February 26-March 1: Advanced machine learning and data analysis for the physical sciences

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February 26-March 1, 2024

Plans for the week February 26-March 1

1. Finalizing discussion of Convolutional Neural Networks (CNNs)
2. Discussion of recurrent neural networks (RNNs)
3. Reading recommendations:
   (a) Goodfellow, Bengio and Courville's chapter 10 from Deep Learning
   (b) Sebastian Rashcka et al, chapter 15, Machine learning with Sickit-Learn and PyTorch
   (c) David Foster, Generative Deep Learning with TensorFlow, see chapter 5

The last two books have codes for RNNs in PyTorch and TensorFlow/Keras.

From FFNNs and CNNs to recurrent neural networks (RNNs)

There are limitation of FFNNs, one of which being that FFNNs are not designed to handle sequential data (data for which the order matters) effectively because they lack the capabilities of storing information about previous inputs; each input is being treated indepen- dently. This is a limitation when dealing with sequential data where past information can be vital to correctly process current and future inputs.

Feedback connections

In contrast to FFNs, recurrent networks introduce feedback connections, meaning the information is al- lowed to be carried to subsequent nodes across different time steps. These cyclic or feedback connections have the objective of providing the network with some kind of memory, making RNNs particularly suited for time- series data, natural language processing, speech recog- nition, and several other problems for which the order of the data is crucial. RNN architectures vary greatly in how they manage information flow and memory in the network. Different architectures often aim at improving some sub-optimal characteristics of the network. The simplest form of recurrent network, commonly called simple or vanilla RNN, for example, is known to suffer from the problem of vanishing gradients. This problem arises due to the nature of backpropagation in time. Gradients of the cost/loss function may get exponentially small (or large) if there are many layers in the network, which is the case of RNN when the sequence gets long.

Recurrent neural networks (RNNs): Overarching view

Till now our focus has been, including convolutional neural networks as well, on feedforward neural networks. The output or the activations flow only in one direction, from the input layer to the output layer.

A recurrent neural network (RNN) looks very much like a feedforward neural network, except that it also has connections pointing backward.

RNNs are used to analyze time series data such as stock prices, and tell you when to buy or sell. In autonomous driving systems, they can anticipate car trajectories and help avoid accidents. More generally, they can work on sequences of arbitrary lengths, rather than on fixed-sized inputs like all the nets we have discussed so far. For example, they can take sentences, documents, or audio samples as input, making them extremely useful for natural language processing systems such as automatic translation and speech-to-text.

A simple example

```
# Start importing packages
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import tensorflow as tf
from tensorflow.keras import datasets, layers, models
from tensorflow.keras.layers import Input
from tensorflow.keras.models import Model, Sequential
from tensorflow.keras.layers import Dense, SimpleRNN, LSTM, GRU
from tensorflow.keras import optimizers
from tensorflow.keras import regularizers
from tensorflow.keras.utils import to_categorical



# convert into dataset matrix
def convertToMatrix(data, step):
```

```
 X, Y =[], []
 for i in range(len(data)-step):
  d=i+step
  X.append(data[i:d,])
  Y.append(data[d,])
 return np.array(X), np.array(Y)

step = 4
N = 1000
Tp = 800

t=np.arange(0,N)
x=np.sin(0.02*t)+2*np.random.rand(N)
df = pd.DataFrame(x)
df.head()

values=df.values
train,test = values[0:Tp,:], values[Tp:N,:]

# add step elements into train and test
test = np.append(test,np.repeat(test[-1,],step))
train = np.append(train,np.repeat(train[-1,],step))

trainX,trainY =convertToMatrix(train,step)
testX,testY =convertToMatrix(test,step)
trainX = np.reshape(trainX, (trainX.shape[0], 1, trainX.shape[1]))
testX = np.reshape(testX, (testX.shape[0], 1, testX.shape[1]))

model = Sequential()
model.add(SimpleRNN(units=32, input_shape=(1,step), activation="relu"))
model.add(Dense(8, activation="relu"))
model.add(Dense(1))
model.compile(loss='mean_squared_error', optimizer='rmsprop')
model.summary()

model.fit(trainX,trainY, epochs=100, batch_size=16, verbose=2)
trainPredict = model.predict(trainX)
testPredict= model.predict(testX)
predicted=np.concatenate((trainPredict,testPredict),axis=0)

trainScore = model.evaluate(trainX, trainY, verbose=0)
print(trainScore)
plt.plot(df)
plt.plot(predicted)
plt.show()
```

Memoryless models

Autoregressive models predict the next term in a sequence from a fixed number of previous terms. David Foster, Generative Deep Learning with TensorFlow, discusses in chapter 5 autoregressive models. We will come back later to autoregressive models.

Feed-forward neural networks. These generalize autoregressive models by using one or more layers of non-linear hidden units.

If we give our generative model some hidden state, and if we give this hidden state its own internal dynamics, we get a much more interesting kind of model.

1. It can store information in its hidden state for a long time.
2. If the dynamics is noisy and the way it generates outputs from its hidden state is noisy, we can never know its exact hidden state.
3. The best we can do is to infer a probability distribution over the

space of hidden state vectors.

This inference is only tractable for two types of hidden state models.

RNNs

RNNs are very powerful, because they combine two properties:

1. Distributed hidden state that allows them to store a lot of information about the past efficiently.
2. Non-linear dynamics that allows them to update their hidden state in complicated ways.

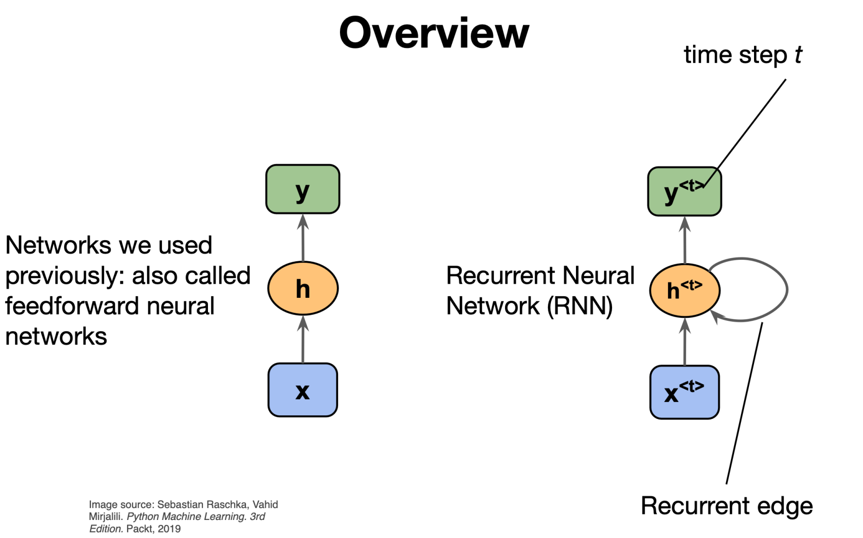
With enough neurons and time, RNNs can compute anything that can be computed by your computer.

What kinds of behaviour can RNNs exhibit?

1. They can oscillate.
2. They can settle to point attractors.
3. They can behave chaotically.
4. RNNs could potentially learn to implement lots of small programs that each capture a nugget of knowledge and run in parallel, interacting to produce very complicated effects.

But the computational power of RNNs makes them very hard to train.

Basic layout, Figures from Sebastian Rashcka et al, Machine learning with Sickit-Learn and PyTorch



We need to specify the initial activity state of all the hidden and output units

1. We could just fix these initial states to have some default value like 0.5.
2. But it is better to treat the initial states as learned parameters.
3. We learn them in the same way as we learn the weights.
4. Start off with an initial random guess for the initial states.
   (a) At the end of each training sequence, backpropagate through time all the way to the initial states to get the gradient of the error function with respect to each initial state.
   (b) Adjust the initial states by following the negative gradient.

We can specify inputs in several ways

1. Specify the initial states of all the units.
2. Specify the initial states of a subset of the units.
3. Specify the states of the same subset of the units at every time step.

This is the natural way to model most sequential data.

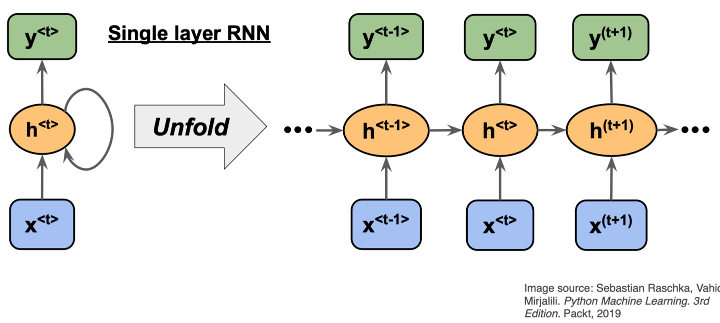
We can specify targets in several ways

1. Specify desired final activities of all the units
2. Specify desired activities of all units for the last few steps
3. Good for learning attractors
4. It is easy to add in extra error derivatives as we backpropagate.
    - Specify the desired activity of a subset of the units.
5. The other units are input or hidden units.

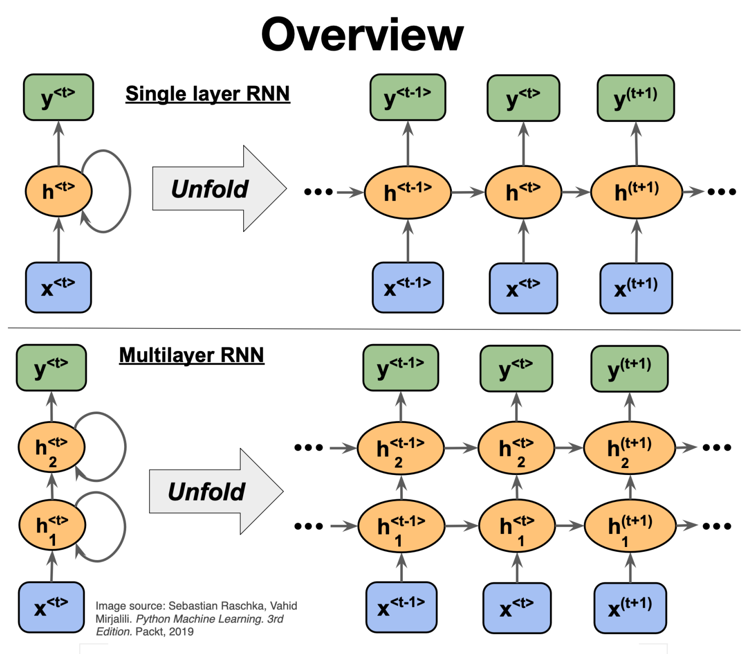
Solving differential equations with RNNs

More material to be added here.

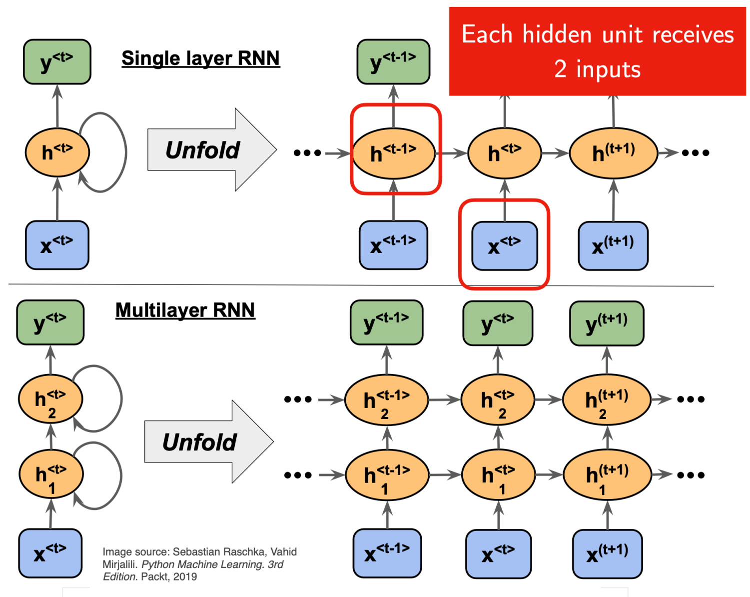
RNNs in mode detail



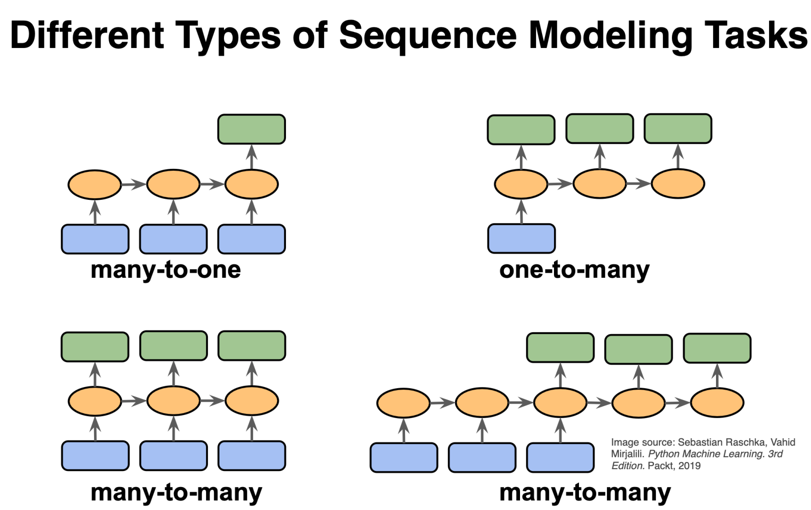
RNNs in mode detail, part 2



RNNs in mode detail, part 3



RNNs in mode detail, part 4



RNNs in mode detail, part 5

Weight matrices in a single-hidden layer RNN

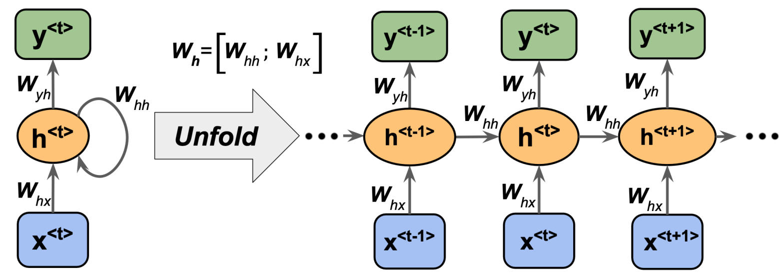


Image source: Sebastian Raschka, Vahid Mirjalili. *Python Machine Learning. 3rd Edition.* Packt, 2019

RNNs in mode detail, part 6

Weight matrices in a single-hidden layer RNN

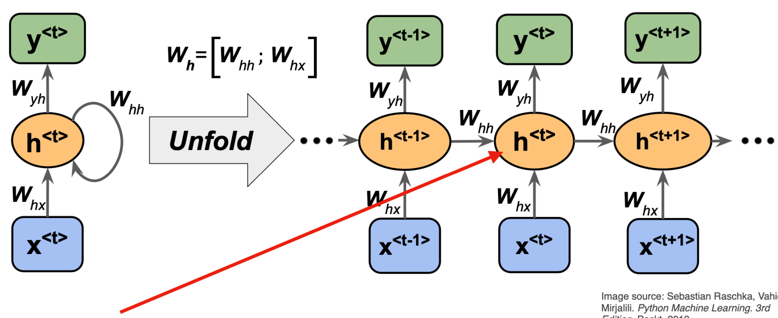
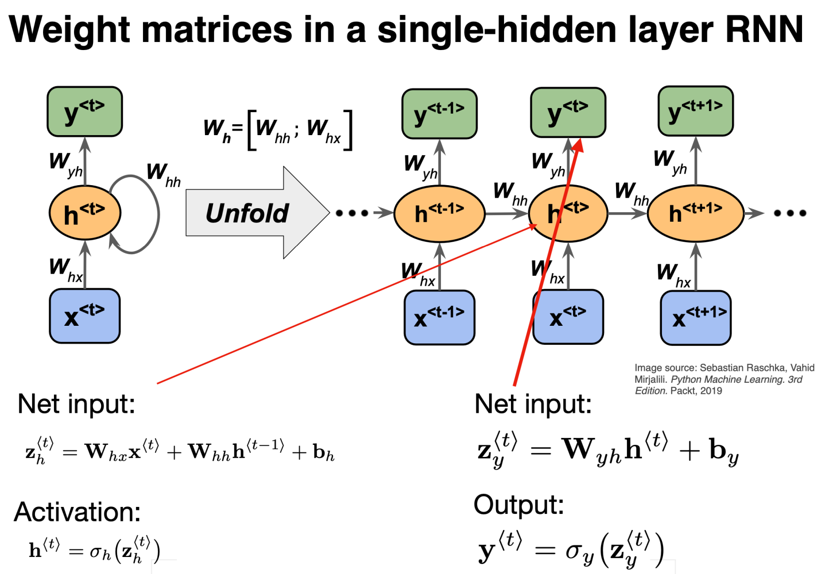


Image source: Sebastian Raschka, Vahid Mirjalili. *Python Machine Learning. 3rd Edition.* Packt, 2019

Net input: $\mathbf{z}_h^{\langle t \rangle} = \mathbf{W}_{hx}\mathbf{x}^{\langle t \rangle} + \mathbf{W}_{hh}\mathbf{h}^{\langle t-1 \rangle} + \mathbf{b}_h$

Activation: $\mathbf{h}^{\langle t \rangle} = \sigma_h\left(\mathbf{z}_h^{\langle t \rangle}\right)$

RNNs in mode detail, part 7



Backpropagation through time

We can think of the recurrent net as a layered, feed-forward net with shared weights and then train the feed-forward net with weight constraints.

We can also think of this training algorithm in the time domain:

1. The forward pass builds up a stack of the activities of all the units at each time step.
2. The backward pass peels activities off the stack to compute the error derivatives at each time step.
3. After the backward pass we add together the derivatives at all the different times for each weight.

The backward pass is linear

1. There is a big difference between the forward and backward passes.
2. In the forward pass we use squashing functions (like the logistic) to prevent the activity vectors from exploding.
3. The backward pass, is completely linear. If you double the error derivatives at the final layer, all the error derivatives will double.

The forward pass determines the slope of the linear function used for backpropagating through each neuron

The problem of exploding or vanishing gradients

- What happens to the magnitude of the gradients as we backpropagate through many layers?

    1. If the weights are small, the gradients shrink exponentially.
    2. If the weights are big the gradients grow exponentially.

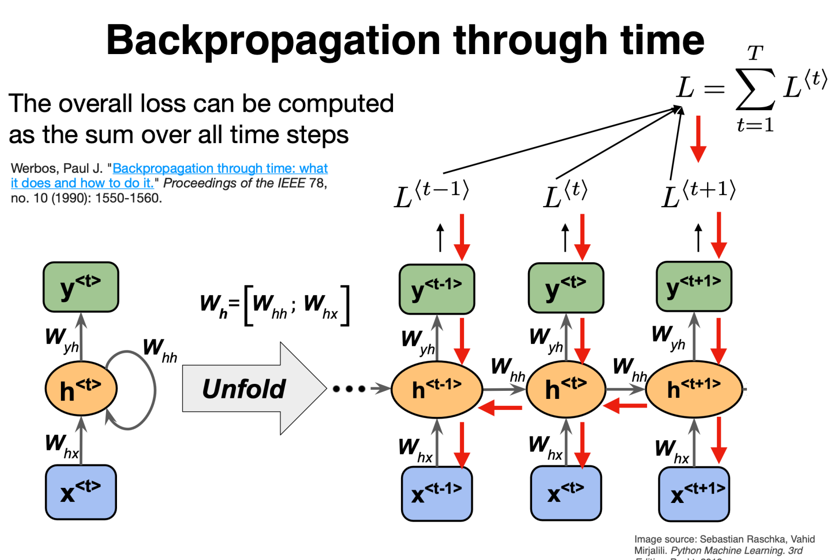
- Typical feed-forward neural nets can cope with these exponential effects because they only have a few hidden layers.
- In an RNN trained on long sequences (e.g. 100 time steps) the gradients can easily explode or vanish.

    1. We can avoid this by initializing the weights very carefully.

- Even with good initial weights, its very hard to detect that the current target output depends on an input from many time-steps ago.

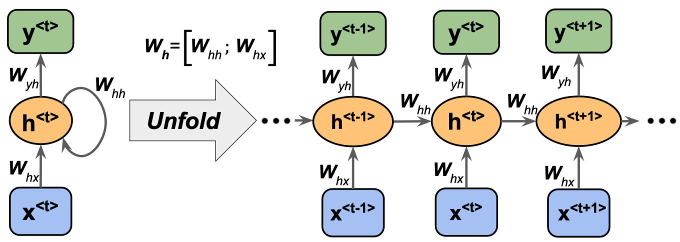
RNNs have difficulty dealing with long-range dependencies.

Back propagation in time, part 1



Back propagation in time, part 2

Backpropagation through time



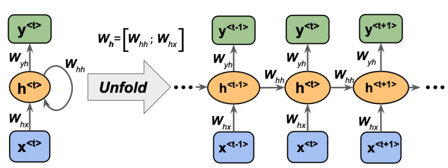
Werbos, Paul J. "Backpropagation through time: what it does and how to do it." *Proceedings of the IEEE* 78, no. 10 (1990): 1550-1560.

$$L = \sum_{t=1}^{T} L^{(t)}$$

$$\frac{\partial L^{(t)}}{\partial \mathbf{W}_{hh}} = \frac{\partial L^{(t)}}{\partial y^{(t)}} \cdot \frac{\partial y^{(t)}}{\partial \mathbf{h}^{(t)}} \cdot \left(\sum_{k=1}^{t} \frac{\partial \mathbf{h}^{(t)}}{\partial \mathbf{h}^{(k)}} \cdot \frac{\partial \mathbf{h}^{(k)}}{\partial \mathbf{W}_{hh}} \right)$$

Back propagation in time, part 3

Backpropagation through time



Werbos, Paul J. "Backpropagation through time: what it does and how to do it." *Proceedings of the IEEE* 78, no. 10 (1990): 1550-1560.

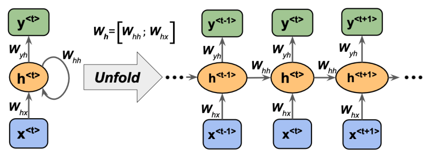
$$\frac{\partial L^{(t)}}{\partial \mathbf{W}_{hh}} = \frac{\partial L^{(t)}}{\partial y^{(t)}} \cdot \frac{\partial y^{(t)}}{\partial \mathbf{h}^{(t)}} \cdot \left(\sum_{k=1}^{t} \boxed{\frac{\partial \mathbf{h}^{(t)}}{\partial \mathbf{h}^{(k)}}} \cdot \frac{\partial \mathbf{h}^{(k)}}{\partial \mathbf{W}_{hh}} \right)$$

computed as a multiplication of adjacent time steps:

$$\frac{\partial \mathbf{h}^{(t)}}{\partial \mathbf{h}^{(k)}} = \prod_{i=k+1}^{t} \frac{\partial \mathbf{h}^{(i)}}{\partial \mathbf{h}^{(i-1)}}$$

Back propagation in time, part 4

Backpropagation through time



Werbos, Paul J. "Backpropagation through time: what it does and how to do it." *Proceedings of the IEEE* 78, no. 10 (1990): 1550-1560.

$$L = \sum_{t=1}^{T} L^{(t)} \qquad \frac{\partial L^{(t)}}{\partial \mathbf{W}_{hh}} = \frac{\partial L^{(t)}}{\partial y^{(t)}} \cdot \frac{\partial y^{(t)}}{\partial \mathbf{h}^{(t)}} \cdot \left(\sum_{k=1}^{t} \boxed{\frac{\partial \mathbf{h}^{(t)}}{\partial \mathbf{h}^{(k)}}} \cdot \frac{\partial \mathbf{h}^{(k)}}{\partial \mathbf{W}_{hh}} \right)$$

computed as a multiplication of adjacent time steps:

This is very problematic:
Vanishing/Exploding gradient problem!

$$\frac{\partial \mathbf{h}^{(t)}}{\partial \mathbf{h}^{(k)}} = \prod_{i=k+1}^{t} \frac{\partial \mathbf{h}^{(i)}}{\partial \mathbf{h}^{(i-1)}}$$

Solving differential equations with RNNs, code examples

Four effective ways to learn an RNN

1. Long Short Term Memory Make the RNN out of little modules that are designed to remember values for a long time.
2. Hessian Free Optimization: Deal with the vanishing gradients problem by using a fancy optimizer that can detect directions with a tiny gradient but even smaller curvature.
3. Echo State Networks: Initialize the input a hidden and hidden-hidden and output-hidden connections very carefully so that the hidden state has a huge reservoir of weakly coupled oscillators which can be selectively driven by the input.
   - ESNs only need to learn the hidden-output connections.
4. Good initialization with momentum Initialize like in Echo State Networks, but then learn all of the connections using momentum

Long Short Term Memory (LSTM)

LSTM uses a memory cell for modeling long-range dependencies and avoid vanishing gradient problems.

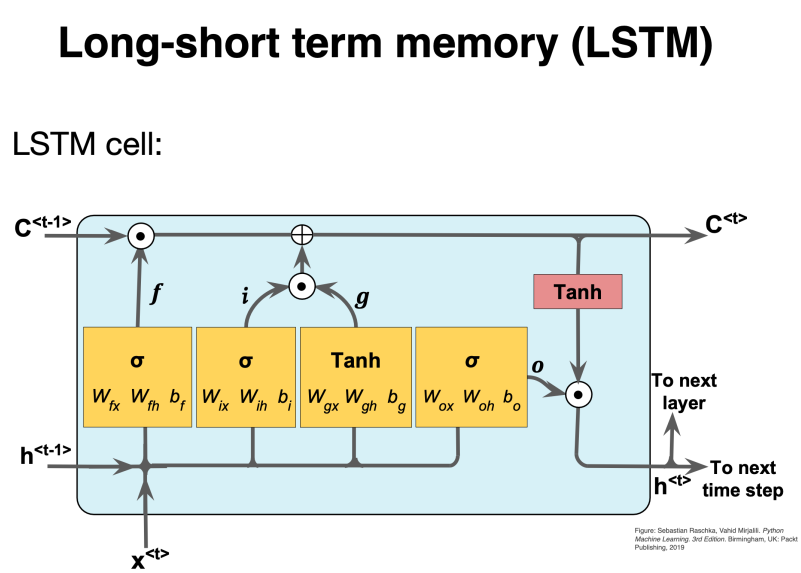
1. Introduced by Hochreiter and Schmidhuber (1997) who solved the problem of getting an RNN to remember things for a long time (like hundreds of time steps).
2. They designed a memory cell using logistic and linear units with multiplicative interactions.
3. Information gets into the cell whenever its “write” gate is on.
4. The information stays in the cell so long as its **keep** gate is on.
5. Information can be read from the cell by turning on its **read** gate.

Implementing a memory cell in a neural network

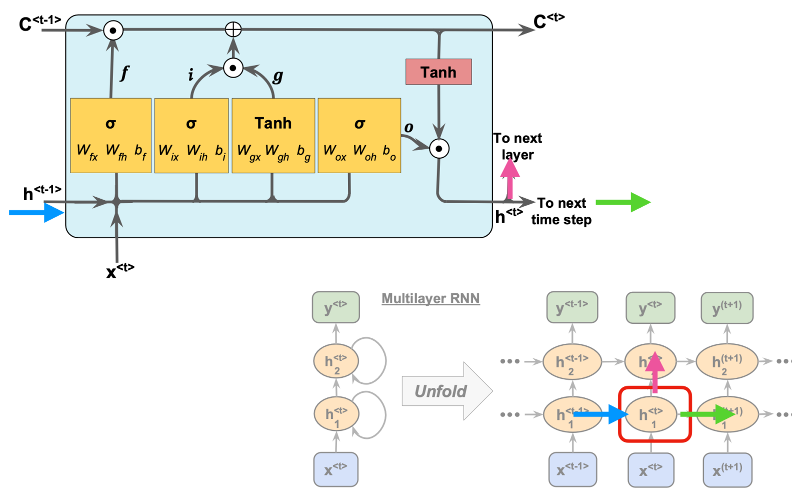
To preserve information for a long time in the activities of an RNN, we use a circuit that implements an analog memory cell.

1. A linear unit that has a self-link with a weight of 1 will maintain its state.
2. Information is stored in the cell by activating its write gate.
3. Information is retrieved by activating the read gate.
4. We can backpropagate through this circuit because logistics are have nice derivatives.

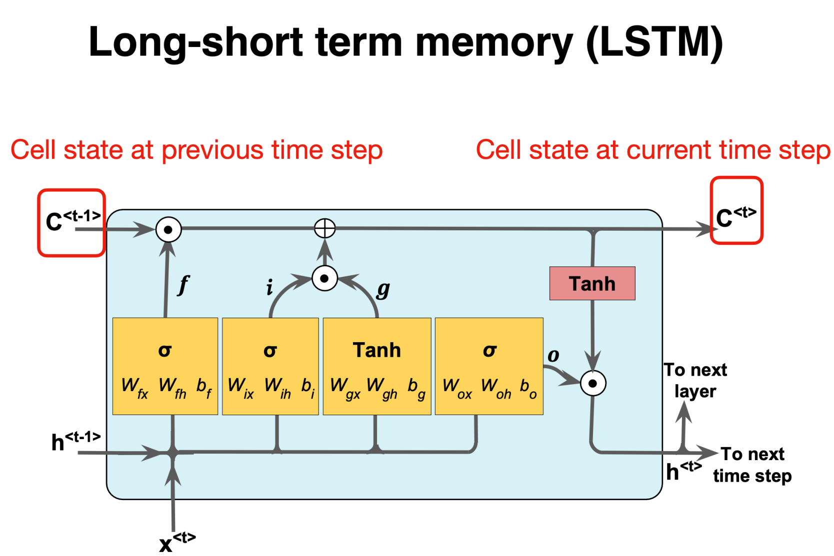
Long Short Term Memory (LSTM), part 1



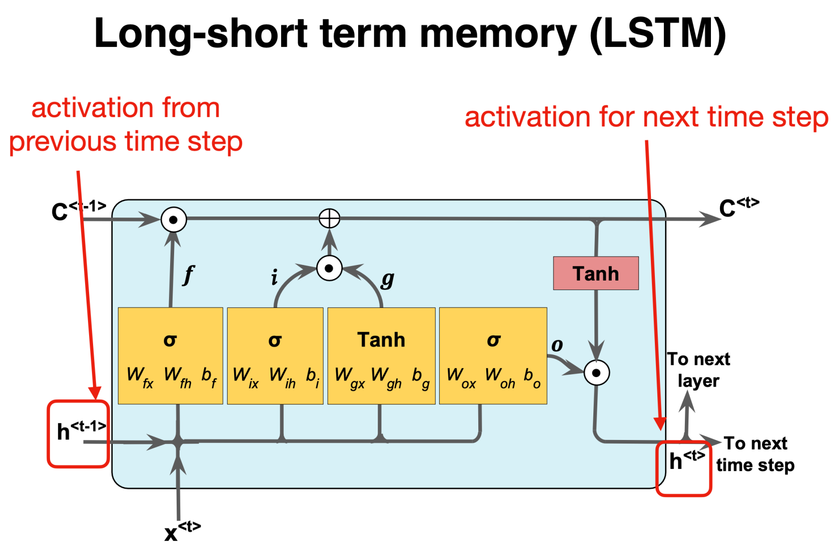
Long Short Term Memory (LSTM), part 2



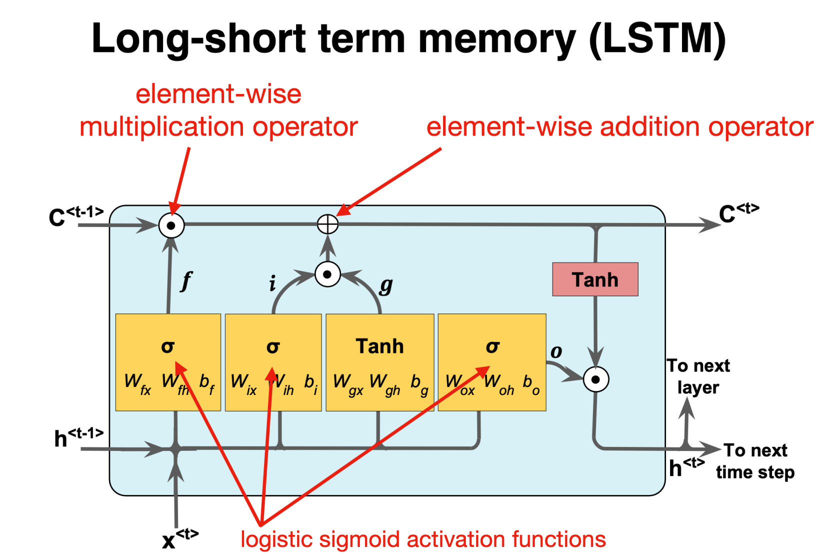
Long Short Term Memory (LSTM), part 3



Long Short Term Memory (LSTM), part 4



Long Short Term Memory (LSTM), part 5



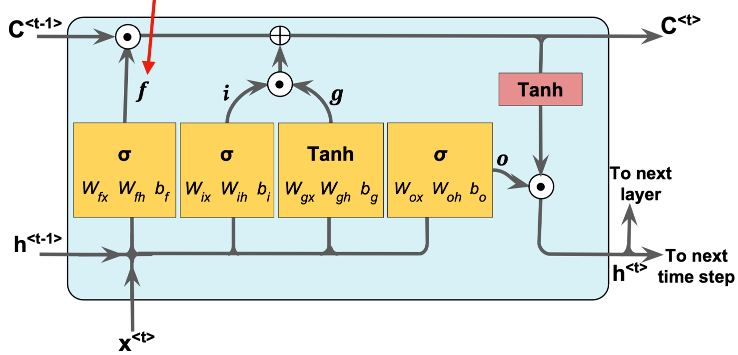
Long Short Term Memory (LSTM), part 6

Long-short term memory (LSTM)

Gers, Felix A., Jürgen Schmidhuber, and Fred Cummins. "Learning to forget: Continual prediction with LSTM." (1999): 850-855.

"Forget Gate": controls which information is remembered, and which is forgotten; can reset the cell state

$$f_t = \sigma\left(\mathbf{W}_{fx}\mathbf{x}^{\langle t\rangle} + \mathbf{W}_{fh}\mathbf{h}^{\langle t-1\rangle} + \mathbf{b}_f\right)$$



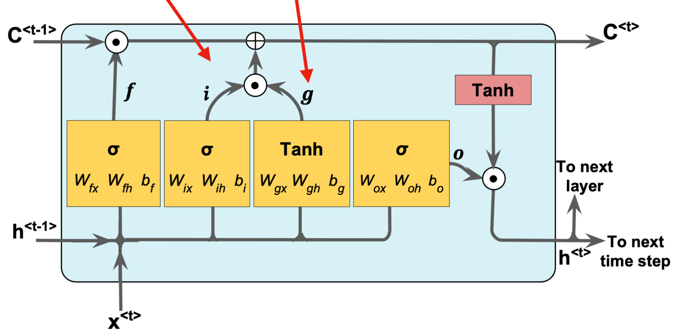
Long Short Term Memory (LSTM), part 7

Long-short term memory (LSTM)

"Input Gate": $\mathbf{i}_t = \sigma\left(\mathbf{W}_{ix}\mathbf{x}^{\langle t\rangle} + \mathbf{W}_{ih}\mathbf{h}^{\langle t-1\rangle} + \mathbf{b}_i\right)$

"Input Node":

$$\mathbf{g}_t = \tanh\left(\mathbf{W}_{gx}\mathbf{x}^{\langle t\rangle} + \mathbf{W}_{gh}\mathbf{h}^{\langle t-1\rangle} + \mathbf{b}_g\right)$$



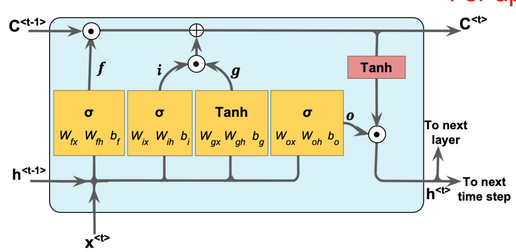
Long Short Term Memory (LSTM), part 8

Long-short term memory (LSTM)

Brief summary of the gates so far ...

Forget Gate Input Node Input Gate

$$C^{\langle t \rangle} = \left(C^{\langle t-1 \rangle} \odot f_t\right) \oplus \underbrace{(i_t \odot g_t)}_{\text{For updating the cell state}}$$

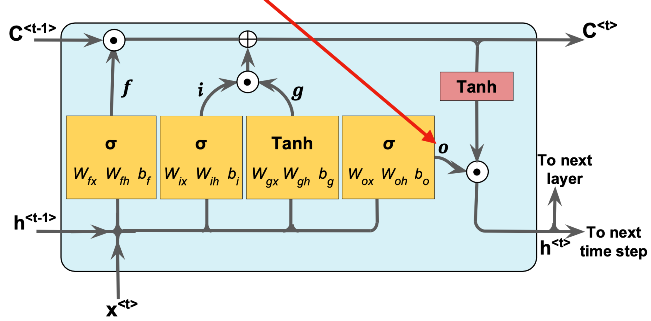


Long Short Term Memory (LSTM), part 9

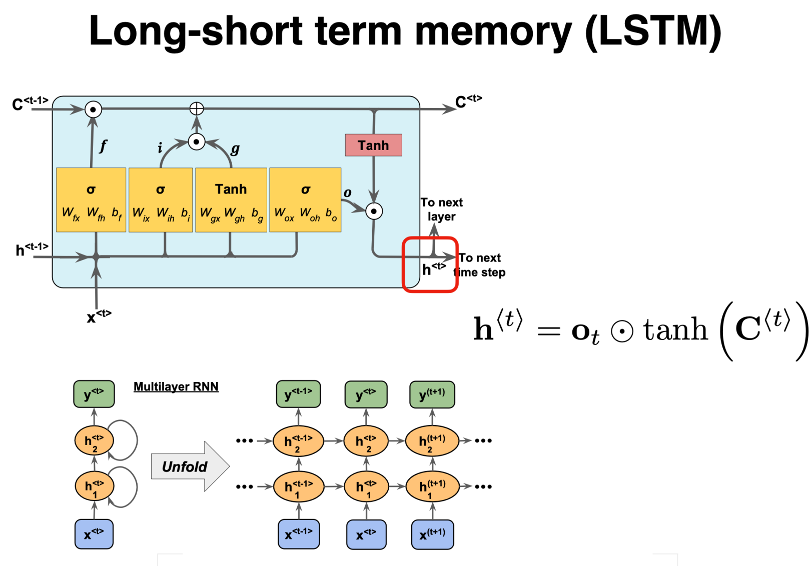
Long-short term memory (LSTM)

Output gate for updating the values of hidden units:

$$\mathbf{o}_t = \sigma\left(\mathbf{W}_{ox}\mathbf{x}^{\langle t \rangle} + \mathbf{W}_{oh}\mathbf{h}^{\langle t-1 \rangle} + \mathbf{b}_o\right)$$



Long Short Term Memory (LSTM), part 10



An extrapolation example

The following code provides an example of how recurrent neural networks can be used to extrapolate to unknown values of physics data sets. Specifically, the data sets used in this program come from a quantum mechanical many-body calculation of energies as functions of the number of particles.

```python
# For matrices and calculations
import numpy as np
# For machine learning (backend for keras)
import tensorflow as tf
# User-friendly machine learning library
# Front end for TensorFlow
import tensorflow.keras
# Different methods from Keras needed to create an RNN
# This is not necessary but it shortened function calls
# that need to be used in the code.
from tensorflow.keras import datasets, layers, models
from tensorflow.keras.layers import Input
from tensorflow.keras import regularizers
from tensorflow.keras.models import Model, Sequential
from tensorflow.keras.layers import Dense, SimpleRNN, LSTM, GRU
# For timing the code
from timeit import default_timer as timer
# For plotting
import matplotlib.pyplot as plt
```

```
# The data set
datatype='VaryDimension'
X_tot = np.arange(2, 42, 2)
y_tot = np.array([-0.03077640549, -0.08336233266, -0.1446729567, -0.2116753732, -0.2830637392, -0
        -0.6019067271, -0.6887363571, -0.7782028952, -0.8702784034, -0.9649652536, -1.062292565, -
        -1.265109911, -1.370782966, -1.479465113, -1.591317992, -1.70653767])
```

Formatting the Data

The way the recurrent neural networks are trained in this program differs from how machine learning algorithms are usually trained. Typically a machine learning algorithm is trained by learning the relationship between the x data and the y data. In this program, the recurrent neural network will be trained to recognize the relationship in a sequence of y values. This is type of data formatting is typically used time series forcasting, but it can also be used in any extrapolation (time series forecasting is just a specific type of extrapolation along the time axis). This method of data formatting does not use the x data and assumes that the y data are evenly spaced.

For a standard machine learning algorithm, the training data has the form of (x,y) so the machine learning algorithm learns to assiciate a y value with a given x value. This is useful when the test data has x values within the same range as the training data. However, for this application, the x values of the test data are outside of the x values of the training data and the traditional method of training a machine learning algorithm does not work as well. For this reason, the recurrent neural network is trained on sequences of y values of the form ((y1, y2), y3), so that the network is concerned with learning the pattern of the y data and not the relation between the x and y data. As long as the pattern of y data outside of the training region stays relatively stable compared to what was inside the training region, this method of training can produce accurate extrapolations to y values far removed from the training data set.

```
# FORMAT_DATA
def format_data(data, length_of_sequence = 2):
    """
        Inputs:
            data(a numpy array): the data that will be the inputs to the recurrent neural
                network
            length_of_sequence (an int): the number of elements in one iteration of the
                sequence patter.  For a function approximator use length_of_sequence = 2.
        Returns:
            rnn_input (a 3D numpy array): the input data for the recurrent neural network.  Its
                dimensions are length of data - length of sequence, length of sequence,
                dimnsion of data
            rnn_output (a numpy array): the training data for the neural network
        Formats data to be used in a recurrent neural network.
    """

    X, Y = [], []
    for i in range(len(data)-length_of_sequence):
        # Get the next length_of_sequence elements
        a = data[i:i+length_of_sequence]
```

```
        # Get the element that immediately follows that
        b = data[i+length_of_sequence]
        # Reshape so that each data point is contained in its own array
        a = np.reshape (a, (len(a), 1))
        X.append(a)
        Y.append(b)
    rnn_input = np.array(X)
    rnn_output = np.array(Y)

    return rnn_input, rnn_output


# ## Defining the Recurrent Neural Network Using Keras
#
# The following method defines a simple recurrent neural network in keras consisting of one input

def rnn(length_of_sequences, batch_size = None, stateful = False):
    """
        Inputs:
            length_of_sequences (an int): the number of y values in "x data".  This is determined
                when the data is formatted
            batch_size (an int): Default value is None.  See Keras documentation of SimpleRNN.
            stateful (a boolean): Default value is False.  See Keras documentation of SimpleRNN.
        Returns:
            model (a Keras model): The recurrent neural network that is built and compiled by thi
                method
        Builds and compiles a recurrent neural network with one hidden layer and returns the mode
    """
    # Number of neurons in the input and output layers
    in_out_neurons = 1
    # Number of neurons in the hidden layer
    hidden_neurons = 200
    # Define the input layer
    inp = Input(batch_shape=(batch_size,
                length_of_sequences,
                in_out_neurons))
    # Define the hidden layer as a simple RNN layer with a set number of neurons and add it to
    # the network immediately after the input layer
    rnn = SimpleRNN(hidden_neurons,
                    return_sequences=False,
                    stateful = stateful,
                    name="RNN")(inp)
    # Define the output layer as a dense neural network layer (standard neural network layer)
    #and add it to the network immediately after the hidden layer.
    dens = Dense(in_out_neurons,name="dense")(rnn)
    # Create the machine learning model starting with the input layer and ending with the
    # output layer
    model = Model(inputs=[inp],outputs=[dens])
    # Compile the machine learning model using the mean squared error function as the loss
    # function and an Adams optimizer.
    model.compile(loss="mean_squared_error", optimizer="adam")
    return model
```

Predicting New Points With A Trained Recurrent Neural Network

```
def test_rnn (x1, y_test, plot_min, plot_max):
    """
        Inputs:
            x1 (a list or numpy array): The complete x component of the data set
            y_test (a list or numpy array): The complete y component of the data set
            plot_min (an int or float): the smallest x value used in the training data
            plot_max (an int or float): the largest x valye used in the training data
        Returns:
            None.
        Uses a trained recurrent neural network model to predict future points in the
        series.  Computes the MSE of the predicted data set from the true data set, saves
        the predicted data set to a csv file, and plots the predicted and true data sets w
        while also displaying the data range used for training.
    """
    # Add the training data as the first dim points in the predicted data array as these
    # are known values.
    y_pred = y_test[:dim].tolist()
    # Generate the first input to the trained recurrent neural network using the last two
    # points of the training data.  Based on how the network was trained this means that it
    # will predict the first point in the data set after the training data.  All of the
    # brackets are necessary for Tensorflow.
    next_input = np.array([[[y_test[dim-2]], [y_test[dim-1]]]])
    # Save the very last point in the training data set.  This will be used later.
    last = [y_test[dim-1]]

    # Iterate until the complete data set is created.
    for i in range (dim, len(y_test)):
        # Predict the next point in the data set using the previous two points.
        next = model.predict(next_input)
        # Append just the number of the predicted data set
        y_pred.append(next[0][0])
        # Create the input that will be used to predict the next data point in the data set.
        next_input = np.array([[last, next[0]]], dtype=np.float64)
        last = next

    # Print the mean squared error between the known data set and the predicted data set.
    print('MSE: ', np.square(np.subtract(y_test, y_pred)).mean())
    # Save the predicted data set as a csv file for later use
    name = datatype + 'Predicted'+str(dim)+'.csv'
    np.savetxt(name, y_pred, delimiter=',')
    # Plot the known data set and the predicted data set.  The red box represents the region that
    # for the training data.
    fig, ax = plt.subplots()
    ax.plot(x1, y_test, label="true", linewidth=3)
    ax.plot(x1, y_pred, 'g-.',label="predicted", linewidth=4)
    ax.legend()
    # Created a red region to represent the points used in the training data.
    ax.axvspan(plot_min, plot_max, alpha=0.25, color='red')
    plt.show()

# Check to make sure the data set is complete
assert len(X_tot) == len(y_tot)

# This is the number of points that will be used in as the training data
dim=12

# Separate the training data from the whole data set
```

```
X_train = X_tot[:dim]
y_train = y_tot[:dim]


# Generate the training data for the RNN, using a sequence of 2
rnn_input, rnn_training = format_data(y_train, 2)


# Create a recurrent neural network in Keras and produce a summary of the
# machine learning model
model = rnn(length_of_sequences = rnn_input.shape[1])
model.summary()

# Start the timer.  Want to time training+testing
start = timer()
# Fit the model using the training data genenerated above using 150 training iterations and a 5%
# validation split.  Setting verbose to True prints information about each training iteration.
hist = model.fit(rnn_input, rnn_training, batch_size=None, epochs=150,
                 verbose=True,validation_split=0.05)

for label in ["loss","val_loss"]:
    plt.plot(hist.history[label],label=label)

plt.ylabel("loss")
plt.xlabel("epoch")
plt.title("The final validation loss: {}".format(hist.history["val_loss"][-1]))
plt.legend()
plt.show()

# Use the trained neural network to predict more points of the data set
test_rnn(X_tot, y_tot, X_tot[0], X_tot[dim-1])
# Stop the timer and calculate the total time needed.
end = timer()
print('Time: ', end-start)
```

Other Things to Try

Changing the size of the recurrent neural network and its parameters can drastically change the results you get from the model. The below code takes the simple recurrent neural network from above and adds a second hidden layer, changes the number of neurons in the hidden layer, and explicitly declares the activation function of the hidden layers to be a sigmoid function. The loss function and optimizer can also be changed but are kept the same as the above network. These parameters can be tuned to provide the optimal result from the network. For some ideas on how to improve the performance of a recurrent neural network.

```
def rnn_2layers(length_of_sequences, batch_size = None, stateful = False):
    """
        Inputs:
            length_of_sequences (an int): the number of y values in "x data".  This is determined
                when the data is formatted
            batch_size (an int): Default value is None.  See Keras documentation of SimpleRNN.
            stateful (a boolean): Default value is False.  See Keras documentation of SimpleRNN.
        Returns:
            model (a Keras model): The recurrent neural network that is built and compiled by thi
```

```
            method
        Builds and compiles a recurrent neural network with two hidden layers and returns the mode
    """
    # Number of neurons in the input and output layers
    in_out_neurons = 1
    # Number of neurons in the hidden layer, increased from the first network
    hidden_neurons = 500
    # Define the input layer
    inp = Input(batch_shape=(batch_size,
                length_of_sequences,
                in_out_neurons))
    # Create two hidden layers instead of one hidden layer.  Explicitly set the activation
    # function to be the sigmoid function (the default value is hyperbolic tangent)
    rnn1 = SimpleRNN(hidden_neurons,
                    return_sequences=True,  # This needs to be True if another hidden layer is to
                    stateful = stateful, activation = 'sigmoid',
                    name="RNN1")(inp)
    rnn2 = SimpleRNN(hidden_neurons,
                    return_sequences=False, activation = 'sigmoid',
                    stateful = stateful,
                    name="RNN2")(rnn1)
    # Define the output layer as a dense neural network layer (standard neural network layer)
    #and add it to the network immediately after the hidden layer.
    dens = Dense(in_out_neurons,name="dense")(rnn2)
    # Create the machine learning model starting with the input layer and ending with the
    # output layer
    model = Model(inputs=[inp],outputs=[dens])
    # Compile the machine learning model using the mean squared error function as the loss
    # function and an Adams optimizer.
    model.compile(loss="mean_squared_error", optimizer="adam")
    return model

# Check to make sure the data set is complete
assert len(X_tot) == len(y_tot)

# This is the number of points that will be used in as the training data
dim=12

# Separate the training data from the whole data set
X_train = X_tot[:dim]
y_train = y_tot[:dim]


# Generate the training data for the RNN, using a sequence of 2
rnn_input, rnn_training = format_data(y_train, 2)


# Create a recurrent neural network in Keras and produce a summary of the
# machine learning model
model = rnn_2layers(length_of_sequences = 2)
model.summary()

# Start the timer.  Want to time training+testing
start = timer()
# Fit the model using the training data genenerated above using 150 training iterations and a 5%
# validation split.  Setting verbose to True prints information about each training iteration.
hist = model.fit(rnn_input, rnn_training, batch_size=None, epochs=150,
                 verbose=True,validation_split=0.05)


# This section plots the training loss and the validation loss as a function of training iteratio
```

```
# This is not required for analyzing the couple cluster data but can help determine if the networ
# being overtrained.
for label in ["loss","val_loss"]:
    plt.plot(hist.history[label],label=label)

plt.ylabel("loss")
plt.xlabel("epoch")
plt.title("The final validation loss: {}".format(hist.history["val_loss"][-1]))
plt.legend()
plt.show()

# Use the trained neural network to predict more points of the data set
test_rnn(X_tot, y_tot, X_tot[0], X_tot[dim-1])
# Stop the timer and calculate the total time needed.
end = timer()
print('Time: ', end-start)
```

Other Types of Recurrent Neural Networks

Besides a simple recurrent neural network layer, there are two other commonly used types of recurrent neural network layers: Long Short Term Memory (LSTM) and Gated Recurrent Unit (GRU). For a short introduction to these layers see https://medium.com/mindboard/lstm-vs-gru-experimental-comparison-955820c21e8b and https://medium.com/mindboard/lstm-vs-gru-experimental-comparison-955820c21e8b.

The first network created below is similar to the previous network, but it replaces the SimpleRNN layers with LSTM layers. The second network below has two hidden layers made up of GRUs, which are preceeded by two dense (feeddorward) neural network layers. These dense layers "preprocess" the data before it reaches the recurrent layers. This architecture has been shown to improve the performance of recurrent neural networks (see the link above and also https://arxiv.org/pdf/1807.02857.pdf.

```
def lstm_2layers(length_of_sequences, batch_size = None, stateful = False):
    """
        Inputs:
            length_of_sequences (an int): the number of y values in "x data".  This is determined
                when the data is formatted
            batch_size (an int): Default value is None.  See Keras documentation of SimpleRNN.
            stateful (a boolean): Default value is False.  See Keras documentation of SimpleRNN.
        Returns:
            model (a Keras model): The recurrent neural network that is built and compiled by thi
                method
        Builds and compiles a recurrent neural network with two LSTM hidden layers and returns th
    """
    # Number of neurons on the input/output layer and the number of neurons in the hidden layer
    in_out_neurons = 1
    hidden_neurons = 250
    # Input Layer
    inp = Input(batch_shape=(batch_size,
                length_of_sequences,
                in_out_neurons))
    # Hidden layers (in this case they are LSTM layers instead if SimpleRNN layers)
    rnn= LSTM(hidden_neurons,
                    return_sequences=True,
                    stateful = stateful,
```

```
                    name="RNN", use_bias=True, activation='tanh')(inp)
    rnn1 = LSTM(hidden_neurons,
                    return_sequences=False,
                    stateful = stateful,
                    name="RNN1", use_bias=True, activation='tanh')(rnn)
    # Output layer
    dens = Dense(in_out_neurons,name="dense")(rnn1)
    # Define the midel
    model = Model(inputs=[inp],outputs=[dens])
    # Compile the model
    model.compile(loss='mean_squared_error', optimizer='adam')
    # Return the model
    return model

def dnn2_gru2(length_of_sequences, batch_size = None, stateful = False):
    """
        Inputs:
            length_of_sequences (an int): the number of y values in "x data".  This is determined
                when the data is formatted
            batch_size (an int): Default value is None.  See Keras documentation of SimpleRNN.
            stateful (a boolean): Default value is False.  See Keras documentation of SimpleRNN.
        Returns:
            model (a Keras model): The recurrent neural network that is built and compiled by thi
                method
        Builds and compiles a recurrent neural network with four hidden layers (two dense followe
        two GRU layers) and returns the model.
    """
    # Number of neurons on the input/output layers and hidden layers
    in_out_neurons = 1
    hidden_neurons = 250
    # Input layer
    inp = Input(batch_shape=(batch_size,
                length_of_sequences,
                in_out_neurons))
    # Hidden Dense (feedforward) layers
    dnn = Dense(hidden_neurons/2, activation='relu', name='dnn')(inp)
    dnn1 = Dense(hidden_neurons/2, activation='relu', name='dnn1')(dnn)
    # Hidden GRU layers
    rnn1 = GRU(hidden_neurons,
                    return_sequences=True,
                    stateful = stateful,
                    name="RNN1", use_bias=True)(dnn1)
    rnn = GRU(hidden_neurons,
                    return_sequences=False,
                    stateful = stateful,
                    name="RNN", use_bias=True)(rnn1)
    # Output layer
    dens = Dense(in_out_neurons,name="dense")(rnn)
    # Define the model
    model = Model(inputs=[inp],outputs=[dens])
    # Compile the mdoel
    model.compile(loss='mean_squared_error', optimizer='adam')
    # Return the model
    return model

# Check to make sure the data set is complete
assert len(X_tot) == len(y_tot)

# This is the number of points that will be used in as the training data
dim=12
```

```
# Separate the training data from the whole data set
X_train = X_tot[:dim]
y_train = y_tot[:dim]


# Generate the training data for the RNN, using a sequence of 2
rnn_input, rnn_training = format_data(y_train, 2)


# Create a recurrent neural network in Keras and produce a summary of the
# machine learning model
# Change the method name to reflect which network you want to use
model = dnn2_gru2(length_of_sequences = 2)
model.summary()

# Start the timer.  Want to time training+testing
start = timer()
# Fit the model using the training data genenerated above using 150 training iterations and a 5%
# validation split.  Setting verbose to True prints information about each training iteration.
hist = model.fit(rnn_input, rnn_training, batch_size=None, epochs=150,
                 verbose=True,validation_split=0.05)


# This section plots the training loss and the validation loss as a function of training iteratio
# This is not required for analyzing the couple cluster data but can help determine if the networ
# being overtrained.
for label in ["loss","val_loss"]:
    plt.plot(hist.history[label],label=label)

plt.ylabel("loss")
plt.xlabel("epoch")
plt.title("The final validation loss: {}".format(hist.history["val_loss"][-1]))
plt.legend()
plt.show()

# Use the trained neural network to predict more points of the data set
test_rnn(X_tot, y_tot, X_tot[0], X_tot[dim-1])
# Stop the timer and calculate the total time needed.
end = timer()
print('Time: ', end-start)


# ### Training Recurrent Neural Networks in the Standard Way (i.e. learning the relationship betw
#
# Finally, comparing the performace of a recurrent neural network using the standard data formatt

# Check to make sure the data set is complete
assert len(X_tot) == len(y_tot)

# This is the number of points that will be used in as the training data
dim=12

# Separate the training data from the whole data set
X_train = X_tot[:dim]
y_train = y_tot[:dim]

# Reshape the data for Keras specifications
X_train = X_train.reshape((dim, 1))
y_train = y_train.reshape((dim, 1))
```

```
# Create a recurrent neural network in Keras and produce a summary of the
# machine learning model
# Set the sequence length to 1 for regular data formatting
model = rnn(length_of_sequences = 1)
model.summary()

# Start the timer.  Want to time training+testing
start = timer()
# Fit the model using the training data genenerated above using 150 training iterations and a 5%
# validation split.  Setting verbose to True prints information about each training iteration.
hist = model.fit(X_train, y_train, batch_size=None, epochs=150,
                 verbose=True,validation_split=0.05)


# This section plots the training loss and the validation loss as a function of training iteratio
# This is not required for analyzing the couple cluster data but can help determine if the networ
# being overtrained.
for label in ["loss","val_loss"]:
    plt.plot(hist.history[label],label=label)

plt.ylabel("loss")
plt.xlabel("epoch")
plt.title("The final validation loss: {}".format(hist.history["val_loss"][-1]))
plt.legend()
plt.show()

# Use the trained neural network to predict the remaining data points
X_pred = X_tot[dim:]
X_pred = X_pred.reshape((len(X_pred), 1))
y_model = model.predict(X_pred)
y_pred = np.concatenate((y_tot[:dim], y_model.flatten()))

# Plot the known data set and the predicted data set.  The red box represents the region that was
# for the training data.
fig, ax = plt.subplots()
ax.plot(X_tot, y_tot, label="true", linewidth=3)
ax.plot(X_tot, y_pred, 'g-.',label="predicted", linewidth=4)
ax.legend()
# Created a red region to represent the points used in the training data.
ax.axvspan(X_tot[0], X_tot[dim], alpha=0.25, color='red')
plt.show()

# Stop the timer and calculate the total time needed.
end = timer()
print('Time: ', end-start)
```

Summary of RNNs

Recurrent neural networks (RNNs) have in general no probabilistic component in a model. With a given fixed input and target from data, the RNNs learn the intermediate association between various layers. The inputs, outputs, and internal representation (hidden states) are all real-valued vectors.

In a traditional NN, it is assumed that every input is independent of each other. But with sequential data, the input at a given stage t depends on the input from the previous stage $t-1$

A typical RNN

1. Weight matrices U, W and V that connect the input layer at a stage t with the hidden layer h_t, the previous hidden layer h_{t-1} with h_t and the hidden layer h_t connecting with the output layer at the same stage and producing an output $\tilde{y}_t$, respectively.

2. The output from the hidden layer h_t is oftem modulated by a $\tanh$ function $h_t = f(x_t, h_{t-1}) = \tanh(Ux_t + Wh_{t-1} + b)$ with b a bias value

3. The output from the hidden layer produces $\tilde{y}_t = g(Vh_t + c)$ where c is a new bias parameter.

4. The output from the training at a given stage is in turn compared with the observation y_t thorugh a chosen cost function.

The function g can any of the standard activation functions, that is a Sigmoid, a Softmax, a ReLU and other. The parameters are trained through the so-called back-propagation through time (BPTT) algorithm.

Gating mechanism: Long Short Term Memory (LSTM)

Besides a simple recurrent neural network layer, as discussed above, there are two other commonly used types of recurrent neural network layers: Long Short Term Memory (LSTM) and Gated Recurrent Unit (GRU). For a short introduction to these layers see `https://medium.com/mindboard/lstm-vs-gru-experimental-comparison-955820c21e8b` and `https://medium.com/mindboard/lstm-vs-gru-experimental-comparison-955820c21e8b`.

LSTM uses a memory cell for modeling long-range dependencies and avoid vanishing gradient problems. Capable of modeling longer term dependencies by having memory cells and gates that controls the information flow along with the memory cells.

1. Introduced by Hochreiter and Schmidhuber (1997) who solved the problem of getting an RNN to remember things for a long time (like hundreds of time steps).

2. They designed a memory cell using logistic and linear units with multiplicative interactions.

3. Information gets into the cell whenever its “write” gate is on.

4. The information stays in the cell so long as its **keep** gate is on.

5. Information can be read from the cell by turning on its **read** gate.

Implementing a memory cell in a neural network

To preserve information for a long time in the activities of an RNN, we use a circuit that implements an analog memory cell.

1. A linear unit that has a self-link with a weight of 1 will maintain its state.
2. Information is stored in the cell by activating its write gate.
3. Information is retrieved by activating the read gate.
4. We can backpropagate through this circuit because logistics are have nice derivatives.