Evaluation and Resampling

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Model Validation

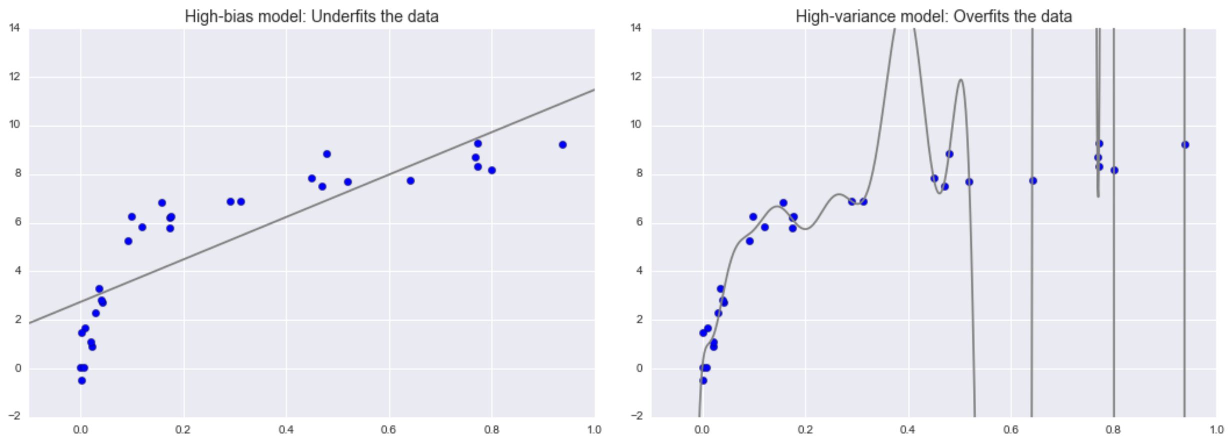
In the previous classes, we saw the basic recipe for applying a supervised machine learning model:

1. Choose the model
2. Choose model hyperparameters
3. Fit the model to the training data
4. Use the model to predict labels for new data

To make an informed choice, we need a way to *validate* that our model and our hyperparameters are a good fit to the data.

The Bias-variance trade-off

The question of "the best model" is about finding a sweet spot in the tradeoff between *bias* and *variance*. Consider the following figure, which presents two regression fits to the same dataset:



It is clear that neither of these models is a particularly good fit to the data, but they fail in different ways.

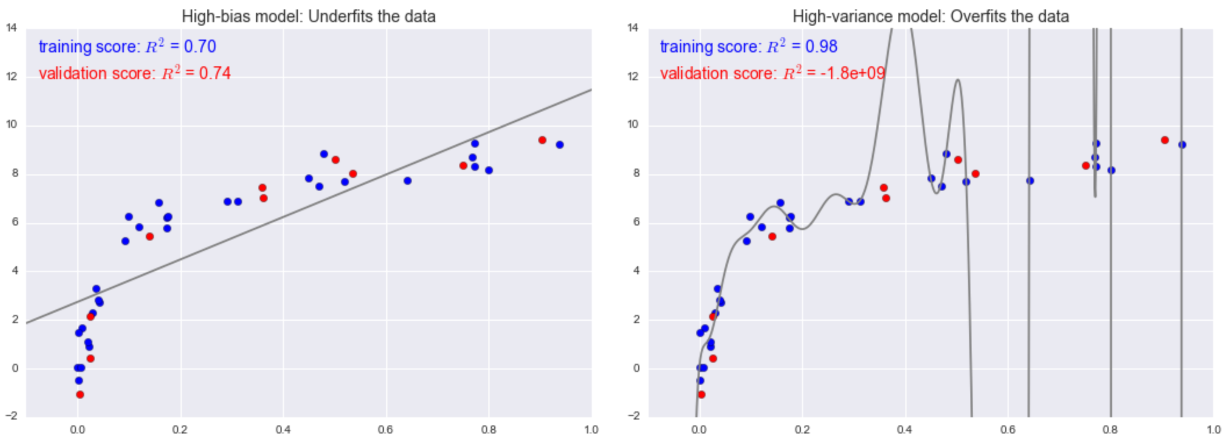
- The model on the left attempts to find a straight-line fit through the data.
  - Because the data are intrinsically more complicated than a straight line, the straight-line model will never be able to describe this dataset well.
  - Such a model is said to *underfit* the data: that is, it does not have enough model flexibility to suitably account for all the features in the data - the model has high *bias*.
- The model on the right attempts to fit a high-order polynomial through the data.

- Here the model fit has enough flexibility to nearly perfectly account for the fine features in the data, but even though it very accurately describes the training data, its precise form seems to be more reflective of the particular noise properties of the data rather than the intrinsic properties of whatever process generated that data.

- Such a model is said to *overfit* the data: it has so much model flexibility that the model ends up accounting for random errors as well as the underlying data distribution - the model has high *variance*.

The Bias-variance trade-off

Consider what happens if we use these two models to predict the y-value for some new data. In the following diagrams, the red/lighter points indicate data that is omitted from the training set:

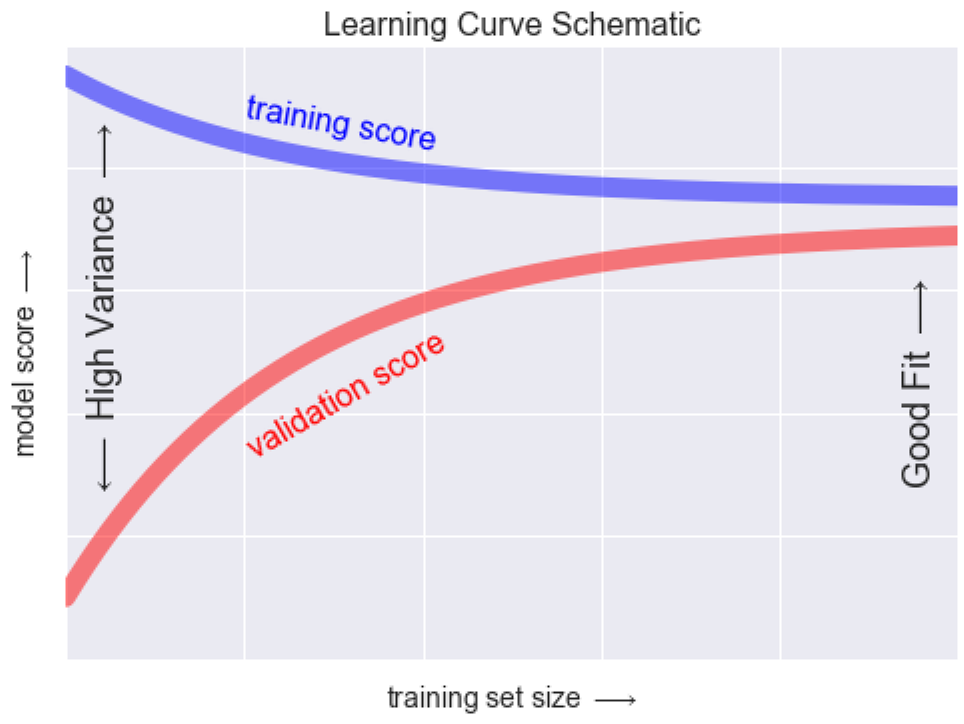


The score here is the R^2 score, or coefficient of determination, which measures how well a model performs relative to a simple mean of the target values. $R^2 = 1$ indicates a perfect match, $R^2 = 0$ indicates the model does no better than simply taking the mean of the data, and negative values mean even worse models. From the scores associated with these two models, we can make an observation that holds more generally:

- For high-bias models, the performance of the model on the validation set is similar to the performance on the training set.
- For high-variance models, the performance of the model on the validation set is far worse than the performance on the training set.

The Bias-variance trade-off

If we imagine that we have some ability to tune the model complexity, we would expect the training score and validation score to behave as illustrated in the following figure:



The diagram shown here is often called a *validation curve*, and we see the following essential features:

- The training score is everywhere higher than the validation score. This is generally the case: the model will be a better fit to data it has seen than to data it has not seen.
- For very low model complexity (a high-bias model), the training data is under-fit, which means that the model is a poor predictor both for the training data and for any previously unseen data.
- For very high model complexity (a high-variance model), the training data is over-fit, which means that the model predicts the training data very well, but fails for any previously unseen data.
- For some intermediate value, the validation curve has a maximum. This level of complexity indicates a suitable trade-off between bias and variance.

Resampling Methods

Resampling methods are an indispensable tool and involve repeatedly drawing samples from a training set and refitting the model on each sample in order to obtain additional information about the fitted model.

For example: To estimate the variability of a linear regression fit

- we can repeatedly draw diferent samples from the training data,
- fit a linear regression to each new sample
- and then examine the extent to which the resulting fits difer.

Resampling

Such an approach may allow us to obtain information that would not be available from fitting the model only once using the original training sample.

Resampling approaches can be computationally expensive

- they involve fitting the same machine learning method multiple times using diferent subsets of the training data.
- due to recent advances in computing power, the computational requirements of resampling methods generally are not prohibitive.

Two of the most commonly used resampling methods

- **Cross-validation**
- **Bootstrap**

Resampling Methods

Cross-validation and the bootstrap.

- These methods refit a model of interest to samples formed from the training set, in order to obtain additional information about the fitted model.

- For example, they provide estimates of test-set prediction error, and the standard deviation and bias of our parameter estimates

Model Evaluation

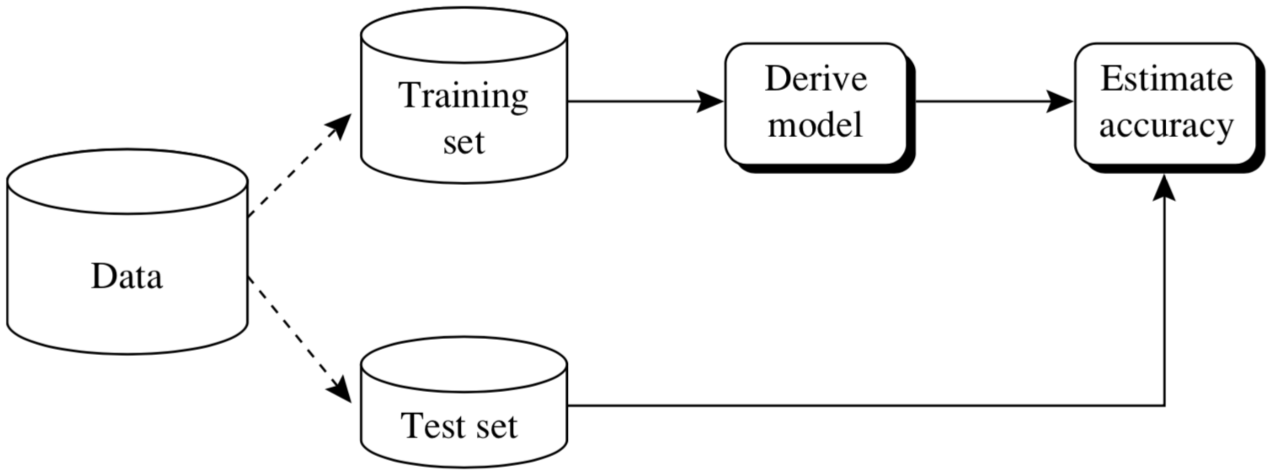
- We want to **estimate** how well the model performs with **unknown** cases
  - makes good predictions
  - makes good diagnoses
  - assigns correctly an email to a folder

Model Evaluation: model selection

- We have, e.g, a classification problem
  - Is Logist Regression **better** than Linear Discriminant Analysys?

- **Model Selection**
  - Obtain a model with each one (on the same data)
  - Identify the model that performs better (on the same data)

Estimating evaluation metrics



- **Option 1**: Estimate accuracy on the training examples
  - Estimate tends to be **optimistic**
  - **Very bad choice!!!**
- **Option 2**: Isolate a subset for testing (**holdout**)
  - Estimate is more **reliable**
  - Estimate tends to be **pessimistic**
  - Depends on **sampling**
  - Depends on the **sizes** of the train and test set

Training Error and Generalization Error

Recall the distinction between the test error and the training error:

- The **training error** can be easily calculated by applying the model to the observations used in its training.

- The **test error** (generalization error) is the average error that results from using a model to predict the response **on a new observation**, one that was not used in training the method.

  - test error rate often is quite different from the training error rate...

Training Error and Generalization Error

- The aim of evaluation is to **estimate** Generalization Error from **observed data** $< X, Y >$
- **Error** is a random variable

  - We want to estimate it as reliably (robustly) as possible
- **Training Error**: average loss over the training sample ($x_i \in X_{train}, y_i \in Y_{train}$)

$$\mathrm{err}_{training} = \frac{1}{N}\sum_{i=1}^{N} L(y_i, \hat{f}(x_i))$$

- **Test Error** or **Generalization Error**: expected prediction error over an independent sample **given** a training set T
  - Notes:
    - We already have a model
    - The test set here is not fixed

$$Err_T = \mathrm{E}[L(y_i, \hat{f}(x_i)) \mid T]$$

- **Expected Test Error**: the training set is not fixed, so we can have different $\hat{f}(x)$

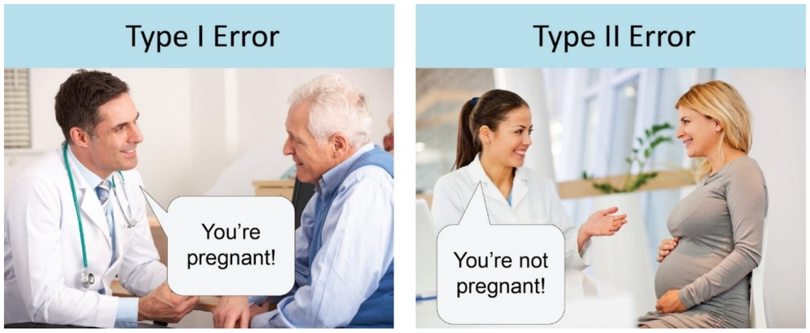
$$Err = \mathrm{E}[L(y_i, \hat{f}(x_i))]$$

Metrics for Evaluating Classifier Performance

- How to **assess** a classifier?
  - many metrics
- Most popular
  - Accuracy
  - Recall
  - Precision
  - F1
  - Sensitivity
  - Specificity

Binary classification

- We have a positive and a negative class
- 2 different kind of errors:
  - False Positive (type I error): model predicts positive while true label is negative
  - False Negative (type II error): model predicts negative while true label is positive
- They are not always equally important
  - Which side do you want to err on for a medical test?



Binary classification

- We have
  - **positive examples**
  - **negative examples**
- Depending on how a model classifies a test case

classified as	Predict Pos	Predicted Neg
Actual Pos	True Positives	False Negatives
Actual Pos	False Positives	True Negatives

An example

- Loans are the core business of loan companies/banks. The main profit comes directly from the loan's interest. The loan companies grant a loan after an intensive process of verification and validation. However, they still don't have assurance if the applicant is able to repay the loan with no difficulties.

classified as	loan	no loan
loan	43	12
no loan	32	21

- **Accuracy** is $(43+21)/(32+12+43+21)=0.59$
- **Recall** ('loan' as positive) is $43/(43+12)=0.78$
  - the bank identifies 78% of the good clients, but 22% are missed
- **Precision** is $43/(43+32)=0.57$
  - 57% of the loans given would fail
- **Specificity** is $21/(21+32)=0.40$
  - the bank only detects 40% of the 'bad' clients
- **F1** is $2\times 0.78\times 0.57/(0.78+0.57)=0.66$
  - there is a relatively good balance of recall and precision

Accuracy

$$Accuracy=\frac{TP+TN}{P+N}$$

- In other words
  - The main diagonal divided by the sum of all the matrix

Recall

$$Recall=\frac{TP}{P}$$

- A.k.a.
  - **True Positive Rate**
  - **Sensitivity**
    - How sensitive is the model to the positive class?

Precision

- Are all our decisions good?
  - If $Precision=1$ we only say right things

$$Precision=\frac{TP}{TP+FP}$$

- **Note the following**
  - Management wants to get more clients and asks for a model with higher **recall**.
  - Data scientists say: "we risk getting more bad clients too"
  - When Recall increases Precision **tends** to go down
  - and vice-versa

Accuracy

- **Accuracy**
  - the test asks $Total$ questions
  - each question is equally important
  - the model gets $Right$ questions right
  - the proportion of right answers

$$Accuracy = \frac{Right}{Total}$$

- **Error**
  - $Error = 1 - Accuracy$

F_1

- How to combine recall and precision?
  - calculate the **harmonic mean**

$$F_1 = \frac{2 \times Recall \times Precision}{Recall + Precision}$$

- F_1 is
  - also known as **F-score**
  - low if **either** recall or precision are low
  - equal to Recall and Precision if $Recall = Precision$
  - generalised by F_β

Specificity

- Are we excluding all the bad clients?
  - If $Specificity = 1$ we identify all bad clients (and hopefully some good ones)

$$Specificity = \frac{TN}{N}$$

- A.k.a.
  - **True Negative Rate**
  - Used in medical applications
    - negatives are patients without the disease

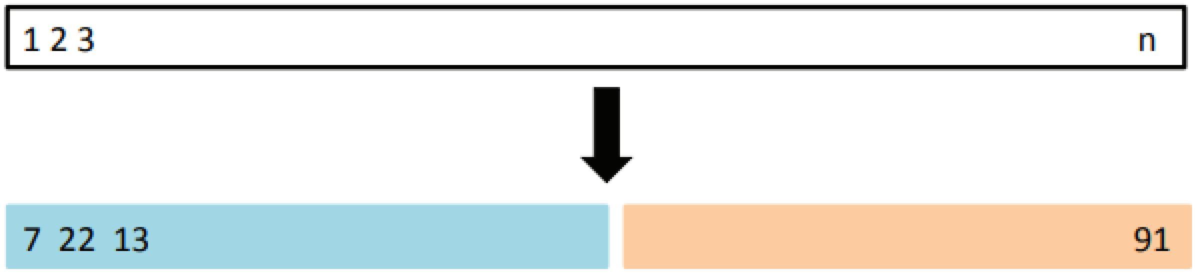
Holdout

- **Holdout** evaluation method

  - separate data set in **train** and **test**
- use **train to learn** the model, and **test to assess** it

In [1]:
```
from IPython.display import Image
Image("cv_5_1.png")
```

Out[1]:



Dealing with assessment variance

- A problem with holdout is **variance** of the evaluation estimates
  - Accuracy is also a **random variable**
  - We do not know its **true value** or **distribution**
- Solutions:
  - Testing with **more data**
    - reduces variance
    - if there is more data
  - **Repeating** the train-test cycle
    - reduces variance
    - enables **studying the distribution** of the measure (e.g. accuracy)
    - but we need a different sample for each iteration

K-fold Cross-validation

- Widely used approach for estimating test error.
- Estimates can be used to select best model, and to give an idea of the test error of the final chosen model.

- Idea:

  - Randomly divide the data into K equal-sized parts.
  - We leave out part k, fit the model to the other $K-1$ parts
  - Obtain predictions for the left-out kth part.

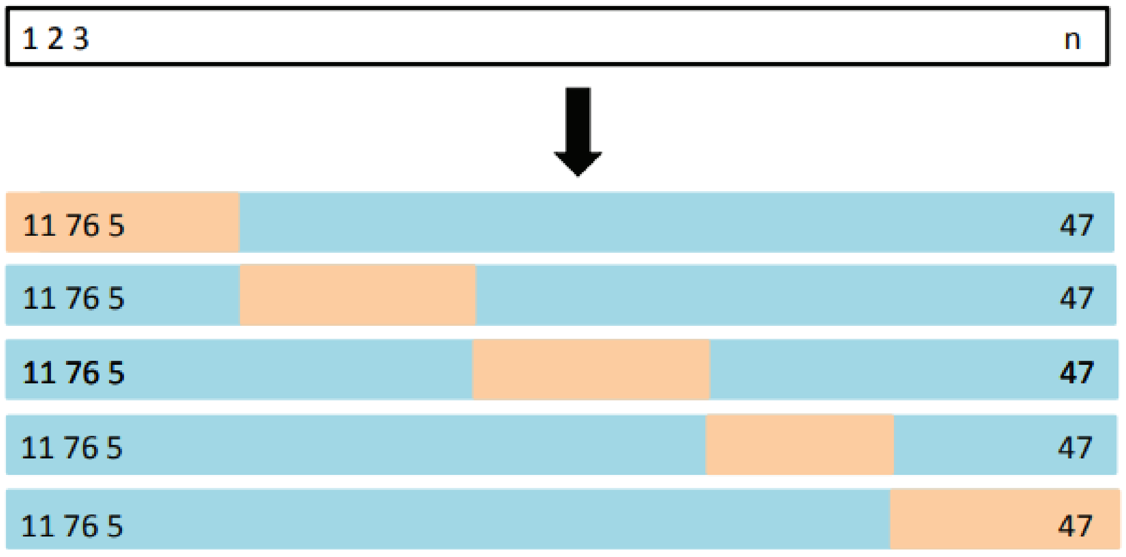
  - This is done in turn for each part $k = 1, 2, \dots K$, and then the results are combined

Repeating train-test: k-fold Cross-validation

- In each iteration $i \in 1 \dots, k$
  - use fold i for testing
  - use the other $k-1$ folds for training
  - obtain Acc_i
- Study the distribution of the Acc_i

In [2]:
```
from IPython.display import Image
Image("cv_5_5.png")
```

Out[2]:



Repeating train-test: k-fold Cross-validation

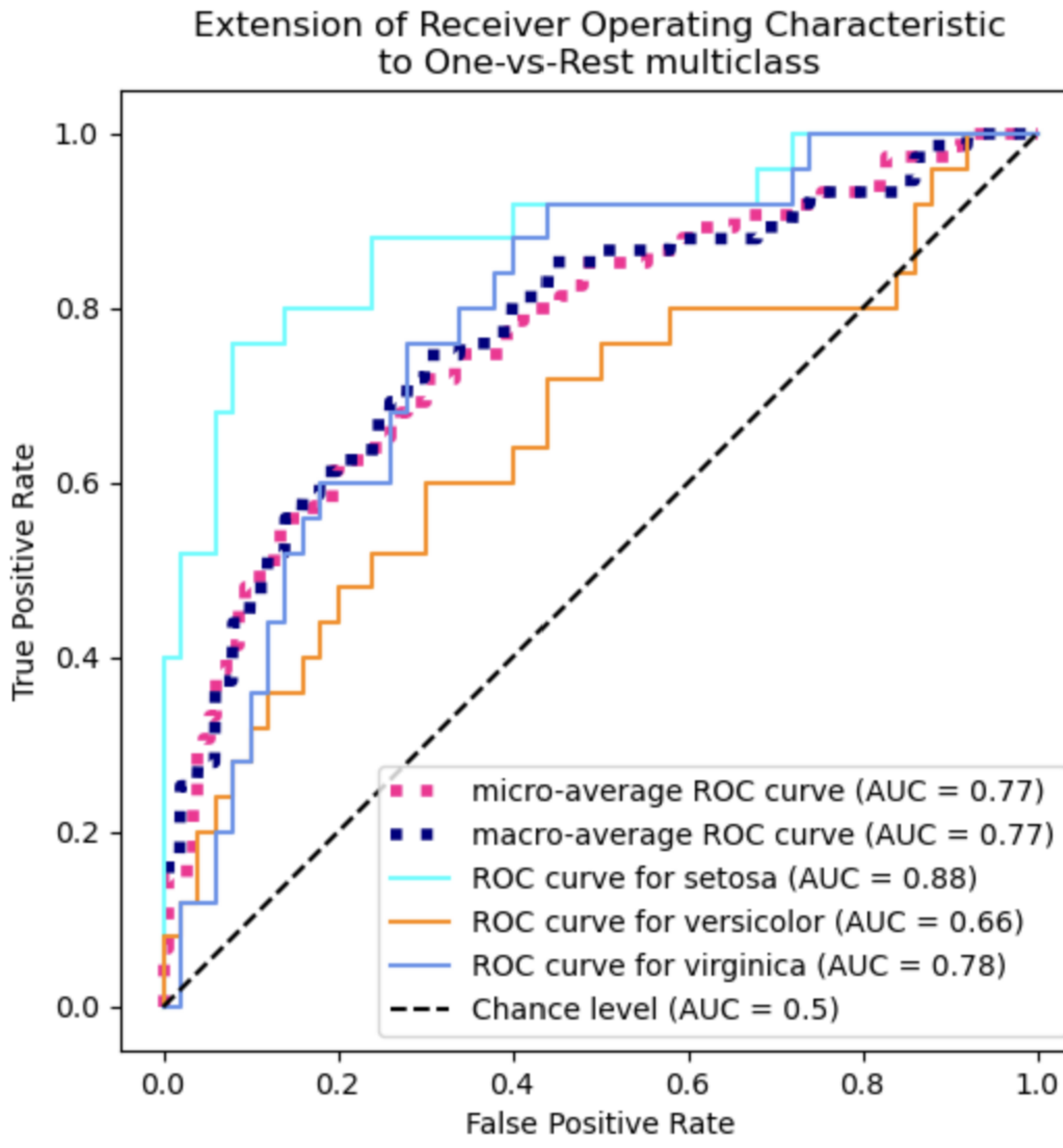
- Each sample is used **exactly once**
- Test sets are **independent**
  - Training sets are not
- What if we have a **small class**?
  - **stratified cross validation** to avoid under representation
- If we have **very few examples**?
  - **leave one out** cross validation
  - also leave p out for other (small) values of p
- **How many** folds should we use?
  - typical: 10 fold cross validation (10 fold CV)
  - (Demsar 2006) 2 times 5 fold CV
- **Shufling** before splitting may be a good idea

Leave-One-Out Cross-Validation (LOOC)

- Leave-one-out
  - If the sample is very small we can make $K = N$
  - We train with **all examples but one** in each iteration
  - Leave-one-out still estimates Expected Test Error

ROC curves

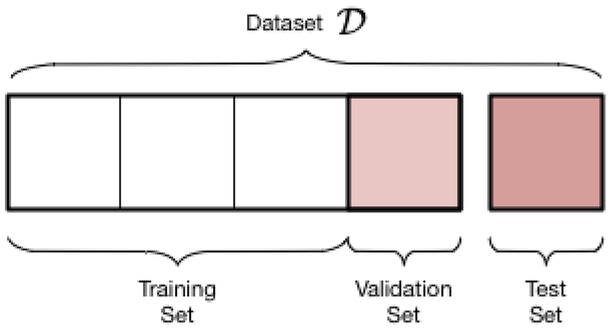
- We can compare the performance of classifiers on the whole spectrum of misclassification costs
- **Receiver operating characteristic curves**
  - plot relation between TPR and FPR
  - the **AUC**, area under the curve, is an assessment measure



(https://scikit-learn.org/stable/auto_examples/model_selection/plot_roc.html)

Validation, Test and deployment

- We can use cross-validation for **tuning**
    - hyperparamater tuning, pre-processing decisions, ...
- In after tuning (and other decisions) use a **new test set**
- The **internal test set** is the **validation set** (or sets)



Validation, Test and deployment

- **Why** do we need **validation and test ?**
  - using the test set to improve results leads to overly **optimistic** results
    - it is like **using the future to make predictions**
    - or **knowing the exam questions** when you study
    - but we do it in the lab as long as comparisons are fair
  - the test set should be for **testing only**
- Which model we use in **deployment** ?
  - We use the approach and hyperparameters that had best test results
  - We can **then** use the whole data to train the model
    - if data is scarce. We can use less data too

Measuring statistical significance

- We compare two algorithms **A** and **B**
  - **A** has 0.8832 accuracy
  - **B** has 0.8845 accuracy
- Is this difference **important**?
  - **Statistical significance**
    - the difference occurs most of the time
    - how likely is it to observe this difference or larger?
  - **Usefulness**
    - st. significant does not imply useful
    - does it save more lifes with fewer secondary effects?

Measuring statistical significance

- Use **Hypothesis testing**
- 10 fold CV example with t-test
  - obtain two samples of the accuracies: Acc_A and Acc_B
  - each sample has size 10
  - calculate the means $mean_A$ and $mean_B$
  - we assume that the accuracy values follow a **t-distribution** with $k-1$ degrees of freedom
  - we can use a paired **t-test**
  - H_0 **or Null hypothesis** is that the difference of means is zero
  - the **paired t-test** checks if we can reject H_0
  - the test **assumes independence** of the samples (not true)

More on statistical significance tests

- t-test with cross validation should be avoided
  - the independence of the values does not exist
  - it gives some information though
- if we have enough data to promote independence
  - t-test is acceptable
- To compare two algorithms on multiple datasets (e.g. 30)
  - cross-validate on each dataset
  - choose a **level of significance** (typically 1% to 5%)
  - if assumptions hold use a parametric test (**t-test**)
  - if not, use non-parametric **wilcoxon signed rank** test
- To compare many algorithms on multiple datasets
  - use **Friedman** test and post-hoc **Nemenyi** with **critical distances**
- Be **careful with multiple comparisons**
  - sometimes we have to **adjust** the p-values

In [3]:
```
# %load ../standard_import.txt
import pandas as pd
import numpy as np
import matplotlib.pyplot as plt
import seaborn as sns

import sklearn.linear_model as skl_lm
from sklearn.metrics import mean_squared_error
from sklearn.model_selection import train_test_split, LeaveOneOut, KFold, cross_val_scor
from sklearn.preprocessing import PolynomialFeatures

%matplotlib inline
#plt.style.use('seaborn-white')
```

Example: Auto dataset

Compare linear vs higher-order polynomial terms in a linear regression

In [4]:
```
df1 = pd.read_csv('Auto.csv', na_values='?').dropna()

df1.info()
```

```
<class 'pandas.core.frame.DataFrame'>
Index: 392 entries, 0 to 396
Data columns (total 9 columns):
 #   Column        Non-Null Count  Dtype  
---  ------        --------------  -----  
 0   mpg           392 non-null    float64
 1   cylinders     392 non-null    int64  
 2   displacement  392 non-null    float64
 3   horsepower    392 non-null    float64
 4   weight        392 non-null    int64  
 5   acceleration  392 non-null    float64
 6   year          392 non-null    int64  
 7   origin        392 non-null    int64  
 8   name          392 non-null    object 
dtypes: float64(4), int64(4), object(1)
memory usage: 30.6+ KB
```

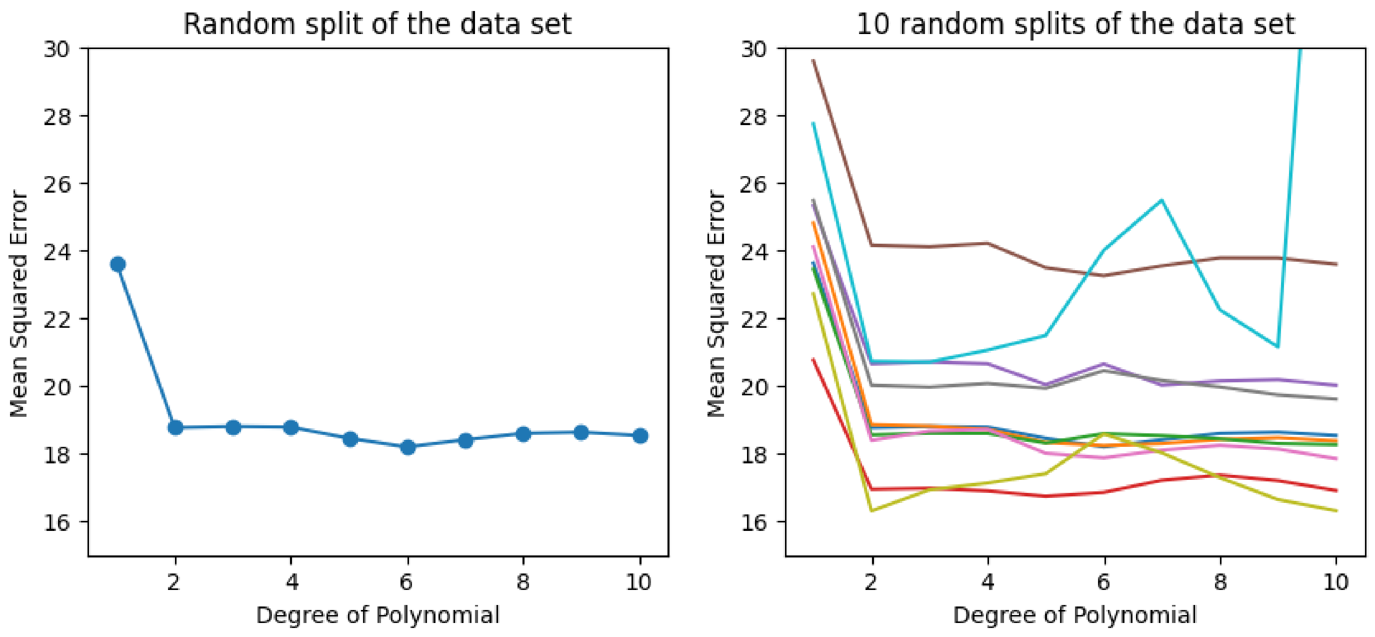
Cross-Validation

Validation Set Approach

- We randomly split the 392 observations into two sets:
    - training set containing 196 of the data points
    - validation set containing the remaining 196 observations.

Using Polynomial feature generation in scikit-learn
http://scikit-learn.org/dev/modules/preprocessing.html#generating-polynomial-features

In [5]:
```
t_prop = 0.5
p_order = np.arange(1,11)
r_state = np.arange(0,10)

X, Y = np.meshgrid(p_order, r_state, indexing='ij')
Z = np.zeros((p_order.size,r_state.size))

regr = skl_lm.LinearRegression()

# Generate 10 random splits of the dataset
for (i,j),v in np.ndenumerate(Z):
    poly = PolynomialFeatures(int(X[i,j]))

    X_poly = poly.fit_transform(df1.horsepower.values.reshape(-1,1))

    X_train, X_test, y_train, y_test = train_test_split(X_poly, df1.mpg.ravel(),
                                                        test_size=t_prop, random_state=Y

    regr.fit(X_train, y_train)
    pred = regr.predict(X_test)
    Z[i,j]= mean_squared_error(y_test, pred)

fig, (ax1, ax2) = plt.subplots(1,2, figsize=(10,4))

# Left plot (first split)
ax1.plot(X.T[0],Z.T[0], '-o')
ax1.set_title('Random split of the data set')

# Right plot (all splits)
ax2.plot(X,Z)
ax2.set_title('10 random splits of the data set')

for ax in fig.axes:
    ax.set_ylabel('Mean Squared Error')
    ax.set_ylim(15,30)
    ax.set_xlabel('Degree of Polynomial')
    ax.set_xlim(0.5,10.5)
    ax.set_xticks(range(2,11,2));
```



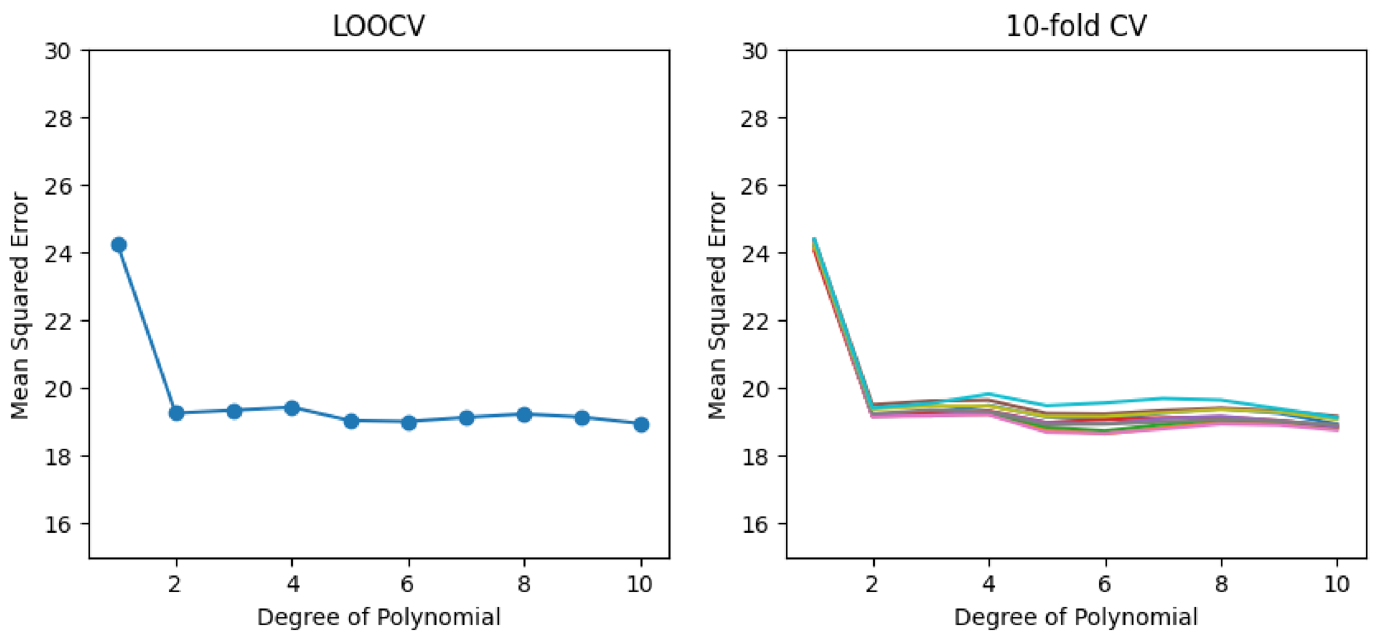
Leave-One-Out Cross-Validation (LOOC)

- Leave-one-out
  - If the sample is very small we can make $K = N$
  - We train with **all examples but one** in each iteration
  - Leave-one-out still estimates Expected Test Error

In [6]:
```
p_order = np.arange(1,11)
r_state = np.arange(0,10)

# LeaveOneOut CV
regr = skl_lm.LinearRegression()
loo = LeaveOneOut()
loo.get_n_splits(df1)
scores = list()

for i in p_order:
    poly = PolynomialFeatures(i)
    X_poly = poly.fit_transform(df1.horsepower.values.reshape(-1,1))
    score = cross_val_score(regr, X_poly, df1.mpg, cv=loo, scoring='neg_mean_squared_err
    scores.append(score)
```

In [7]:
```
# k-fold CV
folds = 10
elements = len(df1.index)

X, Y = np.meshgrid(p_order, r_state, indexing='ij')
Z = np.zeros((p_order.size,r_state.size))

regr = skl_lm.LinearRegression()

for (i,j),v in np.ndenumerate(Z):
    poly = PolynomialFeatures(X[i,j])
    X_poly = poly.fit_transform(df1.horsepower.values.reshape(-1,1))

    kf_10 = KFold(n_splits=folds, random_state=Y[i,j], shuffle=True)
    #kf_10 = KFold(n_splits=folds, random_state=None, shuffle=False)

    Z[i,j] = cross_val_score(regr, X_poly, df1.mpg, cv=kf_10, scoring='neg_mean_squared_
```

In [8]:
```python
fig, (ax1, ax2) = plt.subplots(1,2, figsize=(10,4))

# Note: cross_val_score() method return negative values for the scores.
# https://github.com/scikit-learn/scikit-learn/issues/2439

# Left plot
ax1.plot(p_order, np.array(scores)*-1, '-o')
ax1.set_title('LOOCV')

# Right plot
ax2.plot(X,Z*-1)
ax2.set_title('10-fold CV')

for ax in fig.axes:
    ax.set_ylabel('Mean Squared Error')
    ax.set_ylim(15,30)
    ax.set_xlabel('Degree of Polynomial')
    ax.set_xlim(0.5,10.5)
    ax.set_xticks(range(2,11,2));
```



Choosing the K in KFCV

- $K = N$
  - Provides an approximately **unbiased estimator** of Err
  - High variance
  - Computationally **expensive**
- $K = 5$
  - Lower variance
  - Bias can be a problem
    - Training sets are smaller
    - Easier to overfit
    - Error can be **overestimated**
    - Not a problem with enough data
- 5 or 10 fold-CV are recommended in general

Bootstrap Method

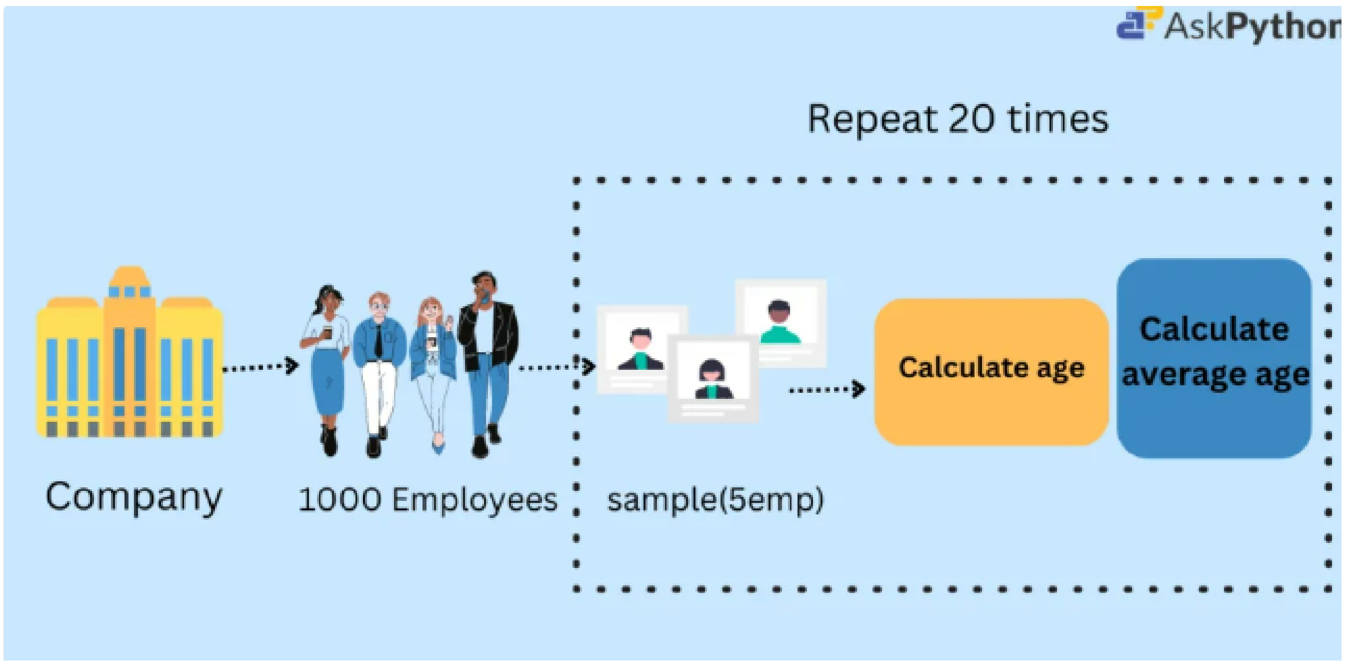
- Is a powerful tool that can be used to quantify the uncertainty associated with a given model.
- It is not the same as the term "bootstrap" used in computer science meaning to "boot" a computer from a set of core instructions, though the derivation is similar.

Boostrap sampling

Example: suppose we want to calculate the average age of 1000 employees working for a particular company

- The first approach could be to ask all the 1000 employees their age and then calculate the mean age.
  - This can be a time-consuming approach
- Another method is to consider a sample of 5 employees and collect their ages
  - This process can be repeated 20 times, and then average the collected age data of 100 employees.
  - This average age would be the estimate of all 1000 employees.

Boostrap sampling



(https://www.askpython.com/python/examples/bootstrap-sampling-introduction)

Repeating train-test: Bootstrapping

- **Bootstrapping** samples the data set with replacement
  - k bootstrap subsamples from the **same** data
    - same size as data, can have **repeated examples**
  - k test sets with the examples left out in each bootstrap
    - on average 63.2% of the data set
  - obtain an accuracy estimate for each subsample
  - calculate average and variance of the k estimates

In [9]:
```
## Bootstrap Resampling
```

```python
# Import numpy
import numpy as np

# Load the breast cancer dataset
from sklearn.datasets import load_breast_cancer
data = load_breast_cancer()

X = data.data # features
y = data.target # labels

# Define the number of bootstrap samples
n_bootstrap = 100

# Define an empty list to store the bootstrap samples
bootstrap_samples = []

# Loop over the number of bootstrap samples
for i in range(n_bootstrap):
    # Draw random indices with replacement
    indices = np.random.choice(len(X), size=len(X), replace=True)
    # Extract the bootstrap sample
    X_bootstrap = X[indices]
    y_bootstrap = y[indices]
    # Append the bootstrap sample to the list
    bootstrap_samples.append((X_bootstrap, y_bootstrap))

#from: https://gpttutorpro.com/machine-learning-evaluation-mastery-how-to-use-bootstrap-
```

References

- Han, Kamber & Pei, Data Mining Concepts and Techniques, Morgan Kaufman.
- Jake VanderPlas, Data Science Handbook, O'Reilly
- Janez Demsar, Statistical Comparisons of Classifiers over Multiple Data Sets, JMLR, 2006.