Introduction to Machine learning with scikit-learn

Important ideas

What is machine learning?

- extracting knowledge from data
- closely related to statistics and optimization.
- What distinguishes machine learning is that it is very focused on prediction.

Types of Machine Learning

- Supervised
- Unsupervised
- Reinforcement
-

Types of ML

- **Supervised** learning: Models that can predict labels based on **labeled data**
  - Classification: Models that predict labels as two or more discrete categories
  - Regression: Models that predict continuous labels
- **Unsupervised** learning: Models that identify structure in unlabeled data
  - Clustering: Models that detect and identify distinct groups in the data
  - Dimensionality reduction: Models that detect and identify lower-dimensional structure in higher-dimensional data.

Supervised Learning

$$(x_i, y_i) \propto p(x, y) \text{ i.i.d.}$$

$$x_i \in \mathbb{R}^p$$

$$y_i \in \mathbb{R}$$

$$f(x_i) \approx y_i$$

- Given an array of test results from a patient, does this patient have diabetes?

The x_i would be the different test results, and y_i would be diabetes or no diabetes.

- Given a piece of a satellite image, what is the terrain in this image?

Here x_i would be the pixels of the image, and y_i would be the terrain types.

Unsupervised Learning

$$x_i \propto p(x) \text{ i.i.d.}$$

Learn about p.

- discovering topics in news articles or on twitter, or grouping data into clusters for easier analysis.
- outlier detection, where you ask "does this data look normal" which is important for fraud detection and security systems.

Classification and Regression

Classification

- target y discrete
- Is this patient sick?

Regression

- target y continuous
- How long will it take for the patient to recover?

Generalization

- Not only $f(x_i) \approx y_i$ for the data seen/used
- also for new data: $f(x) \approx y$

Supervised learning

What is the relationship between input and output variables?

IQ	ClassesAttended	CatsYouOwn	YourFinalGrade
110	14	0	73
105	28	2	99
107	26	1	95

- Input variables
  - Independent variables, predictors, input, features
- Output variables
  - Dependent variables, response, output

The relationship between X and Y

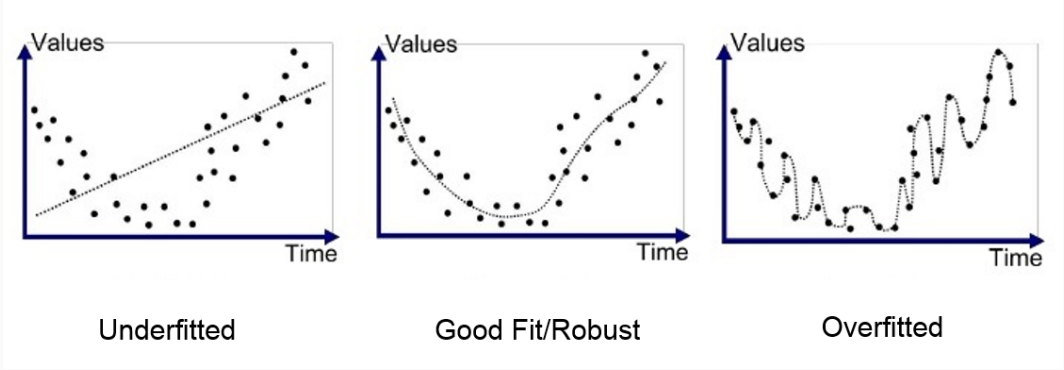
The true relationship is $Y = f(X)$

Our goal is to come up with an *estimate* $\hat{f}$ of the true f

$$\hat{Y} = \hat{f}(X)$$

- Why?
  - So we can plug in values of X and see what $\hat{Y}$ are produced
  - Think of it like a machine.

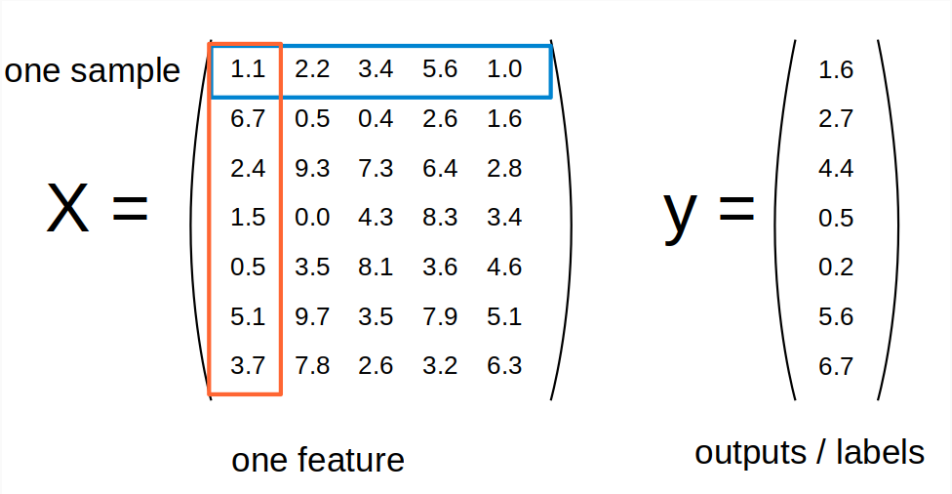
Overfitting



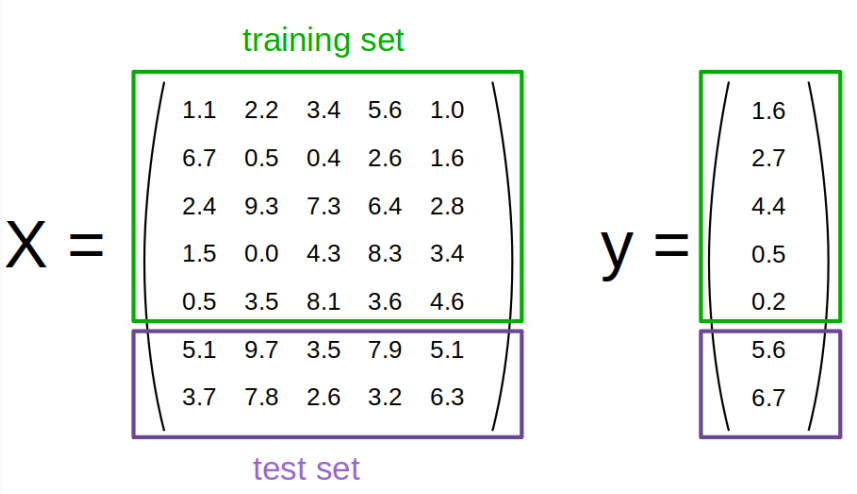
- Worst sin : overfitting

bcos the model works well for data that is seen but does poor job for unseen data

- Split data into Train-Test.


one sample
X =
1.1 2.2 3.4 5.6 1.0
6.7 0.5 0.4 2.6 1.6
2.4 9.3 7.3 6.4 2.8
1.5 0.0 4.3 8.3 3.4
0.5 3.5 8.1 3.6 4.6
5.1 9.7 3.5 7.9 5.1
3.7 7.8 2.6 3.2 6.3
y =
1.6
2.7
4.4
0.5
0.2
5.6
6.7
one feature
outputs / labels

Training and Test Data



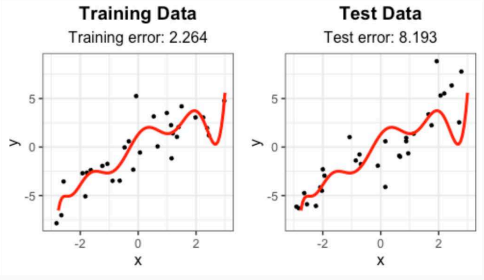
Model evaluation and selection

- train, test
- fit on train
- predict on test
- score the model by how well it does on test

Degree 1 Model

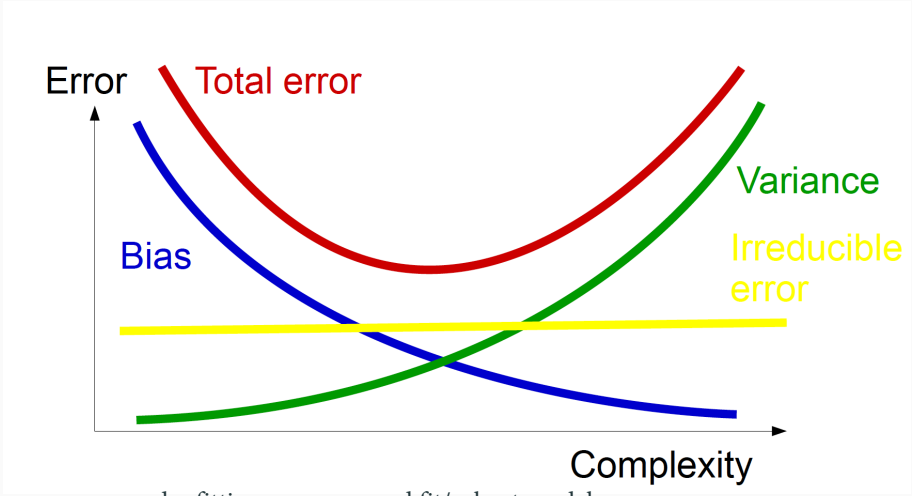
Degree 5 Model

Degree 10 Model



Degree 15 Model

- All data science in one slide: **bias variance tradeoff**



bias variance tradeoff

want the model with least error. As complexity increases, bias goes down but variance increases

- Every estimator has its advantages and drawbacks.
- Its generalization error can be decomposed in terms of bias, variance and noise.
  - The bias of an estimator is its average error for different training sets.
  - The variance of an estimator indicates how sensitive it is to varying training sets.
  - Noise is a property of the data.

Datasets

- Breast Cancer
- Wine
- Iris
- Parkinsons

Team Exercise 1

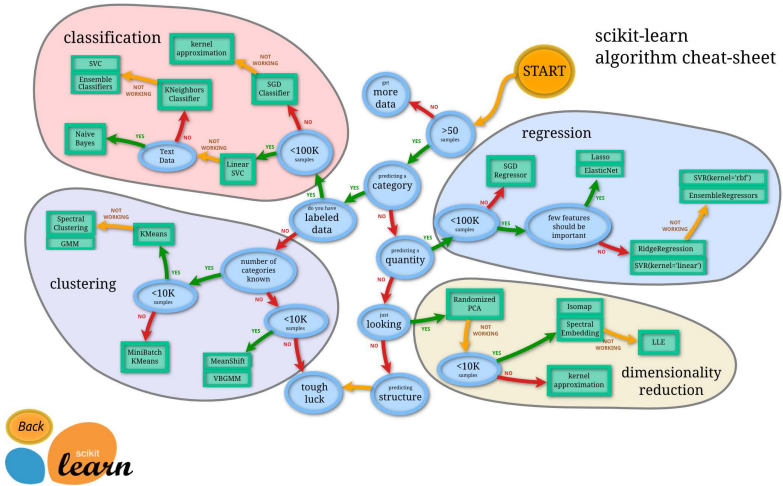
Take a look at the data

Team Exercise 2

Plot the data

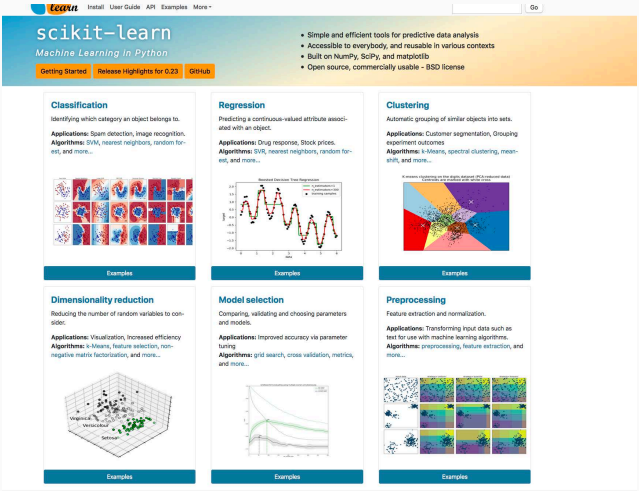
Present : Explain your data set

- Explain the problem you are trying to solve
- Give some preliminary visualizations that are indicative of the difficulty of the problem and possible approaches

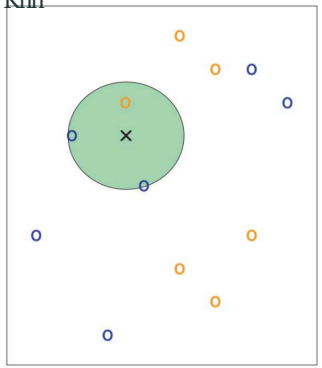


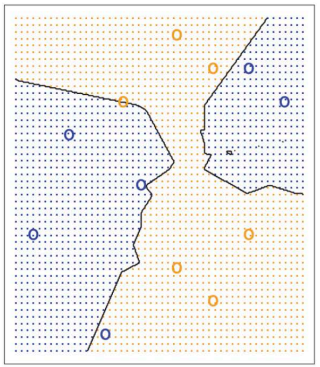
https://scikit-learn.org/stable/tutorial/machine_learning_map/index.html

scikit-learn documentation



Knn





Used for: for regression or classification

How does it work ?

What are parameters to the algorithm if any?

Quick example: picture is fine

Any other relevant information

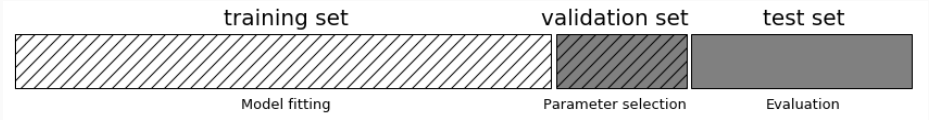
Also, all teams look through pre-processing.

Team Exercise 3

Prepare slides, upload to DSB google drive or Rstudio cloud and share link on status-update. You will present the one of the methods and PCA:

: Knn and kmeans(Team1), LDA(Team 2), SVM(Team 3), Decision trees & if possible Random forests (Team 4), PCA (All)

Threefold split



We use the training set for model building, the validation set for parameter selection and the test set for a final evaluation of the model.

pro: fast, simple

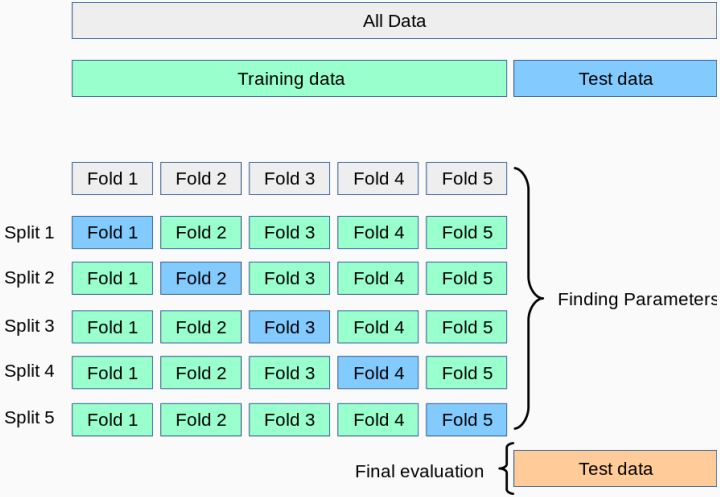
con: high variance, bad use of data

Implementing threefold split

```
X_trainval, X_test, y_trainval, y_test = train_test_split(X, y)
X_train, X_val, y_train, y_val = train_test_split(X_trainval, y_trainval)

val_scores = []
neighbors = np.arange(1, 15, 2)
for i in neighbors:
    knn = KNeighborsClassifier(n_neighbors=i)
    knn.fit(X_train, y_train)
    val_scores.append(knn.score(X_val, y_val))
print("best validation score: {:.3f}".format(np.max(val_scores)))
best_n_neighbors = neighbors[np.argmax(val_scores)]
print("best n_neighbors:", best_n_neighbors)
```

Cross-validation + test set



TimeSeriesSplit

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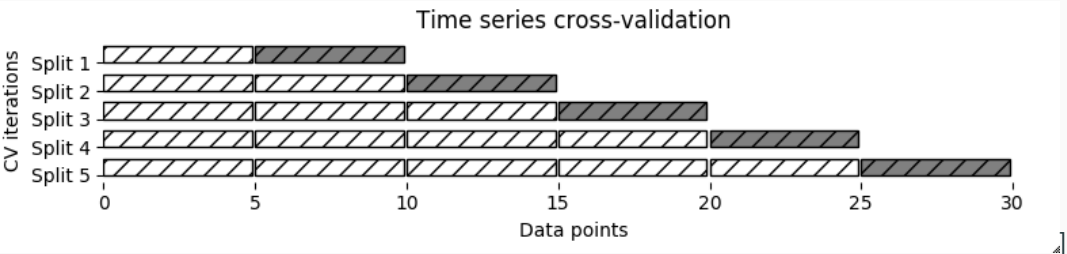

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