# Convolutional (CNN) and Recurrent (RNN) Neural Networks. Start decision trees

**Morten Hjorth-Jensen**[1,2]

[1]Department of Physics, University of Oslo
[2]Department of Physics and Astronomy and National Superconducting Cyclotron Laboratory, Michigan State University

Jan 27, 2021

## Plan for Day 8

Finalize discussions on CNNs and RNNs and start with decision trees.
Reading suggestions: Aurelien Geron's chapters 13 and 14.

**Excellent lectures on CNNs and RNNs.**

- Video on Convolutional Neural Networks from MIT
- Video on Recurrent Neural Networks from MIT

For decision trees we have Geron's chapter 6 which covers decision trees while ensemble models, voting and bagging are discussed in chapter 7. See also lecture from STK-IN4300, lecture 7. Chapter 9.2 of Hastie et al contains also a good discussion.

## Convolutional Neural Networks (recognizing images)

Convolutional neural networks (CNNs) were developed during the last decade of the previous century, with a focus on character recognition tasks. Nowadays, CNNs are a central element in the spectacular success of deep learning methods. The success in for example image classifications have made them a central tool for most machine learning practitioners.

CNNs are very similar to ordinary Neural Networks. They are made up of neurons that have learnable weights and biases. Each neuron receives some inputs, performs a dot product and optionally follows it with a non-linearity. The whole network still expresses a single differentiable score function: from the

raw image pixels on one end to class scores at the other. And they still have a loss function (for example Softmax) on the last (fully-connected) layer and all the tips/tricks we developed for learning regular Neural Networks still apply (back propagation, gradient descent etc etc).

What is the difference? **CNN architectures make the explicit assumption that the inputs are images, which allows us to encode certain properties into the architecture. These then make the forward function more efficient to implement and vastly reduce the amount of parameters in the network.**

Here we provide only a superficial overview, for the more interested, we recommend highly the course IN5400 – Machine Learning for Image Analysis and the slides of CS231.

Another good read is the article here `https://arxiv.org/pdf/1603.07285.pdf`.

## Neural Networks vs CNNs

Neural networks are defined as **affine transformations**, that is a vector is received as input and is multiplied with a matrix of so-called weights (our unknown paramters) to produce an output (to which a bias vector is usually added before passing the result through a nonlinear activation function). This is applicable to any type of input, be it an image, a sound clip or an unordered collection of features: whatever their dimensionality, their representation can always be flattened into a vector before the transformation.

## Why CNNS for images, sound files, medical images from CT scans etc?

However, when we consider images, sound clips and many other similar kinds of data, these data have an intrinsic structure. More formally, they share these important properties:

- They are stored as multi-dimensional arrays (think of the pixels of a figure) .
- They feature one or more axes for which ordering matters (e.g., width and height axes for an image, time axis for a sound clip).
- One axis, called the channel axis, is used to access different views of the data (e.g., the red, green and blue channels of a color image, or the left and right channels of a stereo audio track).

These properties are not exploited when an affine transformation is applied; in fact, all the axes are treated in the same way and the topological information is not taken into account. Still, taking advantage of the implicit structure of the data may prove very handy in solving some tasks, like computer vision and speech recognition, and in these cases it would be best to preserve it. This is where discrete convolutions come into play.

A discrete convolution is a linear transformation that preserves this notion of ordering. It is sparse (only a few input units contribute to a given output unit) and reuses parameters (the same weights are applied to multiple locations in the input).

## Regular NNs don't scale well to full images

As an example, consider an image of size $32 \times 32 \times 3$ (32 wide, 32 high, 3 color channels), so a single fully-connected neuron in a first hidden layer of a regular Neural Network would have $32 \times 32 \times 3 = 3072$ weights. This amount still seems manageable, but clearly this fully-connected structure does not scale to larger images. For example, an image of more respectable size, say $200 \times 200 \times 3$, would lead to neurons that have $200 \times 200 \times 3 = 120,000$ weights.

We could have several such neurons, and the parameters would add up quickly! Clearly, this full connectivity is wasteful and the huge number of parameters would quickly lead to possible overfitting.

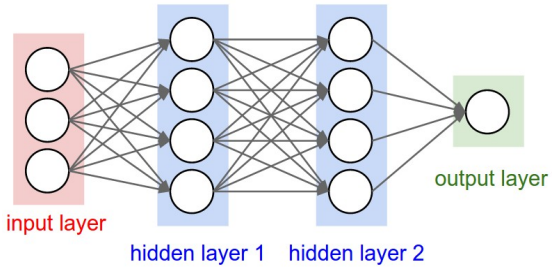



Figure 1: A regular 3-layer Neural Network.

## 3D volumes of neurons

Convolutional Neural Networks take advantage of the fact that the input consists of images and they constrain the architecture in a more sensible way.

In particular, unlike a regular Neural Network, the layers of a CNN have neurons arranged in 3 dimensions: width, height, depth. (Note that the word depth here refers to the third dimension of an activation volume, not to the depth of a full Neural Network, which can refer to the total number of layers in a network.)

To understand it better, the above example of an image with an input volume of activations has dimensions $32 \times 32 \times 3$ (width, height, depth respectively).

The neurons in a layer will only be connected to a small region of the layer before it, instead of all of the neurons in a fully-connected manner. Moreover, the final output layer could for this specific image have dimensions $1 \times 1 \times 10$, because by the end of the CNN architecture we will reduce the full image into a single vector of class scores, arranged along the depth dimension.

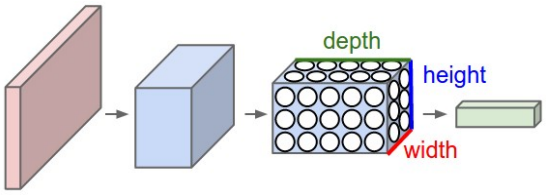



Figure 2: A CNN arranges its neurons in three dimensions (width, height, depth), as visualized in one of the layers. Every layer of a CNN transforms the 3D input volume to a 3D output volume of neuron activations. In this example, the red input layer holds the image, so its width and height would be the dimensions of the image, and the depth would be 3 (Red, Green, Blue channels).

## Layers used to build CNNs

A simple CNN is a sequence of layers, and every layer of a CNN transforms one volume of activations to another through a differentiable function. We use three main types of layers to build CNN architectures: Convolutional Layer, Pooling Layer, and Fully-Connected Layer (exactly as seen in regular Neural Networks). We will stack these layers to form a full CNN architecture.

A simple CNN for image classification could have the architecture:

- **INPUT** ($32 \times 32 \times 3$) will hold the raw pixel values of the image, in this case an image of width 32, height 32, and with three color channels R,G,B.
- **CONV** (convolutional )layer will compute the output of neurons that are connected to local regions in the input, each computing a dot product between their weights and a small region they are connected to in the input volume. This may result in volume such as $[32 \times 32 \times 12]$ if we decided to use 12 filters.
- **RELU** layer will apply an elementwise activation function, such as the $max(0, x)$ thresholding at zero. This leaves the size of the volume unchanged ($[32 \times 32 \times 12]$).
- **POOL** (pooling) layer will perform a downsampling operation along the spatial dimensions (width, height), resulting in volume such as $[16 \times 16 \times 12]$.
- **FC** (i.e. fully-connected) layer will compute the class scores, resulting in volume of size $[1 \times 1 \times 10]$, where each of the 10 numbers correspond to a class score, such as among the 10 categories of the MNIST images we considered above . As with ordinary Neural Networks and as the name implies, each neuron in this layer will be connected to all the numbers in the previous volume.

## Transforming images

CNNs transform the original image layer by layer from the original pixel values to the final class scores.

Observe that some layers contain parameters and other don't. In particular, the CNN layers perform transformations that are a function of not only the activations in the input volume, but also of the parameters (the weights and biases of the neurons). On the other hand, the RELU/POOL layers will implement a fixed function. The parameters in the CONV/FC layers will be trained with gradient descent so that the class scores that the CNN computes are consistent with the labels in the training set for each image.

## CNNs in brief

In summary:

- A CNN architecture is in the simplest case a list of Layers that transform the image volume into an output volume (e.g. holding the class scores)
- There are a few distinct types of Layers (e.g. CONV/FC/RELU/POOL are by far the most popular)
- Each Layer accepts an input 3D volume and transforms it to an output 3D volume through a differentiable function
- Each Layer may or may not have parameters (e.g. CONV/FC do, RELU/POOL don't)
- Each Layer may or may not have additional hyperparameters (e.g. CONV/FC/POOL do, RELU doesn't)

For more material on convolutional networks, we strongly recommend the course IN5400 – Machine Learning for Image Analysis and the slides of CS231 which is taught at Stanford University (consistently ranked as one of the top computer science programs in the world). Michael Nielsen's book is a must read, in particular chapter 6 which deals with CNNs.

## CNNs in more detail, building convolutional neural networks in Tensorflow and Keras

As discussed above, CNNs are neural networks built from the assumption that the inputs to the network are 2D images. This is important because the number of features or pixels in images grows very fast with the image size, and an enormous number of weights and biases are needed in order to build an accurate network.

As before, we still have our input, a hidden layer and an output. What's novel about convolutional networks are the **convolutional** and **pooling** layers stacked in pairs between the input and the hidden layer. In addition, the data is

no longer represented as a 2D feature matrix, instead each input is a number of 2D matrices, typically 1 for each color dimension (Red, Green, Blue).

## Setting it up

It means that to represent the entire dataset of images, we require a 4D matrix or **tensor**. This tensor has the dimensions:

$$(n_{inputs}, n_{pixels,width}, n_{pixels,height}, depth).$$

## The MNIST dataset again

The MNIST dataset consists of grayscale images with a pixel size of $28 \times 28$, meaning we require $28 \times 28 = 724$ weights to each neuron in the first hidden layer.

If we were to analyze images of size $128 \times 128$ we would require $128 \times 128 = 16384$ weights to each neuron. Even worse if we were dealing with color images, as most images are, we have an image matrix of size $128 \times 128$ for each color dimension (Red, Green, Blue), meaning 3 times the number of weights = 49152 are required for every single neuron in the first hidden layer.

## Strong correlations

Images typically have strong local correlations, meaning that a small part of the image varies little from its neighboring regions. If for example we have an image of a blue car, we can roughly assume that a small blue part of the image is surrounded by other blue regions.

Therefore, instead of connecting every single pixel to a neuron in the first hidden layer, as we have previously done with deep neural networks, we can instead connect each neuron to a small part of the image (in all 3 RGB depth dimensions). The size of each small area is fixed, and known as a receptive.

## Layers of a CNN

The layers of a convolutional neural network arrange neurons in 3D: width, height and depth. The input image is typically a square matrix of depth 3.

A **convolution** is performed on the image which outputs a 3D volume of neurons. The weights to the input are arranged in a number of 2D matrices, known as **filters**.

Each filter slides along the input image, taking the dot product between each small part of the image and the filter, in all depth dimensions. This is then passed through a non-linear function, typically the **Rectified Linear (ReLu)** function, which serves as the activation of the neurons in the first convolutional layer. This is further passed through a **pooling layer**, which reduces the size of the convolutional layer, e.g. by taking the maximum or average across some small regions, and this serves as input to the next convolutional layer.

## Systematic reduction

By systematically reducing the size of the input volume, through convolution and pooling, the network should create representations of small parts of the input, and then from them assemble representations of larger areas. The final pooling layer is flattened to serve as input to a hidden layer, such that each neuron in the final pooling layer is connected to every single neuron in the hidden layer. This then serves as input to the output layer, e.g. a softmax output for classification.

## Prerequisites: Collect and pre-process data

```
# import necessary packages
import numpy as np
import matplotlib.pyplot as plt
from sklearn import datasets


# ensure the same random numbers appear every time
np.random.seed(0)

# display images in notebook
%matplotlib inline
plt.rcParams['figure.figsize'] = (12,12)


# download MNIST dataset
digits = datasets.load_digits()

# define inputs and labels
inputs = digits.images
labels = digits.target

# RGB images have a depth of 3
# our images are grayscale so they should have a depth of 1
inputs = inputs[:,:,:,np.newaxis]

print("inputs = (n_inputs, pixel_width, pixel_height, depth) = " + str(inputs.shape))
print("labels = (n_inputs) = " + str(labels.shape))


# choose some random images to display
n_inputs = len(inputs)
indices = np.arange(n_inputs)
random_indices = np.random.choice(indices, size=5)

for i, image in enumerate(digits.images[random_indices]):
    plt.subplot(1, 5, i+1)
    plt.axis('off')
    plt.imshow(image, cmap=plt.cm.gray_r, interpolation='nearest')
    plt.title("Label: %d" % digits.target[random_indices[i]])
plt.show()
```

## Importing Keras and Tensorflow

```
from tensorflow.keras import datasets, layers, models
from tensorflow.keras.layers import Input
from tensorflow.keras.models import Sequential      #This allows appending layers to existing mod
```

```
from tensorflow.keras.layers import Dense           #This allows defining the characteristics of
from tensorflow.keras import optimizers             #This allows using whichever optimiser we wan
from tensorflow.keras import regularizers           #This allows using whichever regularizer we w
from tensorflow.keras.utils import to_categorical   #This allows using categorical cross entropy
#from tensorflow.keras import Conv2D
#from tensorflow.keras import MaxPooling2D
#from tensorflow.keras import Flatten

from sklearn.model_selection import train_test_split

# representation of labels
labels = to_categorical(labels)

# split into train and test data
# one-liner from scikit-learn library
train_size = 0.8
test_size = 1 - train_size
X_train, X_test, Y_train, Y_test = train_test_split(inputs, labels, train_size=train_size,
                                                    test_size=test_size)
```

## Running with Keras

```
def create_convolutional_neural_network_keras(input_shape, receptive_field,
                                              n_filters, n_neurons_connected, n_categories,
                                              eta, lmbd):
    model = Sequential()
    model.add(layers.Conv2D(n_filters, (receptive_field, receptive_field), input_shape=input_shape
              activation='relu', kernel_regularizer=regularizers.l2(lmbd)))
    model.add(layers.MaxPooling2D(pool_size=(2, 2)))
    model.add(layers.Flatten())
    model.add(layers.Dense(n_neurons_connected, activation='relu', kernel_regularizer=regularizers
    model.add(layers.Dense(n_categories, activation='softmax', kernel_regularizer=regularizers.l2

    sgd = optimizers.SGD(lr=eta)
    model.compile(loss='categorical_crossentropy', optimizer=sgd, metrics=['accuracy'])

    return model

epochs = 100
batch_size = 100
input_shape = X_train.shape[1:4]
receptive_field = 3
n_filters = 10
n_neurons_connected = 50
n_categories = 10

eta_vals = np.logspace(-5, 1, 7)
lmbd_vals = np.logspace(-5, 1, 7)
```

## Final part

```
CNN_keras = np.zeros((len(eta_vals), len(lmbd_vals)), dtype=object)

for i, eta in enumerate(eta_vals):
    for j, lmbd in enumerate(lmbd_vals):
        CNN = create_convolutional_neural_network_keras(input_shape, receptive_field,
                                              n_filters, n_neurons_connected, n_categories,
                                              eta, lmbd)
        CNN.fit(X_train, Y_train, epochs=epochs, batch_size=batch_size, verbose=0)
```

```
        scores = CNN.evaluate(X_test, Y_test)

        CNN_keras[i][j] = CNN

        print("Learning rate = ", eta)
        print("Lambda = ", lmbd)
        print("Test accuracy: %.3f" % scores[1])
        print()
```

## Final visualization

```
# visual representation of grid search
# uses seaborn heatmap, could probably do this in matplotlib
import seaborn as sns

sns.set()

train_accuracy = np.zeros((len(eta_vals), len(lmbd_vals)))
test_accuracy = np.zeros((len(eta_vals), len(lmbd_vals)))

for i in range(len(eta_vals)):
    for j in range(len(lmbd_vals)):
        CNN = CNN_keras[i][j]

        train_accuracy[i][j] = CNN.evaluate(X_train, Y_train)[1]
        test_accuracy[i][j] = CNN.evaluate(X_test, Y_test)[1]


fig, ax = plt.subplots(figsize = (10, 10))
sns.heatmap(train_accuracy, annot=True, ax=ax, cmap="viridis")
ax.set_title("Training Accuracy")
ax.set_ylabel("$\eta$")
ax.set_xlabel("$\lambda$")
plt.show()

fig, ax = plt.subplots(figsize = (10, 10))
sns.heatmap(test_accuracy, annot=True, ax=ax, cmap="viridis")
ax.set_title("Test Accuracy")
ax.set_ylabel("$\eta$")
ax.set_xlabel("$\lambda$")
plt.show()
```

## The CIFAR01 data set

The CIFAR10 dataset contains 60,000 color images in 10 classes, with 6,000 images in each class. The dataset is divided into 50,000 training images and 10,000 testing images. The classes are mutually exclusive and there is no overlap between them.

```
import tensorflow as tf

from tensorflow.keras import datasets, layers, models
import matplotlib.pyplot as plt

# We import the data set
(train_images, train_labels), (test_images, test_labels) = datasets.cifar10.load_data()
```

```
# Normalize pixel values to be between 0 and 1 by dividing by 255.
train_images, test_images = train_images / 255.0, test_images / 255.0
```

## Verifying the data set

To verify that the dataset looks correct, let's plot the first 25 images from the training set and display the class name below each image.

```
class_names = ['airplane', 'automobile', 'bird', 'cat', 'deer',
               'dog', 'frog', 'horse', 'ship', 'truck']

plt.figure(figsize=(10,10))
for i in range(25):
    plt.subplot(5,5,i+1)
    plt.xticks([])
    plt.yticks([])
    plt.grid(False)
    plt.imshow(train_images[i], cmap=plt.cm.binary)
    # The CIFAR labels happen to be arrays,
    # which is why you need the extra index
    plt.xlabel(class_names[train_labels[i][0]])
plt.show()
```

## Set up the model

The 6 lines of code below define the convolutional base using a common pattern: a stack of Conv2D and MaxPooling2D layers.

As input, a CNN takes tensors of shape (image$_h eight, image_w idth, color_c hannels), ignoringthebatchsize.If y$

```
model = models.Sequential()
model.add(layers.Conv2D(32, (3, 3), activation='relu', input_shape=(32, 32, 3)))
model.add(layers.MaxPooling2D((2, 2)))
model.add(layers.Conv2D(64, (3, 3), activation='relu'))
model.add(layers.MaxPooling2D((2, 2)))
model.add(layers.Conv2D(64, (3, 3), activation='relu'))

# Let's display the architecture of our model so far.

model.summary()
```

You can see that the output of every Conv2D and MaxPooling2D layer is a 3D tensor of shape (height, width, channels). The width and height dimensions tend to shrink as you go deeper in the network. The number of output channels for each Conv2D layer is controlled by the first argument (e.g., 32 or 64). Typically, as the width and height shrink, you can afford (computationally) to add more output channels in each Conv2D layer.

## Add Dense layers on top

To complete our model, you will feed the last output tensor from the convolutional base (of shape (4, 4, 64)) into one or more Dense layers to perform classification. Dense layers take vectors as input (which are 1D), while the current output is a 3D tensor. First, you will flatten (or unroll) the 3D output to 1D, then add one

or more Dense layers on top. CIFAR has 10 output classes, so you use a final Dense layer with 10 outputs and a softmax activation.

```
model.add(layers.Flatten())
model.add(layers.Dense(64, activation='relu'))
model.add(layers.Dense(10))
Here's the complete architecture of our model.

model.summary()
```

As you can see, our (4, 4, 64) outputs were flattened into vectors of shape (1024) before going through two Dense layers.

## Compile and train the model

```
model.compile(optimizer='adam',
              loss=tf.keras.losses.SparseCategoricalCrossentropy(from_logits=True),
              metrics=['accuracy'])

history = model.fit(train_images, train_labels, epochs=10,
                    validation_data=(test_images, test_labels))
```

## Finally, evaluate the model

```
plt.plot(history.history['accuracy'], label='accuracy')
plt.plot(history.history['val_accuracy'], label = 'val_accuracy')
plt.xlabel('Epoch')
plt.ylabel('Accuracy')
plt.ylim([0.5, 1])
plt.legend(loc='lower right')

test_loss, test_acc = model.evaluate(test_images,  test_labels, verbose=2)

print(test_acc)
```

## Recurrent neural networks: 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.

## Set up of an RNN

## 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()

plt.plot(df)
plt.show()

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)

index = df.index.values
plt.plot(index,df)
plt.plot(index,predicted)
plt.axvline(df.index[Tp], c="r")
plt.show()
```

## 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

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)
```

## Decision trees, overarching aims

We start here with the most basic algorithm, the so-called decision tree. With this basic algorithm we can in turn build more complex networks, spanning from homogeneous and heterogenous forests (bagging, random forests and more) to one of the most popular supervised algorithms nowadays, the extreme gradient boosting, or just XGBoost. But let us start with the simplest possible ingredient.

Decision trees are supervised learning algorithms used for both, classification and regression tasks.

The main idea of decision trees is to find those descriptive features which contain the most **information** regarding the target feature and then split the dataset along the values of these features such that the target feature values for the resulting underlying datasets are as pure as possible.

The descriptive features which reproduce best the target/output features are normally said to be the most informative ones. The process of finding the **most informative** feature is done until we accomplish a stopping criteria where we then finally end up in so called **leaf nodes**.

## Basics of a tree

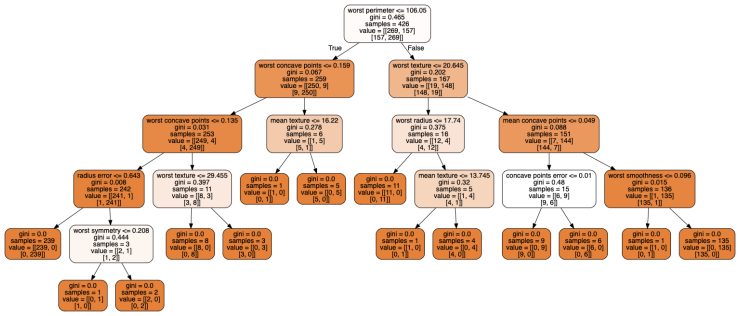
A decision tree is typically divided into a **root node**, the **interior nodes**, and the final **leaf nodes** or just **leaves**. These entities are then connected by so-called **branches**.

The leaf nodes contain the predictions we will make for new query instances presented to our trained model. This is possible since the model has learned the underlying structure of the training data and hence can, given some assumptions, make predictions about the target feature value (class) of unseen query instances.

## A Sketch of a Tree, Regression problem

## A Sketch of a Tree, Classification problem

## A typical Decision Tree with its pertinent Jargon, Classification Problem




This tree was produced using the Wisconsin cancer data (discussed here as well, see code examples below) using **Scikit-Learn**'s decision tree classifier. Here we have used the so-called **gini** index (see below) to split the various branches.

## General Features

The overarching approach to decision trees is a top-down approach.

- A leaf provides the classification of a given instance.
- A node specifies a test of some attribute of the instance.
- A branch corresponds to a possible values of an attribute.
- An instance is classified by starting at the root node of the tree, testing the attribute specified by this node, then moving down the tree branch corresponding to the value of the attribute in the given example.

This process is then repeated for the subtree rooted at the new node.

## How do we set it up?

In simplified terms, the process of training a decision tree and predicting the target features of query instances is as follows:

1. Present a dataset containing of a number of training instances characterized by a number of descriptive features and a target feature

2. Train the decision tree model by continuously splitting the target feature along the values of the descriptive features using a measure of information gain during the training process

3. Grow the tree until we accomplish a stopping criteria create leaf nodes which represent the *predictions* we want to make for new query instances

4. Show query instances to the tree and run down the tree until we arrive at leaf nodes

Then we are essentially done!

## Decision trees and Regression

```
import numpy as np
import matplotlib.pyplot as plt
from sklearn.preprocessing import PolynomialFeatures
from sklearn.linear_model import LinearRegression

steps=250

distance=0
x=0
distance_list=[]
steps_list=[]
while x<steps:
    distance+=np.random.randint(-1,2)
    distance_list.append(distance)
    x+=1
    steps_list.append(x)
plt.plot(steps_list,distance_list, color='green', label="Random Walk Data")

steps_list=np.asarray(steps_list)
distance_list=np.asarray(distance_list)

X=steps_list[:,np.newaxis]

#Polynomial fits

#Degree 2
poly_features=PolynomialFeatures(degree=2, include_bias=False)
X_poly=poly_features.fit_transform(X)

lin_reg=LinearRegression()
poly_fit=lin_reg.fit(X_poly,distance_list)
b=lin_reg.coef_
c=lin_reg.intercept_
print ("2nd degree coefficients:")
print ("zero power: ",c)
print ("first power: ", b[0])
print ("second power: ",b[1])

z = np.arange(0, steps, .01)
z_mod=b[1]*z**2+b[0]*z+c

fit_mod=b[1]*X**2+b[0]*X+c
plt.plot(z, z_mod, color='r', label="2nd Degree Fit")
plt.title("Polynomial Regression")
```

```
plt.xlabel("Steps")
plt.ylabel("Distance")

#Degree 10
poly_features10=PolynomialFeatures(degree=10, include_bias=False)
X_poly10=poly_features10.fit_transform(X)

poly_fit10=lin_reg.fit(X_poly10,distance_list)

y_plot=poly_fit10.predict(X_poly10)
plt.plot(X, y_plot, color='black', label="10th Degree Fit")

plt.legend()
plt.show()


#Decision Tree Regression
from sklearn.tree import DecisionTreeRegressor
regr_1=DecisionTreeRegressor(max_depth=2)
regr_2=DecisionTreeRegressor(max_depth=5)
regr_3=DecisionTreeRegressor(max_depth=7)
regr_1.fit(X, distance_list)
regr_2.fit(X, distance_list)
regr_3.fit(X, distance_list)

X_test = np.arange(0.0, steps, 0.01)[:, np.newaxis]
y_1 = regr_1.predict(X_test)
y_2 = regr_2.predict(X_test)
y_3=regr_3.predict(X_test)

# Plot the results
plt.figure()
plt.scatter(X, distance_list, s=2.5, c="black", label="data")
plt.plot(X_test, y_1, color="red",
         label="max_depth=2", linewidth=2)
plt.plot(X_test, y_2, color="green", label="max_depth=5", linewidth=2)
plt.plot(X_test, y_3, color="m", label="max_depth=7", linewidth=2)

plt.xlabel("Data")
plt.ylabel("Darget")
plt.title("Decision Tree Regression")
plt.legend()
plt.show()
```

## Building a tree, regression

There are mainly two steps

1. We split the predictor space (the set of possible values $x_1, x_2, \ldots, x_p$) into $J$ distinct and non-non-overlapping regions, $R_1, R_2, \ldots, R_J$.

2. For every observation that falls into the region $R_j$ , we make the same prediction, which is simply the mean of the response values for the training observations in $R_j$.

How do we construct the regions $R_1, \ldots, R_J$? In theory, the regions could have any shape. However, we choose to divide the predictor space into high-

dimensional rectangles, or boxes, for simplicity and for ease of interpretation of the resulting predictive model. The goal is to find boxes $R_1, \ldots, R_J$ that minimize the MSE, given by

$$\sum_{j=1}^{J} \sum_{i \in R_j} (y_i - \overline{y}_{R_j})^2,$$

where $\overline{y}_{R_j}$ is the mean response for the training observations within box $j$.

## A top-down approach, recursive binary splitting

Unfortunately, it is computationally infeasible to consider every possible partition of the feature space into $J$ boxes. The common strategy is to take a top-down approach

The approach is top-down because it begins at the top of the tree (all observations belong to a single region) and then successively splits the predictor space; each split is indicated via two new branches further down on the tree. It is greedy because at each step of the tree-building process, the best split is made at that particular step, rather than looking ahead and picking a split that will lead to a better tree in some future step.

## Making a tree

In order to implement the recursive binary splitting we start by selecting the predictor $x_j$ and a cutpoint $s$ that splits the predictor space into two regions $R_1$ and $R_2$

$$\{X | x_j < s\},$$

and

$$\{X | x_j \geq s\},$$

so that we obtain the lowest MSE, that is

$$\sum_{i:x_i \in R_j} (y_i - \overline{y}_{R_1})^2 + \sum_{i:x_i \in R_2} (y_i - \overline{y}_{R_2})^2,$$

which we want to minimize by considering all predictors $x_1, x_2, \ldots, x_p$. We consider also all possible values of $s$ for each predictor. These values could be determined by randomly assigned numbers or by starting at the midpoint and then proceed till we find an optimal value.

For any $j$ and $s$, we define the pair of half-planes where $\overline{y}_{R_1}$ is the mean response for the training observations in $R_1(j, s)$, and $\overline{y}_{R_2}$ is the mean response for the training observations in $R_2(j, s)$.

Finding the values of $j$ and $s$ that minimize the above equation can be done quite quickly, especially when the number of features $p$ is not too large.

Next, we repeat the process, looking for the best predictor and best cutpoint in order to split the data further so as to minimize the MSE within each of the

resulting regions. However, this time, instead of splitting the entire predictor space, we split one of the two previously identified regions. We now have three regions. Again, we look to split one of these three regions further, so as to minimize the MSE. The process continues until a stopping criterion is reached; for instance, we may continue until no region contains more than five observations.

## Pruning the tree

The above procedure is rather straightforward, but leads often to overfitting and unnecessarily large and complicated trees. The basic idea is to grow a large tree $T_0$ and then prune it back in order to obtain a subtree. A smaller tree with fewer splits (fewer regions) can lead to smaller variance and better interpretation at the cost of a little more bias.

The so-called Cost complexity pruning algorithm gives us a way to do just this. Rather than considering every possible subtree, we consider a sequence of trees indexed by a nonnegative tuning parameter $\alpha$.

Read more at the following Scikit-Learn link on pruning.

## Cost complexity pruning

For each value of $\alpha$ there corresponds a subtree $T \in T_0$ such that

$$\sum_{m=1}^{\overline{T}} \sum_{i:x_i \in R_m} (y_i - \overline{y}_{R_m})^2 + \alpha \overline{T},$$

is as small as possible. Here $\overline{T}$ is the number of terminal nodes of the tree $T$ , $R_m$ is the rectangle (i.e. the subset of predictor space) corresponding to the $m$-th terminal node.

The tuning parameter $\alpha$ controls a trade-off between the subtree's complexity and its fit to the training data. When $\alpha = 0$, then the subtree $T$ will simply equal $T_0$, because then the above equation just measures the training error. However, as $\alpha$ increases, there is a price to pay for having a tree with many terminal nodes. The above equation will tend to be minimized for a smaller subtree.

It turns out that as we increase $\alpha$ from zero branches get pruned from the tree in a nested and predictable fashion, so obtaining the whole sequence of subtrees as a function of $\alpha$ is easy. We can select a value of $\alpha$ using a validation set or using cross-validation. We then return to the full data set and obtain the subtree corresponding to $\alpha$.

## Schematic Regression Procedure

### Building a Regression Tree.

1. Use recursive binary splitting to grow a large tree on the training data, stopping only when each terminal node has fewer than some minimum number of observations.

2. Apply cost complexity pruning to the large tree in order to obtain a sequence of best subtrees, as a function of $\alpha$.

3. Use for example $K$-fold cross-validation to choose $\alpha$. Divide the training observations into $K$ folds. For each $k = 1, 2, \ldots, K$ we:

   - repeat steps 1 and 2 on all but the $k$-th fold of the training data.
   - Then we valuate the mean squared prediction error on the data in the left-out $k$-th fold, as a function of $\alpha$.
   - Finally we average the results for each value of $\alpha$, and pick $\alpha$ to minimize the average error.

4. Return the subtree from Step 2 that corresponds to the chosen value of $\alpha$.

## A Classification Tree

A classification tree is very similar to a regression tree, except that it is used to predict a qualitative response rather than a quantitative one. Recall that for a regression tree, the predicted response for an observation is given by the mean response of the training observations that belong to the same terminal node. In contrast, for a classification tree, we predict that each observation belongs to the most commonly occurring class of training observations in the region to which it belongs. In interpreting the results of a classification tree, we are often interested not only in the class prediction corresponding to a particular terminal node region, but also in the class proportions among the training observations that fall into that region.

## Growing a classification tree

The task of growing a classification tree is quite similar to the task of growing a regression tree. Just as in the regression setting, we use recursive binary splitting to grow a classification tree. However, in the classification setting, the MSE cannot be used as a criterion for making the binary splits. A natural alternative to MSE is the **classification error rate**. Since we plan to assign an observation in a given region to the most commonly occurring error rate class of training observations in that region, the classification error rate is simply the fraction of the training observations in that region that do not belong to the most common class.

When building a classification tree, either the Gini index or the entropy are typically used to evaluate the quality of a particular split, since these two approaches are more sensitive to node purity than is the classification error rate.

## Classification tree, how to split nodes

If our targets are the outcome of a classification process that takes for example $k = 1, 2, \dots, K$ values, the only thing we need to think of is to set up the splitting criteria for each node.

We define a PDF $p_{mk}$ that represents the number of observations of a class $k$ in a region $R_m$ with $N_m$ observations. We represent this likelihood function in terms of the proportion $I(y_i = k)$ of observations of this class in the region $R_m$ as

$$p_{mk} = \frac{1}{N_m} \sum_{x_i \in R_m} I(y_i = k).$$

We let $p_{mk}$ represent the majority class of observations in region $m$. The three most common ways of splitting a node are given by

- Misclassification error

$$p_{mk} = \frac{1}{N_m} \sum_{x_i \in R_m} I(y_i \neq k) = 1 - p_{mk}.$$

- Gini index $g$

$$g = \sum_{k=1}^{K} p_{mk}(1 - p_{mk}).$$

- Information entropy or just entropy $s$

$$s = -\sum_{k=1}^{K} p_{mk} \log p_{mk}.$$

## Visualizing the Tree, Classification

```
import os
from sklearn.datasets import load_breast_cancer
from sklearn.tree import DecisionTreeClassifier
from sklearn.model_selection import train_test_split
from sklearn.metrics import confusion_matrix
from sklearn.tree import export_graphviz

from IPython.display import Image
from pydot import graph_from_dot_data
import pandas as pd
import numpy as np


cancer = load_breast_cancer()
X = pd.DataFrame(cancer.data, columns=cancer.feature_names)
print(X)
y = pd.Categorical.from_codes(cancer.target, cancer.target_names)
y = pd.get_dummies(y)
print(y)
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state=1)
```

```
tree_clf = DecisionTreeClassifier(max_depth=5)
tree_clf.fit(X_train, y_train)

export_graphviz(
    tree_clf,
    out_file="DataFiles/cancer.dot",
    feature_names=cancer.feature_names,
    class_names=cancer.target_names,
    rounded=True,
    filled=True
)
cmd = 'dot -Tpng DataFiles/cancer.dot -o DataFiles/cancer.png'
os.system(cmd)
```

## Visualizing the Tree, The Moons

```
# Common imports
import numpy as np
from sklearn.model_selection import  train_test_split
from sklearn.tree import DecisionTreeClassifier
from sklearn.datasets import make_moons
from sklearn.tree import export_graphviz
from pydot import graph_from_dot_data
import pandas as pd
import os

np.random.seed(42)
X, y = make_moons(n_samples=100, noise=0.25, random_state=53)
X_train, X_test, y_train, y_test = train_test_split(X,y,random_state=0)
tree_clf = DecisionTreeClassifier(max_depth=5)
tree_clf.fit(X_train, y_train)

export_graphviz(
    tree_clf,
    out_file="DataFiles/moons.dot",
    rounded=True,
    filled=True
)
cmd = 'dot -Tpng DataFiles/moons.dot -o DataFiles/moons.png'
os.system(cmd)
```

## Other ways of visualizing the trees

**Scikit-Learn** has also another way to visualize the trees which is very useful, here with the Iris data.

```
from sklearn.datasets import load_iris
from sklearn import tree
X, y = load_iris(return_X_y=True)
tree_clf = tree.DecisionTreeClassifier()
tree_clf = tree_clf.fit(X, y)
# and then plot the tree
tree.plot_tree(tree_clf)
```

## Printing out as text

Alternatively, the tree can also be exported in textual format with the function exporttext. This method doesn't require the installation of external libraries and is more compact:

```
from sklearn.datasets import load_iris
from sklearn.tree import DecisionTreeClassifier
from sklearn.tree import export_text
iris = load_iris()
decision_tree = DecisionTreeClassifier(random_state=0, max_depth=2)
decision_tree = decision_tree.fit(iris.data, iris.target)
r = export_text(decision_tree, feature_names=iris['feature_names'])
print(r)
```

## Algorithms for Setting up Decision Trees

Two algorithms stand out in the set up of decision trees:

1. The CART (Classification And Regression Tree) algorithm for both classification and regression

2. The ID3 algorithm based on the computation of the information gain for classification

We discuss both algorithms with applications here. The popular library **Scikit-Learn** uses the CART algorithm. For classification problems you can use either the **gini** index or the **entropy** to split a tree in two branches.

## The CART algorithm for Classification

For classification, the CART algorithm splits the data set in two subsets using a single feature $k$ and a threshold $t_k$. This could be for example a threshold set by a number below a certain circumference of a malign tumor.

How do we find these two quantities? We search for the pair $(k, t_k)$ that produces the purest subset using for example the **gini** factor $G$. The cost function it tries to minimize is then

$$C(k, t_k) = \frac{m_{\text{left}}}{m} G_{\text{left}} + \frac{m_{\text{right}}}{m} G_{\text{right}},$$

where $G_{\text{left/right}}$ measures the impurity of the left/right subset and $m_{\text{left/right}}$ is the number of instances in the left/right subset

Once it has successfully split the training set in two, it splits the subsets using the same logic, then the subsubsets and so on, recursively. It stops recursing once it reaches the maximum depth (defined by the $max\_depth$ hyperparameter), or if it cannot find a split that will reduce impurity. A few other hyperparameters control additional stopping conditions such as the $min\_samples\_split$, $min\_samples\_leaf$, $min\_weight\_fraction\_leaf$, and $max\_leaf\_nodes$.

## The CART algorithm for Regression

The CART algorithm for regression works is similar to the one for classification except that instead of trying to split the training set in a way that minimizes say the **gini** or **entropy** impurity, it now tries to split the training set in a way that minimizes our well-known mean-squared error (MSE). The cost function is now

$$C(k, t_k) = \frac{m_{\text{left}}}{m}\text{MSE}_{\text{left}} + \frac{m_{\text{right}}}{m}\text{MSE}_{\text{right}}.$$

Here the MSE for a specific node is defined as

$$\text{MSE}_{\text{node}} = \frac{1}{m_{\text{node}}}\sum_{i\in\text{node}}(\overline{y}_{\text{node}} - y_i)^2,$$

with

$$\overline{y}_{\text{node}} = \frac{1}{m_{\text{node}}}\sum_{i\in\text{node}} y_i,$$

the mean value of all observations in a specific node.

Without any regularization, the regression task for decision trees, just like for classification tasks, is prone to overfitting.

## Cancer Data again now with Decision Trees and other Methods

```
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.svm import SVC
from sklearn.linear_model import LogisticRegression
from sklearn.tree import DecisionTreeClassifier

# Load the data
cancer = load_breast_cancer()

X_train, X_test, y_train, y_test = train_test_split(cancer.data,cancer.target,random_state=0)
print(X_train.shape)
print(X_test.shape)
# Logistic Regression
logreg = LogisticRegression(solver='lbfgs')
logreg.fit(X_train, y_train)
print("Test set accuracy with Logistic Regression: {:.2f}".format(logreg.score(X_test,y_test)))
# Support vector machine
svm = SVC(gamma='auto', C=100)
svm.fit(X_train, y_train)
print("Test set accuracy with SVM: {:.2f}".format(svm.score(X_test,y_test)))
# Decision Trees
deep_tree_clf = DecisionTreeClassifier(max_depth=None)
deep_tree_clf.fit(X_train, y_train)
print("Test set accuracy with Decision Trees: {:.2f}".format(deep_tree_clf.score(X_test,y_test)))
#now 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)
# Logistic Regression
logreg.fit(X_train_scaled, y_train)
print("Test set accuracy Logistic Regression with scaled data: {:.2f}".format(logreg.score(X_test_
# Support Vector Machine
svm.fit(X_train_scaled, y_train)
print("Test set accuracy SVM with scaled data: {:.2f}".format(logreg.score(X_test_scaled,y_test))
# Decision Trees
deep_tree_clf.fit(X_train_scaled, y_train)
print("Test set accuracy with Decision Trees and scaled data: {:.2f}".format(deep_tree_clf.score(X
```

## Another example, the moons again

```
from __future__ import division, print_function, unicode_literals

# Common imports
import numpy as np
import os

# to make this notebook's output stable across runs
np.random.seed(42)

# To plot pretty figures
import matplotlib
import matplotlib.pyplot as plt
from matplotlib.colors import ListedColormap
plt.rcParams['axes.labelsize'] = 14
plt.rcParams['xtick.labelsize'] = 12
plt.rcParams['ytick.labelsize'] = 12


from sklearn.svm import SVC
from sklearn import datasets
from sklearn.tree import DecisionTreeClassifier
from sklearn.datasets import make_moons
from sklearn.tree import export_graphviz

Xm, ym = make_moons(n_samples=100, noise=0.25, random_state=53)

deep_tree_clf1 = DecisionTreeClassifier(random_state=42)
deep_tree_clf2 = DecisionTreeClassifier(min_samples_leaf=4, random_state=42)
deep_tree_clf1.fit(Xm, ym)
deep_tree_clf2.fit(Xm, ym)


def plot_decision_boundary(clf, X, y, axes=[0, 7.5, 0, 3], iris=True, legend=False, plot_training=
    x1s = np.linspace(axes[0], axes[1], 100)
    x2s = np.linspace(axes[2], axes[3], 100)
    x1, x2 = np.meshgrid(x1s, x2s)
    X_new = np.c_[x1.ravel(), x2.ravel()]
    y_pred = clf.predict(X_new).reshape(x1.shape)
    custom_cmap = ListedColormap(['#fafab0','#9898ff','#a0faa0'])
    plt.contourf(x1, x2, y_pred, alpha=0.3, cmap=custom_cmap)
    if not iris:
        custom_cmap2 = ListedColormap(['#7d7d58','#4c4c7f','#507d50'])
        plt.contour(x1, x2, y_pred, cmap=custom_cmap2, alpha=0.8)
    if plot_training:
        plt.plot(X[:, 0][y==0], X[:, 1][y==0], "yo", label="Iris-Setosa")
```

```
            plt.plot(X[:, 0][y==1], X[:, 1][y==1], "bs", label="Iris-Versicolor")
            plt.plot(X[:, 0][y==2], X[:, 1][y==2], "g^", label="Iris-Virginica")
            plt.axis(axes)
        if iris:
            plt.xlabel("Petal length", fontsize=14)
            plt.ylabel("Petal width", fontsize=14)
        else:
            plt.xlabel(r"$x_1$", fontsize=18)
            plt.ylabel(r"$x_2$", fontsize=18, rotation=0)
        if legend:
            plt.legend(loc="lower right", fontsize=14)
    plt.figure(figsize=(11, 4))
    plt.subplot(121)
    plot_decision_boundary(deep_tree_clf1, Xm, ym, axes=[-1.5, 2.5, -1, 1.5], iris=False)
    plt.title("No restrictions", fontsize=16)
    plt.subplot(122)
    plot_decision_boundary(deep_tree_clf2, Xm, ym, axes=[-1.5, 2.5, -1, 1.5], iris=False)
    plt.title("min_samples_leaf = {}".format(deep_tree_clf2.min_samples_leaf), fontsize=14)
    plt.show()
```

## Playing around with regions

```
np.random.seed(6)
Xs = np.random.rand(100, 2) - 0.5
ys = (Xs[:, 0] > 0).astype(np.float32) * 2

angle = np.pi/4
rotation_matrix = np.array([[np.cos(angle), -np.sin(angle)], [np.sin(angle), np.cos(angle)]])
Xsr = Xs.dot(rotation_matrix)

tree_clf_s = DecisionTreeClassifier(random_state=42)
tree_clf_s.fit(Xs, ys)
tree_clf_sr = DecisionTreeClassifier(random_state=42)
tree_clf_sr.fit(Xsr, ys)

plt.figure(figsize=(11, 4))
plt.subplot(121)
plot_decision_boundary(tree_clf_s, Xs, ys, axes=[-0.7, 0.7, -0.7, 0.7], iris=False)
plt.subplot(122)
plot_decision_boundary(tree_clf_sr, Xsr, ys, axes=[-0.7, 0.7, -0.7, 0.7], iris=False)

plt.show()
```

## Regression trees

```
# Quadratic training set + noise
np.random.seed(42)
m = 200
X = np.random.rand(m, 1)
y = 4 * (X - 0.5) ** 2
y = y + np.random.randn(m, 1) / 10

from sklearn.tree import DecisionTreeRegressor

tree_reg = DecisionTreeRegressor(max_depth=2, random_state=42)
tree_reg.fit(X, y)
```

## Final regressor code

```
from sklearn.tree import DecisionTreeRegressor

tree_reg1 = DecisionTreeRegressor(random_state=42, max_depth=2)
tree_reg2 = DecisionTreeRegressor(random_state=42, max_depth=3)
tree_reg1.fit(X, y)
tree_reg2.fit(X, y)

def plot_regression_predictions(tree_reg, X, y, axes=[0, 1, -0.2, 1], ylabel="$y$"):
    x1 = np.linspace(axes[0], axes[1], 500).reshape(-1, 1)
    y_pred = tree_reg.predict(x1)
    plt.axis(axes)
    plt.xlabel("$x_1$", fontsize=18)
    if ylabel:
        plt.ylabel(ylabel, fontsize=18, rotation=0)
    plt.plot(X, y, "b.")
    plt.plot(x1, y_pred, "r.-", linewidth=2, label=r"$\hat{y}$")

plt.figure(figsize=(11, 4))
plt.subplot(121)
plot_regression_predictions(tree_reg1, X, y)
for split, style in ((0.1973, "k-"), (0.0917, "k--"), (0.7718, "k--")):
    plt.plot([split, split], [-0.2, 1], style, linewidth=2)
plt.text(0.21, 0.65, "Depth=0", fontsize=15)
plt.text(0.01, 0.2, "Depth=1", fontsize=13)
plt.text(0.65, 0.8, "Depth=1", fontsize=13)
plt.legend(loc="upper center", fontsize=18)
plt.title("max_depth=2", fontsize=14)

plt.subplot(122)
plot_regression_predictions(tree_reg2, X, y, ylabel=None)
for split, style in ((0.1973, "k-"), (0.0917, "k--"), (0.7718, "k--")):
    plt.plot([split, split], [-0.2, 1], style, linewidth=2)
for split in (0.0458, 0.1298, 0.2873, 0.9040):
    plt.plot([split, split], [-0.2, 1], "k:", linewidth=1)
plt.text(0.3, 0.5, "Depth=2", fontsize=13)
plt.title("max_depth=3", fontsize=14)

plt.show()

tree_reg1 = DecisionTreeRegressor(random_state=42)
tree_reg2 = DecisionTreeRegressor(random_state=42, min_samples_leaf=10)
tree_reg1.fit(X, y)
tree_reg2.fit(X, y)

x1 = np.linspace(0, 1, 500).reshape(-1, 1)
y_pred1 = tree_reg1.predict(x1)
y_pred2 = tree_reg2.predict(x1)

plt.figure(figsize=(11, 4))

plt.subplot(121)
plt.plot(X, y, "b.")
plt.plot(x1, y_pred1, "r.-", linewidth=2, label=r"$\hat{y}$")
plt.axis([0, 1, -0.2, 1.1])
plt.xlabel("$x_1$", fontsize=18)
plt.ylabel("$y$", fontsize=18, rotation=0)
plt.legend(loc="upper center", fontsize=18)
plt.title("No restrictions", fontsize=14)
```

```
plt.subplot(122)
plt.plot(X, y, "b.")
plt.plot(x1, y_pred2, "r.-", linewidth=2, label=r"$\hat{y}$")
plt.axis([0, 1, -0.2, 1.1])
plt.xlabel("$x_1$", fontsize=18)
plt.title("min_samples_leaf={}".format(tree_reg2.min_samples_leaf), fontsize=14)

plt.show()
```

## Pros and cons of trees, pros

- White box, easy to interpret model. Some people believe that decision trees more closely mirror human decision-making than do the regression and classification approaches discussed earlier (think of support vector machines)
- Trees are very easy to explain to people. In fact, they are even easier to explain than linear regression!
- No feature normalization needed
- Tree models can handle both continuous and categorical data (Classification and Regression Trees)
- Can model nonlinear relationships
- Can model interactions between the different descriptive features
- Trees can be displayed graphically, and are easily interpreted even by a non-expert (especially if they are small)

## Disadvantages

- Unfortunately, trees generally do not have the same level of predictive accuracy as some of the other regression and classification approaches
- If continuous features are used the tree may become quite large and hence less interpretable
- Decision trees are prone to overfit the training data and hence do not well generalize the data if no stopping criteria or improvements like pruning, boosting or bagging are implemented
- Small changes in the data may lead to a completely different tree. This issue can be addressed by using ensemble methods like bagging, boosting or random forests
- Unbalanced datasets where some target feature values occur much more frequently than others may lead to biased trees since the frequently occurring feature values are preferred over the less frequently occurring ones.

- If the number of features is relatively large (high dimensional) and the number of instances is relatively low, the tree might overfit the data
- Features with many levels may be preferred over features with less levels since for them it is *more easy* to split the dataset such that the sub datasets only contain pure target feature values. This issue can be addressed by preferring for instance the information gain ratio as splitting criteria over information gain

However, by aggregating many decision trees, using methods like bagging, random forests, and boosting, the predictive performance of trees can be substantially improved.