Nonparametric Models: kNN, Decision Trees and Local Regression

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Author: Omar Ghattas

Introduction ¶

In this lab we will look at nonparametric modelling, which is an alternative to parametric modelling that has been our focus in the last few weeks. We'll work through kNN, Linear Smoothing and Decision Trees in detail. We will implement these algorithms from scratch, and we'll also explore existing implementations in sklearn. We will also work with Pandas a bit more heavily to see how it can be used for data analysis.

Nonparametric vs. Parametric Models

Surprisingly, it is difficult to have a good definition for nonparametric models and there is often disagreement about which models are nonparametric rather than parametric. Here we will try to build intuition for the differences between the two types of modelling regimes. First, let's recall our data generating process (DGP) set-up from tutorials, we assume that the data are generated independently according to the following process:

$$y = f(x) + \epsilon$$
,

where ϵ is some random noise, and f is the true data function that we wish to estimate.

Parametric Modelling

In parametric modelling, we place a strong assumption on what kind of function f really is, and we assume that this structure is known when we do our estimation. For example, in linear regression, we assume that $f(x) = w^T x$, i.e. that f is a linear function parameterized by a vector w. We then proceed by estimating w from the data. Parametric models tend to have a relatively small number of parameters. They are also usually high bias because of the strong assumptions placed on the underlying model.

Nonparametric Modelling

In contrast to parametric models, here we place little to no assumptions on the underlying function f. Nonparametric models (the number of parameters) often grow as the size of the observed data grows.

Regression \& Classification

There are Nonparametric versions of both regression and classification models, and we will explore many of them throughout the course. Here is a short list to keep in mind:

Parametric:

- 1. Linear Regression
- 2. Ridge Regression
- 3. Lasso Regression
- 4. Perceptron (classification)
- 5. Logistic Regression (both regression and classification)

Nonparametric:

- 1. Decision Trees (both regression and classification)
- 2. k-Nearest Neighbours (kNN) (both regression and classification)
- 3. Local Linear Regression
- 4. Support Vector Machines (both regression and classification)
- 5. Random Forests (both regression and classification)

kNN

We begin with the simplest nonparametric model, kNN, and we will explore both kNN classification and kNN regression. Both classification and regression variants require an understanding of the k-neighbour function: $\mathcal{N}_k(x)$. The k-neighbour function simply returns the k points in the dataset that are nearest to the input x. We can define 'nearest' here quite broadly, and it is up to the modeler to come up with a distance function that they would like to use; the most common choice is the Euclidean distance $\|\cdot\|_2$.

Toy Regression Example

Let's assume we have data X = [-1, 0, 1, 2, 3, 4], y = [0.5, 0.25, 1, 0.2, 0.8, 3], and we choose k = 3. Given an input point x = 0.25, we have:

$$\mathcal{N}_3(0.25) = \{-1, 0, 1\}.$$

Now that we have identified the 3-NN of x, we need to return a prediction for it. The idea in kNN is just to use an average over the neighbours, so:

$$\hat{y}(0.25) = rac{1}{3}[0.5 + 0.25 + 1] pprox 0.58$$

is our prediction for this input. More rigorously, an average over the k-nearest neighbours can be written:

$$egin{aligned} \hat{y}(x) &= rac{1}{k} \sum_{i \in \mathcal{N}_k(x)} Y_i \ &= \sum_{i=1}^n rac{1}{k} \mathbf{1}\{X_i ext{ is a kNN of } x\}Y_i. \end{aligned}$$

Toy Classification Example

The kNN classifier works in the same was as kNN regression, except that instead of averaging, we take a majority vote of the class labels. This works for multi-class classification as well.

Note

The examples we showed here use numerical data, as in X is comprised of numbers. However, kNN works whenever you have a way of measuring distance between objects. For example, if X represented words in the alphabet that you were trying to classify into given classes, you could use kNN with Levenshtein (edit) distance.

In this lab we'll work with some of the same code used in Lab2 for sampling. For regression problems we'll simulate toy data from the model:

$$y=f(x)+\epsilon, \qquad f(x)=0.3\cos(x)+0.4\ln(10x), \quad \epsilon\sim N(0,\sigma^2), \quad \sigma=0.5.$$

The following code loads in the required packages and defines the f sampler function used in Lab2.

In [6]:

```
import numpy as np
import matplotlib.pyplot as plt

def f_sampler(f, n=100, sigma=0.5, seed=123):
    np.random.seed(seed)

# sample points from function f with Gaussian noise (0,sigma**2)
    xvals = np.random.uniform(low=1, high=10, size=n)
    yvals = f(xvals) + sigma * np.random.normal(0,1,size=n)

# build dataset D
    D = np.zeros(shape=(n, 2))
    D[:,0] = xvals; D[:,1] = yvals;

return D
```

Exercise:

In this exercise, we will write code to implement kNN regression from scratch. Generate data using the following code:

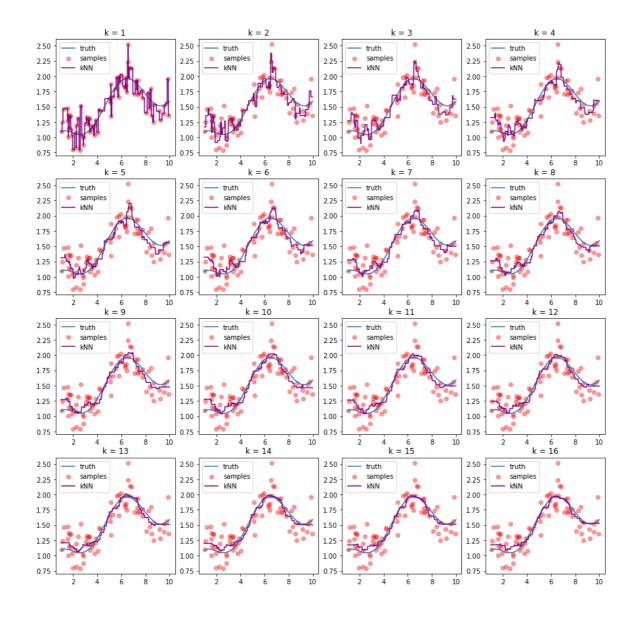
```
f = lambda x: 0.3 * np.cos(x) + 0.4 * np.log(10*x)
fsamples = f_sampler(f, 80, sigma=0.2, seed=100)
X = fsamples[:, 0]
y = fsamples[:, 1]
```

Write a function kNNRegression(x, X, y, k) that implements kNN regression (i.e., predicts a value for x where x is potentially an array of inputs based on data X, y) using k neighbours and using euclidean distance. Run the algorithm with $k=1,\ldots,16$ and p=2 and plot each fit on a 4×4 grid plot, one plot for each k. Be sure to plot the original function and the samples on the same plot as well.

Hint: the function np.argsort might be useful here.

In [14]:

```
#### Solution
f = lambda x: 0.3 * np.cos(x) + 0.4 * np.log(10*x)
fsamples = f_sampler(f, 80, sigma=0.2, seed=120)
X = fsamples[:, 0]
y = fsamples[:, 1]
def kNNRegression_(x0, X, y, k):
    # given single point x0, returns knn prediction
    # indices of k nearest neighbours of x0
    kNearestIdx = np.argsort(np.sqrt((X-x0)**2))[:k]
    # y values of k nearest neighbours of x0
    kNearesty = y[kNearestIdx]
    return kNearesty.mean()
def kNNRegression(x, X, y, k):
    # generalize kNNRegression_ to work on array of inputs
    return np.apply_along_axis(kNNRegression_, 1, x.reshape(-1,1), X, y, k)
# generate plot
fig, axes = plt.subplots(4,4,figsize=(15,15))
xx = np.linspace(1,10,1000)
for i, ax in enumerate(axes.flat):
    ax.plot(xx, f(xx), label="truth")
    ax.scatter(*fsamples.T, color="red", label="samples", alpha=0.4)
    ax.plot(xx, kNNRegression(xx, X, y, k=i+1), color='purple', label='kNN')
    ax.set_title(f"k = {i+1}")
    ax.legend()
plt.show()
```



kNN with sklearn

Of course, sklearn has existing implementations of both kNN classification and kNN regression. These can be found by running:

from sklearn.neighbors import KNeighborsClassifier, KNeighborsRegressor

Their usage follows the same standard sklearn approach we have seen in previous labs.

Linear Smoothing

From the previous exercise, you will most likely notice that the fitted regression function using kNN is quite jagged, especially for smaller values of k. To understand this behaviour, it helps to look at the specific form of kNN predictions which we wrote down earlier:

$$\hat{y}(x) = \sum_{i=1}^n rac{1}{k} \mathbf{1}\{X_i ext{ is a kNN of } x\}Y_i.$$

Note that this is of the form: $\hat{y}(x) = \sum_{i=1}^n w_i(x) Y_i$, so we can think of kNN as producing a weighted average of the responses Y_i , where the weights are chosen based on the given x. The 'weighting' scheme in kNN is rather crude; it looks at the closest k elements and cuts out the rest, resulting in a jagged fit. We can improve the kNN regression model by incorporating other weight functions that will induce a smoother fit this is the idea behind Linear smoothing, and we use special functions called kernels to define the weighting schemes. Specifically, we first define some common kernel functions:

- 1. Box-car Kernel: $K(u)=\mathbf{1}\{|u|\leq 1/2\}$ 2. Gaussian Kernel: $K(u)=rac{1}{\sqrt{2\pi}}\mathrm{exp}(-u^2/2)$
- 3. Epanechnikov Kernel: $K(u) = \frac{3}{4}(1-u^2)\mathbf{1}\{|u| \leq 1\}$

We then use a chosen kernel to construct a linear smoother which is defined by:

$$\hat{y}(x) = \sum_{i=1}^n rac{K\left(rac{\|x-X_i\|_2}{h}
ight)}{\sum_{j=1}^n K\left(rac{\|x-X_j\|_2}{h}
ight)} Y_i.$$

In words, the i-th weight (the weight assigned to the i-th response Y_i) is the kernel function evaluated at the distance of X_i from the input point x, and divided by a normalizing term to ensure that the weight add up to 1. The parameter h is called the bandwidth, and plays a similar role as k in kNN regression. Larger values of h>0 means we incorporate more information from points that are further away.

Exercise:

Implement the three kernels defined above.

In [16]:

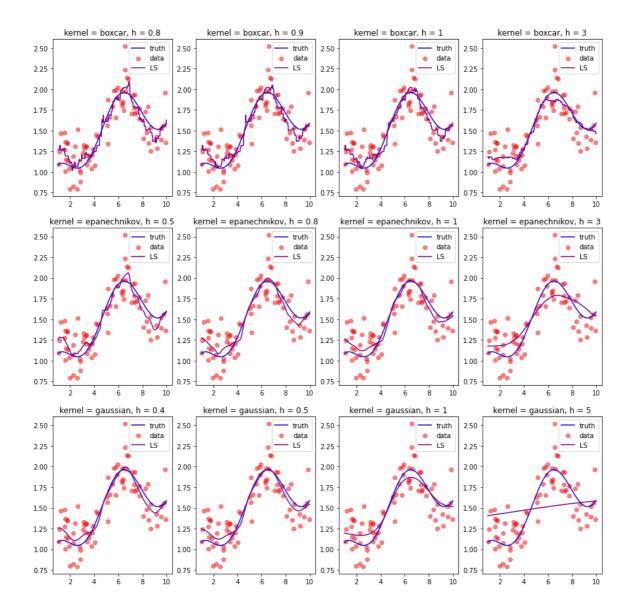
```
#### Solution
def boxcar(u):
    cond = abs(u) <= 0.5
    return 1 * cond
def gaussian(u):
    t1 = 1/np.sqrt(2 * np.pi)
    return t1 * np.exp(-0.5 * u**2)
def epanechnikov(u):
    cond = abs(u) <= 1
    return cond * 0.75 * (1-u**2)
```

Exercise:

Write a function LinearSmoother(X, y, kernel, h) that implements LinearSmoother using the data from the previous kNN regression exercise. Demonstrate your code by plotting your fitted functions for various bandwidth values and the three kernels defined above. Use the bandwidths [0.8, 0.9, 1, 3] for the boxcar kernel, [0.5, 0.8, 1, 3] for the Epanechnikov kernel and [0.4, 0.5, 1, 5] for the Gaussian kernel. What do you notice happens to the fits as you vary the bandwidth?

In [22]:

```
#### Solution
def LS_(x0, X, y, kernel, h):
    # given single point x0, returns linear smoother prediction
    # compute K(|x-X_i|/h) terms
    K = kernel(np.sqrt((X - x0)**2)/h)
    # sum to get normalization constant for weights
    Ksum = K.sum()
    # compute weights by dividing the K terms by their sum
   weights = K/Ksum if Ksum > 0 else np.zeros_like(y)
    return weights @ y
def LinearSmoother(x, X, y, kernel, h):
    # generalize LS_ to work on array of inputs
    return np.apply_along_axis(LS_, 1, x.reshape(-1,1), X, y, kernel, h)
bandwidth_grid = {
    boxcar: [0.8, 0.9, 1, 3],
    epanechnikov: [0.5, 0.8, 1, 3],
    gaussian: [0.4, 0.5, 1, 5]
fig, axes = plt.subplots(3, 4, figsize=(15, 15))
xx = np.linspace(1, 10, 1000)
for i, (kern, h_grid) in enumerate(bandwidth_grid.items()):
    for j, h in enumerate(h_grid):
        axes[i,j].plot(xx, f(xx), label="truth", color="blue")
        axes[i,j].scatter(X, y, label="data", color="red", alpha=0.5)
        axes[i,j].plot(xx, LinearSmoother(xx, X, y, kern, h), label="LS", color="purpl
e")
        axes[i,j].set_title(f"kernel = {kern.__name__}, h = {h}")
        axes[i,j].legend()
plt.show()
```



Existing Implementations

Unfortunately, there are no sklearn implementations of the linear smoother, however a good implementation does exist in scipy.statsmodels.nonparametric.kernel_regression, (kernel regression, Nadaraya-Watson) are two different names commonly used for linear smoothing. You can read more about it here:

https://www.statsmodels.org/dev/generated/statsmodels.nonparametric.kernel_regression.KernelReg.html (https://www.statsmodels.org/dev/generated/statsmodels.nonparametric.kernel_regression.KernelReg.html)

The curse of dimensionality

The algorithms we have seen so far (kNN and Linear Smoothing) are quite straight forward to construct, even more so than the parametric models we have dealt with in the past. One problem that arises however is the curse of dimensionality, which is a problem that plagues much of nonparametric modelling. The problem is the following: distances break down in high dimensional spaces.

What this means is that when we are dealing with high dimensional data (such as MNIST), the distances between objects in high dimensional space are not very informative. So an image with class label '0' will have similar distance to an image with class label '8' as it does to other images in class '0'. Since kNN and LS rely on finding neighbouring points, their performance is affected negatively, to the point that they become useless.

We can demonstrate this breakdown of distances through the following simulation experiment:

The set $[0,1]^d$ consists of d-dimensional vectors with elements between 0 and 1 and is called the d-dimensional unit cube. We can generate n independent samples uniformly distributed on $[0,1]^d$ using the code: np.random.random(low=0.0, high=1.0, size=(n,d)).

The idea will be to sample n=1000 points on $[0,1]^d$ for increasing values of d. For each d, we will compute the pairwise Euclidean distances between the n points and plot a histogram. As the dimension increases, we will see that the distribution of the distances becomes more and more concentrated. This is bad because it means that all the points have similar distance to each other, and so we cannot really figure out different labels for these points.

Note: that the 2-norm has min value zero, and max value $\sqrt{2}$, so for dimension 2, the maximum 2-norm is \sqrt{d} , for dim=100, the maximum is 10, etc, which is why the x-axis range changes from plot to plot.

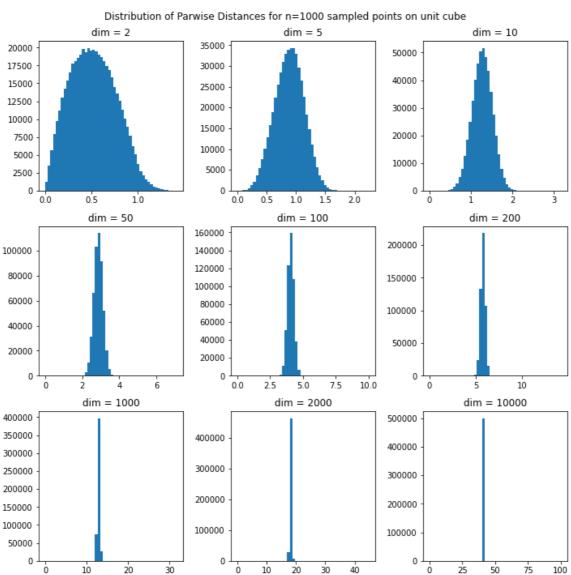
In [5]:

```
n = 1000
dims = [2, 5, 10, 50, 100, 200, 1000, 2000, 10000]
fig, axs = plt.subplots(3,3, figsize=(10,10))
for i, ax in enumerate(axs.flat):
    d = dims[i]

# randomly sample N points from [0,1]^dim
    X = np.random.uniform(low=0., high=1., size=(n, d))

# compute pairwise distances between the points
    pdists = np.array([np.linalg.norm(X[i]-X[j], ord=2) for i in range(n) for j in range(in))

# plot histogram
    ax.hist(pdists, range=[0, np.sqrt(d)], bins=50)
    ax.set_title(f"dim = {d}")
plt.suptitle(f"Distribution of Parwise Distances for n={n} sampled points on unit cube")
plt.tight_layout()
```



Decision Trees for Classification

An important nonparametric model is the decision tree, which is the building block for more complex models such as the random forest and adaptive boosting algorithms we will encounter later on in the course. Decision trees can be thought of as a large set of if-then-else statements. They are also referred to as recursive partitioning algorithms, since they repeatedly partition the input space into smaller and smaller subsets or regions. In this section we will focus on decision trees for classification, but note that they are also able to be used for regression problems.

Recursive Partitioning and visualizing classifiers

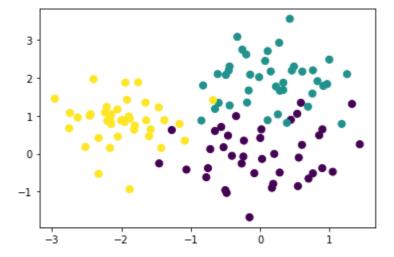
We first aim to understand decision trees as a partitioning estimator. To do so, we'll need the following helper function that allows us to visualize the classifier, and you can use it as a black box for the remainder of the lab.

In [8]:

```
# Helper function for visualising classifiers and decision surfaces
def visualize_classifier(model, X, y, ax=None, cmap='rainbow', title=None):
    # reference: Python Data Science Handbook by Jake VanderPlas
   ax = ax or plt.gca()
   # Plot the training points
   if np.any(y==-1):
       y[y==-1] = 0. # fix to get scatter c=y arg working when we use -1,1 coding
    ax.scatter(X[:, 0], X[:, 1], c=y, s=30, cmap=cmap,
                        clim=(y.min(), y.max()), zorder=3)
    ax.axis('tight')
    xlim = ax.get_xlim()
   ylim = ax.get_ylim()
    # compute predictions on grid
    xx, yy = np.meshgrid(np.linspace(*xlim, num=200),
                         np.linspace(*ylim, num=200))
    Z = model.predict(np.c [xx.ravel(), yy.ravel()]).reshape(xx.shape)
    if np.any(Z==-1): # fix to get c=y working
       Z[Z==-1] = 0
    # Create a color plot with the results
    n classes = len(np.unique(y))
    contours = ax.contourf(xx, yy, Z, alpha=0.3,
                           levels=np.arange(n_classes + 1) - 0.5,
                           cmap=cmap, zorder=1)
    ax.set(xlim=xlim, ylim=ylim)
    if title:
        ax.set_title(title)
```

The sklearn.datasets.make_blobs function gives us a quick way to create toy data for classification. In the following we'll create a 3 class classification problem

In [9]:

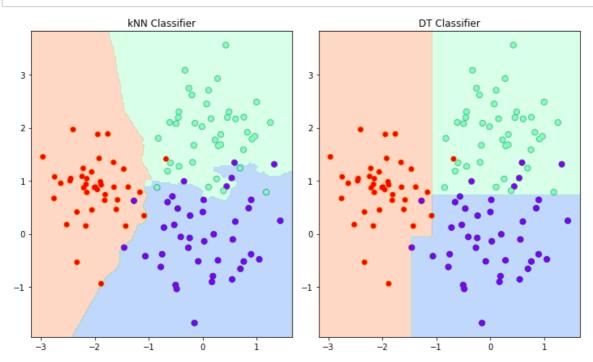


We will also use the sklearn.neighbors.KNeighborsClassifier and

sklearn.tree.DecisionTreeClassifier objects to demonstrate the visualize_classifier function. The shaded regions correspond to how the classifier would classify a point that falls in that region. Note that for the kNN classifier, the regions are quite jagged, whereas the regions for the DT are always constructed by splitting using straight lines.

In [19]:

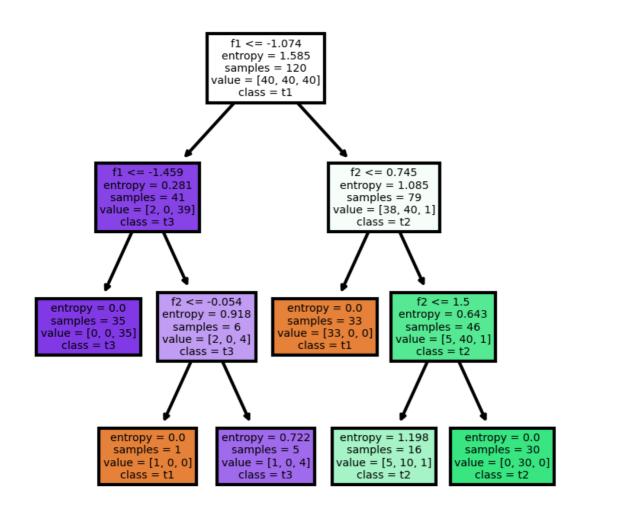
```
from sklearn.tree import DecisionTreeClassifier
from sklearn.neighbors import KNeighborsClassifier
# kNN with 5 neighbours and euclidean distance (p=2)
model0 = KNeighborsClassifier(n_neighbors=5, p=2)
# DT with max depth of 3 and entropy criterion (this is information gain from lectures/
tutorials)
model1 = DecisionTreeClassifier(max_depth=3, criterion='entropy', random_state=3)
# fit both models
model0.fit(X,y)
model1.fit(X,y)
# visualize classifiers
fig, axes = plt.subplots(1,2, figsize=(10,6))
# scatter data
axes[0].scatter(X[:, 0], X[:, 1], c=y, s=50)
axes[1].scatter(X[:, 0], X[:, 1], c=y, s=50)
# classifier plot
visualize_classifier(model0, X, y, ax=axes[0], title="kNN Classifier")
visualize_classifier(model1, X, y, ax=axes[1], title="DT Classifier")
plt.tight_layout()
plt.show()
```



Another good way to visualize a tree is to look directly at the rules it uses to perform the splits at each depth. Recall that for a classification decision tree, we pass an input down the tree and look at the majority class in the child node that it falls into to find its predicted class. In regression, we do something identical, except that instead of taking a majority, we can use an average (or weighted average) of the points in the child node (similar to kNN regression)

Note that the color of the labels correspond to the majority class at that particular point. The plot also gives us the distribution of the three classes at each node (value), and tells us the number of samples that falls into a particular node. We also can see the information gain (entropy) (see tutorials for details) for each node.

In [20]:



Exercise:

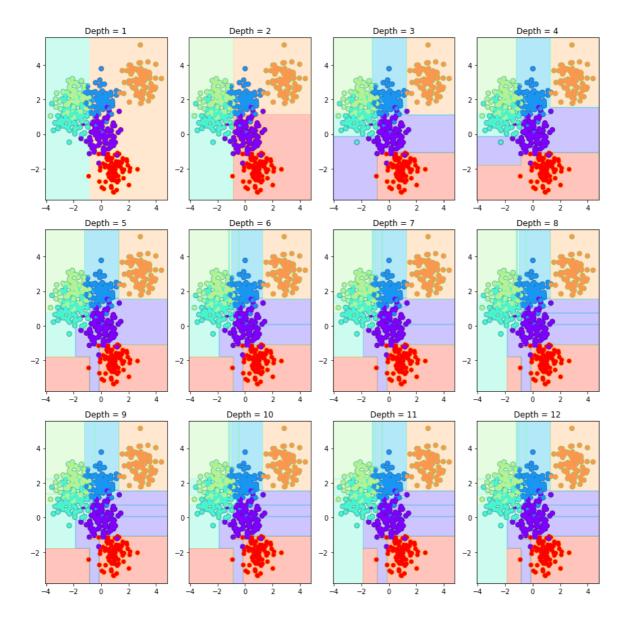
Generate data using the following code:

Then fit a decision tree (using information gain for splits) with \max_{depth} set to $1, 2, \ldots, 12$ and visualize the classifier (use a 3×4 grid). What do you observe? Why do you think decision trees are described as performing 'recursive partitioning'?

When depth=1, the tree is just a decision stump (a single if/else statement) and so it can only choose a single feature to split on (either feature 1 which we can call f1 (x axis) or f2 (y axis)). Here we see that it splits on f1, and classifies everything to the left of the split as aqua blue, and everything to the right of the split as purple, since these are the majority classes on each side. This is a partition of the 2d space into two rectangles.

When we increase the depth by 2, the tree has more flexibility (chained if/else), and can now partition the original partition. It does so in this case by splitting on f2 to isolate the red cluster. In depth 3 it partitions the previous partition. This is why we say that trees perform recursive partitioning, at each depth they simply look at the partition from the previous depth and partition it in a way to isolate new clusters. As we keep increasing the depth, the partitions become finer and finer (of course in practice, we need to trade-off the fine-ness of the partition with the risk of over fitting).

In [21]:



Extended Data Exercise

In this exercise, we'll work with the titanic.csv dataset which you should have available in the same working directory where this notebook is located. If you get stuck at any point, the first thing to do will be to google your question - when it comes to data analysis in Python it is almost impossible to remember all the different commands, and https://stackoverflow.com/ (https://stackoverflow.com/) is your best friend.

- 1. Using pandas, load in the dataset and call the dataframe df. Run df.info() to gain an understanding of the different features.
- 2. Remove the following columns 'PassengerId','Name', 'Ticket','Cabin', 'Embarked' from the data, as we won't be using them for this exercise.
- 3. Use the dropna() method to remove any missing rows.
- 1. We would like to treat all attributes as numeric, so convert the Sex feature to numeric, and code males as 0 and females as 1. Hint: a good approach is to use the df.Sex.map() method.
- 2. We will be interested in predicting Survived as a function of the remaining features. Create X,y numPy arrays to use for this problem. Be sure to also save a copy of the names of the columns. Hint: use iloc to index pandas dataframes, and use to_numpy() to convert pandas dataframes to numpy arrays.
- 3. Create train/test datasets using 70\% of your data for training.
- 4. Fit decision trees to your training dataset: do this for <code>max_depth =1,...,20</code>. For each depth, record the train and test classification error (1-accuracy). Create a plot of error against depth, and plot both the train and test errors. What do you notice?
- 5. Re-fit the model on the entire dataset with a depth 3 tree. Plot the decision tree and interpret the results.

In [22]:

```
#### Solution Q1
import pandas as pd
df = pd.read_csv('titanic.csv')
# df.info()
#### Solution Q2
cols_to_drop = [
    'PassengerId',
    'Name',
    'Ticket',
    'Cabin',
    'Embarked',
]
df = df.drop(cols_to_drop, axis=1)
#### Solution Q3
df = df.dropna()
#### Solution Q4
df.Sex = df.Sex.map(lambda x: 0 if x=='male' else 1)
#### Solution Q5
fnames = df.columns[1:].to_list()
                                             # feature names
tname = df.columns[0]
                                              # target name
X = df.iloc[:, 1:].to_numpy()
y = df.iloc[:, 0].to_numpy()
#### Solution 06
from sklearn.model_selection import train_test_split
Xtrain, Xtest, ytrain, ytest = train_test_split(X, y, test_size=0.3, shuffle=True)
#### Solution Q7
from sklearn.metrics import accuracy_score, log_loss
N = 20
train_errs = np.empty(N)
test_errs = np.empty(N)
for d in range(N):
    model = DecisionTreeClassifier(max depth=d+1, criterion='entropy')
   model.fit(Xtrain, ytrain)
    train_errs[d] = 1-accuracy_score(ytrain, model.predict(Xtrain))
    test_errs[d] = 1-accuracy_score(ytest, model.predict(Xtest))
ds = np.linspace(1,N, N)
plt.plot(ds, train_errs, color='red', label='train error')
plt.plot(ds, test_errs, color='blue', label='test error')
plt.xlabel("Depth")
plt.legend()
plt.show()
#### Solution Q8
model = DecisionTreeClassifier(max_depth=3, criterion='entropy').fit(X, y)
fig, axes = plt.subplots(1, 1, figsize = (4,4), dpi=300)
tree.plot tree(model, feature names=fnames, class names=['Died', 'Survived'], filled=Tr
```

ue)
plt.show()

