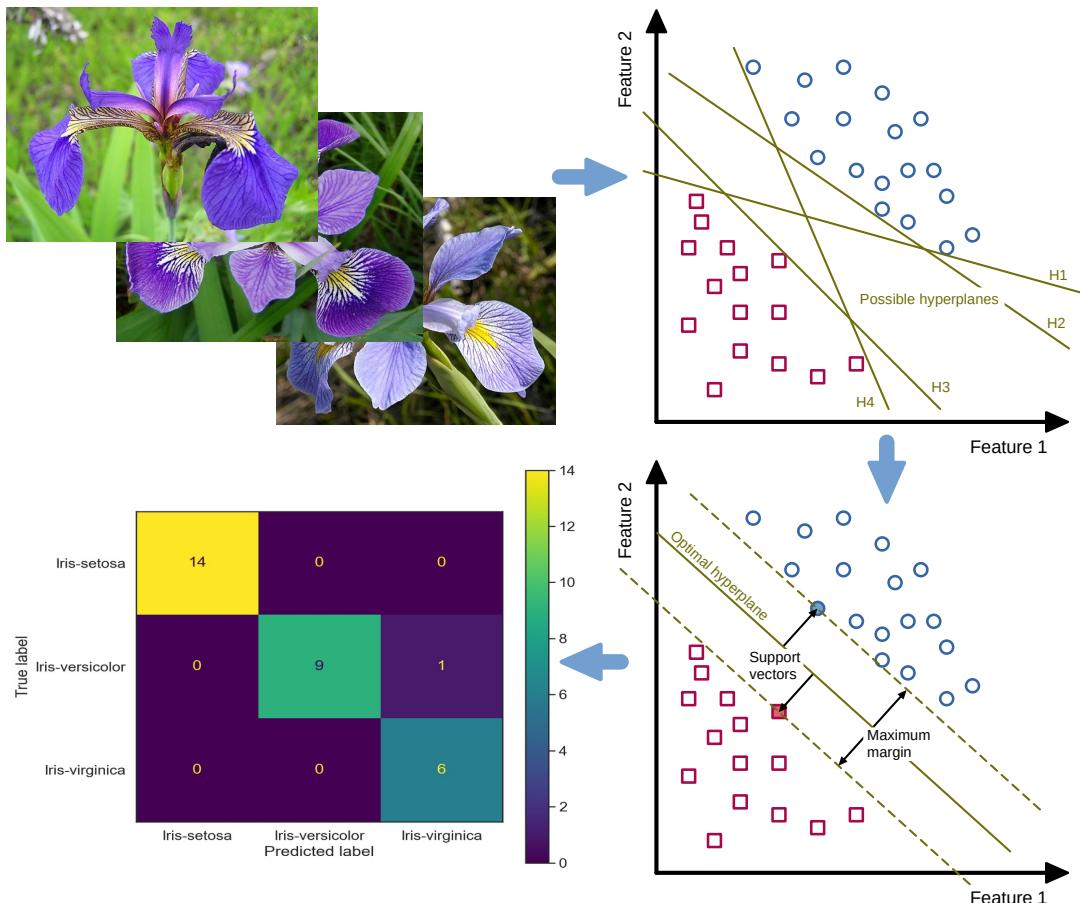


# Getting started with Machine Learning (ML) and Support Vector Classifiers (SVC) - A systematic step-by-step approach

Dipl.-Ing. Björn Kasper ([kasper.bjoern@bgetem.de](mailto:kasper.bjoern@bgetem.de))

*Test and Certification Body for Electrical Engineering at BG ETEM*

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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.



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# 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** or **Machine Learning**. 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**. 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 **Sprachassistentensystemen** (ähnlich z. B. Siri oder Alexa aus dem privaten Umfeld) bis hin zu teil- oder gar **vollautonomen Systemen**. Solche vollautonomen Systeme sind beispielsweise sogenannte **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 **Zuverlässigkeit** 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** bzw. **Maschinellem Lernen**. 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**. 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 sogenannte **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:

- **STEP 0:** Select hardware and software suitable for ML
- **STEP 1:** Acquire the ML dataset
- **STEP 2:** Explore the ML dataset
- **STEP 3:** Choose and create the ML model
- **STEP 4:** Prepare the dataset for training
- **STEP 5:** Carry out training, prediction and testing
- **STEP 6:** Evaluate model's performance
- **STEP 7:** Vary parameters of the ML model manually
- **STEP 8:** Tune the ML model systematically

## 2 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.

This is a test citation (Kasper 2019) and another (Barney 2012).

### 2.1 Hardware

When considering hardware requirements, two systems and their use cases must be taken into account: the **training system** and the **application system**.

#### 2.1.1 Training system

The **training phase** requires a lot of **computational power** and **memory (RAM)**, depending on the **amount of data** to be processed and the **ML algorithm (so-called estimator)** chosen.

Depending on the estimator model, highly parallel processing on a **Graphics Processing Unit (GPU)** can provide significant **speed advantages** over processing on a **Central Processing Unit (CPU)** (e.g., when training deep neural networks in the area of **deep learning**). To take advantage of this speed benefit, the AI application must be suitable in terms of **parallelizability** of the estimator model used as well as **GPU support** through special driver layers (so-called Operating System Abstraction Layer (OSAL)).

Such GPUs are installed on powerful **3D graphics cards**. However, these must be explicitly qualified for the application for AI - not every game-suitable 3D graphics card from any manufacturer can be used. The manufacturer **Nvidia** offers GPUs suitable for AI in its high-performance graphics cards with **CUDA architecture**. **CUDA** stands for “Compute Unified Device Architecture” and is a **programming interface** (API) developed by Nvidia, with which program parts can be processed by the graphics processor (GPU). The GPU works significantly faster than the CPU, especially with highly parallelizable program sequences (high data parallelism). This speed advantage can be considerable despite currently available CPU technologies like **Multicore** and **Hyper-Threading** with Intel CPUs!

However, it should be mentioned that currently only the manufacturer Nvidia offers 3D graphics cards with CUDA implementation, since CUDA is a **proprietary** framework. In addition, there is also the much less well-known **open source** alternative **OpenCL**, which has now been implemented by a large number of graphics card manufacturers. Since OpenCL is an **open industry standard**, Intel and AMD chips and their GPUs, ATI Radeon cards of the 5, 6, 7 and R9 series as well as various Nvidia GeForce cards are supported, for example.

Nvidia graphics cards with CUDA-supporting GPUs can be found listed by their **compute capability** (the higher the value, the better) here: [CUDA GPUs - Compute Capability](#).

Regarding the **code execution performance** of both alternatives in direct comparison, there are different statements in the technical literature. While the 2010 paper [A Performance Comparison of CUDA and OpenCL](#) sees the CUDA implementation as the clear favorite, more recent publications point out the strong dependence of performance on **code quality**, **algorithm type** and the **GPU hardware** used, among other things (see e.g. here: [CUDA vs OpenCL: Which to Use for GPU Programming](#)).

It is therefore recommended that the decision for **CUDA or OpenCL** should depend on the extent to which most of the applications employed and the GPU hardware used are better supported by one of the two approaches in each case.

The **state of the art** should be also taken into account when selecting the rest of the training system's hardware. Otherwise, seemingly (price-wise) inexpensive components could very quickly nullify the speed advantage of the GPU. In addition to a mainboard suitable for one (or more) high-performance 3D graphics cards with a correspondingly powerful BUS system (e.g. PCI Express), the RAM should be as large as possible (min. 64 GB) and fast. A large RAM allows, for example, the **virtualization** of several parallel systems (see [Virtual machine](#)) and thus a significantly better utilization of the available computing capacity. The permanent memory should also be as large and fast as possible - high-performance **solid-state drives (SSDs)** should be clearly preferred over classic hard disks (HDDs).

### 2.1.2 Application system

In the **application phase** of the trained estimator model, considerably less computing power and RAM are usually required. If the concrete application does not require **continuous learning during operation**, significantly less expensive systems (in terms of acquisition costs, power consumption, etc.) can also be used. Such application-specific **embedded systems** have only one CPU (usually in **ARM architecture**), comparatively limited RAM (e.g. 1 - 8 GB) and usually no GPU. A popular **embedded computer** that is very well supported in terms of ML software is the **Raspberry Pi**. In addition to its ARM CPU, the Raspberry Pi also has a GPU installed on the same processor in the so-called **System on a Chip design (SoC)**. However, the SoC manufacturer **Broadcom** does not support the CUDA API.

There are references in the technical literature that the open source alternative **OpenCL** can be installed on the Raspberry Pi and that the AI framework **TensorFlow** (see section "Software") can be compiled with **SYCL** support (SYCL stands for "Single Source OpenCL"). However, a first rough review gives the impression that support for this approach is still very experimental at the moment. Therefore, parallelizing the AI application on the GPU of the Raspberry Pi does not seem to be an option (yet).

Here are some links for further reading:

- Deep learning with Raspberry Pi and alternatives in 2022
- Benchmarking Machine Learning on the New Raspberry Pi 4, Model B
- Portable Computer Vision: TensorFlow 2.0 on a Raspberry Pi
- Install OpenCL on Raspberry Pi 3 B+
- Does TensorFlow Support OpenCL ?
- TensorFlow for OpenCL using SYCL

## 2.2 Software

### 2.2.1 Operating system

@TODO: Rephrase and translate!!

These are general requirements to the operating system:

- Offenheit (Verfügbarkeit sehr guter Schnittstellen-Dokumentation und idealerweise quelloffener Software)
- Verfügbarkeit (Installations- und Konfigurationsrechte)
- Kommunikation (ungefilterte und bidirektionale Kommunikation im lokalen Netzwerk sowie ins Internet auf allen notwendigen Protokollen)

- leichte Erweiterbarkeit
  - SW-Installation + Updates über zentrale Paketmanagementsysteme wie z. B. apt, pip oder conda
  - Einbindung zusätzlicher SW-Bibliotheken oder externer HW-Sensoren

### 2.2.2 Programming IDEs

**RStudio (based on R language)**

**JupyterLab (Python language used)**

### 2.2.3 Packages for data analytics and libraries for ML (Python only)

#### Data analytics

NumPy

Pandas

#### Data visualization

matplotlib

seaborn

#### Machine learning

Scikit-Learn

**TensorFlow, Keras, CUDA Toolkit** 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>.

## 2.3 Community Support

When selecting and deciding for or against the use of certain hardware and software components, in addition to purely technical or financial characteristics, significant attention should be paid to broad **support from a well-networked community**. This community should consist of a balanced share of **manufacturers** of hardware components (e.g. GPU suppliers, manufacturers of embedded systems or sensors), **software developers** ideally from the **open source** ecosystem, and an active **user community** (e.g. for reporting hardware and software bugs or providing help in forums).

The author's many years of development experience show that the technically best hardware or software component is worthless if you are (apparently) the only user. This impression arises either because the component is actually very exotic and has only a few users or because the development takes place "behind closed doors", i.e. in the company's internal **closed source** domain.

Without the support of an active community, you are (almost) on your own when it comes to questions or problems. Progress in the development and maintenance of an AI application is therefore very difficult! The clear recommendation is therefore: Go for the (technically, price-wise) **second-best alternative** with an even bigger **community**.

## 2.4 Import Python packages

The aim of this section is to import globally used Python packages for data analysis and ML, such as Pandas, NumPY, matplotlib and Scikit-Learn.

```
[16]: import time

from IPython.display import HTML

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

## 3 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 Iris dataset for exploration
irisdata_df = pd.read_csv('./datasets/IRIS_flower_dataset_kaggle.csv')
```

## 4 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.

### 4.1 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 need 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

## 4.2 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)

## 4.3 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:

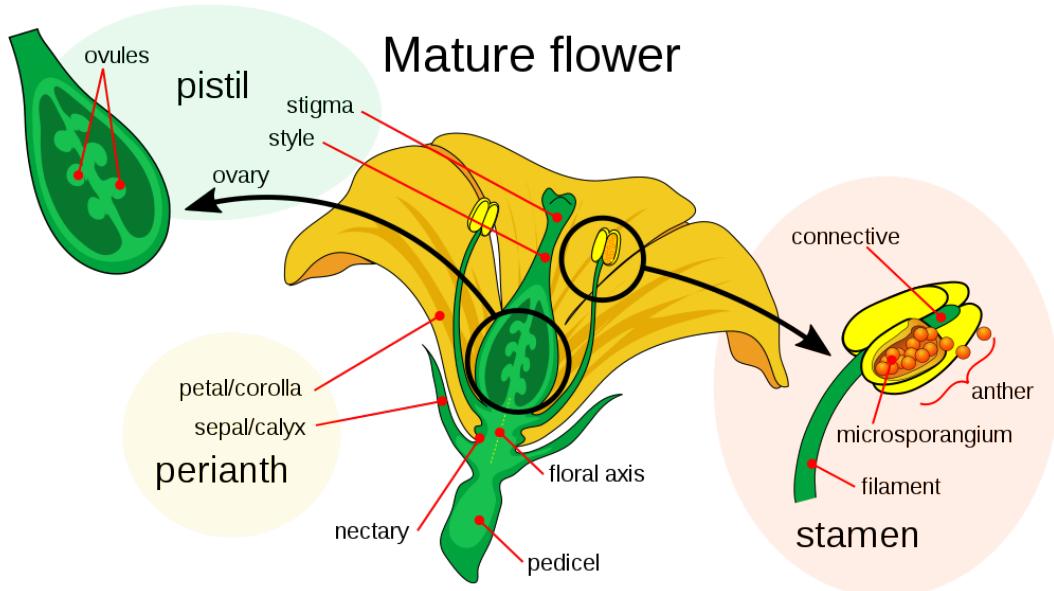


Figure 1: Principle illustration of a flower with sepals and petals (source: [Mature\\_flower\\_diagram.svg](#), license: public domain)

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)

#### 4.3.1 Inspect structure of dataframe

Print first or last 5 rows of dataframe:

```
[3]: irisdata_df.head(10)
```

	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

```
[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

### 4.3.2 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()`

	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

### 4.3.3 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()

```

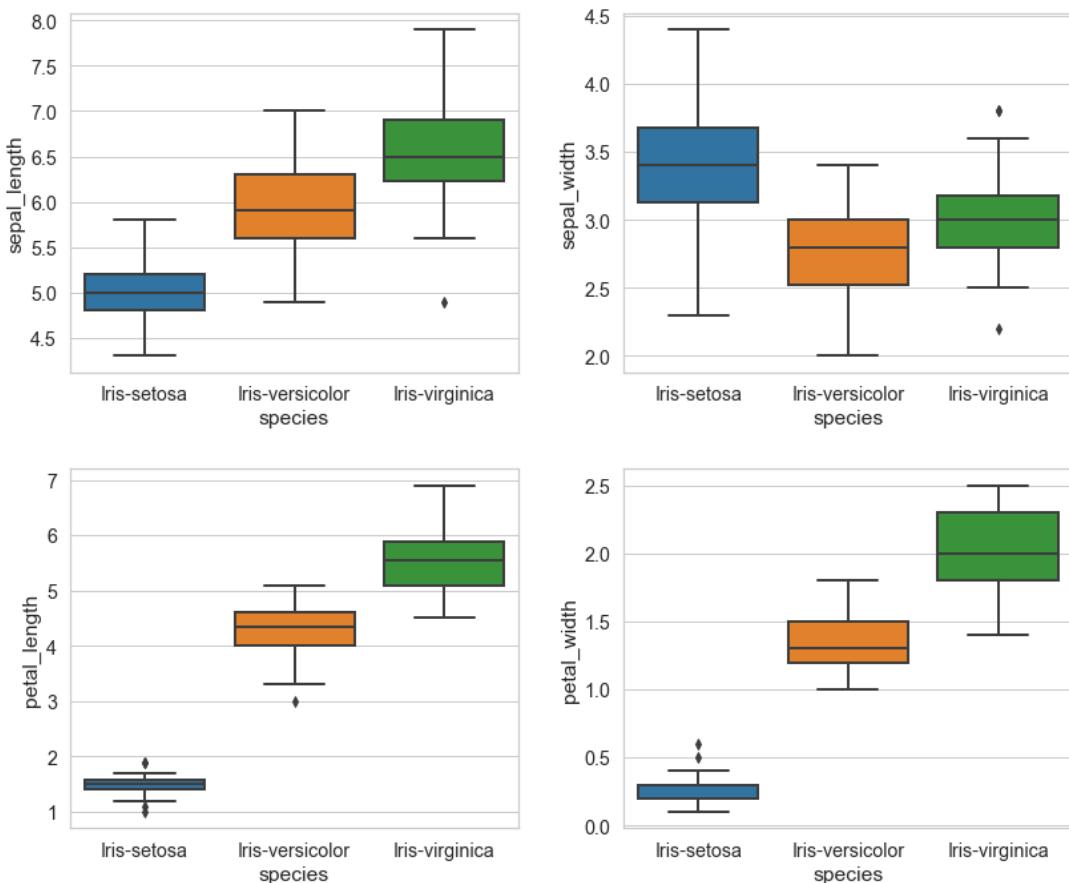


Figure 3: Boxplots used to explore the data ranges in the Iris dataset

## 4.4 Identify anomalies in the datasets

### 4.4.1 Find and repair gaps in dataset

This section was inspired by [Working with Missing Data in Pandas](#).

**Check 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
 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: [employees.csv](#)

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

# highlight cells with nan values
#employees_df_hl = employees_df.style.highlight_null('yellow')
#employees_df_hl

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)]

# highlight cells with nan values
#employees_df_gaps = employees_df_gaps.style.highlight_null('yellow')

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 in missing string values with fillna()** Now all null values (NaN) in the column “Gender” of the data type String are filled with “No gender”.

**Warning:** 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)

# highlight cells by condition
#employees_df_hl = employees_df.style.apply(lambda x: ["background: yellow" if v == "No Gender" else "" for v in x], axis = 1)
#employees_df_hl

employees_df
```

	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]

**Fill in missing *numerical* values with mean values** Missing integer or float values can be filled with the mean values of the corresponding column.

**@TODO:**

Incorporate section “4.1.3 Fehlende Werte ergänzen” of the book mitp\_Praxishandbuch\_Machine\_Learning\_Python\_Scikit-learn\_TensorFlow\_2018\_Anm\_bk.pdf.

**Drop 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).

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

```
[11]:   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
...
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
...	...	...
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
```

#### 4.4.2 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](#)

**Check 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**:

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

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

	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

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

	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**:

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

	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

```
[16]: # 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
```

```
[16]: 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

**Drop 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'])`

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

Remove duplicate rows across **all columns**:

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

```
[17]:   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
...
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
...
999                 ...             ...
1000                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**:

```
[18]: # 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
```

```
[18]:   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
...
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
...
999        False   Distribution
1000       False   Finance
1001       False   Product
1002      False Business Development
1003       True    Sales

[994 rows x 8 columns]

```

#### 4.4.3 Compare the edited dataset with the original dataset side-by-side

@TODO:

Incorporate following sources: - Compare two DataFrames and output their differences side-by-side - pandas compare two data frames and highlight the differences - How to Compare Two Pandas DataFrames and Get Differences

#### 4.4.4 Save edited dataset to new CSV file

@TODO:

Add explanation and python code here.

### 4.5 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?

#### 4.5.1 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

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

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

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

```
[21]: # 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)
```

```
[21]: 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

```

#### 4.5.2 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**.

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

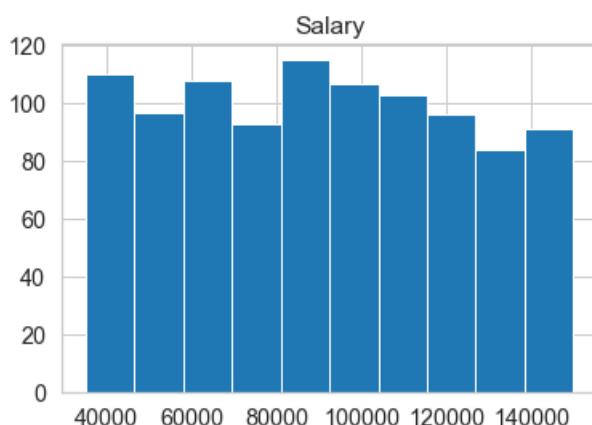


Figure 4: Histogram for frequency distribution of the salary

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

#### 4.6 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**.

##### 4.6.1 Visualise data with correlation heatmap

This section was inspired by [How to Create a Seaborn Correlation Heatmap in Python?](#).

**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

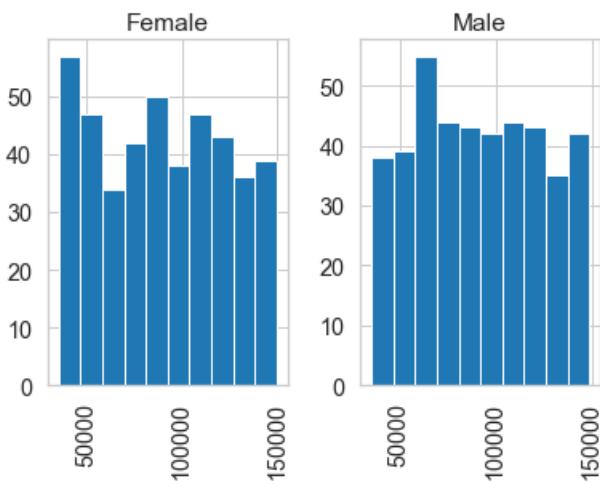


Figure 5: Histogram for the frequency distribution of the salary in comparison between men and women

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:

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

#irisdata_df_enc
```

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

	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.

```
[26]: # 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()
```

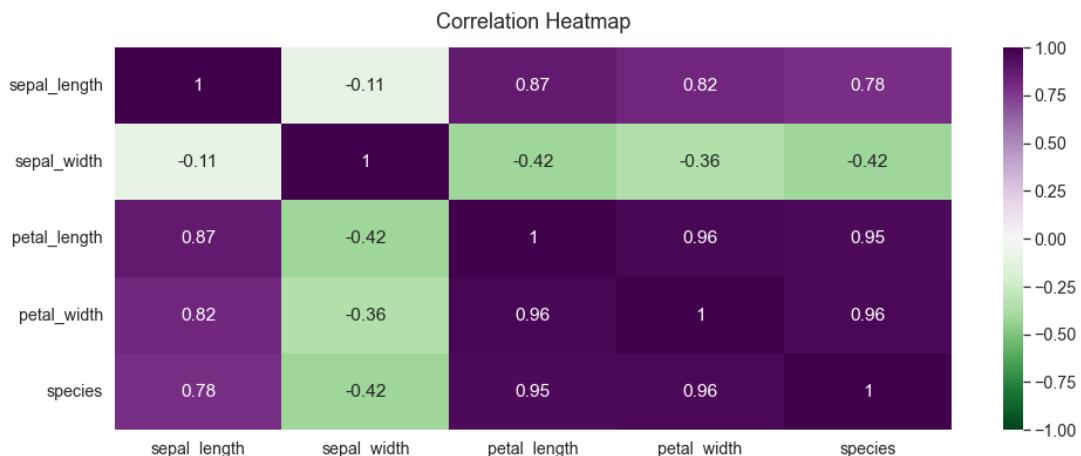


Figure 6: Correlation heatmap to explore coherences between single variables in the iris dataset

**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.

```
[27]: np.triu(np.ones_like(irisdata_df_enc.corr()))
```

```
[27]: 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:

```
[28]: 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 correlated columns** (0.96) with the **type of flowers** (species classes).

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

#### 4.6.2 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**.

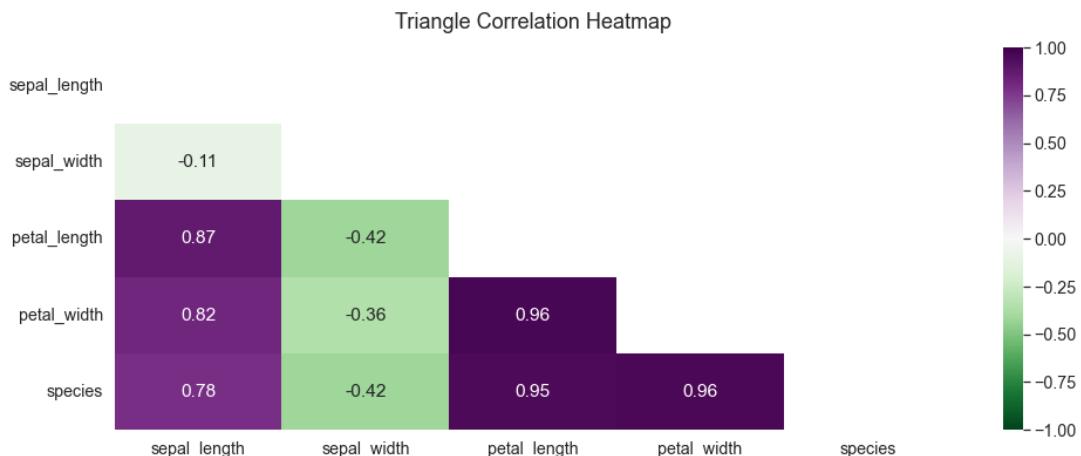


Figure 7: Correlation heatmap, which was cut at its main diagonal without losing any information

```
[29]: # 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()
```

#### 4.6.3 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 be shared in the y-axis across a single row and in the x-axis across a single column.

```
[30]: 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)

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()
```

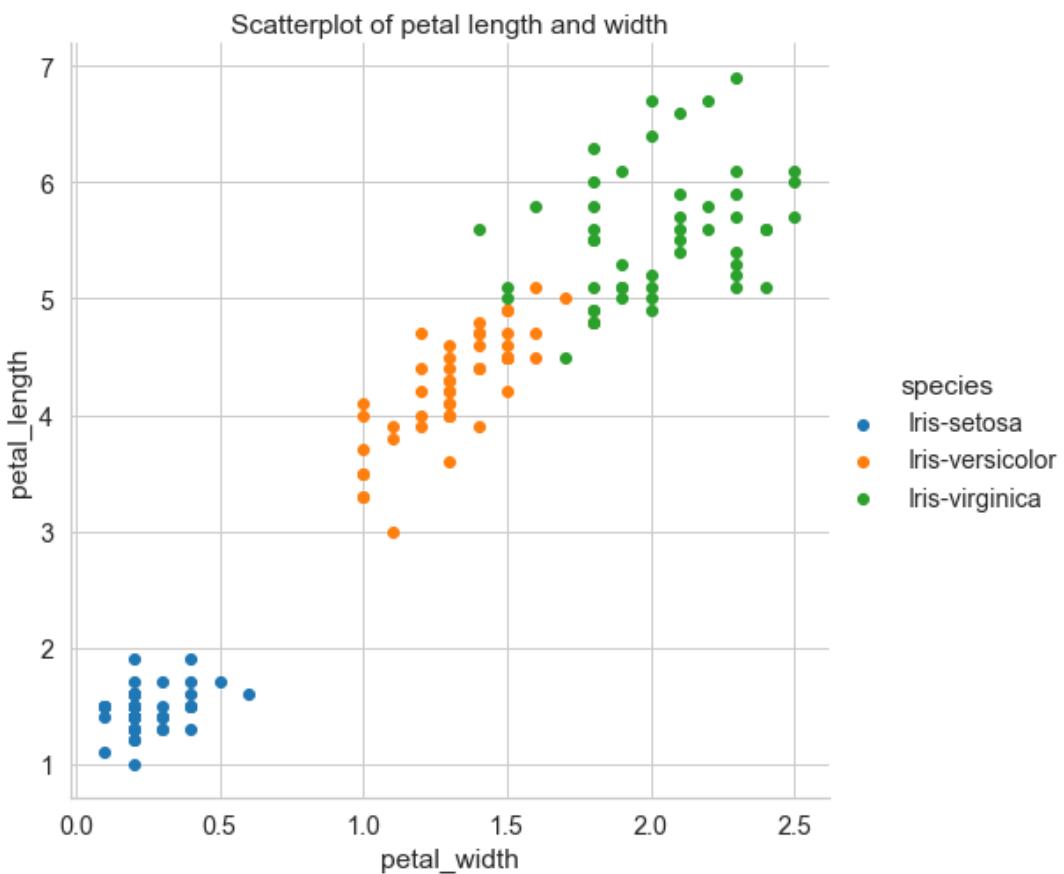


Figure 8: Plotting two individual variables of the iris dataset in the scatterplot to explore the relationships between these two

## 5 STEP 3: Choose and 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.

However, since the AI or ML world is so huge and impossible for a ML novice to overlook, a brief description of the **relationship between AI and ML** is given in the following sections. Furthermore, a **taxonomy** of the different **learning types** is presented by also providing some example algorithms.

### 5.1 Short overview of the AI world and its ML algorithms

#### 5.1.1 Relationship between AI, ML and others

**@TODO:** Include in this section the presentation IFA\_Steimers\_KI\_Grundlagen\_Neuronaler\_Netze\_2021-03-22.pdf by Prof. Steimers (IFA): - slides 6-7 “Definition of KI” - slides 10-12 “ML: Categories based on the data, task and algorithms”

In the **science world**, the term **artificial intelligence (AI)** refers to machines and systems that are capable of performing tasks that are characteristic of human intelligence.

In the **business world**, on the other hand, AI typically refers to mechanisms that perceive environmental factors and take autonomous actions. This is seen as an opportunity to achieve **predefined goals** with maximum success - without human intervention. Ultimately, this view is a mapping of **input information** to controlled **output actions** of a system. This expectation of AI-driven systems is thus hardly higher than what can be expected from today’s modern automation systems.

**Machine Learning (ML)**, on the other hand, addresses the mathematical models and algorithms that enable a computer system to recognize (new) correlations in huge amounts of sample data from various

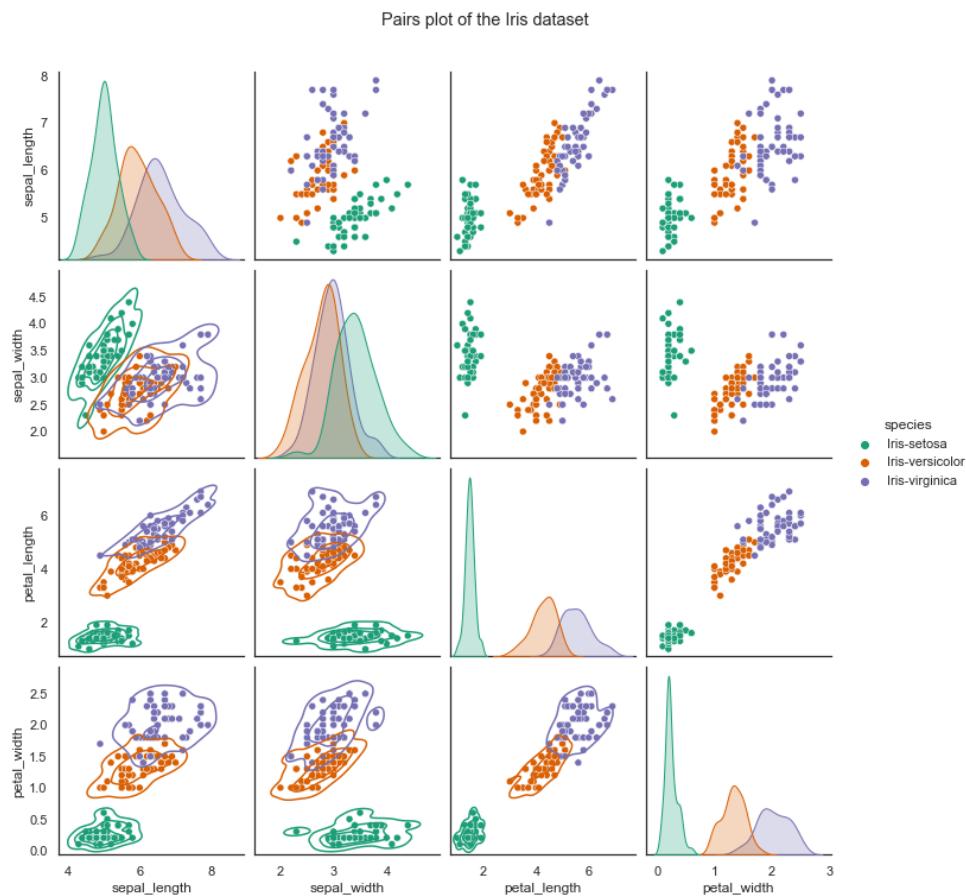


Figure 9: Plot all individual variables of the Iris dataset in pairs plot to see both the relationships between two variables and the distribution of the individual variables

sources by inferring them independently. For scientists, machine learning is a subset of AI.

The umbrella term AI covers a very large research area. It includes a number of techniques that enable computers to learn independently and solve complex problems:

- Computer-Vision (CV)
- Supervised and Unsupervised Learning
- Reinforcement Learning and Genetic Algorithms
- Computational Linguistics
- Robotics
- etc.

The following Venn diagram shows the relationship between Artificial Intelligence (AI), Machine Learning (ML) and other integrated technologies. The quantities that do not belong to the main category represent techniques that can function as stand-alone techniques and do not necessarily fall into the artificial intelligence group in all cases (for further details see [Emerging technologies based on artificial intelligence to assess quality and consumer preference of beverages](#)).

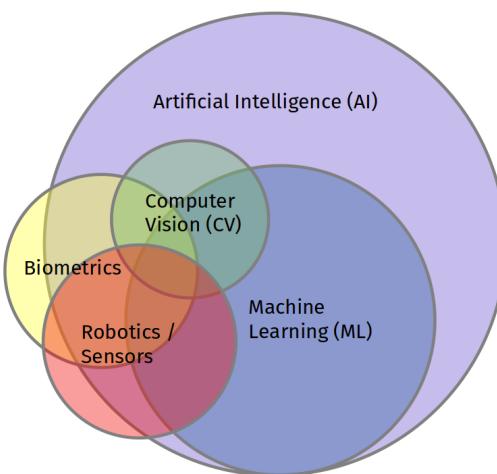


Figure 10: Venn diagram showing the relationship between Artificial Intelligence (AI), Machine Learning (ML) and other integrated technologies (source: Kasper, adapted from [Emerging technologies based on artificial intelligence to assess quality and consumer preference of beverages](#), license: CC-BY-SA 4.0)

### 5.1.2 Taxonomy of machine learning

The field of machine learning can be divided into the following **types of learning**:

- Supervised learning
- Unsupervised learning
- Semi-supervised learning
- Reinforcement learning

Here are some further sources:

- [Taxonomy of machine learning algorithms](#)
- [Comprehensive Survey of Machine Learning Approaches in Cognitive Radio-Based Vehicular Ad Hoc Networks](#)
- [A Taxonomy of Machine Learning Techniques](#)
- [ML Algorithms: One SD](#)
- [Machine Learning Map](#)

**Supervised learning** The goal of **supervised learning (SL)** is to learn a **function** that maps a **input to an output**, based on example input-output pairs. This involves inferring a relationship describable by a mathematical function from **labeled training data** consisting of a set of training examples (see [Supervised Learning](#)).

A few well-known algorithms from the field of **supervised learning** are mentioned here:

- Naive Bayes
- Linear Regression
- Logistic Regression
- Artificial Neural Networks (ANN)
- Support Vector Classifier (SVC)
- Decision Trees
- Random Forests

**Unsupervised learning** The algorithms of this category look for internal structures in the data of a dataset, such as **grouping** or **clustering of data points**. These algorithms can thus learn relationships from test data that have not been labeled, classified, or categorized. Rather than responding to feedback (as in supervised learning), unsupervised learning algorithms detect **commonalities in the data** and respond based on the presence or absence of such commonalities in each new dataset (see [Unsupervised learning](#)).

Here are some algorithms from the field of **unsupervised learning**:

- K-means Clustering
- Spectral Clustering
- Hierarchical Clustering
- Principal Component Analysis (PCA)

**Semi-supervised learning** This type of learning falls between **unsupervised** learning (without any labeled training data) and **supervised** learning (with completely labeled training data). Some of the training examples are missing training labels, yet many machine-learning researchers have found that unlabeled data, when used in conjunction with a small amount of labeled data, can produce a considerable improvement in learning accuracy (source: [Semi-supervised learning](#)).

**Reinforcement learning** This is an area of machine learning concerned with how **intelligent agents** ought to **take actions in an environment** in order to maximize the notion of cumulative **reward**. Due to its generality, the field is studied in many other disciplines, such as **game theory** and **control theory**.

Reinforcement learning differs from supervised learning in **not needing labeled input/output pairs** be presented, and in not needing sub-optimal actions to be explicitly corrected. Instead the focus is on **finding a balance** between **exploration** (of uncharted territory) and **exploitation** (of current knowledge) (source: [Reinforcement learning](#)).

Here are some algorithms from the field of **reinforcement learning**:

- Iterative Policy
- Q-Learning
- SARSA
- Learning Classifiers
- Stochastic Gradient
- Genetic Algorithm

## 5.2 Decision graph for selecting an suitable 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. The good news is that the ML software package **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.

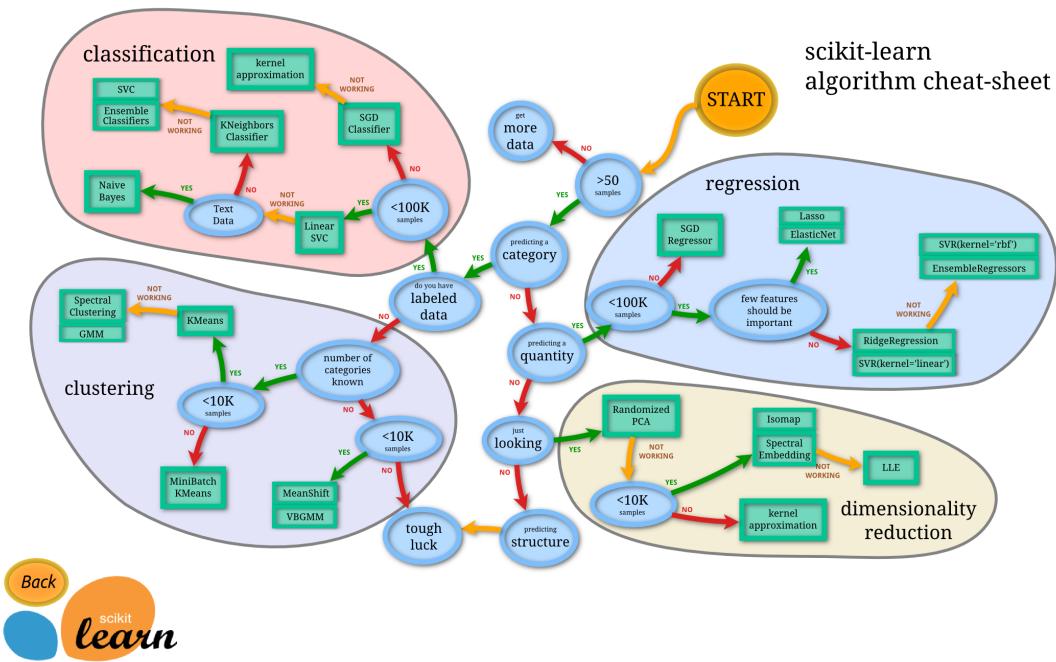


Figure 11: Decision graph for choosing an appropriate ML algorithm (source: [Choosing the right estimator](#), license: unknown)

### 5.3 Reasons for choosing Support Vector Classifier (SVC)

Among other ML algorithms suitable for the Iris dataset (such as the decision-tree-based **random-forests classifier**), the reasoned choice here in this tutorial falls on the **support vector classifier (SVC)**.

The following **reasons** led to the decision for the **Support Vector Classifier (SVC)**:

- the aim is to predict the species using unlabeled test data, so the task is to **classify**
- the iris dataset is **fully labeled** (by designating the iris species)
- the dataset contains significantly **less than 100k samples**

But the most important reason is that it is **easy to understand** how it works - so it is exactly suitable for a beginner tutorial ;)

### 5.4 Operating principle of SVC

Support Vector 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 principle of the SVC algorithm: the hyperplanes  $H_1$  till  $H_4$  (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.

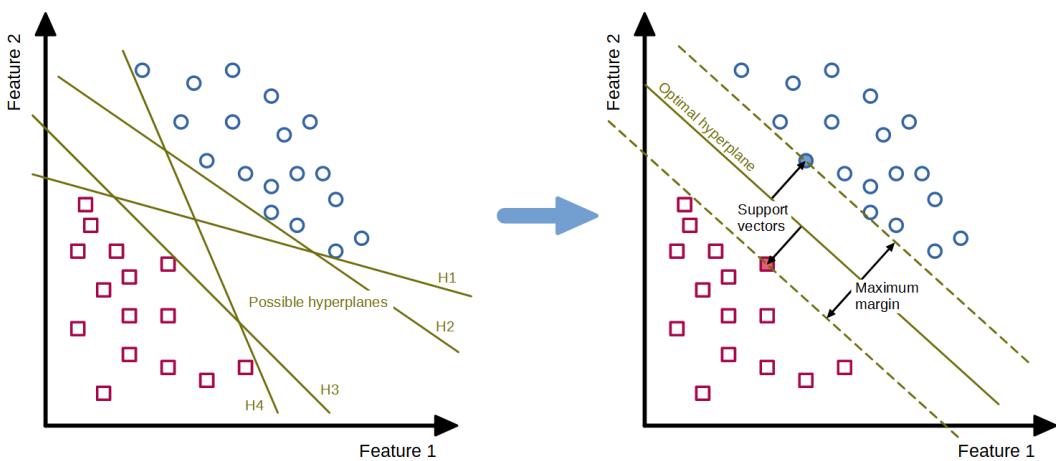


Figure 12: Support Vector Classifiers (SVC) separate the data points in classes by finding the best hyperplane by maximizing the margin to its support vectors (source: Kasper, license: CC-BY-SA 4.0)

## 5.5 Create the SVC model

In this step we create the SVC model choosing a **linear kernel** with default parameters.

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

## 6 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: 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.

For further details about **Standardization** and **Normalization** read here: [What are standardization and normalization? Test with iris data set in Scikit-learn.](#)

```
[32]: # import Iris dataset for exploration (again)
irisdata_df = pd.read_csv('./datasets/IRIS_flower_dataset_kaggle.csv')
```

### 6.1 Standardization

Standardize the feature values by computing the **mean**, subtracting the mean from the data points, and then dividing by the **standard deviation**.

**@TODO:**

Incorporate section “Skalieren von Merkmalen” of the book [O'Reilly\\_Praxiseinstieg\\_Machine\\_Learning\\_Scikit-Learn](#)

```
[39]: from sklearn.preprocessing import StandardScaler
```

```
#scaler = StandardScaler()
#X_train = scaler.fit_transform(X_train)
#X_test = scaler.transform(X_test)
irisdata_df

#X_train
```

[39]:

	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]

## 6.2 Normalization

# 7 STEP 5: Carry out training, prediction and testing

### 7.1 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.

In particular, to **avoid bias** in the sorted iris dataset due to splitting, the **order** of the data rows must be **randomized**. This is done with the parameter `shuffle=True`.

[35]:

```
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, u
→shuffle=True)
```

Check that the split datasets are still balanced and that no **bias** has been created by the splitting.

For this test, the previously separated labels `y_train` must be added back to the training dataset `X_train`.

[37]:

```
# make a deep copy of 'X_train'
X_train_bias_test_df = X_train.copy(deep=True)

# add list of labels to test dataframe
X_train_bias_test_df['species'] = y_train

# count unique values without missing values in a column,
# ordered descending and normalized
```

```
X_train_bias_test_df['species'].value_counts(ascending=False, dropna=False, normalize=True)
```

```
-----  
TypeError Traceback (most recent call last)  
Input In [37], in <cell line: 2>()  
 1 # make a deep copy of 'X_train'  
----> 2 X_train_bias_test_df = X_train.copy(deep=True)  
 3 # add list of labels to test dataframe  
 4 X_train_bias_test_df['species'] = y_train  
  
TypeError: copy() got an unexpected keyword argument 'deep'
```

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)
```

## 7.2 Train the SVC

In this step the SVC is trained with the training data. Training means to **fit** the SVC to the **training data**.

```
[39]: # fit the model for the data  
classifier.fit(X_train, y_train)
```

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

## 7.3 Make predictions

In this step the aim is to **predict the species** using unlabeled test data.

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

# 8 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**.

## 8.1 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](#).

```
[41]: 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: 80.00 %

## 8.2 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](#)).

[42]: `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	5
Iris-versicolor	0.86	0.75	0.80	16
Iris-virginica	0.64	0.78	0.70	9
accuracy			0.80	30
macro avg	0.83	0.84	0.83	30
weighted avg	0.81	0.80	0.80	30

## 8.3 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](#)).

@TODO:

Incorporate section “Bessere Auswertung mittels Kreuzvalidierung” of the book OReilly\_Praxiseinstieg\_Machine\_Learning\_Scikit-Learn\_TensorFlow\_2018\_Anm\_bk.pdf.

[43]: `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: 82.50 %

Standard Deviation: 14.65 %

## 8.4 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?](#)).

### 8.4.1 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.

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

```
[[ 6  0  0]
 [ 0  9  1]
 [ 0  0 14]]
```

#### 8.4.2 Colored confusion matrix

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

```
[44]: 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()
```

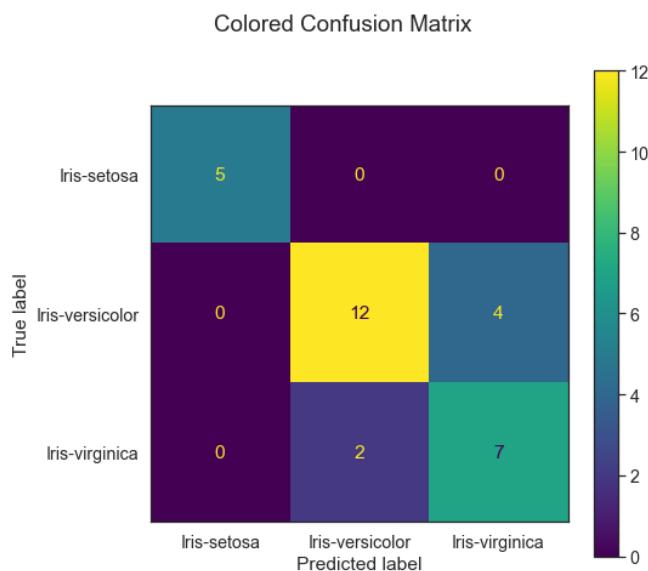


Figure 13: Checking the accuracy of the model by using the confusion matrix for cross-validation

## 9 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.

**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.

## 9.1 Prepare dataset

```
[ ]: 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
```

### 9.1.1 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.

```
[ ]: # 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

[ ]: # 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
```

### 9.1.2 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.

```
[ ]: 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, ↴
                                                    shuffle=True)
```

## 9.2 Plotting functions

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

```
[ ]: 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:

```
[ ]: 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**:

```
[ ]: 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()
```

### 9.3 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`.

```
[ ]: 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)
```

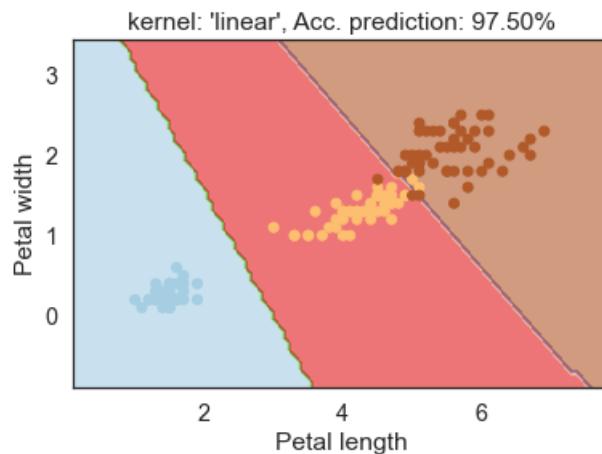


Figure 14: This group of images shows the effect on the classification by the choice of the different SVC kernels ('linear', 'rbf', 'poly' and 'sigmoid')

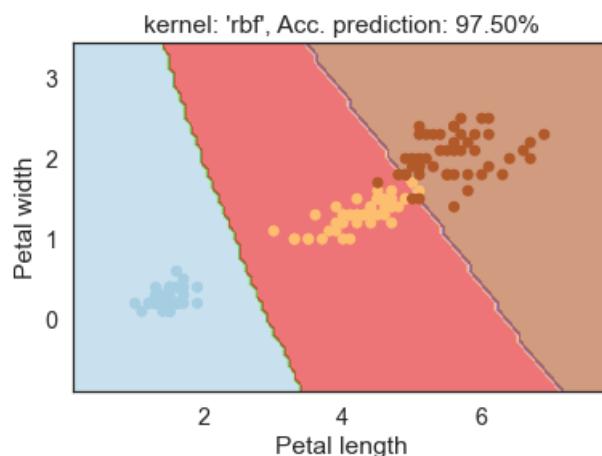


Figure 15: This group of images shows the effect on the classification by the choice of the different SVC kernels ('linear', 'rbf', 'poly' and 'sigmoid')

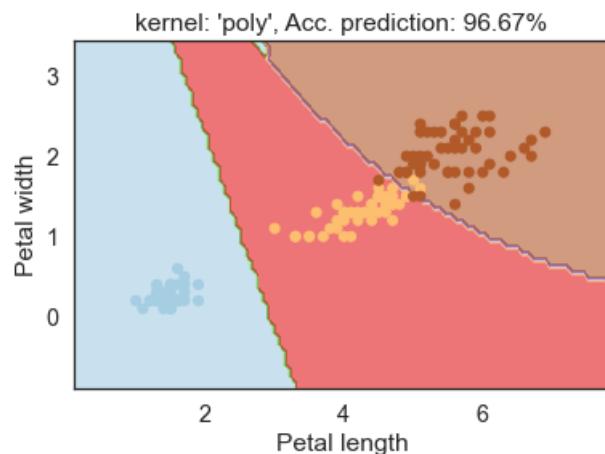


Figure 16: This group of images shows the effect on the classification by the choice of the different SVC kernels ('linear', 'rbf', 'poly' and 'sigmoid')

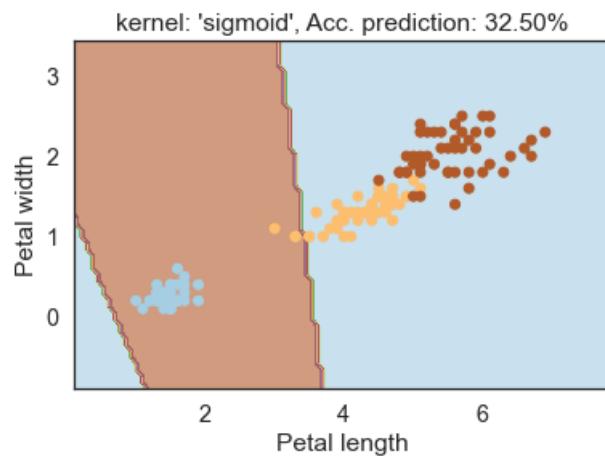


Figure 17: This group of images shows the effect on the classification by the choice of the different SVC kernels ('linear', 'rbf', 'poly' and 'sigmoid')

#### 9.4 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'`.

```
[ ]: 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)
```

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.

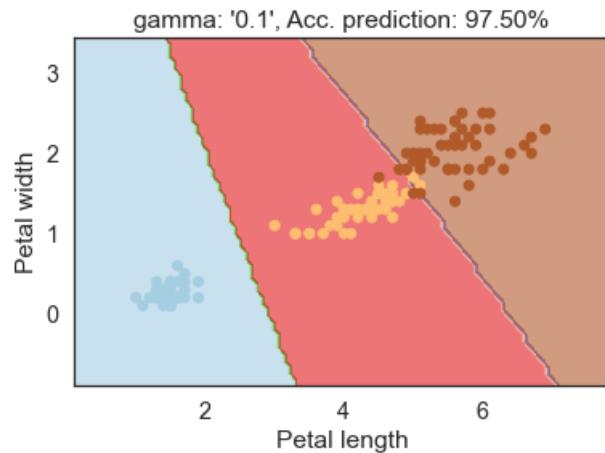


Figure 18: This group of images shows the effect on the classification by the variation of the parameter 'gamma' of the 'rbf' kernel

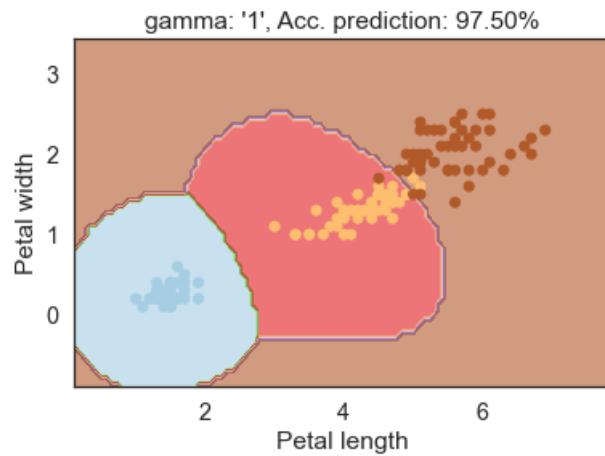


Figure 19: This group of images shows the effect on the classification by the variation of the parameter 'gamma' of the 'rbf' kernel

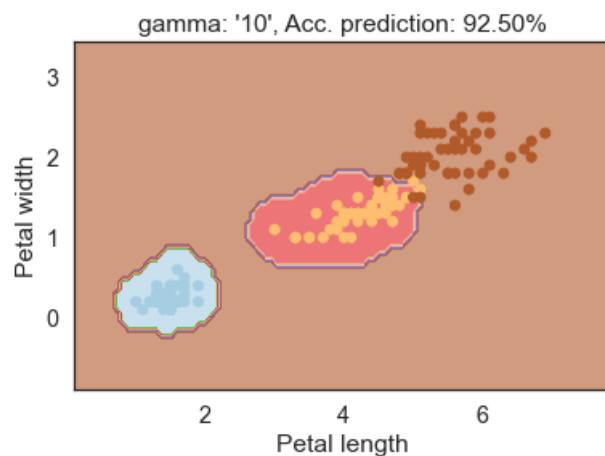


Figure 20: This group of images shows the effect on the classification by the variation of the parameter 'gamma' of the 'rbf' kernel

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

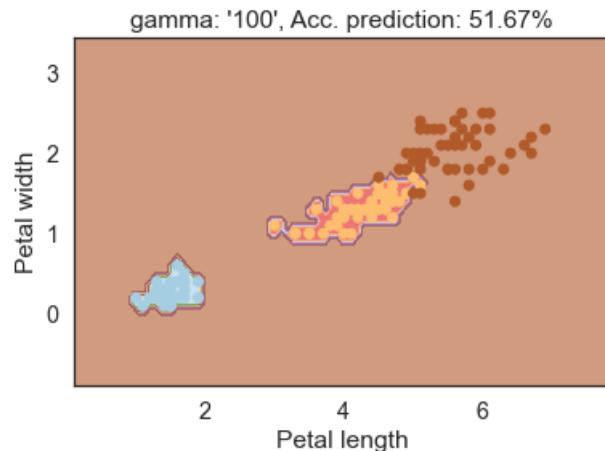


Figure 21: This group of images shows the effect on the classification by the variation of the parameter 'gamma' of the 'rbf' kernel

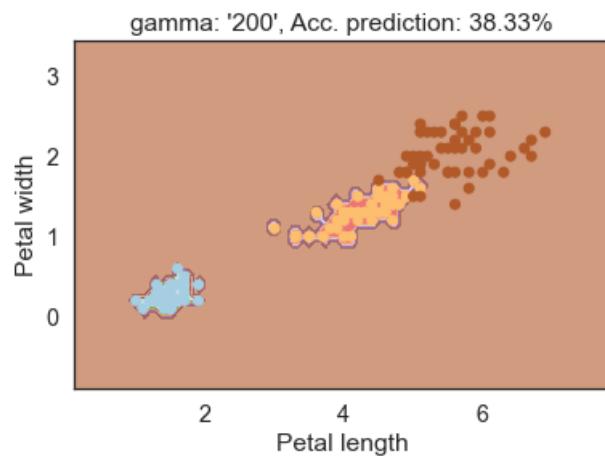


Figure 22: This group of images shows the effect on the classification by the variation of the parameter 'gamma' of the 'rbf' kernel

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

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

## 9.5 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.

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

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

for c in cs:
```

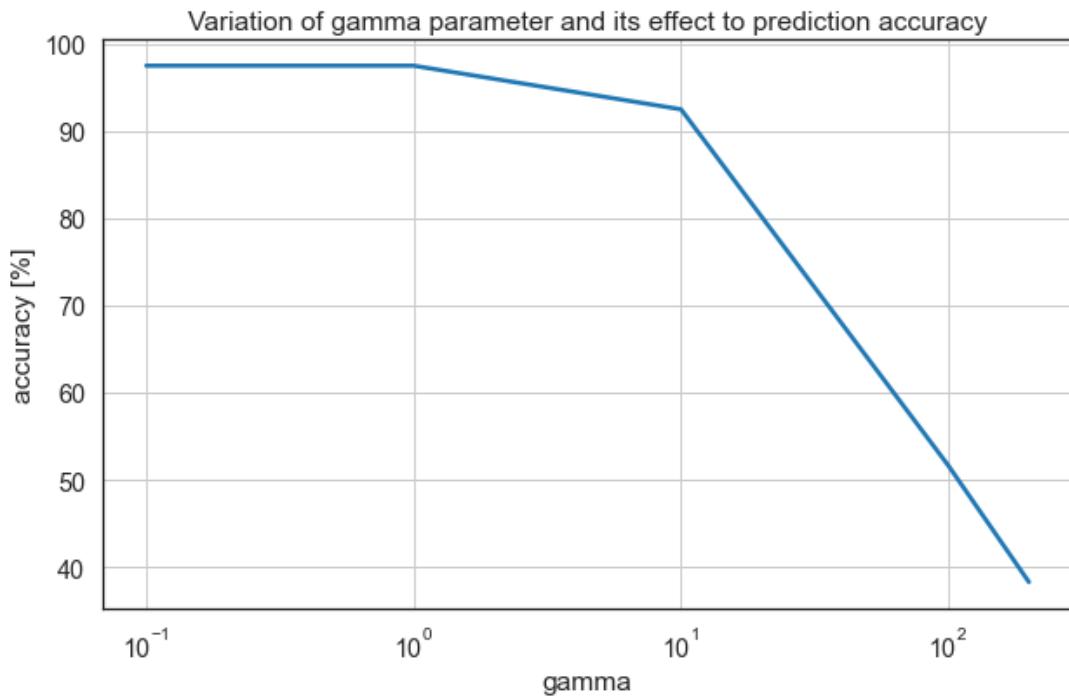


Figure 23: The plot shows the variation of the SVC parameter 'gamma' against the prediction accuracy

```
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)
```

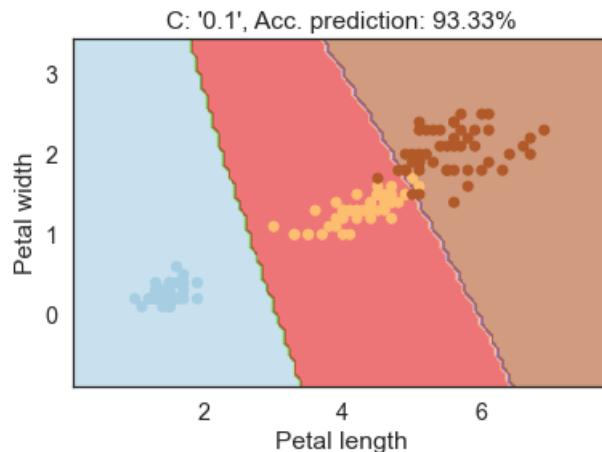


Figure 24: This group of images shows the effect on the classification by the variation of the parameter 'C' of the 'rbf' kernel

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.

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

accuracy_list = []
for c in cs:
```

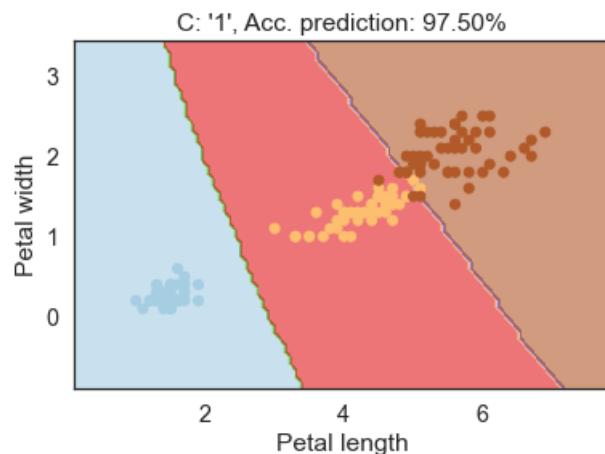


Figure 25: This group of images shows the effect on the classification by the variation of the parameter 'C' of the 'rbf' kernel

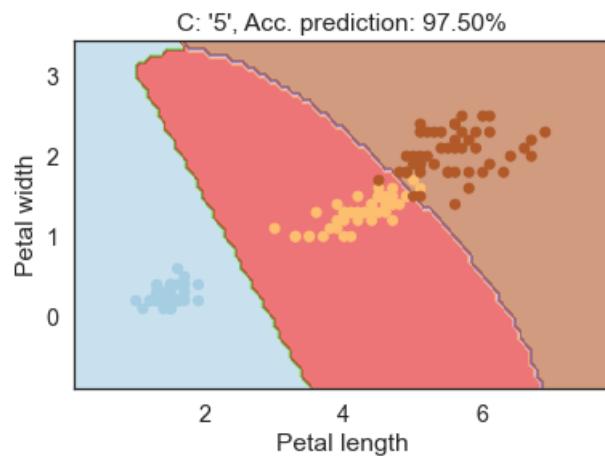


Figure 26: This group of images shows the effect on the classification by the variation of the parameter 'C' of the 'rbf' kernel

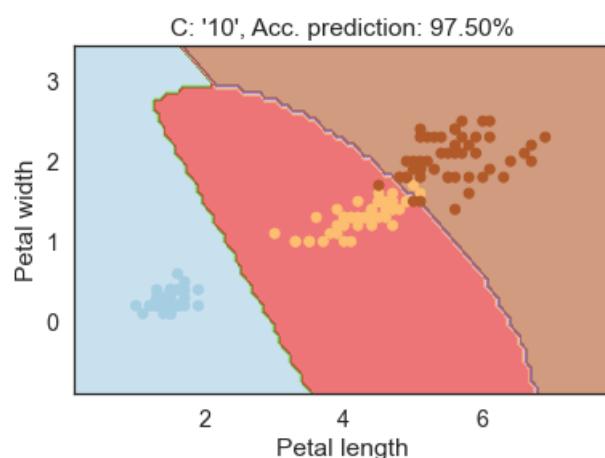


Figure 27: This group of images shows the effect on the classification by the variation of the parameter 'C' of the 'rbf' kernel

```
accuracy = crossValSVC(X_train, y_train, kernel='rbf', C=c)
```

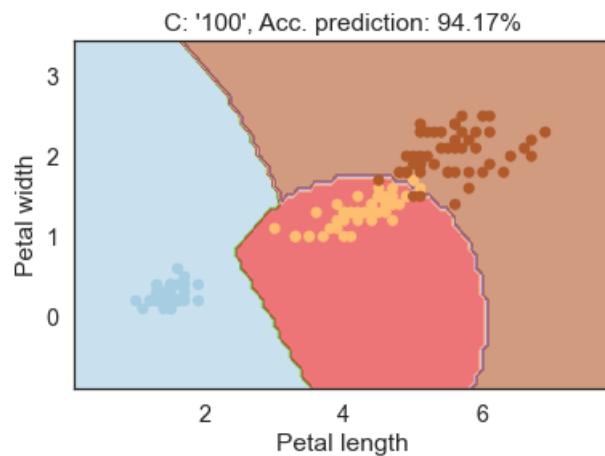


Figure 28: This group of images shows the effect on the classification by the variation of the parameter 'C' of the 'rbf' kernel

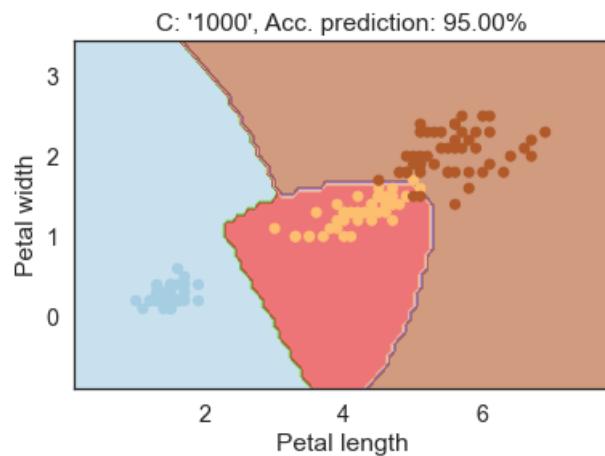


Figure 29: This group of images shows the effect on the classification by the variation of the parameter 'C' of the 'rbf' kernel

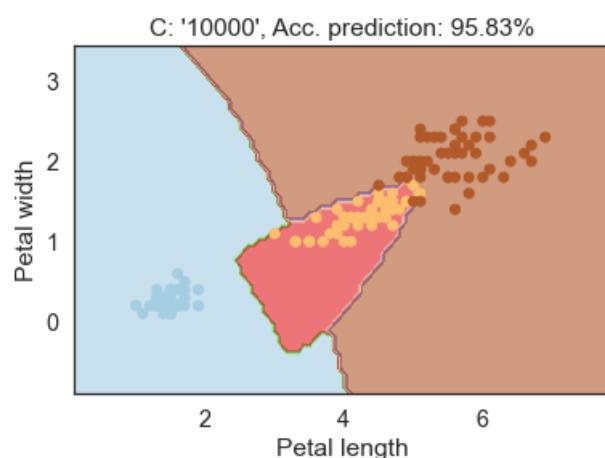


Figure 30: This group of images shows the effect on the classification by the variation of the parameter 'C' of the 'rbf' kernel

```
accuracy_list.append(accuracy)
```

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

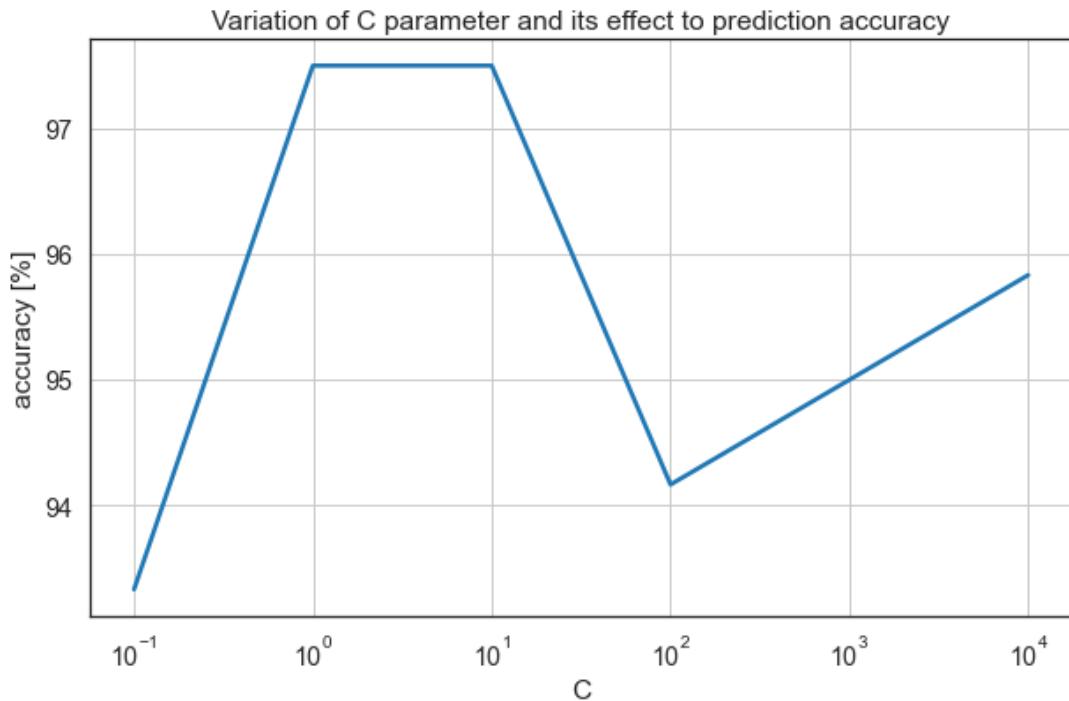


Figure 31: The plot shows the variation of the SVC parameter 'C' against the prediction accuracy

## 9.6 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 `degree=3`.

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

```
[ ]: 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 data.

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

accuracy_list = list()
```

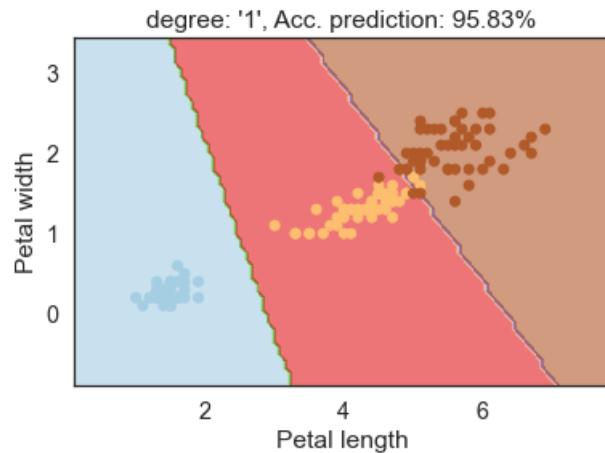


Figure 32: This group of images shows the effect on the classification by the variation of the parameter 'degree' of the 'poly' kernel

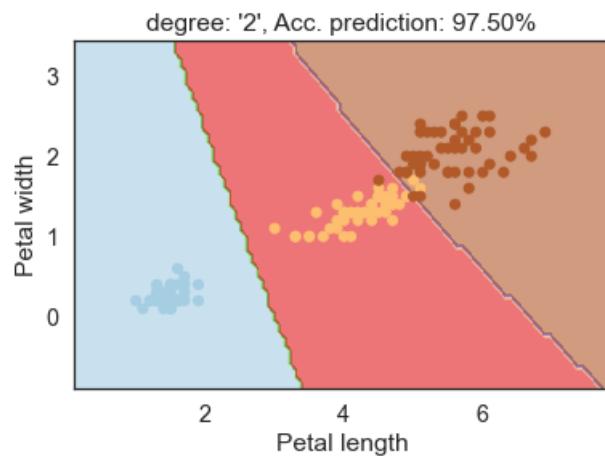


Figure 33: This group of images shows the effect on the classification by the variation of the parameter 'degree' of the 'poly' kernel

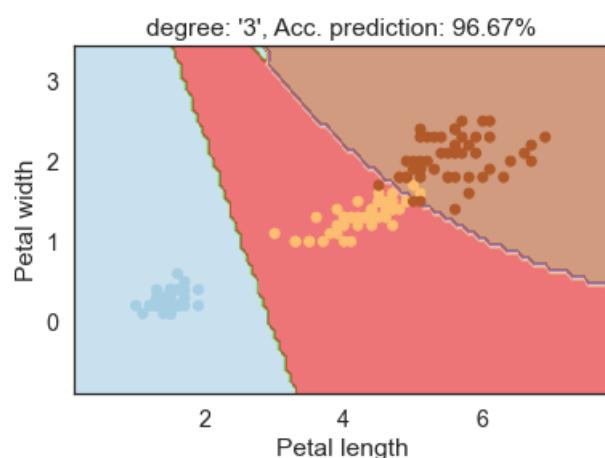


Figure 34: This group of images shows the effect on the classification by the variation of the parameter 'degree' of the 'poly' kernel

```
for degree in degrees:
```

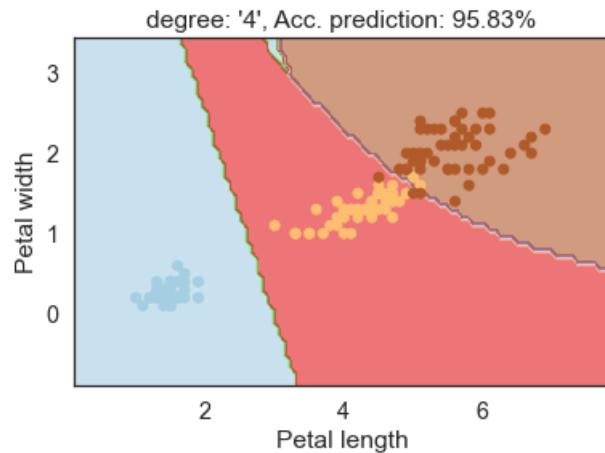


Figure 35: This group of images shows the effect on the classification by the variation of the parameter 'degree' of the 'poly' kernel

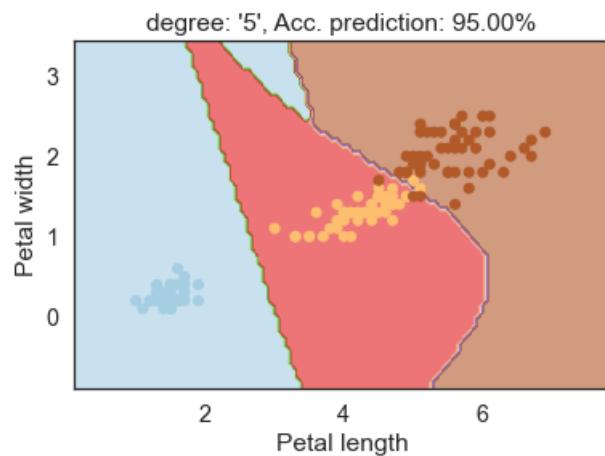


Figure 36: This group of images shows the effect on the classification by the variation of the parameter 'degree' of the 'poly' kernel

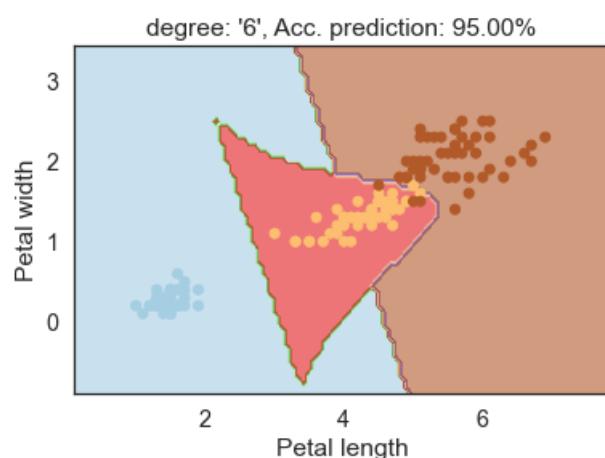


Figure 37: This group of images shows the effect on the classification by the variation of the parameter 'degree' of the 'poly' kernel

```
accuracy = crossValSVC(X_train, y_train, kernel='poly', degree=degree)
```

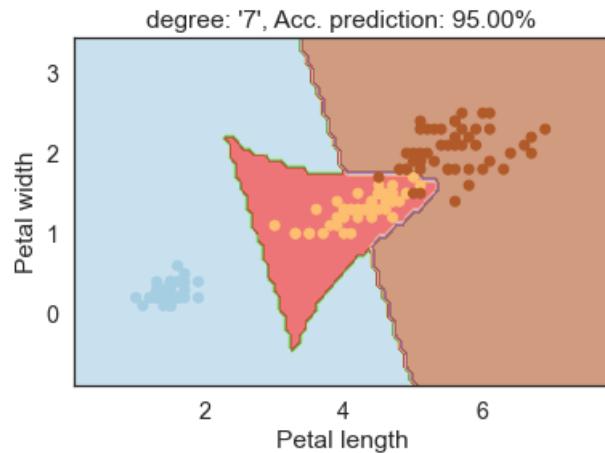


Figure 38: This group of images shows the effect on the classification by the variation of the parameter 'degree' of the 'poly' kernel

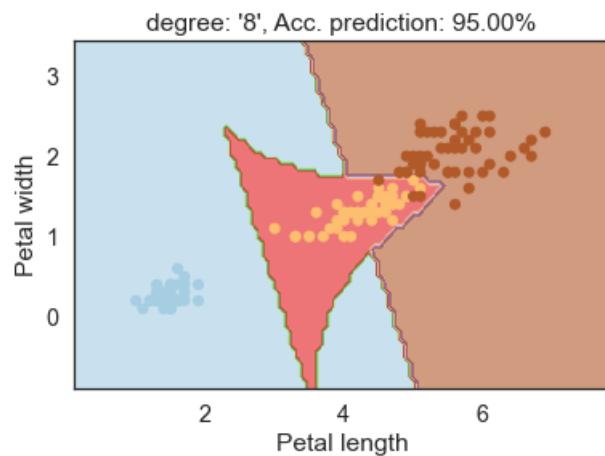


Figure 39: This group of images shows the effect on the classification by the variation of the parameter 'degree' of the 'poly' kernel

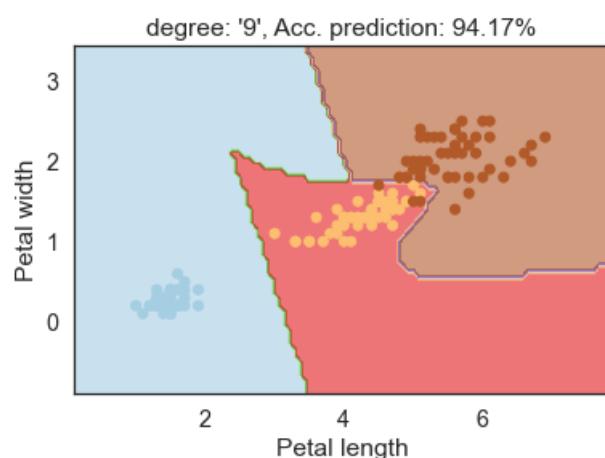


Figure 40: This group of images shows the effect on the classification by the variation of the parameter 'degree' of the 'poly' kernel

```
accuracy_list.append(accuracy)
```

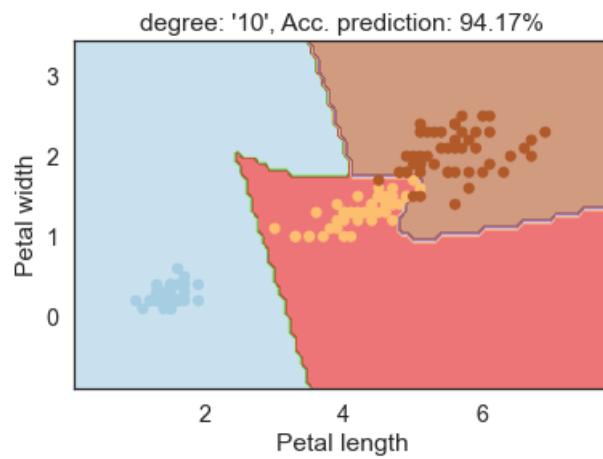


Figure 41: This group of images shows the effect on the classification by the variation of the parameter 'degree' of the 'poly' kernel

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

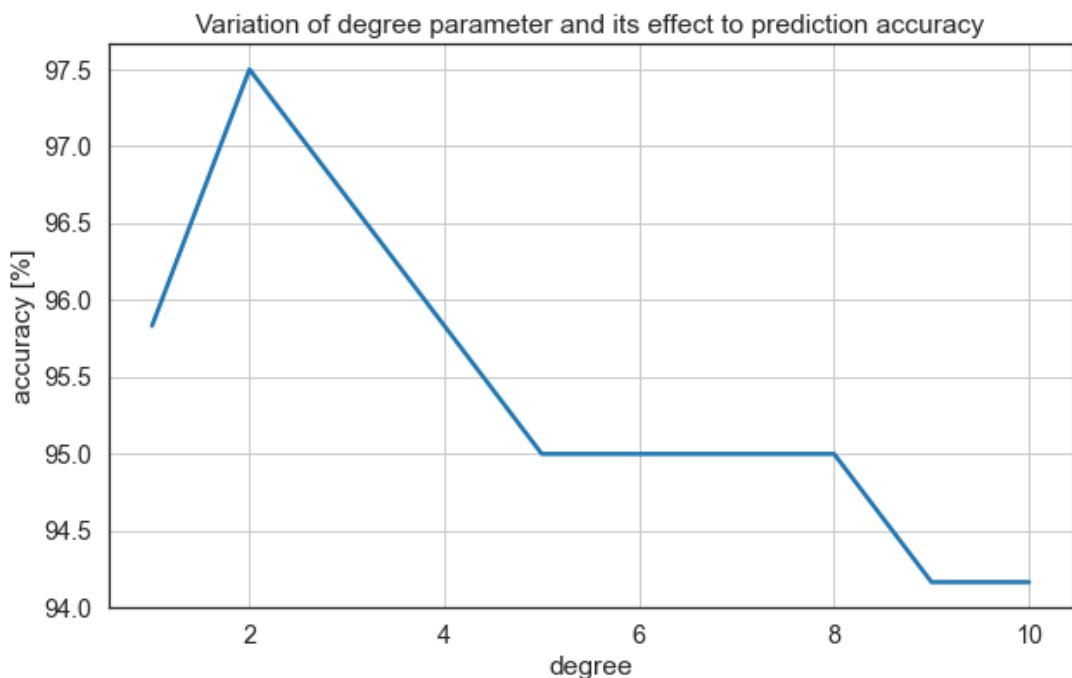


Figure 42: The plot shows the variation of the SVC parameter 'degree' against the prediction accuracy

## 10 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`
- Introduction to hyperparameter tuning with scikit-learn and Python
  - Abalone Dataset
- Hyperparameter tuning using Grid Search and Random Search: A Conceptual Guide

Import the necessary packages:

```
[47]: # general packages
from sklearn.preprocessing import StandardScaler
from sklearn.model_selection import train_test_split
from sklearn.model_selection import cross_val_score
from sklearn.metrics import accuracy_score
from sklearn.metrics import classification_report
#from sklearn.svm import SVC
from sklearn import svm, metrics
import pandas as pd
import seaborn as sns
import matplotlib.pyplot as plt
%matplotlib inline

# additional packages for grid search
from sklearn.model_selection import RepeatedKFold
from sklearn.model_selection import GridSearchCV

# additional packages for randomized search
from sklearn.model_selection import RandomizedSearchCV
from sklearn.model_selection import RepeatedKFold

# import class MeasExecTimeOfProgram from python file MeasExecTimeOfProgramclass.py
from MeasExecTimeOfProgram_class import MeasExecTimeOfProgram
```

Set path and columns of the Iris dataset for import:

```
[2]: # specify the path of the dataset
CSV_PATH = "./datasets/IRIS_flower_dataset_kaggle.csv"
```

Load dataset and split it into subsets for training and testing in the ratio 80% to 20%:

```
[23]: # load the dataset, separate the features and labels, and perform a
# training and testing split using 80% of the data for training and
# 20% for evaluation
irisdata_df = pd.read_csv(CSV_PATH)

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, □
→shuffle=True)
```

Check that the split datasets are still balanced and that no **bias** has been created by the splitting.

For this test, the previously separated labels `y_train` must be added back to the training dataset `X_train`.

```
[24]: # make a deep copy of 'X_train'
X_train_bias_test_df = X_train.copy(deep=True)

# add list of labels to test dataframe
X_train_bias_test_df['species'] = y_train
```

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

[24]: Iris-versicolor 0.358333  
Iris-virginica 0.333333  
Iris-setosa 0.308333  
Name: species, dtype: float64

Standardize the feature values by computing the **mean**, subtracting the mean from the data points, and then dividing by the **standard deviation**:

```
[ ]: scaler = StandardScaler()
X_train = scaler.fit_transform(X_train)
X_test = scaler.transform(X_test)

#X_train
```

## 10.1 Finding a baseline

The aim of this sub-step is to establish a baseline on the Iris dataset by training a **Support Vector Classifier (SVC)** with no hyperparameter tuning.

Train the model with **no tuning of hyperparameters** to find the baseline for later improvements:

[54]: classifier = svm.SVC(kernel = 'linear', random\_state = 0)

# initiate measuring execution time
execTime = MeasExecTimeOfProgram()
execTime.start()

classifier.fit(X\_train, y\_train)

# print time delta
print('Execution time: {:.4f} ms'.format(execTime.stop()))

Execution time: 1.6954 ms

Evaluate our model using accuracy score:

[55]: # predict labels
y\_pred = classifier.predict(X\_test)

[56]: # calculate cross validation score
# HINT: do NOT use the accuracy score - it's too inaccurate!
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: 97.50 %

Standard Deviation: 3.82 %

[57]: # print classification report
print(classification\_report(y\_test, y\_pred))

	precision	recall	f1-score	support
Iris-setosa	1.00	1.00	1.00	13
Iris-versicolor	1.00	0.86	0.92	7
Iris-virginica	0.91	1.00	0.95	10
accuracy			0.97	30
macro avg	0.97	0.95	0.96	30
weighted avg	0.97	0.97	0.97	30

```
[58]: 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

plt.tight_layout()
plt.show()
```

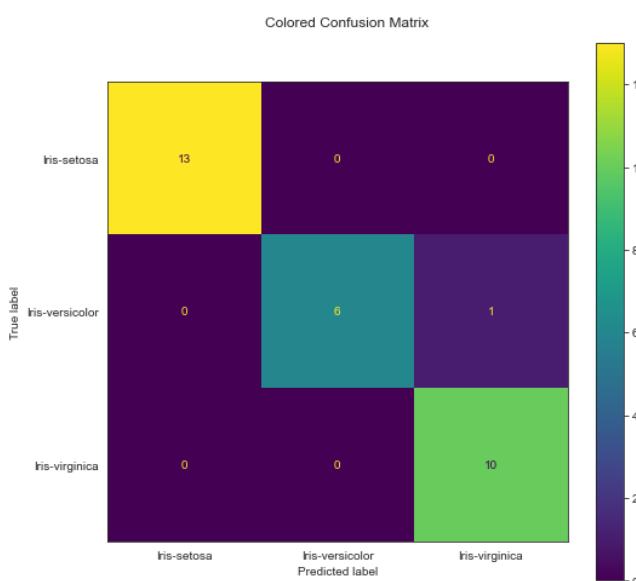


Figure 43:

```
[42]: classifier.get_params()
```

```
[42]: {'C': 1.0,
'break_ties': False,
'cache_size': 200,
'class_weight': None,
'coef0': 0.0,
'decision_function_shape': 'ovr',
'degree': 3,
'gamma': 'scale',
'kernel': 'linear',
```

```
'max_iter': -1,
'probability': False,
'random_state': 0,
'shrinking': True,
'tol': 0.001,
'verbose': False}
```

## 10.2 Grid Search

Initialize the SVC model and define the **space of the hyperparameters** to perform the **grid-search** over:

```
[45]: classifier = svm.SVC()

kernels = ["linear", "rbf", "sigmoid", "poly"]
gammas = [0.1, 1, 10, 100, 200]
cs = [0.1, 1, 5, 10, 100, 1000, 10000]

# reduce the possible polynomial degrees to reasonable values,
# since with higher degrees the calculation time increases exponentially
degrees = [1, 2, 3, 4, 5]

grid = dict(kernel=kernels, gamma=gammas, C=cs, degree=degrees)
```

Initialize a **cross-validation fold** and **perform a grid-search** to tune the hyperparameters:

```
[59]: cvFold = RepeatedKFold(n_splits=10, n_repeats=3, random_state=1)

gridSearch = GridSearchCV(estimator=classifier, param_grid=grid, n_jobs=-1,
                           cv=cvFold, scoring="accuracy")

# initiate measuring execution time
execTime = MeasExecTimeOfProgram()
execTime.start()

searchResults = gridSearch.fit(X_train, y_train)

# print time delta
print('Execution time: {:.2f} s'.format(execTime.stop()/1000))
```

Execution time: 39.64 s

Extract the best model and evaluate it:

```
[61]: # predict labels by best model
bestModel = searchResults.best_estimator_

y_pred = bestModel.predict(X_test)
```

```
[62]: # calculate cross validation score from the best model
# HINT: do NOT use the accuracy score - it's too inaccurate!
accuracies = cross_val_score(estimator = bestModel, 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 %

```
[63]: 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	13
Iris-versicolor	1.00	0.86	0.92	7
Iris-virginica	0.91	1.00	0.95	10
accuracy			0.97	30
macro avg	0.97	0.95	0.96	30
weighted avg	0.97	0.97	0.97	30

```
[64]: 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

plt.tight_layout()
plt.show()
```

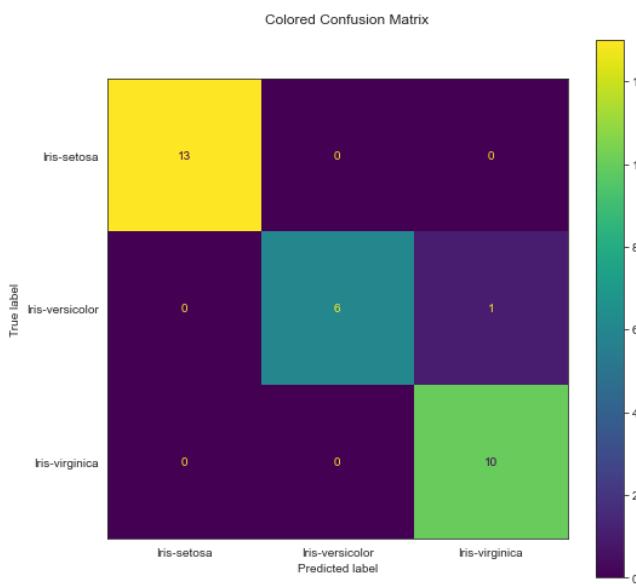


Figure 44:

```
[ ]: bestModel.get_params()
```

```
[ ]: {'C': 5,
      'break_ties': False,
```

```
'cache_size': 200,
'class_weight': None,
'coef0': 0.0,
'decision_function_shape': 'ovr',
'degree': 1,
'gamma': 0.1,
'kernel': 'poly',
'max_iter': -1,
'probability': False,
'random_state': None,
'shrinking': True,
'tol': 0.001,
'verbose': False}
```

### 10.3 Randomized Search

Initialize the SVC model and define the **space of the hyperparameters** to perform the **randomized-search** over:

```
[72]: classifier = svm.SVC()

kernels = ["linear", "rbf", "sigmoid", "poly"]
gammas = [0.1, 1, 10, 100, 200]
cs = [0.1, 1, 5, 10, 100, 1000, 10000]

# reduce the possible polynomial degrees to reasonable values,
# since with higher degrees the calculation time increases exponentially
degrees = [1, 2, 3, 4, 5]

grid = dict(kernel=kernels, gamma=gammas, C=cs, degree=degrees)
```

Initialize a **cross-validation fold** and **perform a randomized-search** to tune the hyperparameters:

```
[73]: cvFold = RepeatedKFold(n_splits=10, n_repeats=3, random_state=1)

randomSearch = RandomizedSearchCV(estimator=classifier, n_jobs=-1,
                                    cv=cvFold, param_distributions=grid,
                                    scoring="accuracy")

# initiate measuring execution time
execTime = MeasExecTimeOfProgram()
execTime.start()

searchResults = randomSearch.fit(X_train, y_train)

# print time delta
print('Execution time: {:.3f} s'.format(execTime.stop()/1000))
```

Execution time: 0.720 s

Extract the best model and evaluate it:

```
[74]: # predict labels by best model
bestModel = searchResults.best_estimator_

y_pred = bestModel.predict(X_test)
```

```
[75]: # calculate cross validation score from the best model
# HINT: do NOT use the accuracy score - it's too inaccurate!
accuracies = cross_val_score(estimator = bestModel, 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: 97.50 %

Standard Deviation: 3.82 %

```
[76]: 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	13
Iris-versicolor	1.00	0.86	0.92	7
Iris-virginica	0.91	1.00	0.95	10
accuracy			0.97	30
macro avg	0.97	0.95	0.96	30
weighted avg	0.97	0.97	0.97	30

```
[77]: 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

plt.tight_layout()
plt.show()
```

```
[78]: bestModel.get_params()
```

```
[78]: {'C': 10,
      'break_ties': False,
      'cache_size': 200,
      'class_weight': None,
      'coef0': 0.0,
      'decision_function_shape': 'ovr',
      'degree': 1,
      'gamma': 0.1,
      'kernel': 'rbf',
      'max_iter': -1,
      'probability': False,
      'random_state': None,
      'shrinking': True,
      'tol': 0.001,
      'verbose': False}
```

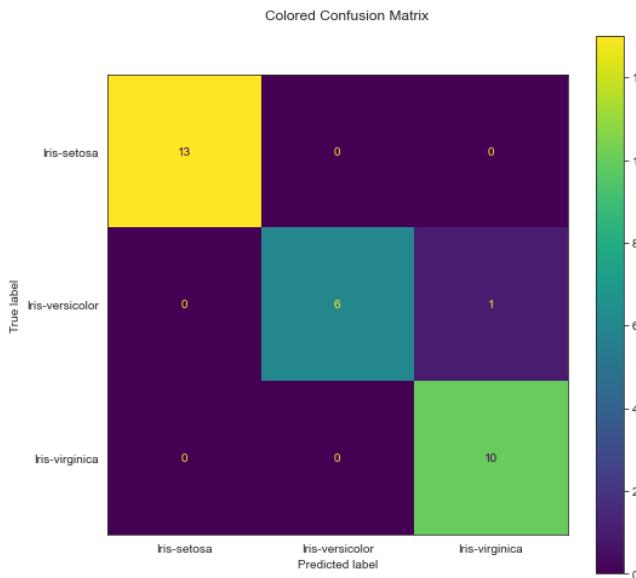


Figure 45:

## 11 Summary and conclusions

### 11.1 English summary

### 11.2 German summary

[ ]:

## 12 References

### Online references

Barney, Blaise (June 27, 2012). *Introduction to Parallel Computing*. Lawrence Livermore National Laboratory. URL: <https://csis.pace.edu/~marchese/SE765/L0/Introduction%20to%20Parallel%20Computing.htm> (visited on 08/29/2022) (cit. on p. 7).

### Books, technical reports and others

Kasper, Björn (Feb. 22, 2019). *Industrie 4.0: Technologieentwicklung und sicherheitstechnische Bewertung von Anwendungsszenarien*. Tech. rep. Gd96. Bundesanstalt für Arbeitsschutz und Arbeitsmedizin (BAuA). 98 pp. DOI: [10.21934/baua:bericht20190204](https://doi.org/10.21934/baua:bericht20190204). URL: <https://www.baua.de/DE/Angebote/Publikationen/Berichte/Gd96.html> (visited on 10/25/2020) (cit. on p. 7).