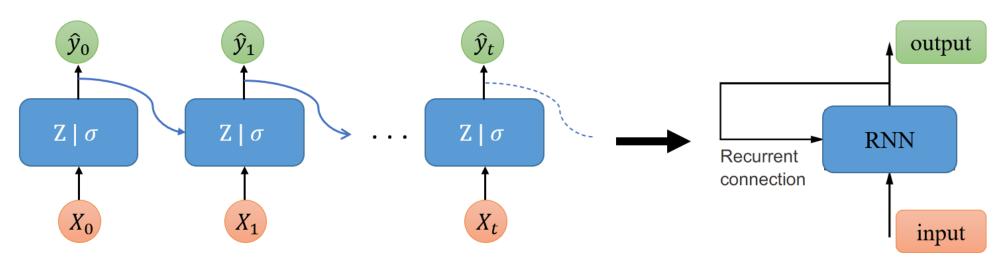
Module 7 – Part I Deep Sequence Modeling Recurrent Neural Networks (RNN)







Road map!

- Module 1- Introduction to Deep Forecasting
- Module 2- Setting up Deep Forecasting Environment
- Module 3- Exponential Smoothing
- Module 4- ARIMA models
- Module 5- Machine Learning for Time series Forecasting
- Module 6- Deep Neural Networks
- Module 7- Deep Sequence Modeling (RNN, LSTM)
- Module 8- Transformers (Attention is all you need!)
- Module 9- Prophet and Neural Prophet

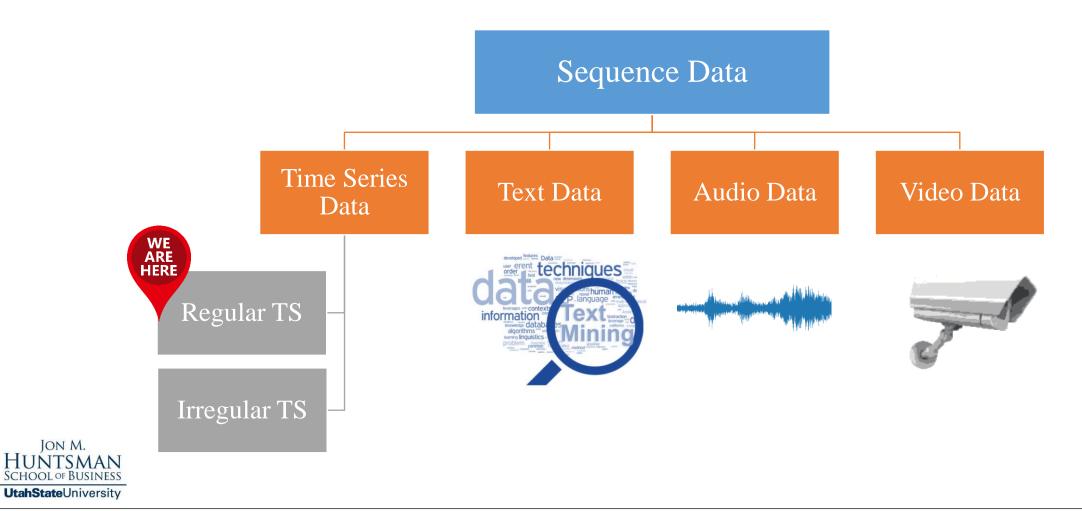






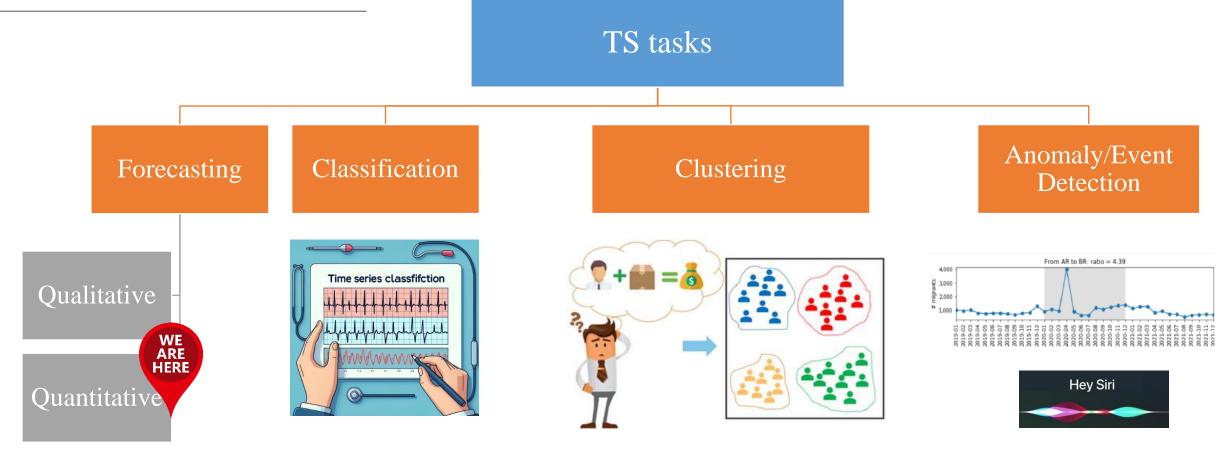
What is Sequence Data?

• Sequence data refers to any data that has a specific **order** or sequence to it!





Time series Tasks

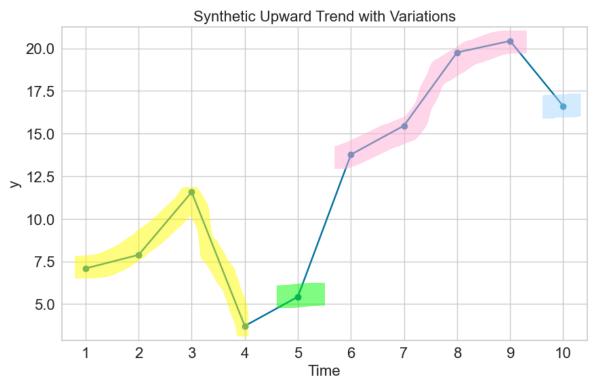








ML Data Transformation (Single-output)



Features (X)				Target (y)
y_{t-4}	y_{t-3}	y_{t-2}	y_{t-1}	y_t
y_1	y_2	y_3	y_4	y_5
y_2	y_3	y_4	y_5	y_6
y_3	y_4	y_5	y_6	y_7
y_4	y_5	y_6	y_7	y_8
y_5	y_6	y_7	y_8	y_9
y_6	y_7	y_8	<i>y</i> ₉	y_{10}

TS raw data									
y_1	y_2	y_3	y_4	y_5	y_6	y_7	y_8	y_9	y_{10}

→ TS Supervised data



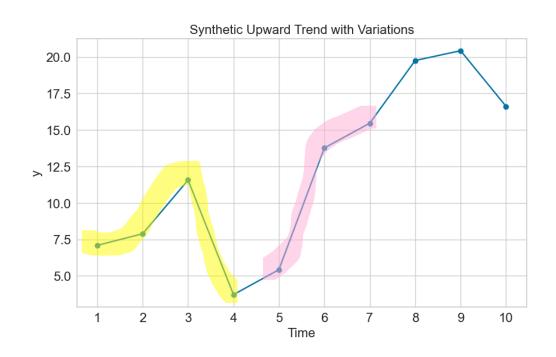




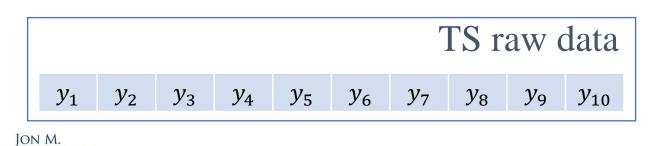
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ML Data Transformation (Multi-output)



Features (X)			Target (y)			
y_{t-4}	y_{t-3}	y_{t-2}	y_{t-1}	y_t	y_{t+1}	y_{t+2}
y_1	y_2	y_3	y_4	y_5	<i>y</i> ₆	y_7
y_2	y_3	y_4	y_5	y_6	<i>y</i> ₇	y_8
y_3	y_4	y_5	y_6	y_7	y_8	y_9
y_4	y_5	y_6	y_7	y_8	<i>y</i> ₉	y ₁₀

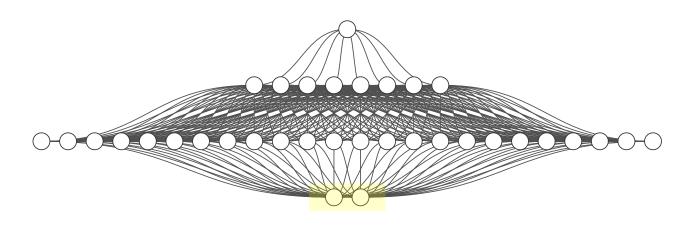


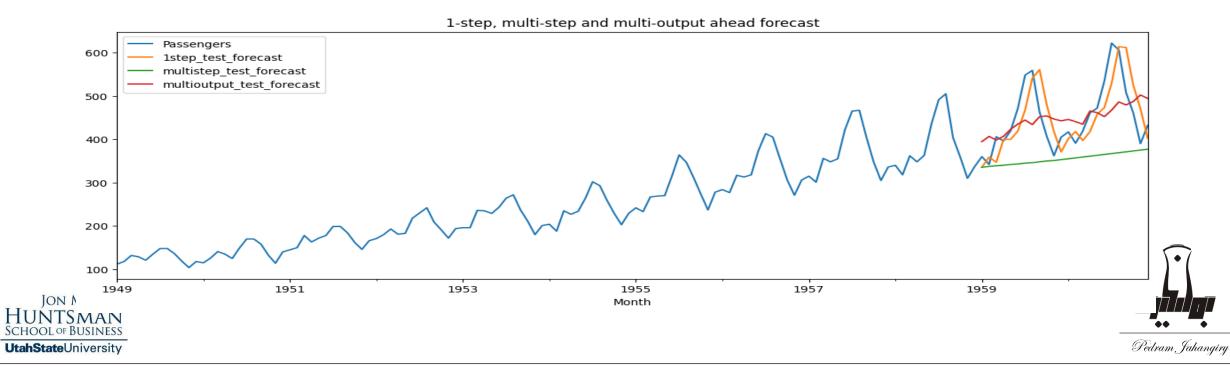
TS Supervised data (h=3)





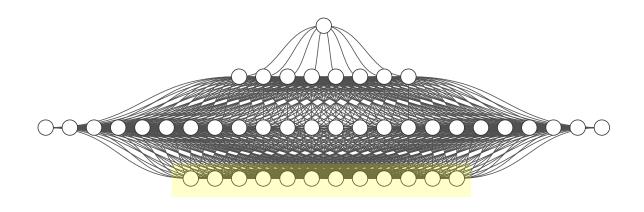
DL Example: DNN with 2 lags

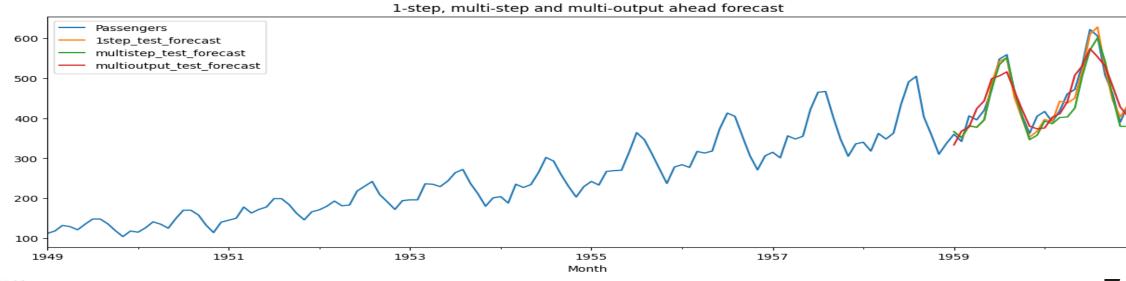






DL Example: DNN with 12 lags



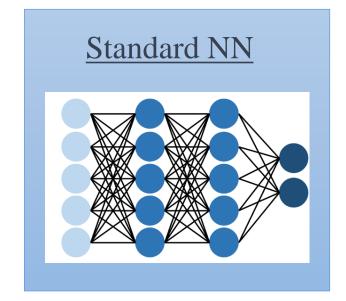


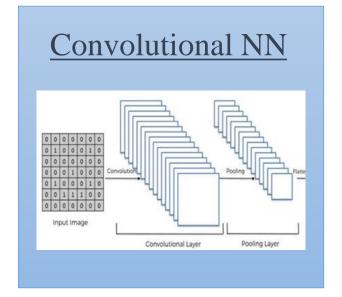


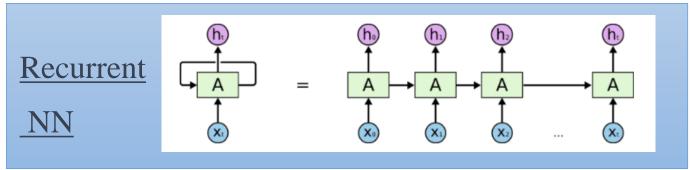


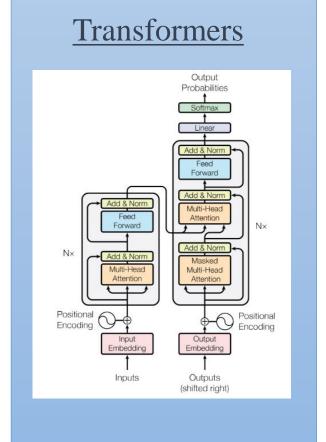


Deep Learning Architectures







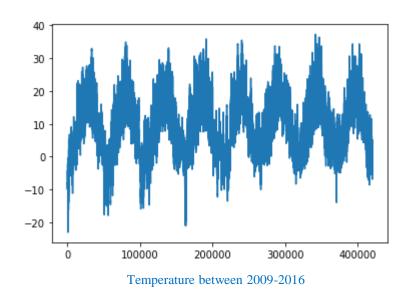


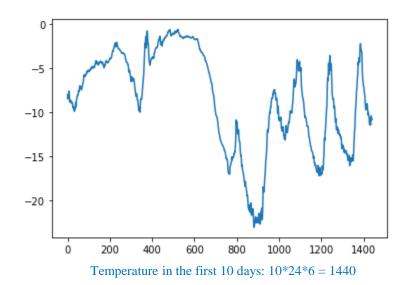




A simple timeseries example

- A temperature forecasting example: <u>deep-learning-with-python-notebooks</u>
- Predicting the temperature 24 hours in the future
 - Target: temperature
 - Features: 14 different variables including pressure, humidity, wind direction and etc
 - Data recorded every 10 minutes from 2009-2016











Preparing the data

- Given the previous 5 days (120 hours) and samples once per hour, can we predict temperature in 24 hours (after the end of the sequence)?
- Data batches:
 - Sequence length = 120
 - [1,2,3,...,120][144]
 - [2,3,4,...,121][**145**]
 - [3,4,5,...,122][146]
 - Bath size: 256 of these samples are shuffled and batched
 - Sample shape: (256, 120, 14)
 - Target shape: (256,)







Naïve forecaster: common-sense baseline

- Temperature 24 hours from now = Temperature right now
- This is our random walk with no drift forecaster.



- Validation MAE = 2.44 degrees Celsius
- Test MAE = 2.62 degrees Celsius
- The baseline model is off by about 2.5 degrees on average. Not bad!!







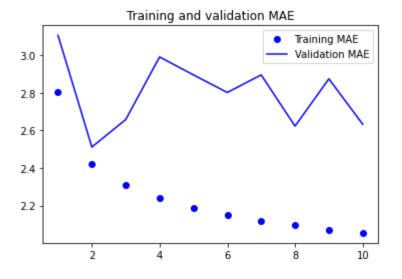


Let's try DNN (Deep Neural Networks)

```
inputs = keras.Input(shape=(sequence_length, raw_data.shape[-1]))
x = layers.Flatten()(inputs)
x = layers.Dense(16, activation="relu")(x)
outputs = layers.Dense(1)(x)
model = keras.Model(inputs, outputs)
```

Layer (type)	Output Shape	Param #
input_1 (InputLayer)	[(None, 120, 14)]	0
flatten (Flatten)	(None, 1680)	0
dense (Dense)	(None, 16)	26896
dense_1 (Dense)	(None, 1)	17

Total params: 26,913 Trainable params: 26,913 Non-trainable params: 0



- Test MAE = 2.62 degrees Celsius
- No improvement!!
- Flattening a timeseries data is not a good idea!





Let's try CNN (Convolutional Neural Networks)

• Motivation: Maybe a temporal convnet could reuse the same representations across different days, much like a spatial convnet can reuse the same representations across different locations in an image!

```
inputs = keras.Input(shape=(sequence_length, raw_data.shape[-1]))
x = layers.Conv1D(8, 24, activation="relu")(inputs)
x = layers.MaxPooling1D(2)(x)
x = layers.Conv1D(8, 12, activation="relu")(x)
x = layers.MaxPooling1D(2)(x)
x = layers.Conv1D(8, 6, activation="relu")(x)
x = layers.GlobalAveragePooling1D()(x)
outputs = layers.Dense(1)(x)
model = keras.Model(inputs, outputs)
```

Layer (type)	Output Shape	Param #
input_2 (InputLayer)	[(None, 120, 14)]	0
conv1d (Conv1D)	(None, 97, 8)	2696
<pre>max_pooling1d (MaxPooling1D)</pre>	(None, 48, 8)	0
conv1d_1 (Conv1D)	(None, 37, 8)	776
<pre>max_pooling1d_1 (MaxPooling 1D)</pre>	(None, 18, 8)	0
conv1d_2 (Conv1D)	(None, 13, 8)	392
<pre>global_average_pooling1d (G lobalAveragePooling1D)</pre>	(None, 8)	0
dense_2 (Dense)	(None, 1)	9

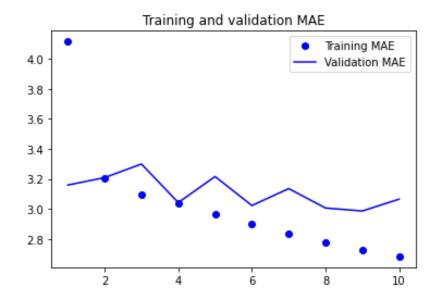
Total params: 3,873 Trainable params: 3,873 Non-trainable params: 0





CNN performance

- Test MAE = 3.10 degrees Celsius
- Even worse than the densely connected model!!
 - CNN treats every segment of the data the same way!
 - Pooling layers are destroying order information.









Sequence Modeling

To model sequence data efficiently, we need a new architecture that:

- Preserve the order
- Account for long-term dependencies
- Handle input-length
- Share parameters across the sequence

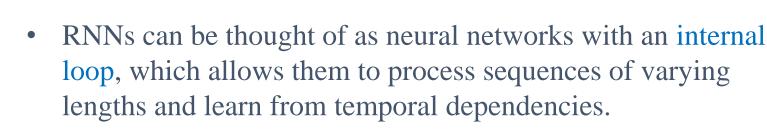


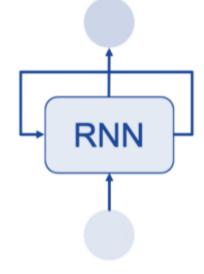




What is RNN (Recurrent Neural Network)?

- The architecture of RNNs is inspired by the way biological intelligence processes information incrementally while maintaining an internal model of what it is processing.
- This ability to remember previous inputs and <u>incorporate them</u> into the current output allows RNNs to model sequential data.
- RNN maintains a state that contains information relative to what it has seen so far
- loop, which allows them to process sequences of varying lengths and learn from temporal dependencies.

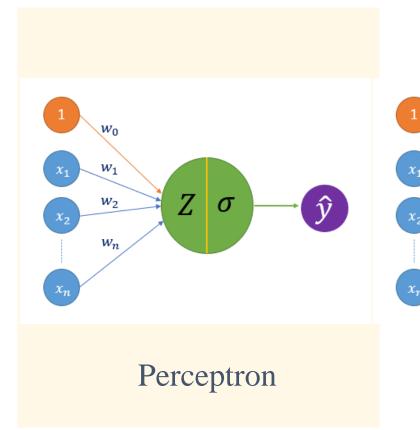


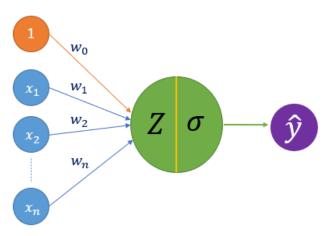


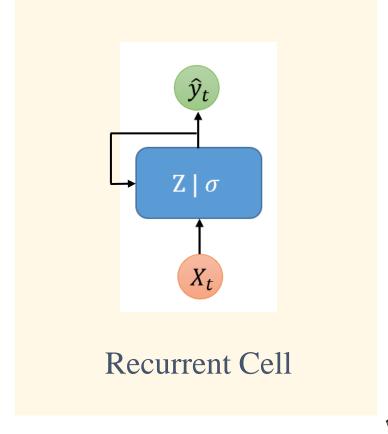




Perceptron vs Recurrent Cell



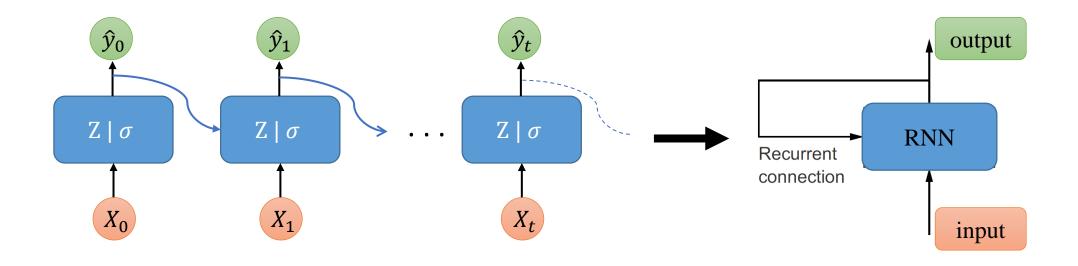








Unrolling the Recurrent Cell

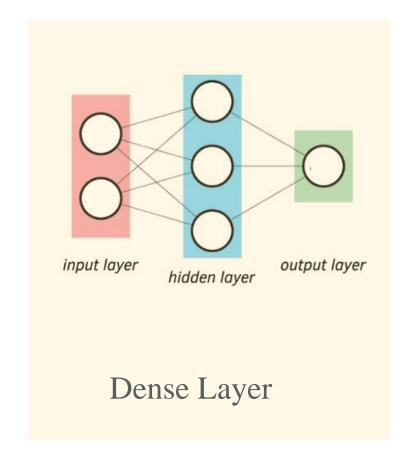


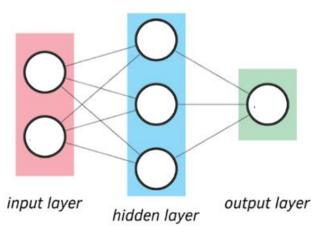


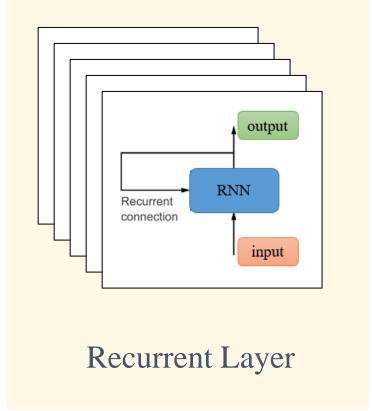




Dense Layer vs Recurrent Layer





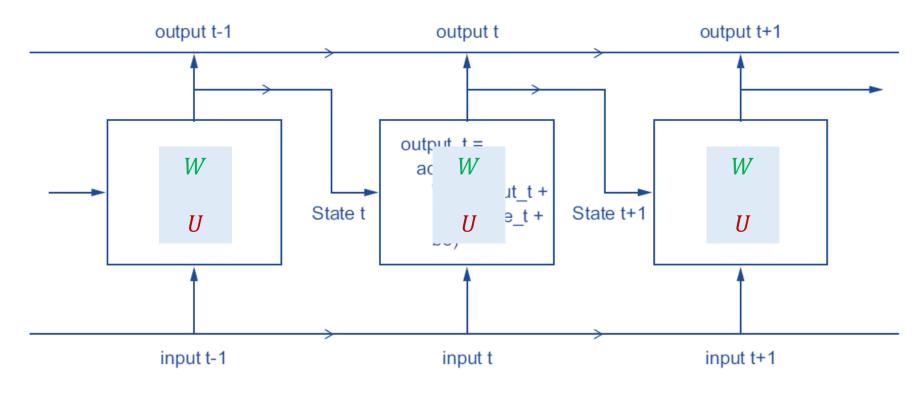






Inside the Recurrent Cell

$output_t = f(input_t, State_t)$



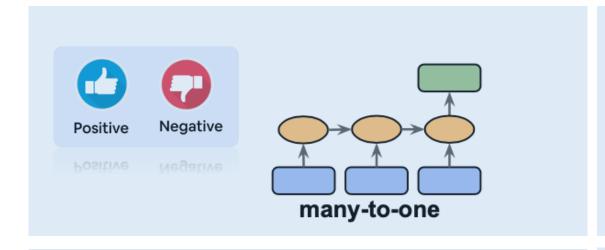


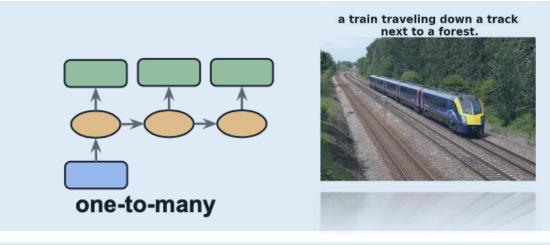
$$s_{t+1} = activation(WX_t + Us_t + b)$$

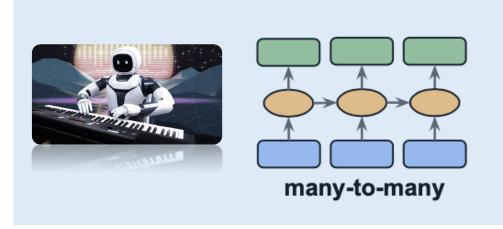


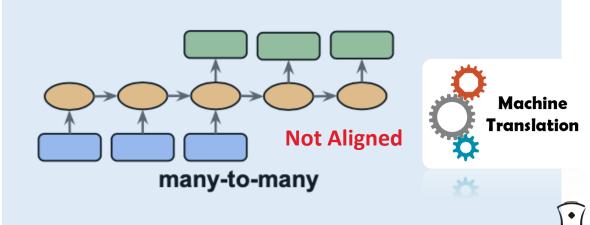


RNN architectures













How does RNN learn representations?

- Backpropagation Through Time (BPTT)
- $\frac{\partial J}{\partial P}$ P are the parameters

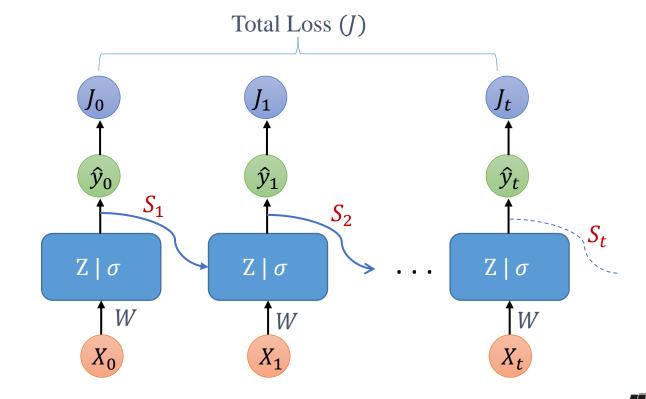
•
$$\frac{\partial J}{\partial W} = \frac{\partial J_0}{\partial W} + \frac{\partial J_1}{\partial W} + \dots$$

$$\bullet \quad \frac{\partial J_0}{\partial W} = \frac{\partial J_0}{\partial y_0} \frac{\partial y_0}{\partial S_0} \frac{\partial S_0}{\partial W}$$

•
$$\frac{\partial J_1}{\partial W} = \frac{\partial J_1}{\partial y_1} \frac{\partial y_1}{\partial S_1} \frac{\partial S_1}{\partial W}$$
 , $\frac{\partial S_1}{\partial W} = \frac{\partial S_1}{\partial S_0} \frac{\partial S_0}{\partial W}$

•

•
$$\frac{\partial J_t}{\partial W} = \sum_{k=0}^t \frac{\partial J_t}{\partial y_t} \frac{\partial y_t}{\partial S_t} \frac{\partial S_t}{\partial S_k} \frac{\partial S_k}{\partial W}$$



Pedram, Jahangiry





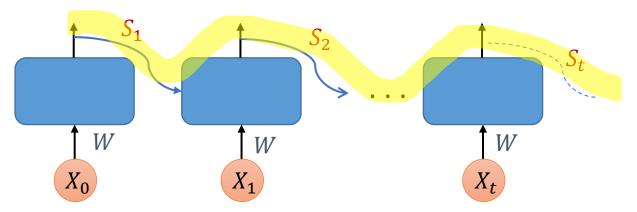
Vanishing Gradient Problem

- As the time horizon gets bigger, this product gets longer and longer.
- We are multiplying a lot of <u>small numbers</u> \rightarrow <u>smaller gradients</u> \rightarrow <u>biased parameters</u> unable to capture long term dependencies.

•
$$\frac{\partial J_t}{\partial W} = \sum_{k=0}^t \frac{\partial J_t}{\partial y_t} \frac{\partial y_t}{\partial S_t} \frac{\partial S_t}{\partial S_k} \frac{\partial S_k}{\partial W}$$

•
$$\frac{\partial S_{10}}{\partial S_0} = \frac{\partial S_{10}}{\partial S_9} \frac{\partial S_9}{\partial S_8} \frac{\partial S_8}{\partial S_7} \frac{\partial S_7}{\partial S_6} \dots \frac{\partial S_1}{\partial S_0}$$

$$S_t = activation(WX_{t_1} + US_{t-1})$$









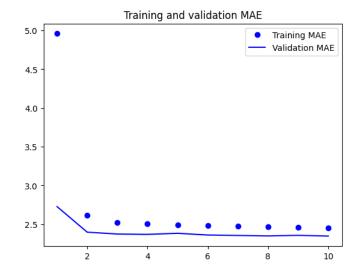
Let's try a simple RNN

```
inputs = keras.Input(shape=(sequence_length, raw_data.shape[-1]))
x = layers.SimpleRNN(16)(inputs)
outputs = layers.Dense(1)(x)
model = keras.Model(inputs, outputs)
```

Layer (type)	Output Shape	Param #
input_3 (InputLayer)	[(None, 120, 14)]	0
simple_rnn (SimpleRNN)	(None, 16)	496
dense_3 (Dense)	(None, 1)	17

Total params: 513 (2.00 KB)
Trainable params: 513 (2.00 KB)

Non-trainable params: 0 (0.00 Byte)



- Baseline Test MAE = 2.62
- Simple RNN Test MAE = 2.51
- beats the naïve forecaster.

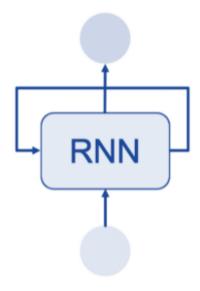




Beyond RNN

RNN can handle the following sequence modeling criteria:

- Preserve the order
- Handle input-length
- Share parameters across the sequence



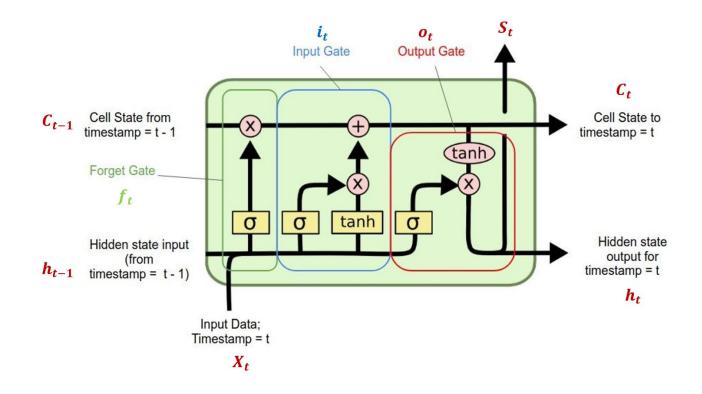
RNN limitations:

- Does not account for long-term dependencies (only remember short term history)
- Vanishing Gradient Problem





Module 7 – Part II Deep Sequence Modeling (Gated cells, LSTM)





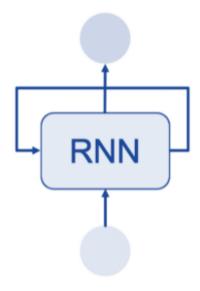




Beyond RNN

RNN can handle the following sequence modeling criteria:

- Preserve the order
- Handle input-length
- Share parameters across the sequence



RNN limitations:

- Does not account for long-term dependencies (only remember short term history)
- Vanishing Gradient Problem

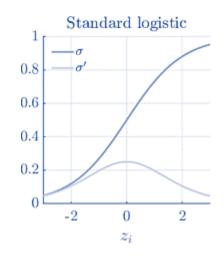


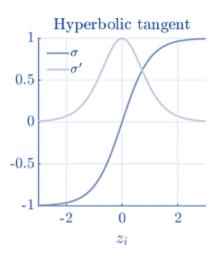


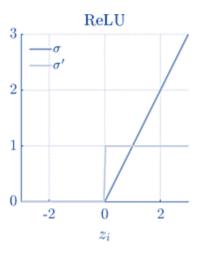


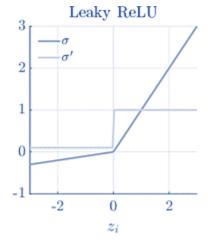
How to solve vanishing gradient problem

1. Use Activation Function that prevents fast shrinkage of gradient











$$S_t = activation(WX_{t-1} + US_{t-1})$$





How to solve vanishing gradient problem

- 1. Use Activation Function that prevents fast shrinkage of gradient
- 2. Use weight initialization techniques that ensure that the initial weights are not too small
- 3. Use gradient clipping which limits the magnitude of the gradients from becoming too small (vanishing gradient) or too large (exploding gradient)
- 4. Use batch normalization, which normalizes the input to each layer and helps to reduce the range of activation values and thus the likelihood of vanishing gradients.
- 5. Use a different optimization algorithm that is more resilient to vanishing gradients, such as Adam or RMSprop.
- **6. Gated cells:** Use some sort of **skip connections**, which allow gradients to bypass some of the layers in the network and thus prevent them from becoming too small.

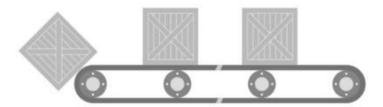


Pedram, Jahangiry



Gated cells

- Instead of using a simple RNN cell, let's use a more complex cell with gates which control the flow of information.
- Think of a conveyer belt running parallel to the sequence being processed:
 - Information can jump on \rightarrow transported to a later timestep \rightarrow jump off when needed.
 - This is what a gated cell does! Analogous to residual connections we saw before.

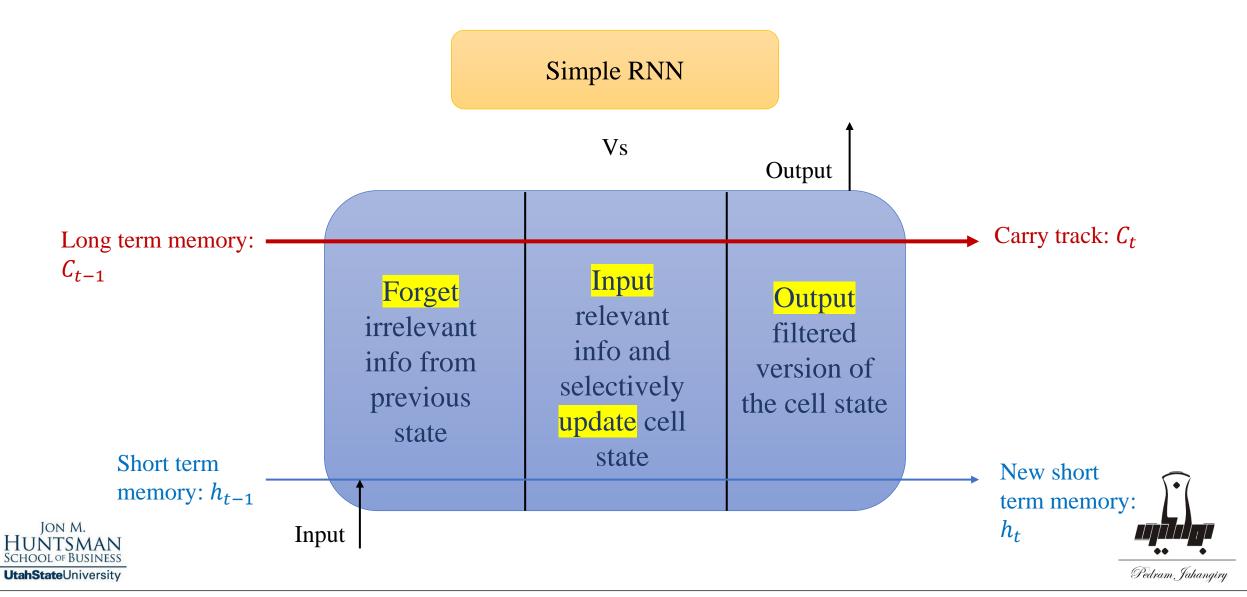


• Long Short-Term Memory (LSTM) and Gated Recurrent Unit (GRU) are two examples of gated cells that can keep track of information throughout many timesteps.





Inside the LSTM cell

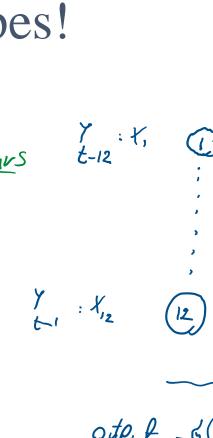




All about shapes!

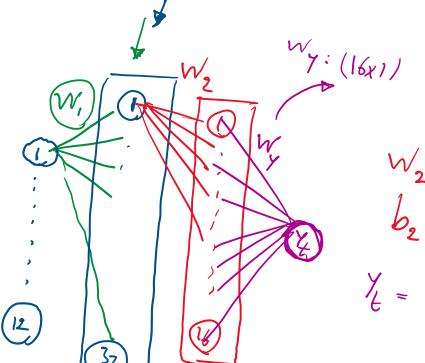
DNN
univariate to with loop hours
X: 12 lags

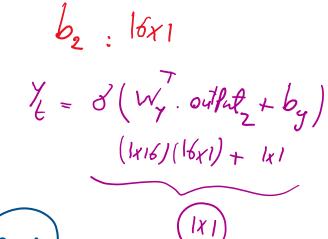
$$X: (12 \times 1)$$
 $W_1: (12 \times 32)$
 $b_1: (32 \times 1)$



otput, =
$$G(W_1, X + b_1)$$
: (32x1)

outlity =
$$6(W_2 \cdot \text{outlit}, + b_2)$$
 - $(16x32)(32x1) + 16x1$





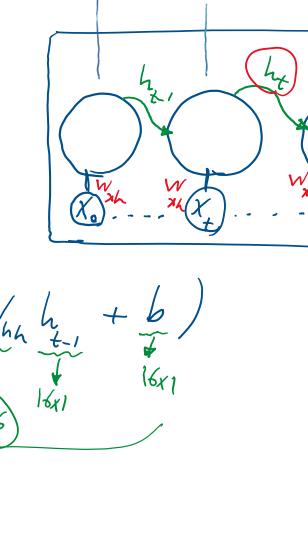
W2: 32x16

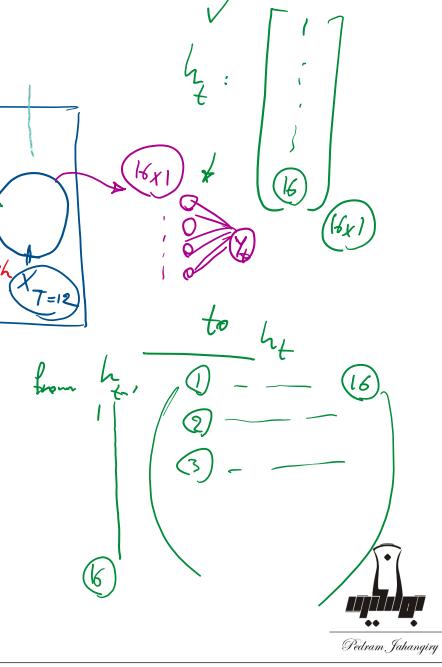






All about shapes!





Jon M. HUNTSMAN

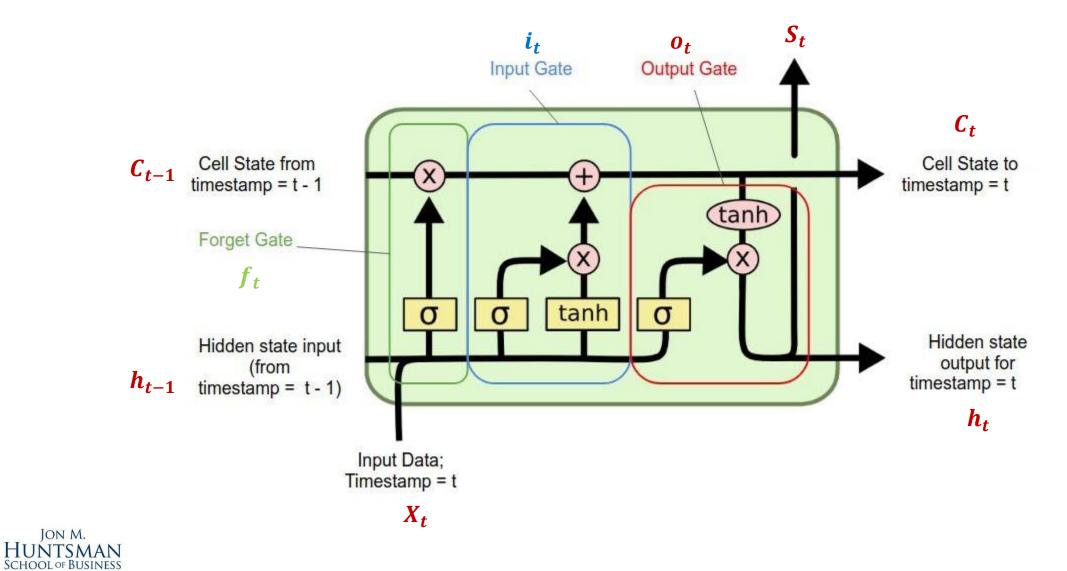
RM, : (None, 12, 16)

RNN2: (None, 32)



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LSTM details

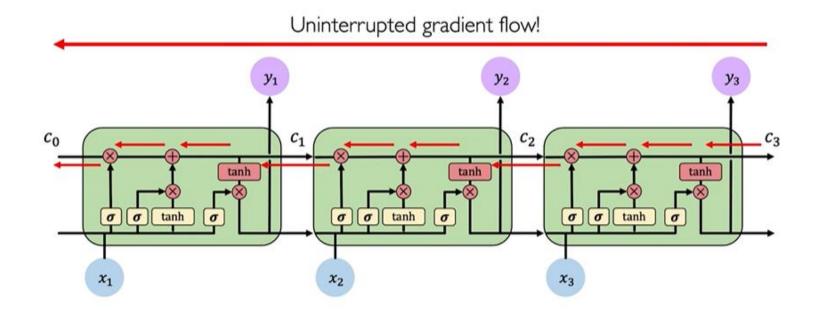






LSTM takeaway

- LSTM uses gates to regulate the information flow (allows past information to be reinjected later)
- This new cell state (carry) can better capture longer term dependencies
- LSTM fights the vanishing gradient problem









Let's try LSTM on the temperature example

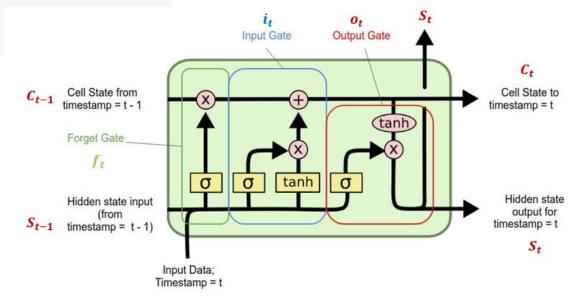
inputs = keras.Input(shape=(sequence_length, raw_data.shape[-1]))
x = layers.LSTM(16)(inputs)

outputs = layers.Dense(1)(x)

model = keras.Model(inputs, outputs)

Layer (type)	Output Shape	Param #
input_3 (InputLayer)	[(None, 120, 14)]	0
lstm (LSTM)	(None, 16)	1984
dense_3 (Dense)	(None, 1)	17

Total params: 2,001 Trainable params: 2,001 Non-trainable params: 0



 X_t

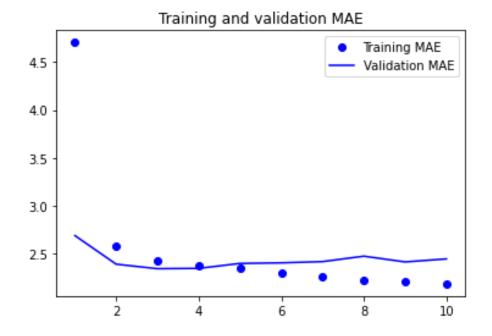
```
output_t = activation(dot(state_t, Uo) + dot(input_t, Wo) + dot(c_t, Vo) + bo)
i_t = activation(dot(state_t, Ui) + dot(input_t, Wi) + bi)
f_t = activation(dot(state_t, Uf) + dot(input_t, Wf) + bf)
k_t = activation(dot(state_t, Uk) + dot(input_t, Wk) + bk)
```





LSTM performance

- Baseline Test MAE = 2.62
- Simple LSTM Test MAE = 2.53
- Also beats the naïve forecaster.
- Overfitting?







Can we do better?







Improving the simple LSTM model

- We can improve the performance of the simple LSTM model by:
- 1. Recurrent Dropout: use drop out to fight overfitting in the recurrent layers (in addition to drop out for the dense layers)
- 2. Stacking recurrent layers: increase model complexity to boost representation power
- 3. Using bidirectional RNN: processing the same information differently! Mostly used in NLP.





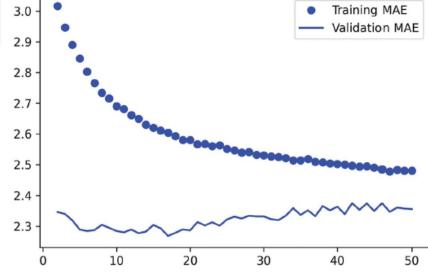


Recurrent Drop out

• The same dropout pattern should be applied at every timestep

```
inputs = keras.Input(shape=(sequence_length, raw_data.shape[-1]))
x = layers.LSTM(32, recurrent_dropout=0.25)(inputs)
x = layers.Dropout(0.5)(x)
outputs = layers.Dense(1)(x)
model = keras.Model(inputs, outputs)
3.0
0.29
```

- Baseline Test MAE = 2.62
- Simple RNN, Test MAE = 2.51
- Simple LSTM, Test MAE = 2.53
- LSTM with dropout, Test MAE = 2.45









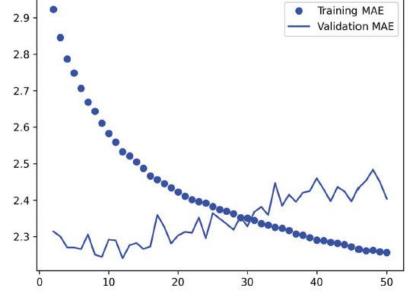
Stacking Recurrent Layers

- Let's train a dropout-regulated, stacked GRU model.
- GRU is a slightly simpler version (hence, faster) of LSTM architecture

```
inputs = keras.Input(shape=(sequence_length, raw_data.shape[-1]))
x = layers.GRU(32, recurrent_dropout=0.5, return_sequences=True)(inputs)
x = layers.GRU(32, recurrent_dropout=0.5)(x)
x = layers.Dropout(0.5)(x)
outputs = layers.Dense(1)(x)
model = keras.Model(inputs, outputs)
```

- Baseline Test MAE = 2.62
- Simple RNN, Test MAE = 2.51
- Simple LSTM, Test MAE = 2.53
- Stacking GRU, Test MAE = 2.39







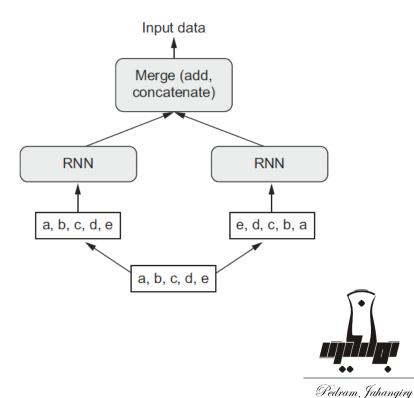


Bidirectional RNN

- Bidirectional RNN process the input sequence both chronologically and antichronologically.
- Idea: capturing patterns (representations) that might be overlooked by a unidirectional RNN.
- For the temperature example, the bidirectional LSTM strongly underperforms even the common-sense baseline.

```
inputs = keras.Input(shape=(sequence_length, raw_data.shape[-1]))
x = layers.Bidirectional(layers.LSTM(16))(inputs)
outputs = layers.Dense(1)(x)
model = keras.Model(inputs, outputs)
```







Final message

- Deep learning is more an art than science! Too many moving part!
 - Number of units in each recurrent layer
 - Number of stacked layers
 - Amount of dropout and recurrent dropout
 - Number of dense layers
 - Sequence horizon!
 - Optimizers, learning rates and etc
 - •







Road map!

- ✓ Module 1- Introduction to Deep Forecasting
- ✓ Module 2- Setting up Deep Forecasting Environment
- ✓ Module 3- Exponential Smoothing
- ✓ Module 4- ARIMA models
- ✓ Module 5- Machine Learning for Time series Forecasting
- ✓ Module 6- Deep Neural Networks
- ✓ Module 7- Deep Sequence Modeling (RNN, LSTM)
- Module 8- Transformers (Attention is all you need!)
- Module 9- Prophet and Neural Prophet



