March 4-8: Advanced machine learning and data analysis for the physical sciences

Morten Hjorth-Jensen[1,2]

[1]Department of Physics and Center for Computing in Science Education, University of Oslo, Norway
[2]Department of Physics and Astronomy and Facility for Rare Isotope Beams, Michigan State University, East Lansing, Michigan, USA

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Plans for the week March 4-8

1. RNNs and discussion of Long-Short-Term memory
2. Discussion of specific examples relevant for project 1, see project from last year by Daniel and Keran
3. Start discussion of Autoencoders (AEs) if we get time.

Reading recommendations

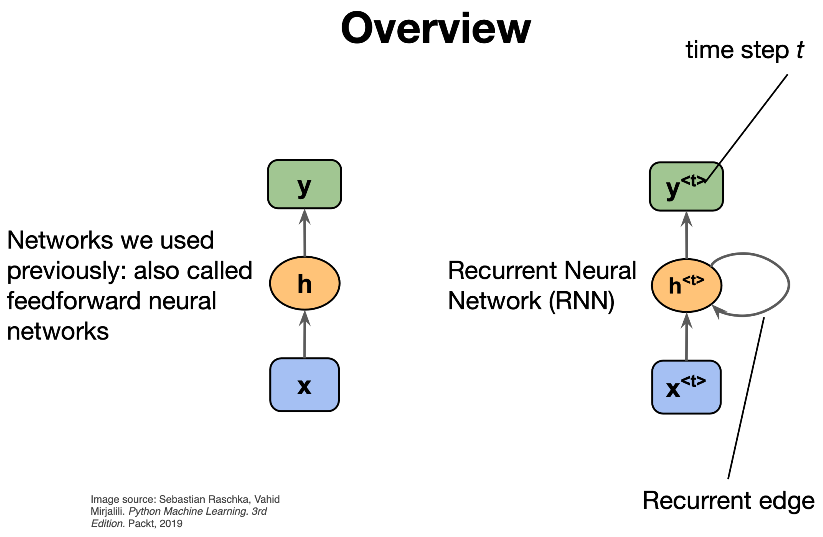
1. For RNNs see Goodfellow et al chapter 10.
2. For AEs, see chapter 14 of same book
3. Reading suggestions for implementation of RNNs in PyTorch: Rashcka et al's text, chapter 15
4. Reading suggestions for implementation of RNNs in TensorFlow: Aurelien Geron's chapter 14.

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 $t-1$

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


Overview
time step *t*
y
h
x
Networks we used previously: also called feedforward neural networks
Recurrent Neural Network (RNN)
y<t>
h<t>
x<t>
Recurrent edge
Image source: Sebastian Raschka, Vahid Mirjalili. *Python Machine Learning. 3rd Edition.* Packt, 2019

Solving differential equations with RNNs

To gain some intuition on how we can use RNNs for time series, let us tailor the representation of the solution of a differential equation as a time series.

Consider the famous differential equation (Newton's equation of motion for damped harmonic oscillations, scaled in terms of dimensionless time)

$$\frac{d^2x}{dt^2}+\eta\frac{dx}{dt}+x(t)=F(t),$$

where η is a constant used in scaling time into a dimensionless variable and $F(t)$ is an external force acting on the system. The constant η is a so-called damping.

Two first-order differential equations

In solving the above second-order equation, it is common to rewrite it in terms of two coupled first-order equations with the velocity

$$v(t) = \frac{dx}{dt},$$

and the acceleration

$$\frac{dv}{dt} = F(t) - \eta v(t) - x(t).$$

With the initial conditions $v_0 = v(t_0)$ and $x_0 = x(t_0)$ defined, we can integrate these equations and find their respective solutions.

Velocity only

Let us focus on the velocity only. Discretizing and using the simplest possible approximation for the derivative, we have Euler's forward method for the updated velocity at a time step $i+1$ given by

$$v_{i+1} = v_i + \Delta t \frac{dv}{dt}_{|v=v_i} = v_i + \Delta t \left(F_i - \eta v_i - x_i\right).$$

Defining a function

$$h_i(x_i, v_i, F_i) = v_i + \Delta t \left(F_i - \eta v_i - x_i\right),$$

we have

$$v_{i+1} = h_i(x_i, v_i, F_i).$$

Linking with RNNs

The equation

$$v_{i+1} = h_i(x_i, v_i, F_i).$$

can be used to train a feed-forward neural network with inputs v_i and outputs v_{i+1} at a time t_i. But we can think of this also as a recurrent neural network with inputs v_i, x_i and F_i at each time step t_i, and producing an output v_{i+1}.

Noting that

$$v_i = v_{i-1} + \Delta t \left(F_{i-1} - \eta v_{i-1} - x_{i-1}\right) = h_{i-1}.$$

we have

$$v_i = h_{i-1}(x_{i-1}, v_{i-1}, F_{i-1}),$$

and we can rewrite

$$v_{i+1} = h_i(x_i, h_{i-1}, F_i).$$

Minor rewrite

We can thus set up a recurring series which depends on the inputs x_i and F_i and the previous values h_{i-1}. We assume now that the inputs at each step (or time t_i) is given by x_i only and we denote the outputs for $\tilde{y}_i$ instead of v_{i_1}, we have then the compact equation for our outputs at each step t_i

$$y_i = h_i(x_i, h_{i-1}).$$

We can think of this as an element in a recurrent network where our network (our model) produces an output y_i which is then compared with a target value through a given cost/loss function that we optimize. The target values at a given step t_i could be the results of a measurement or simply the analytical results of a differential equation.

RNNs in more detail

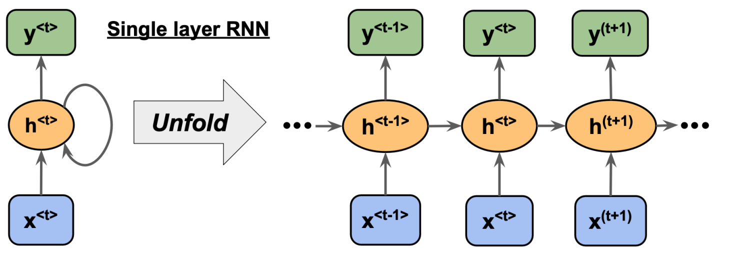
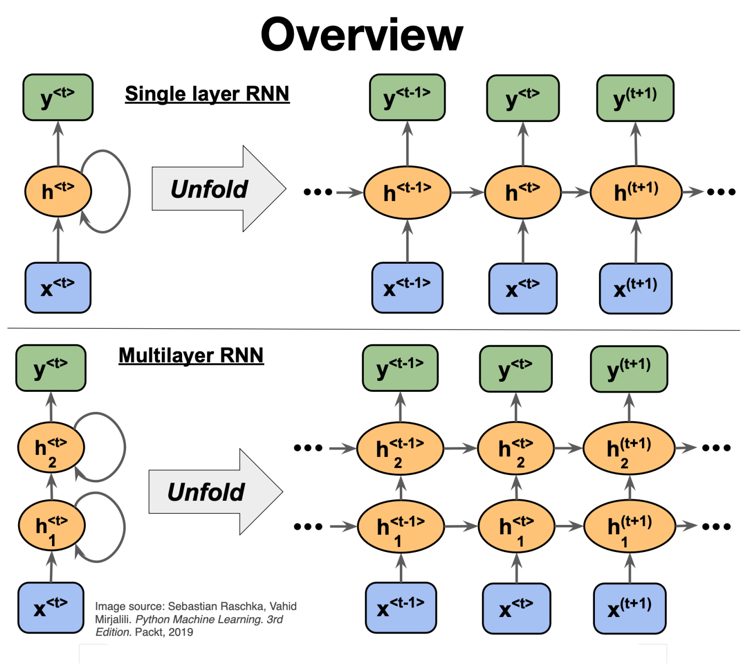
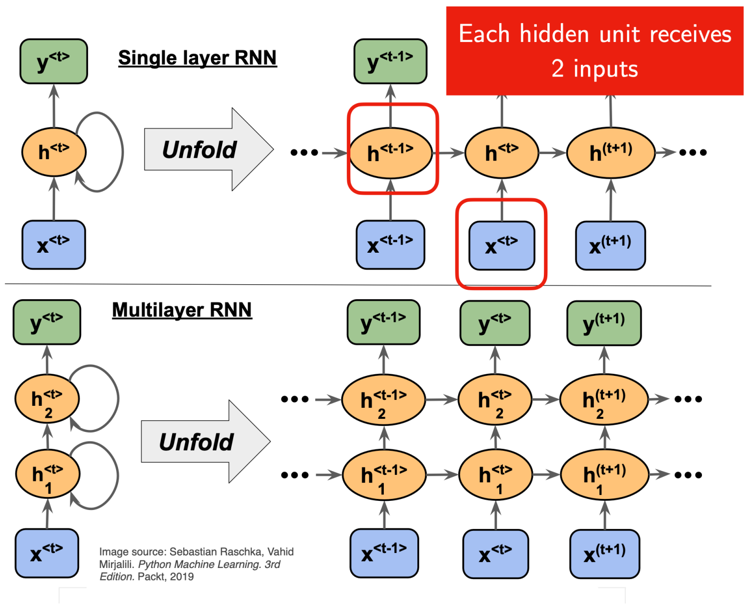


Image source: Sebastian Raschka, Vahid Mirjalili. *Python Machine Learning. 3rd Edition.* Packt, 2019

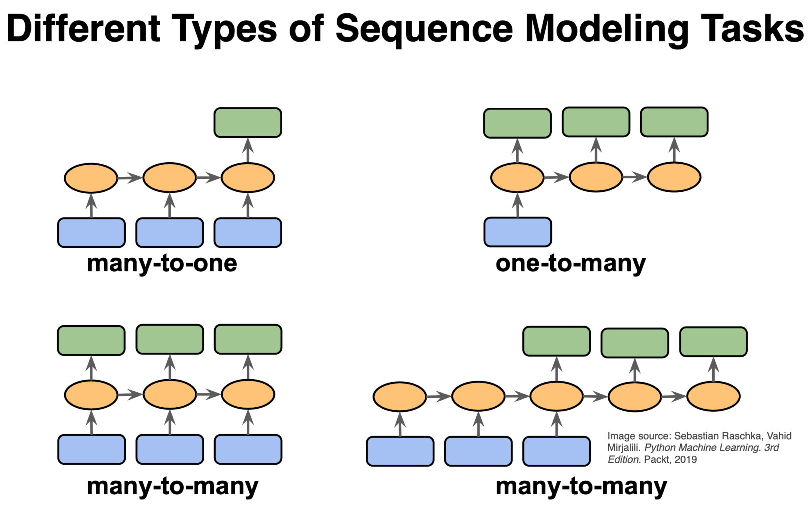
RNNs in more detail, part 2



RNNs in more detail, part 3


Single layer RNN
Unfold
Each hidden unit receives 2 inputs
Multilayer RNN
Unfold
Image source: Sebastian Raschka, Vahid Mirjalili. Python Machine Learning. 3rd Edition. Packt, 2019

RNNs in more detail, part 4


Different Types of Sequence Modeling Tasks
many-to-one
one-to-many
many-to-many
many-to-many
Image source: Sebastian Raschka, Vahid Mirjalili. Python Machine Learning. 3rd Edition. Packt, 2019

RNNs in more detail, part 5

Weight matrices in a single-hidden layer RNN

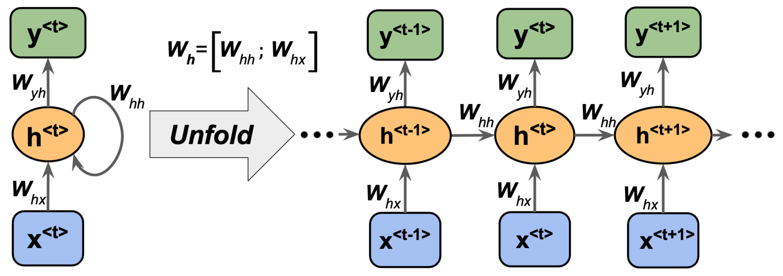


Image source: Sebastian Raschka, Vahid Mirjalili. *Python Machine Learning. 3rd Edition.* Packt, 2019

RNNs in more detail, part 6

Weight matrices in a single-hidden layer RNN

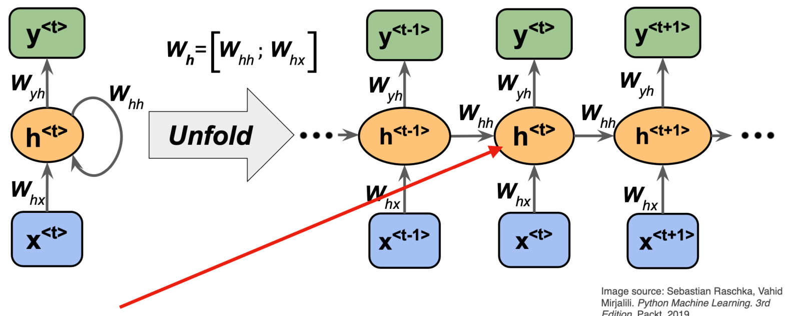


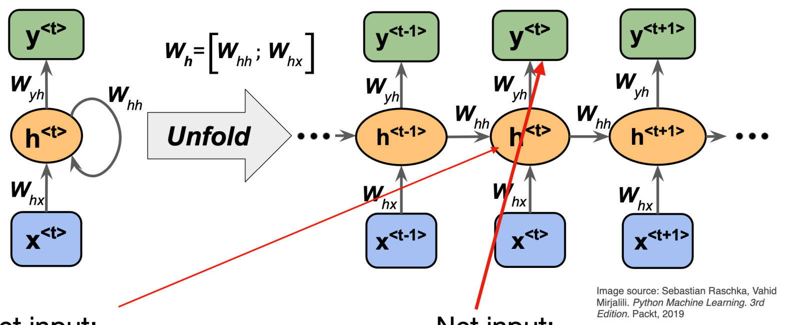
Image source: Sebastian Raschka, Vahid Mirjalili. *Python Machine Learning. 3rd Edition.* Packt, 2019

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 more detail, part 7

Weight matrices in a single-hidden layer RNN



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:

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

Net input:

$$\mathbf{z}_y^{\langle t\rangle} = \mathbf{W}_{yh}\mathbf{h}^{\langle t\rangle} + \mathbf{b}_y$$

Output:

$$\mathbf{y}^{\langle t\rangle} = \sigma_y\left(\mathbf{z}_y^{\langle t\rangle}\right)$$

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.

Mathematical setup

The expression for the simplest Recurrent network resembles that of a regular feed-forward neural network, but now with the concept of temporal dependencies

$$
\begin{aligned}
\mathbf{a}^{(t)} &= U * \mathbf{x}^{(t)} + W * \mathbf{h}^{(t-1)} + \mathbf{b}, \\
\mathbf{h}^{(t)} &= \sigma_h(\mathbf{a}^{(t)}), \\
\mathbf{y}^{(t)} &= V * \mathbf{h}^{(t)} + \mathbf{c}, \\
\hat{\mathbf{y}}^{(t)} &= \sigma_y(\mathbf{y}^{(t)}).
\end{aligned}
$$

Back propagation in time through figures, part 1

Backpropagation through time

The overall loss can be computed as the sum over all time steps

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

$$L = \sum_{t=1}^{T} L^{\langle t \rangle}$$

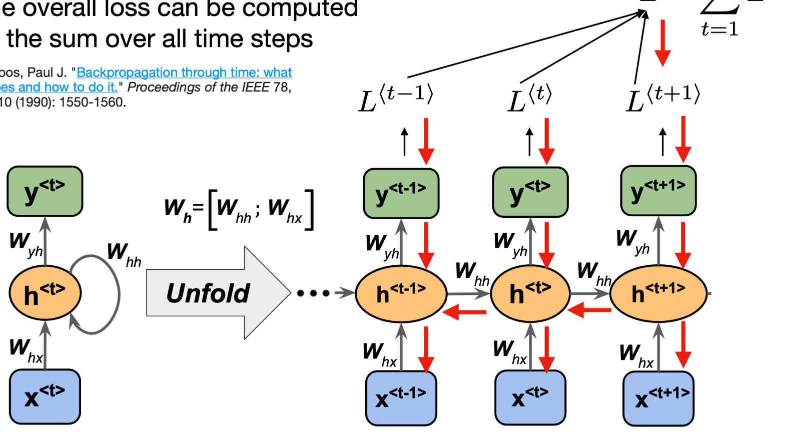
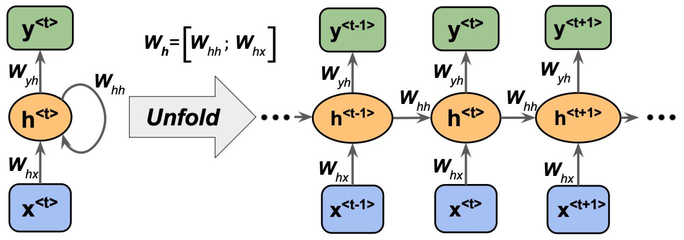


Image source: Sebastian Raschka, Vahid Mirjalili. *Python Machine Learning. 3rd Edition.* Packt, 2019

Back propagation in time, part 2

Backpropagation through time



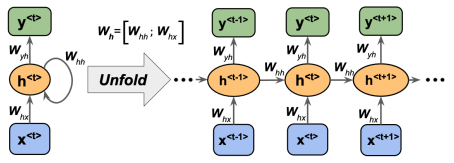
Werbos, Paul J. "Backpropagation through time: what it does and how to do it." *Proceedings of the IEEE* 78, no. 10 (1990): 1550-1560.

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

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

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.

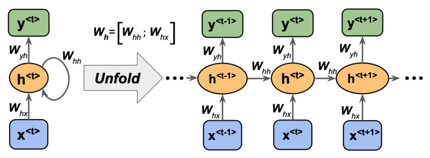
$$\frac{\partial L^{(t)}}{\partial \mathbf{W}_{hh}} = \frac{\partial L^{(t)}}{\partial y^{(t)}} \cdot \frac{\partial y^{(t)}}{\partial \mathbf{h}^{(t)}} \cdot \left(\sum_{k=1}^{t} \boxed{\frac{\partial \mathbf{h}^{(t)}}{\partial \mathbf{h}^{(k)}}} \cdot \frac{\partial \mathbf{h}^{(k)}}{\partial \mathbf{W}_{hh}}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

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!

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

Back propagation in time in equations

To derive the expression of the gradients of $\mathcal{L}$ for the RNN, we need to start recursively from the nodes closer to the output layer in the temporal unrolling scheme - such as $\mathbf{y}$ and $\mathbf{h}$ at final time $t = \tau$,

$$
\begin{aligned}
(\nabla_{\mathbf{y}^{(t)}} \mathcal{L})_i &= \frac{\partial \mathcal{L}}{\partial L^{(t)}} \frac{\partial L^{(t)}}{\partial y_i^{(t)}}, \\
\nabla_{\mathbf{h}^{(\tau)}} \mathcal{L} &= \mathbf{V}^{\mathsf{T}} \nabla_{\mathbf{y}^{(\tau)}} \mathcal{L}.
\end{aligned}
$$

Chain rule again

For the following hidden nodes, we have to iterate through time, so by the chain rule,

$$
\nabla_{\mathbf{h}^{(t)}} \mathcal{L} = \left(\frac{\partial \mathbf{h}^{(t+1)}}{\partial \mathbf{h}^{(t)}} \right)^{\mathsf{T}} \nabla_{\mathbf{h}^{(t+1)}} \mathcal{L} + \left(\frac{\partial \mathbf{y}^{(t)}}{\partial \mathbf{h}^{(t)}} \right)^{\mathsf{T}} \nabla_{\mathbf{y}^{(t)}} \mathcal{L}.
$$

Gradients of loss functions

Similarly, the gradients of $\mathcal{L}$ with respect to the weights and biases follow,

$$
\begin{aligned}
\nabla_{\mathbf{c}} \mathcal{L} &= \sum_t \left(\frac{\partial \mathbf{y}^{(t)}}{\partial \mathbf{c}} \right)^{\mathsf{T}} \nabla_{\mathbf{y}^{(t)}} \mathcal{L} \\
\nabla_{\mathbf{b}} \mathcal{L} &= \sum_t \left(\frac{\partial \mathbf{h}^{(t)}}{\partial \mathbf{b}} \right)^{\mathsf{T}} \nabla_{\mathbf{h}^{(t)}} \mathcal{L} \\
\nabla_{\mathbf{V}} \mathcal{L} &= \sum_t \sum_i \left(\frac{\partial \mathcal{L}}{\partial y_i^{(t)}} \right) \nabla_{\mathbf{V}^{(t)}} y_i^{(t)} \\
\nabla_{\mathbf{W}} \mathcal{L} &= \sum_t \sum_i \left(\frac{\partial \mathcal{L}}{\partial h_i^{(t)}} \right) \nabla_{\mathbf{w}^{(t)}} h_i^{(t)} \\
\nabla_{\mathbf{U}} \mathcal{L} &= \sum_t \sum_i \left(\frac{\partial \mathcal{L}}{\partial h_i^{(t)}} \right) \nabla_{\mathbf{U}^{(t)}} h_i^{(t)}.
\end{aligned}
$$

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 $t-1$

Summary of 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 $h_t = \sigma_h(x_t, h_{t-1}) = \tanh(Ux_t + Wh_{t-1} + b)$ with b a bias value

3. The output from the hidden layer produces $\tilde{y}_t = \sigma_y(Vh_t + c)$ 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.

Four effective ways to learn an RNN and preparing for next week

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

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.

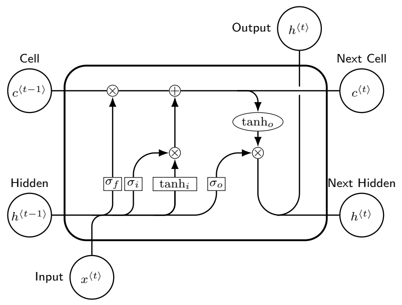
LSTM details

The LSTM is a unit cell that is made of three gates:

1. the input gate,
2. the forget gate,
3. and the output gate.

It also introduces a cell state c, which can be thought of as the long-term memory, and a hidden state h which can be thought of as the short-term memory.

Basic layout



More LSTM details

The first stage is called the forget gate, where we combine the input at (say, time t), and the hidden cell state input at $t-1$, passing it through the Sigmoid activation function and then performing an element-wise multiplication, denoted by $\otimes$.

It follows
$$\mathbf{f}^{(t)} = \sigma(W_f \mathbf{x}^{(t)} + U_f \mathbf{h}^{(t-1)} + \mathbf{b}_f)$$
where W and U are the weights respectively.

The forget gate

This is called the forget gate since the Sigmoid activation function's outputs are very close to 0 if the argument for the function is very negative, and 1 if the argument is very positive. Hence we can control the amount of information we want to take from the long-term memory.

Input gate

The next stage is the input gate, which consists of both a Sigmoid function (σ_i), which decide what percentage of the input will be stored in the long-term memory, and the $\tanh_i$ function, which decide what is the full memory that can be stored in the long term memory. When these results are calculated and multiplied together, it is added to the cell state or stored in the long-term memory, denoted as $\oplus$.

We have
$$\mathbf{i}^{(t)} = \sigma_g(W_i \mathbf{x}^{(t)} + U_i \mathbf{h}^{(t-1)} + \mathbf{b}_i),$$
and
$$\tilde{\mathbf{c}}^{(t)} = \tanh(W_c \mathbf{x}^{(t)} + U_c \mathbf{h}^{(t-1)} + \mathbf{b}_c),$$
again the W and U are the weights.

Forget and input

The forget gate and the input gate together also update the cell state with the following equation,
$$\mathbf{c}^{(t)} = \mathbf{f}^{(t)} \otimes \mathbf{c}^{(t-1)} + \mathbf{i}^{(t)} \otimes \tilde{\mathbf{c}}^{(t)},$$
where $f^{(t)}$ and $i^{(t)}$ are the outputs of the forget gate and the input gate, respectively.

Output gate

The final stage of the LSTM is the output gate, and its purpose is to update the short-term memory. To achieve this, we take the newly generated long-term memory and process it through a hyperbolic tangent (tanh) function creating a potential new short-term memory. We then multiply this potential memory by the output of the Sigmoid function (σ_o). This multiplication generates the final output as well as the input for the next hidden cell ($h^{\langle t\rangle}$) within the LSTM cell.

We have

$$\mathbf{o}^{(t)} = \sigma_g(W_o\mathbf{x}^{(t)} + U_o\mathbf{h}^{(t-1)} + \mathbf{b}_o),$$
$$\mathbf{h}^{(t)} = \mathbf{o}^{(t)} \otimes \sigma_h(\mathbf{c}^{(t)}).$$

where $\mathbf{W_o}, \mathbf{U_o}$ are the weights of the output gate and $\mathbf{b_o}$ is the bias of the output gate.

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.

```
# 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 mod
    """
    # 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

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
```

```python
    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)
```

Autoencoders: Overarching view

Autoencoders are artificial neural networks capable of learning efficient representations of the input data (these representations are called codings) without any supervision (i.e., the training set is unlabeled). These codings typically have a much lower dimensionality than the input data, making autoencoders useful for dimensionality reduction.

More importantly, autoencoders act as powerful feature detectors, and they can be used for unsupervised pretraining of deep neural networks.

Lastly, they are capable of randomly generating new data that looks very similar to the training data; this is called a generative model. For example, you could train an autoencoder on pictures of faces, and it would then be able to generate new faces. Surprisingly, autoencoders work by simply learning to copy their inputs to their outputs. This may sound like a trivial task, but we will see that constraining the network in various ways can make it rather difficult. For example, you can limit the size of the internal representation, or you can add noise to the inputs and train the network to recover the original inputs. These constraints prevent the autoencoder from trivially copying the inputs directly to the outputs, which forces it to learn efficient ways of representing the data. In short, the codings are byproducts of the autoencoder's attempt to learn the identity function under some constraints.

First introduction of AEs

Autoencoders were first introduced by Rumelhart, Hinton, and Williams in 1986 with the goal of learning to reconstruct the input observations with the lowest error possible.

Why would one want to learn to reconstruct the input observations? If you have problems imagining what that means, think of having a dataset made of images. An autoencoder would be an algorithm that can give as output an image that is as similar as possible to the input one. You may be confused, as there is no apparent reason of doing so. To better understand why autoencoders are useful we need a more informative (although not yet unambiguous) definition.

An autoencoder is a type of algorithm with the primary purpose of learning an "informative" representation of the data that can be used for different applications (see Bank, D., Koenigstein, N., and Giryes, R., Autoencoders) by learning to reconstruct a set of input observations well enough.

Autoencoder structure

Autoencoders are neural networks where the outputs are its own inputs. They are split (see whiteboard drawing) into an **encoder part** which maps the input $\boldsymbol{x}$ via a function $f(\boldsymbol{x},\boldsymbol{W})$ (this is the encoder part) to a **so-called code part** (or intermediate part) with the result $\boldsymbol{h}$

$$\boldsymbol{h} = f(\boldsymbol{x},\boldsymbol{W})),$$

where $\boldsymbol{W}$ are the weights to be determined. The **decoder** parts maps, via its own parameters (weights given by the matrix $\boldsymbol{V}$ and its own biases) to the final ouput

$$\tilde{\boldsymbol{x}} = g(\boldsymbol{h},\boldsymbol{V})).$$

The goal is to minimize the construction error.

Dimensionality reduction and links with Principal component analysis

The hope is that the training of the autoencoder can unravel some useful properties of the function f. They are often trained with only single-layer neural networks (although deep networks can improve the training) and are essentially given by feed forward neural networks.

If the function f and g are given by a linear dependence on the weight matrices $\boldsymbol{W}$ and $\boldsymbol{V}$, we can show that for a regression case, by miminizing the mean squared error between $\boldsymbol{x}$ and $\tilde{\boldsymbol{x}}$, the autoencoder learns the same subspace as the standard principal component analysis (PCA).

In order to see this, we define then

$$\boldsymbol{h} = f(\boldsymbol{x},\boldsymbol{W})) = \boldsymbol{W}\boldsymbol{x},$$

and

$$\tilde{\boldsymbol{x}} = g(\boldsymbol{h},\boldsymbol{V})) = \boldsymbol{V}\boldsymbol{h} = \boldsymbol{V}\boldsymbol{W}\boldsymbol{x}.$$

AE mean-squared error

With the above linear dependence we can in turn define our optimization problem in terms of the optimization of the mean-squared error, that is we wish to optimize

$$\min_{\boldsymbol{W},\boldsymbol{V}\in\mathbb{R}\frac{1}{n}\sum_{i=0}^{n-1}(x_i-\tilde{x}_i)^2=\frac{1}{n}||\boldsymbol{x}-\boldsymbol{V}\boldsymbol{W}\boldsymbol{x}||_2^2,}$$

where we have used the definition of a norm-2 vector, that is

$$||\boldsymbol{x}||_2 = \sqrt{\sum_i x_i^2}.$$

This is equivalent to our functions learning the the same subspace as the PCA method. This means that we can interpret AEs as a dimensionality reduction method. To see this, we need to remind ourselves about the PCA method.

Basic ideas of the Principal Component Analysis (PCA)

The principal component analysis deals with the problem of fitting a low-dimensional affine subspace S of dimension d much smaller than the total dimension D of the problem at hand (our data set). Mathematically it can be formulated as a statistical problem or a geometric problem. In our discussion of the theorem for the classical PCA, we will stay with a statistical approach. Historically, the PCA was first formulated in a statistical setting in order to estimate the principal component of a multivariate random variable.

We have a data set defined by a design/feature matrix $\boldsymbol{X}$ (see below for its definition)

- Each data point is determined by p extrinsic (measurement) variables
- We may want to ask the following question: Are there fewer intrinsic variables (say $d << p$) that still approximately describe the data?
- If so, these intrinsic variables may tell us something important and finding these intrinsic variables is what dimension reduction methods do.

A good read is for example Vidal, Ma and Sastry.

Introducing the Covariance and Correlation functions

Before we discuss the PCA theorem, we need to remind ourselves about the definition of the covariance and the correlation function. These are quantities

Suppose we have defined two vectors $\hat{x}$ and $\hat{y}$ with n elements each. The covariance matrix $\boldsymbol{C}$ is defined as

$$\boldsymbol{C}[\boldsymbol{x},\boldsymbol{y}] = \begin{bmatrix} \mathrm{cov}[\boldsymbol{x},\boldsymbol{x}] & \mathrm{cov}[\boldsymbol{x},\boldsymbol{y}] \\ \mathrm{cov}[\boldsymbol{y},\boldsymbol{x}] & \mathrm{cov}[\boldsymbol{y},\boldsymbol{y}] \end{bmatrix},$$

where for example

$$\mathrm{cov}[\boldsymbol{x},\boldsymbol{y}] = \frac{1}{n}\sum_{i=0}^{n-1}(x_i-\overline{x})(y_i-\overline{y}).$$

With this definition and recalling that the variance is defined as

$$\mathrm{var}[\boldsymbol{x}] = \frac{1}{n}\sum_{i=0}^{n-1}(x_i-\overline{x})^2,$$

we can rewrite the covariance matrix as

$$
\boldsymbol{C}[\boldsymbol{x},\boldsymbol{y}] = \begin{bmatrix} \mathrm{var}[\boldsymbol{x}] & \mathrm{cov}[\boldsymbol{x},\boldsymbol{y}] \\ \mathrm{cov}[\boldsymbol{x},\boldsymbol{y}] & \mathrm{var}[\boldsymbol{y}] \end{bmatrix}.
$$

More on the covariance

The covariance takes values between zero and infinity and may thus lead to problems with loss of numerical precision for particularly large values. It is common to scale the covariance matrix by introducing instead the correlation matrix defined via the so-called correlation function

$$
\mathrm{corr}[\boldsymbol{x},\boldsymbol{y}] = \frac{\mathrm{cov}[\boldsymbol{x},\boldsymbol{y}]}{\sqrt{\mathrm{var}[\boldsymbol{x}]\mathrm{var}[\boldsymbol{y}]}}.
$$

The correlation function is then given by values $\mathrm{corr}[\boldsymbol{x},\boldsymbol{y}] \in [-1,1]$. This avoids eventual problems with too large values. We can then define the correlation matrix for the two vectors $\boldsymbol{x}$ and $\boldsymbol{y}$ as

$$
\boldsymbol{K}[\boldsymbol{x},\boldsymbol{y}] = \begin{bmatrix} 1 & \mathrm{corr}[\boldsymbol{x},\boldsymbol{y}] \\ \mathrm{corr}[\boldsymbol{y},\boldsymbol{x}] & 1 \end{bmatrix},
$$

In the above example this is the function we constructed using **pandas**.

Reminding ourselves about Linear Regression

In our derivation of the various regression algorithms like **Ordinary Least Squares** or **Ridge regression** we defined the design/feature matrix $\boldsymbol{X}$ as

$$
\boldsymbol{X} = \begin{bmatrix}
x_{0,0} & x_{0,1} & x_{0,2} & \dots & \dots x_{0,p-1} \\
x_{1,0} & x_{1,1} & x_{1,2} & \dots & \dots x_{1,p-1} \\
x_{2,0} & x_{2,1} & x_{2,2} & \dots & \dots x_{2,p-1} \\
\dots & \dots & \dots & \dots\dots & \dots \\
x_{n-2,0} & x_{n-2,1} & x_{n-2,2} & \dots & \dots x_{n-2,p-1} \\
x_{n-1,0} & x_{n-1,1} & x_{n-1,2} & \dots & \dots x_{n-1,p-1}
\end{bmatrix},
$$

with $\boldsymbol{X} \in \mathbb{R}^{n\times p}$, with the predictors/features p refering to the column numbers and the entries n being the row elements. We can rewrite the design/feature matrix in terms of its column vectors as

$$
\boldsymbol{X} = \begin{bmatrix} \boldsymbol{x}_0 & \boldsymbol{x}_1 & \boldsymbol{x}_2 & \dots & \dots & \boldsymbol{x}_{p-1} \end{bmatrix},
$$

with a given vector

$$
\boldsymbol{x}_i^T = \begin{bmatrix} x_{0,i} & x_{1,i} & x_{2,i} & \dots & \dots x_{n-1,i} \end{bmatrix}.
$$

Simple Example

With these definitions, we can now rewrite our 2×2 correlation/covariance matrix in terms of a moe general design/feature matrix $\boldsymbol{X} \in \mathbb{R}^{n \times p}$. This leads to a $p \times p$ covariance matrix for the vectors $\boldsymbol{x}_i$ with $i = 0, 1, \dots, p-1$

$$\boldsymbol{C}[\boldsymbol{x}] = \begin{bmatrix} \mathrm{var}[\boldsymbol{x}_0] & \mathrm{cov}[\boldsymbol{x}_0, \boldsymbol{x}_1] & \mathrm{cov}[\boldsymbol{x}_0, \boldsymbol{x}_2] & \dots & \dots & \mathrm{cov}[\boldsymbol{x}_0, \boldsymbol{x}_{p-1}] \\ \mathrm{cov}[\boldsymbol{x}_1, \boldsymbol{x}_0] & \mathrm{var}[\boldsymbol{x}_1] & \mathrm{cov}[\boldsymbol{x}_1, \boldsymbol{x}_2] & \dots & \dots & \mathrm{cov}[\boldsymbol{x}_1, \boldsymbol{x}_{p-1}] \\ \mathrm{cov}[\boldsymbol{x}_2, \boldsymbol{x}_0] & \mathrm{cov}[\boldsymbol{x}_2, \boldsymbol{x}_1] & \mathrm{var}[\boldsymbol{x}_2] & \dots & \dots & \mathrm{cov}[\boldsymbol{x}_2, \boldsymbol{x}_{p-1}] \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \mathrm{cov}[\boldsymbol{x}_{p-1}, \boldsymbol{x}_0] & \mathrm{cov}[\boldsymbol{x}_{p-1}, \boldsymbol{x}_1] & \mathrm{cov}[\boldsymbol{x}_{p-1}, \boldsymbol{x}_2] & \dots & \dots & \mathrm{var}[\boldsymbol{x}_{p-1}] \end{bmatrix},$$

The Correlation Matrix

and the correlation matrix

$$\boldsymbol{K}[\boldsymbol{x}] = \begin{bmatrix} 1 & \mathrm{corr}[\boldsymbol{x}_0, \boldsymbol{x}_1] & \mathrm{corr}[\boldsymbol{x}_0, \boldsymbol{x}_2] & \dots & \dots & \mathrm{corr}[\boldsymbol{x}_0, \boldsymbol{x}_{p-1}] \\ \mathrm{corr}[\boldsymbol{x}_1, \boldsymbol{x}_0] & 1 & \mathrm{corr}[\boldsymbol{x}_1, \boldsymbol{x}_2] & \dots & \dots & \mathrm{corr}[\boldsymbol{x}_1, \boldsymbol{x}_{p-1}] \\ \mathrm{corr}[\boldsymbol{x}_2, \boldsymbol{x}_0] & \mathrm{corr}[\boldsymbol{x}_2, \boldsymbol{x}_1] & 1 & \dots & \dots & \mathrm{corr}[\boldsymbol{x}_2, \boldsymbol{x}_{p-1}] \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \dots & \dots & \dots & \dots & \dots & \dots \\ \mathrm{corr}[\boldsymbol{x}_{p-1}, \boldsymbol{x}_0] & \mathrm{corr}[\boldsymbol{x}_{p-1}, \boldsymbol{x}_1] & \mathrm{corr}[\boldsymbol{x}_{p-1}, \boldsymbol{x}_2] & \dots & \dots & 1 \end{bmatrix},$$

Numpy Functionality

The Numpy function **np.cov** calculates the covariance elements using the factor $1/(n-1)$ instead of $1/n$ since it assumes we do not have the exact mean values. The following simple function uses the **np.vstack** function which takes each vector of dimension $1 \times n$ and produces a $2 \times n$ matrix $\boldsymbol{W}$

$$\boldsymbol{W}^T = \begin{bmatrix} x_0 & y_0 \\ x_1 & y_1 \\ x_2 & y_2 \\ \dots & \dots \\ x_{n-2} & y_{n-2} \\ x_{n-1} & y_{n-1} \end{bmatrix},$$

which in turn is converted into into the 2×2 covariance matrix $\boldsymbol{C}$ via the Numpy function **np.cov()**. We note that we can also calculate the mean value of each set of samples $\boldsymbol{x}$ etc using the Numpy function **np.mean(x)**. We can also extract the eigenvalues of the covariance matrix through the **np.linalg.eig()** function.

```
# Importing various packages
import numpy as np
n = 100
x = np.random.normal(size=n)
print(np.mean(x))
```

```
y = 4+3*x+np.random.normal(size=n)
print(np.mean(y))
W = np.vstack((x, y))
C = np.cov(W)
print(C)
```

Correlation Matrix again

The previous example can be converted into the correlation matrix by simply scaling the matrix elements with the variances. We should also subtract the mean values for each column. This leads to the following code which sets up the correlations matrix for the previous example in a more brute force way. Here we scale the mean values for each column of the design matrix, calculate the relevant mean values and variances and then finally set up the 2×2 correlation matrix (since we have only two vectors).

```
import numpy as np
n = 100
# define two vectors
x = np.random.random(size=n)
y = 4+3*x+np.random.normal(size=n)
#scaling the x and y vectors
x = x - np.mean(x)
y = y - np.mean(y)
variance_x = np.sum(x@x)/n
variance_y = np.sum(y@y)/n
print(variance_x)
print(variance_y)
cov_xy = np.sum(x@y)/n
cov_xx = np.sum(x@x)/n
cov_yy = np.sum(y@y)/n
C = np.zeros((2,2))
C[0,0]= cov_xx/variance_x
C[1,1]= cov_yy/variance_y
C[0,1]= cov_xy/np.sqrt(variance_y*variance_x)
C[1,0]= C[0,1]
print(C)
```

We see that the matrix elements along the diagonal are one as they should be and that the matrix is symmetric. Furthermore, diagonalizing this matrix we easily see that it is a positive definite matrix.

The above procedure with **numpy** can be made more compact if we use **pandas**.

Using Pandas

We whow here how we can set up the correlation matrix using **pandas**, as done in this simple code

```
import numpy as np
import pandas as pd
n = 10
```

```
x = np.random.normal(size=n)
x = x - np.mean(x)
y = 4+3*x+np.random.normal(size=n)
y = y - np.mean(y)
X = (np.vstack((x, y))).T
print(X)
Xpd = pd.DataFrame(X)
print(Xpd)
correlation_matrix = Xpd.corr()
print(correlation_matrix)
```

And then the Franke Function

We expand this model to the Franke function discussed above.

```
# Common imports
import numpy as np
import pandas as pd


def FrankeFunction(x,y):
        term1 = 0.75*np.exp(-(0.25*(9*x-2)**2) - 0.25*((9*y-2)**2))
        term2 = 0.75*np.exp(-((9*x+1)**2)/49.0 - 0.1*(9*y+1))
        term3 = 0.5*np.exp(-(9*x-7)**2/4.0 - 0.25*((9*y-3)**2))
        term4 = -0.2*np.exp(-(9*x-4)**2 - (9*y-7)**2)
        return term1 + term2 + term3 + term4


def create_X(x, y, n ):
        if len(x.shape) > 1:
                x = np.ravel(x)
                y = np.ravel(y)

        N = len(x)
        l = int((n+1)*(n+2)/2)                # Number of elements in beta
        X = np.ones((N,l))

        for i in range(1,n+1):
                q = int((i)*(i+1)/2)
                for k in range(i+1):
                        X[:,q+k] = (x**(i-k))*(y**k)

        return X


# Making meshgrid of datapoints and compute Franke's function
n = 4
N = 100
x = np.sort(np.random.uniform(0, 1, N))
y = np.sort(np.random.uniform(0, 1, N))
z = FrankeFunction(x, y)
X = create_X(x, y, n=n)

Xpd = pd.DataFrame(X)
# subtract the mean values and set up the covariance matrix
Xpd = Xpd - Xpd.mean()
covariance_matrix = Xpd.cov()
print(covariance_matrix)
```

We note here that the covariance is zero for the first rows and columns since all matrix elements in the design matrix were set to one (we are fitting the function in terms of a polynomial of degree n). We would however not include the intercept and wee can simply drop these elements and construct a correlation matrix without them by centering our matrix elements by subtracting the mean of each column.

Lnks with the Design Matrix

We can rewrite the covariance matrix in a more compact form in terms of the design/feature matrix $\boldsymbol{X}$ as

$$\boldsymbol{C}[\boldsymbol{x}] = \frac{1}{n}\boldsymbol{X}^T\boldsymbol{X} = \mathbb{E}[\boldsymbol{X}^T\boldsymbol{X}].$$

To see this let us simply look at a design matrix $\boldsymbol{X} \in \mathbb{R}^{2\times 2}$

$$\boldsymbol{X} = \begin{bmatrix} x_{00} & x_{01} \\ x_{10} & x_{11} \end{bmatrix} = \begin{bmatrix} \boldsymbol{x}_0 & \boldsymbol{x}_1 \end{bmatrix}.$$

Computing the Expectation Values

If we then compute the expectation value

$$\mathbb{E}[\boldsymbol{X}^T\boldsymbol{X}] = \frac{1}{n}\boldsymbol{X}^T\boldsymbol{X} = \begin{bmatrix} x_{00}^2 + x_{01}^2 & x_{00}x_{10} + x_{01}x_{11} \\ x_{10}x_{00} + x_{11}x_{01} & x_{10}^2 + x_{11}^2 \end{bmatrix},$$

which is just

$$\boldsymbol{C}[\boldsymbol{x}_0, \boldsymbol{x}_1] = \boldsymbol{C}[\boldsymbol{x}] = \begin{bmatrix} \mathrm{var}[\boldsymbol{x}_0] & \mathrm{cov}[\boldsymbol{x}_0, \boldsymbol{x}_1] \\ \mathrm{cov}[\boldsymbol{x}_1, \boldsymbol{x}_0] & \mathrm{var}[\boldsymbol{x}_1] \end{bmatrix},$$

where we wrote

$$\boldsymbol{C}[\boldsymbol{x}_0, \boldsymbol{x}_1] = \boldsymbol{C}[\boldsymbol{x}]$$

to indicate that this the covariance of the vectors $\boldsymbol{x}$ of the design/feature matrix $\boldsymbol{X}$.

It is easy to generalize this to a matrix $\boldsymbol{X} \in \mathbb{R}^{n\times p}$.

Towards the PCA theorem

We have that the covariance matrix (the correlation matrix involves a simple rescaling) is given as

$$\boldsymbol{C}[\boldsymbol{x}] = \frac{1}{n}\boldsymbol{X}^T\boldsymbol{X} = \mathbb{E}[\boldsymbol{X}^T\boldsymbol{X}].$$

Let us now assume that we can perform a series of orthogonal transformations where we employ some orthogonal matrices $\boldsymbol{S}$. These matrices are defined as $\boldsymbol{S} \in \mathbb{R}^{p\times p}$ and obey the orthogonality requirements $\boldsymbol{S}\boldsymbol{S}^T = \boldsymbol{S}^T\boldsymbol{S} = \boldsymbol{I}$. The matrix can be written out in terms of the column vectors $\boldsymbol{s}_i$ as $\boldsymbol{S} = [\boldsymbol{s}_0, \boldsymbol{s}_1, \dots, \boldsymbol{s}_{p-1}]$ and $\boldsymbol{s}_i \in \mathbb{R}^p$.

Assume also that there is a transformation $\boldsymbol{S}^T\boldsymbol{C}[\boldsymbol{x}]\boldsymbol{S} = \boldsymbol{C}[\boldsymbol{y}]$ such that the new matrix $\boldsymbol{C}[\boldsymbol{y}]$ is diagonal with elements $[\lambda_0, \lambda_1, \lambda_2, \dots, \lambda_{p-1}]$.

That is we have

$$\boldsymbol{C}[\boldsymbol{y}] = \mathbb{E}[\boldsymbol{S}^T\boldsymbol{X}^T\boldsymbol{X}T\boldsymbol{S}] = \boldsymbol{S}^T\boldsymbol{C}[\boldsymbol{x}]\boldsymbol{S},$$

since the matrix $\boldsymbol{S}$ is not a data dependent matrix. Multiplying with $\boldsymbol{S}$ from the left we have

$$\boldsymbol{S}\boldsymbol{C}[\boldsymbol{y}] = \boldsymbol{C}[\boldsymbol{x}]\boldsymbol{S},$$

and since $\boldsymbol{C}[\boldsymbol{y}]$ is diagonal we have for a given eigenvalue i of the covariance matrix that

$$\boldsymbol{S}_i\lambda_i = \boldsymbol{C}[\boldsymbol{x}]\boldsymbol{S}_i.$$

More on the PCA Theorem

In the derivation of the PCA theorem we will assume that the eigenvalues are ordered in descending order, that is $\lambda_0 > \lambda_1 > \dots > \lambda_{p-1}$.

The eigenvalues tell us then how much we need to stretch the corresponding eigenvectors. Dimensions with large eigenvalues have thus large variations (large variance) and define therefore useful dimensions. The data points are more spread out in the direction of these eigenvectors. Smaller eigenvalues mean on the other hand that the corresponding eigenvectors are shrunk accordingly and the data points are tightly bunched together and there is not much variation in these specific directions. Hopefully then we could leave it out dimensions where the eigenvalues are very small. If p is very large, we could then aim at reducing p to $l << p$ and handle only l features/predictors.

The Algorithm before the Theorem

Here's how we would proceed in setting up the algorithm for the PCA, see also discussion below here.

- Set up the datapoints for the design/feature matrix $\boldsymbol{X}$ with $\boldsymbol{X} \in \mathbb{R}^{n\times p}$, with the predictors/features p referring to the column numbers and the entries n being the row elements.

$$\boldsymbol{X} = \begin{bmatrix} x_{0,0} & x_{0,1} & x_{0,2} & \dots & \dots x_{0,p-1} \\ x_{1,0} & x_{1,1} & x_{1,2} & \dots & \dots x_{1,p-1} \\ x_{2,0} & x_{2,1} & x_{2,2} & \dots & \dots x_{2,p-1} \\ \dots & \dots & \dots & \dots\dots & \dots \\ x_{n-2,0} & x_{n-2,1} & x_{n-2,2} & \dots & \dots x_{n-2,p-1} \\ x_{n-1,0} & x_{n-1,1} & x_{n-1,2} & \dots & \dots x_{n-1,p-1} \end{bmatrix},$$

- Center the data by subtracting the mean value for each column. This leads to a new matrix $\boldsymbol{X} \rightarrow \overline{\boldsymbol{X}}$.

- Compute then the covariance/correlation matrix $\mathbb{E}[\overline{\boldsymbol{X}}^T\overline{\boldsymbol{X}}]$.
- Find the eigenpairs of $\boldsymbol{C}$ with eigenvalues $[\lambda_0, \lambda_1, \dots, \lambda_{p-1}]$ and eigenvectors $[\boldsymbol{s}_0, \boldsymbol{s}_1, \dots, \boldsymbol{s}_{p-1}]$.
- Order the eigenvalue (and the eigenvectors accordingly) in order of decreasing eigenvalues.
- Keep only those l eigenvalues larger than a selected threshold value, discarding thus $p-l$ features since we expect small variations in the data here.

Writing our own PCA code

We will use a simple example first with two-dimensional data drawn from a multivariate normal distribution with the following mean and covariance matrix (we have fixed these quantities but will play around with them below):

$$\mu = (-1, 2) \qquad \Sigma = \begin{bmatrix} 4 & 2 \\ 2 & 2 \end{bmatrix}$$

Note that the mean refers to each column of data. We will generate $n = 10000$ points $X = \{x_1, \dots, x_N\}$ from this distribution, and store them in the 1000×2 matrix $\boldsymbol{X}$. This is our design matrix where we have forced the covariance and mean values to take specific values.

Implementing it

The following Python code aids in setting up the data and writing out the design matrix. Note that the function **multivariate** returns also the covariance discussed above and that it is defined by dividing by $n-1$ instead of n.

```python
import numpy as np
import pandas as pd
import matplotlib.pyplot as plt
from IPython.display import display
n = 10000
mean = (-1, 2)
cov = [[4, 2], [2, 2]]
X = np.random.multivariate_normal(mean, cov, n)
```

Now we are going to implement the PCA algorithm. We will break it down into various substeps.

First Step

The first step of PCA is to compute the sample mean of the data and use it to center the data. Recall that the sample mean is

$$\mu_n = \frac{1}{n}\sum_{i=1}^{n} x_i$$

and the mean-centered data $\bar{X} = \{\bar{x}_1, \dots, \bar{x}_n\}$ takes the form

$$\bar{x}_i = x_i - \mu_n.$$

When you are done with these steps, print out μ_n to verify it is close to μ and plot your mean centered data to verify it is centered at the origin! The following code elements perform these operations using **pandas** or using our own functionality for doing so. The latter, using **numpy** is rather simple through the **mean()** function.

```
df = pd.DataFrame(X)
# Pandas does the centering for us
df = df -df.mean()
# we center it ourselves
X_centered = X - X.mean(axis=0)
```

Scaling

Alternatively, we could use the functions we discussed earlier for scaling the data set. That is, we could have used the **StandardScaler** function in **Scikit-Learn**, a function which ensures that for each feature/predictor we study the mean value is zero and the variance is one (every column in the design/feature matrix). You would then not get the same results, since we divide by the variance. The diagonal covariance matrix elements will then be one, while the non-diagonal ones need to be divided by $2\sqrt{2}$ for our specific case.

Centered Data

Now we are going to use the mean centered data to compute the sample covariance of the data by using the following equation

$$\Sigma_n = \frac{1}{n-1}\sum_{i=1}^{n} \bar{x}_i^T \bar{x}_i = \frac{1}{n-1}\sum_{i=1}^{n}(x_i - \mu_n)^T(x_i - \mu_n)$$

where the data points $x_i \in \mathbb{R}^p$ (here in this example $p = 2$) are column vectors and x^T is the transpose of x. We can write our own code or simply use either the functionaly of **numpy** or that of **pandas**, as follows

```
print(df.cov())
print(np.cov(X_centered.T))
```

Note that the way we define the covariance matrix here has a factor $n-1$ instead of n. This is included in the **cov()** function by **numpy** and **pandas**. Our own code here is not very elegant and asks for obvious improvements. It is tailored to this specific 2×2 covariance matrix.

```
# extract the relevant columns from the centered design matrix of dim n x 2
x = X_centered[:,0]
y = X_centered[:,1]
Cov = np.zeros((2,2))
Cov[0,1] = np.sum(x.T@y)/(n-1.0)
Cov[0,0] = np.sum(x.T@x)/(n-1.0)
Cov[1,1] = np.sum(y.T@y)/(n-1.0)
Cov[1,0]= Cov[0,1]
print("Centered covariance using own code")
print(Cov)
plt.plot(x, y, 'x')
plt.axis('equal')
plt.show()
```

Exploring

Depending on the number of points n, we will get results that are close to the covariance values defined above. The plot shows how the data are clustered around a line with slope close to one. Is this expected? Try to change the covariance and the mean values. For example, try to make the variance of the first element much larger than that of the second diagonal element. Try also to shrink the covariance (the non-diagonal elements) and see how the data points are distributed.

Diagonalize the sample covariance matrix to obtain the principal components

Now we are ready to solve for the principal components! To do so we diagonalize the sample covariance matrix Σ. We can use the function **np.linalg.eig** to do so. It will return the eigenvalues and eigenvectors of Σ. Once we have these we can perform the following tasks:

- We compute the percentage of the total variance captured by the first principal component
- We plot the mean centered data and lines along the first and second principal components
- Then we project the mean centered data onto the first and second principal components, and plot the projected data.
- Finally, we approximate the data as

$$x_i \approx \tilde{x}_i = \mu_n + \langle x_i, v_0 \rangle v_0$$

where v_0 is the first principal component.

Collecting all Steps

Collecting all these steps we can write our own PCA function and compare this with the functionality included in **Scikit-Learn**.

The code here outlines some of the elements we could include in the analysis. Feel free to extend upon this in order to address the above questions.

```python
# diagonalize and obtain eigenvalues, not necessarily sorted
EigValues, EigVectors = np.linalg.eig(Cov)
# sort eigenvectors and eigenvalues
#permute = EigValues.argsort()
#EigValues = EigValues[permute]
#EigVectors = EigVectors[:,permute]
print("Eigenvalues of Covariance matrix")
for i in range(2):
    print(EigValues[i])
FirstEigvector = EigVectors[:,0]
SecondEigvector = EigVectors[:,1]
print("First eigenvector")
print(FirstEigvector)
print("Second eigenvector")
print(SecondEigvector)
#thereafter we do a PCA with Scikit-learn
from sklearn.decomposition import PCA
pca = PCA(n_components = 2)
X2Dsl = pca.fit_transform(X)
print("Eigenvector of largest eigenvalue")
print(pca.components_.T[:, 0])
```

This code does not contain all the above elements, but it shows how we can use **Scikit-Learn** to extract the eigenvector which corresponds to the largest eigenvalue. Try to address the questions we pose before the above code. Try also to change the values of the covariance matrix by making one of the diagonal elements much larger than the other. What do you observe then?

Classical PCA Theorem

We assume now that we have a design matrix $\boldsymbol{X}$ which has been centered as discussed above. For the sake of simplicity we skip the overline symbol. The matrix is defined in terms of the various column vectors $[\boldsymbol{x}_0, \boldsymbol{x}_1, \dots, \boldsymbol{x}_{p-1}]$ each with dimension $\boldsymbol{x} \in \mathbb{R}^n$.

The PCA theorem states that minimizing the above reconstruction error corresponds to setting $\boldsymbol{W} = \boldsymbol{S}$, the orthogonal matrix which diagonalizes the empirical covariance(correlation) matrix. The optimal low-dimensional encoding of the data is then given by a set of vectors $\boldsymbol{z}_i$ with at most l vectors, with $l << p$, defined by the orthogonal projection of the data onto the columns spanned by the eigenvectors of the covariance(correlations matrix).

The PCA Theorem

To show the PCA theorem let us start with the assumption that there is one vector $\boldsymbol{s}_0$ which corresponds to a solution which minimized the reconstruction error J. This is an orthogonal vector. It means that we now approximate the reconstruction error in terms of $\boldsymbol{w}_0$ and $\boldsymbol{z}_0$ as

We are almost there, we have obtained a relation between minimizing the reconstruction error and the variance and the covariance matrix. Minimizing the error is equivalent to maximizing the variance of the projected data.

We could trivially maximize the variance of the projection (and thereby minimize the error in the reconstruction function) by letting the norm-2 of $\boldsymbol{w}_0$ go to infinity. However, this norm since we want the matrix $\boldsymbol{W}$ to be an orthogonal matrix, is constrained by $||\boldsymbol{w}_0||_2^2 = 1$. Imposing this condition via a Lagrange multiplier we can then in turn maximize

$$J(\boldsymbol{w}_0) = \boldsymbol{w}_0^T \boldsymbol{C}[\boldsymbol{x}]\boldsymbol{w}_0 + \lambda_0(1 - \boldsymbol{w}_0^T \boldsymbol{w}_0).$$

Taking the derivative with respect to $\boldsymbol{w}_0$ we obtain

$$\frac{\partial J(\boldsymbol{w}_0)}{\partial \boldsymbol{w}_0} = 2\boldsymbol{C}[\boldsymbol{x}]\boldsymbol{w}_0 - 2\lambda_0 \boldsymbol{w}_0 = 0,$$

meaning that

$$\boldsymbol{C}[\boldsymbol{x}]\boldsymbol{w}_0 = \lambda_0 \boldsymbol{w}_0.$$

The direction that maximizes the variance (or minimizes the construction error) is an eigenvector of the covariance matrix! If we left multiply with $\boldsymbol{w}_0^T$ we have the variance of the projected data is

$$\boldsymbol{w}_0^T \boldsymbol{C}[\boldsymbol{x}]\boldsymbol{w}_0 = \lambda_0.$$

If we want to maximize the variance (minimize the construction error) we simply pick the eigenvector of the covariance matrix with the largest eigenvalue. This establishes the link between the minimization of the reconstruction function J in terms of an orthogonal matrix and the maximization of the variance and thereby the covariance of our observations encoded in the design/feature matrix $\boldsymbol{X}$.

The proof for the other eigenvectors $\boldsymbol{w}_1, \boldsymbol{w}_2, \dots$ can be established by applying the above arguments and using the fact that our basis of eigenvectors is orthogonal, see Murphy chapter 12.2. The discussion in chapter 12.2 of Murphy's text has also a nice link with the Singular Value Decomposition theorem. For categorical data, see chapter 12.4 and discussion therein.

For more details, see for example Vidal, Ma and Sastry, chapter 2.

Geometric Interpretation and link with Singular Value Decomposition

For a detailed demonstration of the geometric interpretation, see Vidal, Ma and Sastry, section 2.1.2.

Principal Component Analysis (PCA) is by far the most popular dimensionality reduction algorithm. First it identifies the hyperplane that lies closest to the data, and then it projects the data onto it.

The following Python code uses NumPy's **svd()** function to obtain all the principal components of the training set, then extracts the first two principal components. First we center the data using either **pandas** or our own code

```
import numpy as np
import pandas as pd
from IPython.display import display
np.random.seed(100)
# setting up a 10 x 5 vanilla matrix
rows = 10
cols = 5
X = np.random.randn(rows,cols)
df = pd.DataFrame(X)
# Pandas does the centering for us
df = df -df.mean()
display(df)

# we center it ourselves
X_centered = X - X.mean(axis=0)
# Then check the difference between pandas and our own set up
print(X_centered-df)
#Now we do an SVD
U, s, V = np.linalg.svd(X_centered)
c1 = V.T[:, 0]
c2 = V.T[:, 1]
W2 = V.T[:, :2]
X2D = X_centered.dot(W2)
print(X2D)
```

PCA assumes that the dataset is centered around the origin. Scikit-Learn's PCA classes take care of centering the data for you. However, if you implement PCA yourself (as in the preceding example), or if you use other libraries, don't forget to center the data first.

Once you have identified all the principal components, you can reduce the dimensionality of the dataset down to d dimensions by projecting it onto the hyperplane defined by the first d principal components. Selecting this hyperplane ensures that the projection will preserve as much variance as possible.

```
W2 = V.T[:, :2]
X2D = X_centered.dot(W2)
```

PCA and scikit-learn

Scikit-Learn's PCA class implements PCA using SVD decomposition just like we did before. The following code applies PCA to reduce the dimensionality of the dataset down to two dimensions (note that it automatically takes care of centering the data):

```
#thereafter we do a PCA with Scikit-learn
from sklearn.decomposition import PCA
```

```
pca = PCA(n_components = 2)
X2D = pca.fit_transform(X)
print(X2D)
```

After fitting the PCA transformer to the dataset, you can access the principal components using the components variable (note that it contains the PCs as horizontal vectors, so, for example, the first principal component is equal to

```
pca.components_.T[:, 0]
```

Another very useful piece of information is the explained variance ratio of each principal component, available via the *explained_variance_ratio* variable. It indicates the proportion of the dataset's variance that lies along the axis of each principal component.

Back to the Cancer Data

We can now repeat the above but applied to real data, in this case our breast cancer data. Here we compute performance scores on the training data using logistic regression.

```
import matplotlib.pyplot as plt
import numpy as np
from sklearn.model_selection import  train_test_split
from sklearn.datasets import load_breast_cancer
from sklearn.linear_model import LogisticRegression
cancer = load_breast_cancer()

X_train, X_test, y_train, y_test = train_test_split(cancer.data,cancer.target,random_state=0)

logreg = LogisticRegression()
logreg.fit(X_train, y_train)
print("Train set accuracy from Logistic Regression: {:.2f}".format(logreg.score(X_train,y_train))
# We scale the data
from sklearn.preprocessing import StandardScaler
scaler = StandardScaler()
scaler.fit(X_train)
X_train_scaled = scaler.transform(X_train)
X_test_scaled = scaler.transform(X_test)
# Then perform again a log reg fit
logreg.fit(X_train_scaled, y_train)
print("Train set accuracy scaled data: {:.2f}".format(logreg.score(X_train_scaled,y_train)))
#thereafter we do a PCA with Scikit-learn
from sklearn.decomposition import PCA
pca = PCA(n_components = 2)
X2D_train = pca.fit_transform(X_train_scaled)
# and finally compute the log reg fit and the score on the training data
logreg.fit(X2D_train,y_train)
print("Train set accuracy scaled and PCA data: {:.2f}".format(logreg.score(X2D_train,y_train)))
```

We see that our training data after the PCA decomposition has a performance similar to the non-scaled data.

Instead of arbitrarily choosing the number of dimensions to reduce down to, it is generally preferable to choose the number of dimensions that add up to a sufficiently large portion of the variance (e.g., 95%). Unless, of course, you are reducing dimensionality for data visualization — in that case you will generally want to reduce the dimensionality down to 2 or 3. The following code computes PCA without reducing dimensionality, then computes the minimum number of dimensions required to preserve 95% of the training set's variance:

```
pca = PCA()
pca.fit(X)
cumsum = np.cumsum(pca.explained_variance_ratio_)
d = np.argmax(cumsum >= 0.95) + 1
```

You could then set *n_components* $= d$ and run PCA again. However, there is a much better option: instead of specifying the number of principal components you want to preserve, you can set *n_components* to be a float between 0.0 and 1.0, indicating the ratio of variance you wish to preserve:

```
pca = PCA(n_components=0.95)
X_reduced = pca.fit_transform(X)
```

Incremental PCA

One problem with the preceding implementation of PCA is that it requires the whole training set to fit in memory in order for the SVD algorithm to run. Fortunately, Incremental PCA (IPCA) algorithms have been developed: you can split the training set into mini-batches and feed an IPCA algorithm one minibatch at a time. This is useful for large training sets, and also to apply PCA online (i.e., on the fly, as new instances arrive).

Randomized PCA. Scikit-Learn offers yet another option to perform PCA, called Randomized PCA. This is a stochastic algorithm that quickly finds an approximation of the first d principal components. Its computational complexity is $O(m \times d^2) + O(d^3)$, instead of $O(m \times n^2) + O(n^3)$, so it is dramatically faster than the previous algorithms when d is much smaller than n.

Kernel PCA. The kernel trick is a mathematical technique that implicitly maps instances into a very high-dimensional space (called the feature space), enabling nonlinear classification and regression with Support Vector Machines. Recall that a linear decision boundary in the high-dimensional feature space corresponds to a complex nonlinear decision boundary in the original space. It turns out that the same trick can be applied to PCA, making it possible to perform complex nonlinear projections for dimensionality reduction. This is called Kernel PCA (kPCA). It is often good at preserving clusters of instances after projection, or sometimes even unrolling datasets that lie close to a twisted manifold. For example, the following code uses Scikit-Learn's KernelPCA class to perform kPCA with an

```
from sklearn.decomposition import KernelPCA
rbf_pca = KernelPCA(n_components = 2, kernel="rbf", gamma=0.04)
X_reduced = rbf_pca.fit_transform(X)
```

Other techniques

There are many other dimensionality reduction techniques, several of which are available in Scikit-Learn.

Here are some of the most popular:

- **Multidimensional Scaling (MDS)** reduces dimensionality while trying to preserve the distances between the instances.
- **Isomap** creates a graph by connecting each instance to its nearest neighbors, then reduces dimensionality while trying to preserve the geodesic distances between the instances.
- **t-Distributed Stochastic Neighbor Embedding** (t-SNE) reduces dimensionality while trying to keep similar instances close and dissimilar instances apart. It is mostly used for visualization, in particular to visualize clusters of instances in high-dimensional space (e.g., to visualize the MNIST images in 2D).
- Linear Discriminant Analysis (LDA) is actually a classification algorithm, but during training it learns the most discriminative axes between the classes, and these axes can then be used to define a hyperplane onto which to project the data. The benefit is that the projection will keep classes as far apart as possible, so LDA is a good technique to reduce dimensionality before running another classification algorithm such as a Support Vector Machine (SVM) classifier discussed in the SVM lectures.