Listing 7.18. The covariance of encoded features

```
encoder_model = Model(inputs=autoencoder.inputs,
                      outputs=autoencoder.get_layer(
                         'encoder').output)
encoded_features = np.array(encoder_model.predict(X)
   )
print('Encoded feature covariance\n',
      np.round(np.cov(encoded_features.T), 3))

# Encoded feature covariance
#   [[ 0.01 -0.     0.    -0.02]
#   [-0.     0.     0.    -0.02]
#   [ 0.     0.     0.02 -0.02]
#   [-0.02 -0.02 -0.02  4.36]]
```

7.8 Rules-of-thumb

- **Autoencoder Construction**.
  - Add unit-norm constraint on the weights. This prevents ill-conditioning of the model.
  - Add a linearly activated dense layer at the end of the encoder and decoder for calibration in most autoencoders.
  - The activation on the decoder output layer should be based on the range of the input. For example, `linear` if the input $\boldsymbol{x}$ is in $(-\infty, \infty)$ (scaled with `StandardScaler`) or `sigmoid` if $\boldsymbol{x}$ is in $(0, 1)$ (scaled with `MinMaxScaler`).
- **Sparse autoencoder**.
  - A sparsity constraint should be added to the encoder's output. Typically, it is a dense layer. The sparsity can be added as `activity_regularizer=tf.keras.regularizers.L1(l1=0.01)`.
  - The encoding size should be equal to the original data dimension (overcomplete). The sparsity penalty ensures that the encodings are useful and not trivial.
  - Sparse encodings are best suited for use in other tasks such as classification.

- **Denoising autoencoder**.
  - Unlike sparse autoencoders, denoising autoencoders regularize the decoder output to make them insensitive to minor changes in the input.
  - Train a denoising autoencoder by adding small gaussian noise to the input. Ensure that the loss function minimizes the difference of the original data $\boldsymbol{x}$ with the decodings of the noisy data $g(f(\boldsymbol{x}+\boldsymbol{\epsilon}))$ where $\boldsymbol{\epsilon}$ is Gaussian(0,σ).
  - They are useful for denoising or reconstruction objectives. But their encodings are typically not useful for classification tasks.
- **LSTM autoencoder**.
  - Use `tanh` activation in the LSTM layers in both encoder and decoder.
  - Works better for translation tasks, for example, English to Spanish text translation. Typically, they do not work well for data reconstruction.
- **Convolutional autoencoder**.
  - Encoder module has a stack of `Conv` and `Pooling` layers. They perform summarization of the useful features of the data.
  - Decoder module has a stack of `ConvTranspose` and `BatchNormalization` layers.
  - Decoder module should **not** have `Conv` or `Pooling` layers.

7.9 Exercises

1. At the beginning of the chapter it is mentioned that autoencoders were conceptualized with inspiration from an older concept of principal component analysis (PCA) in statistics.

   (a) A PCA model is linear. It was mentioned in § 4.2 that a dense layer network is equivalent to a linear model if the activations on each layer are linear (proved in Appendix A). Extending this to a dense autoencoder, does it become the same as a principal component analysis (PCA) model if the activations are linear? Refer to § 7.7.1.

   (b) Under what conditions an autoencoder becomes equivalent to PCA? Refer to § 7.2 and § 7.7.1.

2. In § 7.6.1 and 7.6.2 it is mentioned that a linearly activated dense layer should be added at the end of encoder and decoder modules.

   (a) What is the benefit of the linear dense layers?

   (b) When is it not essential?

   (c) Is it more essential in decoder than encoder? Explain.

3. The chapter provides examples of shallow autoencoders. In building a deep autoencoder what would you do in the following scenario?

   (a) In constructing a Sparse autoencoder would you consider adding sparsity penalty on the activations (output) of the intermediate layers in the encoder versus only on the last encoder layer?

   (b) An autoencoder is essentially a special case of a feed-forward network where both the predictors and the response are the same. Looking at an autoencoder from this perspective sometimes makes it difficult to separate encoder and decoder. Essentially, to tell the boundary. This becomes even harder in a deep network. How would you distinguish where an encoder ends and a decoder begins?

4. In § 7.7.1 a few aspects of regularizing autoencoder by constraining encoder and decoder are discussed. Based on them,

   (a) Should you consider regularizing the encoder or decoder functions f and g, respectively? Why?

   (b) If following the structure of the principal component of analysis, what is the difference in constraining weights on encoder and decoder to be unit-norm in a dense autoencoder? Why?

   (c) Why is it difficult to strictly enforce weights orthogonality in an autoencoder? Why is it present by default in PCA? Refer to § 7.7.3.

   (d) Orthogonal weights in PCA leads to independent features. However, an autoencoder even with orthogonal encoder weights does not guarantee independent encodings. Why? The answer to this question also answers Q 1a.

5. The goal of an autoencoder is to learn the essential properties of the data while training to reconstruct the input. There are different types of regularization available to improve learning. Broadly, regularization can be applied to either the encoding $f(\boldsymbol{x})$ or the decoding $g(f(\boldsymbol{x}))$. Refer to § 7.3 and answer the following.

   (a) Among them, when is regularizing the encoding $f(\boldsymbol{x})$ better?

   (b) When is regularizing the decoder $g(f(\boldsymbol{x}))$ better?

   (c) (Optional) Refer to § 14.2.1 in Goodfellow, Bengio, and Courville 2016 to show that a sparse autoencoder approximates a generative model and that the sparsity penalty arrives as a result of this framework.

6. (Optional) The encoder module in an autoencoder can be incorporated in a classifier network. There are several ways it can be incorporated. Appendix K provides a flexible implementation to try different approaches.

   (a) Run the model in the appendix to train a classifier by transferring the encoder weights learned in autoencoder training to a classifier.

(b) Make the transferred encoder weights trainable. Note the change in the number of trainable parameters compared to in Q 6a. Train the model.

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Appendix A

Importance of Nonlinear Activation

It is mentioned a few times in this book that a nonlinear activation is essential for the nonlinearity of a deep learning model. Specifically, this is emphasized in § 4.7 in Chapter 4. In this appendix, it is shown that a linear activation makes a multi-layer network a simple linear regression model.

In the following, Equation A.1 applies the activation successively from input to the output in an illustrative two-layer network in Chapter 4. It shows that if the activation is linear, i.e., $g(x) = x$, then any multi-layer network becomes equivalent to a linear model.

$$\begin{aligned}
\hat{y} &= g(\mathbf{w}^T \mathbf{z}^{(2)}) && \text{(A.1a)}\\
&= g(\mathbf{w}^T g(W^{(2)T} g(W^{(1)T}\mathbf{x}))) && \text{(A.1b)}\\
&= \mathbf{w}^T W^{(2)T} W^{(1)T}\mathbf{x}, \text{if activation } g \text{ is linear.} && \text{(A.1c)}\\
&= \tilde{W}^T \mathbf{x} && \text{(A.1d)}
\end{aligned}$$

where, $\tilde{W}^T = \mathbf{w}^T W^{(2)T} W^{(1)T}$.

Appendix B

Curve Shifting

Curve shifting is used to learn relationships between the variables at a certain time with an event at a different time. The event can be either from the past or the future.

For a rare event prediction, where the objective is to predict an event in advance, the event is shifted back in time. This approach is similar to developing a model to predict a transition state which ultimately leads to an event.

In Listing B.1, a user-defined function (UDF) for curve-shifting a binary response data is shown. In the UDF, an input argument `shift_by` corresponds to the time units we want to shift `y`. `shift_by` can be a positive or negative integer.

Listing B.1. Curve Shifting.

```
import numpy as np

def sign(x):
    return (1, -1)[x < 0]


def curve_shift(df, shift_by):
    '''
    This function will shift the binary labels in a
        dataframe.
    The curve shift will be with respect to the 1s.
    For example, if shift is -2, the following
        process
    will happen: if row n is labeled as 1, then
    - Make row (n+shift_by):(n+shift_by-1) = 1.
    - Remove row n.
    i.e. the labels will be shifted up to 2 rows up.

    Inputs:
    df       A pandas dataframe with a binary
        labeled column.
             This labeled column should be named as
                 'y'.
    shift_by An integer denoting the number of rows
        to shift.

    Output
    df       A dataframe with the binary labels
        shifted by shift.
    '''

    vector = df['y'].copy()
    for s in range(abs(shift_by)):
        tmp = vector.shift(sign(shift_by))
        tmp = tmp.fillna(0)
        vector += tmp
    labelcol = 'y'
    # Add vector to the df
    df.insert(loc=0, column=labelcol + 'tmp', value=
        vector)
    # Remove the rows with labelcol == 1.
    df = df.drop(df[df[labelcol] == 1].index)
    # Drop labelcol and rename the tmp col as
        labelcol
    df = df.drop(labelcol, axis=1)
    df = df.rename(columns={labelcol + 'tmp':
        labelcol})
    # Make the labelcol binary
    df.loc[df[labelcol] > 0, labelcol] = 1

    return df
```

`curve_shift` assumes the response is binary with `(0, 1)` labels, and for any row `t` where `y==1` it,

1. makes the `y` for rows `(t+shift_by):(t+shift_by-1)` equal to 1. Mathematically, this is $y_{(t-k):t} \leftarrow 1$, if $y_t = 1$ and k is the `shift_by`. And,

2. remove row `t`.

Step 1 shifts the curve. Step 2 removes the row when the event (sheet-break) occurred. As also mentioned in § 2.1.2, we are not interested in teaching the model to predict an event when it has already occurred.

The effect of the curve shifting is shown using Listing B.2.

Listing B.2. Testing Curve Shift.

```
import pandas as pd
import numpy as np

'''Download data here:
https://docs.google.com/forms/d/e/1
    FAIpQLSdyUk3lfDl7I5KYK_pw285LCApc-
    _RcoC0Tf9cnDnZ_TWzPAw/viewform
'''
df = pd.read_csv("data/processminer-sheet-break-rare
    -event-dataset.csv")
df.head(n=5)  # visualize the data.

# Hot encoding
hotencoding1 = pd.get_dummies(df['Grade&Bwt'])
hotencoding1 = hotencoding1.add_prefix('grade_')
hotencoding2 = pd.get_dummies(df['EventPress'])
hotencoding2 = hotencoding2.add_prefix('eventpress_'
    )

df = df.drop(['Grade&Bwt', 'EventPress'], axis=1)

df = pd.concat([df, hotencoding1, hotencoding2],
    axis=1)

df = df.rename(columns={'SheetBreak': 'y'})  #
    Rename response column name for ease of
    understanding
```

```
'''
Shift the data by 2 units, equal to 4 minutes.

Test: Testing whether the shift happened correctly.
'''
print('Before shifting')  # Positive labeled rows
    before shifting.
one_indexes = df.index[df['y'] == 1]
display(df.iloc[(one_indexes[0]-3):(one_indexes
    [0]+2), 0:5].head(n=5))

# 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))
```

The outputs of the listing are visualized in Figure 4.3 in Chapter 4.

Appendix C

Simple Plots

The result plots in every chapter are made using the definitions in Listing C.1.

Listing C.1. Simple plot definitions.

```
##############################
#####  Plotting functions #####
##############################

import matplotlib.pyplot as plt
import seaborn as sns
import numpy as np

def plot_metric(model_history, metric,
    ylim=None, grid=False):
    sns.set()

    if grid is False:
        sns.set_style("white")
        sns.set_style("ticks")

    train_values = [
        value for key, value in model_history.items
            ()
        if metric in key.lower()
    ][0]
    valid_values = [
            value for key, value in model_history.items
                ()
            if metric in key.lower()
        ][1]

    fig, ax = plt.subplots()

    color = 'tab:blue'
    ax.set_xlabel('Epoch', fontsize=16)
    ax.set_ylabel(metric, color=color, fontsize=16)

    ax.plot(train_values, '--', color=color,
        label='Train ' + metric)
    ax.plot(valid_values, color=color,
        label='Valid ' + metric)
    ax.tick_params(axis='y', labelcolor=color)
    ax.tick_params(axis='both',
        which='major', labelsize=14)

    if ylim is None:
        ylim = [
            min(min(train_values),
                min(valid_values), 0.),
            max(max(train_values),
                max(valid_values))
        ]
    plt.yticks(np.round(np.linspace(ylim[0],
        ylim[1], 6), 1))
    plt.legend(loc='upper left', fontsize=16)

    if grid is False:
        sns.despine(offset=1, trim=True)

    return plt, fig


def plot_model_recall_fpr(model_history, grid=False)
    :
    sns.set()

    if grid is False:
        sns.set_style("white")
```

```python
        sns.set_style("ticks")

    train_recall = [
        value for key, value in model_history.items()
        if 'recall' in key.lower()
    ][0]
    valid_recall = [
        value for key, value in model_history.items()
        if 'recall' in key.lower()
    ][1]

    train_fpr = [
        value for key, value in model_history.items()
        if 'false_positive_rate' in key.lower()
    ][0]
    valid_fpr = [
        value for key, value in model_history.items()
        if 'false_positive_rate' in key.lower()
    ][1]

    fig, ax = plt.subplots()

    color = 'tab:red'
    ax.set_xlabel('Epoch', fontsize=16)
    ax.set_ylabel('value', fontsize=16)
    ax.plot(train_recall, '--', color=color, label='Train Recall')
    ax.plot(valid_recall, color=color, label='Valid Recall')
    ax.tick_params(axis='y', labelcolor='black')
    ax.tick_params(axis='both', which='major', labelsize=14)
    plt.legend(loc='upper left', fontsize=16)

    color = 'tab:blue'
    ax.plot(train_fpr, '--', color=color, label='Train FPR')
    ax.plot(valid_fpr, color=color, label='Valid FPR
        ')
    plt.yticks(np.round(np.linspace(0., 1., 6), 1))

    fig.tight_layout()
    plt.legend(loc='upper left', fontsize=16)

    if grid is False:
        sns.despine(offset=1, trim=True)

    return plt, fig
```

Appendix D

Backpropagation Gradients

Think of the two-layer neural network shown in Figure 4.2 illustrated in Chapter 4. We used a `binary_crossentropy` loss for this model shown in Equation 4.7. Without any loss of generality (w.l.o.g.), it can be expressed for a single sample as,

$$\mathcal{L}(\theta) = y \log(\hat{y}) + (1 - y) \log(1 - \hat{y}) \tag{D.1}$$

where, $\hat{y}$ is the prediction for y, i.e. the $\Pr_\theta[y = 1]$ (denoted by p in Eq. 4.7) and θ is the set of all parameters $\{W^{(1)}, W^{(2)}, \mathbf{w}^{(o)}\}$. Here the bias parameters are assumed as 0 w.l.o.g.

The parameter update in an iterative estimation vary for different optimizers such as `adam` and `sgd` in TensorFlow. However, as they are all Gradient Descent based, the update rule generalizes as,

$$\theta \leftarrow \theta - \eta \frac{\partial \mathcal{L}}{\partial \theta} \tag{D.2}$$

where η is a learning parameter.

As seen in the equation, the gradient guides the parameter estimation to reach its optimal value.

The gradient expression for a weight parameter can be derived as,

$$\frac{\partial \mathcal{L}}{\partial W^T} = \frac{\partial \mathcal{L}}{\partial \hat{y}} \frac{\partial \hat{y}}{\partial W^T} \tag{D.3}$$

A derivative of the weight transpose is used for mathematical convenience. Besides, $\frac{\partial \mathcal{L}}{\partial \hat{y}}$ will always be the same and, therefore, can be ignored to express,

$$\frac{\partial \mathcal{L}}{\partial W^T} \propto \frac{\partial \hat{y}}{\partial W^T} \tag{D.4}$$

Additionally, the relationship between the layers' inputs and outputs are,

$$\hat{y} = \sigma(\mathbf{w}^{(o)T}\mathbf{z}^{(2)}) \tag{D.5a}$$
$$\mathbf{z}^{(2)} = g(W^{(2)T}\mathbf{z}^{(1)}) \tag{D.5b}$$
$$\mathbf{z}^{(1)} = g(W^{(1)T}\mathbf{x}) \tag{D.5c}$$

where σ is the activation on the output layer and g on the hidden layers. Note that g can be different across layers but shown to be the same here for simplicity.

Using Equation D.4-D.5, we can express the gradients for each weight parameter as,

Output Layer.

$$\frac{\partial \mathcal{L}}{\partial \mathbf{w}^{(o)T}} \propto \frac{\partial \sigma(\mathbf{w}^{(o)T}\mathbf{z}^{(2)})}{\partial \mathbf{w}^{(o)T}} \tag{D.6}$$

Hidden Layer-2.

$$\begin{aligned}\frac{\partial \mathcal{L}}{\partial W^{(2)T}} &\propto \frac{\partial \sigma(\mathbf{w}^{(o)T}\mathbf{z}^{(2)})}{\partial W^{(2)T}} \\ &\propto \frac{\partial}{\partial W^{(2)T}}\sigma(\mathbf{w}^{(o)T}g(W^{(2)T}\mathbf{z}^{(1)})) \\ &\propto \frac{\partial \sigma(\mathbf{w}^{(o)T}g(W^{(2)T}\mathbf{z}^{(1)}))}{\partial g(W^{(2)T}\mathbf{z}^{(1)})}\frac{\partial g(W^{(2)T}\mathbf{z}^{(1)})}{\partial W^{(2)T}} \end{aligned} \tag{D.7}$$

Hidden Layer-1.

$$\begin{aligned}\frac{\partial \mathcal{L}}{\partial W^{(1)T}} &\propto \frac{\partial \sigma(\mathbf{w}^{(o)T}\mathbf{z}^{(2)})}{\partial W^{(1)T}} \\ &\propto \frac{\partial}{\partial W^{(1)T}}\sigma(\mathbf{w}^{(o)T}g(W^{(2)T}g(W^{(1)T}\mathbf{x}))) \\ &\propto \frac{\partial \sigma(\mathbf{w}^{(o)T}g(W^{(2)T}g(W^{(1)T}\mathbf{x})))}{\partial g(W^{(2)T}g(W^{(1)T}\mathbf{x}))}\frac{\partial g(W^{(2)T}g(W^{(1)T}\mathbf{x}))}{\partial g(W^{(1)T}\mathbf{x})}\frac{\partial g(W^{(1)T}\mathbf{x})}{\partial W^{(1)T}} \end{aligned} \tag{D.8}$$

Appendix E

Data Temporalization

Temporal models such as LSTM and convolutional networks are a bit more demanding than other models. A significant amount of time and attention goes into preparing the data that fits them.

First, we will create the three-dimensional tensors of shape: (*samples*, *timesteps*, *features*) in Listing E.1. *Samples* mean the number of data points. *Timesteps* is the number of time steps we look back at any time t to make a prediction. This is also referred to as the `lookback` period. The *features* are the number of features the data has, in other words, the number of predictors in multivariate data.

Listing E.1. Data temporalization

```
def temporalize(X, y, lookback):
    '''
    Inputs
    X           A 2D numpy array ordered by time of
       shape: (n_observations x n_features)
    y           A 1D numpy array with indexes aligned
       with X, i.e. y[i] should correspond to X[i].
        Shape: n_observations.
    lookback   The window size to look back in the
       past records. Shape: a scalar.

    Output
    output_X   A 3D numpy array of shape: ((
       n_observations-lookback-1) x lookback x
```

```
        n_features)
    output_y   A 1D array of shape: (n_observations-lookback-1), aligned with X.
    '''
    output_X = []
    output_y = []
    for i in range(len(X) - lookback - 1):
        t = []
        for j in range(1, lookback + 1):
            # Gather the past records upto the lookback period
            t.append(X[[(i + j + 1)], :])
        output_X.append(t)
        output_y.append(y[i + lookback + 1])
    return np.squeeze(np.array(output_X)), np.array(output_y)


def flatten(X):
    '''
    Flatten a 3D array.

    Input
    X            A 3D array for lstm, where the array is sample x timesteps x features.

    Output
    flattened_X   A 2D array, sample x features.
    '''
    flattened_X = np.empty(
        (X.shape[0], X.shape[2]))  # sample x features array.
    for i in range(X.shape[0]):
        flattened_X[i] = X[i, (X.shape[1] - 1), :]
    return flattened_X


def scale(X, scaler):
    '''
    Scale 3D array.

    Inputs
    X               A 3D array for lstm, where the
        array is sample x timesteps x features.
    scaler          A scaler object, e.g., sklearn.
        preprocessing.StandardScaler, sklearn.
        preprocessing.normalize

    Output
    X               Scaled 3D array.
    '''
    for i in range(X.shape[0]):
        X[i, :, :] = scaler.transform(X[i, :, :])

    return X
```

Additional helper functions, `flatten()` and `scale()`, are defined to make it easier to work with the tensors.

Testing

Since temporalization is an error-prone transformation, it is important to test the input tensors as shown in Listing E.2.

Listing E.2. Testing data temporalization.

```
"""### Temporalized data scale testing"""

from sklearn.preprocessing import StandardScaler
from sklearn.model_selection import train_test_split

# Sort by time and drop the time column.
df['DateTime'] = pd.to_datetime(df.DateTime)
df = df.sort_values(by='DateTime')
df = df.drop(['DateTime'], axis=1)

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

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

# Temporalize the data
lookback = 5
```

```python
X, y = temporalize(X=input_X,
                   y=input_y,
                   lookback=lookback)

X_train, X_test, y_train, y_test = train_test_split(
    np.array(X),
    np.array(y),
    test_size=0.2,
    random_state=123)
X_train, X_valid, y_train, y_valid = train_test_split(
    X_train,
    y_train,
    test_size=0.2,
    random_state=123)

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

X_train_scaled = scale(X_train, scaler)

'''
Test: Check if the scaling is correct.

The test succeeds if all the column means
and variances are 0 and 1, respectively, after
flattening.
'''
print('==== Column-wise mean ====\n', np.mean(flatten(X_train_scaled), axis=0).round(6))
print('==== Column-wise variance ====\n', np.var(flatten(X_train_scaled), axis=0))

# ==== Column-wise mean ====
#  [-0.  0.  0. -0. -0. -0. -0.  0. -0. -0.  0. -0. -0.  0.  0.  0.  0.  0.
#  -0. -0. -0. -0.  0.  0. -0. -0.  0.  0. -0.  0.  0.  0.  0.  0. -0.  0.
#   0.  0. -0.  0.  0. -0. -0.  0. -0.  0.  0.  0.  0. -0. -0. -0.  0.  0.
#   0.  0.  0. -0. -0.  0. -0. -0. -0. -0.  0.  0. -0.  0.  0.]
# ==== Column-wise variance ====
#  [1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1.
    1. 1. 1. 1. 1. 1. 1. 1.
#   1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1.
    1. 1. 1. 1. 1. 1. 1. 1.
#   1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1. 1.
    1. 1. 1. 0. 0.]
```

The temporalization output is shown in Figure 5.8 in Chapter 5.

Besides, the `scale()` function is tested and the outputs are shown in the listing. As expected, the mean and variances become 0 and 1 after using a `StandardScaler()` on the temporalized data.

Appendix F

Stateful LSTM

A typical *stateless* LSTM cell illustrated in Chapter 5 processes only as much "past" in the data as defined by the timesteps. This could be restrictive because:

> "Ideally, we want to expose the network to the entire sequence and let it learn the inter-dependencies, rather than we define those dependencies explicitly in the framing of the problem.
>
> ...
>
> This is truly how the LSTM networks are intended to be used."
>
> – Jason Brownlee

It is, in fact, learned in temporal modeling with LSTMs and convolutional neural networks in Chapter 5 and 6 that a larger lookback (timesteps) typically improves a model's accuracy. This is logical because there are lagged dependencies. And, a larger timestep allows the model to look farther in the past to have more context for prediction.

If going farther back in time improves accuracy then can we go all the way in the past? The answer is yes. This can be done with *stateful* LSTMs.

Using a stateful LSTM is a simple approach. This approach requires the input samples to be ordered by time. Also, unlike typical model fitting that resets the model every training iteration, with the stateful LSTM it is reset every epoch.

The implementation in this appendix shows that a stateful LSTM cell processes the entire input training data sequentially and learns the dependencies from anywhere in the past.

However, as lucrative as the stateful LSTM appears, it does not always work. This approach tends to work better if the data is stationary. For example, text documents. The writing pattern does not change significantly and therefore, the process is stationary.

But most time series processes are non-stationary. The dependencies in them are confounded due to the non-stationarity. Therefore, a window of timesteps in which the process is assumed to be stationary tends to work better. For the same reason, a large time step should be carefully chosen in non-stationary processes.

Stateful LSTM is suitable if the data is stationary, i.e., the patterns do not change with time.

Implementing a stateful LSTM is different from traditional models. In the following, the implementation steps are given.

Data Preparation

In a stateful LSTM network, it is necessary to have the size of the input data as a multiple of the batch size. The data preparation is thus slightly different. In Listing F.1 the number of samples for train, valid, and test is taken as a multiple of the batch size which is closest to their original size.

Listing F.1. Stateful LSTM model data preparation.

```python
# Time ordered original data.
lookback_stateful = 1
# Temporalize the data
X, y = temporalize(X=input_X,
                   y=input_y,
                   lookback=lookback_stateful)

batch_size = 128

# Train, valid and test size set
# to match the previous models.
train_size = 13002
valid_size = 3251
test_size = 3251

X_train_stateful, y_train_stateful =
    np.array(
        X[0:int(train_size / batch_size) *
            batch_size]),
            np.array(
        y[0:int(train_size / batch_size) *
            batch_size])
X_valid_stateful, y_valid_stateful = np.array(
    X[int(train_size / batch_size) *
      batch_size:int((train_size + valid_size) /
          batch_size) *
      batch_size]), np.array(
          y[int(train_size / batch_size) *
            batch_size:int((train_size +
                valid_size) / batch_size) *
            batch_size])
X_test_stateful, y_test_stateful = np.array(
    X[int((train_size + test_size) / batch_size) *
        batch_size:]), np.array(
        y[int((train_size + test_size) /
            batch_size) * batch_size:])

X_train_stateful =
    X_train_stateful.reshape(
        X_train_stateful.shape[0],
        lookback_stateful,
        n_features)
X_valid_stateful =
    X_valid_stateful.reshape(
        X_valid_stateful.shape[0],
        lookback_stateful,
        n_features)
X_test_stateful =
    X_test_stateful.reshape(
        X_test_stateful.shape[0],
        lookback_stateful,
        n_features)

scaler_stateful =
    StandardScaler().fit(flatten(
        X_train_stateful))

X_train_stateful_scaled =
    scale(X_train_stateful,
          scaler_stateful)

X_valid_stateful_scaled =
    scale(X_valid_stateful,
          scaler_stateful)
X_test_stateful_scaled =
    scale(X_test_stateful,
          scaler_stateful)
```

The question is, why the batch size is required in a stateful model?

It is because when the model is stateless, TensorFlow allocates a tensor for the states of size `output_dim` based on the number of LSTM cells. At each sequence processing, this state tensor is reset.

On the other hand, TensorFlow propagates the previous states for each sample across the batches in a stateful model. In this case, the structure to store the states is of shape `(batch_size, output_dim)`. Due to this, it is necessary to provide the batch size while constructing the network.

Stateful Model

A stateful LSTM model is designed to traverse the entire past in the data for the model to self-learn the distant inter-dependencies instead of limiting it in a lookback window. This is achieved with a specific training procedure shown in Listing F.2.

The LSTM layer is made stateful by setting its argument `stateful=True`.

Listing F.2. Stateful LSTM model.

```python
# Stateful model.

timesteps_stateful =
    X_train_stateful_scaled.shape[1]
n_features_stateful =
    X_train_stateful_scaled.shape[2]

model = Sequential()
model.add(
    Input(shape=(timesteps_stateful,
                 n_features_stateful),
          batch_size=batch_size,
          name='input'))
model.add(
    LSTM(8,
         activation='relu',
         return_sequences=True,
         stateful=True,
         name='lstm_layer_1'))
model.add(Flatten())
model.add(Dense(units=1,
                activation='sigmoid',
                name='output'))

model.summary()

model.compile(optimizer='adam',
              loss='binary_crossentropy',
              metrics=[
                  'accuracy',
                  tf.keras.metrics.Recall(),
                  performancemetrics.F1Score(),
                  performancemetrics.
                      FalsePositiveRate()
              ])
```

Unlike stateless LSTM, the cell states are preserved at every training iteration in a stateful LSTM. This allows it to learn the dependencies between the batches and, therefore, long-term patterns in significantly long sequences. However, we do not want the state to be transferred from one epoch to the next. To avoid this, we have to manually reset the state after each epoch.

A custom operation during training iterations can be performed by overriding the definitions in `tf.keras.callbacks.Callback`[1]. The `Callback()` class has definitions to perform operations at the beginning and/or end of a `batch` or `epoch` for both `test` and `train`. Since we require to reset the model states at the end of every epoch, we override the `on_epoch_end()` in Listing F.3 with `model.reset_states()`.

Listing F.3. Custom Callback() for Stateful LSTM model.

```
class ResetStatesCallback(
    tf.keras.callbacks.Callback):

    def on_epoch_end(self, epoch, logs={}):
        self.model.reset_states()
```

We now train the model in Listing F.4. In the `model.fit()`, we set the argument `callbacks` equal to our custom defined `ResetStatesCallback()`. Also, we set `shuffle=False` to maintain the time ordering of the samples during the training.

Listing F.4. Stateful LSTM model fitting.

```
history = model.fit(
    x=X_train_stateful_scaled,
    y=y_train_stateful,
    callbacks=[ResetStatesCallback()],
    batch_size=batch_size,
    epochs=100,
    shuffle=False,
    validation_data=(X_valid_stateful_scaled,
                     y_valid_stateful),
    verbose=0).history
```

The results from stateful LSTM on the sheet-break time series is poorer than the other LSTM models in Chapter 5. As alluded to earlier, a potential reason is that the process is non-stationary. Due to this, the dependencies change over time and are difficult to learn.

[1] /api_docs/python/tf/keras/callbacks/Callback

Appendix G

Null-Rectified Linear Unit

Rectified Linear Units (`relu`) is one of the most common activation functions. It is expressed as,

$$g(x) = \begin{cases} x, & \text{if } x > 0 \\ 0, & \text{otherwise.} \end{cases} \tag{G.1}$$

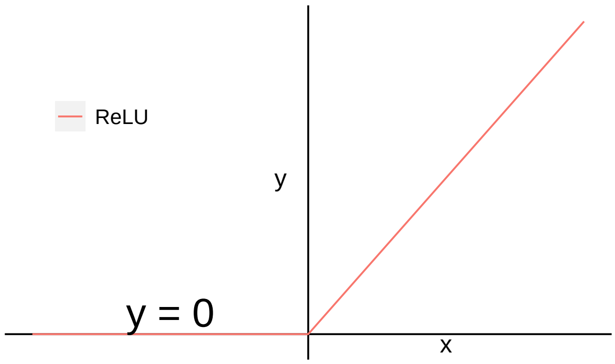
As shown in the equation, `relu` makes any non-positive x as 0. This brings nonlinearity to the model but at the cost of feature manipulation.

Such manipulation affects the pooling operation in convolutional networks (see § 6.12.2 in Chapter 6). The manipulation distorts the original distribution of the features which makes some pooling statistics, e.g., average, inefficient.

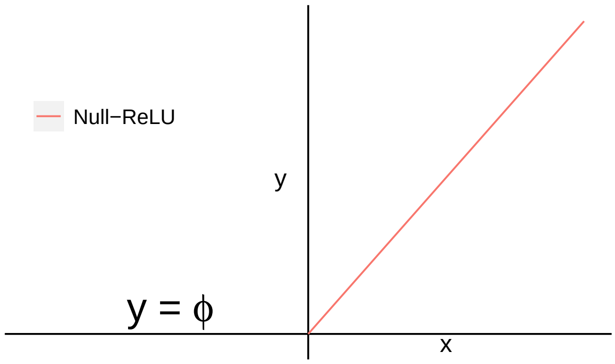
A resolution mentioned in § 6.13.3 is replacing `relu` activation with null-`relu`, which is defined as,

$$g(x) = \begin{cases} x, & \text{if } x > 0 \\ \phi, & \text{otherwise} \end{cases} \tag{G.2}$$

where ϕ denotes *null*. Unlike Equation G.1, null-`relu` acts as dropping the non-positive x's instead of treating them as 0. Both are visualized in Figure G.1a and G.1b, respectively.



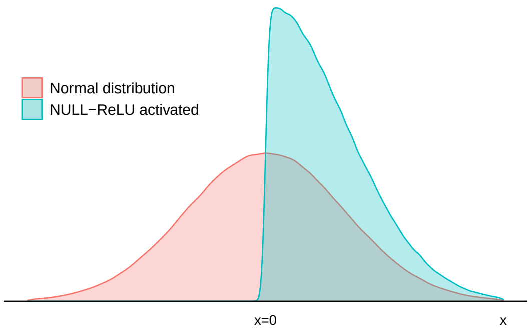
(a) *Traditional **`relu`** activation.*



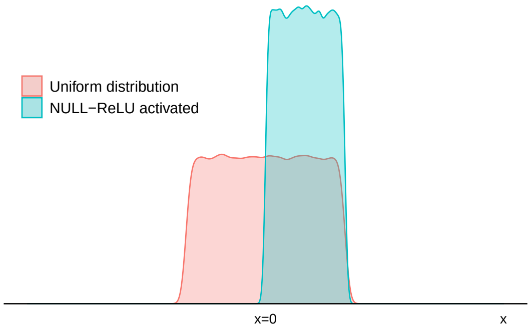
(b) *A variant null-**`relu`** activation.*

Figure G.1. *The traditional Rectified Linear Unit (**`relu`**) activation (top) transforms any non-positive x to zero. This is a nonlinear operation essential in most deep learning layers. However, in between a convolutional and pooling operation, the **`relu`** transformation can have an unwanted effect. The pooling attempts to draw a summary statistic from convolution output. But **`relu`** brings artificial* 0*'s that subvert summary information. A Null-**`relu`** activation (bottom) mitigates this by replacing the non-positive x's with ϕ (null). Unlike* 0*s in **`relu`**, nulls do not add any artificial information; they only mask the non-positive x's.*

Null-`relu`'s impact on the activated features for normal and uniform distributions are shown in Figure G.2a and G.2b, respectively. As opposed to the `relu` effect shown in Figure 6.28a and 6.28b, the activated feature distributions are still known—half-gaussian and uniform. Therefore, efficient pooling statistics such as in Kobayashi 2019a can be used.



(a) *Normal Distribution after null-`relu` activation.*



(b) *Uniform Distribution after null-`relu` activation.*

Figure G.2. *The distribution of the feature map is distorted by a `relu` activation. While any nonlinear activation distorts the original distribution, `relu`'s is severe because it artificially adds zeros for every non-positive x. Due to this, the activated x's distribution becomes extremely heavy at zero. Such distributions do not belong to known or well-defined distribution families. A variant of `relu` called null-`relu` transforms the non-positive x to null (ϕ). This is equivalent to throwing the non-positive x's instead of assuming them to be zero. If the original distribution is normal (top) or uniform (bottom), the null-`relu` activated are half-Gaussian and Uniform, respectively. Therefore, it has a less severe effect on distribution.*