CS5785 Homework 3

The homework is generally split into programming exercises and written exercises.
This homework is due on **November 10, 2020, at 11:59 PM EST**. Upload your homework to Gradescope (Canvas->Gradescope). A complete submission should include:

1. A write-up as a single `.pdf` file. Submit to "Homework 3 - Write Up".

2. Source code for all of your experiments (AND figures)zipped into a single .zip file, in `.py` files if you use Python or `.ipynb` files if you use the IPython Notebook. If you use some other language, include all build scripts necessary to build and run your project along with instructions on how to compile and run your code. **If you use the IPython Notebook to create any graphs, please make sure you also include them in your write-up.** Submit to "Homework 3 - Code".

The write-up should contain a general summary of what you did, how well your solution works, any insights you found, etc. On the cover page, include the class name, homework number, and team member names. You are responsible for submitting clear, organized answers to the questions. You could use online LaTeX templates from Overleaf, under "Homework Assignment" and "Project / Lab Report".
Please include all relevant information for a question, including text response, equations, figures, graphs, output, etc. If you include graphs, be sure to include the source code that generated them. Please pay attention to Canvas for relevant information regarding updates, tips, and policy changes.

IF YOU NEED HELP

There are several strategies available to you.

- If you ever get stuck, post your question on the Discussions section in Canvas. That way, your solutions will be available to the other students in the class.

- Your instructor and TAs will offer office hours, which are a great way to get some one-on-one help.

- You are allowed to use well-known libraries such as `scikit-learn`, `scikit-image`, `numpy`, `scipy`, etc. in this assignment. Any reference or copy of public code repositories should be properly cited in your submission (examples include Github, Wikipedia, Blogs).

PROGRAMMING EXERCISES

1. **Convolutional Neural Networks**

   We will work with the MNIST dataset for this question. This dataset contains 60,000 images of handwritten numbers from 0 to 9 and you need to recognize the handwritten numbers by building a CNN.

   You will use the Keras library for this. You might have to install the library if it hasn't been installed already. Please check the installation by printing out the version of Keras inside the python shell as follows.

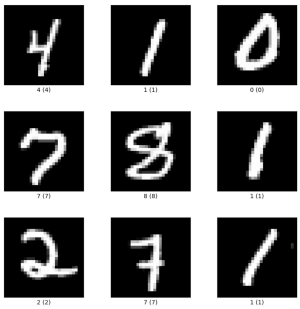
   ```
   import keras
   keras.__version__
   ```

   The above lines will give you the current version of Keras you are using. Once this works, you can proceed with the assignment.

   (a) **Loading Dataset** For using this dataset, you will need to import mnist and use it as follows.

   ```
   from keras.datasets import mnist
   (train_X, train_Y), (test_X, test_Y) = mnist.load_data()
   ```

   To verify that you have loaded the dataset correctly, try printing out the shape of your train and test dataset matrices. Also, try to visualize individual images in this dataset by using imshow() function in pyplot. Below are some example images from the Tensorflow datasets catalog.

   (b) **Preprocessing** The data has images with 28×28 pixel values. Since we use just one grayscale color channel, you need to reshape the matrix such that we have a $28 \times 28 \times 1$ sized matrix holding each input data-point in the training and testing dataset. The output variable can be converted into a one-hot vector by using the function to_categorical (make sure you import to_categorical from keras.utils). For example, if the output label for a given image is the digit 2, then the one-hot representation for this consists of a 10-element vector, where the element at index 2 is set to 1 and all the other elements are zero.

   For preprocessing, scale the pixel values such that they lie between 0.0 and 1.0. Make sure that you use the appropriate conversion to float wherever required while scaling.

   You can include all these steps into a single python function that loads your dataset appropriately. Once you finish this, visualize some images using imshow() function.

(c) **Implementation**

Now, to define a CNN model, we will use the Sequential module in Keras. We are providing you with the code for creating a simple CNN here. We use Conv2D (for declaring 2D convolutional networks), MaxPooling2D (for maxpooling layer), Dense (for densely connected neural network layers) and Flatten (for flattening the input for next layer).

```
from keras.models import Sequential
from keras.layers import Conv2D
from keras.layers import MaxPooling2D
from keras.layers import Dense
from keras.layers import Flatten
from keras.optimizers import SGD

def create_cnn():
        # define using Sequential
        model = Sequential()
        # Convolution layer
        model.add(
                Conv2D(32, (3, 3),
                activation='relu',
                kernel_initializer='he_uniform',
                input_shape=(28, 28, 1))
                )
        # Maxpooling layer
        model.add(MaxPooling2D((2, 2)))
        # Flatten output
        model.add(Flatten())
        # Dense layer of 100 neurons
        model.add(
                Dense(100,
                activation='relu',
                kernel_initializer='he_uniform')
                )
        model.add(Dense(10, activation='softmax'))
        # initialize optimizer
        opt = SGD(lr=0.01, momentum=0.9)
        # compile model
        model.compile(
                optimizer=opt,
                loss='categorical_crossentropy',
                metrics=['accuracy']
                )
        return model
```

Specifically, we have added the following things in this code.

i. A single convolutional layer with 3×3 sized window for computing the convolution, with 32 filters
ii. Maxpooling layer with 2×2 window size.
iii. Flatten resulting features to reshape your output appropriately.
iv. Dense layer on top of this (100 neurons) with ReLU activation
v. Dense layer with 10 neurons for calculating softmax output (Our classification result will output one of the ten possible classes, corresponding to our digits)

After defining this model, we use Stochastic Gradient Descent (SGD) optimizer and cross-entropy loss to compile the model. We are using a learning rate of 0.01 and a momentum of 0.9 here. We have added this to the given code stub already. Please see that this code stub works for you. Try to print model.layers in your interactive shell to see that the model is generated as we defined.

(d) **Training and Evaluating CNN**

Now we will train the network. You can see some examples here. Look at the fit() and evaluate() methods.

You will call the fit method with a validation split of 0.1 (i.e. 10% of data will be used for validation in every epoch). Please use 10 epochs and a batch size of 32. When you evaluate the trained model, you can call the evaluate method on the test data-set. Please report the accuracy on test data after you have trained it as above. You can refer to the following while you write code for training and evaluating your CNN.

```
model.fit(train_x, train_y, batch_size=32,
    epochs=10, validation_split=0.1)

score = model.evaluate(test_x, test_y, verbose=0)
```

(e) **Experimentation**

i. Run the above training for 50 epochs. Using pyplot, graph the validation and training accuracy after every 10 epochs. Is there a steady improvement for both training and validation accuracy?
For accessing the required values while plotting, you can store the output of the fit method while training your network. Please refer to the code below.

```
epoch_history = model.fit(train_x, train_y, batch_size=32,
   epochs=10, validation_split=0.1)

# print validation and training accuracy over epochs
print(epoch_history.history['accuracy'])
print(epoch_history.history['val_accuracy'])
```

Make sure that your plot has a meaningful legend, title, and labels for X/Y axes.

ii. To avoid over-fitting in neural networks, we can 'drop out' a certain fraction of units randomly during the training phase. You can add the following layer (before the dense layer with 100 neurons) to your model defined in the function create_cnn.

```
model.add(Dropout(0.5))
```

Make sure you import Dropout from keras.layers! Now, train this CNN for 50 epochs. Graph the validation and train accuracy after every 10 epochs.
This tutorial might be helpful if you want to see more examples of dropout with Keras.

iii. Add another convolution layer and maxpooling layer to the create_cnn function defined above (immediately following the existing maxpooling layer). For the additional convolution layer, use 64 output filters. Train this for 10 epochs and report the test accuracy.

iv. We used a learning rate of 0.01 in the given create_cnn function. Using learning rates of 0.001 and 0.1 respectively, train the model and report accuracy on test data-set. To be sure, we are working with 2 convolution layers and training for 10 epochs while doing this experiment

(f) **Analysis**

i. Explain how the trends in validation and train accuracy change after using the dropout layer in the experiments.

ii. How does the performance of CNN with two convolution layers differ as compared to CNN with a single convolution layer in your experiments?

iii. How did changing learning rates change your experimental results in part (iv)?

2. **Random forests for image approximation** In this question, you will use random forest regression to approximate an image by learning a function, $f : \mathbb{R}^2 \to \mathbb{R}$, that takes *image* (x, y) *coordinates* as input and outputs *pixel brightness*. This way, the function learns to approximate areas of the image that it has not seen before.

(a) Start with an image of the Mona Lisa. If you don't like the Mona Lisa, pick another interesting image of your choice.

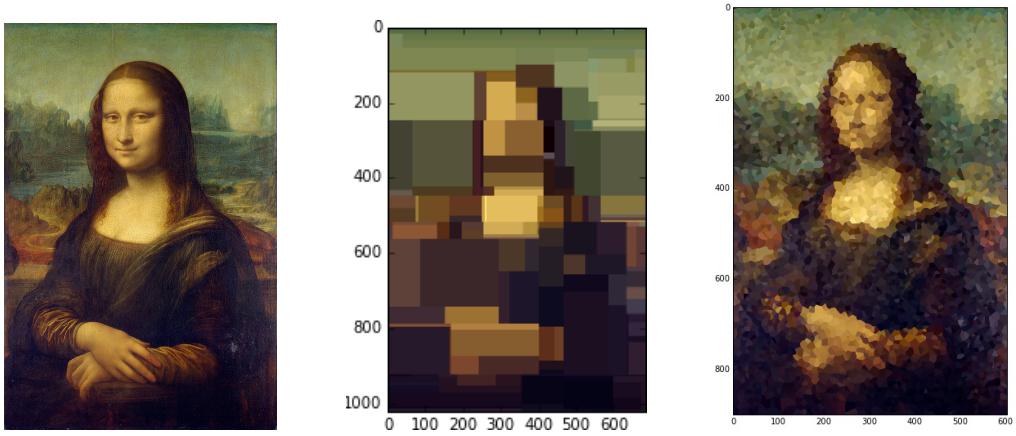


Figure 1: **Left**: http://tinyurl.com/mona-lisa-small *Mona Lisa*, Leonardo da Vinci, via Wikipedia. Licensed under Public Domain. **Middle**: Example output of a decision tree regressor. The input is a "feature vector" containing the (x, y) coordinates of the pixel. The output at each point is an (r, g, b) tuple. This tree has a depth of 7. **Right**: Example output of a k-NN regressor, where $k = 1$. The output at each pixel is equal to its closest sample from the training set.

(b) **Preprocessing the input.** To build your "training set," uniformly sample 5,000 random (x, y) coordinate locations.

- What other preprocessing steps are necessary for random forests inputs? Describe them, implement them, and justify your decisions. In particular, do you need to perform mean subtraction, standardization, or unit-normalization?

(c) **Preprocessing the output.** Sample pixel values at each of the given coordinate locations. Each pixel contains red, green, and blue intensity values, so decide how you want to handle this. There are several options available to you:

- Convert the image to grayscale
- Regress all three values at once, so your function maps (x, y) coordinates to (r, g, b) values: $f : \mathbb{R}^2 \to \mathbb{R}^3$
- Learn a different function for each channel, $f_{Red} : \mathbb{R}^2 \to \mathbb{R}$, and likewise for f_{Green}, f_{Blue}.

Note that you may need to rescale the pixel intensities to lie between 0.0 and 1.0. (The default for pixel values may be between 0 and 255, but your image library may have different defaults.)

What other preprocessing steps are necessary for random regression forest outputs? Describe them, implement them, and justify your decisions.

(d) To build the final image, for each pixel of the output, feed the pixel coordinate through the random forest and color the resulting pixel with the output prediction. You can then use `imshow` to view the result. (If you are using grayscale, try `imshow(Y, cmap='gray')` to avoid fake-coloring). You may use any implementation of random forests, but you should understand the implementation and you must cite your sources.

(e) **Experimentation.**

i. Repeat the experiment for a random forest containing a single decision tree, but with depths 1, 2, 3, 5, 10, and 15. How does depth impact the result? Describe in detail why.

ii. Repeat the experiment for a random forest of depth 7, but with number of trees equal to 1, 3, 5, 10, and 100. How does the number of trees impact the result? Describe in detail why.

iii. As a simple baseline, repeat the experiment using a k-NN regressor, for $k = 1$. This means that every pixel in the output will equal the nearest pixel from the "training set." Compare and contrast the outlook: why does this look the way it does?

iv. Experiment with different pruning strategies of your choice.

(f) **Analysis.**

i. What is the decision rule at each split point? Write down the 1-line formula for the split point at the root node for one of the trained decision trees inside the forest. Feel free to define any variables you need.

ii. Why does the resulting image look the way it does? What shape are the patches of color, and how are they arranged?

iii. *Straightforward:* How many patches of color may be in the resulting image if the forest contains a single decision tree? Define any variables you need.

iv. *Tricky:* How many patches of color might be in the resulting image if the forest contains n decision trees? Define any variables you need.

WRITTEN EXERCISES

(a) **Decision trees.**

i. A. Consider a 2D rectangular input space containing points X^1 and X^2. Is it possible to create an example such that X^1 and X^2 are not separable by decision stump (i.e. decision tree with a single node)?
For example, $X = (X_0, X_1)$ is a data-point such that X_0 corresponds to the 0-th dimension and X_1 corresponds to the 1st dimension in the 2D input space. Decision stump could classify point X as positive if $X_0 > 0$ and negative otherwise.
Does adding another data-point change your answer? Draw a diagram and write a short explanation to support your answers.
In both the cases above, can you separate these data-points with a linear classifier?

B. Is it possible to add more data-points to the first example such they are not separable by a two-level decision tree? (Each level of the decision tree can look at just one axis of the input data point)

C. Is it possible to construct an example such that the data-points are separable by a 2-level decision tree but not by a linear classifier? If yes, try to construct the example with minimum number of data-points. Otherwise, explain why this is not possible.

ii. Lucy wants to rent a house for herself. She makes some inquiries and arrives at the following data based on the availability and her preferences.

Location	*Pollution*	*Area*	*Windows*	*Preference*
Rural	low	large	large	yes
Rural	high	large	small	no
Rural	med	small	large	yes
Rural	low	small	small	no
Urban	high	small	small	no
Urban	high	small	large	yes
Urban	med	large	small	no
Urban	med	small	small	yes
Semi-rural	low	large	small	yes
Semi-rural	high	small	large	no
Semi-rural	med	large	large	yes

Considering the preference as binary output variable that we want to predict, which attribute should be at the root of this decision tree? Answer using cross-entropy and Gini index.

(b) **Neural networks as function approximators.** Design a feed-forward neural network to approximate the 1-dimensional function given in Fig. 2. The output should match exactly. How many hidden layers do you need? How many units are there within each layer? Show the hidden layers, units, connections, weights, and biases.

Use the ReLU nonlinearity for every unit. Every possible path from input to output must pass through the same number of layers. This means each layer should have the form

$$Y_i = \sigma(W_i Y_{i-1}^T + \beta_i), \tag{1}$$

where $Y_i \in \mathbb{R}^{d_i \times 1}$ is the output of the ith layer, $W_i \in \mathbb{R}^{d_i \times d_{i-1}}$ is the weight matrix for that layer,

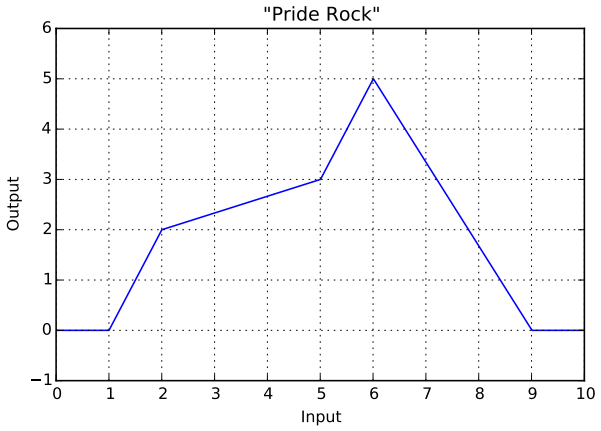


Figure 2: Example function to approximate using a neural network.

$Y_0 = x \in \mathbb{R}^{1\times 1}$, and the ReLU nonlinearity is defined as

$$\sigma(x) \triangleq \begin{cases} x & x \geq 0, \\ 0 & \text{otherwise} \end{cases}. \tag{2}$$

Hint 1: Try to express the input function as a sum of weighted and scaled ReLU units. Once you can do this, it should be straightforward to turn your final equation into a series of neural network layers with individual weights and biases.

Hint 2: If you're not convinced neural networks can approximate this function, see http://neuralnetworksanddeeplearning.com/chap4.html for an example of the flavor of the solution we're looking for. (If you rely on this source, cite it!) However, keep in mind that your output must match the given input *exactly*.

Ordinarily, such a network could be learned via backpropagation, but we're instead asking you to figure out the weights to this simple network by hand.

(c) **Bootstrap aggregation ("bagging")** Suppose we have a training set of N examples, and we use bagging to create a bootstrap replicate by drawing N samples **with replacement** to form a new training set. Because each sample is drawn with replacement, some examples may be included in this bootstrap replicate multiple times, and some examples will be omitted from it entirely.

As a function of N, compute the expected fraction of the training set that does not appear at all in the bootstrap replicate. What is the limit of this expectation as $N \to \infty$?

Hint: You can use the limit $\lim_{n\to\infty}\left(1+\frac{x}{n}\right)^n = e^x$