Machine Learning Engineer Nanodegree

Capstone Project

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I. Definition

Project Overview

Given an integer sequence: 1, 2, 3, 4, 5, ? So what is the next number?

If your answer is 7, You read that correctly. That's the start to a real integer sequence, the powers of primes[1]. Continuously, how about the next number in 0, 1, 1, 2, 3, 5, 8, 13, 21, 34, 55, ? If you answered 89, you may enjoy this challenge. In this project, a machine learning solution will be demonstated to predict the next number of a given integer sequence.

A number in a sequence is equivalent to a word. Based on this observation, we try to predict the last number based on the preceding numbers. Hence, the problem can be treated as the Natural Language Processing (NLP)[2] domain.

NLP is the computerized approach to analyzing text that is based on both a set of theories and a set of technologies. Definitionally speaking, NLP is a theoretically motivated range of computational techniques for analyzing and representing naturally occurring texts at one or more levels of linguistic analysis for the purpose of achieving human-like language processing for a range of tasks or applications.

The history of NLP generally started in the 1950s, although work can be found from earlier periods. During the 1970s, many programmers began to write "conceptual ontologies", which structured real-world information into computer-understandable data. Up to the 1980s, most NLP systems were based on complex sets of hand-written rules.

Recent research has increasingly focused on unsupervised and semi-supervised learning algorithms. Such algorithms are able to learn from data that has not been hand-annotated with the desired answers, or using a combination of annotated and non-annotated data.

In recent years, there has been a flurry of results showing deep learning techniques achieving state-of-the-art results in many natural language tasks, for example in language modeling, parsing and many others, among which, sequence prediction is different from traditional classification and regression problems. It is required to take the order of observations into account and apply models that have memory and that can learn any temporal dependence between observations.

The dataset[3] of this project contains the majority of the integer sequences from the On-Line Encyclopedia of Integer Sequences® (OEIS®)[4]. It is split into a training set, where you are given the full sequence, and a test set, where we have removed the last number from the sequence. The task is to predict this removed integer.

Note that some sequences may have identical beginnings (or even be identical altogether). They have not been removed these from the dataset.

File descriptions

- train.csv - the training set, contains full sequences
- test.csv - the test set, missing the last number in each sequence

Problem Statement

This problem at hand is defined by Kaggle[5] team's competition named Integer Sequence Learning[6]. It challenges you create a machine learning algorithm capable of guessing the next number in an integer sequence. While this sounds like pattern recognition in its most basic form, a quick look at the data will convince you this is anything but basic!

The Recurrent Neural Networks[7] approach – usually just called "RNNs" - is applied to solve this problem. This task particularly interests me as it's analogous to word prediction. Hence integers are treated as words in the solution.

Metrics

The evaluation metric for this problem is based on the accuracy of the predictions (the percentage of sequences where the next number is predicted correctly). It can be defined as follows:

$$Pr = \frac{Nc}{Nt}$$

Where,

- *Pr*: the accuracy rate of the predictions
- *Nc*: the number of sequences where the next number is predicted correctly
- *Nt*: the total number of sequences to be tested in test set

The target of the problem is to predict each sequence's last element of the test set which has been removed, hence the metric defined above should be the most straightforward way to evaluate the performance of the designed predictive model which generates the final item of each sequence.

II. Analysis

Data Exploration

The input datasets of this project are two CSV files for `train` and `test`. It's known that for the training set, we are given the entire sequence and for the test set the final element has been removed, which is the target we are trying to predict.

Firstly, we explore the training set to understand the details using R.

```
train <- read.csv("train.csv")
str(train)
```

```
## 'data.frame':    113845 obs. of  2 variables:
##  $ Id      : int  3 7 8 11 13 15 16 18 20 21 ...
##  $ Sequence: Factor w/ 112880 levels "-1,-1,-1,-1,-1,-1,-1,-1,8,-1,-10,-19,-28,-37,-46,-55,-64,-73,17,8,-1,-10,-19,-28,-37,-46,-55,-64,2
```

```
head(train)
```

```
##   Id
## 1  3
## 2  7
## 3  8
## 4 11
## 5 13
## 6 15
##   Sequence
## 1  1,3,13,87,1053,28576,2141733,508147108,402135275365,1073376057490373,9700385489355970183,298434346895322960005291,314793600959079080
## 2  1,2,1,5,5,1,11,16,7,1,23,44,30,9,1,47,112,104,48,11,1,95,272,320,200,70,13,1,191,640,912,720,340,96,15,1,383,1472,2464,2352,1400,532,
## 3  1,2,4,5,8,10,16,20,32,40,64,80,128,160,256,320,512,640,1024,1280,2048,2560,4096,5120,8192,10240,16384,20480,32768,40960,65536,81920,1
## 4  1,8,25,83,274,2275,132224,1060067,3312425,10997342,36304451,301432950,17519415551,140456757358,438889687625,1457125820233,4810267148
## 5  1,111,12211,1343211,147753211,16252853211,1787813853211,196659523853211,21632547623853211,2379580238623853211,2617538262486238532112
## 6  1,1,1,1,1,1,1,1,1,5,1,1,1,1,5,5,1,1,1,1,11,5,5,11,5,1,1,1,1,5,23,5,23,5,5,1,1,1,1,21,5,39,5,5,39,5,21,5,1,1,1,1,5,1,17,1,17,1,1,5,1,1
```

It's obersed that each row of the data contains `Id` and `Sequence`. There are totally 113,845 sequences indicated by `Id`.

```
# Count all numbers in training set
train_numbers_count = str_count(train$Sequence, ',') + 1
summary(train_numbers_count)
```

```
Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
1.00   19.00   34.00   41.67   59.00  348.00
```

From above table, we find that of all the sequences in the training set the minimum length is 1, the maximum length is 348 meanwhile the mean value of the length is 41.67.

For the test set, we use the same method to explore it.

```
test <- read.csv("test.csv")
str(test)
```

```
## 'data.frame':    113845 obs. of  2 variables:
##  $ Id      : int  1 2 4 5 6 9 10 12 14 17 ...
##  $ Sequence: Factor w/ 112743 levels "-1,-1,-1,-1,-1,-1,-1,-1,0,-1,-1,-1,-1,1,-1,-1,-1,-1,0,1,-1,-1,-1,-1,-1,1,0,-1,-1,-1,-1,0,2,-1,-
```

```
head(test)
```

```
##   Id
## 1  1
## 2  2
## 3  4
## 4  5
## 5  6
## 6  9
##   Sequence
## 1  1,0,0,2,24,552,21280,103760,70299264,5792853248,587159944704
## 2  1,1,5,11,35,93,269,747,2115,5933,16717,47003,132291,372157,1047181,2946251,8289731,23323853,65624397,184640891,519507267,1461688413,4
## 3  0,1,101,2,15,102,73,3,40,16,47,103,51,74,116,4,57,41,125,17,12,48,9,104,30,52,141,75,107,117,69,5,148,58,88,42,33,126,152,18,160,13,3
## 4  1,4,14,23,42,33,35,34,63,66,87,116,84,101,126,164,128,102,135,143,149,155,203,224,186,204,210,237,261,218,219,286,257,266,361,355,336
## 5  1,1,2,5,4,2,6,13,11,4,10,10,12,6,8,29,16,11,18,20,12,10,22,26,29,12,38,30,28,8,30,61,20,16,24,55,36,18,24,52,40,12,42,50,44,22,46,58,
## 6  0,31,59,90,120,151,181,212,243,273,304,334,365,396,424,455,485,516,546,577,608,638,669,699,730,761,789,820,850,881,911,942,973,1003,1
```

We can see that the test set also has 113,845 sequences indicated by `Id` .

Hence, it's learned that we are provided with 227,690 sequences in total from the OEIS, split 50% to 50% into a training and test set.

```
# Count all numbers in test set
test_numbers_count  = str_count(test$Sequence, ',') + 1
summary(test_numbers_count)
```

```
Min. 1st Qu.  Median    Mean 3rd Qu.    Max.
1.00   18.00   33.00   40.54   57.00  347.00
```

From above table, we find that of all the sequences in the training set the minimum length is 1, the maximum length is 347 meanwhile the mean value of the length is 40.54.

To further understand the features of the provided data sets, we merge both data sets to explore more info.

```
# Merge training and test data sets
dat = rbind(test, train)
dat = dat[order(dat$Id), ]
head(dat$Id, 20)
```

```
[1]  1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 20
```

```
print(object.size(dat), units = "Mb")
```

```
51.8 Mb
```

After that we will find the range of the merged data set.

```
# Extract the actual numbers
nums = strsplit(as.character(dat$Sequence), ',')
```

```
max(unlist(lapply(nums, FUN = max)))
```

```
[1] "99999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999
```

```
min(unlist(lapply(nums, FUN = min)))
```

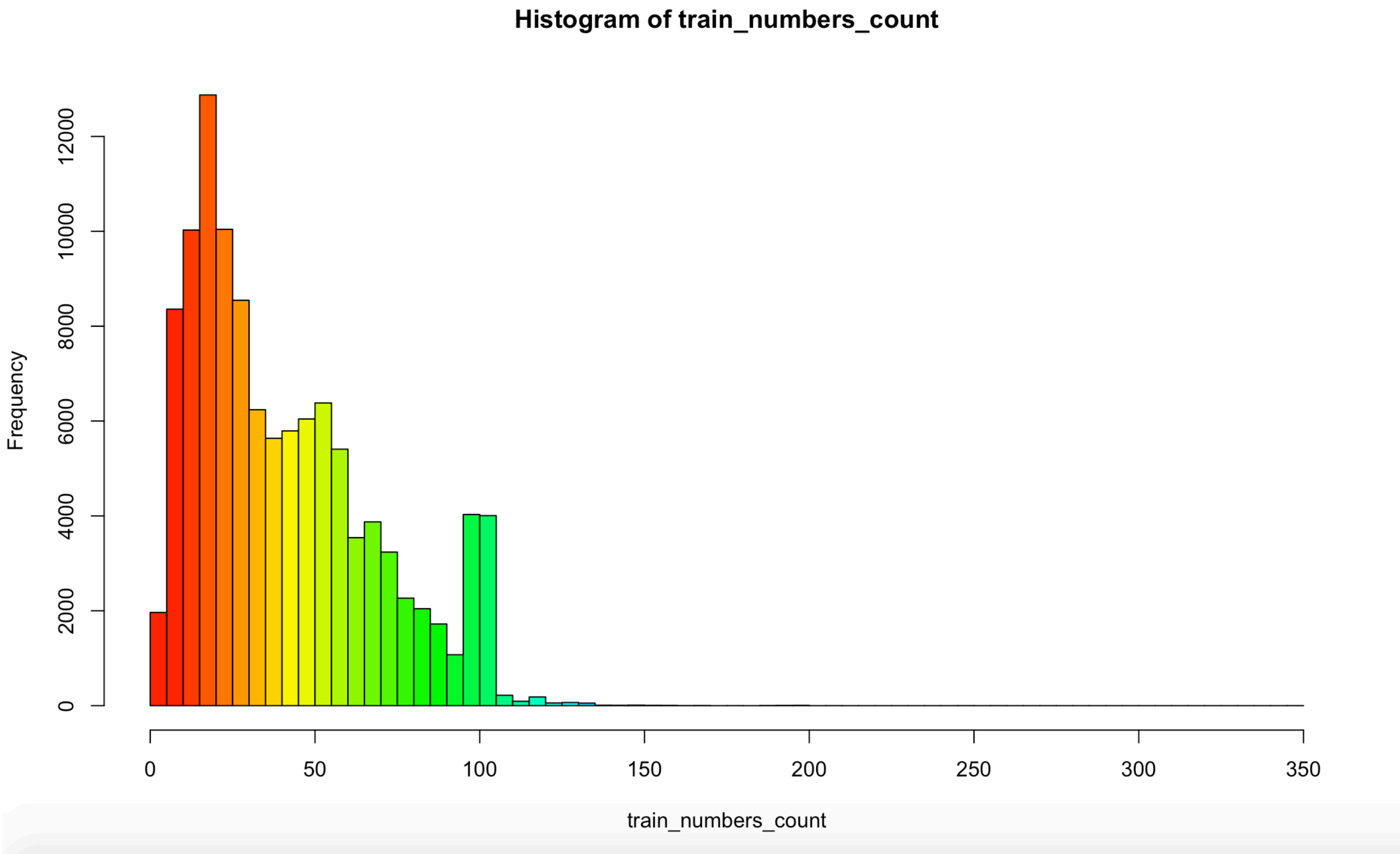
```
[1] "-1"
```

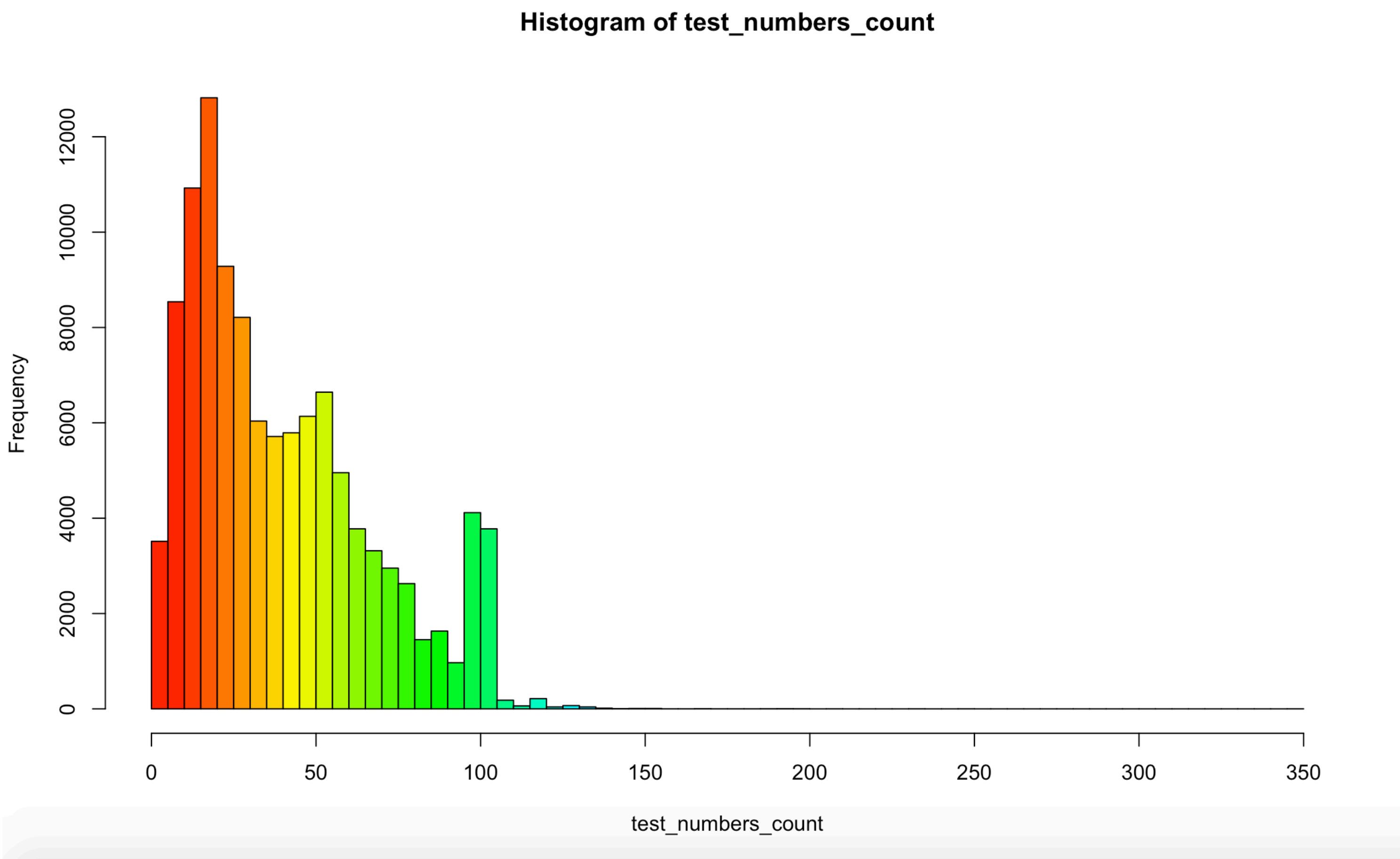
As shown above the input numbers of the sequences are ranging from "-1" to "99999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999999".

Exploratory Visualization

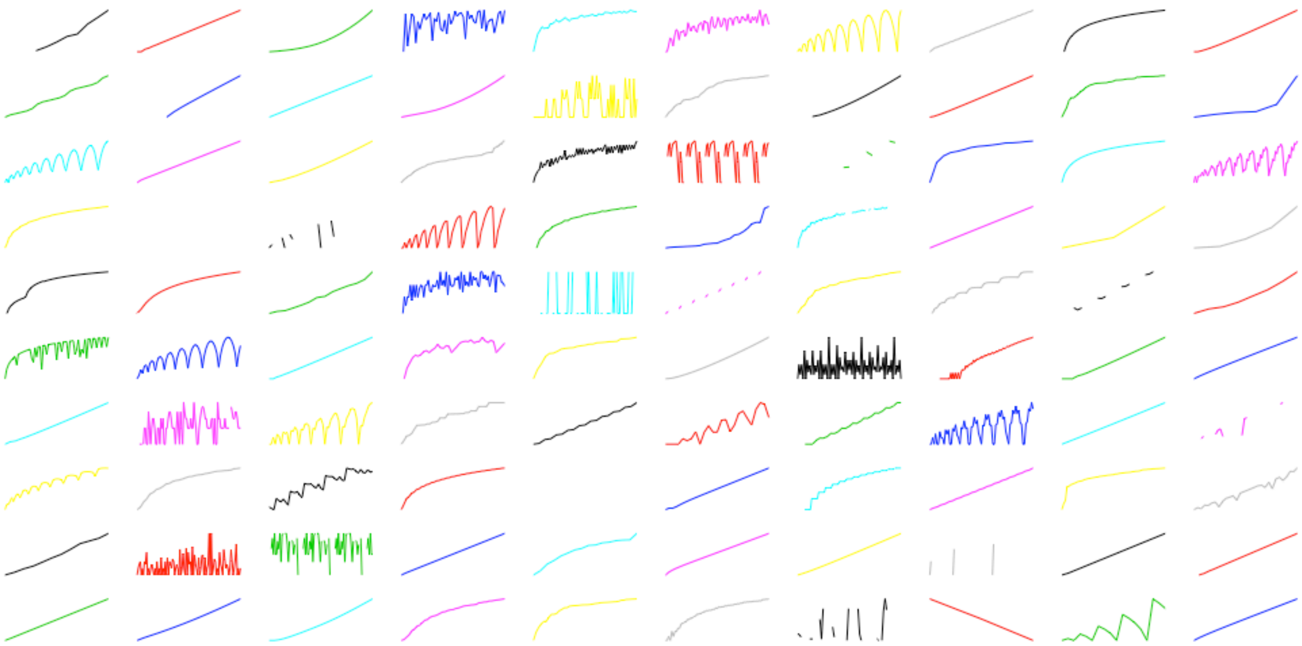
The sequences are made up of a linear sequences, logarithmic sequences, sequences with a modulus, and many other oddities. Firstly, we count all numbers in both sets, and then based on that to generate the illustrations regarding the count of numbers in each sequence versus its frequency in the dataset.

The details of this feature of both training set and test set are shown as follows:





To get an idea of what kind of dataset we are working with, we can illustrate some of these sequences after merging training set and test set together and making all the sequences sorted by Id in ascending order. The first 100 sequences are shown below. Please note that the data is on a log scale.



Algorithms and Techniques

As mentioned above, a number in a sequence is equivalent to a word. Based on this observation, we try to predict the last number based on the preceding numbers. Hence, the problem can be treated as the Natural Language Processing (NLP) domain.

It's known that RNNs can use their internal memory to process arbitrary sequences of inputs. This makes them applicable to tasks such as unsegmented, connected handwriting recognition or speech recognition.

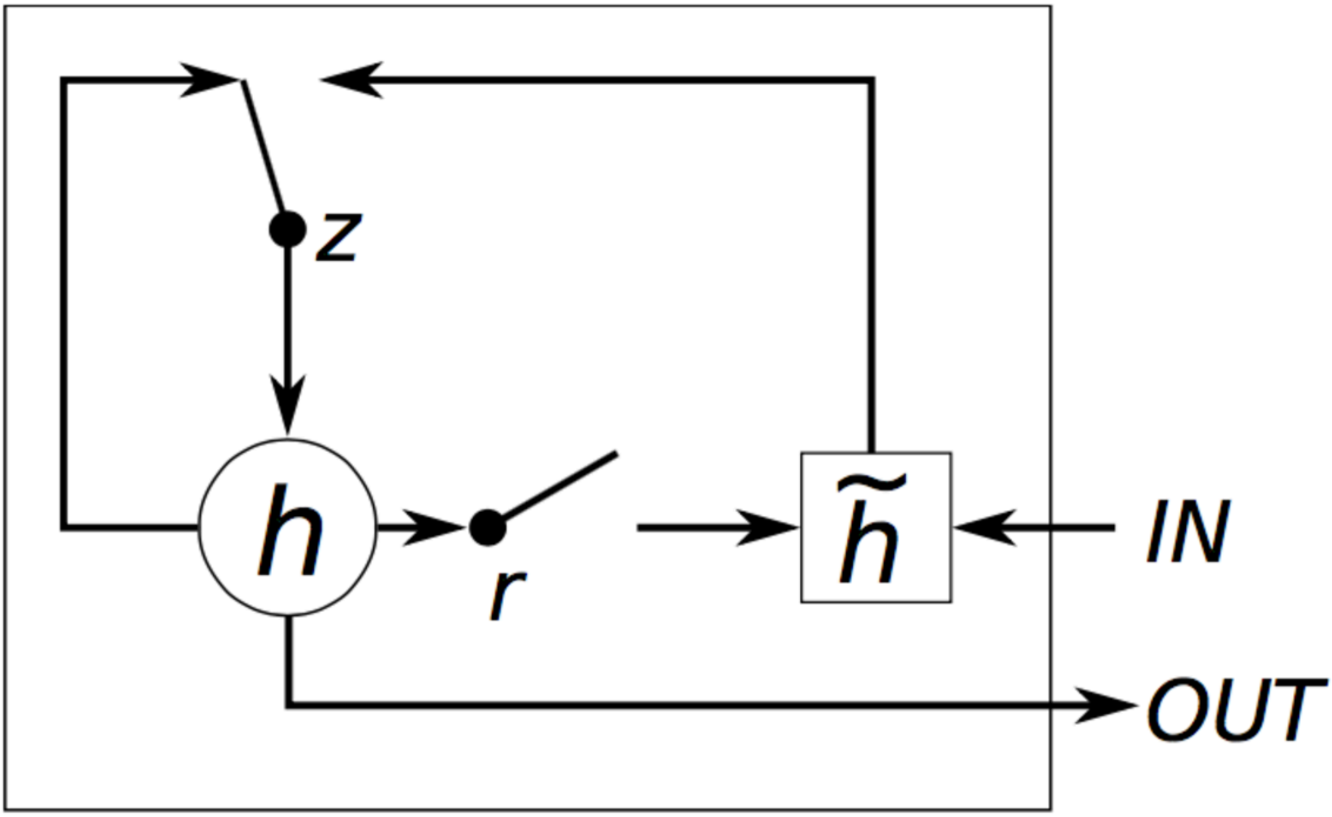
Training a RNN is similar to training a traditional Neural Network. Considering the parameters are shared by all time steps in the network, the gradient at each output depends not only on the calculations of the current time step, but also the previous time steps, we use the backpropagation algorithm to deal with it. For example, in order to calculate the gradient at the 4th step, we would need to backpropagate 3 steps and sum up the gradients. This is called Backpropagation Through Time (BPTT). For now, just be aware of the fact that vanilla RNNs trained with BPTT have difficulties learning long-term dependencies (e.g., dependencies between steps that are far apart) due to what is called the vanishing/exploding gradient problem.

To solve the problem, based on plain RNNs the Gated Recurrent Units (GRUs)[8] - a gating mechanism RNNs - will be used as the classifier to see if it can give reasonable prediction of a given sequence's last term in the test set (Long Short Term Memory (LSTM) networks[9] is also applicable but not used and discussed here).

The idea behind a GRU layer is quite similar to that of a LSTM layer, the equations are shown as follows.

$$
\begin{aligned}
z &= \sigma(x_t U^z + s_{t-1} W^z) \\
r &= \sigma(x_t U^r + s_{t-1} W^r) \\
h &= tanh(x_t U^h + (s_{t-1} \circ r) W^h) \\
s_t &= (1 - z) \circ h + z \circ s_{t-1}
\end{aligned}
$$

A GRU has two gates, a reset gate `r`, and an update gate `z`. Intuitively, the reset gate determines how to combine the new input with the previous memory, and the update gate defines how much of the previous memory to keep around. If we set the reset to all 1's and update gate to all 0's we again arrive at the plain RNN model.



There's just an additional `tanh` that squashes the output a bit. The gating mechanism is what allows GRUs to explicitly model long-term dependencies. By learning the parameters for its gates, the network learns how its memory should behave.

Benchmark

The `Mode` methodology is used as the benchmark model for the last number prediction in a certain sequence. For this, we simply find the mode in a given sequence, and that will be our guess for the last term in the sequence. The Mode Benchmark (implemented in R) seen on the competiton leaderboard[10] has an accuracy of `0.05746`.

```
Mode <- function(x) {
    ux <- unique(x)
    ux[which.max(tabulate(match(x, ux)))]
}
```

The top 20 accuracy scores of the competition leaderboard range between 0.20 - 0.59 (excluding an outlier in first place with a score of 0.98).

To be able to predict the last term with an accuracy score above 0.20 would be satisfactory, above 0.30 (top 10) would be great, and above 0.40 (top 3) would be outstanding.

III. Methodology

Data Preprocessing

Reading the provided CSV file produces a data frame of two variables, Id and Sequence. The Id variables are integers, and are exactly how we want them. The Sequence variable is in strings, so we will need to convert that to a list of numbers. Combining the use of `splitlines()` and `split()` function is a simple way to make it (refer to Implementation section for details).

Implementation

During the training classifer stage, the classifier was trained on the preprocessed training data. The specific implementation is shown below. The dataset is read from the CSV file and then saved to disk as Python pickle file to be loaded for training the model subsequently.

```python
# Map each character with the indicated index
def load_vocab():
    vocab = 'E,-0123456789'
    digit2idx = {digit:idx for idx, digit in enumerate(vocab)}
    idx2digit = {idx:digit for idx, digit in enumerate(vocab)}

    return digit2idx, idx2digit

def create_train_data():
    digit2idx, idx2digit = load_vocab()

    # Vectorize
    train_lines = [line.split('"')[1] for line in \
    open('../data/train.csv', 'r').read().splitlines()[1:]]
    test_lines = [line.split('"')[1] for line in \
    open('../data/test.csv', 'r').read().splitlines()[1:]]

    xs0, xs1, xs2, xs3 = [], [], [], []
    ys0, ys1, ys2, ys3 = [], [], [], []
    for i, line in enumerate(train_lines + test_lines):
        digits = line[-400:]

        # Numbers consisting of more than five digits are excluded
        # to avoid disturbing the training process
        isvalid = True
        for num in digits.split(","):
            if len(num) > 5:
                isvalid = False
                break
        if not isvalid:
            continue

        x = [digit2idx[digit] for digit in digits]
        y = [digit2idx[digit] for digit in (digits[1:] + ",")]

        # Data Bucketing
        if len(x) <= 100:
            x += [0] * (100 - len(x)) # Zero postpadding
            y += [0] * (100 - len(y)) # Zero postpadding
            xs0.append(x); ys0.append(y)
        elif len(x) <= 200:
            x += [0] * (200 - len(x)) # Zero postpadding
            y += [0] * (200 - len(y)) # Zero postpadding
            xs1.append(x); ys1.append(y)
        elif len(x) <= 300:
            x += [0] * (300 - len(x)) # Zero postpadding
            y += [0] * (300 - len(y)) # Zero postpadding
            xs2.append(x); ys2.append(y)
        else:
            x += [0] * (400 - len(x)) # Zero postpadding
            y += [0] * (400 - len(y)) # Zero postpadding
            xs3.append(x); ys3.append(y)

    X = [np.array(xs0), np.array(xs1), np.array(xs2), np.array(xs3)]
    Y = [np.array(ys0), np.array(ys1), np.array(ys2), np.array(ys3)]

    pickle.dump((X, Y), open('../data/train.pkl', 'wb'))

def load_train_data(num):
    X, Y = pickle.load(open('../data/train.pkl', 'rb'))
    return X[num], Y[num]
```

The training model is implemented in Python as shown below.

```
def build_model(seqlen):
    sequence = Input(shape=(seqlen,), dtype="int32")
    embedded = Embedding(13, 300, mask_zero=True)(sequence)
    gru1 = GRU(1000, return_sequences=True)(embedded)
    after_dp = Dropout(0.5)(gru1)
    gru2 = GRU(1000, return_sequences=True)(after_dp)
    after_dp = Dropout(0.5)(gru2)
    output = TimeDistributed(Dense(13, activation="softmax"))(after_dp)

    model = Model(inputs=sequence, outputs=output)

    return model
```

It's really a complication to achieve a proper training model to effectively solve the problem. For instance, the following questions were involved during the coding process:

- What kind of KNN layer to use.
- How to set relative hyperparameters (e.g., how many hidden layers should be selected).
- Which technique to include to reduce overfitting.

After serious consideration and repeated experiments, we could get the training model for this problem. The network architecture is "Inputs -> GRU Layer 1 of 1000 hidden units -> Dropout -> GRU Layer 2 of 1000 hidden units -> Dropout -> Time distributed dense -> Outputs".

After that, the classifier is trained on the preprocessed training data as described above. And then we do necessary predictions based on the training model.

```
for epoch in range(0, 30):
    for subepoch in range(4):
        num = epoch % 4

        # Load training set
        X, Y = load_train_data(num)
        Y = np.expand_dims(Y, -1)

        # Build model
        seqlen = X.shape[1]
        model = build_model(seqlen)

        # Compile model
        model.compile('adam', 'sparse_categorical_crossentropy', \
        metrics=['accuracy'])

        # Train model
        model.fit(X, Y, batch_size=64, epochs=1)
```

Refinement

As mentioned in the Implementation section, the network architecture includes two GRU layers with dropout after each one. But initially the network architecture just has one GRU layer without dropout, which will have an accuracy of below 0.10. To deal with this, one more GRU layer is added while appending dropout function after each GRU layer. Dropout will randomly drop weights in the layer it’s applied to during training and scales the weights so that the network keeps working during inference.

After the optimization, the final model is derived by subsequent training process which will have an accuracy of around 0.13 (the details will be discussed in next section).

IV. Results

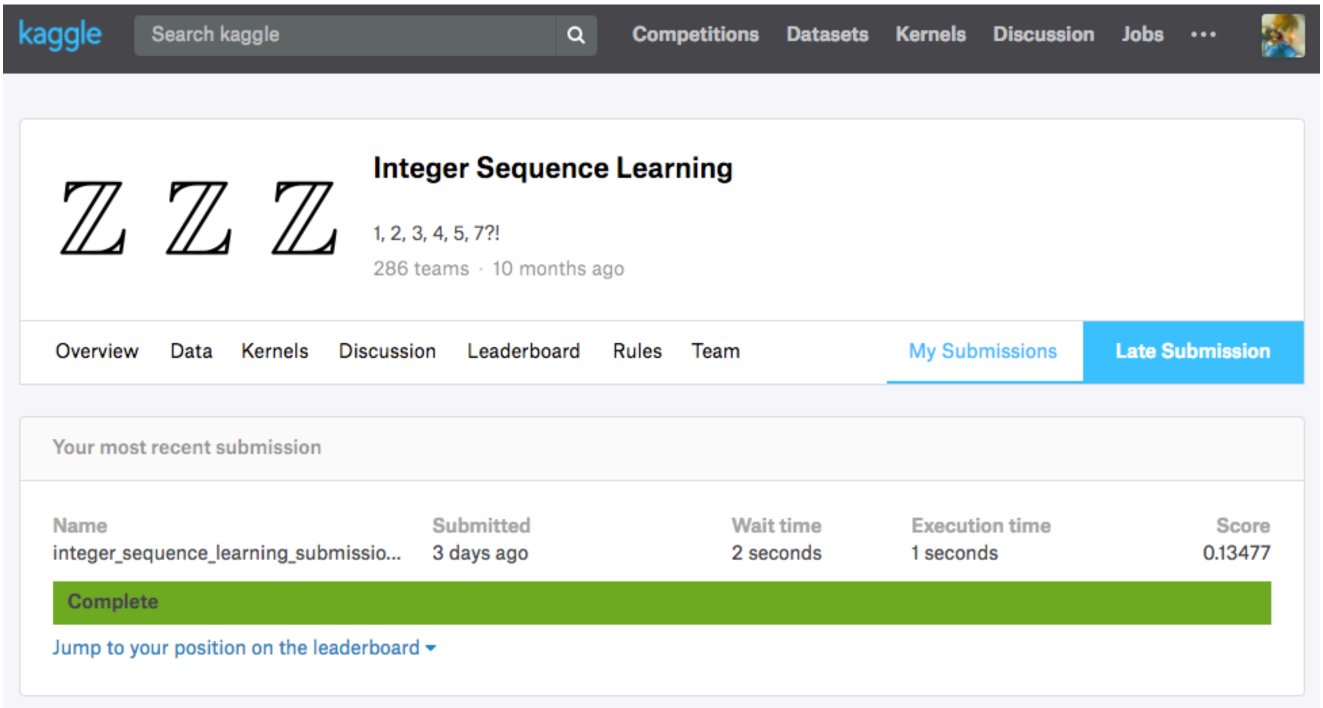
Model Evaluation and Validation

The metrics discussed at the beginning of the investigation (the prdiction accuracy, i.e., the percentage of sequences where the next number is predicted correctly) can be applied to judge the health and validate the designed model.

Based on multiple experiments, the final model used to implement predition in terms of architecture and hyperparameters is "Inputs -> GRU Layer 1 of 1000 hidden units -> Dropout -> GRU Layer 2 of 1000 hidden units -> Dropout -> Time distributed dense -> Outputs".

As for the test set the final element has been removed, which is the target we are trying to predict. Based on above model, we will try to generate the last item of each sequence of the test set.

The big question of this investigation, is whether this model can be used to predict the last term of a given sequence accurately. As the nature of the challenge was a contest, the predictions created by the model were submitted online on Kaggle for a blind evaluation and received a decent score `0.13477`.



Kaggle's evaluation system gave a well formed tests covering a variety of test cases (113,845 scenarios), which is a objective way to test and prove the robustness of the model. Therefore, given the score generated by Kaggle, we can say that the model does generalize well to unseen data and it's not sensitive to small changes in the data or to outliers. Essentially, we trust this model as well as its predition results.

Justification

In the Benchmark section the `Mode` methodology is discussed as the benchmark model for the last number prediction in a certain sequence. Compared with the Mode Benchmark with an accuracy of `0.05746`, the predictions generated by the designed model can be regarded as meeting the specification considering only the top 20 accuracy scores of the competition leaderboard are greater than 0.20.

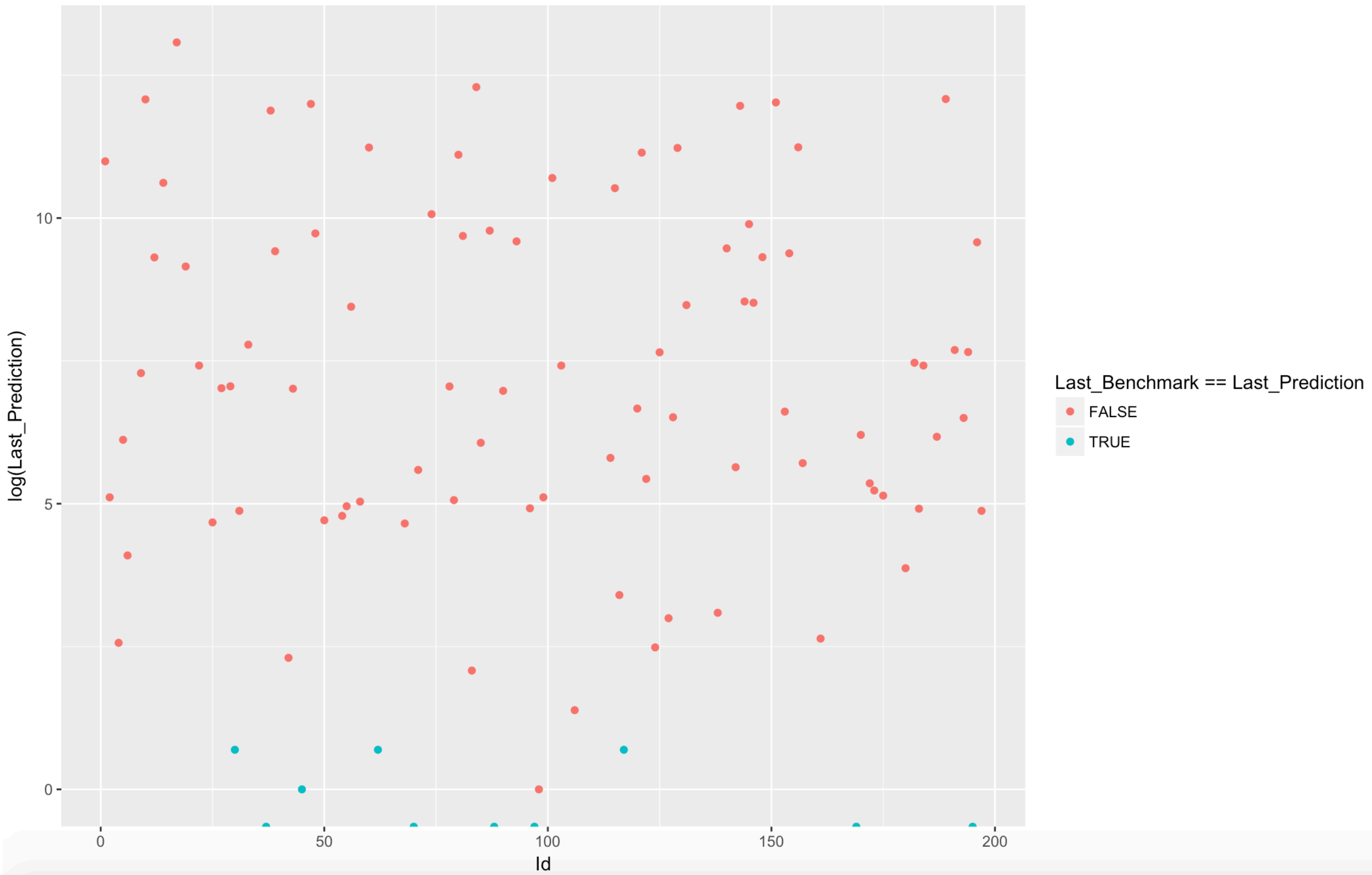
V. Conclusion

Free-Form Visualization

Based on the predictions created by the final model and the results generated by benchmark model, we would like to make a plot to get a clear and straightforward understanding about the designed model's performance.

Considering the big volume of the datasets, we only take the first 100 rows as data input to plot. The plot shown below is plotted with `Id` as x-axis and the predicted last term by the training model as y-axis (on a log scale). All the values which are the same as benchmark model are marked by `blue` color.

It's observed that there are only measly points share the same prediction results, the training model has improved the prediction capability to some degree.



Reflection

During solving the problem, many standard techniques were applied: first, a data cleaning step to identify the dataset's features programmatically, then transforming the strings into numbers via the vectorization method, and finally building a specific model based on the dataset's characteristics.

I found that training the classifier using the data input was the most difficult part. It's very difficult to decide the consisting layer and the hyperparameters to build the model. Some empirically-derived rules-of-thumb were taken into consideration to handle it meanwhile the final model structure was also based on multiple experiments. It's exciting to see that the final model designed for the problem achieves decent accuracy score.

As for the most interesting aspects of the project, I'm very delighted that I used RNNs to deal with this problem as I think it will be quite useful for later projects/experiments. I'm also happy about getting to use TensorFlow and Keras, as they are the most popular deep learning libraries in AI field.

Improvement

With ample time, this investigation could be expanded by experimenting with the effects of adding more GRU layers to the classifier until it starts to overfit the training set there and arrive at a tipping point at which it loses accuracy.

In addition, the parameters such as the dimensionality of the output space, activation function can be modified to achieve the optimal training model.

Other classifiers are always fair contestants when trying to tackle such scale issues with larger datasets. For instance, Long Short Term Memory (LSTM) networks would be a good candidate to investigate. In addition, [Natural Language Toolkit (NLTK)][11] would be a good choice to implement NLP related projects.

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1. "Powers of primes. Alternatively, 1 and the prime powers (p^k, p prime, k >= 1). (Formerly M0517 N0185)", *https://oeis.org/A000961* ↩
2. Natural language processing from Wikipedia, the free encyclopedia, *https://en.wikipedia.org/wiki/Natural*language*processing* ↩
3. Kaggle Integer Sequence Learning Dataset, *https://www.kaggle.com/c/integer-sequence-learning/data* ↩
4. On-Line Encyclopedia of Integer Sequences® (OEIS®) Official Website, *https://oeis.org* ↩
5. Kaggle Official Website, *https://www.kaggle.com* ↩
6. Kaggle Integer Sequence Learning Competition, *https://www.kaggle.com/c/integer-sequence-learning* ↩
7. Recurrent Neural Networks from Wikipedia, the free encyclopedia, *https://en.wikipedia.org/wiki/Recurrent*neural*network* ↩

8. Gated Recurrent Units (GRUs), *https://en.wikipedia.org/wiki/Gated*recurrent*unit* ↩

9. Long Short Term Memory (LSTM) networks, *https://en.wikipedia.org/wiki/Long*short-term*memory* ↩

10. Kaggle Integer Sequence Learning Competition Leaderboard, *https://www.kaggle.com/c/integer-sequence-learning/leaderboard* ↩

11. Natural Language Toolkit (NLTK), *http://www.nltk.org* ↩