HW1 report

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Answer to the problems:

- mostly in pdf of ipython notebook for TAs
- more clarification of problem 1-c(experiments):
  To find the important factors, I think removing one at once to see how much does the RMS error change is a good way if the given data features are independent with each other(which can be checked by other methods like covariance matrix).
  The more the corresponding RMS rises the more important should the factor be.
  This idea is implemented with ipython notebook files.

Discussion:

- Data Preprocessing:
  - regression:
    - drop one-hot features and y(heating load)
    - make one-hot features(orientation, etc.) (considered as a feature n-d vector of unit norm)
    - normalize non-one-hot features(important if there is one-hot feature)
    - combine
  - classification:
    - drop y is enough
    - the features seem already normalized
  - implementation : pandas + numpy
  - dataframe.drop([comlum names], axis=1)
  - dataframe.values
  - implementation of one-hot encoding and normalization
  - np.c_[a,b,c]

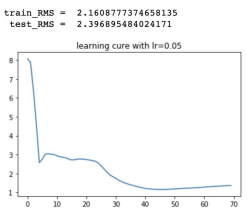
- Model Topology Design:
  - Overview:
    - follow my intuition at first and try some different models
    - not complicated task + small training data size
      => should use lower VC dimension models
      => less hidden units(layers)
    - extract useful information during the model
      =>decreasing hidden units(neurons)
  - Regression:
    NN([in, 10, 5, 1],activations=['sigmoid', 'sigmoid', 'relu'])
  - Classification:
    NN([in, 17, dim, 1],activations=['selu', ‘selu’, 'sigmoid'])

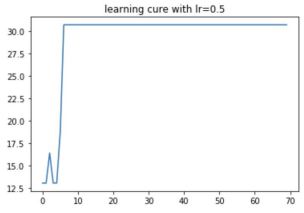
- Weight Initialization:
    - Xavier initialization / HE initialization
    - np.random.randn(layers[i+1], layers[i])*np.sqrt(2./layers[i]) for RELU-like activiations
    - np.random.randn(layers[i+1], layers[i])*np.sqrt(1./layers[i])) for Sigmoid-like activations
    - In the beginning, my model is quite sensitive to initial weights.
      And the model would stop working if bad init values are chosen.
      So I google for “weight initialization” and find the two heuristics depends on activation and the input size of the layer

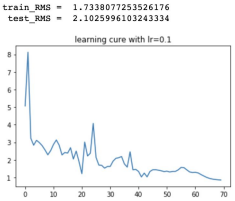
- Activation Functions:
    - relu:
      zero gradient problem => try leaky relu/selu/sigmoid
      good enough for classification problem
    - sigmoid:
      force the output to be in (0,1)
      not a good choice generally, but add a lot non-linearity in my opinion
      perform well in my regression task than relu/selu for zero gradient
    - selu:
      A better version of relu-like functions, math background, self-normalizing.
      However, in my task, it seems that it just does similar job with RELU.

- Gradient Descent:
  Just the naive gradient descent with minibatch (~78*10)(~35*10).
  Nothing fancy.
  May add features of :
    - reuse data/emphasis data that didn’t perform well,
      which is a similar idea to priority experience replay.
    - momentum/Adagrad/RMSprop/Adam...etc.

- Learning Rate:
    - 0.1(default): stable, generally better convergence results
    - 0.5(too large): unstable and cause concussion and divergence
    - 0.05-0.08(trial): almost always good, smoother than 0.1
    - 0.01(too small): plausible in regression task, but cause a lot lower accuracy(0.9 compared to 0.98 training accuracy) in the classification task. I think it’s because that classification task is of fewer data.



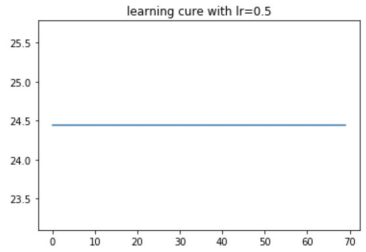




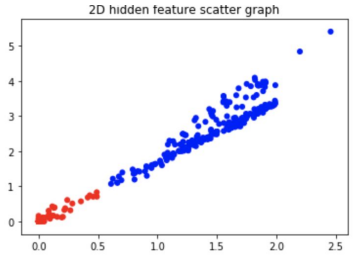
    - In conclusion, 0.08-0.1 is good for both tasks in most cases

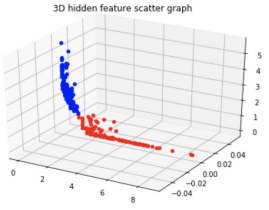
- About regression task:
  Zero gradients for some init values remain unsolved.
  It will need to try several times before getting a good model.
  So in the experiments about problem1(c), it is required to write a program that retries automatically.

```
train_RMS =  24.612000827283875
 test_RMS =  24.081340383946653
```



- Interesting facts about classification task:
  - it seems that the well-trained NN(because of better initialization) tends to form a line with a red-blue cut in 2D/3D space
    i.e. It is actually linear-separable!

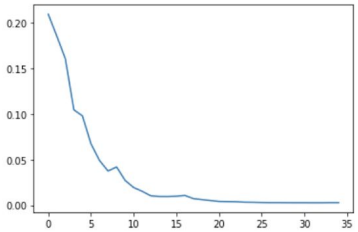




so I tried to set the last layer length to 1, and the result is good as I guess

```
In [79]: nn2 = NN([34, 17, 1, 1],activations=['selu', 'selu',  'sigmoid'], usage = 'classification')
         #the network architecture is as the constructer

         learning_curve = nn2.train(train_X, train_y, epochs=35, batch_size=10, lr = .1)

         train_CE = nn2.calc_error(train_X, train_y)
         train_accuracy = nn2.calc_accuracy(train_X, train_y)
         test_CE = nn2.calc_error(test_X, test_y)
         test_accuracy = nn2.calc_accuracy(test_X, test_y)

         plt.plot(np.arange(len(learning_curve)), learning_curve)

         print('train_CE = ', train_CE, '\n', 'test_RMS = ', test_CE)
         print('train_Accuracy = ', train_accuracy, '\n', 'test_Accuracy = ', test_accuracy)
         print('train_ErrorRate = ', 1-train_accuracy, '\n', 'test_ErrorRate = ', 1-test_accuracy)
```

```
train_CE =  0.005769448506493566
 test_RMS =  0.02004422382835881
train_Accuracy =  0.9857142857142858
 test_Accuracy =  0.8591549295774648
train_ErrorRate =  0.014285714285714235
 test_ErrorRate =  0.14084507042253525
```



Moreover, as I remove the hidden layer (same as linear regression model with gradient descent) the accuracy is still quite high(92%/80%)
and one 3-node hidden layer can rise to (97%/85%)

In conclusion, I think the data is quite a trivial task: however, adding hidden layers can explore more inside properties and achieve a more precise result to determine “special cases” while preventing overfitting meanwhile.

Some Problems Encountered and Implementation Details:

- Numerical Issues:
    - exponential explosion
      => use numpy.clip(z, -500, 500) to avoid huge or close to zero values
    - division by zero(classification)
      => use numpy.clip(epsilon, 1-epsilon) to avoid 0 value of denominator
- Zero gradient:
    - Wright initialization with HE/X => better result but still have zero gradient sometimes(on regression task)
    - SELU activation function => not working when bad init happens
    - use numpy.clip(z, -10, 10) to avoid zero gradient of exp related => not working
    - batch normalization layer is too complicated to implement

- @staticmethod decorator
- misunderstaning of np.linalg.norm(a-b) => corret RMS formula to np.linalg.norm(y-yhat)/np.sqrt(y.shape[1])
- np.where is useful :)
- save_res(name) function for Neural Network and prediction.csv saving

Other Issue:

- all work by myself with some Internet references, and TA consultation
- noticed that the NN is sensitive to the initial value for the naive gradient method
- to run, need to move the corresponding data(.csv) and model(model.py) to the directory of ipython file
- pdf of ipython is already run with data and model for fast evaluation of TAs