Business 4720 - Class 17

Recurrent Neural Networks using Python

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This Class

What You Will Learn:

- Deep Learning Concepts
  - Recurrent Neural Networks
  - GRU cells and layers
  - LSTM cells and layers
  - Time series prediction with RNN
  - Business process prediction with RNN

Based On

Gareth James, Daniel Witten, Trevor Hastie and Robert Tibshirani: *An Introduction to Statistical Learning with Applications in R*. 2nd edition, corrected printing, June 2023. (ISLR2)

`https://www.statlearning.com`

Chapter 10

Kevin P. Murphy: *Probabilistic Machine Learning – An Introduction*. MIT Press 2022.

`https://probml.github.io/pml-book/book1.html`

Chapter 15

Based On

Tensorflow and Keras Tutorials

- https://www.tensorflow.org/tutorials/structured_data/time_series
- https://www.tensorflow.org/guide/keras/working_with_rnns
- https://www.tensorflow.org/text/tutorials/text_generation
- https://keras.io/examples/timeseries/timeseries_weather_forecasting/

Other Tutorials

- https://colah.github.io/posts/2015-08-Understanding-LSTMs/
- https://karpathy.github.io/2015/05/21/rnn-effectiveness/

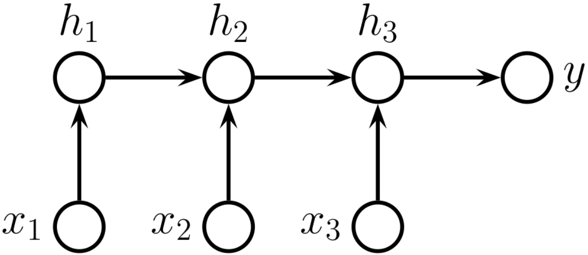
Predictions from Sequences

Application Examples

- Text classification
- Next-word or next-character prediction
- Text translation
- Time series forecasting (financial, ecological, metereological, etc.)
- Business process prediction
- Speech translation or transcription
- Audio or sound generation
- Video captioning

RNN – Seq2Vec

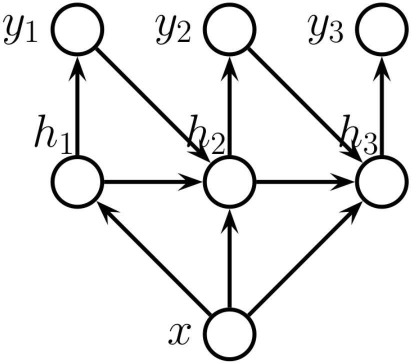
- Predict (regression or classification) from a sequence
- Inputs *x*, output *y* and hidden layers *h*



Source: Murphy Fig. 15.4

RNN – Vec2Seq

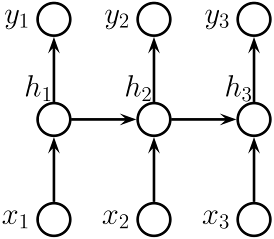
- Generate a sequence from initial input
- Input *x*, outputs *y* and hidden layers *h*

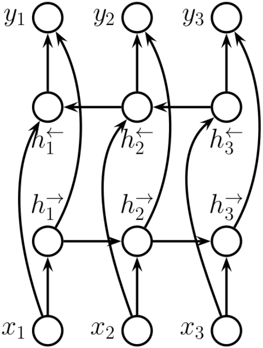


Source: Murphy Fig. 15.1

RNN – Seq2Seq

- Predict sequence from a sequence
- Inputs x, outputs y and hidden layers h

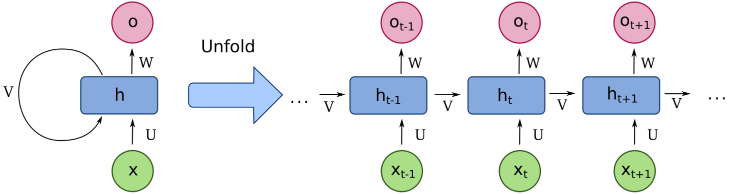




Source: Murphy Fig 15.5

Recurrent Neural Networks (RNN)

- A neural network block occurs multiple times in sequence
- **Input**: Sequence or single (initial) input
- **Output**: Sequence or single (final) output
- **State**: Hidden, passed from one step to the next



`https://commons.wikimedia.org/wiki/File:Recurrent_neural_network_unfold.svg`

Backpropagation Through Time

$$h_t = \sigma(W_x \cdot x_t + W_h \cdot h_{t-1} + B_h)$$
$$o_t = \sigma(W_o \cdot h_t + B_o)$$

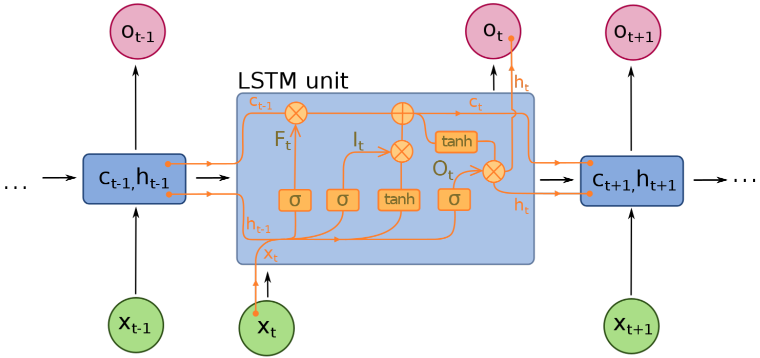
- Unfolding and truncating to make computationally tractable
- Train on short input subsequences

Vanishing Gradient Problem

- Multiplicative updates of state through time
- Loss of memory about inputs in distant past
- *Solution*: Additive updates of state

Long-Short-Term Memory (LSTM) Cells

- "Input gate" I, "Forget gate" F, "Output gate" O
- Hidden state h, Cell memory c



https://en.wikipedia.org/wiki/File:Long_Short-Term_Memory.svg

LSTM Cells

$$
\begin{aligned}
F_t &= \sigma(W_f \cdot [x_t, h_{t-1}] + b_f) \\
I_t &= \sigma(W_i \cdot [x_t, h_{t-1}] + b_i) \\
O_t &= \sigma(W_o \cdot [x_t, h_{t-1}] + b_o) \\
\tilde{c}_t &= \phi(W_c \cdot [x_t, h_{t-1}] + b_c) \\
c_t &= F_t \otimes c_{t-1} + I_t \otimes \tilde{c}_t \\
h_t &= O_t \otimes \phi(c_t)
\end{aligned}
$$

Here $\cdot$ is the dot-product (vector product), $\otimes$ is element-wise multiplication, and [.] denotes vector concatenation. σ is the sigmoid/logistic function and ϕ is the hyperbolic tangent.

LSTM Cell Parameters

- Let h_t and c_t be vectors of size n and x_t be a vector of size m and
- The input to each gate is of size $n + m$, the output is of size n
- Then W_f, W_i, W_o and W_c must be matrices of size $n \times (n + m)$
- Then b_f, b_i, b_o and b_c must be vectors of size n.
- Then for each gate there are $n \times (n + m) + n$ parameters
- Then for all four gates, there are $4 \times (n \times (n + m) + n)$ parameters

Important: Parameters are "re-used" for each unrolled step.

Example: Let the unit size (state size) be 16 and the input size be 8.
Then the total number of parameters for the LSTM cell is
$4 \times (16 \times (8 + 16) + 16) = 1600$

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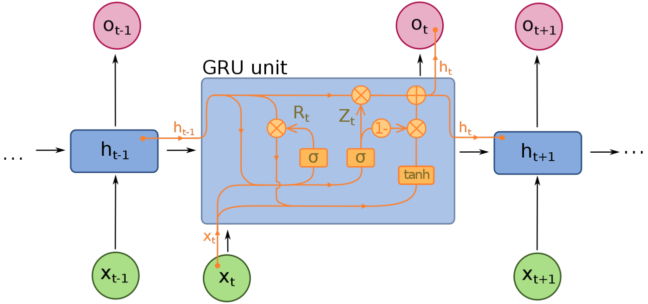
Gated Recurrent Unit (GRU) Cells

- ”Update gate” Z, ”Reset gate gate” R
- Hidden state h



https://en.wikipedia.org/wiki/File:Gated_Recurrent_Unit.svg

- Fewer parameters than, and similar performance to LSTM

GRU Cells

$$
\begin{aligned}
Z_t &= \sigma(W_z \cdot [x_t, h_{t-1}] + b_z) \\
R_t &= \sigma(W_r \cdot [x_t, h_{t-1}] + b_r) \\
\hat{h}_t &= \phi(W_h \cdot [x_t, R_t \otimes h_{t-1}] + b_h) \\
h_t &= (1 - Z_t) \otimes h_{t-1} + Z_t \otimes \hat{h}_t
\end{aligned}
$$

Here $\cdot$ is the dot-product (vector product), $\otimes$ is element-wise multiplication, and [.] denotes vector concatenation. σ is the sigmoid/logistic function and ϕ is the hyperbolic tangent.

GRU Cell Parameters

- Let h_t be a vector of size n and x_t be a vector of size m and
- The input to each gate is of size $n + m$, the output is of size n
- Then W_z, W_r, and W_h must be matrices of size $n \times (n + m)$
- Then b_z, b_r, and b_h must be vectors of size n.
- Then for each gate there are $n \times (n + m) + n$ parameters
- Then for all three gates, there are $3 \times (n \times (n + m) + n)$ parameters

Important: Parameters are "re-used" for each unrolled step.

Example: Let the unit size (state size) be 16 and the input size be 8. Then the total number of parameters for the GRU cell is
$3 \times (16 \times (8 + 16) + 16) = 1200$

With Keras GRU layer option `reset_after=False`.

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Statefulness of RNN

Stateless LSTM/GRU

- Forget internal hidden state and cell memory after each training batch
- Allows shuffling of data between epochs
- No ”long-term memory” for the LSTM/GRU

Stateful LSTM/GRU

- Retain internal state and cell memory between training batches
- Must not shuffle training data, data must be presented for learning in ”correct” order
- Allows ”long-term memory” for the LSTM/GRU across multiple batches

Stock Market Prediction

Using historic stock market data, predict future performance.

- DJIA performance
- "Seq2Vec" task: From a sequence of values, predict one following value
- Data exported from the R package `quarks`
- 2000 to 2021 (converted to EUR)
- Limited to open, low, high, close, and volume data

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Stock Market Prediction [cont'd]

Load packages and read data file:

```
import math
import tensorflow as tf
from tensorflow import keras
from keras import layers
import pandas as pd

tf.random.set_seed(123)
n_steps = 20
n_epochs = 25

data = \
pd.read_csv('https://evermann.ca/busi4720/djia.data.csv')
```

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Add useful features for timeseries models:

- Successive differences
- Percentage changes

```
data = pd.concat([
    data,
    data.diff().add_suffix('diff'),
    data.pct_change().add_suffix('pct')],
    axis=1).iloc[1:,]
# Split data to train and validation set
# No random shuffling for time series
train = data[:math.floor(0.8*data.shape[0])]
valid = data.drop(train.index)
# Normalize data using only info from training
# set. Prevent information 'leakage'
train_mean = train.mean()
train_sd = train.std()
train = (train - train_mean)/train_sd
valid = (valid - train_mean)/train_sd
```

Create `tf.Dataset` objects:

```
dataset_train = keras.preprocessing \
    .timeseries_dataset_from_array(
    train.drop('price.closediff', axis=1),
    train['price.closediff'],
    sequence_length=n_steps,
    batch_size=32,
    shuffle=True)

dataset_valid = keras.preprocessing \
    .timeseries_dataset_from_array(
    valid.drop('price.closediff', axis=1),
    valid['price.closediff'],
    sequence_length=n_steps,
    batch_size=32,
    shuffle=True)
```

Interlude – Dataset Objects

Dataset objects feed inputs and targets to the `fit` function.

See how this works with simple example data:

```
test = pd.DataFrame([[0, 0], [1, 1], [2, 2,], [3, 3],
                     [4, 4], [5, 5], [6, 6], [7, 7]])
inputs = test.iloc[:-1,0]
targets = test.iloc[2:,1]

pd.DataFrame([inputs, targets])
     0    1    2    3    4    5    6    7
0  0.0  1.0  2.0  3.0  4.0  5.0  6.0  NaN
1  NaN  NaN  2.0  3.0  4.0  5.0  6.0  7.0
```

Interlude – Dataset Objects

Do not shuffle data:

- Each batch continues from the previous batch
- Suitable for stateful RNN architectures

```
ds = keras.preprocessing \
    .timeseries_dataset_from_array(inputs, targets, \
     batch_size=2, sequence_length=2, \
     sequence_stride=1, shuffle=False)
for element in ds.as_numpy_iterator():
     print(element)

(array([[0, 1],
       [1, 2]]), array([2, 3]))
(array([[2, 3],
       [3, 4]]), array([4, 5]))
(array([[4, 5],
       [5, 6]]), array([6, 7]))
```

Interlude – Dataset Objects

Shuffle data:

- Batches do not continue sequence
- Suitable for stateless NN architectures

```
ds = keras.preprocessing \
    .timeseries_dataset_from_array(inputs, targets, \
     batch_size=2, sequence_length=2, \
     sequence_stride=1, shuffle=True)
for element in ds.as_numpy_iterator():
     print(element)

(array([[4, 5],
       [2, 3]]), array([6, 4]))
(array([[5, 6],
       [0, 1]]), array([7, 2]))
(array([[3, 4],
       [1, 2]]), array([5, 3]))
```

Sequence stride:

```
ds = keras.preprocessing \
    .timeseries_dataset_from_array(inputs, targets, \
     batch_size=1, sequence_length=2, \
     sequence_stride=2, shuffle=False)
for element in ds.as_numpy_iterator():
     print(element)

(array([[0, 1]]), array([2]))
(array([[2, 3]]), array([4]))
(array([[4, 5]]), array([6]))
```

Hands-On Exercise – Dataset Objects

Using example data as in the previous slides,

1. Experiment with different values for `batch_size`,
2. Experiment with different values for `sequence_length`,
3. Experiment with different values for `sequence_stride`.

Do the results match your expectations?

Stock Market Prediction [cont'd]

Build a sequential model using an input layer, one LSTM layer and a dense (fully-connected) layer with a single output:

- Hidden state and cell memory size: `units=16`
- "Seq2Vec" model: `return_sequences=False`
- Stateless model: `stateful=False`

```
model = keras.Sequential()
model.add(layers.InputLayer(
    input_shape=(n_steps, len(train.columns)-1)))
model.add(layers.LSTM(
    units=16,
    return_sequences=False,
    return_state=False,
    stateful=False))
model.add(layers.Dense(1))
model.summary()
```

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Compile and fit the model:

```
model.compile(loss='mean_squared_error',
              optimizer='Adagrad')

model.fit(dataset_train,
          epochs=n_epochs,
          validation_data=dataset_valid)
```

Results:

```
Model: "sequential_4"
_______________________________________________
 Layer (type)          Output Shape      Param #
===============================================
 lstm_1 (LSTM)         (None, 16)        1984
 dense_8 (Dense)       (None, 1)         17
===============================================
Total params: 2001 (7.82 KB)
Trainable params: 2001 (7.82 KB)
Non-trainable params: 0 (0.00 Byte)
_______________________________________________

Epoch 1/25
138/138 [==============================] - 4s 14ms/step
loss: 1.1351 - val_loss: 7.2034

Epoch 25/25
138/138 [==============================] - 1s 9ms/step
loss: 0.9916 - val_loss: 7.1444
```

Hands-On Exercises

Download the Python code from `https://evermann.ca/busi4720/ts_prediction_s2v_stateless.py`

1. Predict the percentage change of the closing value (column `price.closepct`)
2. Predict the actual closing value (column `price.close`)
3. Comment on the model performance results. Are these values more or less predictable than the differenced closing values?

Experiment with different model characteristics:

1. Vary the size of the LSTM state (`unit=16`).
2. Swap the LSTM layer for a GRU layer (`layers.GRU`). The GRU layer takes the same arguments as the LSTM layer.
3. Comment on the model performance results.

Stock Market Prediction [cont'd]

Can we do better with more layers?

```
model = keras.Sequential()
model.add(layers.InputLayer(
    input_shape=(n_steps, len(train.columns)-1)))
model.add(layers.LSTM(
    units=16,
    return_sequences=True,
    stateful=False))
model.add(layers.Dropout(rate=0.25))
model.add(layers.LSTM(
    units=16,
    return_sequences=False,
    stateful=False))
model.add(layers.Dense(32))
model.add(layers.Dropout(rate=0.25))
model.add(layers.Dense(1))
model.summary()
```

The first LSTM returns sequences, the second one does not.

Results of more complex model:

```
Model: "sequential"
_______________________________________________________________
 Layer (type)              Output Shape          Param #
===============================================================
 lstm (LSTM)               (None, 20, 16)        2048
 dropout (Dropout)         (None, 20, 16)        0
 lstm_1 (LSTM)             (None, 16)            2112
 dense (Dense)             (None, 32)            544
 dropout_1 (Dropout)       (None, 32)            0
 dense_1 (Dense)           (None, 1)             33
===============================================================
Total params: 4737 (18.50 KB)
Trainable params: 4737 (18.50 KB)
Non-trainable params: 0 (0.00 Byte)

Epoch 25/25
138/138 [==============================] - 1s 8ms/step
- loss: 0.9966 - val_loss: 0.9486
```

Stock Market Prediction [cont'd]

Does a stateful LSTM perform better?

Change batch size to a single batch of continuous sequence:

```
dataset_train = keras.preprocessing \
    .timeseries_dataset_from_array(
    train.drop('price.closediff', axis=1),
    train['price.closediff'],
    sequence_length=n_steps,
    sampling_rate=1, batch_size=1, shuffle=False)

dataset_valid = keras.preprocessing \
    .timeseries_dataset_from_array(
    valid.drop('price.closediff', axis=1),
    valid['price.closediff'],
    sequence_length=n_steps,
    sampling_rate=1, batch_size=1, shuffle=False)
```

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Stock Market Prediction [cont'd]

```
model = keras.Sequential()
model.add(layers.InputLayer(
    batch_input_shape=(
        1, None, len(train.columns)-1)))
model.add(layers.LSTM(
    units=16,
    return_sequences=False,
    return_state=False,
    stateful=True))
model.add(layers.Dense(1))
model.summary()
```

Results of stateful model:

```
 Layer (type)     Output Shape     Param #
=========================================
 lstm (LSTM)      (1, 16)          2048
 dense (Dense)    (1, 1)           17
=========================================
Total params: 2065 (8.07 KB)
Trainable params: 2065 (8.07 KB)
Non-trainable params: 0 (0.00 Byte)
_________________________________________
Epoch 1/25
4407/4407 [==============================]
- 14s 3ms/step - loss: 1.0094 - val_loss: 1.4701

Epoch 25/25
4407/4407 [==============================]
- 13s 3ms/step - loss: 0.9909 - val_loss: 1.1229
```

Hands-On Exercises

1. Download the stateful LSTM from `https://evermann.ca/busi4720/ts_prediction_s2v_stateful.py`
2. Extend the stateful model to a multi-layer network and include dropout layers
3. How does this change the predictive performance of the model?

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Stock Market Prediction [cont'd]

How does a "Vec2Vec" model perform?
Treat the entire input as one large feature vector, without expressing any time-ordering in the model:

```
model = keras.Sequential()
model.add(layers.InputLayer(
    input_shape=(n_steps,
                 len(train.columns)-1)))
model.add(layers.Flatten())
model.add(layers.Dense(256))
model.add(layers.Dropout(rate=0.25))
model.add(layers.Dense(64))
model.add(layers.Dropout(rate=0.25))
model.add(layers.Dense(1))
model.summary()
```

The `Flatten` layer flattens its input tensor.

Results of "Vec2Vec" model. Note the large number of parameters.

```
 Layer (type)              Output Shape     Param #
==============================================
 flatten (Flatten)         (None, 300)      0
 dense (Dense)             (None, 256)      77056
 dropout (Dropout)         (None, 256)      0
 dense_1 (Dense)           (None, 64)       16448
 dropout_1 (Dropout)       (None, 64)       0
 dense_2 (Dense)           (None, 1)        65
==============================================
Total params: 93569 (365.50 KB)
Trainable params: 93569 (365.50 KB)
Non-trainable params: 0 (0.00 Byte)

Epoch 1/25  - loss: 3.5692 - val_loss: 2.3847
Epoch 25/25 - loss: 1.5864 - val_loss: 1.0902
```

Next Activity Prediction of a Business Process

Using an event log, train a model to predict the next activity from a prefix sequence of 5 activities that have already occured.

Download the complete Python file here: https://evermann.ca/busi4720/process_prediction.py
Download the example event log here: https://evermann.ca/busi4720/BPI_Challenge_2012.xes.gz

```
import numpy
from tensorflow import keras
from keras import layers
import pandas as pd
import pm4py
# Length of sequences to predict from
prefix_len= 5
# Read the log
log = pm4py.read_xes('BPI_Challenge_2012.xes.gz')
```

Next Activity Prediction of a Business Process [cont'd]

Fix the data types:

```
log['time:timestamp'] = \
    pd.to_datetime(log['time:timestamp'], utc=True)
log['case:REG_DATE'] = \
    pd.to_datetime(log['case:REG_DATE'], utc=True)
log['case:AMOUNT_REQ'] = \
    pd.to_numeric(log['case:AMOUNT_REQ'])
log['org:resource'] = \
    log['org:resource'].astype(str)
```

Filter the log for completion events:

```
# Retain only activity completion events
log = log[log['lifecycle:transition'] == 'COMPLETE']
```

Next Activity Prediction of a Business Process [cont'd]

Filter and sort the log for sequences of length *k*:

```python
# Find the case start time as time of the
# first event in case
log = log.merge(
    log.groupby('case:concept:name',as_index=False) \
    ['time:timestamp'].min() \
    .rename(columns={'time:timestamp':'case:start'}),
    how='left')
# Find the number of events for each case
log = log.merge(
    log.groupby('case:concept:name', as_index=False) \
    ['time:timestamp'].count(). \
    rename(columns={'time:timestamp':'num_events'}),
    how='left')
# Filter log for minimum 6 events (5 input, 1 target)
log = log[log['num_events'] > prefix_len]
# Sort log by case start, then by event time
log.sort_values(['case:start', 'time:timestamp'], \
    inplace=True)
```

Next Activity Prediction of a Business Process [cont'd]

Identify feature to predict from:

```python
# This is the feature we predict (from)
f_name = 'concept:name'
# Vocabulary
vocab = list(log[f_name].unique()) + ['EOC']
v_size = len(vocab)
# Dictionaries to convert to/from integers
f2int = dict([(s, vocab.index(s)) for s in vocab])
int2f = dict([(v, k) for (k, v) in f2int.items()])
# Make sequences of feature names for each case
features = log.groupby(['case:concept:name'])[f_name] \
    .apply(list).reset_index(name='features')
```

Next Activity Prediction of a Business Process [cont'd]

Add end-of-case marker and convert to numeric:

```
sequences=[l+['EOC'] for l in list(features['features'])]
sequences=[[f2int[i] for i in seq] for seq in sequences]
```

Split sequences into prefix and target using a sliding window over each sequence:

```
data = pd.DataFrame([(seq[i:i+prefix_len], \
    seq[i+prefix_len]) for seq in sequences \
    for i in range(len(seq)-prefix_len)])
# Split the lists into dataframe columns
data = data.assign(**data[0] \
    .apply(pd.Series).add_prefix('index_'))
```

Next Activity Prediction of a Business Process [cont'd]

Create training and validation sets:

```
# Divide into train and test set
train = data.sample(frac=0.8)
valid = data.drop(train.index)
# Separate X and Y
train_x = train.iloc[:,2:]
train_y = train.iloc[:,1]
valid_x = valid.iloc[:,2:]
valid_y = valid.iloc[:,1]
```

Define the model:

```
model = keras.Sequential()
model.add(layers.InputLayer(input_shape=(5,)))
model.add(layers.Embedding(input_dim=v_size,
                           output_dim=16))
model.add(layers.LSTM(units=32,
                      return_sequences=False,
                      return_state=False,
                      stateful=False))
model.add(layers.Dense(v_size, activation='softmax'))
```

Note: `units` specifies the size of the h and c vectors

Next Activity Prediction of a Business Process [cont'd]

Compile and fit the model:

```
# Compile with loss and optimizer
model.compile(loss='sparse_categorical_crossentropy',
              optimizer='Adagrad',
              metrics=['sparse_categorical_accuracy'])
# Train the model and validate on
model.fit(train_x, train_y,
          validation_data=(valid_x, valid_y),
          epochs=25, shuffle=True)
```

Results:

```
 Layer (type)              Output Shape    Param #
===============================================
 embedding (Embedding)    (None, 5, 16)    384
 lstm (LSTM)              (None, 32)       6272
 dense (Dense)            (None, 24)       792
===============================================
Total params: 7448 (29.09 KB)
Trainable params: 7448 (29.09 KB)

Epoch 25/25
2875/2875 [==============================] - 6s 2ms/step
- loss: 1.3819 - sparse_categorical_accuracy: 0.6295
- val_loss: 1.3825 - val_sparse_categorical_accuracy: 0.6241
```

Next Activity Prediction of a Business Process [cont'd]

Predict activities from the model until end-of-case:

```
input = train_x.iloc[2:3,:].copy()
print(input)
probs = model.predict(input)[0]
# pred = probs.argmax()
pred = numpy.random.choice(a=range(v_size), p=probs)
print(int2f[pred])
while int2f[pred] != 'EOC':
    for i in range(4):
        input.iat[0,i] = input.iat[0, i+1]
    input.iat[0,4] = pred
    print(input)
    probs = model.predict(input)[0]
    # pred = probs.argmax()
    pred = numpy.random.choice(a=range(v_size),p=probs)
    print(int2f[pred])
```

Next Activity Prediction of a Business Process [cont'd]

Results:

```
        index_0  index_1  index_2  index_3  index_4
109280        6        7        8       10        9
1/1 [==============================] - 0s 197ms/step
W_Nabellen offertes
         index_0  index_1  index_2  index_3  index_4
109280         7        8       10        9        9
1/1 [==============================] - 0s 11ms/step
W_Nabellen offertes
         index_0  index_1  index_2  index_3  index_4
109280         8       10        9        9        9
1/1 [==============================] - 0s 11ms/step
W_Nabellen offertes
         index_0  index_1  index_2  index_3  index_4
109280        10        9        9        9        9
1/1 [==============================] - 0s 11ms/step
EOC
```

Hands-On Exercises

Download the complete Python file here:
`https://evermann.ca/busi4720/process_prediction.py`
Download the example event log here: `https://://evermann.ca/busi4720/BPI_Challenge_2012.xes.gz`

Adapt the network architecture to identify the impact on training and validation performance of the following:

1. Dropouts in the LSTM layer (use the `dropout=0.x` option when defining the LSTM layer)
2. GRU instead of LSTM layers (use `layers.GRU()`)
3. Embedding size (originally 16, note: vocabulary size is 23+1)
4. Further training epochs (originally 25)

Comment on your findings and identify the best model.