that is, iterations:



[26]: <IPython.core.display.HTML object>

Remark: recall that we are visualizing what is happening in the first layer.

</video>'''.format(encoded.decode('ascii')))

Let's analize this video more carefully: it seems that the weights on $W^{(1)}[i]$ for $i \ge 2$ are getting more negative through "time"(i.e., iterations) while $W^{(1)}[0]$ is getting bigger. Let's plot it

<source src="data:video/mp4;base64,{0}" type="video/mp4" />

```
[27]: plt.figure(figsize=(15,8))
for i in range(k):
    plt.plot(Movie[0,i,:],label="W^{(1)}["+str(i)+"]")
plt.legend(loc=2)
plt.xlabel('Iteration',size=22)
plt.ylabel('Weight value',size=22)
plt.show()
```



Whaaaat?!! Why are the weights not getting separated??!! Yes, they are, but in AVERAGE!

```
[28]: plt.figure(figsize=(15,5))

cop_Movie = np.copy(Movie)
v_0 = np.copy(Movie[0,0,:])
v_1 = np.copy(Movie[0,1,:])
cop_Movie[0,0,:]=0*Movie[0,0,:]
cop_Movie[0,1,:]=0*Movie[0,1,:]

plt.plot(v_0,label="$W^{(1)}$["+str(0)+"]")
plt.plot(v_1,label="$W^{(1)}$["+str(1)+"]")
plt.plot(np.squeeze(np.mean(cop_Movie,1)),label="average of rest")
plt.xlabel('Iteration',size=22)
plt.ylabel('Weight value',size=22)
plt.legend(loc=2)
plt.show()
```



Note that there is node that is a bit different from others: that's the first one! It is exactly the one responsible for capturing the behavior of the first coordinate. Further, note that in half of Y = 0 or Y = 1 cases one can expect the second coordinate to be either positive or negative, for it is normally distributed. The "best way" to avoid any issue with this coordinate is by "shutting it off": that's why we see it converging to zero. Curiously, the model does not turn off the weight on the other coordinates, showing that it gets affected by the noise we have added.

You can certainly do the same for larger NN, but the shallowest model is the best to see the effect of mass shuffling on the weights: as the video goes you start seeing less mass on the weights $W^{(i)}$ for $i \ge 1$. It is also possible to wonder what are the possible ways to shuffle mass in a NN, because backpropagation is one of them (indeed, a very effecient one!). We could also think of other methods, but let's not worry about that for these notes: I will investigate that a bit further in future notebooks.

```
[29]: np.mean(Movie[:,:,[1,2]],1)
```

```
[29]: array([[-0.13295904, -0.13375863]], dtype=float32)
```

```
[30]: Movie_averaged= np.zeros([1,3,Movie.shape[-1]])
Movie_averaged[0,0,:] = Movie[0,0,:]
Movie_averaged[0,1,:] = Movie[0,1,:]
Movie_averaged[0,2,:] = np.mean(Movie[0,2:,:],0)
```

[30]: (1, 3, 750)

```
[31]: global Movie_averaged
```

ani.save('NN_shallow_averaged.mp4')



[32]: <IPython.core.display.HTML object>

3 Non linear prediction boundaries

The boundary between classes in the previous model was linear, thus one could exepect a good performance of even a shallow NN (a logit model is the simplest possible NN you can imagine). But let's see what happens if we change the boundary a bit. By doing so we also bring in the second coordinate, making it "slightly" relevant fot the prediction, but not that much: on average, the model still "separates well" with a simple linear boundary.

```
[34]: fig = plt.figure()
plt.figure(figsize=(10,8))
ax = plt.axes(projection='3d')
colors =['red','blue']
vec_color = [colors[i] for i in Y[:]]
ax.scatter3D(X[0,:1000],X[1,:1000],X[2,:1000],color=vec_color[:1000]);
ax.set_xlim3d(-30, 30)
ax.set_ylim3d(-30, 30)
ax.set_zlim3d(-30, 30)
ax.view_init(40, 60) # This sets the angle by which we rotate the axis
```

<Figure size 432x288 with 0 Axes>





```
}
k = 2 + additional_dimension
nodes_per_layer = np.array([k,1],ndmin=1)
type_activation = ['sigmoid']
ntwk_settings={
    'number_nodes':nodes_per_layer,
    'activation_type':type_activation
}
```

```
[36]: _,_,_,Movie=
```

--full_model(optimization_parameters,ntwk_settings,X_train,Y_train,X_test,Y_test)

```
Cost at 0th iterate: 1.3417832
Cost at 1000th iterate: 0.79833853
Cost at 2000th iterate: 0.47583246
Cost at 3000th iterate: 0.32199946
Cost at 3000th iterate: 0.2611546
Cost at 4000th iterate: 0.23907354
Cost at 5000th iterate: 0.23003292
Cost at 6000th iterate: 0.22525847
Cost at 8000th iterate: 0.22249818
Cost at 9000th iterate: 0.2209907
```



```
Accuracy of training: 0.890625
Accuracy of test/validation: 0.85
```

It is clear that the accuracy of the model has decayed, in both the training and in the test set. As before, let's plot the dynamic behavior of the weights

```
[37]: plt.figure(figsize=(15,5))

cop_Movie = np.copy(Movie)
v_0 = np.copy(Movie[0,0,:])
v_1 = np.copy(Movie[0,1,:])
cop_Movie[0,0,:]=0*Movie[0,0,:]
cop_Movie[0,1,:]=0*Movie[0,1,:]

plt.plot(v_0,label="W^{(1)}["+str(0)+"]")
plt.plot(v_1,label="W^{(1)}["+str(1)+"]")
plt.plot(np.squeeze(np.mean(cop_Movie,1)),label="average of rest")
plt.xlabel('Iteration',size=22)
plt.ylabel('Weight value',size=22)
plt.legend(loc=2)
plt.show()
```

