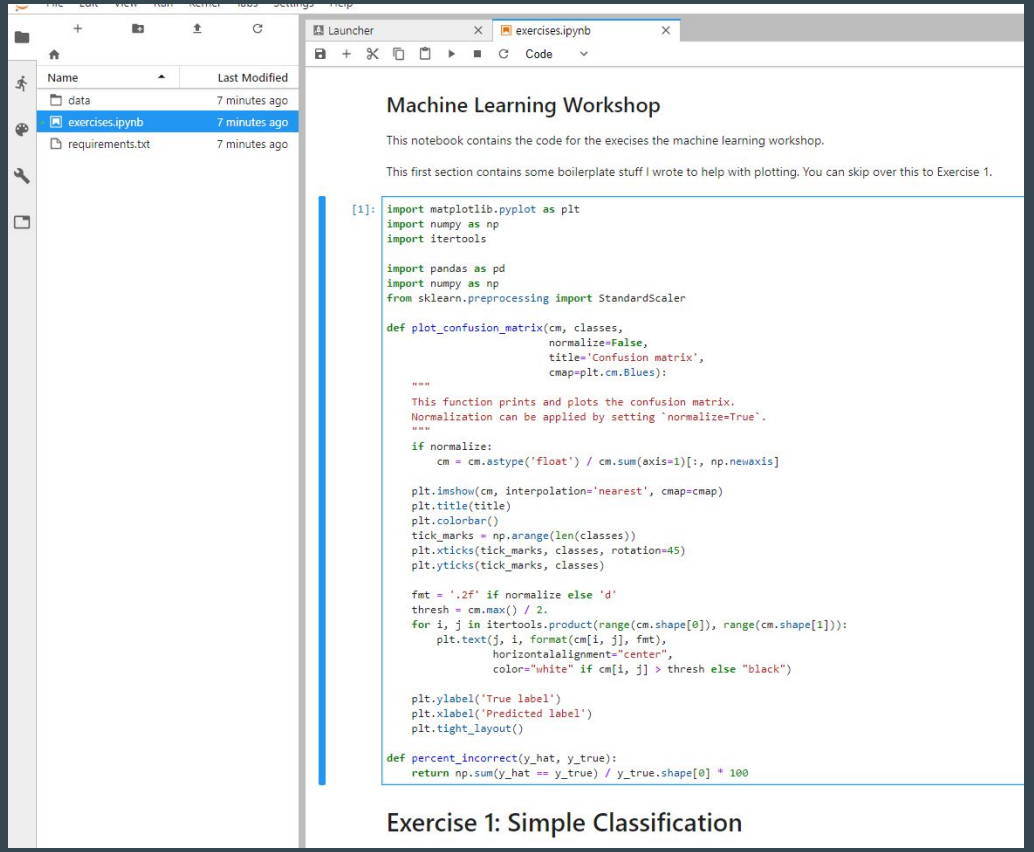
Machine Learning

Go to:
https://mybinder.org/v2/gh/samueljackson92/ml-workshop/master?urlpath=lab

Binder

- Interactive Jupyter Lab environment
- Open exercises.ipynb
- Can run code in each of the boxes
- Data should already be there

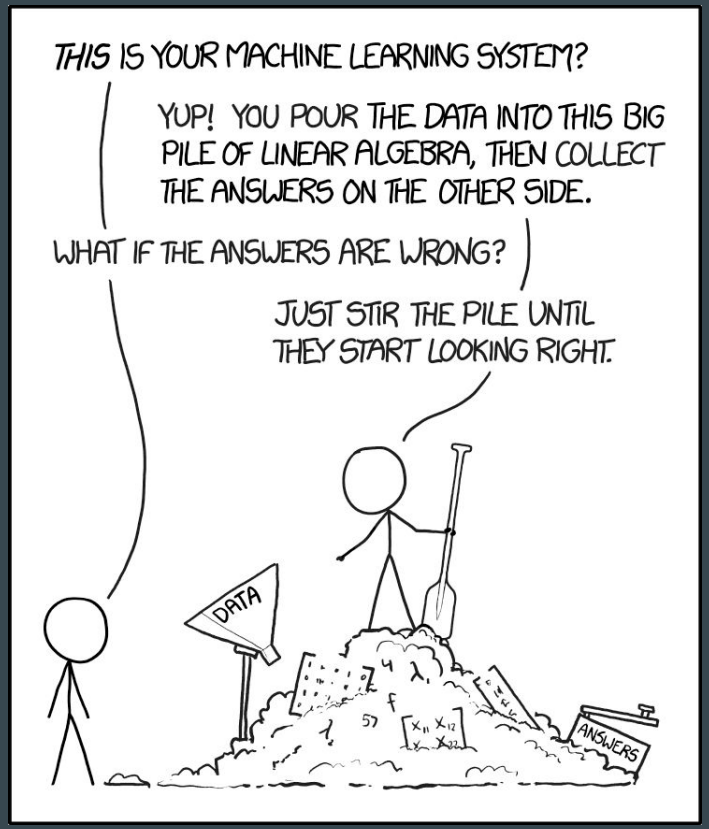


What We'll Cover:

- What is machine learning?
- Using scikit-learn for:
  - Classification
  - Clustering
  - Model Selection
- 30 seconds of Pandas

What We Won't Cover:

- Lots of math
- Neural Networks
- Tensorflow
- ...

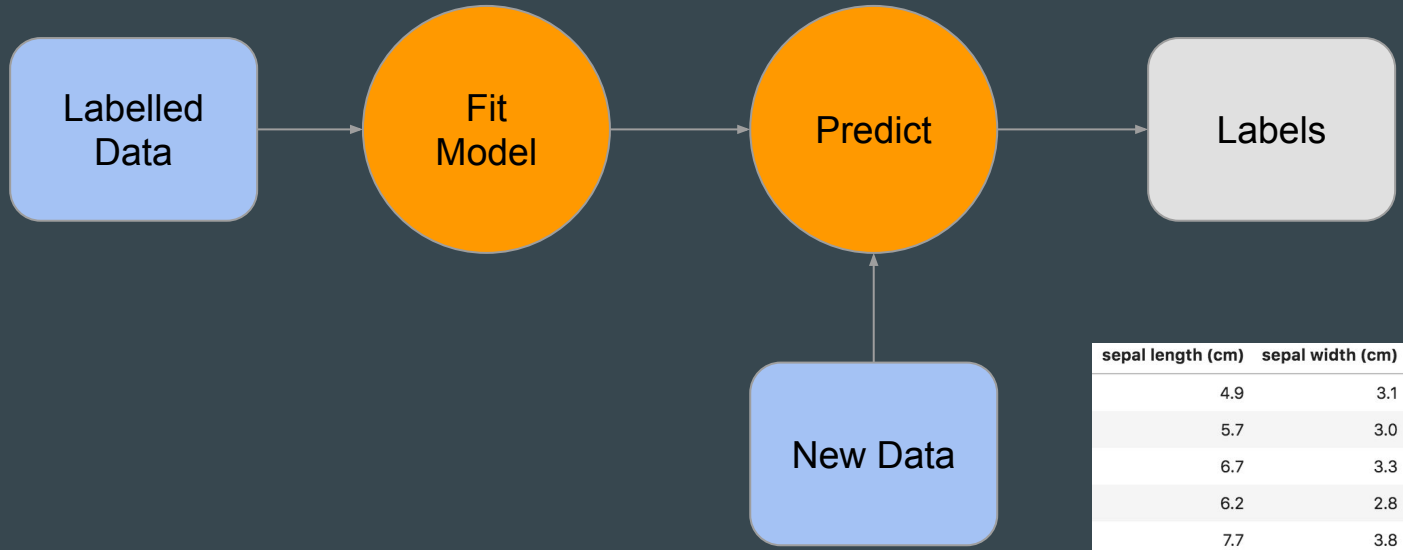


Machine Learning definition

“A set of methods that can automatically detect patterns in data, then use the uncovered pattern to predict future data”

Murphy, Kevin P. "Machine Learning: A Probabilistic Perspective." (2012).

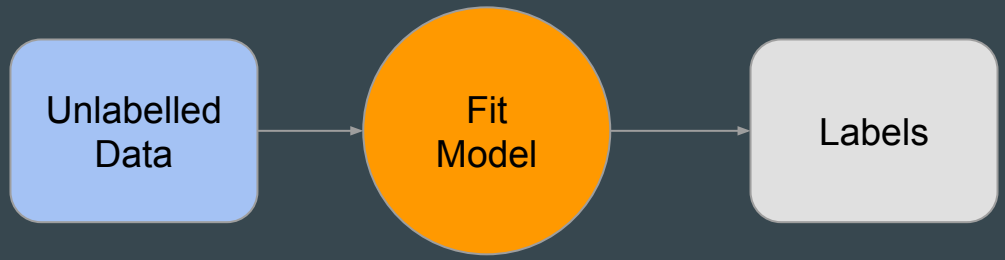
Types of Machine Learning: Supervised



sepal length (cm)	sepal width (cm)	petal length (cm)	petal width (cm)	labels
4.9	3.1	1.5	0.1	0
5.7	3.0	4.2	1.2	1
6.7	3.3	5.7	2.5	2
6.2	2.8	4.8	1.8	2
7.7	3.8	6.7	2.2	2
5.5	2.6	4.4	1.2	1
5.6	3.0	4.5	1.5	1
6.1	2.8	4.7	1.2	1
5.5	3.5	1.3	0.2	0
6.7	3.3	5.7	2.1	2

- Classification: which one is this?
- Regression: predicting a value.

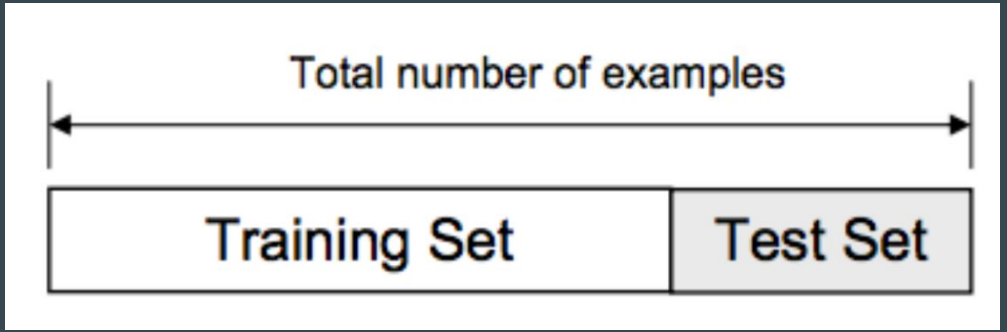
Types of Machine Learning: Unsupervised



- Clustering: group together “similar” data into one label.

Model Evaluation - Supervised

- How good are our predictions?
- How do we know?
- Training/test split:
  - Split data into training and test set
  - Train only on the test set
  - Compare predictions to known label
  - There are other strategies...
- KFold Cross Validation:
  - Split data into K-folds
  - Use one fold as “test” and train on others
  - Repeat



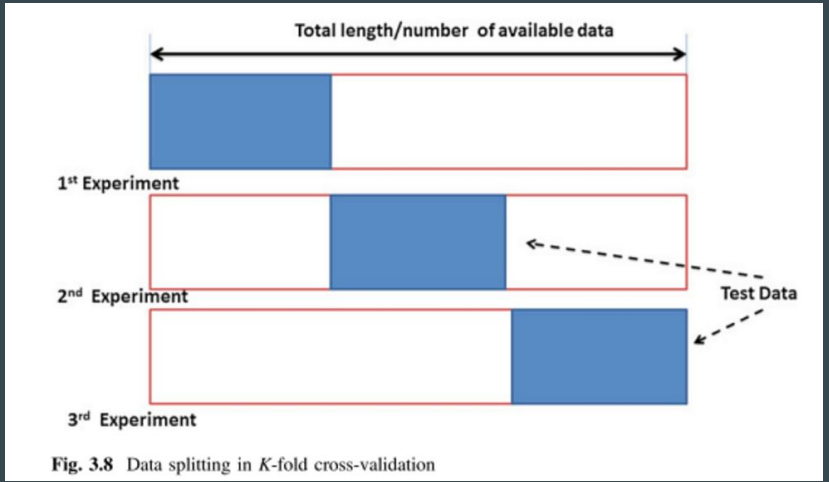
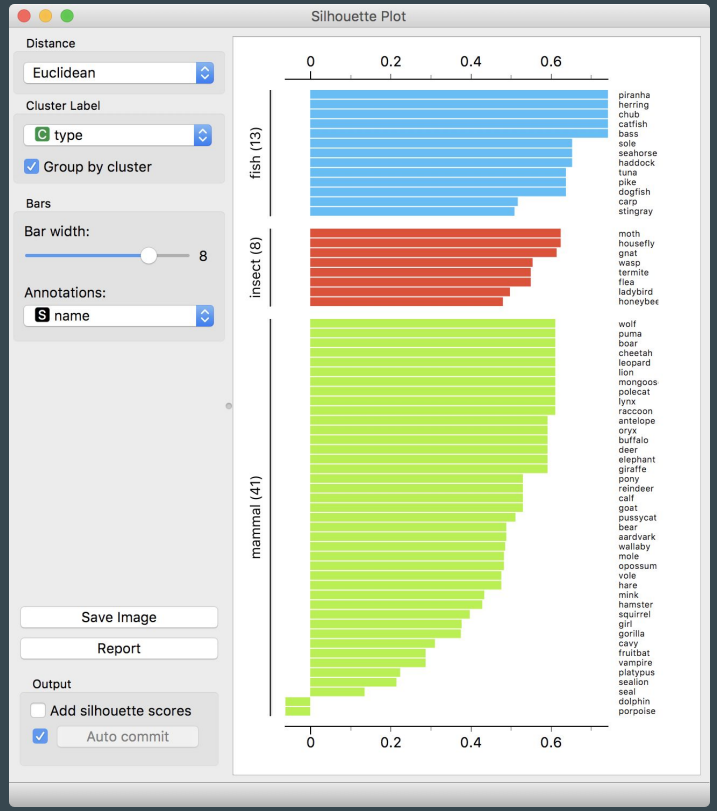


Fig. 3.8 Data splitting in *K*-fold cross-validation

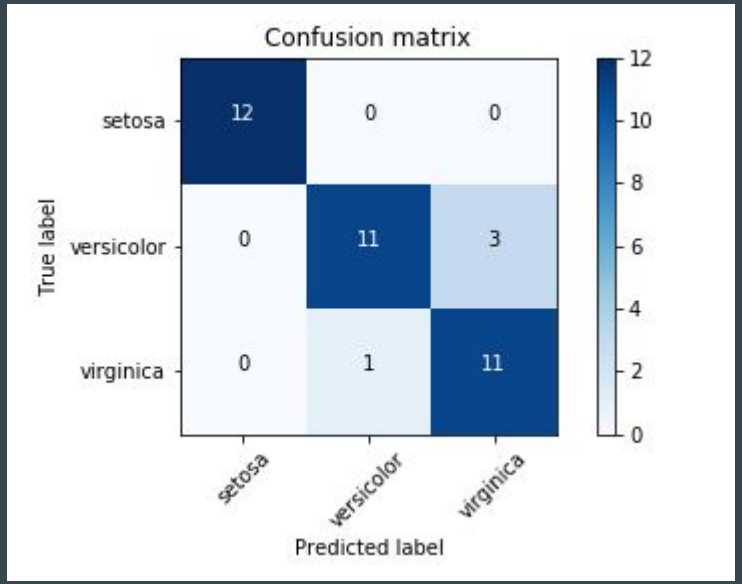
Model Evaluation - Unsupervised

- Harder to know
- We don't have any labels!
- Silhouette score
  - a measure of how close each point in one cluster is to points in the neighboring clusters
  - Higher == More consistent



Model Evaluation

- So how do we compare labels?
- Simple percentage of what we got wrong (accuracy)
- Confusion matrix

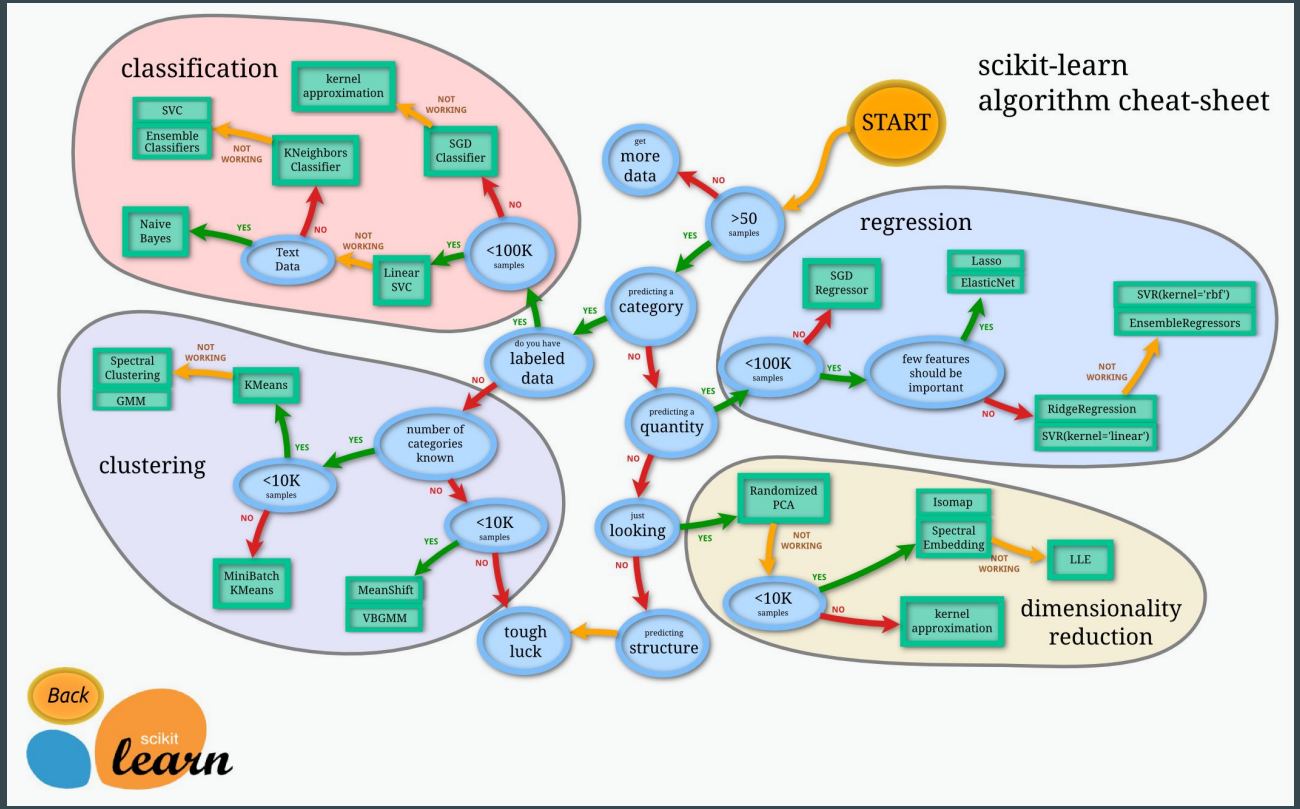


Scikit-learn

- Python library for machine learning
- Consists of a bunch of *Estimator* classes.
  - These have methods *fit*, and *predict*

```
from sklearn import linear_model
from sklearn import datasets

iris = datasets.load_iris()
clf = linear_model.LogisticRegression(solver='lbfgs')
X, y = iris.data, iris.target
clf.fit(X, y)
y_predicted = clf.predict(X)
```

Scikit-learn Estimators

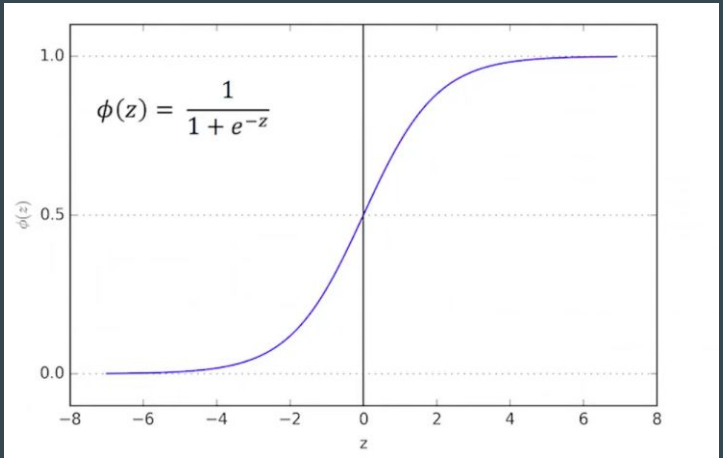


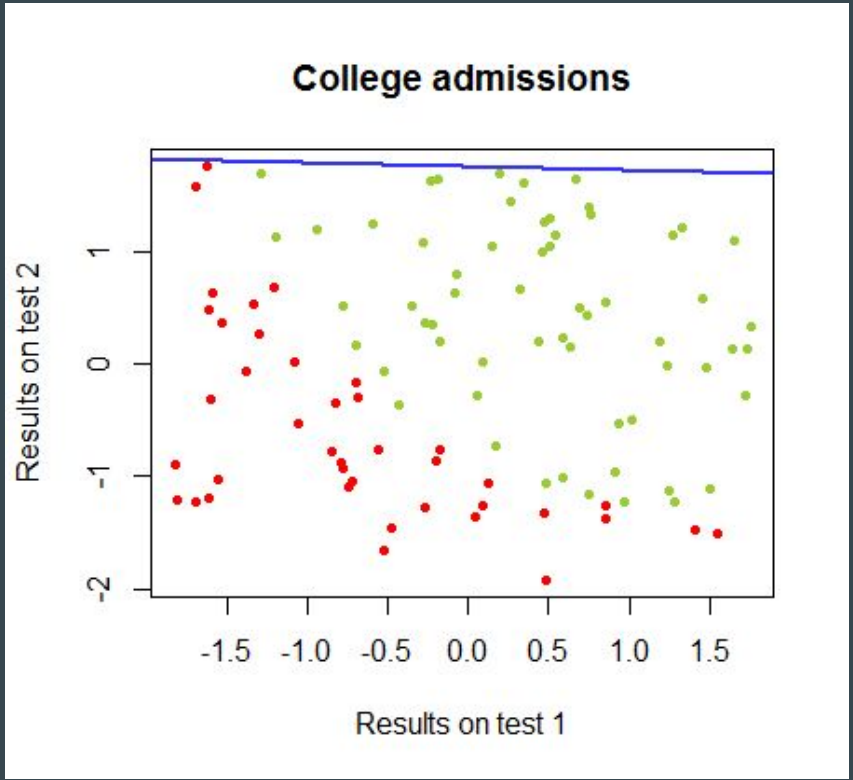
Model Selection

```
from sklearn.model_selection import train_test_split

X_train, X_test, y_train, y_test = \
    train_test_split(iris.data, iris.target, test_size=0.25)

...

from sklearn.metrics import confusion_matrix
cm = confusion_matrix(y_predicted, y_test)
```

Logistic Regression

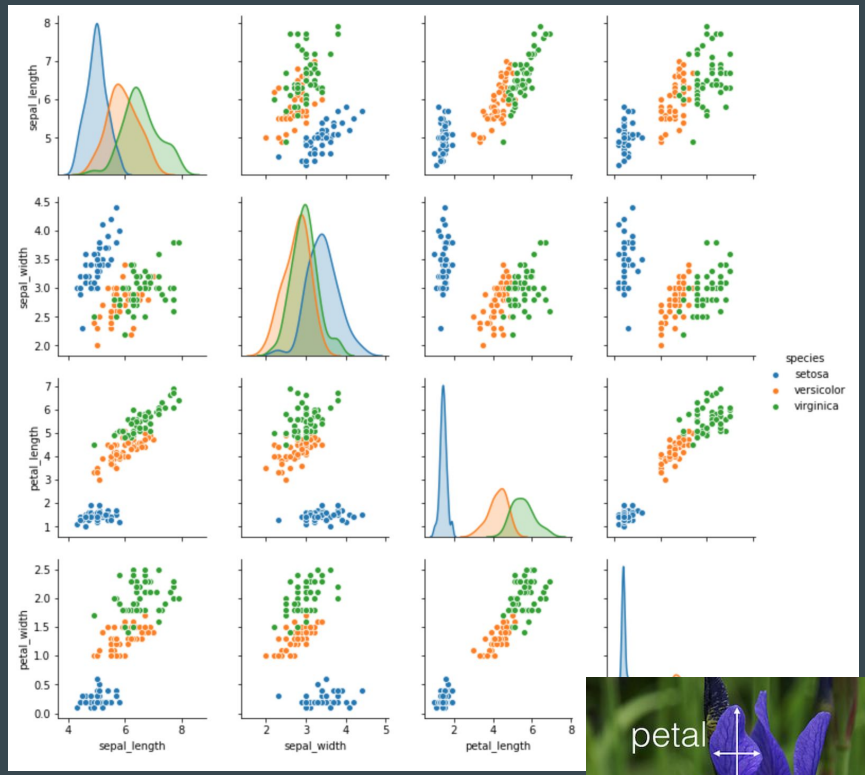
- Try to find a line that *separates* the data
- Then for each point
  - Use distance from line compute probability of class

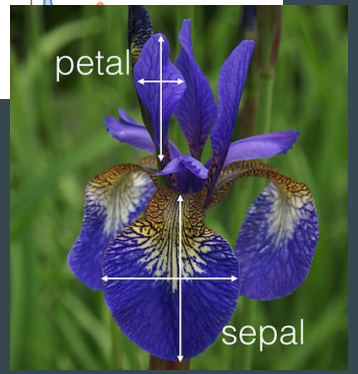




Exercise 1: Classifying Flowers

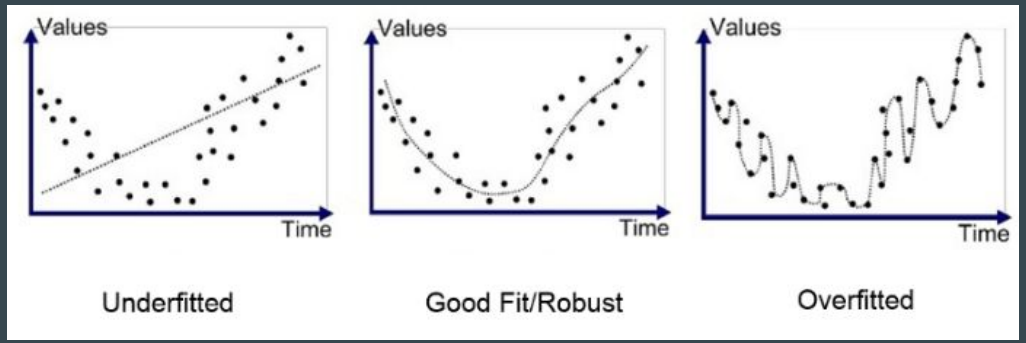
- The Iris Dataset has a 3 classes
  - Setosa, versicolor, virginica
- Run exercise 1 to train the classifier
  - Check what percentage correct do you get?
  - Run it multiple times, does it change?
  - Why? What could we do instead?
- Change the train/test split value
  - Change it to .97
  - What happens to the results?
- Change the code to use KFold cross validation
- Change the Estimator to use *SVC* from the *svm* module.
  - Repeat the above.





Underfitting & Overfitting

- Underfitting - Model cannot capture the underlying trend of the data
  - Try a more complex model, probably with more parameters
- Overfitting - Model fits too well and starts fitting to the noise in the data
  - Try a simpler model
  - Try getting more data
  - Try regularizing you model ...

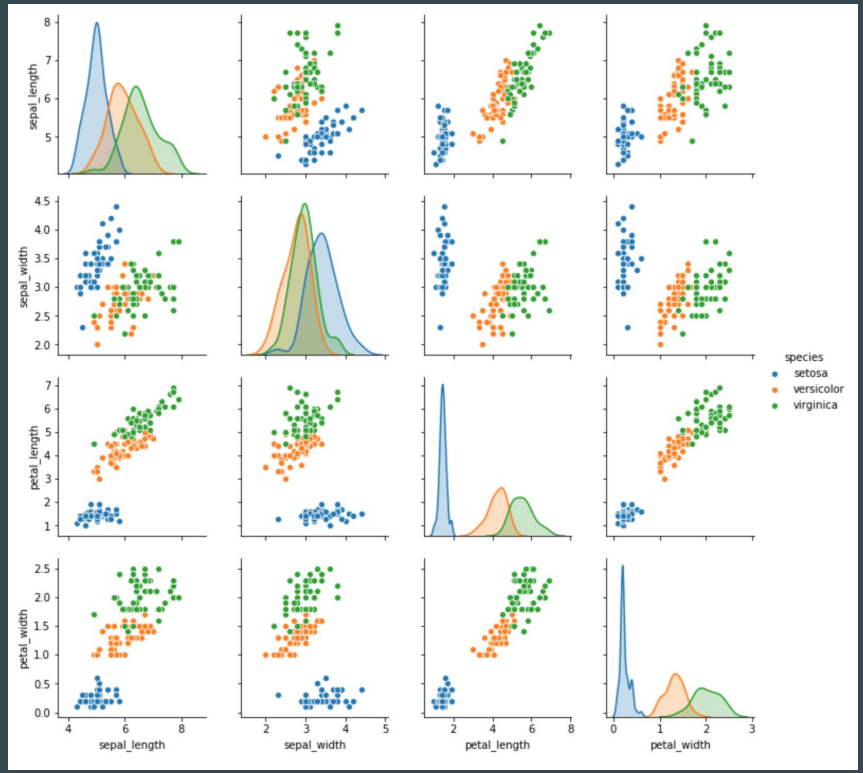


Regularization

- Add a penalty term to the cost function of the model
- L2 regularisation
  - Aka: Ridge regression.
  - Penalises very large weights.
  - Sklearn has *sklearn.linear_model.Ridge*
- **Exercise 2**: Underfitting & Overfitting
  - Polynomial model for a cosine wave.
  - Play with the number of degrees (this increases model complexity)
  - Play with the number of number of samples
  - Try swapping the model to ridge regression

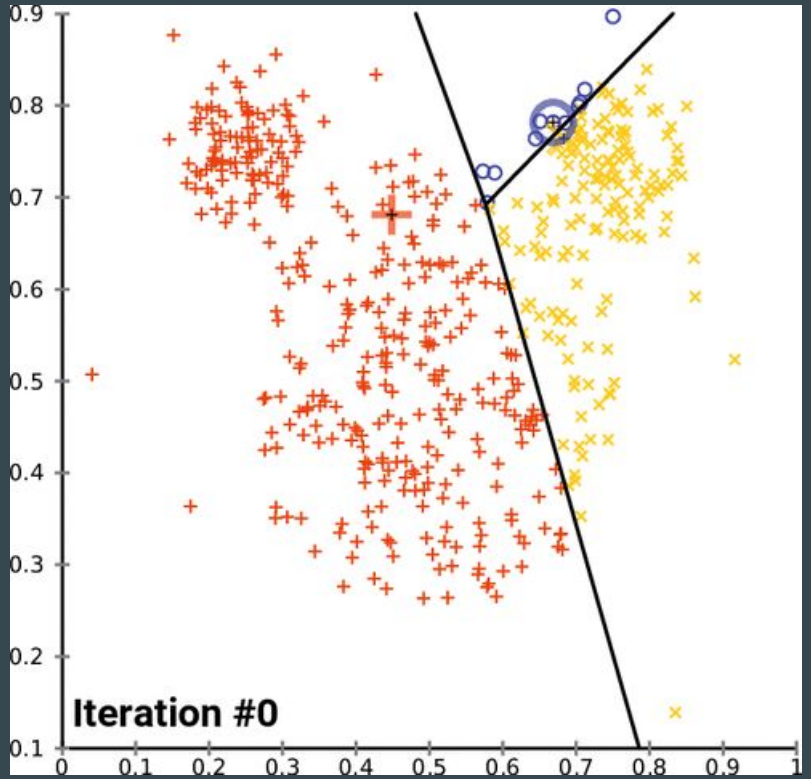
Clustering

- What if we didn't have the labels?
- The classes form clusters in the data
  - *Virginica* and *versicolor* overlap a little
- Cluster can infer structure without labels



K-Means Classifier

- Pick *k* points randomly
- Calculate mean distance from center points to every other point
- Classify points by whatever center is closest
- Calculate mean of those clusters
- Use mean as new center
- Rinse and repeat



Exercise 3: Clustering

- Write some code to cluster the Iris dataset
  - Using the KMeans Classifier
- Hint: cluster classifiers have a method called *fit_predict* to fit and predict in one step
- Try a different clustering technique:
  - https://scikit-learn.org/stable/modules/clustering.html
- Try measuring the consistency of the cluster with the silhouette score

Aside: 30 seconds of Pandas

- Awesome library for handling raw data.
- Allows us to create *DataFrames* which store data in table like structures.

```
import pandas as pd
df = pd.read_csv("data/titanic/train.csv")
df.head() # get the top n rows
df.tail() # get the bottom n rows
df['Age'] # get the column with the heading "Age"
df.drop("Name", axis=1) # drop the column called name
df.values # get the entries as a numpy matrix
df.fillna('Age': 0) # fill all NaN entries in the Age column with 0.
```

Exercise 4: Titanic Data

- For the final exercise we'll try a Kaggle Competition dataset
- Given a set of (labelled) data try and predict who survives on the titanic
- Play with different classifiers
- Play with different parameters
- Investigate what the variables mean?
  - Can we make new ones?
  - Representation is key!

You may also like:

- SciML Seminars
  - 12:30 - 13:30 Weekly.
  - 1hr presentation on a variety of ML topics (with free pizza!)
  - Workshops on practical ML are coming soon.
  - https://indico.stfc.ac.uk/category/15/
- Slides & code for this session:
  - https://github.com/samueljackson92/ml-workshop

Thank You