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

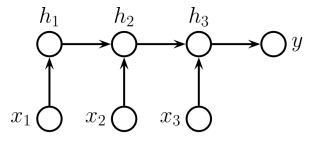
Application Examples

- ► 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

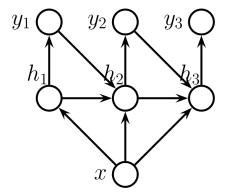
- ▶ Predict (regression or classification) from a sequence
- ► Inputs *x*, output *y* and hidden layers *h*



Source: Murphy Fig. 15.4

RNN – Vec2Seq

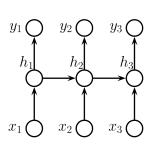
- Generate a sequence from initial input
- ► Input *x*, outputs *y* and hidden layers *h*

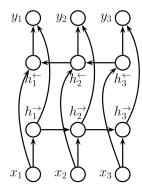


Source: Murphy Fig. 15.1

RNN – Seq2Seq

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



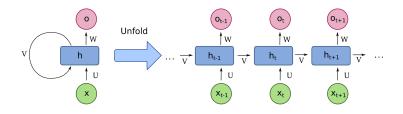


Source: Murphy Fig 15.5



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

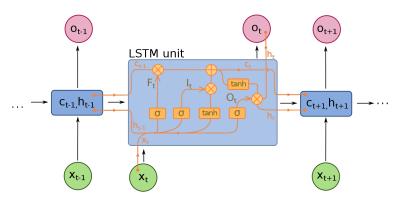
- Multiplicative updates of state through time
- Loss of memory about inputs in distant past
- ► Solution: Additive updates of state



Long-Short-Term Memory (LSTM) Cells

- Input gate I, "Forget gate F, "Output gate O, candidate new memory c

 t
- ► Hidden state *h*, Cell memory *c*



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

LSTM Cells

$$F_{t} = \sigma(W_{f} \cdot [x_{t}, h_{t-1}] + b_{f})$$

$$I_{t} = \sigma(W_{i} \cdot [x_{t}, h_{t-1}] + b_{i})$$

$$O_{t} = \sigma(W_{o} \cdot [x_{t}, h_{t-1}] + b_{o})$$

$$\tilde{c}_{t} = \phi(W_{c} \cdot [x_{t}, h_{t-1}] + b_{c})$$

$$c_{t} = F_{t} \otimes c_{t-1} + I_{t} \otimes \tilde{c}_{t}$$

$$h_{t} = O_{t} \otimes \phi(c_{t})$$

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_t , 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

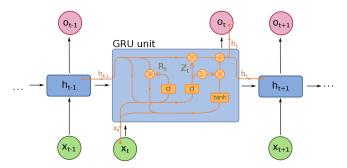
Important: Parameters are "re-used" for each unrolled step.

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 $4 \times (16 \times (8+16)+16) = 1600$



Gated Recurrent Unit (GRU) Cells

- "Update gate" Z, "Reset gate gate" R, candidate new memory ĥ_t
- ► Hidden state h



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

Fewer parameters than, and similar performance to LST

GRU Cells

$$Z_t = \sigma(W_z \cdot [x_t, h_{t-1}] + b_z)$$

$$R_t = \sigma(W_r \cdot [x_t, h_{t-1}] + b_r)$$

$$\hat{h}_t = \phi(W_h \cdot [x_t, R_t \otimes h_{t-1}] + b_h)$$

$$h_t = (1 - Z_t) \otimes h_{t-1} + Z_t \otimes \hat{h}_t$$

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.



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

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')
```

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)
```

Dataset objects feed inputs and targets to the fit function.

See how this works with simple example data:

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

Shuffle data:

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

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,
- Experiment with different values for sequence_length,
- 3 Experiment with different values for sequence_stride.

Do the results match your expectations?



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()
```

Compile and fit the model:

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)
- 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.



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.summarv()
```

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
- loss: 0.9966 - val loss: 0.9486
```

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)
```



```
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
- 14s 3ms/step - loss: 1.0094 - val_loss: 1.4701
Epoch 25/25
- 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
- Extend the stateful model to a multi-layer network and include dropout layers
- 3 How does this change the predictive performance of the model?



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:

The Flatten layer flattens its input tensor.



Stock Market Prediction [cont'd]

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)
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
```

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')
```



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']
```



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

```
# 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)
```

Identify feature to predict from:

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:



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:

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



Compile and fit the model:

Results:

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])
```

Results:

```
index_0 index_1 index_2 index_3 index_4
109280 6 7
                 8 10 9
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
            1.0
1/1 [======] - 0s 11ms/step
W Nabellen offertes
     index_0 index_1 index_2 index_3 index_4
109280 10 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.

