

LSTM Autoencoder for Extreme Rare Event Classification in Keras

Here we will learn the details of data preparation for LSTM models, and build an LSTM Autoencoder for rare-event classification.



This post is a continuation of my previous post Extreme Rare Event Classification using Autoencoders. In the previous post, we talked about the challenges in an extremely rare event data with less than 1% positively labeled data. We built an Autoencoder Classifier for such processes using the concepts of Anomaly Detection.

However, the data we have is a time series. But earlier we used a Dense layer Autoencoder that does not use the temporal features in the data. Therefore, in this post, we will improve on our approach by building an LSTM Autoencoder.

Here, we will learn:

- data preparation steps for an LSTM model,
- · building and implementing LSTM autoencoder, and
- using LSTM autoencoder for rare-event classification.

Quick recap on LSTM:

- LSTM is a type of Recurrent Neural Network (RNN). RNNs, in general, and LSTM, specifically, are used on sequential or time series data.
- These models are capable of automatically extracting effect of past events.
- LSTM are known for its ability to extract both long- and short- term effects of pasts event.

In the following, we will go directly to developing an LSTM Autoencoder. It is recommended to read <u>Step-by-step understanding LSTM Autoencoder layers</u> to better understand and further improve the network below.

About the data problem in brief, we have real-world data on sheet breaks from a paper manufacturing. Our objective is to predict the break in advance. Please refer to Extreme Rare Event Classification using Autoencoders for the details on the data, problem, and the classification approach.

LSTM Autoencoder for Multivariate Data

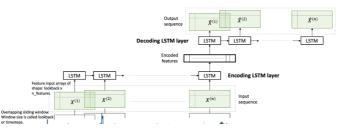


Figure 1. An LSTM Autoencoder.

In our problem, we have a multivariate time-series data. A multivariate time-series data contains multiple variables observed over a period of time. We will build an LSTM autoencoder on this multivariate time-series to perform rare-event classification. As described in [1], this is achieved by using an anomaly detection approach:

- we build an autoencoder on the normal (negatively labeled) data,
- · use it to reconstruct a new sample,
- if the reconstruction error is high, we label it as a sheet-break.

LSTM requires few special data-preprocessing steps. In the following, we will give sufficient attention to these steps.

Let's get to the implementation.

Libraries

I like to put together the libraries and global constants first.

```
%matplotlib inline
import matplotlib.pyplot as plt
import seaborn as sns
import pandas as pd
import numpy as np
from pylab import rcParams
import tensorflow as tf
Import tensorIoW as tr
from keras import optimizers, Sequential
from keras.models import Model
from keras.utils import plot_model
from keras.layers import Dense, LSTM, RepeatVector, TimeDistributed
from keras.callbacks import ModelCheckpoint, TensorBoard
from sklearn.preprocessing import StandardScaler
from sklearn.model_selection import train test_split
from sklearn.metrics import confusion_matrix, precision_recall_curve
from sklearn.metrics import recall_score, classification_report, auc,
from sklearn.metrics import precision_recall_fscore_support, f1_score
from numpy.random import seed
from tensorflow import set_random_seed
set_random_seed(11
from sklearn.model_selection import train_test_split
SEED = 123 #used to help randomly select the data points
DATA SPLIT PCT = 0.2
rcParams['figure.figsize'] = 8, 6
LABELS = ["Normal", "Break"]
```

Data Preparation

As mentioned before, LSTM requires a few specific steps in the data preparation. The input to LSTMs are 3-dimensional arrays created from the time-series data. This is an **error prone step** so we will look at the details.

Read data

The data is taken from [2]. The link to the data is here.

```
df = pd.read_csv("data/processminer-rare-event-mts - data.csv")
df.head(n=5)  # visualize the data.
```

```
| This |
```

```
4 5/1/99 0 0.265578 -4.749928 -4.333150 15.267340 -0.155314 -17.505913 0.000732 -0.061114 ... 10.109054 0.091121 -4.939414
5 rows x 63 columns
```

Curve Shifting

As also mentioned in [1], the objective of this rare-event problem is to predict a sheet-break before it occurs. We will try to predict the break up to 4 minutes in advance. For this data, this is equivalent to shifting the labels up by two rows. It can be done directly with df.y=df.y.shift(-2). However, here we require to do the following,

- For any row *n* with label 1, make (*n*-2):(*n*-1) as 1. With this, we are teaching the classifier to predict **up to** 4 minutes ahead. And,
- remove row n. Row n is removed because we are not interested in teaching the classifier to predict a break when it has already happened.

We develop the following function to perform this curve shifting.

We will now shift our data and verify if the shifting is correct. In the subsequent sections, we have few more test steps. It is recommended to use them to ensure the data preparation steps are working as expected.

```
print('Before shifting')  # Positive labeled rows before shifting.
one_indexes = df.index[df['y'] == 1]
display(df.iloc[(np.where(np.array(input_y) == 1)[0][0]-5):
(np.where(np.array(input_y) == 1)[0][0]+1), ])

# Shift the response column y by 2 rows to do a 4-min ahead prediction.
df = curve_shift(df, shift_by = -2)
print('After shifting')  # Validating if the shift happened correctly.
display(df.iloc[(one_indexes[0]-4):(one_indexes[0]+1),
0:5].head(n=5))
```

Before shifting

```
| 256 | 5/1/99 8:32 | 0 | 1.016235 | -4.058394 | -1.097158 |
| 257 | 5/1/99 8:32 | 0 | 1.005602 | -3.876199 | -1.074373 |
| 258 | 5/1/99 8:38 | 0 | 0.933933 | -3.868467 | -1.249954 |
| 259 | 5/1/99 8:38 | 1 | 0.892311 | -13.332664 | -10.006578 |
| 260 | 5/1/99 10:50 | 0 | 0.020062 | -3.987897 | -1.248529 |
| 261 | 1 | 1 | 1 | 1 | 1 | 1 |
| 262 | 1 | 1 | 1 | 1 | 1 | 1 |
| 263 | 5/1/99 8:30 | 0 | 0 | 0.997107 | -3.865720 | -1.133779 |
```



If we note here, we moved the positive label at 5/1/99~8:38 to n-1 and n-2 timestamps, and dropped row n. Also, there is a time difference of more than 2 minutes between a break row and the next row. This is because, when a break occurs, the machine stays in the break status for a while. During this time, we have y=1 for consecutive rows. In the provided data, these consecutive break rows are deleted to prevent the classifier from learning to predict a break **after** it has already happened. Refer [2] for details.

Before moving forward, we clean up the data by dropping the time, and two other categorical columns.

```
# Remove time column, and the categorical columns
df = df.drop(['time', 'x28', 'x61'], axis=1)
```

Prepare Input Data for LSTM

LSTM is a bit more demanding than other models. Significant amount of time and attention may go in preparing the data that fits an LSTM. However, it is generally worth the effort.

The input data to an LSTM model is a 3-dimensional array. The shape of the array is *samples* x *lookback* x *features*. Let's understand them,

- *samples*: This is simply the number of observations, or in other words, the number of data points.
- lookback: LSTM models are meant to look at the past. Meaning, at time t
 the LSTM will process data up to (t-lookback) to make a prediction.
- features: It is the number of features present in the input data.

First, we will extract the features and response.

```
input_X = df.loc[:, df.columns != 'y'].values # converts the df to a
numpy array
input_y = df['y'].values

n_features = input_X.shape[1] # number of features
```

The $input_x$ here is a 2-dimensional array of size *samples* x *features*. We want to be able to transform such a 2D array into a 3D array of size: *samples* x *lookback* x *features*. Refer to Figure 1 above for a visual understanding.

For that, we develop a function ${\scriptsize \texttt{temporalize}}$.

```
output_X.append(t)
  output_y.append(y[i + lookback + 1])
return np.squeeze(np.array(output_X)), np.array(output_y)
```

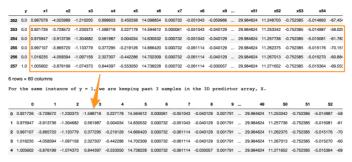
To test and demonstrate this function, we will look at an example below with lookback = 5.

```
print('First instance of y = 1 in the original data')
display(df.iloc[(np.where(np.array(input_y) == 1)[0][0]-5):
    (np.where(np.array(input_y) == 1)[0][0]+1), ])

lookback = 5  # Equivalent to 10 min of past data.
# Temporalize the data
X, y = temporalize(X = input_X, y = input_y, lookback = lookback)

print('For the same instance of y = 1, we are keeping past 5 samples in the 3D predictor array, X.')
display(pd.DataFrame(np.concatenate(X[np.where(np.array(y) == 1)[0][0]], axis=0)))
```

First instance of y = 1 in the original data



What we are looking for here is,

- In the original data, y = 1 at row 257.
- With lookback = 5 we want the LSTM to look at the 5 rows before row 257 (including itself).
- In the 3D array, x, each 2D block at x[i,:,:] denotes the prediction data that corresponds to y[i]. To draw an analogy, in regression y[i] corresponds to a 1D vector x[i,:]; in LSTM y[i] corresponds to a 2D array x[i,:,:].
- This 2D block x[i,:,:] should have the predictors at $input_x[i,:]$ and the previous rows up to the given lookback.
- As we can see in the output above, the x[i,:,:] block in the bottom is
 the same as the five past rows of y=1 shown on the top.
- Similarly, this is applied for the entire data, for all y's. The example here
 is shown for an instance of y=1 for easier visualization.

Split into train, valid, and test

This is straightforward with the sklearn function.

```
X_train, X_test, y_train, y_test = train_test_split(np.array(X),
np.array(y), test_size=DATA_SPLIT_PCT, random_state=SEED)

X_train, X_valid, y_train, y_valid = train_test_split(X_train,
y_train, test_size=DATA_SPLIT_PCT, random_state=SEED)
```

For training the autoencoder, we will be using the X coming from only the negatively labeled data. Therefore, we separate the X corresponding to y=0

```
X_train_y0 = X_train[y_train==0]
X_train_y1 = X_train[y_train==1]
```

```
X_valid_y0 = X_valid[y_valid==0]
X_valid_y1 = X_valid[y_valid==1]
```

We will reshape the X's into the required 3D dimension: $sample \times lookback \times features$.

```
X_train = X_train.reshape(X_train.shape[0], lookback, n_features)
X_train_y0 = X_train_y0.reshape(X_train_y0.shape[0], lookback,
n_features)
X_train_y1 = X_train_y1.reshape(X_train_y1.shape[0], lookback,
n_features)

X_valid = X_valid.reshape(X_valid.shape[0], lookback, n_features)
X_valid_y0 = X_valid_y0.reshape(X_valid_y0.shape[0], lookback,
n_features)
X_valid_y1 = X_valid_y1.reshape(X_valid_y1.shape[0], lookback,
n_features)

X_test = X_test.reshape(X_test.shape[0], lookback, n_features)
```

Standardize the Data

It is usually better to use a standardized data (transformed to Gaussian with mean 0 and standard deviation 1) for autoencoders.

One common standardization mistake is: we normalize the entire data and then split into train-test. This is incorrect. Test data should be completely unseen to anything during the modeling. We should, therefore, normalize the training data, and use its summary statistics to normalize the test data (for normalization, these statistics are the mean and variances of each feature).

Standardizing this data is a bit tricky. This is because the X matrices are 3D, and we want the standardization to happen with respect to the original 2D data.

To do this, we will require two UDFs.

- flatten: This function will re-create the original 2D array from which the 3D arrays were created. This function is the inverse of temporalize, meaning x = flatten(temporalize(x)).
- scale: This function will scale a 3D array that we created as inputs to the LSTM.

```
def flatten(X):
     Flatten a 3D array.
                A 3D array for 1stm, where the array is sample \boldsymbol{x}
timesteps x features.
     Output
     flattened_X A 2D array, sample x features.
     {\tt flattened\_X = np.empty((X.shape[0], X.shape[2]))} \  \  \# \  \  {\tt sample \ } x
flattened_
features array.
for i in range(X.shape[0]):
    flattened_X[i] = X[i, (X.shape[1]-1), :]
def scale(X, scaler):
     Scale 3D array.
                      A 3D array for 1stm, where the array is sample x
timesteps x features.
scaler A scaler object, e.g.,
sklearn.preprocessing.StandardScaler, sklearn.preprocessing.normalize
     Output
                      Scaled 3D array.
     for i in range(X.shape[0]):
    X[i, :, :] = scaler.transform(X[i, :, :])
     return X
```

Why didn't we first normalize the original 2D data and then create the 3D arrays? Because, to do this we will: split the data into train and test, followed by their normalization. However, when we create the 3D arrays on the test

data, we lose the initial rows of samples up till the lookback. Splitting into train-valid-test will cause this for both the validation and test sets.

We will fit a Standardization object from $_{\tt sklearn}$. This function standardizes the data to Normal(0, 1). Note that we require to flatten the $x_{\tt train_y0}$ array to pass to the $_{\tt fit}$ function.

```
# Initialize a scaler using the training data.
scaler = StandardScaler().fit(flatten(X_train_y0))
```

We will use our UDF, scale, to standardize x_train_y0 with the fitted transform object scaler.

```
X_train_y0_scaled = scale(X_train_y0, scaler)
```

Make sure the scale worked correctly?

A correct transformation of $x_{\tt train}$ will ensure that the means and variances of each column of the flattened $x_{\tt train}$ are 0 and 1, respectively. We test this.

```
a = flatten(X_train_y0_scaled)
print('colwise mean', np.mean(a, axis=0).round(6))
print('colwise variance', np.var(a, axis=0))
```

All the means and variances outputted above are 0 and 1, respectively. Therefore, the scaling is correct. We will now scale the validation and test sets. We will again use the <code>scaler</code> object on these sets.

```
X_valid_scaled = scale(X_valid, scaler)
X_valid_y0_scaled = scale(X_valid_y0, scaler)

X_test_scaled = scale(X_test, scaler)
```

LSTM Autoencoder Training

We will, first, initialize few variables.

```
timesteps = X_train_y0_scaled.shape[1] # equal to the lookback
n_features = X_train_y0_scaled.shape[2] # 59
epochs = 200
batch = 64
lr = 0.0001
```

We, now, develop a simple architecture.

```
lstm_autoencoder = Sequential()
# Encoder
lstm_autoencoder.add(LSTM(32, activation='relu', input_shape=
(timesteps, n_features), return_sequences=True))
lstm_autoencoder.add(LSTM(16, activation='relu',
return_sequences=False))
lstm_autoencoder.add(RepeatVector(timesteps))
# Decoder
lstm_autoencoder.add(LSTM(16, activation='relu',
return_sequences=True))
lstm_autoencoder.add(LSTM(32, activation='relu',
return_sequences=True))
lstm_autoencoder.add(TimeDistributed(Dense(n_features)))
lstm_autoencoder.summary()
```

| Layer (type) | Output | Shape | Param # |
|-----------------------------------------------------------------------------|--------|--------|---------|
| Lstm_23 (LSTM) | (None, | 5, 32) | 11776 |
| stm_24 (LSTM) | (None, | 16) | 3136 |
| epeat_vector_7 (RepeatVecto | (None, | 5, 16) | 0 |
| stm_25 (LSTM) | (None, | 5, 16) | 2112 |
| stm_26 (LSTM) | (None, | 5, 32) | 6272 |
| time_distributed_6 (TimeDist | (None, | 5, 59) | 1947 |
| Cotal params: 25,243 Crainable params: 25,243 Non-trainable params: 0 | | | |

From the summary(), the total number of parameters are 5,331. This is about half of the training size. Hence, this is an appropriate model to fit. To have a bigger architecture, we will need to add regularization, e.g. Dropout, which will be covered in the next post.

Now, we will train the autoencoder.

```
Train on 11691 samples, validate on 2923 samples
Epoch 1/500
- 8s - loss: 0.9955 - val_loss: 1.0305
Epoch 2/500
- 2s - loss: 0.9949 - val_loss: 1.0282
Epoch 3/500
- 2s - loss: 0.9709 - val_loss: 0.9869
Epoch 4/500
- 2s - loss: 0.9382 - val_loss: 0.9601
Epoch 5/500
- 2s - loss: 0.9399 - val_loss: 0.9326
```

Plotting the change in the loss over the epochs.

```
plt.plot(lstm_autoencoder_history['loss'], linewidth=2,
label='Train')
plt.plot(lstm_autoencoder_history['val_loss'], linewidth=2,
label='Valid')
plt.legend(loc='upper right')
plt.title('Model loss')
plt.ylabel('Loss')
plt.ylabel('Loss')
plt.xlabel('Epoch')
plt.show()
```

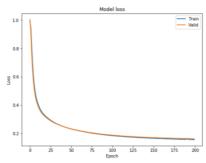


Figure 2. Loss function over the epochs.

Classification

Similar to the <u>previous post</u> [1], here we show how we can use an Autoencoder reconstruction error for the rare-event classification. We

follow this concept: the autoencoder is expected to reconstruct a noif the reconstruction error is high, we will classify it as a sheet-break.

We will need to determine the threshold for this. Also, note that here we will be using the entire validation set containing both y=0 or 1.

Note that we have to flatten the arrays to compute the mse.

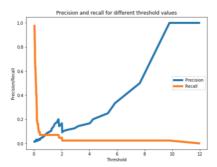


Figure 3. A threshold of 0.3 should provide a reasonable trade-off between precision and recall, as we want to higher recall.

Now, we will perform classification on the test data.

We should not estimate the classification threshold from the test data. It will result in overfitting.

Figure 4. Using threshold = 0.8 for classification. The orange and blue dots above the threshold line represents the True Positive and False Positive, respectively.

In Figure 4, the orange and blue dot above the threshold line represents the True Positive and False Positive, respectively. As we can see, we have good number of false positives.

Let's see the accuracy results.

Test Accuracy

Confusion Matrix

```
pred_y = [1 if e > threshold_fixed else 0 for e in
error_df.Reconstruction_error.values]

conf_matrix = confusion_matrix(error_df.True_class, pred_y)

plt.figure(figsize=(6, 6))
sns.heatmap(conf_matrix, xticklabels=LABELS, yticklabels=LABELS,
annot=True, fmt="d");
plt.title("Confusion matrix")
plt.ylabel('True class')
plt.ylabel('True class')
plt.show()
```



Figure 5. Confusion matrix showing the True Positives and False Positives.

ROC Curve and AUC

```
false_pos_rate, true_pos_rate, thresholds =
roc_curve(error_df.True_class, error_df.Reconstruction_error)
roc_auc = auc(false_pos_rate, true_pos_rate,)

plt.plot(false_pos_rate, true_pos_rate, linewidth=5, label='AUC =
%0.3f'% roc_auc
plt.plot([0,1],[0,1], linewidth=5)

plt.xlim([-0.01, 1])
plt.ylim([0, 1.01])
plt.legend(loc='lower right')
plt.title('Receiver operating characteristic curve (ROC)')
plt.ylabel('True Positive Rate')
plt.xlabel('False Positive Rate')
plt.show()
```



Figure 6. The ROC curve.

We see approximately 10% improvement in the AUC compared to the dense layer Autoencoder in $[\underline{1}]$. From the Confusion Matrix in Figure 5, we could predict 10 out of 39 break instances. As also discussed in $[\underline{1}]$, this is significant for a paper mill. However, the improvement we achieved in comparison to the dense layer Autoencoder is minor.

The primary reason is LSTM model has more parameters to estimate. It becomes important to use regularization with LSTMs. Regularization and other model improvements will be discussed in the next post.

Github repository

cran2367/lstm_autoencoder_classifier

An LSTM Autoencoder for rare event classification. Contribute to cran2367/lstm_autoencoder_classifier development by...





What can be done better?

In the next article, we will learn tuning an Autoencoder. We will go over,

- · CNN LSTM Autoencoder,
- · Dropout layer,
- LSTM Dropout (Dropout_U and Dropout_W)
- · Gaussian-dropout layer
- · SELU activation, and
- alpha-dropout with SELU activation.

Conclusion

This post continued the work on extreme rare event binary labeled data in [1]. To utilize the temporal patterns, LSTM Autoencoders is used to build a rare event classifier for a multivariate time-series process. Details about the data preprocessing steps for LSTM model are discussed. A simple LSTM Autoencoder model is trained and used for classification. Some improvement in the accuracy over a Dense Autoencoder is found. For further improvement, we will look at ways to improve an Autoencoder with Dropout and other techniques in the next post.

. . .

Follow-up Read

It is recommended to read <u>Step-by-step understanding LSTM Autoencoder layers</u> to clear the LSTM network concepts.

References

- 1. Extreme Rare Event Classification using Autoencoders in Keras
- 2. Ranjan, C., Mustonen, M., Paynabar, K., & Pourak, K. (2018). Dataset: Rare Event Classification in Multivariate Time Series. <u>arXiv preprint</u> <u>arXiv:1809.10717</u>
- 3. Time-series forecasting with deep learning & LSTM autoencoders
- 4. Complete code: LSTM Autoencoder

Disclaimer: The scope of this post is limited to a tutorial for building an LSTM Autoencoder and using it as a rare-event classifier. A practitioner is expected to achieve better results for this data by network tuning. The purpose of the article is helping Data Scientists implement an LSTM Autoencoder.

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