Getting started with Machine Learning (ML) and Support Vector Classifiers (SVC) - A systematic step-by-step approach

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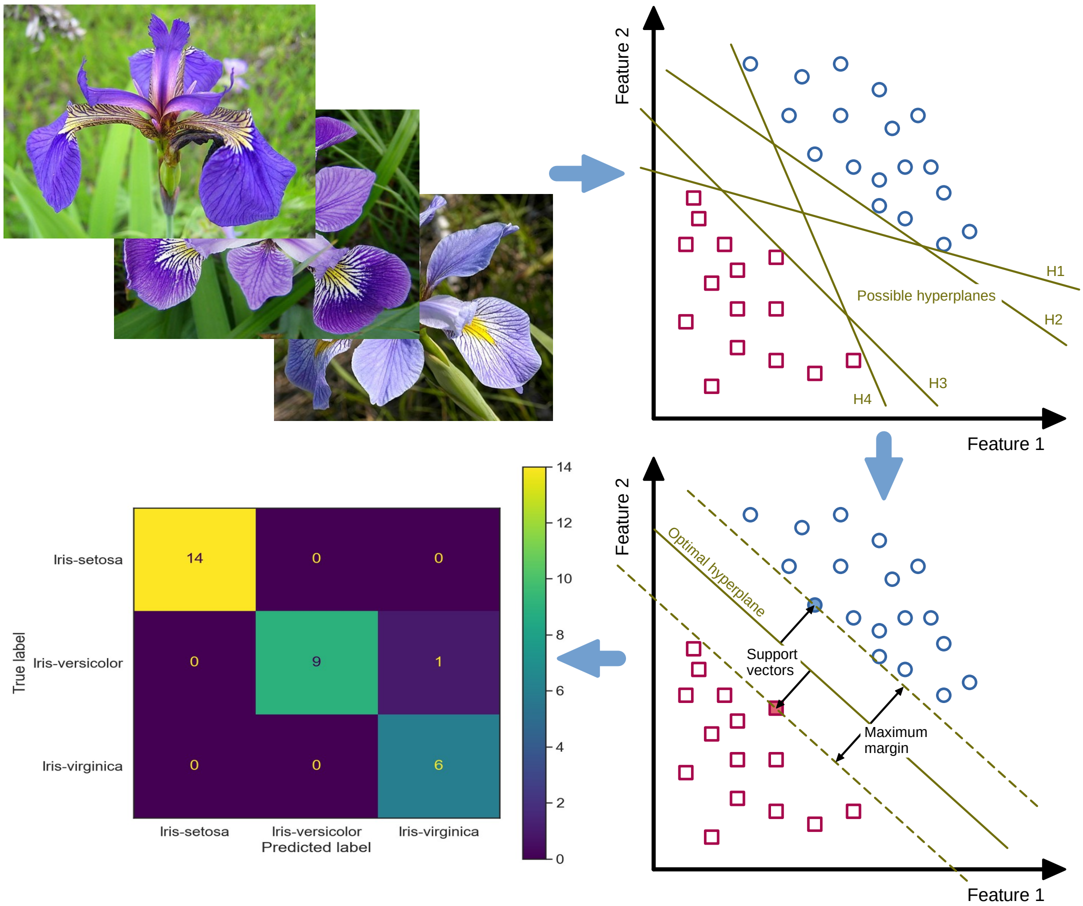

Anyone who wants to seriously deal with the hypothetical topic of our time "Artificial Intelligence (AI)" or "Machine Learning (ML)" cannot avoid dealing with the basic ML algorithms, corresponding software tools, libraries and programming systems. However, someone who opens the door for the first time to this equally very exciting as well as arbitrarily complex and, at first glance, confusing world will very quickly be overwhelmed. Here, it is a good idea to consult introductory and systematic tutorials. Therefore, this Getting Started tutorial systematically demonstrates the typical ML work process step-by-step using the very powerful and performant "Support Vector Classifier (SVC)" and the widely known and exceptionally beginner-friendly "Iris Dataset". Furthermore, the selection of the "correct" SVC kernel and its parameters are described and their effects on the classification result are shown.

Contents

1 Introduction

1.1 English introduction

In the **digitized work environment**, there is an increasing demand for **Work equipment** to be able to adapt independently and in a task-related manner to changing work situations. This **situational adaptivity** can often only be realized through the use of **Artificial Intelligence (AI)** or **Machine Learning (ML)**, depending on the degree of flexibility.

Examples of such AI applications in work environments can range from comparatively simple **voice assistance systems** (similar, for example, to Siri or Alexa from the private sphere) to partially or even **fully autonomous systems**. Such fully autonomous systems are, for example, so-called **driverless transport systems**, which are autonomously driving logistics vehicles in larger industrial plants.

In addition to the numerous very interesting advantages in terms of economic efficiency, workload reduction, etc., such fully autonomous systems are characterized by a very high level of technical complexity. This concerns both their **operating functions** (e.g. autonomous navigation through complex industrial environments with shared use of the roadways by other human-controlled vehicles) and their **safety functions** (e.g. evaluation of interlinked imaging and non-imaging safety sensors for monitoring the driving space to avoid collisions).

Very high requirements are placed on such autonomous systems and the AI algorithms used for this purpose with regard to **functional safety**. However, the requirements for safety evaluability in terms of **transparency** and **explainability** of decisions made by AI are very difficult or impossible to meet, depending on the AI algorithms applied. For example, current research projects are investigating the transparency and explainability of **deep neural networks**. Furthermore, today's AI algorithms, in terms of their **recognition rates** and thus their **reliabilities**, very often do not meet the functional safety requirements to achieve higher safety levels (e.g. Performance Level d (PLd) according to ISO 13849), even under the most convenient conditions.

An appropriate assessment or even **testing** with regard to the required functional safety according to uniform and ideally standardized criteria has numerous consequences for the future orientation and organization of technical **occupational safety and health (OSH)** in Germany and in Europe. In addition to the currently still very difficult safety-related assessability, an important point is that the previous clear separation between **placing on the market law** (see e.g. Machinery Directive) and **occupational safety and health law** (see European Framework Directive for Occupational Safety and Health and German Ordinance on Occupational Safety and Health) can no longer be continued in this way. The reason for this is that the **safety-relevant properties** of the autonomous systems will change due to new or **adapted behaviors** learned during operation.

For these reasons, especially the actors of technical occupational safety and health who will deal with the evaluation of such adaptive, autonomous systems or system components with AI algorithms in the future should familiarize themselves with the AI or ML algorithms in depth as early as possible. This is the only way to ensure that the rapid development of adaptive systems capable of learning can be accompanied by OSH and their testing authorities in a constructive, critical and technically appropriate manner. If this is omitted, it must be assumed on the basis of the experiences of recent years that the OSH system will be ruthlessly circumvented or undermined by the economic interests of globally operating software giants. This would have the consequence that serious or fatal occupational accidents are likely to occur due to inadequately designed AI-based work systems.

The safety-related evaluation of such learning-capable systems requires a deeper technical entry into the world of **Artificial Intelligence (AI)** or **Machine Learning (ML)**. For this purpose, it is necessary to deal with the basic operation of typical ML algorithms, corresponding software tools, libraries and programming systems.

However, someone who opens the door for the first time to this equally very exciting as well as arbitrarily complex and, at first glance, confusing world will very quickly be overwhelmed. In addition to reading general technical literature, it is advisable to consult introductory and systematic tutorials.

This Getting Started tutorial has exactly this goal, demonstrating systematically and step-by-step the typical ML workflow using the very powerful **Support Vector Classifier (SVC)** as an example.

This tutorial will be presented in the context of a workshop at the **Conference "Artificial Intelligence"**, hosted by the German Social Accident Insurance (DGUV), probably in November 2022 in Dresden. The workshop addresses interested ML novices in the technical occupational safety and health of the social accident insurance institutions.

Besides the **deep neural networks**, which are very present in the media, there is a very rich diversity of other very powerful ML algorithms - suitable for the particular use case. For a more generally comprehensible introduction, the SVC algorithm was deliberately chosen for the target audience of the workshop. Its operating principles are easy to convey to ML novices as well as in the time frame given for the workshop - quite in contrast to the entry into the world of deep neural networks.

The following main sections will demonstrate the typical ML workflow step-by-step. In **Step 0**, specific guidance is provided for selecting hardware and software suitable for machine learning. To allow an ML novice to first familiarize themselves with the ML algorithms, tools, libraries, and programming systems, the ready-made and very beginner-friendly **Iris dataset** is involved in **Step 1**. Only after a comprehensive acquaintance with the application of ML tools would it make sense to examine one's own environment for ML-suitable applications and to obtain suitable datasets from them. However, this is beyond the scope of this introductory tutorial.

One of the most important steps in the entire ML process is **Step 2**, in which the dataset included in Step 1 is examined using typical data analysis tools. In addition to exploring the **data structure** and **internal correlations** in the dataset, errors such as gaps, duplications, or obvious misentries must also be found and corrected where possible. This is enormously important so that the classification can later provide plausible results.

After exploring the dataset, in **step 3** one has to decide on a specific ML algorithm based on certain selection criteria. Among other ML algorithms suitable for the Iris dataset (such as the decision-tree-based **random-forests classifier**), the reasoned choice here in the tutorial falls on the **support vector classifier (SVC)**. A dedicated SVC model is now being implemented.

In **step 4** the dataset is prepared for the actual classification by SVC. Depending on the selected ML algorithm as well as the data structure, it may be necessary to prepare the data before training (e.g., by standardization, normalization, or binarization based on thresholds). After splitting the dataset into a training and test dataset, the SVC model is trained with the training dataset in **step 5**. Subsequently, classification predictions are made with the trained SVC model based on the test data. In **step 6**, the quality of the classification result is evaluated using known **metrics** such as the **confusion matrix**.

Since the classification in step 5 was initially performed with standard parameters (so-called **hyper-parameters**), their meaning is explained in **step 7** and then their effect on the classification result is demonstrated by manually varying the individual hyper-parameters.

In the final **Step 8**, two approaches to systematic hyper-parameter search are presented: **Grid Search** and **Randomized Search**. While the former exhaustively considers all parameter combinations for given values, the latter selects a number of candidates from a parameter space with a particular random distribution.

1.2 German introduction

Von den **Arbeitsmitteln** in der **digitalisierten Arbeitswelt** wird immer stärker gefordert, dass sie sich selbstständig und aufgabenbezogen an sich ändernde Arbeitssituationen anpassen können. Diese **situative Adaptivität** kann je nach Stärke des Flexibilisierungsgrades oft nur durch Anwendung von **Künstlicher Intelligenz (KI)** bzw. **Maschinellem Lernen (ML)** realisiert werden.

Beispiele für solche KI-Anwendungen in der Arbeitswelt reichen von vergleichsweise einfachen **Sprachassistenzsystemen** (ähnlich z. B. Siri oder Alexa aus dem privaten Umfeld) bis hin zu teil- oder gar **vollautonomen Systemen**. Solche vollautonomen Systeme sind beispielsweise sog. **fahrerlose Transportsysteme**, bei denen es sich um autonom fahrende Logistikfahrzeuge in größeren Industrieanlagen handelt.

Neben den vielen sehr interessanten Vorteilen bzgl. Wirtschaftlichkeit, Arbeitserleichterung usw. kennzeichnet solche vollautonomen Systeme eine sehr hohe technische Komplexität. Diese betrifft sowohl ihre **Betriebsfunktionen** (z. B. autonome Navigation durch komplexe industrielle Umgebungen bei gemeinsamer Nutzung der Fahrwege durch andere menschlich gesteuerte Fahrzeuge) als auch ihre **Sicherheitsfunktionen** (z. B. Auswertung miteinander verknüpfter bildgebender und nicht-bildgebender Sicherheitssensorik zur Überwachung des Fahrraums zur Kollisionsvermeidung).

An solche autonomen Systeme und die hierfür eingesetzten KI-Algorithmen werden sehr hohe Anforderungen hinsichtlich der **funktionalen Sicherheit** gestellt. Jedoch sind die Anforderungen für eine sicherheitstechnische Bewertbarkeit bezüglich der **Transparenz** und **Erklärbarkeit** der durch KI getroffenen Entscheidungen je nach verwendeten KI-Algorithmen sehr schwer bis unmöglich erreichbar. Beispielsweise werden durch aktuell laufende Forschungsprojekte die Transparenz und Erklärbarkeit von **tiefen neuronalen Netzen** untersucht. Weiterhin erfüllen heutige KI-Algorithmen hinsichtlich ihrer **Erkennungsraten** und damit ihrer **Zuverlässigkeiten** selbst unter günstigsten Bedingungen sehr oft nicht die Anforderungen an die funktionale Sicherheit, um höhere Safety-Level (z. B. Performance Level d (PLd) nach ISO 13849) zu erreichen.

Eine hinsichtlich der geforderten funktionalen Sicherheit angemessene Bewertung oder gar **Prüfung** nach einheitlichen und idealerweise genormten Maßstäben hat viele Konsequenzen für die zukünftige Ausrichtung und Gestaltung des **technischen Arbeitsschutzes** in Deutschland und in Europa. Neben der derzeit noch sehr schwierigen sicherheitstechnischen Bewertbarkeit von KI-Algorithmen ist ein wichtiger Punkt, dass die bisherige klare Trennung zwischen **Inverkehrbringensrecht** (siehe z. B. Maschinenrichtlinie) und **betrieblichem Arbeitsschutzrecht** (siehe Arbeitsschutz-Rahmenrichtlinie und Betriebssicherheitsverordnung) so nicht mehr aufrechterhalten werden kann. Grund hierfür ist, dass sich auch die **sicherheitsrelevanten Eigenschaften** der autonomen Systeme durch während des Betriebs erlernte, neue oder **angepasste Verhaltensweisen** verändern werden.

Aus diesen Gründen sollten sich insbesondere die Akteure des technischen Arbeitsschutzes, die sich zukünftig mit der Prüfung solcher lernfähigen, autonomen Systeme oder Systemkomponenten mit KI-Algorithmen befassen werden, möglichst frühzeitig mit den KI- bzw. ML-Algorithmen vertieft auseinandersetzen. Nur dadurch lässt sich erreichen, dass die stürmische Entwicklung lernfähiger, adaptiver Systeme durch den Arbeitsschutz und dessen Prüfinstitute konstruktiv, kritisch und fachlich angemessen begleitet werden kann. Wird dies versäumt, muss aufgrund der Erfahrungen der vergangenen Jahre davon ausgegangen werden, dass das Arbeitsschutzsystem durch die wirtschaftlichen Interessen global agierender Softwaregiganten skrupellos umgangen oder ausgehebelt werden wird. Dies hätte die Folge, dass schwere oder tödliche Arbeitsunfälle wegen unzulänglich gestalteter KI-basierter Arbeitssysteme wahrscheinlich werden.

Allerdings erfordert die sicherheitstechnische Bewertung solcher lernfähigen Systeme einen tiefer gehenden fachlichen Einstieg in die Welt von **Künstlicher Intelligenz (KI)** bzw. **Maschinellem Lernen (ML)**. Hierzu muss sich mit den grundlegenden Funktionsweisen typischer ML-Algorithmen, entsprechenden Software-Werkzeugen, Bibliotheken und Programmiersystemen auseinander gesetzt werden.

Wer jedoch zum ersten Mal die Tür zu dieser ebenso spannenden wie beliebig komplexen und auf den ersten Blick verwirrenden Welt öffnet, wird sehr schnell überfordert sein. Hier empfiehlt es sich neben dem Lesen allgemeiner Fachliteratur, einführende und systematische Anleitungen zu Rate zu ziehen.

Genau dieses Ziel verfolgt das vorliegende Getting-Started-Tutorial, indem systematisch und Schritt-für-Schritt der typische ML-Arbeitsablauf am Beispiel des sehr leistungsfähigen **Support Vector Classifier (SVC)** demonstriert wird.

Dieses Tutorial wird im Rahmen eines Workshops auf der **Fachtagung "Künstliche Intelligenz"**, ausgerichtet durch die Deutsche Gesetzliche Unfallversicherung (DGUV), voraussichtlich im November 2022 in Dresden vorgestellt. Der Workshop richtet sich an interessierte ML-Neulinge im technischen Arbeitsschutz der gesetzlichen Unfallversicherungsträger.

Neben den medial sehr präsenten **tiefen neuronalen Netzen** gibt es eine sehr reichhaltige Auswahl anderer sehr leistungsfähiger ML-Algorithmen - passend für den jeweiligen Anwendungsfall. Für einen allgemein verständlicheren Einstieg wurde für die Zielgruppe des Workshops der SVC-Algorithmus bewusst gewählt. Dessen Arbeitsweise ist sowohl für ML-Neulinge als auch in dem für den Workshop vorgegebenen Zeitrahmen leicht vermittelbar - ganz im Gegensatz zum Einstieg in die Welt der tiefen neuronalen Netze.

Die folgenden Hauptabschnitte demonstrieren den typischen ML-Arbeitsablauf Schritt-für-Schritt. Im **Schritt 0** werden konkrete Hinweise für die Auswahl der für das maschinelle Lernen geeigneten Hardware und Software gegeben. Damit sich ein ML-Neuling zunächst mit den ML-Algorithmen, Werkzeugen, Bibliotheken und Programmiersystemen vertraut machen kann, wird im **Schritt 1** der fertige und sehr einsteigerfreundliche **Iris-Datensatz** hinzugezogen. Erst nach einer umfassenden Einarbeitung in die Anwendung der ML-Werkzeuge wäre es sinnvoll, die eigene Umgebung auf ML-taugliche Anwendungen hin zu untersuchen und daraus geeignete Datensätze zu gewinnen. Dies geht jedoch über den Rahmen dieses einführenden Tutorials hinaus.

Mit der wichtigste Schritt im gesamten ML-Prozess ist **Schritt 2**, in dem der in Schritt 1 einbezogene Datensatz mit Hilfe typischer Datenanalyse-Werkzeuge untersucht wird. Neben der Erkundung der **Datenstruktur** sowie **innerer Zusammenhänge** im Datensatz müssen auch Fehler wie z. B. Lücken, Dopplungen oder offensichtliche Fehleingaben gefunden und nach Möglichkeit behoben werden. Dies ist enorm wichtig, damit die Klassifikation später plausible Ergebnisse liefern kann.

Nach der Erkundung des Datensatzes muss man sich im **Schritt 3** anhand bestimmter Auswahlkriterien für einen konkreten ML-Algorithmus entscheiden. Neben anderen für den Iris-Datensatz passenden ML-Algorithmen (wie z. B. der entscheidungsbaum-basierte **Random-forests-Classifier**) fällt die begründete Auswahl hier im Tutorial auf den **Support-Vector-Classifier (SVC)**. Ein entsprechendes SVC-Modell wird nun implementiert.

Im **Schritt 4** wird der Datensatz für die eigentliche Klassifikation per SVC vorbereitet. Je nach gewähltem ML-Algorithmus sowie der Datenstruktur kann es erforderlich sein, dass die Daten vor dem Training aufbereitet werden müssen (z. B. durch Standardisierung, Normalisierung oder Binärisierung anhand von Schwellwerten). Nach der Aufteilung des Datensatzes in einen Trainings- und Testdatensatz, wird das SVC-Modell im **Schritt 5** mit dem Trainingsdatensatz trainiert. Anschließend werden mit dem trainierten SVC-Modell anhand der Testdaten Klassifikationsvorhersagen getroffen. Im **Schritt 6** wird die Güte des Klassifikationsergebnisses anhand bekannter **Metriken** wie z. B. der **Konfusionsmatrix** evaluiert.

Da die Klassifikation im Schritt 5 zunächst mit Standard-Parametern (den sog. **Hyper-Parametern**) durchgeführt wurde, wird ihre Bedeutung im **Schritt 7** erklärt und danach ihr Einfluss auf das Klassifikationsergebnis durch manuelle Variation der einzelnen Hyper-Parameter demonstriert.

Im abschließenden **Schritt 8** werden zwei Ansätze zur systematischen Hyper-Parameter-Suche vorgestellt: **Grid Search** und **Randomized Search**. Während bei ersterer für gegebene Werte erschöpfend alle Parameterkombinationen betrachtet werden, wird beim zweiten Ansatz eine Anzahl von Kandidaten aus einem Parameterraum mit einer bestimmten zufälligen Verteilung ausgewählt.

1.3 Steps of the systematic ML process

The following **steps of the systematic ML process** are covered in the next main sections:

2 Load globally used libraries and set plot parameters

[1]:
```python
import time

from IPython.display import HTML

import pandas as pd
import matplotlib.pyplot as plt
from sklearn import svm, metrics
import seaborn as sns
%matplotlib inline
```

3 STEP 0: Select hardware and software suitable for ML

In this step, specific guidance is provided for selecting hardware and software suitable for machine learning.

3.1 Hardware

3.1.1 General hardware requirements

3.1.2 Desktop or server based

3.1.3 Embedded application

3.2 Software

3.2.1 General requirements to the operating system

3.2.2 Programming IDEs

R and RStudio

Python and JupyterLab

3.2.3 Packages for data analytics and libraries for ML (Python only)

`NumPy`

`Pandas`

`matplotlib` and `seaborn`

`Scikit-Learn`

`TensorFlow` The package `TensorFlow` offers, among other things, the possibility to create and train **artificial neural networks (ANN)** based on Google AI. However, the installation and application is very much beyond the scope of this beginner tutorial. Further information can be found here: `https://www.tensorflow.org`.

4 STEP 1: Acquire the ML dataset

To allow an ML novice to first familiarize themselves with the ML algorithms, tools, libraries, and programming systems, the ready-made and very beginner-friendly **Iris dataset** is involved in this step. Only after a comprehensive acquaintance with the application of ML tools would it make sense to examine one's own environment for ML-suitable applications and to obtain suitable datasets from them. However, this is beyond the scope of this introductory tutorial.

Several details, for example, on the history of the creation of the Iris dataset can be found here: Iris flower datasets.

It can be downloaded on Kaggle: Iris Flower Dataset. Furthermore, the dataset is available via Python in the machine learning package Scikit-learn, so that users can access it without having to find a special source for it.

[2]:
```
# import some data to play with
irisdata_df = pd.read_csv('./datasets/IRIS_flower_dataset_kaggle.csv')
```

5 STEP 2: Explore the ML dataset

One of the most important steps in the entire ML process is this step, in which the dataset included in Step 1 is examined using typical data analysis tools. In addition to exploring the **data structure** and **internal correlations** in the dataset, errors such as **gaps**, **duplications**, or obvious **misentries** must also be found and corrected where possible. This is enormously important so that the classification can later provide plausible results.

5.1 Goals of exploration

The objectives of the exploration of the dataset are as follows:

1. Clarify the **origins history**:
   - Where did the data come from? => Contact persons and licensing permissions?
   - Who obtained the data and with which (measurement) methods? => Did systematic errors occur during the acquisition?
   - What were they originally intended for? => Can they be used for my application?
2. Overview of the internal **structure and organisation** of the data:
   - Which columns are there? => With which methods can they be read in (e.g. import of CSV files)?
   - What do they contain for (physical) measured variables? => Which technical or physical correlations exist?
   - Which data formats or types are there? => Do they have to be converted?
   - In which value ranges do the measurement data vary? => Are normalizations necessary?
3. Identify **anomalies** in the datasets:
   - Do the data have **gaps** or **duplicates**? => Does the dataset needs to be cleaned?
   - Are there obvious erroneous entries or measurement outliers? => Does (statistical) filtering have to be carried out?
4. Avoidance of **tendencies due to bias**:
   - Are all possible classes included in the dataset and equally distributed? => Does the dataset need to be enriched with additional data for balance?
5. Find a first rough **idea of which correlations** could be in the dataset

5.2 Clarify the origins history

> The ***Iris* flower datasets** is a multivariate dataset introduced by the British statistician and biologist *Ronald Fisher* in his paper "The use of multiple measurements in taxonomic problems as an example of linear discriminant analysis" (1936). It is sometimes called *Anderson's Iris dataset* because Edgar Anderson collected the data to quantify the morphologic variation of Iris flowers of three related species (source: Iris flower dataset).

The dataset is published in Public Domain with a CC0-License.

This dataset became a typical test case for many statistical classification techniques in machine learning such as **support vector machines**.

> [..] measurements of the flowers of fifty plants each of the two species *Iris setosa* and *I. versicolor*, found **growing together in the same colony** and measured by Dr E. Anderson [..] (source: R. A. Fisher (1936). "The use of multiple measurements in taxonomic problems". Annals of Eugenics)

> [..] *Iris virginica*, differs from the two other samples in **not being taken from the same natural colony** [..] (source: ibidem)

5.3 Overview of the internal structure and organisation of the data

The dataset consists of 50 samples from each of three species of Iris (*Iris setosa*, *Iris virginica* and *Iris versicolor*), so there are 150 total samples. Four features were measured from each sample: the length and the width of the sepals and petals, in centimetres.
Here is a principle illustration of a flower with sepal and petal:

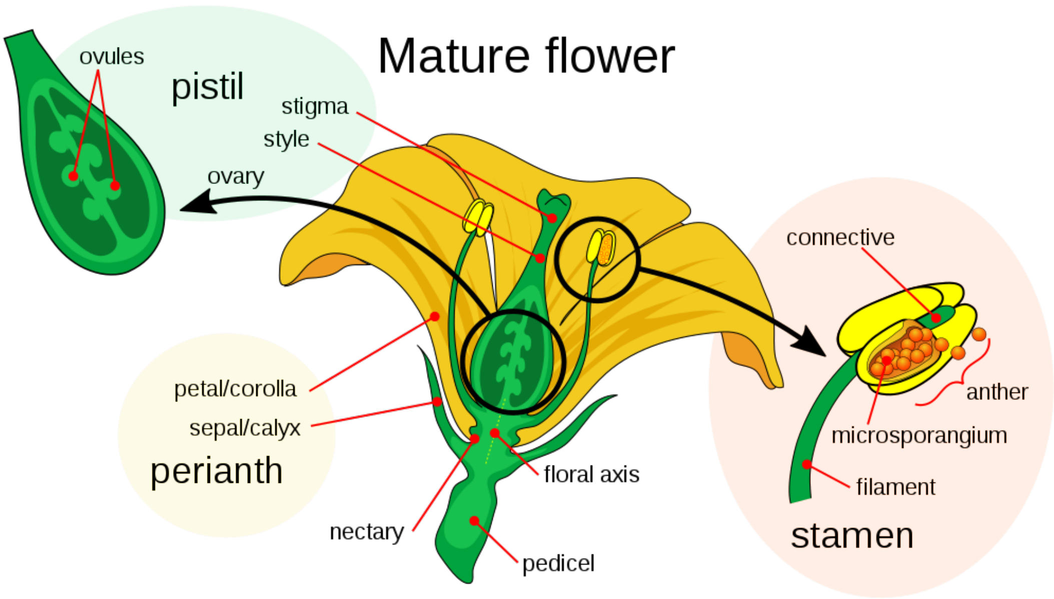

Figure 1: Principle illustration of a flower with sepal and petal (source: Mature_flower_diagram.svg, license: public domain)

Here are pictures of the three different Iris species (*Iris setosa*, *Iris virginica* and *Iris versicolor*). Given the dimensions of the flower, it will be possible to predict the class of the flower.

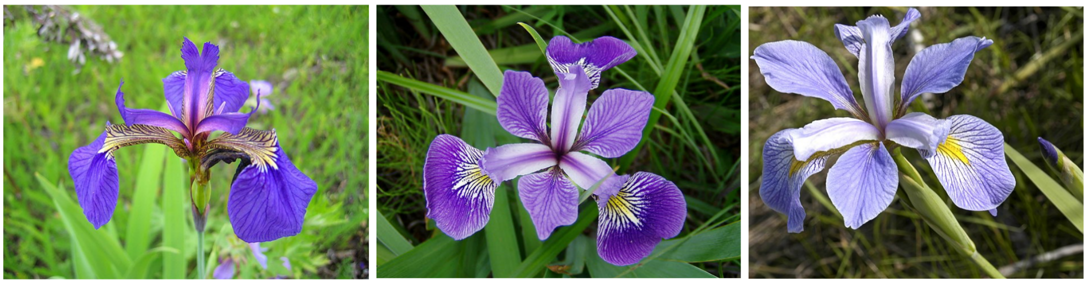

Figure 2: Left: *Iris setosa* (source: Irissetosa1.jpg, license: public domain); middle: *Iris versicolor* (source: Iris_versicolor_3.jpg, license: CC-SA 3.0); right: *Iris virginica* (source: Iris_virginica.jpg, license: CC-SA 2.0)

5.3.1 Inspect structure of dataframe

Print first or last 5 rows of dataframe:

[3]:
```
irisdata_df.head()
```

[3]:
```
   sepal_length  sepal_width  petal_length  petal_width      species
0           5.1          3.5           1.4          0.2  Iris-setosa
1           4.9          3.0           1.4          0.2  Iris-setosa
2           4.7          3.2           1.3          0.2  Iris-setosa
3           4.6          3.1           1.5          0.2  Iris-setosa
4           5.0          3.6           1.4          0.2  Iris-setosa
```

[4]:
```
irisdata_df.tail()
```

[4]:
```
     sepal_length  sepal_width  petal_length  petal_width         species
145           6.7          3.0           5.2          2.3  Iris-virginica
146           6.3          2.5           5.0          1.9  Iris-virginica
147           6.5          3.0           5.2          2.0  Iris-virginica
148           6.2          3.4           5.4          2.3  Iris-virginica
149           5.9          3.0           5.1          1.8  Iris-virginica
```

While printing a dataframe - only an abbreviated view of the dataframe is shown :(
Default setting in the pandas library makes it to display only 5 lines from head and from tail.

[5]:
```
irisdata_df
```

[5]:
```
     sepal_length  sepal_width  petal_length  petal_width         species
0             5.1          3.5           1.4          0.2     Iris-setosa
1             4.9          3.0           1.4          0.2     Iris-setosa
2             4.7          3.2           1.3          0.2     Iris-setosa
3             4.6          3.1           1.5          0.2     Iris-setosa
4             5.0          3.6           1.4          0.2     Iris-setosa
..            …            …             …            …               …
145           6.7          3.0           5.2          2.3  Iris-virginica
146           6.3          2.5           5.0          1.9  Iris-virginica
147           6.5          3.0           5.2          2.0  Iris-virginica
148           6.2          3.4           5.4          2.3  Iris-virginica
149           5.9          3.0           5.1          1.8  Iris-virginica

[150 rows x 5 columns]
```

To print all rows of a dataframe, the option `display.max_rows` has to set to `None` in pandas:

[6]:
```
pd.set_option('display.max_rows', None)
irisdata_df
```

[6]:

	sepal_length	sepal_width	petal_length	petal_width	species
0	5.1	3.5	1.4	0.2	Iris-setosa
1	4.9	3.0	1.4	0.2	Iris-setosa
2	4.7	3.2	1.3	0.2	Iris-setosa
3	4.6	3.1	1.5	0.2	Iris-setosa
4	5.0	3.6	1.4	0.2	Iris-setosa
5	5.4	3.9	1.7	0.4	Iris-setosa
6	4.6	3.4	1.4	0.3	Iris-setosa
7	5.0	3.4	1.5	0.2	Iris-setosa
8	4.4	2.9	1.4	0.2	Iris-setosa
9	4.9	3.1	1.5	0.1	Iris-setosa
10	5.4	3.7	1.5	0.2	Iris-setosa
11	4.8	3.4	1.6	0.2	Iris-setosa
12	4.8	3.0	1.4	0.1	Iris-setosa
13	4.3	3.0	1.1	0.1	Iris-setosa
14	5.8	4.0	1.2	0.2	Iris-setosa
15	5.7	4.4	1.5	0.4	Iris-setosa
16	5.4	3.9	1.3	0.4	Iris-setosa
17	5.1	3.5	1.4	0.3	Iris-setosa
18	5.7	3.8	1.7	0.3	Iris-setosa
19	5.1	3.8	1.5	0.3	Iris-setosa
20	5.4	3.4	1.7	0.2	Iris-setosa
21	5.1	3.7	1.5	0.4	Iris-setosa
22	4.6	3.6	1.0	0.2	Iris-setosa
23	5.1	3.3	1.7	0.5	Iris-setosa
24	4.8	3.4	1.9	0.2	Iris-setosa
25	5.0	3.0	1.6	0.2	Iris-setosa
26	5.0	3.4	1.6	0.4	Iris-setosa
27	5.2	3.5	1.5	0.2	Iris-setosa
28	5.2	3.4	1.4	0.2	Iris-setosa
29	4.7	3.2	1.6	0.2	Iris-setosa
30	4.8	3.1	1.6	0.2	Iris-setosa
31	5.4	3.4	1.5	0.4	Iris-setosa
32	5.2	4.1	1.5	0.1	Iris-setosa
33	5.5	4.2	1.4	0.2	Iris-setosa
34	4.9	3.1	1.5	0.1	Iris-setosa
35	5.0	3.2	1.2	0.2	Iris-setosa
36	5.5	3.5	1.3	0.2	Iris-setosa
37	4.9	3.1	1.5	0.1	Iris-setosa
38	4.4	3.0	1.3	0.2	Iris-setosa
39	5.1	3.4	1.5	0.2	Iris-setosa
40	5.0	3.5	1.3	0.3	Iris-setosa
41	4.5	2.3	1.3	0.3	Iris-setosa
42	4.4	3.2	1.3	0.2	Iris-setosa
43	5.0	3.5	1.6	0.6	Iris-setosa
44	5.1	3.8	1.9	0.4	Iris-setosa
45	4.8	3.0	1.4	0.3	Iris-setosa
46	5.1	3.8	1.6	0.2	Iris-setosa
47	4.6	3.2	1.4	0.2	Iris-setosa
48	5.3	3.7	1.5	0.2	Iris-setosa
49	5.0	3.3	1.4	0.2	Iris-setosa
50	7.0	3.2	4.7	1.4	Iris-versicolor
51	6.4	3.2	4.5	1.5	Iris-versicolor
52	6.9	3.1	4.9	1.5	Iris-versicolor

53	5.5	2.3	4.0	1.3	Iris-versicolor
54	6.5	2.8	4.6	1.5	Iris-versicolor
55	5.7	2.8	4.5	1.3	Iris-versicolor
56	6.3	3.3	4.7	1.6	Iris-versicolor
57	4.9	2.4	3.3	1.0	Iris-versicolor
58	6.6	2.9	4.6	1.3	Iris-versicolor
59	5.2	2.7	3.9	1.4	Iris-versicolor
60	5.0	2.0	3.5	1.0	Iris-versicolor
61	5.9	3.0	4.2	1.5	Iris-versicolor
62	6.0	2.2	4.0	1.0	Iris-versicolor
63	6.1	2.9	4.7	1.4	Iris-versicolor
64	5.6	2.9	3.6	1.3	Iris-versicolor
65	6.7	3.1	4.4	1.4	Iris-versicolor
66	5.6	3.0	4.5	1.5	Iris-versicolor
67	5.8	2.7	4.1	1.0	Iris-versicolor
68	6.2	2.2	4.5	1.5	Iris-versicolor
69	5.6	2.5	3.9	1.1	Iris-versicolor
70	5.9	3.2	4.8	1.8	Iris-versicolor
71	6.1	2.8	4.0	1.3	Iris-versicolor
72	6.3	2.5	4.9	1.5	Iris-versicolor
73	6.1	2.8	4.7	1.2	Iris-versicolor
74	6.4	2.9	4.3	1.3	Iris-versicolor
75	6.6	3.0	4.4	1.4	Iris-versicolor
76	6.8	2.8	4.8	1.4	Iris-versicolor
77	6.7	3.0	5.0	1.7	Iris-versicolor
78	6.0	2.9	4.5	1.5	Iris-versicolor
79	5.7	2.6	3.5	1.0	Iris-versicolor
80	5.5	2.4	3.8	1.1	Iris-versicolor
81	5.5	2.4	3.7	1.0	Iris-versicolor
82	5.8	2.7	3.9	1.2	Iris-versicolor
83	6.0	2.7	5.1	1.6	Iris-versicolor
84	5.4	3.0	4.5	1.5	Iris-versicolor
85	6.0	3.4	4.5	1.6	Iris-versicolor
86	6.7	3.1	4.7	1.5	Iris-versicolor
87	6.3	2.3	4.4	1.3	Iris-versicolor
88	5.6	3.0	4.1	1.3	Iris-versicolor
89	5.5	2.5	4.0	1.3	Iris-versicolor
90	5.5	2.6	4.4	1.2	Iris-versicolor
91	6.1	3.0	4.6	1.4	Iris-versicolor
92	5.8	2.6	4.0	1.2	Iris-versicolor
93	5.0	2.3	3.3	1.0	Iris-versicolor
94	5.6	2.7	4.2	1.3	Iris-versicolor
95	5.7	3.0	4.2	1.2	Iris-versicolor
96	5.7	2.9	4.2	1.3	Iris-versicolor
97	6.2	2.9	4.3	1.3	Iris-versicolor
98	5.1	2.5	3.0	1.1	Iris-versicolor
99	5.7	2.8	4.1	1.3	Iris-versicolor
100	6.3	3.3	6.0	2.5	Iris-virginica
101	5.8	2.7	5.1	1.9	Iris-virginica
102	7.1	3.0	5.9	2.1	Iris-virginica
103	6.3	2.9	5.6	1.8	Iris-virginica
104	6.5	3.0	5.8	2.2	Iris-virginica
105	7.6	3.0	6.6	2.1	Iris-virginica
106	4.9	2.5	4.5	1.7	Iris-virginica
107	7.3	2.9	6.3	1.8	Iris-virginica
108	6.7	2.5	5.8	1.8	Iris-virginica
109	7.2	3.6	6.1	2.5	Iris-virginica

```
110          6.5         3.2          5.1         2.0   Iris-virginica
111          6.4         2.7          5.3         1.9   Iris-virginica
112          6.8         3.0          5.5         2.1   Iris-virginica
113          5.7         2.5          5.0         2.0   Iris-virginica
114          5.8         2.8          5.1         2.4   Iris-virginica
115          6.4         3.2          5.3         2.3   Iris-virginica
116          6.5         3.0          5.5         1.8   Iris-virginica
117          7.7         3.8          6.7         2.2   Iris-virginica
118          7.7         2.6          6.9         2.3   Iris-virginica
119          6.0         2.2          5.0         1.5   Iris-virginica
120          6.9         3.2          5.7         2.3   Iris-virginica
121          5.6         2.8          4.9         2.0   Iris-virginica
122          7.7         2.8          6.7         2.0   Iris-virginica
123          6.3         2.7          4.9         1.8   Iris-virginica
124          6.7         3.3          5.7         2.1   Iris-virginica
125          7.2         3.2          6.0         1.8   Iris-virginica
126          6.2         2.8          4.8         1.8   Iris-virginica
127          6.1         3.0          4.9         1.8   Iris-virginica
128          6.4         2.8          5.6         2.1   Iris-virginica
129          7.2         3.0          5.8         1.6   Iris-virginica
130          7.4         2.8          6.1         1.9   Iris-virginica
131          7.9         3.8          6.4         2.0   Iris-virginica
132          6.4         2.8          5.6         2.2   Iris-virginica
133          6.3         2.8          5.1         1.5   Iris-virginica
134          6.1         2.6          5.6         1.4   Iris-virginica
135          7.7         3.0          6.1         2.3   Iris-virginica
136          6.3         3.4          5.6         2.4   Iris-virginica
137          6.4         3.1          5.5         1.8   Iris-virginica
138          6.0         3.0          4.8         1.8   Iris-virginica
139          6.9         3.1          5.4         2.1   Iris-virginica
140          6.7         3.1          5.6         2.4   Iris-virginica
141          6.9         3.1          5.1         2.3   Iris-virginica
142          5.8         2.7          5.1         1.9   Iris-virginica
143          6.8         3.2          5.9         2.3   Iris-virginica
144          6.7         3.3          5.7         2.5   Iris-virginica
145          6.7         3.0          5.2         2.3   Iris-virginica
146          6.3         2.5          5.0         1.9   Iris-virginica
147          6.5         3.0          5.2         2.0   Iris-virginica
148          6.2         3.4          5.4         2.3   Iris-virginica
149          5.9         3.0          5.1         1.8   Iris-virginica
```

5.3.2 Get data types

[7]:
```
irisdata_df.info()
```

```
<class 'pandas.core.frame.DataFrame'>
RangeIndex: 150 entries, 0 to 149
Data columns (total 5 columns):
 #   Column        Non-Null Count  Dtype
---  ------        --------------  -----
 0   sepal_length  150 non-null    float64
 1   sepal_width   150 non-null    float64
 2   petal_length  150 non-null    float64
 3   petal_width   150 non-null    float64
 4   species       150 non-null    object
dtypes: float64(4), object(1)
memory usage: 6.0+ KB
```

[8]:
```
irisdata_df.describe()
```

[8]:
```
       sepal_length  sepal_width  petal_length  petal_width
count    150.000000   150.000000    150.000000   150.000000
mean       5.843333     3.054000      3.758667     1.198667
std        0.828066     0.433594      1.764420     0.763161
min        4.300000     2.000000      1.000000     0.100000
25%        5.100000     2.800000      1.600000     0.300000
50%        5.800000     3.000000      4.350000     1.300000
75%        6.400000     3.300000      5.100000     1.800000
max        7.900000     4.400000      6.900000     2.500000
```

5.3.3 Get data ranges with Boxplots

Boxplots can be used to explore the data ranges in the dataset. These also provide information about **outliers**.

[9]:
```
sns.set_context("notebook", font_scale=1.3, rc={"lines.linewidth": 2.0})
sns.set_style("whitegrid")
#sns.set_style("white")

fig, axs = plt.subplots(2, 2, figsize=(12, 10))

fn = ['sepal_length', 'sepal_width', 'petal_length', 'petal_width']
cn = ['Iris-setosa', 'Iris-versicolor', 'Iris-virginica']
box1 = sns.boxplot(x = 'species', y = 'sepal_length',
                   data = irisdata_df, order = cn, ax = axs[0,0])
box2 = sns.boxplot(x = 'species', y = 'sepal_width',
                   data = irisdata_df, order = cn, ax = axs[0,1])
box3 = sns.boxplot(x = 'species', y = 'petal_length',
                   data = irisdata_df, order = cn, ax = axs[1,0])
box4 = sns.boxplot(x = 'species', y = 'petal_width',
                   data = irisdata_df,  order = cn, ax = axs[1,1])

# add some spacing between subplots
fig.tight_layout(pad=2.0)

plt.show()
```

5.4 Identify anomalies in the datasets

5.4.1 Find gaps in dataset

This section was inspired by Working with Missing Data in Pandas.

Checking for missing values using `isnull()` In order to check for missing values in Pandas DataFrame, we use the function `isnull()`. This function returns a dataframe of Boolean values which are True for **NaN values**.

[10]:
```
pd.set_option('display.max_rows', 40)
pd.set_option('display.min_rows', 30)
```

[11]:
```
irisdata_df.isnull()
```

[11]:
```
     sepal_length  sepal_width  petal_length  petal_width  species
0           False        False         False        False    False
```

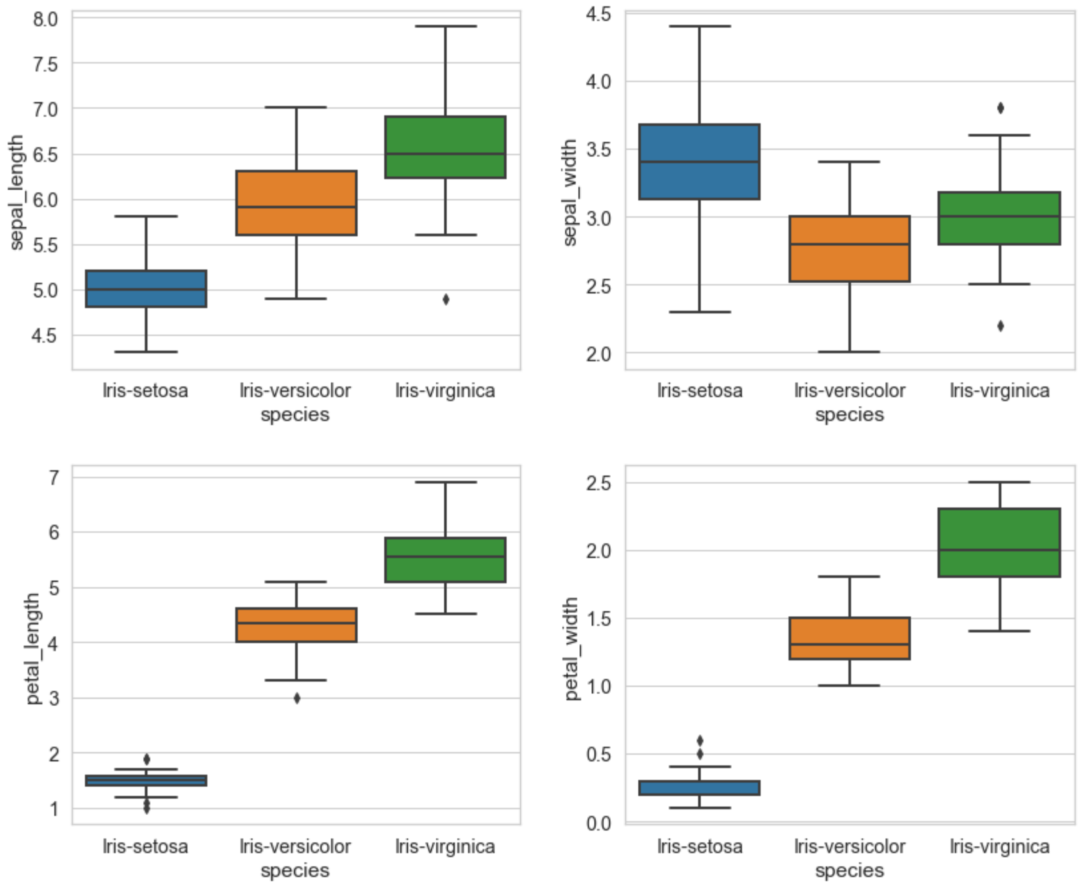

Figure 3: Boxplots used to explore the data ranges in the Iris dataset

1	False	False	False	False	False
2	False	False	False	False	False
3	False	False	False	False	False
4	False	False	False	False	False
5	False	False	False	False	False
6	False	False	False	False	False
7	False	False	False	False	False
8	False	False	False	False	False
9	False	False	False	False	False
10	False	False	False	False	False
11	False	False	False	False	False
12	False	False	False	False	False
13	False	False	False	False	False
14	False	False	False	False	False
..	…	…	…	…	…
135	False	False	False	False	False
136	False	False	False	False	False
137	False	False	False	False	False
138	False	False	False	False	False
139	False	False	False	False	False
140	False	False	False	False	False
141	False	False	False	False	False
142	False	False	False	False	False
143	False	False	False	False	False
144	False	False	False	False	False
145	False	False	False	False	False

```
146        False        False        False        False    False
147        False        False        False        False    False
148        False        False        False        False    False
149        False        False        False        False    False

[150 rows x 5 columns]
```

Show only the gaps:

[12]:
```
irisdata_df_gaps = irisdata_df[irisdata_df.isnull().any(axis=1)]
irisdata_df_gaps
```

[12]:
```
Empty DataFrame
Columns: [sepal_length, sepal_width, petal_length, petal_width, species]
Index: []
```

Fine - this dataset seems to be complete :)

So let's look for something else for exercise: employes.csv

[13]:
```
# import data to dataframe from csv file
employees_df = pd.read_csv("./datasets/employees_edit.csv")

employees_df
```

[13]:
```
     First Name  Gender  Start Date Last Login Time  Salary   Bonus %  \
0       Douglas    Male    8/6/1993        12:42 PM   97308   6945.00
1        Thomas    Male   3/31/1996         6:53 AM   61933      4.17
2         Maria  Female   4/23/1993        11:17 AM  130590  11858.00
3         Jerry    Male    3/4/2005         1:00 PM  138705      9.34
4         Larry    Male   1/24/1998         4:47 PM  101004   1389.00
5        Dennis    Male   4/18/1987         1:35 AM  115163  10125.00
6          Ruby  Female   8/17/1987         4:20 PM   65476  10012.00
7           NaN  Female   7/20/2015        10:43 AM   45906  11598.00
8        Angela  Female  11/22/2005         6:29 AM   95570  18523.00
9       Frances  Female    8/8/2002         6:51 AM  139852   7524.00
10       Louise  Female   8/12/1980         9:01 AM   63241  15132.00
11        Julie  Female  10/26/1997         3:19 PM  102508  12637.00
12      Brandon    Male   12/1/1980         1:08 AM  112807  17492.00
13         Gary    Male   1/27/2008        11:40 PM  109831   5831.00
14     Kimberly  Female   1/14/1999         7:13 AM   41426  14543.00
…           …     …          …           …      …       …
989     Stephen     NaN   7/10/1983         8:10 PM   85668   1909.00
990       Donna  Female  11/26/1982         7:04 AM   82871  17999.00
991      Gloria  Female   12/8/2014         5:08 AM  136709  10331.00
992       Alice  Female   10/5/2004         9:34 AM   47638  11209.00
993      Justin     NaN   2/10/1991         4:58 PM   38344   3794.00
994       Robin  Female   7/24/1987         1:35 PM  100765  10982.00
995        Rose  Female   8/25/2002         5:12 AM  134505  11051.00
996     Anthony    Male  10/16/2011         8:35 AM  112769  11625.00
997        Tina  Female   5/15/1997         3:53 PM   56450     19.04
998      George    Male   6/21/2013         5:47 PM   98874   4479.00
999       Henry     NaN  11/23/2014         6:09 AM  132483  16655.00
1000    Phillip    Male   1/31/1984         6:30 AM   42392  19675.00
1001    Russell    Male   5/20/2013        12:39 PM   96914   1421.00
1002      Larry    Male   4/20/2013         4:45 PM   60500  11985.00
1003     Albert    Male   5/15/2012         6:24 PM  129949  10169.00
```

```
     Senior Management                 Team
0                 True            Marketing
1                 True                  NaN
2                False              Finance
3                 True              Finance
4                 True      Client Services
5                False                Legal
6                 True              Product
7                  NaN              Finance
8                 True          Engineering
9                 True Business Development
10                True                  NaN
11                True                Legal
12                True      Human Resources
13               False                Sales
14                True              Finance
…                    …                    …
989              False                Legal
990              False            Marketing
991               True              Finance
992              False      Human Resources
993              False                Legal
994               True      Client Services
995               True            Marketing
996               True              Finance
997               True          Engineering
998               True            Marketing
999              False         Distribution
1000             False              Finance
1001             False              Product
1002             False Business Development
1003              True                Sales

[1004 rows x 8 columns]
```

Show only the gaps from this gappy dataset again:

[14]:
```
employees_df_gaps = employees_df[employees_df.isnull().any(axis=1)]
employees_df_gaps
```

[14]:
```
    First Name  Gender  Start Date Last Login Time  Salary   Bonus %  \
1       Thomas    Male   3/31/1996         6:53 AM   61933      4.17
7          NaN  Female   7/20/2015        10:43 AM   45906  11598.00
10      Louise  Female   8/12/1980         9:01 AM   63241  15132.00
20        Lois     NaN   4/22/1995         7:18 PM   64714   4934.00
22      Joshua     NaN    3/8/2012         1:58 AM   90816  18816.00
23         NaN    Male   6/14/2012         4:19 PM  125792   5042.00
25         NaN    Male   10/8/2012         1:12 AM   37076  18576.00
27       Scott     NaN   7/11/1991         6:58 PM  122367   5218.00
31       Joyce     NaN   2/20/2005         2:40 PM   88657  12752.00
32         NaN    Male   8/21/1998         2:27 PM  122340   6417.00
39         NaN    Male   1/29/2016         2:33 AM  122173   7797.00
41   Christine     NaN   6/28/2015         1:08 AM   66582  11308.00
49       Chris     NaN   1/24/1980        12:13 PM  113590   3055.00
51         NaN     NaN  12/17/2011         8:29 AM   41126  14009.00
53        Alan     NaN    3/3/2014         1:28 PM   40341  17578.00
..           …       …           …               …       …         …
916        Joe    Male   12/8/1998        10:28 AM  126120      1.02
```

```
927       Irene     NaN   2/28/1991        10:23 PM  135369      4.38
929         NaN  Female   8/23/2000         4:19 PM   95866  19388.00
941       Aaron     NaN   1/22/1986         7:39 PM   63126  18424.00
942        Mark     NaN    9/9/2006        12:27 PM   44836   2657.00
943       Ralph     NaN   7/28/1995         6:53 PM   70635   2147.00
949      Gerald     NaN   4/15/1989        12:44 PM   93712  17426.00
950         NaN  Female   9/15/1985         1:50 AM  133472  16941.00
951         NaN    Male   7/30/2012         3:07 PM  107351   5329.00
955         NaN  Female   9/14/2010         5:19 AM  143638   9662.00
965     Antonio     NaN   6/18/1989         9:37 PM  103050      3.05
976      Victor     NaN   7/28/2006         2:49 PM   76381  11159.00
989     Stephen     NaN   7/10/1983         8:10 PM   85668   1909.00
993      Justin     NaN   2/10/1991         4:58 PM   38344   3794.00
999       Henry     NaN  11/23/2014         6:09 AM  132483  16655.00

    Senior Management                  Team
1                True                   NaN
7                 NaN               Finance
10               True                   NaN
20               True                 Legal
22               True       Client Services
23                NaN                   NaN
25                NaN       Client Services
27              False                 Legal
31              False               Product
32                NaN                   NaN
39                NaN       Client Services
41               True  Business Development
49              False                 Sales
51                NaN                 Sales
53               True               Finance
..                ...                   ...
916             False                   NaN
927             False  Business Development
929               NaN                 Sales
941             False       Client Services
942             False       Client Services
943             False       Client Services
949              True          Distribution
950               NaN          Distribution
951               NaN             Marketing
955               NaN                   NaN
965             False                 Legal
976              True                 Sales
989             False                 Legal
993             False                 Legal
999             False          Distribution

[237 rows x 8 columns]
```

Fill the missing values with `fillna()` Now we are going to fill all the null (NaN) values in Gender column with *"No Gender"*.

Attention: We are doing that directly in this dataframe with `inplace = True` - we don't make a deep copy!

[15]:
```
# filling a null values using fillna()
employees_df["Gender"].fillna("No Gender", inplace = True)
employees_df
```

[15]:
```
     First Name     Gender  Start Date Last Login Time  Salary   Bonus %  \
0       Douglas       Male    8/6/1993        12:42 PM   97308  6945.00
1        Thomas       Male   3/31/1996         6:53 AM   61933     4.17
2         Maria     Female   4/23/1993        11:17 AM  130590 11858.00
3         Jerry       Male    3/4/2005         1:00 PM  138705     9.34
4         Larry       Male   1/24/1998         4:47 PM  101004  1389.00
5        Dennis       Male   4/18/1987         1:35 AM  115163 10125.00
6          Ruby     Female   8/17/1987         4:20 PM   65476 10012.00
7           NaN     Female   7/20/2015        10:43 AM   45906 11598.00
8        Angela     Female  11/22/2005         6:29 AM   95570 18523.00
9       Frances     Female    8/8/2002         6:51 AM  139852  7524.00
10       Louise     Female   8/12/1980         9:01 AM   63241 15132.00
11        Julie     Female  10/26/1997         3:19 PM  102508 12637.00
12      Brandon       Male   12/1/1980         1:08 AM  112807 17492.00
13         Gary       Male   1/27/2008        11:40 PM  109831  5831.00
14     Kimberly     Female   1/14/1999         7:13 AM   41426 14543.00
…             …          …           …               …       …       …
989     Stephen  No Gender   7/10/1983         8:10 PM   85668  1909.00
990       Donna     Female  11/26/1982         7:04 AM   82871 17999.00
991      Gloria     Female   12/8/2014         5:08 AM  136709 10331.00
992       Alice     Female   10/5/2004         9:34 AM   47638 11209.00
993      Justin  No Gender   2/10/1991         4:58 PM   38344  3794.00
994       Robin     Female   7/24/1987         1:35 PM  100765 10982.00
995        Rose     Female   8/25/2002         5:12 AM  134505 11051.00
996     Anthony       Male  10/16/2011         8:35 AM  112769 11625.00
997        Tina     Female   5/15/1997         3:53 PM   56450    19.04
998      George       Male   6/21/2013         5:47 PM   98874  4479.00
999       Henry  No Gender  11/23/2014         6:09 AM  132483 16655.00
1000    Phillip       Male   1/31/1984         6:30 AM   42392 19675.00
1001    Russell       Male   5/20/2013        12:39 PM   96914  1421.00
1002      Larry       Male   4/20/2013         4:45 PM   60500 11985.00
1003     Albert       Male   5/15/2012         6:24 PM  129949 10169.00

     Senior Management                  Team
0                 True             Marketing
1                 True                   NaN
2                False               Finance
3                 True               Finance
4                 True       Client Services
5                False                 Legal
6                 True               Product
7                  NaN               Finance
8                 True           Engineering
9                 True  Business Development
10                True                   NaN
11                True                 Legal
12                True       Human Resources
13               False                 Sales
14                True               Finance
…                    …                     …
989              False                 Legal
990              False             Marketing
991               True               Finance
```

```
992            False       Human Resources
993            False                 Legal
994             True       Client Services
995             True             Marketing
996             True               Finance
997             True           Engineering
998             True             Marketing
999            False          Distribution
1000           False               Finance
1001           False               Product
1002           False  Business Development
1003            True                 Sales

[1004 rows x 8 columns]
```

Dropping missing values using `dropna()` In order to drop null values from a dataframe, we use `dropna()` function. This function drops rows or columns of datasets with NaN values in different ways.

Default is to drop rows with at least 1 null value (NaN). Giving the parameter `how = 'all'` the function drops rows with all data missing or contain null values (NaN).

[16]:
```
# making a new dataframe with dropped NaN values
employees_df_dropped = employees_df.dropna(axis = 0, how ='any')
employees_df_dropped
```

[16]:
```
     First Name     Gender  Start Date Last Login Time  Salary   Bonus %  \
0       Douglas       Male    8/6/1993        12:42 PM   97308   6945.00
2         Maria     Female   4/23/1993        11:17 AM  130590  11858.00
3         Jerry       Male    3/4/2005         1:00 PM  138705      9.34
4         Larry       Male   1/24/1998         4:47 PM  101004   1389.00
5        Dennis       Male   4/18/1987         1:35 AM  115163  10125.00
6          Ruby     Female   8/17/1987         4:20 PM   65476  10012.00
8        Angela     Female  11/22/2005         6:29 AM   95570  18523.00
9       Frances     Female    8/8/2002         6:51 AM  139852   7524.00
11        Julie     Female  10/26/1997         3:19 PM  102508  12637.00
12      Brandon       Male   12/1/1980         1:08 AM  112807  17492.00
13         Gary       Male   1/27/2008        11:40 PM  109831   5831.00
14     Kimberly     Female   1/14/1999         7:13 AM   41426  14543.00
15      Lillian     Female    6/5/2016         6:09 AM   59414   1256.00
16       Jeremy       Male   9/21/2010         5:56 AM   90370   7369.00
17        Shawn       Male   12/7/1986         7:45 PM  111737   6414.00
…           …         …          …           …       …       …
989     Stephen  No Gender   7/10/1983         8:10 PM   85668   1909.00
990       Donna     Female  11/26/1982         7:04 AM   82871  17999.00
991      Gloria     Female   12/8/2014         5:08 AM  136709  10331.00
992       Alice     Female   10/5/2004         9:34 AM   47638  11209.00
993      Justin  No Gender   2/10/1991         4:58 PM   38344   3794.00
994       Robin     Female   7/24/1987         1:35 PM  100765  10982.00
995        Rose     Female   8/25/2002         5:12 AM  134505  11051.00
996     Anthony       Male  10/16/2011         8:35 AM  112769  11625.00
997        Tina     Female   5/15/1997         3:53 PM   56450     19.04
998      George       Male   6/21/2013         5:47 PM   98874   4479.00
999       Henry  No Gender  11/23/2014         6:09 AM  132483  16655.00
1000    Phillip       Male   1/31/1984         6:30 AM   42392  19675.00
1001    Russell       Male   5/20/2013        12:39 PM   96914   1421.00
1002      Larry       Male   4/20/2013         4:45 PM   60500  11985.00
1003     Albert       Male   5/15/2012         6:24 PM  129949  10169.00
```

```
     Senior Management                Team
0                 True           Marketing
2                False             Finance
3                 True             Finance
4                 True     Client Services
5                False               Legal
6                 True             Product
8                 True         Engineering
9                 True  Business Development
11                True               Legal
12                True     Human Resources
13               False               Sales
14                True             Finance
15               False             Product
16               False     Human Resources
17               False             Product
…                    …                   …
989              False               Legal
990              False           Marketing
991               True             Finance
992              False     Human Resources
993              False               Legal
994               True     Client Services
995               True           Marketing
996               True             Finance
997               True         Engineering
998               True           Marketing
999              False        Distribution
1000             False             Finance
1001             False             Product
1002             False  Business Development
1003              True               Sales

[903 rows x 8 columns]
```

Finally we compare the sizes of dataframes so that we learn how many rows had at least 1 Null value.

[17]:
```
print("Old data frame length:", len(employees_df))
print("New data frame length:", len(employees_df_dropped))
print("Number of rows with at least 1 NaN value: ",
      (len(employees_df)-len(employees_df_dropped)))
```

```
Old data frame length: 1004
New data frame length: 903
Number of rows with at least 1 NaN value:  101
```

5.4.2 Find and remove duplicates in dataset

This section was inspired by: - How to Find Duplicates in Pandas DataFrame (With Examples) - How to Drop Duplicate Rows in a Pandas DataFrame

Checking for duplicate values using `duplicated()` In order to check for duplicate values in Pandas DataFrame, we use a function `duplicated()`. This function can be used in two ways: - find duplicate rows across **all columns** with `duplicateRows = df[df.duplicated()]` - find duplicate rows across **specific columns** `duplicateRows = df[df.duplicated(subset=['col1', 'col2'])]`

Find duplicate rows across **all columns**:

[18]:
```
# import (again) data to dataframe from csv file
employees_df = pd.read_csv("./datasets/employees_edit.csv")
```

[19]:
```
# find duplicate rows across all columns
duplicateRows = employees_df[employees_df.duplicated()]
duplicateRows
```

[19]:
```
    First Name  Gender  Start Date Last Login Time  Salary  Bonus %  \
112      Karen  Female  11/30/1999         7:46 AM  102488  17653.0
127      Linda  Female   5/25/2000         5:45 PM  119009  12506.0
296    Brandon     NaN   11/3/1997         8:17 PM  121333  15295.0
580   Nicholas    Male    3/1/2013         9:26 PM  101036   2826.0

    Senior Management                  Team
112              True               Product
127              True  Business Development
296             False  Business Development
580              True       Human Resources
```

[20]:
```
# argument keep='last' displays the first duplicate rows instead of the last
duplicateRows = employees_df[employees_df.duplicated(keep='last')]
duplicateRows
```

[20]:
```
    First Name  Gender  Start Date Last Login Time  Salary  Bonus %  \
55       Karen  Female  11/30/1999         7:46 AM  102488  17653.0
92       Linda  Female   5/25/2000         5:45 PM  119009  12506.0
153    Brandon     NaN   11/3/1997         8:17 PM  121333  15295.0
442   Nicholas    Male    3/1/2013         9:26 PM  101036   2826.0

    Senior Management                  Team
55               True               Product
92               True  Business Development
153             False  Business Development
442              True       Human Resources
```

Find duplicate rows across **specific columns**:

[21]:
```
# identify duplicate rows across 'First Name' and 'Last Login Time' columns
duplicateRows = employees_df[employees_df.duplicated(
                    subset=['First Name', 'Last Login Time'])]
duplicateRows
```

[21]:
```
    First Name  Gender  Start Date Last Login Time  Salary  Bonus %  \
112      Karen  Female  11/30/1999         7:46 AM  102488  17653.0
127      Linda  Female   5/25/2000         5:45 PM  119009  12506.0
296    Brandon     NaN   11/3/1997         8:17 PM  121333  15295.0
577        NaN  Female   1/13/2009         1:01 PM  118736   7421.0
580   Nicholas    Male    3/1/2013         9:26 PM  101036   2826.0
632        NaN     NaN    9/2/1988        12:49 PM  147309   1702.0
881        NaN    Male    9/5/1980         7:36 AM  114896  13823.0
929        NaN  Female   8/23/2000         4:19 PM   95866  19388.0
934      Nancy  Female   9/10/2001        11:57 PM   85213   2386.0
973      Linda  Female    2/4/2010         8:49 PM   44486  17308.0

    Senior Management                  Team
112              True               Product
127              True  Business Development
```

```
296             False  Business Development
577               NaN       Client Services
580              True       Human Resources
632               NaN          Distribution
881               NaN       Client Services
929               NaN                 Sales
934              True             Marketing
973              True           Engineering
```

[22]:
```
# argument keep='last' displays the first duplicate rows instead of the last
duplicateRows = employees_df[employees_df.duplicated(
                    subset=['First Name', 'Last Login Time'], keep='last')]
duplicateRows
```

[22]:
```
    First Name  Gender  Start Date Last Login Time  Salary   Bonus %  \
23         NaN    Male   6/14/2012         4:19 PM  125792   5042.00
37       Linda  Female  10/19/1981         8:49 PM   57427   9557.00
55       Karen  Female  11/30/1999         7:46 AM  102488  17653.00
66       Nancy  Female  12/15/2012        11:57 PM  125250   2672.00
92       Linda  Female   5/25/2000         5:45 PM  119009  12506.00
153    Brandon     NaN   11/3/1997         8:17 PM  121333  15295.00
222        NaN  Female   6/17/1991        12:49 PM   71945      5.56
269        NaN    Male    2/4/2005         1:01 PM   40451  16044.00
442   Nicholas    Male    3/1/2013         9:26 PM  101036   2826.00
778        NaN  Female   6/18/2000         7:36 AM  106428  10867.00

    Senior Management                  Team
23                NaN                   NaN
37               True       Client Services
55               True               Product
66               True  Business Development
92               True  Business Development
153             False  Business Development
222               NaN             Marketing
269               NaN          Distribution
442              True       Human Resources
778               NaN                   NaN
```

Dropping duplicate values using `drop_duplicates()` In order to drop duplicate values from a dataframe, we use `drop_duplicates()` function.

This function can be used in two ways: - remove duplicate rows across **all columns** with `df.drop_duplicates()` - find duplicate rows across **specific columns** `df.drop_duplicates(subset=['col1', 'col2'])`

Attention: We are doing that directly in this dataframe with `inplace = True` - we don't make a deep copy!

Remove duplicate rows across **all columns**:

[23]:
```
# remove duplicate rows across all columns
employees_df.drop_duplicates(inplace=True)
employees_df
```

[23]:
```
  First Name  Gender  Start Date Last Login Time  Salary   Bonus %  \
0    Douglas    Male    8/6/1993        12:42 PM   97308   6945.00
1     Thomas    Male   3/31/1996         6:53 AM   61933      4.17
2      Maria  Female   4/23/1993        11:17 AM  130590  11858.00
```

```
3         Jerry    Male    3/4/2005         1:00 PM  138705      9.34
4         Larry    Male   1/24/1998         4:47 PM  101004   1389.00
5        Dennis    Male   4/18/1987         1:35 AM  115163  10125.00
6          Ruby  Female   8/17/1987         4:20 PM   65476  10012.00
7           NaN  Female   7/20/2015        10:43 AM   45906  11598.00
8        Angela  Female  11/22/2005         6:29 AM   95570  18523.00
9       Frances  Female    8/8/2002         6:51 AM  139852   7524.00
10       Louise  Female   8/12/1980         9:01 AM   63241  15132.00
11        Julie  Female  10/26/1997         3:19 PM  102508  12637.00
12      Brandon    Male   12/1/1980         1:08 AM  112807  17492.00
13         Gary    Male   1/27/2008        11:40 PM  109831   5831.00
14     Kimberly  Female   1/14/1999         7:13 AM   41426  14543.00
…           …      …          …         …        …        …
989     Stephen     NaN   7/10/1983         8:10 PM   85668   1909.00
990       Donna  Female  11/26/1982         7:04 AM   82871  17999.00
991      Gloria  Female   12/8/2014         5:08 AM  136709  10331.00
992       Alice  Female   10/5/2004         9:34 AM   47638  11209.00
993      Justin     NaN   2/10/1991         4:58 PM   38344   3794.00
994       Robin  Female   7/24/1987         1:35 PM  100765  10982.00
995        Rose  Female   8/25/2002         5:12 AM  134505  11051.00
996     Anthony    Male  10/16/2011         8:35 AM  112769  11625.00
997        Tina  Female   5/15/1997         3:53 PM   56450     19.04
998      George    Male   6/21/2013         5:47 PM   98874   4479.00
999       Henry     NaN  11/23/2014         6:09 AM  132483  16655.00
1000    Phillip    Male   1/31/1984         6:30 AM   42392  19675.00
1001    Russell    Male   5/20/2013        12:39 PM   96914   1421.00
1002      Larry    Male   4/20/2013         4:45 PM   60500  11985.00
1003     Albert    Male   5/15/2012         6:24 PM  129949  10169.00

     Senior Management                  Team
0                 True             Marketing
1                 True                   NaN
2                False               Finance
3                 True               Finance
4                 True       Client Services
5                False                 Legal
6                 True               Product
7                  NaN               Finance
8                 True           Engineering
9                 True  Business Development
10                True                   NaN
11                True                 Legal
12                True       Human Resources
13               False                 Sales
14                True               Finance
…                    …                  …
989              False                 Legal
990              False             Marketing
991               True               Finance
992              False       Human Resources
993              False                 Legal
994               True       Client Services
995               True             Marketing
996               True               Finance
997               True           Engineering
998               True             Marketing
999              False          Distribution
```

```
1000             False                Finance
1001             False                Product
1002             False   Business Development
1003              True                  Sales

[1000 rows x 8 columns]
```

Remove duplicate rows across **specific columns**:

[24]:
```
# remove duplicate rows across 'First Name' and 'Last Login Time' columns
employees_df.drop_duplicates(
    subset=['First Name', 'Last Login Time'], keep='last', inplace=True)
employees_df
```

[24]:
```
     First Name  Gender  Start Date Last Login Time  Salary   Bonus %  \
0       Douglas    Male    8/6/1993        12:42 PM   97308   6945.00
1        Thomas    Male   3/31/1996         6:53 AM   61933      4.17
2         Maria  Female   4/23/1993        11:17 AM  130590  11858.00
3         Jerry    Male    3/4/2005         1:00 PM  138705      9.34
4         Larry    Male   1/24/1998         4:47 PM  101004   1389.00
5        Dennis    Male   4/18/1987         1:35 AM  115163  10125.00
6          Ruby  Female   8/17/1987         4:20 PM   65476  10012.00
7           NaN  Female   7/20/2015        10:43 AM   45906  11598.00
8        Angela  Female  11/22/2005         6:29 AM   95570  18523.00
9       Frances  Female    8/8/2002         6:51 AM  139852   7524.00
10       Louise  Female   8/12/1980         9:01 AM   63241  15132.00
11        Julie  Female  10/26/1997         3:19 PM  102508  12637.00
12      Brandon    Male   12/1/1980         1:08 AM  112807  17492.00
13         Gary    Male   1/27/2008        11:40 PM  109831   5831.00
14     Kimberly  Female   1/14/1999         7:13 AM   41426  14543.00
…           …      …          …              …       …        …
989     Stephen     NaN   7/10/1983         8:10 PM   85668   1909.00
990       Donna  Female  11/26/1982         7:04 AM   82871  17999.00
991      Gloria  Female   12/8/2014         5:08 AM  136709  10331.00
992       Alice  Female   10/5/2004         9:34 AM   47638  11209.00
993      Justin     NaN   2/10/1991         4:58 PM   38344   3794.00
994       Robin  Female   7/24/1987         1:35 PM  100765  10982.00
995        Rose  Female   8/25/2002         5:12 AM  134505  11051.00
996     Anthony    Male  10/16/2011         8:35 AM  112769  11625.00
997        Tina  Female   5/15/1997         3:53 PM   56450     19.04
998      George    Male   6/21/2013         5:47 PM   98874   4479.00
999       Henry     NaN  11/23/2014         6:09 AM  132483  16655.00
1000    Phillip    Male   1/31/1984         6:30 AM   42392  19675.00
1001    Russell    Male   5/20/2013        12:39 PM   96914   1421.00
1002      Larry    Male   4/20/2013         4:45 PM   60500  11985.00
1003     Albert    Male   5/15/2012         6:24 PM  129949  10169.00

     Senior Management                  Team
0                 True             Marketing
1                 True                   NaN
2                False               Finance
3                 True               Finance
4                 True       Client Services
5                False                 Legal
6                 True               Product
7                  NaN               Finance
8                 True           Engineering
9                 True  Business Development
```

```
10              True                    NaN
11              True                  Legal
12              True        Human Resources
13             False                  Sales
14              True                Finance
…                  …                      …
989            False                  Legal
990            False              Marketing
991             True                Finance
992            False        Human Resources
993            False                  Legal
994             True        Client Services
995             True              Marketing
996             True                Finance
997             True            Engineering
998             True              Marketing
999            False           Distribution
1000           False                Finance
1001           False                Product
1002           False   Business Development
1003            True                  Sales

[994 rows x 8 columns]
```

5.5 Avoidance of tendencies due to bias

The description of the Iris dataset says, that it consists of **50 samples** from **each of three species** of Iris (Iris setosa, Iris virginica and Iris versicolor), so there are **150 total samples**.

But how to prove it?

5.5.1 Count occurrences of unique values

To prove whether all possible classes included in the dataset and equally distributed, you can use the function `df.value_counts`.

Following parameters can be used for fine tuning: - `dropna=False` causes that NaN values are included - `normalize=True`: relative frequencies of the unique values are returned - `ascending=False`: sort resulting classes descending

[25]:
```
# import (again) data to dataframe from csv file
employees_df = pd.read_csv("./datasets/employees_edit.csv")
```

[26]:
```
# count unique values without missing values in a column,
# ordered descending and normalized
irisdata_df['species'].value_counts(ascending=False, dropna=False, normalize=True)
```

[26]:
```
Iris-setosa        0.333333
Iris-versicolor    0.333333
Iris-virginica     0.333333
Name: species, dtype: float64
```

[27]:
```
# count unique values and missing values in a column,
# ordered descending and not absolute values
employees_df['Team'].value_counts(ascending=False, dropna=False, normalize=False)
```

[27]:
```
Client Services         106
Business Development    103
Finance                 102
Marketing                98
Product                  96
Sales                    94
Engineering              92
Human Resources          92
Distribution             90
Legal                    88
NaN                      43
Name: Team, dtype: int64
```

5.5.2 Display Histogram

This section was inspired by: Pandas Histogram – DataFrame.hist().

Histograms represent **frequency distributions** graphically. This requires the separation of the data into classes (so-called **bins**).

These classes are represented in the histogram as rectangles of equal or variable width. The height of each rectangle then represents the (relative or absolute) **frequency density**.

[28]:
```
employees_df.hist(column=['Salary'])
plt.show()
```

Figure 4: Histogram for frequency distribution of the salary

[29]:
```
employees_df.hist(column='Salary', by='Gender')
plt.show()
```

5.6 First idea of correlations in dataset

To get a rough idea of the **dependencies** and **correlations** in the dataset, it can be helpful to visualize the whole dataset in a **correlation heatmap**. They show in a glance which variables are correlated, to what degree and in which direction.

Later, 2 particularly well correlated variables are selected from the dataset and plotted in a **scatterplot**.

5.6.1 Visualise data with correlation heatmap

This section was inspired by How to Create a Seaborn Correlation Heatmap in Python?.

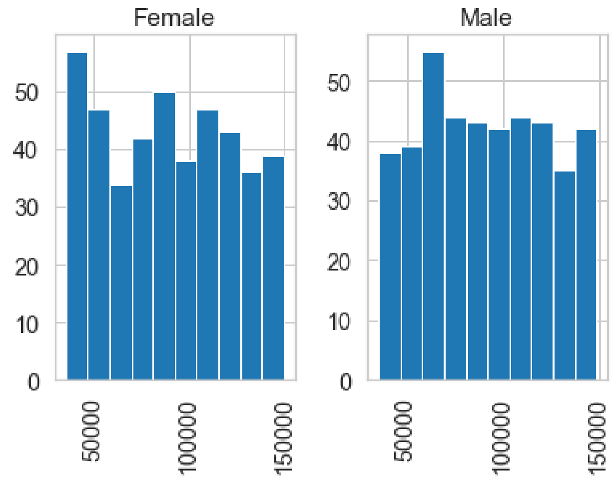

Figure 5: Histogram for the frequency distribution of the salary in comparison between men and women

> **Correlation matrices** are an **essential tool of exploratory data analysis**. Correlation heatmaps contain the same information in a visually appealing way. What more: they show in a glance which variables are correlated, to what degree, in which direction, and alerts us to potential multicollinearity problems (source: ibidem).

Simple correlation matrix Because **string values can never be correlated**, the class names (species) have to be converted first:

[30]:
```
# encoding the class column
irisdata_df_enc = irisdata_df.replace({"species":  {"Iris-setosa":0,
                                                    "Iris-versicolor":1,
                                                    "Iris-virginica":2}})
#irisdata_df_enc
```

[31]:
```
irisdata_df_enc.corr()
```

[31]:

	sepal_length	sepal_width	petal_length	petal_width	species
sepal_length	1.000000	-0.109369	0.871754	0.817954	0.782561
sepal_width	-0.109369	1.000000	-0.420516	-0.356544	-0.419446
petal_length	0.871754	-0.420516	1.000000	0.962757	0.949043
petal_width	0.817954	-0.356544	0.962757	1.000000	0.956464
species	0.782561	-0.419446	0.949043	0.956464	1.000000

Correlation heatmap Choose the color sets from color map.

[32]:
```
# increase the size of the heatmap
plt.figure(figsize=(16, 6))

# store heatmap object in a variable to easily access it
# when you want to include more features (such as title)
# set the range of values to be displayed on the colormap from -1 to 1,
# and set 'annotation=True' to display the correlation values on the heatmap
heatmap = sns.heatmap(irisdata_df_enc.corr(), vmin=-1, vmax=1,
                      annot=True, cmap='PRGn_r')

# give a title to the heatmap
# 'pad=12' defines the distance of the title from the top of the heatmap
```

```
heatmap.set_title('Correlation Heatmap', fontdict={'fontsize':18}, pad=16)
plt.show()
```

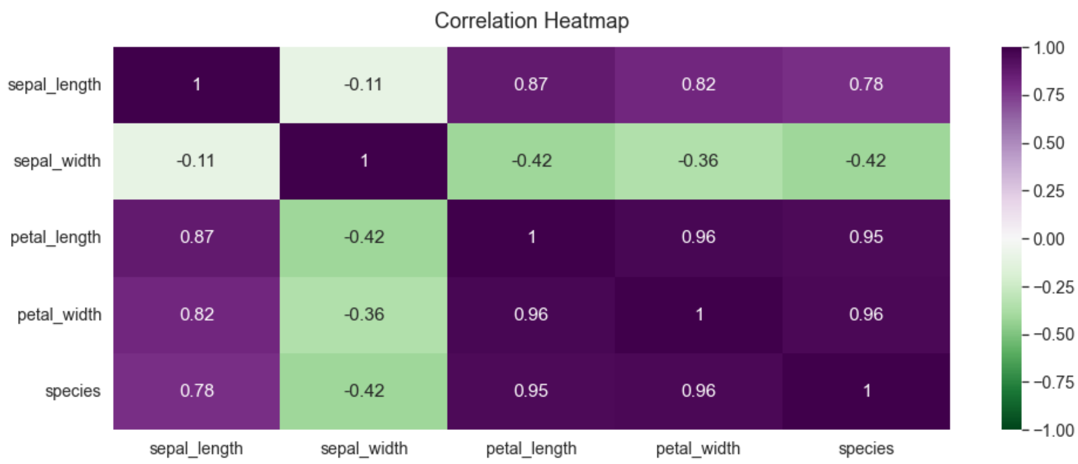

Figure 6: Correlation heatmap to explore coherences between single variables in the iris dataset

Triangle correlation heatmap When looking at the correlation heatmaps above, you would not lose any information by **cutting** away half of it **along the diagonal** line marked by 1-s.

The **numpy** function `np.triu()` can be used to isolate the upper triangle of a matrix while turning all the values in the lower triangle into 0.

[33]:
```
import numpy as np

np.triu(np.ones_like(irisdata_df_enc.corr()))
```

[33]:
```
array([[1., 1., 1., 1., 1.],
       [0., 1., 1., 1., 1.],
       [0., 0., 1., 1., 1.],
       [0., 0., 0., 1., 1.],
       [0., 0., 0., 0., 1.]])
```

Use this mask to cut the heatmap along the diagonal:

[34]:
```
plt.figure(figsize=(16, 6))

# define the mask to set the values in the upper triangle to 'True'
mask = np.triu(np.ones_like(irisdata_df_enc.corr(), dtype=bool))

heatmap = sns.heatmap(irisdata_df_enc.corr(), mask=mask,
                      vmin=-1, vmax=1, annot=True, cmap='PRGn_r')

heatmap.set_title('Triangle Correlation Heatmap', fontdict={'fontsize':18}, pad=16)
plt.show()
```

As a result from the **heatmaps** we can see, that the shape of the **petals** are the **most correlationed columns** (0.96) with the **type of flowers** (species classes).

Somewhat lower correlates **sepal length** with **petal length** (0.87).

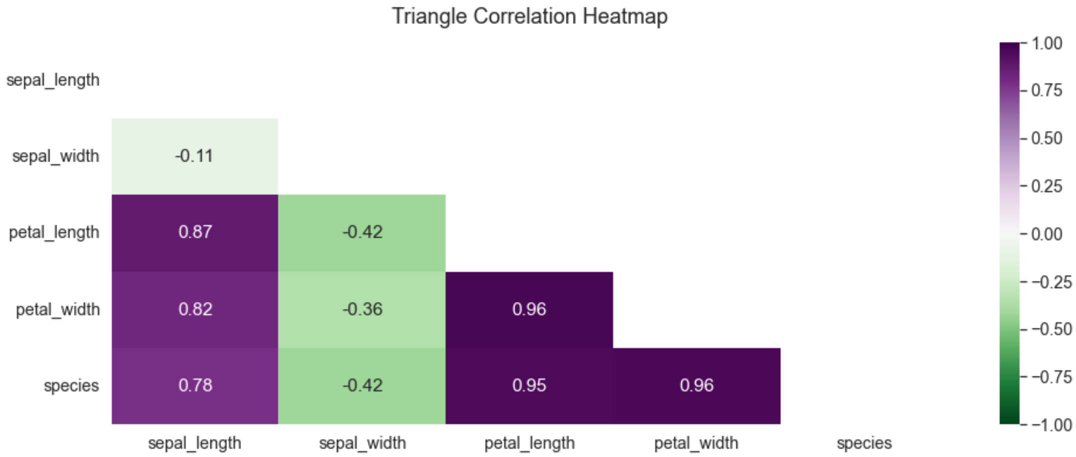

Figure 7: Correlation heatmap, which was cut at its main diagonal without losing any information

5.6.2 Visualise data with scatter plot

In the following, Seaborn is applied which is a library for making statistical graphics in Python. It is built on top of matplotlib and closely integrated with pandas data structures.

To investigate whether there are dependencies (e.g. correlations) in `irisdata_df` between individual variables in the dataset, it is advisable to plot them in a **scatter plot**.

[35]:
```
# There are five preset seaborn themes: darkgrid, whitegrid, dark, white, and ticks.
sns.set_style("whitegrid")
# set scale of fonts
sns.set_context("notebook", font_scale=1.3, rc={"lines.linewidth": 2.5})

# 'sepal_length', 'petal_length' are iris feature data
# 'height' used to define height of graph
# 'hue' stores the class/label of iris dataset
sns.FacetGrid(irisdata_df, hue ="species",
              height = 7).map(plt.scatter,
                              'petal_width',
                              'petal_length').add_legend()


plt.title('Scatterplot of petal length and width')
plt.show()
```

5.6.3 Visualise data with pairs plot

For systematic investigation of dependencies, all variables (each against each) are plotted in separate scatter plots.

With this so called **pairs plot** it is possible to see both **relationships** between two variables and **distribution** of single variables.

This function will create a grid of Axes such that **each numeric variable** in `irisdata_df` will by shared in the y-axis across a single row and in the x-axis across a single column.

[36]:
```
sns.set(font_scale=1.0)
sns.set_style("white")

g = sns.pairplot(irisdata_df, diag_kind="kde", hue='species',
                 palette='Dark2', height=2.5)
```

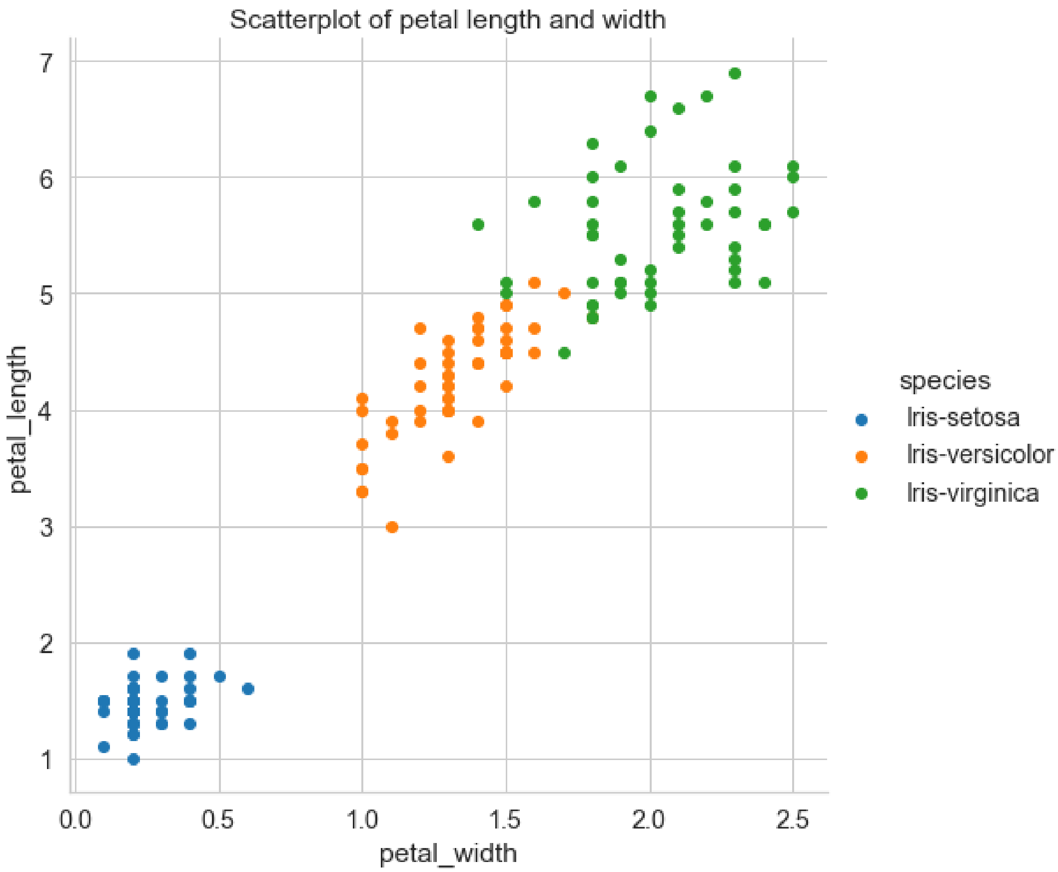

Figure 8: Plotting two individual variables of the iris dataset in the scatterplot to explore the relationships between these two

```
g.map_lower(sns.kdeplot, levels=4, color=".2")
# y .. padding between title and plot
g.fig.suptitle('Pairs plot of the Iris dataset', y=1.05)
plt.show()
```

6 STEP 3: Create the ML model

After exploring the dataset, in this step one has to decide on a specific ML algorithm based on certain selection criteria. Among other ML algorithms suitable for the Iris dataset (such as the decision-tree-based **random-forests classifier**), the reasoned choice here in the tutorial falls on the **support vector classifier (SVC)**. A dedicated SVC model is now being implemented.

6.1 Relationship between AI, ML and others

Sources:

- Emerging technologies based on artificial intelligence to assess quality and consumer preference of beverages, Figure 5

6.2 Taxonomy of machine learning

Sources:

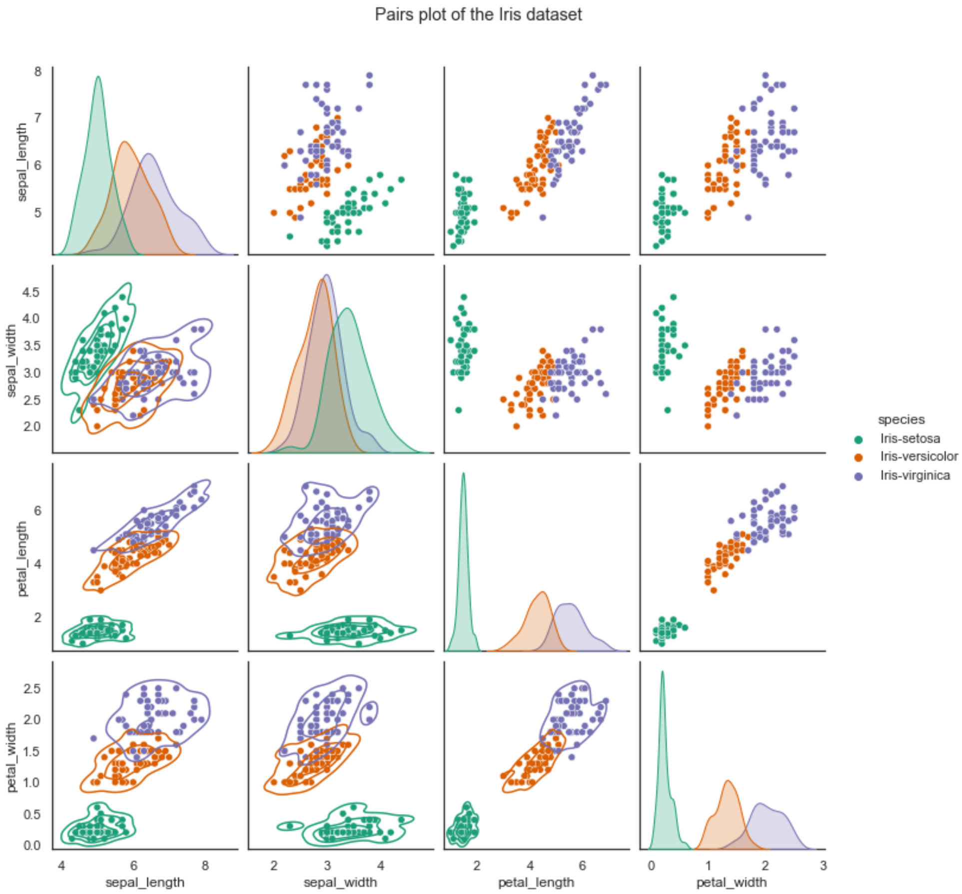

Figure 9: Plot all individual variables of the Iris dataset in pairs plot to see both the relationships between two variables and the distribution of the individual variables

- Taxonomy of machine learning algorithms
- Comprehensive Survey of Machine Learning Approaches in Cognitive Radio-Based Vehicular Ad Hoc Networks, Figure 3
- A Taxonomy of Machine Learning Techniques, Figure 2
- ML Algorithms: One SD
- Machine Learning Map

6.2.1 Supervised learning

6.2.2 Unsupervised learning

6.2.3 Semi-supervised learning

6.2.4 Reinforcement learning

6.3 Decision graph for selecting an ML algorithm

Now that the iris dataset has been analyzed in terms of its data structure and internal correlations, the most difficult task on the way to solving a problem using machine learning arises: finding the “right” ML algorithm (also called **estimator**).

The diverse estimators available are more or less well qualified for the respective problems with their partly very different data types.

Scikit-Learn provides the following **flowchart** as a rough **guide** in choosing the right estimator for the particular task (see: Choosing the right estimator).

However, it must also be emphasized that a considerable level of experience through systematic trial and error is crucial to be successful in finding an “optimal” estimator.

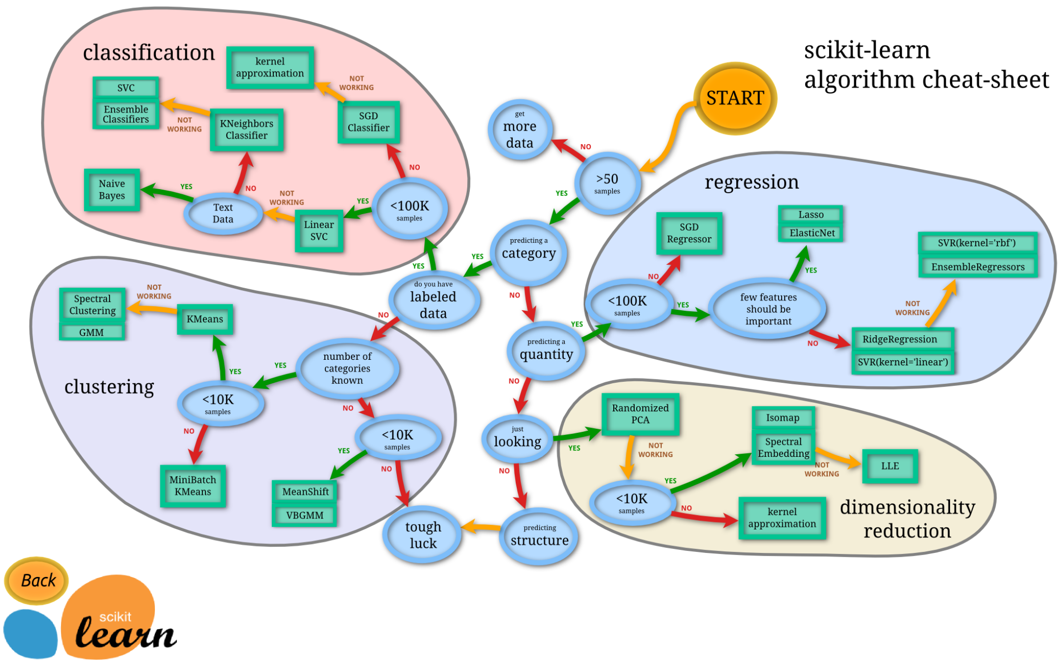

Figure 10: Decision graph for choosing an appropriate ML algorithm (source: Choosing the right estimator, license: unknown)

7 STEP 4: Prepare the dataset for training

In this step the dataset is prepared for the actual classification by SVC. Depending on the selected ML algorithm as well as the data structure, it may be necessary to prepare the data before training (e.g., by **standardization**, **normalization**, or **binarization** based on thresholds). Furthermore, errors in the dataset (e.g. **data gaps**, **duplicates** or obvious **misentries**) should be corrected now at the latest.

Through the intensive exploration of the data in Step 2 (STEP 2: Explore the ML dataset), we know that special **preparation** of the data is **not necessary**. The values are complete and without gaps and there are no duplicates. The values are in similar ranges, which **does not require normalization** of the data.

Furthermore, we know that the **classes** are very **evenly distributed** and thus bias tendencies should be avoided.

8 STEP 5: Carry out training, prediction and testing

8.1 Operating principal of SVC

> Support Vectors Classifiers (SVC) try to **find the best hyperplane to separate** the different classes by maximizing the distance between sample points and the hyperplane (source: In Depth: Parameter tuning for SVC).

The figure **??** shows the operating principal of the SVC algorithm: the hyperplanes *H1* till *H4* (left graphic) do separate the classes. A good separation is achieved by the hyperplane that has the largest distance to the nearest training-data point of any class (so-called functional margin), since in general the larger the margin, the lower the generalization error of the classifier (source: Support-vector machine).

The right graphic shows the optimal hyperplane characterized by maximizing the margin between the classes. The perpendicular distance of the closest data points to the hyperplane determines their position and orientation. These perpendicular distances are the **support vectors** of the hyperplane - this is how the algorithm got its name.

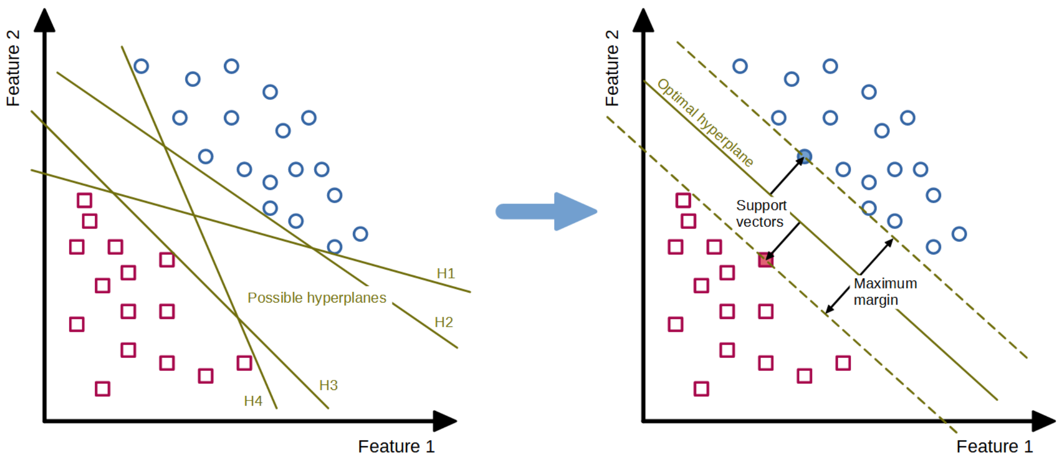

Figure 11: Support Vectors Classifiers (SVC) separate the data points in classes by finding the best hyperplane by maximizing the margin to its support vectors

8.2 Split the dataset

In the next very important step, the dataset is split into **2 subsets**: a **training dataset** and a **test dataset**. As the names suggest, the training dataset is used to train the ML algorithm. The test dataset is then used to check the quality of the trained ML algorithm (here the **recognition rate**). For this purpose, the **class labels** are **removed** from the training dataset - after all, these are to be predicted.

Typically, the **test dataset** should contain about **20%** of the entire dataset.

[40]:
```
from sklearn.model_selection import train_test_split

X = irisdata_df.drop('species', axis=1)
y = irisdata_df['species']

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size = 0.20)
```

For training, do not use only the variables that correlate best with each other, but all of them.

Otherwise, the result of the prediction would be significantly worse. Maybe this is already an indication of **overfitting** of the ML model.

[38]:
```
# DO NOT USE THIS!!
X_train, X_test, y_train, y_test = train_test_split(X[['sepal_length',
                                                       'sepal_width']],
                                                    y, test_size = 0.20)
```

8.3 Create the SVM model

In this step we create the SVC model and fit it to our training data.

[41]:
```
from sklearn.svm import SVC
classifier = SVC(kernel = 'linear', random_state = 0)

# fit the model for the data
classifier.fit(X_train, y_train)
```

[41]:
```
SVC(kernel='linear', random_state=0)
```

8.4 Make predictions

[42]:
```
y_pred = classifier.predict(X_test)
#X_test
```

9 STEP 6: Evaluate model's performance

Subsequently to the training of the SVC model and the classification predictions made based on the test data, this step evaluates the **quality of the classification result** using known **metrics** such as the **accuracy score** as well as the **confusion matrix**.

9.1 Accuracy Score

In a multilabel classification (such as the Iris dataset), this **Accuracy classification score** computes the subset accuracy. For further details see sklearn.metrics.accuracy_score.

[54]:
```
from sklearn.metrics import accuracy_score

acc_score = accuracy_score(y_test, y_pred)

print("Accuracy score: {:.2f} %".format(acc_score.mean()*100))
```

```
Accuracy score: 96.67 %
```

9.2 Classification Report

The classification report shows a representation of the main **classification metrics on a per-class basis**. This gives a deeper intuition of the classifier behavior over global accuracy which can mask functional weaknesses in one class of a multiclass problem (see Classification Report).

[52]:
```
from sklearn.metrics import classification_report

print(classification_report(y_test, y_pred))
```

```
                 precision    recall  f1-score   support

    Iris-setosa       1.00      1.00      1.00         4
Iris-versicolor       1.00      0.92      0.96        13
 Iris-virginica       0.93      1.00      0.96        13

       accuracy                           0.97        30
      macro avg       0.98      0.97      0.97        30
   weighted avg       0.97      0.97      0.97        30
```

9.3 Cross-validation score

The function `cross_val_score()` from the Scikit-learn package **trains and tests a model over multiple folds** of your dataset. This cross validation method gives a better **understanding of model performance** over the whole dataset instead of just a single train/test split (see Using cross_val_score in sklearn, simply explained).

[49]:
```
from sklearn.model_selection import cross_val_score

accuracies = cross_val_score(estimator = classifier, X = X_train,
                             y = y_train, cv = 10)

print("Cross-validation score: {:.2f} %".format(accuracies.mean()*100))
print("Standard Deviation: {:.2f} %".format(accuracies.std()*100))
```

```
Cross-validation score: 98.33 %
Standard Deviation: 3.33 %
```

9.4 Confusion matrix

The **confusion matrix** measures the quality of predictions from a classification model by looking at how many **predictions** are **True** and how many are **False** (see What the Confusion Matrix Measures?.

9.4.1 Textual confusion matrix

For checking the accuracy of the model, the **confusion matrix** can be used for the **cross validation**.

By using the function `sklearn.metrics.confusion_matrix()` a confusion matrix of the true iris class labels versus the predicted class labels is plotted.

[44]:
```
cm = metrics.confusion_matrix(y_test, y_pred)
print(cm)
```

```
[[ 4  0  0]
 [ 0 12  1]
 [ 0  0 13]]
```

9.4.2 Colored confusion matrix

The function `sklearn.metrics.ConfusionMatrixDisplay()` plots a colored confusion matrix.

[45]:
```
sns.set_style("white")

# print colored confusion matrix
cm_colored = metrics.ConfusionMatrixDisplay.from_predictions(y_test, y_pred)

cm_colored.figure_.suptitle("Colored Confusion Matrix")
cm_colored.figure_.set_figwidth(8)
cm_colored.figure_.set_figheight(7)

cm_colored.confusion_matrix

# save figure as PNG
plt.tight_layout()
plt.savefig('images/confusion_matrix.png', dpi=150, pad_inches=5)
plt.show()
```

10 STEP 7: Vary parameters of the ML model manually

This section was inspired by In Depth: Parameter tuning for SVC

In this section, the 4 SVC parameters `kernel`, `gamma`, `C` and `degree` will be introduced one by one. Furthermore, their influence on the classification result by varying these single parameters will be shown.

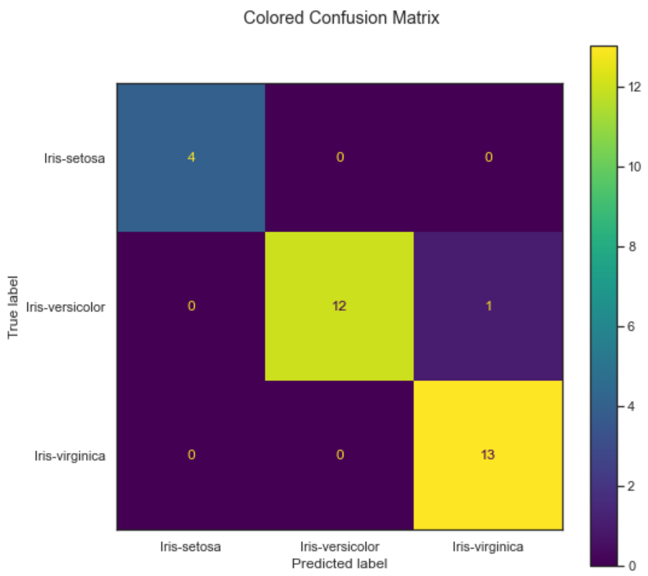

Figure 12: Checking the accuracy of the model by using the confusion matrix for cross-validation

Disclaimer: In order to show the effects of varying the individual parameters in 2D graphs, only the best correlating variables `petal_length` and `petal_width` are used to train the SVC.

10.1 Prepare dataset

[142]:
```
from sklearn.svm import SVC
from sklearn.model_selection import train_test_split
from sklearn.model_selection import cross_val_score
import numpy as np

# import iris dataset again
irisdata_df = pd.read_csv('./datasets/IRIS_flower_dataset_kaggle.csv')

# encode the class column from class strings to integer equivalents
irisdata_df_enc = irisdata_df.replace({"species":  {"Iris-setosa":0,
                                                     "Iris-versicolor":1,
                                                     "Iris-virginica":2}})
#irisdata_df_enc
```

10.1.1 Prepare datasets for parameter variation and plotting

These datasets will be used for parameter variation and plotting only. In particular, for later **2D plotting** of the effects of parameter variation, only **2 variables** of the iris dataset can be used.

However, as seen in the previous section, this selection is very much at the expense of detection accuracy. Therefore, it is not useful to make predictions with this subset of data - it is not necessary to divide it into a training and a test dataset.

[143]:
```
# copy only 2 feature columns
# and convert pandas dataframe to numpy array
X_plot = irisdata_df_enc[['petal_length', 'petal_width']].to_numpy(copy=True)
#X_plot = irisdata_df_enc[['sepal_length', 'sepal_width']].to_numpy(copy=True)
#X_plot
```

[144]:
```
# convert pandas dataframe to numpy array
# and get a flat 1D copy of 2D numpy array
y_plot = irisdata_df_enc[['species']].to_numpy(copy=True).flatten()
#y_plot
```

10.1.2 Prepare dataset for prediction and evaluation

To **evaluate the recognition accuracy** by parameter variation, the complete iris dataset with all variables must be used. To make predictions with test data, the dataset is again divided into a training and a test dataset.

[145]:
```
X = irisdata_df.drop('species', axis=1)
y = irisdata_df['species']

X_train, X_test, y_train, y_test = train_test_split(X, y, test_size = 0.20)
```

10.2 Plotting functions

This function helps to visualize the modifications by varying the individual SVC parameters:

[146]:
```
def plotSVC(title, svc, X, y, xlabel, ylabel):
    # create a mesh to plot in
    x_min, x_max = X[:, 0].min() - 1, X[:, 0].max() + 1
    y_min, y_max = X[:, 1].min() - 1, X[:, 1].max() + 1

    # prevent division by zero
    if x_min == 0.0:
        x_min = 0.1

    h = (x_max / x_min)/1000
    xx, yy = np.meshgrid(np.arange(x_min, x_max, h), np.arange(y_min, y_max, h))

    plt.subplot(1, 1, 1)
    Z = svc.predict(np.c_[xx.ravel(), yy.ravel()])
    Z = Z.reshape(xx.shape)

    plt.contourf(xx, yy, Z, cmap=plt.cm.Paired, alpha=0.6)
    plt.scatter(X[:, 0], X[:, 1], c=y, cmap=plt.cm.Paired)
    plt.xlabel(xlabel)
    plt.ylabel(ylabel)
    plt.xlim(xx.min(), xx.max())
    plt.title(title)
    plt.show()
```

This function cares for cross validation:

[168]:
```
def crossValSVC(X_train, y_train, kernel='rbf', gamma='scale', C=1.0, degree=3):
    # train the SVC
    svc = svm.SVC(kernel=kernel,
                  gamma=gamma,
                  C=C,
                  degree=degree).fit(X_train, y_train)
    # calculate accuracies
    accuracies = cross_val_score(estimator = svc, X = X_train,
                                 y = y_train, cv = 10)

    accuracy = accuracies.mean()*100
```

```
    return accuracy
```

This function plots the variation of the SVC parameters against the prediction accuracy to show the effect of variation and its limits regarding the phenomenon **overfitting**:

[182]:
```
def plotParamsAcc(param_list, acc_list, param_name, log_scale=False):
    fig, ax = plt.subplots(figsize=(10,6))
    title_str = 'Variation of {} parameter '.format(param_name) \
                +'and its effect to prediction accuracy'
    plt.title(title_str)
    ax.plot(param_list, accuracy_list)
    if log_scale:
        # set the X axis scale to logarithmic
        ax.set_xscale('log')
    plt.xlabel(param_name)
    plt.ylabel('accuracy [%]')
    plt.grid()
    plt.show()
```

10.3 Vary `kernel` of SVC

The `kernel` parameter selects the type of hyperplane that is used to separate the data. Using `linear` (linear classifier) kernel will use a linear hyperplane (a line in the case of 2D data). The `rbf` (radial basis function kernel) and `poly` (polynomial kernel) kernel use non linear hyperplanes. The **default** is `kernel=rbf`.

[149]:
```
kernels = ['linear', 'rbf', 'poly', 'sigmoid']

xlabel = 'Petal length'
ylabel = 'Petal width'

for kernel in kernels:
    svc_plot = svm.SVC(kernel=kernel).fit(X_plot, y_plot)
    accuracy = crossValSVC(X_train, y_train, kernel=kernel)
    title_str = 'kernel: \''+str(kernel)+'\', '+'Acc. prediction: {:.2f}%'.
 ↪format(accuracy)
    plotSVC(title_str, svc_plot, X_plot, y_plot, xlabel, ylabel)
```

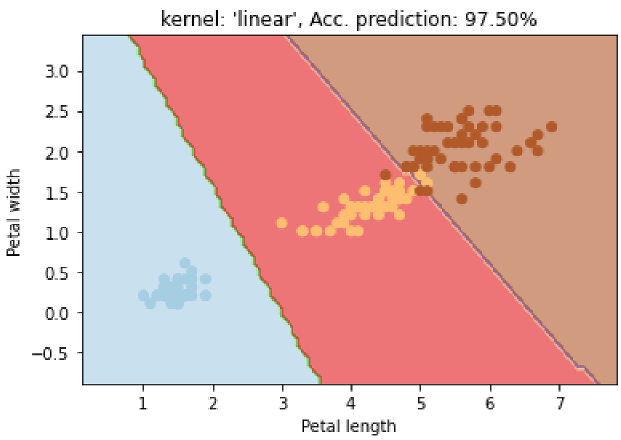

Figure 13: This group of images shows the effect on the classification by the choice of the different SVC kernels ('linear', 'rbf', 'poly' and 'sigmoid')

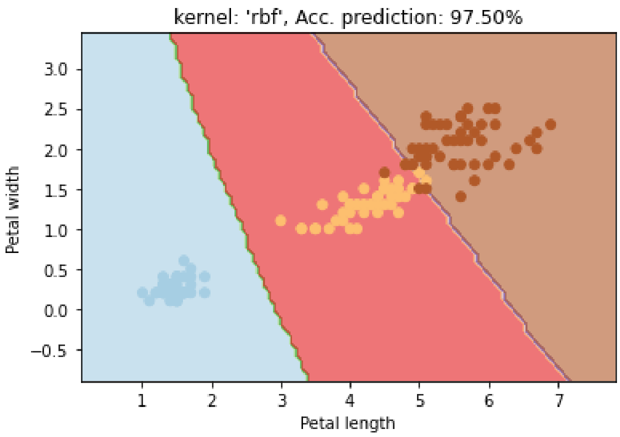

Figure 14: This group of images shows the effect on the classification by the choice of the different SVC kernels ('linear', 'rbf', 'poly' and 'sigmoid')

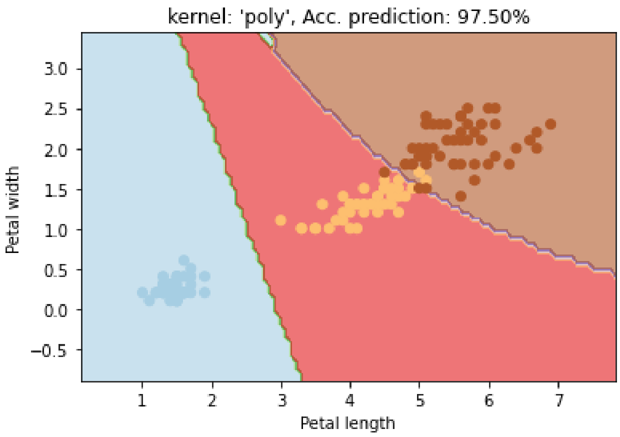

Figure 15: This group of images shows the effect on the classification by the choice of the different SVC kernels ('linear', 'rbf', 'poly' and 'sigmoid')

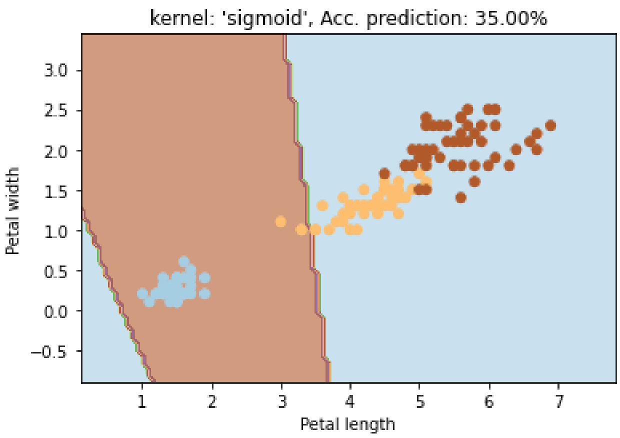

Figure 16: This group of images shows the effect on the classification by the choice of the different SVC kernels ('linear', 'rbf', 'poly' and 'sigmoid')

10.4 Vary `gamma` parameter

The `gamma` parameter is used for **non linear hyperplanes**. The higher the `gamma` float value it tries to exactly fit the training dataset. The **default** is `gamma='scale'`.

[175]:
```python
gammas = [0.1, 1, 10, 100, 200]

xlabel = 'Petal length'
ylabel = 'Petal width'

for gamma in gammas:
    svc_plot = svm.SVC(kernel='rbf', gamma=gamma).fit(X_plot, y_plot)
    accuracy = crossValSVC(X_train, y_train, kernel='rbf', gamma=gamma)
    title_str = 'gamma: \''+str(gamma)+'\', ' \
                +'Acc. prediction: {:.2f}%'.format(accuracy)
    plotSVC(title_str, svc_plot, X_plot, y_plot, xlabel, ylabel)
```

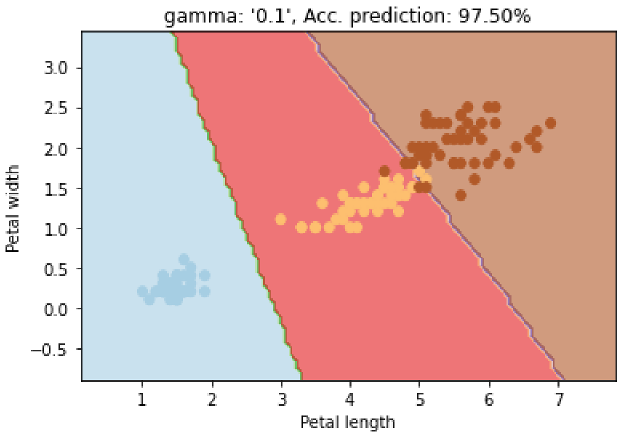

Figure 17: This group of images shows the effect on the classification by the variation of the parameter 'gamma' of the 'rbf' kernel

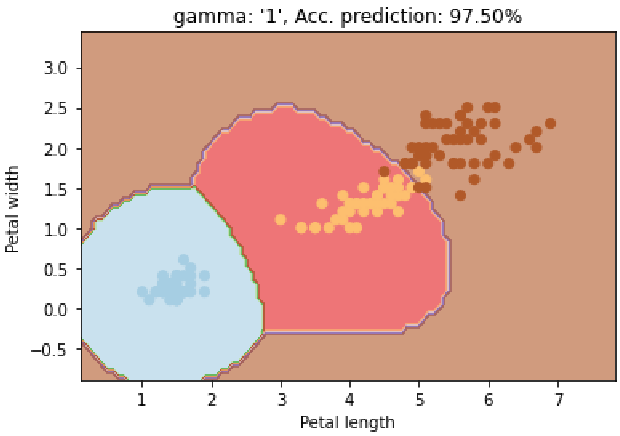

Figure 18: This group of images shows the effect on the classification by the variation of the parameter 'gamma' of the 'rbf' kernel

Show the variation of the SVC parameter `gamma` against the **prediction accuracy**.

As we can see, increasing `gamma` leads to **overfitting** as the classifier tries to perfectly fit the training data.

[184]:
```python
gammas = [0.1, 0.2, 0.3, 0.4, 0.5, 0.6, 0.7, 0.8, 0.9, 1, 10, 100, 200]

accuracy_list = list()
for gamma in gammas:
    accuracy = crossValSVC(X_train, y_train, kernel='rbf', gamma=gamma)
```

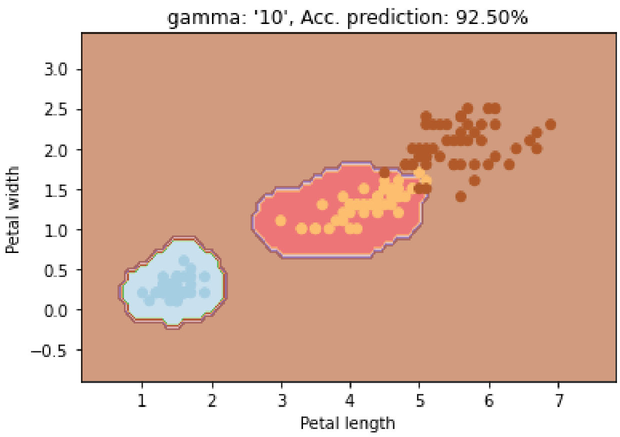

Figure 19: This group of images shows the effect on the classification by the variation of the parameter 'gamma' of the 'rbf' kernel

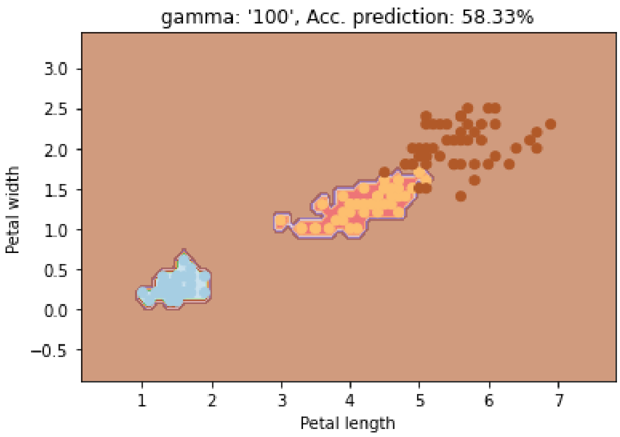

Figure 20: This group of images shows the effect on the classification by the variation of the parameter 'gamma' of the 'rbf' kernel

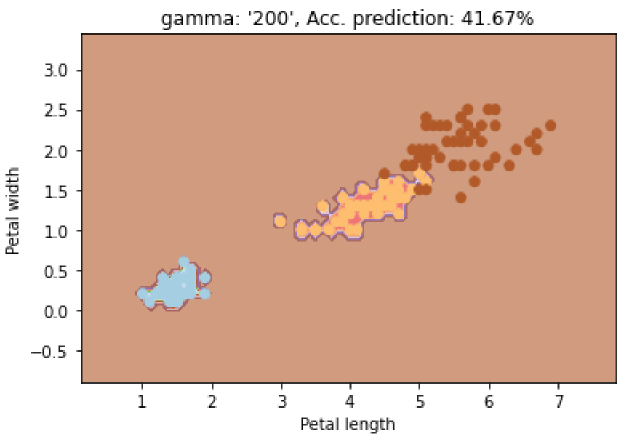

Figure 21: This group of images shows the effect on the classification by the variation of the parameter 'gamma' of the 'rbf' kernel

```
    accuracy_list.append(accuracy)

plotParamsAcc(gammas, accuracy_list, 'gamma', log_scale=True)
```

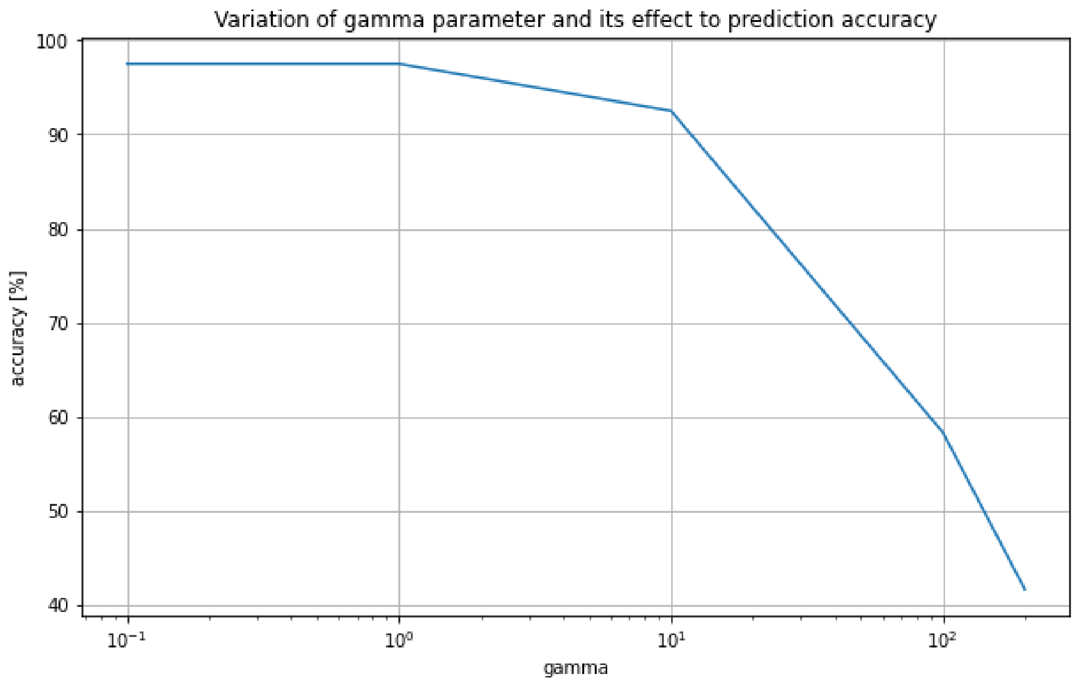

Figure 22: The plot shows the variation of the SVC parameter 'gamma' against the prediction accuracy

10.5 Vary C parameter

The C parameter is the **penalty** of the error term. It controls the trade off between smooth decision boundary and classifying the training points correctly. The **default** is C=1.0.

[172]:
```
cs = [0.1, 1, 5, 10, 100, 1000, 10000]

xlabel = 'Petal length'
ylabel = 'Petal width'

for c in cs:
    svc_plot = svm.SVC(kernel='rbf', C=c).fit(X_plot, y_plot)
    accuracy = crossValSVC(X_train, y_train, kernel='rbf', C=c)
    title_str = 'C: \''+str(c)+'\', ' \
                +'Acc. prediction: {:.2f}%'.format(accuracy)
    plotSVC(title_str, svc_plot, X_plot, y_plot, xlabel, ylabel)
```

Show the variation of the SVC parameter C against the **prediction accuracy**.

But be careful: to high C values may lead to **overfitting** the training data.

[185]:
```
cs = [0.1, 1, 5, 6, 7, 8, 10, 100, 1000, 10000]

accuracy_list = list()
for c in cs:
    accuracy = crossValSVC(X_train, y_train, kernel='rbf', C=c)
    accuracy_list.append(accuracy)

plotParamsAcc(cs, accuracy_list, 'C', log_scale=True)
```

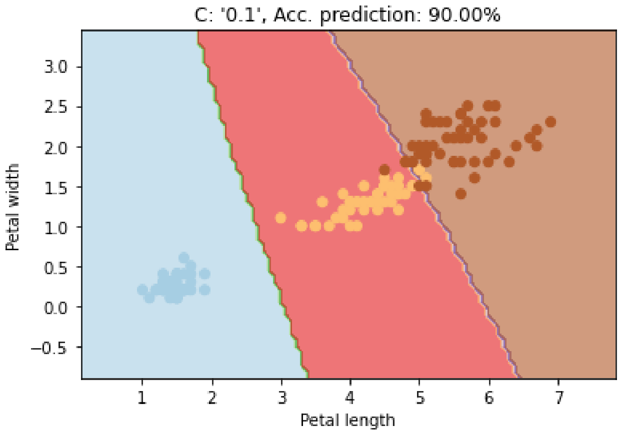

Figure 23: This group of images shows the effect on the classification by the variation of the parameter 'C' of the 'rbf' kernel

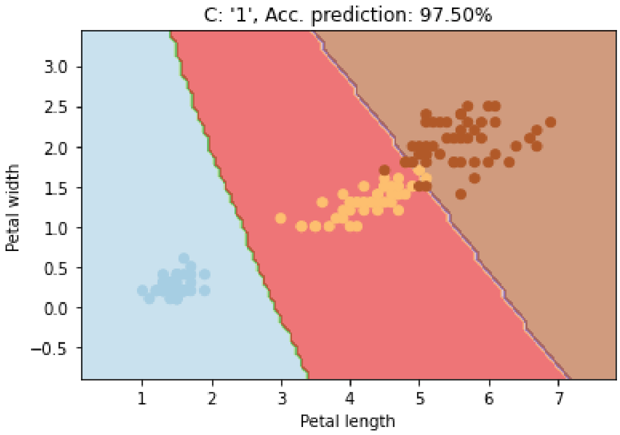

Figure 24: This group of images shows the effect on the classification by the variation of the parameter 'C' of the 'rbf' kernel

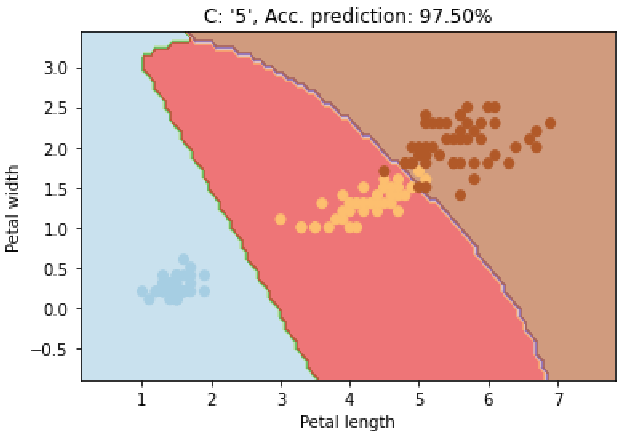

Figure 25: This group of images shows the effect on the classification by the variation of the parameter 'C' of the 'rbf' kernel

10.6 Vary `degree` parameter

The `degree` parameter is used when the `kernel` is set to `poly` and is ignored by all other kernels. It's basically the **degree of the polynomial** used to find the hyperplane to split the data. The **default** is

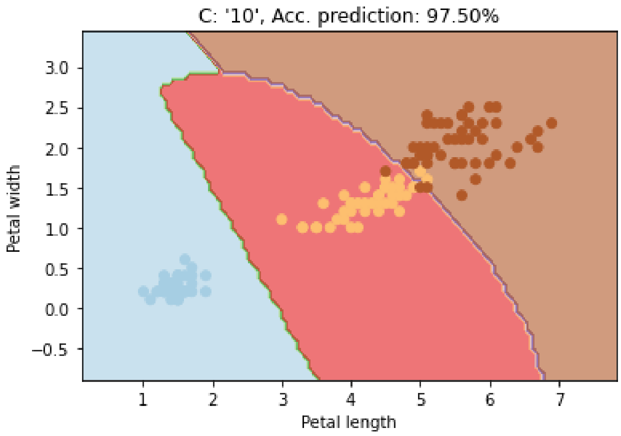

Figure 26: This group of images shows the effect on the classification by the variation of the parameter 'C' of the 'rbf' kernel

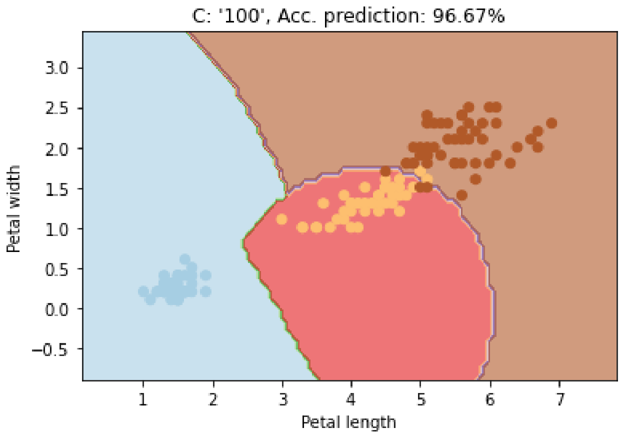

Figure 27: This group of images shows the effect on the classification by the variation of the parameter 'C' of the 'rbf' kernel

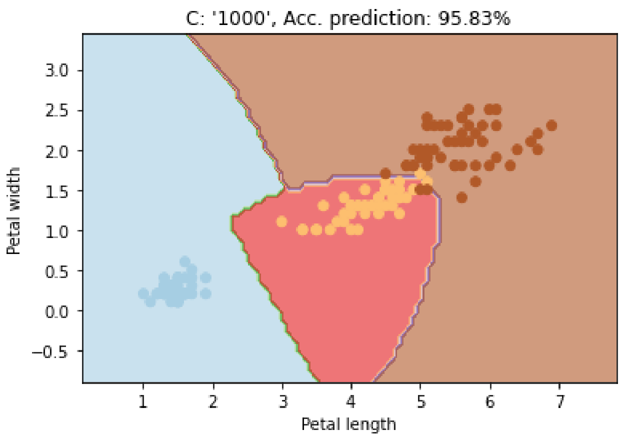

Figure 28: This group of images shows the effect on the classification by the variation of the parameter 'C' of the 'rbf' kernel

`degree=3`.

Using `degree = 1` is the same as using a `linear` kernel. Also, increasing this parameters leads to **higher training times**.

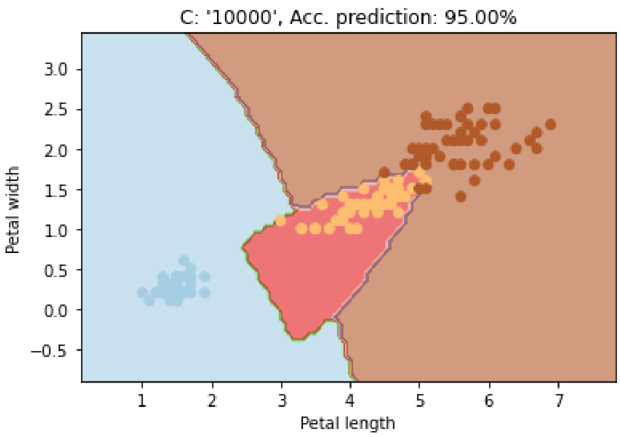

Figure 29: This group of images shows the effect on the classification by the variation of the parameter 'C' of the 'rbf' kernel

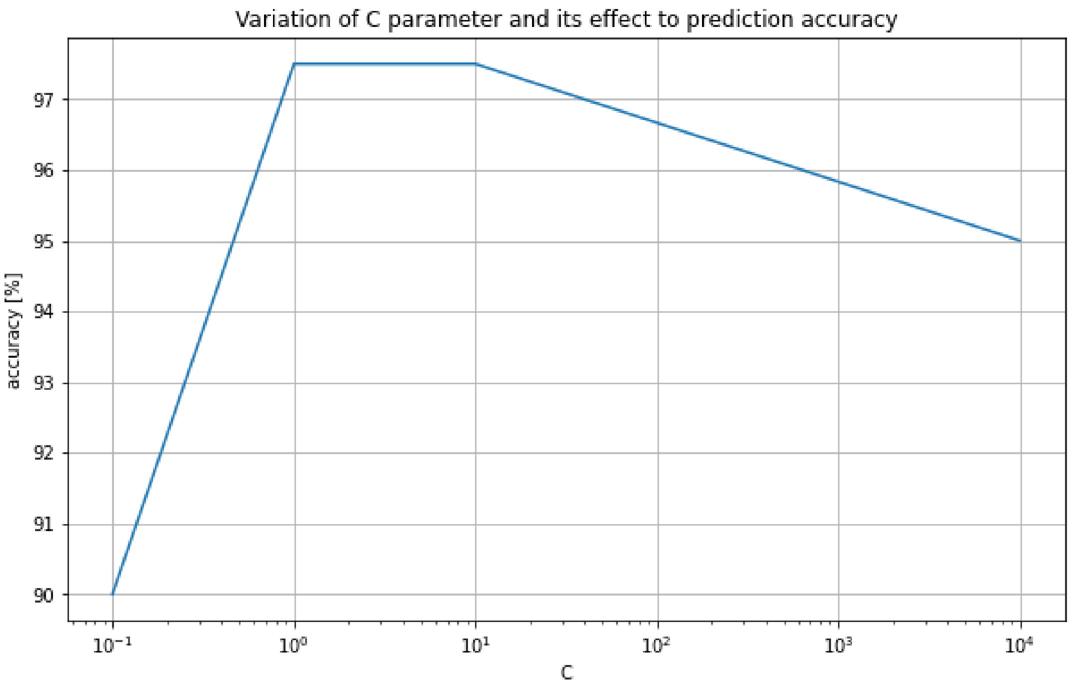

Figure 30: The plot shows the variation of the SVC parameter 'C' against the prediction accuracy

[173]:
```
degrees = [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]

xlabel = 'Petal length'
ylabel = 'Petal width'

for degree in degrees:
    svc_plot = svm.SVC(kernel='poly', degree=degree).fit(X_plot, y_plot)
    accuracy = crossValSVC(X_train, y_train, kernel='poly', degree=degree)
    title_str = 'degree: \''+str(degree)+'\', ' \
                +'Acc. prediction: {:.2f}%'.format(accuracy)
    plotSVC(title_str, svc_plot, X_plot, y_plot, xlabel, ylabel)
```

Show the variation of the SVC parameter `degree` against the **prediction accuracy**.

As we can see, increasing the `degree` of the polynomial hyperplane leads to **overfitting** the training

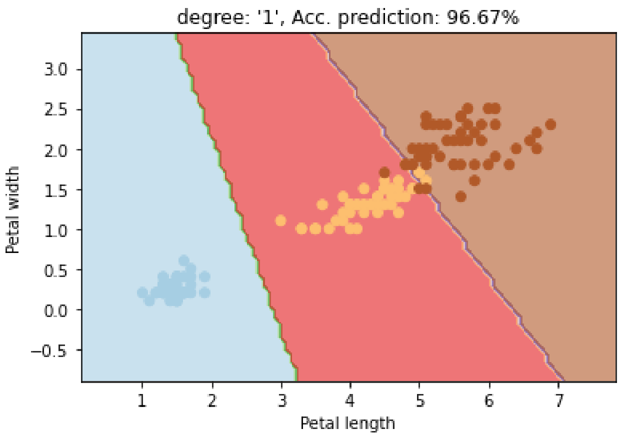

Figure 31: This group of images shows the effect on the classification by the variation of the parameter 'degree' of the 'poly' kernel

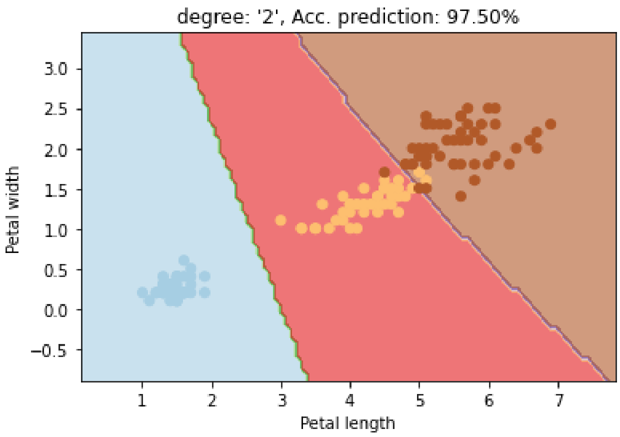

Figure 32: This group of images shows the effect on the classification by the variation of the parameter 'degree' of the 'poly' kernel

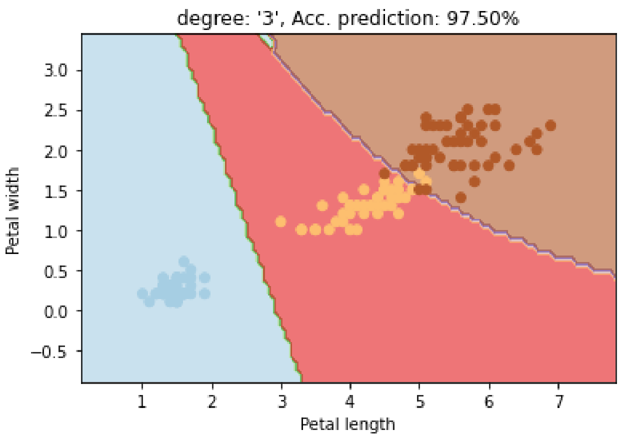

Figure 33: This group of images shows the effect on the classification by the variation of the parameter 'degree' of the 'poly' kernel

data.

[186]:
```
degrees = [1, 2, 3, 4, 5, 6, 7, 8, 9, 10]
```

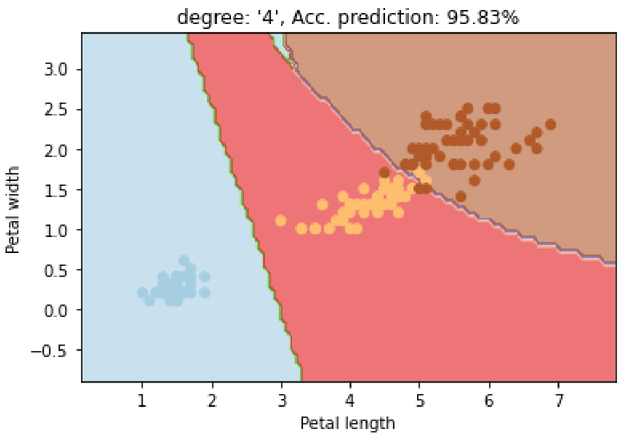

Figure 34: This group of images shows the effect on the classification by the variation of the parameter 'degree' of the 'poly' kernel

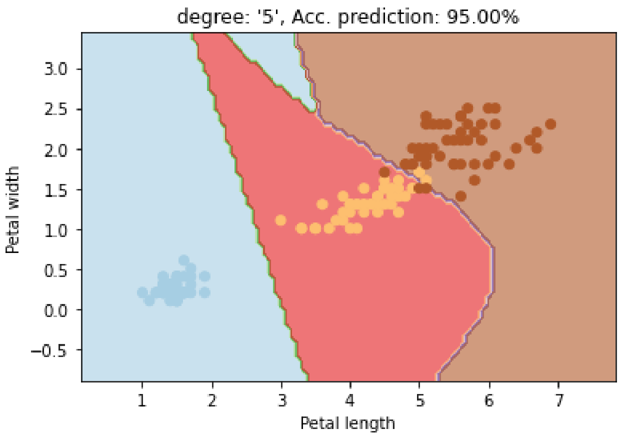

Figure 35: This group of images shows the effect on the classification by the variation of the parameter 'degree' of the 'poly' kernel

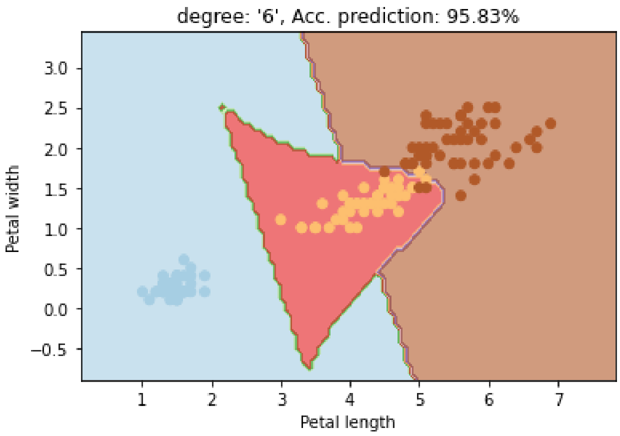

Figure 36: This group of images shows the effect on the classification by the variation of the parameter 'degree' of the 'poly' kernel

```
accuracy_list = list()
for degree in degrees:
    accuracy = crossValSVC(X_train, y_train, kernel='poly', degree=degree)
```

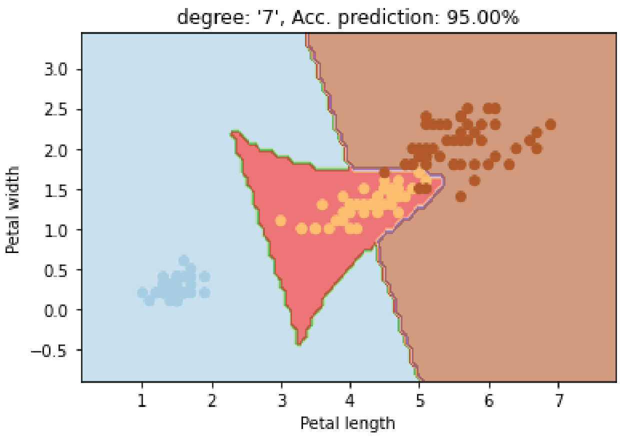

Figure 37: This group of images shows the effect on the classification by the variation of the parameter 'degree' of the 'poly' kernel

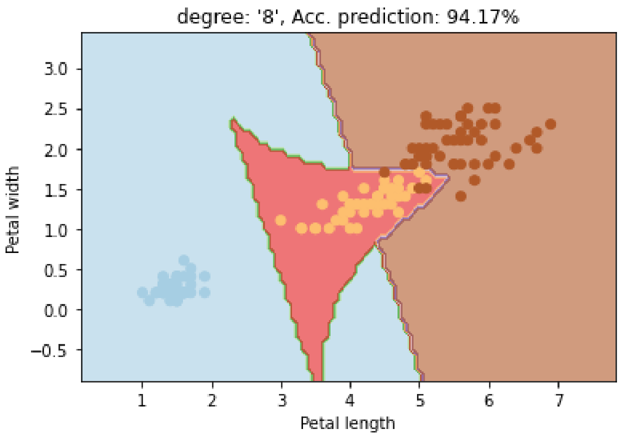

Figure 38: This group of images shows the effect on the classification by the variation of the parameter 'degree' of the 'poly' kernel

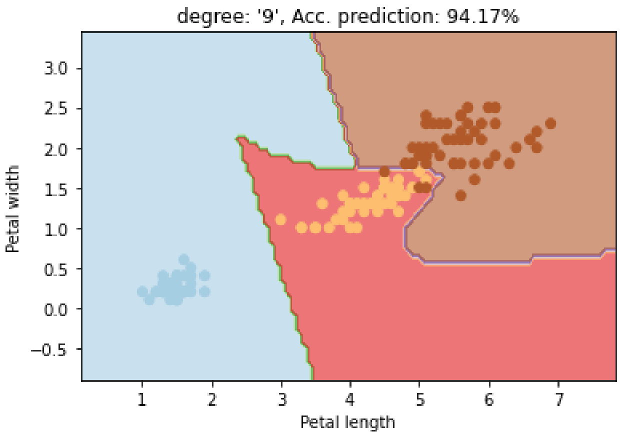

Figure 39: This group of images shows the effect on the classification by the variation of the parameter 'degree' of the 'poly' kernel

```
    accuracy_list.append(accuracy)

plotParamsAcc(degrees, accuracy_list, 'degree', log_scale=False)
```

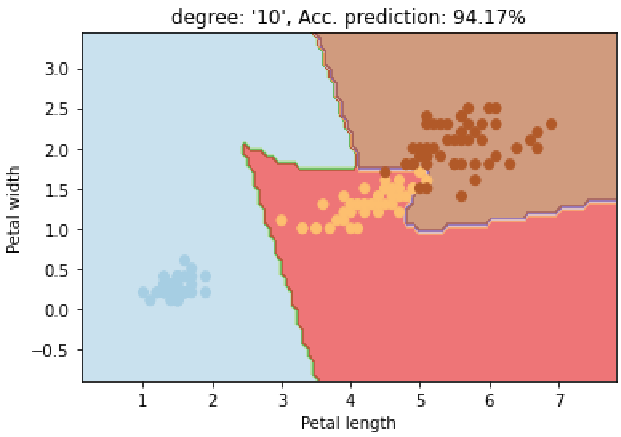

Figure 40: This group of images shows the effect on the classification by the variation of the parameter 'degree' of the 'poly' kernel

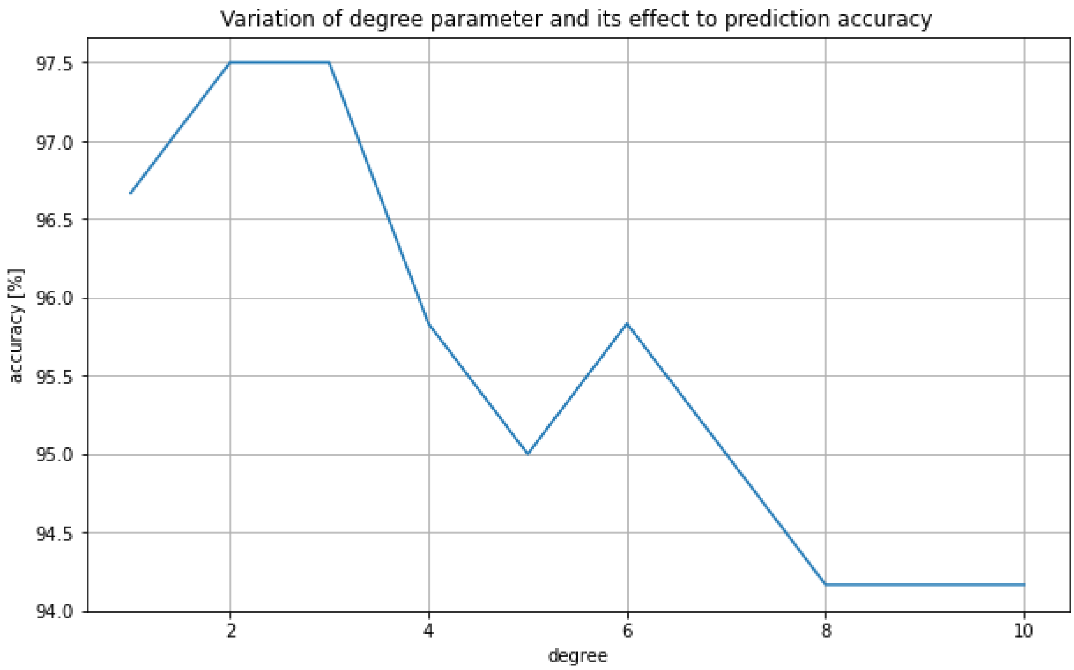

Figure 41: The plot shows the variation of the SVC parameter 'degree' against the prediction accuracy

11 STEP 8: Tune the ML model systematically

In the final step, two approaches to systematic hyper-parameter search are presented: **Grid Search** and **Randomized Search**. While the former exhaustively considers all parameter combinations for given values, the latter selects a number of candidates from a parameter space with a particular random distribution.

Sources:

- 3.2. Tuning the hyper-parameters of an estimator
  - sklearn.model_selection.GridSearchCV
  - sklearn.model_selection.RandomizedSearchCV

11.1 Grid Search

11.2 Randomized Search

12 Summary and conclusions

```
[ ]:
```