# 6. Predictions and Machine Learning

- We have seen in chapter 2 that regressions are a powerful tool to approximate the Conditional Expectation Function $E\left[Y_i \middle| X_i\right]$
- But: In a regression we impose assumptions on the functional form of the CEF
- For instance: When we estimate a model

$$Y_i = \alpha + \beta_1 \cdot X_{i1} + \beta_2 \cdot X_{i2} + \varepsilon_i$$

  we approximate the CEF with a linear function

- We can estimate much more complex functions and can for instance add interaction terms, quadratic terms etc…
  - … but this will always be assumptions that we impose
  - … & we cannot be sure about the true functional form of the CEF
- Here: Use more general machine learning techniques to estimate the CEF relaxing assumptions about its functional form

# Regression and Classification

- In „machine learning speak“ people distinguish between regression and classification
- In this terminology:
  - Regression means solving a prediction problem where the dependendent variable is a continuous variable (a quantity like age, income, job satisfaction,…)
  - Classification means solving a prediction problem where the dependendent variable is a discrete variable (a “label“ or a “class“ such as employee turnover (yes/no), , …)
- Here we will only cover regression problems
- Classification methods are often very similar (and sometimes you can also apply a regression method for binary classification problems)

# Recall: Basic Properties of the CEF

**Result: CEF Prediction Property**

Let $m(X_i)$ be any function of $X_i$. The CEF solves

$$E\left[Y_i\middle|X_i\right] = \arg\min_{m(X_i)} E\left[\left(Y_i - m(X_i)\right)^2\right]$$

so it is the best predictor of $Y_i$ given $X_i$ in the sense that it solves the minimum mean square error (MMSE) prediction problem.

**Result: CEF Decomposition Property**

We can decompose $Y_i$ such that $Y_i = E\left[Y_i\middle|X_i\right] + \varepsilon_i$

(i) where $\varepsilon_i$ is mean independent of $X_i$ that is $E\left[\varepsilon_i\middle|X_i\right] = 0$

(ii) and therefore $\varepsilon_i$ is uncorrelated with any function of $X_i$

# Supervised Learning

- The part of ML we are interested in is **supervised learning** as the task of learning a function $\hat{f}(X)$ ("training an algorithm") that maps an input $X$ to an output $Y$ based on a sample
- The learning method learns from a training sample consisting of a set of input-output observations
- Hence, we have (as before) a data set $D$ with $N$ observations and $M$ explanatory variables

$$(y_1, x_{11}, x_{12}, x_{13}, \ldots x_{1M}),$$
$$(y_2, x_{21}, x_{22}, x_{23}, \ldots x_{2M}), \ldots$$

- In ML the vector $x_i$ of explanatory variables is called the **feature vector** and the matrix $X$ of the feature vectors of all observations the **feature matrix**
- We want to estimate a function $\hat{f}_D(X)$ that approximates the CEF

# Parametric and Non-Parametric Approaches

- An OLS Regression is a specific **parametric** ML algorithm
  - Easy to fit as only few parameters need to be estimated
  - Easy to interpret
- But:
  - Makes strong assumptions on functional form
  - May perform poorly in prediction task when underlying CEF is non-linear and when the number of independent variables is large
- Other **non-parametric** Algorithms may then be more flexible:
  - Do not assume a specific functional form
  - Are thus more flexible to adapt to complex forms of the CEF
  - But are harder to interpret and may perform worse on small data sets

# k-Nearest Neighbor Regression

**Key idea:**

- For a given value $x_i$ we could approximate the CEF $E[Y_i|X_i = x_i]$ by computing the average of $Y_i$ across observations with $X_i = x_i$

**Problem:** We might have very few or no other observations with $X_i = x_i$

- Instead, use the average value of $Y_i$ of the k nearest neighbors of $x_i$:

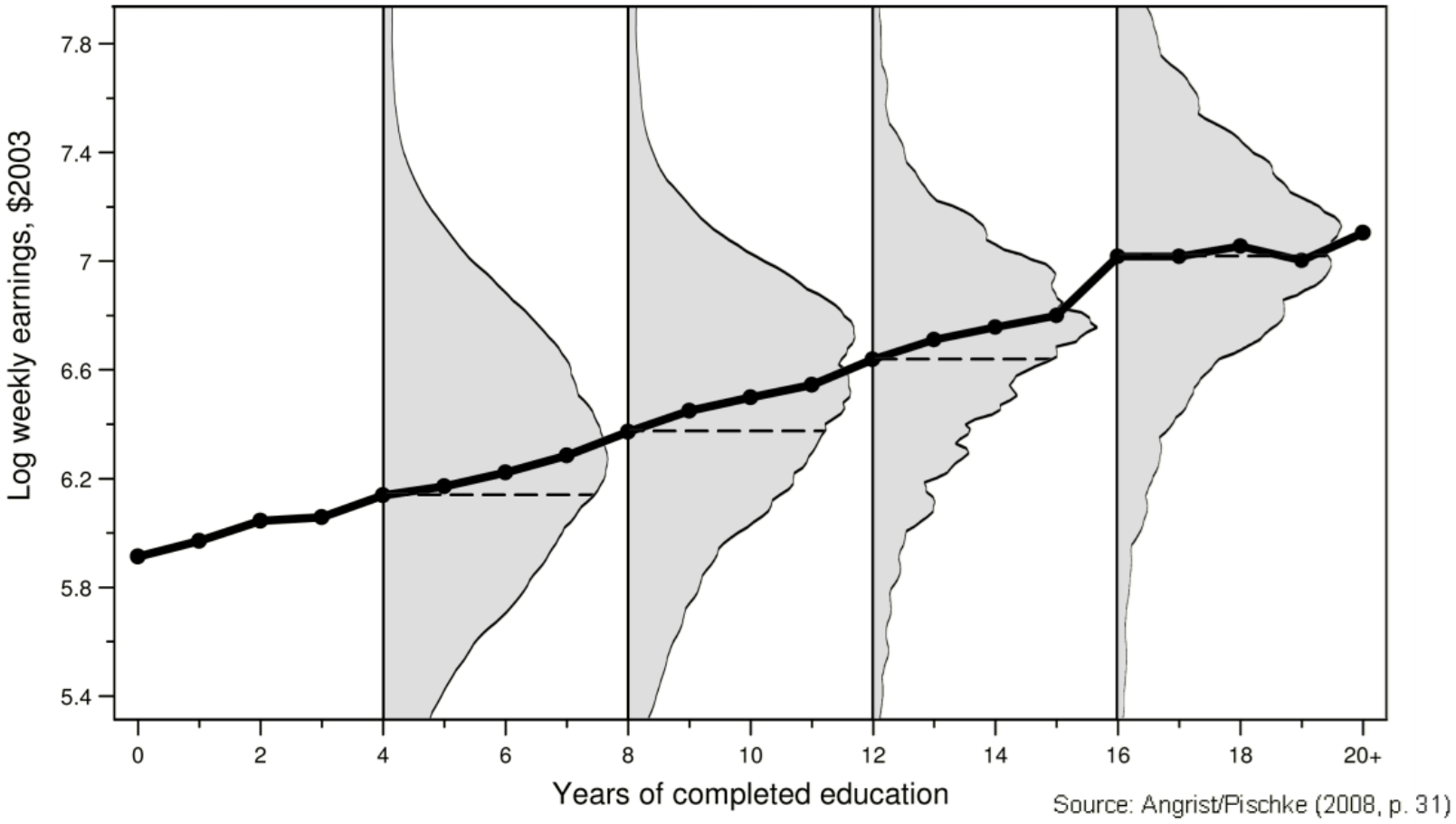
$$\hat{f}_D(x_0) = \frac{1}{K} \sum_{j \in N_k(x_0)} y_j$$

where $N_k(x)$ is a neighborhood containing the indices of the K closest $x$ values in the training data

- Closest neighbors for instance those with smallest Euclidean distance

$$\sqrt{\sum_{j=1}^{M} (x_{0j} - x_{1j})^2}$$

## Recall: The CEF of earnings as a function of years of education




Source: Angrist/Pischke (2008, p. 31)

# k-Nearest Neighbor Regression: Standardization

**Note:**

- When the $x_i$ vector consists of multiple variables measured in different units the measured distance will depend on the unit of measurement
  - If there is, for instance, a wage variable the chosen currency unit will affect the assignment of neighbors
  - Or, if there is a tenure variable measuring the time an employee has been with a firm it will matter whether it is measured in months or years
  - In other words: variables where there are large nominal distances will have stronger effects on "who is an observation's neighbor"

**Hence:**

- When the $x_i$ vector consists of multiple variables measured in different units, then it is useful to standardize all independent variables/features

$$x_{ij}^{Std} = \frac{x_{ij} - \bar{x}_j}{std(x_j)}$$

where $\bar{x}_j$ is the mean of the variable and $std(x_j)$ its standard deviation

# The Loss Function and Mean Squared Error

An important concept in ML is the **loss function**

$$L(Y_i, \hat{f}_D(X_i, D))$$

- The loss function measures the "loss" of approximating $Y_i$ by $\hat{f}(X_i, D)$
- Common choice: Squared error

$$L\left(Y_i, \hat{f}_D(X_i)\right) = \left(Y_i - \hat{f}_D(X_i)\right)^2$$

**Central Goal:**

Find an algorithm $\hat{f}_D(X_i)$ that minimizes the expected loss

**Recall:**

- When estimating a linear regression we did exactly that, being restricted to the class of linear functions
- In ML more general and flexible functional forms atre often considered (sometimes at the expense of interpretability)

# The Loss Function and Mean Squared Error

**Hence:**

- When assessing the predictive performance of an algorithm for a regression problem (i.e. one with a continuous outcome variable), we often use the **mean squared error (MSE)**

- That is, we use the data set (or part of it) to compute the squared deviation between actual values of $y$ and predicted values $\hat{y}$

$$MSE = \frac{1}{N}\sum_{i=1}^{N}\left(y_i - \hat{f}_D(x_i)\right)^2$$

- This can, for instance, we used to compare the performance of different algorithms

# Mean Squared Error and $R^2$

**Note: The Mean Squared Error is directly connected to $R^2$**

- The coefficient of determination $R^2$ is the proportion of the variance in the dependent variable that is predictable from the independent variables
- It is given by

$$R^2 = 1 - \frac{\frac{1}{N}\sum_{i=1}^{N}\left(y_i - \hat{f}_D(x_i)\right)^2}{\frac{1}{N}\sum_{i=1}^{N}(y_i - \bar{y})^2}$$

  where $\bar{y} = \frac{1}{N}\sum_{i=1}^{N} y_i$ is the mean of the $y_i$

- Hence

$$R^2 = 1 - \frac{MSE}{V[y_i]}$$

- As the variance of the dependent variable $V[y_i]$ is given, minimizing the MSE corresponds to maximizing the $R^2$

Python

## Data Cleaning and Preparation

- Typically, you start a project by inspecting the data, cleaning it, and preparing it for the analysis
- To do so you first pick two subsets of the variables in your data frame:
  - A (one dimensional) array containing the dependent variable to be predicted, which you typically name `y`
  - A two dimensional array or data frame containing the explanatory variables (features) of each observation, which you typically name `X`
- For instance, you can define `y=df['JobSatis']`
- To define the feature matrix `X`, for instance
  - include all other variables: `X=df.drop(columns='JobSatis')`
  - or include a subset of the variables: `X=df[['age','wage']]`
- Sometimes there are missing values shown in a data frame as `NaN`
  - Rows with `NaN` can be dropped using `df = df.dropna()`

Python

## Using scikit-learn (sklearn)

- Key ML methods are implemente in package scikit-learn
- Starting point: we can also run a linear regression
- Import:

```
from sklearn.linear_model import LinearRegression
```

- Then we can perform a regression with the following code:

```
lreg = LinearRegression().fit(X,y)
```

  - `X` is a (two dimensional) array containing the explanatory variables (features) of each observation
  - `y` is a (one dimensional) array containing the dependent variable to be predicted

- We can then use the results to make predictions

  `lreg.predict([[50]])` predicts the $y$ for $X = 50$

- Note: As Sci-kit Learn rather aims at making predictions, we do not easily get nice regression tables. To obtain these rather use `statsmodels`

Python

## k-Nearest Neighbor Regression

- To fit a k-Nearest Neighbor Regression import:

```
from sklearn.neighbors import KNeighborsRegressor
```

- Then we can perform a knn regression with the following code:

```
knn=KneighborsRegressor(n_neighbors=8).fit(X,y)
```

  - where `X` is again the feature matrix and `y` the variable to be predicted
  - `n_neighbors` specifies the number of neighbors considered

- The method `mean_squared_error` computes the MSE:

```
from sklearn.metrics import mean_squared_error
y_pred = knn.predict(X)
print(mean_squared_error(y, y_pred))
```

- The method `r2_score` computes the $R^2$:

```
from sklearn.metrics import r2_score
print(r2_score(y, y_pred))
```

## Your Task — Predicting performance

- The dataset `data_performance.csv` contain data on employees in a call center of a Chinese travel agency (taken from Bloom et al. (2015))
- Your task is to train an algorithm to predict the performance of these call center workers
- The variable `z_performance` is a standardized performance measure, which is based on employee performance on their main task (e.g. phone calls answered, calls answered per minute, weekly minutes on the phone)
- Import the data from `https://raw.githubusercontent.com/dsliwka/EEMP2022/main/datasets/data_performance.csv'`
- Please first inspect the data and look at the variables (`df.columns`)
- Plot a histogram of the performance variable with `sns.histplot`

## Your Task — Predicting performance

- Then prepare the data:
  - Drop all rows with missing values
  - Define your y vector `y=..`
  - Define your feature matrix `X=..` omitting the dependent variable as well as the variable `personid`
- Then perform a k-Nearest Neighbor Regression to predict `z_performance` with $k = 5$ neighbors
- Compute the mean squared error and the $R^2$ of this prediction
- Save the notebook as `PerformancePrediction`

# Hyperparameters

- **Parameters** are learned by the algorithm during training (like regression coefficients)
- **Hyperparameters** refers to something that is passed to the algorithm, i.e. is set by the user and determines how the algorithm works
  - The number of neighbors to inspect in a KNN model is a hyperparameter that we have to specify when we create the model
- We can compare the prediction accuracy of a model to determine the best values for the hyperparameters
- In order to understand this further we will consider:
  - The problem of overfitting
  - The importance of separating training and test data
  - The bias-variance trade-off

# Overfitting, Training Error, and Test Error

**Recall:** Quality of the prediction often assesed by *mean squared error* (MSE):

$$MSE = \frac{1}{N}\sum_{i=1}^{N}\left(y_i - \hat{f}_D(x_i)\right)^2$$

**A key problem:**

- When the estimated functional form is very flexible, we will overestimate the predictive power of our algorithm when computing the MSE on the **same data** which we used to train the algorithm

**This is due to *Overfitting:***

- The function $\hat{f}_D(X)$ estimated on a sample $D$ will tend to follow patterns too closely that by chance occur in $D$ rather than the whole population!
- When overfitting plays a big role, then $\hat{f}_D(X)$ will be a bad predictor for observations that are not part of the training sample $D$

# Overfitting, Training Error, and Test Error

**Key element of ML:**

- Assess the prediction quality **out-of-sample**!
- In order to do so: Use only a subset of the data to train the algorithm
- Use the remainder to assess the quality of the prediction

**Important distinction: Training error and test error**

- *Training error*: Average of loss function over the *training data* $D_{train}$

$$\overline{err}_{train} = \frac{1}{|D_{train}|} \sum_{j \in D_{train}} L(y_j , \hat{f}_{D_{train}}(x_j))$$

- *Test error/generalization error*: Average loss when applying $\hat{f}_{D_{train}}(X)$ for observations that are not part of the training data

$$\overline{err}_{test} = \frac{1}{|D_{test}|} \sum_{j \in D_{test}} L(y_j, \hat{f}_{D_{train}}(x_j))$$

## Python — Splitting Training and Test Data

- First import:

```
from sklearn.model_selection import train_test_split
```

- The method `train_test_split` conveniently splits the data set into training and test data:

```
X_train, X_test, y_train, y_test
 = train_test_split(X,y,train_size=0.7,random_state=181)
```

**Note:**

- The `train_size` parameter determines the share of observations used for the training data set, the remaining observations are the test set
- The method returns four arrays: `X_train` and `X_test` are the feature matrices for the observations in the train and test sets
- `y_train` and `y_test` are the outcome variables in the two data sets
- As the data sets are randomly sampled you will get a different sample each time → fix the sampling with the parameter `random_state=181`

Python

## Training and Test Error

- We can then train the algorithm on our test data:

```
knn = KNeighborsRegressor(n_neighbors=10).fit(X_tr,y_tr)
```

- Recall: The method `mean_squared_error` computes the MSE:

```
from sklearn.metrics import mean_squared_error
```

- Print the training mean squared error:

```
print(mean_squared_error(y_tr, knn.predict(X_tr)))
```

- Print the test mean squared error:

```
print(mean_squared_error(y_test, knn.predict(X_test)))
```

## Your Task

## Predicting performance

- Open again your notebook `PerformancePrediction`
- Now split the data in a training and a test set where the test set should comprise 70% of the observations and set the `random_state=181`
- Train the knn Algorithm on the training set
- Compute the mean squared error and $R^2$
  - on the training set and
  - on the test set
- Interpret your findings. Did we obtain a good prediction?
- Save the notebook

Python

## Standardizing Variables

- We have seen in section 1 of the course how to "manually" standardize variables (substracting the mean and dividing by the standard deviation)
- Scikit-Lean provides a convenient way to standardize all variables in $X$

```
from sklearn.preprocessing import StandardScaler
scaler=StandardScaler()
scaler.fit(X_train)
X_trainS=scaler.transform(X_train)
X_testS=scaler.transform(X_test)
```

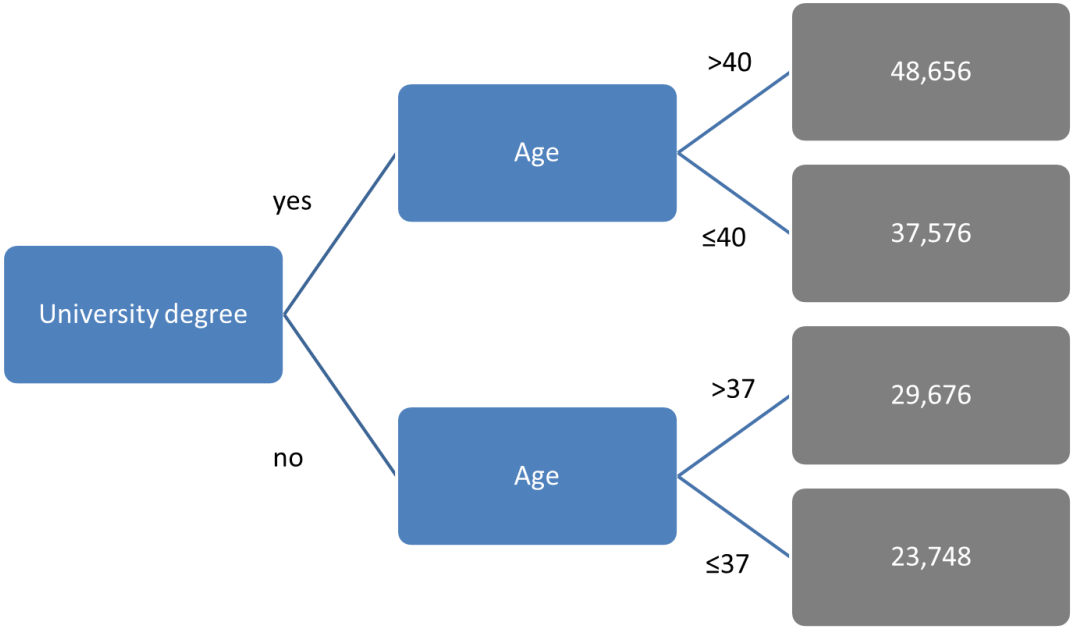
- Then `X_trainS` and `X_testS` are standardized versions of `X_train` and `X_test`
- The standardization is done with the mean and standard deviation of the respective variables in the training set

## Your Task — Predicting performance

- Open the `PerformancePrediction` notebook
- Now standardize the variables in the feature matrix $X$ with the `StandardScaler`
- Then perform a k-Nearest Neighbor Regression to predict `z_performance` with $k = 5$ neighbors training the algorithm on the standardized data
- Again, compute the test mean squared error and the $R^2$ of this prediction
- Save the notebook

# Decision Trees

- Decision trees are the building block of powerful ML algorithms
- The key idea of a decision tree is simple:
  - Sequentially partition the data
  - At each step generate two subsets
  - Base the split in each step on a specific condition on one variable
  - Choose the splits by mimizing the expected loss (MSE)



# Decision Trees: How it works

**Top-down, greedy approach known as *recursive binary splitting***

(Compare James/Witten/Hastie/Tibshirani (2022, pp. 327)

- Begin at the top of the tree & successively split the predictor space
- Each split generates two new branches
- Called “greedy” because at each step, the best split is made at that particular step (rather than looking ahead)
- To perform recursive binary splitting,
  - select a feature $j$ and cutpoint $s$ such that splitting the predictor space into the “regions” $\{X|X_j < s\}$ and $\{X|X_j \geq s\}$ leads to the smallest loss
  - repeat the process, looking within each region generated in the previous step for the best predictor and cutpoint minimizing the loss within the respective region
  - …

# Decision Trees: How it works

**More formally, at each step:**

- For each branch look at the set of observations in this branch
- Within this set, define two subsets for feature $j$ and cutpoint $s$

$$R_1(j,s) = \{X | X_j < s\} \text{ and } R_2(j,s) = \{X | X_j \geq s\}$$

- Let $\hat{y}_{R_k}$ be the average value of $y_i$ across all observations in $R_k(j,s)$

  Note: This $\hat{y}_{R_k}$ is the *predicted value* for this region

- Seek the values of $j$ and $s$ that minimize

$$\sum_{i:i \in R_1(j,s)} (y_i - \hat{y}_{R_1})^2 + \sum_{i:i \in R_2(j,s)} (y_i - \hat{y}_{R_2})^2$$

- Repeat the steps until a certain (predetermined) depth of the tree is attained
- The depth of the tree is a hyperparameter to be tuned

## Python — Decision Trees

- To fit a decision tree import:

```
from sklearn.tree import DecisionTreeRegressor
```

- Then we can fit the tree with:

```
dtree = DecisionTreeRegressor(max_depth=3).
                fit(X_train, y_train)
```

  - where `max_depth` is a hyperparameter that gives the maximal depth of the tree (the number of layers)
  - Note: Restricting `max_depth` prevents overfitting as a tree without a maximum depth will simply map out the whole data set

- Another hyperparameter is `min_samples_leaf` specifying a minimal number of observation that have to be in each leaf

## Python — Decision Trees

- For a (not too large) tree it is convenient to plot the tree

```
from sklearn.tree import plot_tree
```

- To set the plot size

```
plt.figure(figsize=(20, 10))
```

- Plot the tree and show it

```
plot_tree(dtree, feature_names=X.columns,
                 fontsize =10)
plt.show()
```

- Note:
  - `feature_names` is a parameter with which you specify the names of the features to be displayed
  - `X.columns` gives back a list of the variable names in the dataframe containing the features

## Your Task

## Predicting performance

- Open again your notebook `PerformancePrediction` and save it under a different name `PerformancePredictionTree`
- Now instead of the Knn regression train a decision tree with a maximum depth of 3 (note: here you do not need to standardize the X matrix)
- Plot the tree and interpet your findings
- Compute the mean squared error and $R^2$
  - on the training set and
  - on the test set
- Save the notebook

# Optimizing Prediction Quality

- But one can go beyond merely assessing the quality of an algorithm by measuring the accuracy of the prediction out-of-sample
- We should aim at finding a specification (i.e. a version of the algorithm) that yields the best out-of-sample prediction
- That is, for instance, find the specification that yields the lowest MSE when applied to new data
- To do so it is useful to consider different splits of the data into training and test data
- An algorithm performs well when it consistently produces good out-of-sample predictions across different splits
- This can be done using so-called *cross validation*

# Cross-Validation

**Basic idea:** Single split validation

- Randomly split the data set in two two halves $D_1$ and $D_2$
- Train algorithm on one half of the data $D_1$ to obtain $\hat{f}_{D_1}(X)$
- Estimate error on the other half $D_2$ by computing

$$\frac{1}{|D_2|}\sum_{j\in D_2} L(y_j, \hat{f}_{D_1}(x_j))$$

- Key approach: To find the best algorithm
  - train different particular forms of an algorithm (such as regressions with a different number of parameters)
  - determine test error for these different forms
  - pick the form that produces the lowest test error
- But: With single split validation results depend very much on specific split

# Cross-Validation

**K-fold Cross Validation:** Split multiple times and compute the average test error

- First split data into K roughly equal-sized folds (subsets) $D_1, D_2, \ldots D_K$
- Repeat for $k = 1, 2, \ldots, K$:
  - For k-th fold, train the model on data from all other folds, i.e. $D \backslash D_k$
  - Calculate prediction error on $D_{\mathrm{k}}$ to obtain $MSE_k$

$$MSE_k = \frac{1}{|D_k|} \sum_{j \in D_k} L(y_j, \hat{f}_{D \backslash D_k}(x_j))$$

- Compute the average prediction error

$$MSE^{K-fold} = \frac{1}{K} \sum_{k=1}^{K} MSE_k$$

- Then again pick the specification of an algorithm that minimizes $MSE^{K-fold}$
- It is common to use k=5 or k=10

# Tuning Hyperparameters

- Often, we consider models with hyperparameters $\alpha$ such as the number of neighbors in KNN regression or the depth of a tree
- We train an algorithm for a specific hyperparameter $\alpha$ (or vector of hyperparameters if there are more than one)
- Key question: But what are the "best" values for the hyperparameters?

Again: Find the hyperparameters that minimize expected loss **out-of-sample**

- Let $\hat{f}(X, \alpha)$ be the algorithm trained with hyperparameters $\alpha$
- We can now estimate the K-Fold cross validation (CV) mean squared error

$$MSE^{K-fold}(\hat{f}, \alpha)$$

- And then choose the value of $\alpha$ that minimizes this
- Note: Some also advocate the random standard error rule: Pick the least complex model that is in a range of one standard error from the best model

Python

## Cross Validation and Hyperparameter Tuning

- Scikit-Learn provides a convenient tool to perform cross validation:

```
from sklearn.model_selection import cross_val_score
```

- Then perform K-fold cross-validation:

```
cv = cross_val_score(knn, X_train, y_train, cv=5,
      scoring='neg_mean_squared_error')
```

- Returns an array of $k$ (here 5) estimates for the generalization error (one for each of the $k$ folds)
- We can just look at the mean of these with `cv.mean()`
- To find (near) optimal values of the hyperparameters:
  - We can write a python loop to vary $k$ and look for the value of $k$ that minimizes the CV mean squared error
  - But Scikit-Learn can also do that automatically with grid search

Python

## Grid Search

- Scikit-Learn also provides a class for automatic hyperparameter tuning

```
from sklearn.model_selection import GridSearchCV
```

- You only have to specify the model that you want to apply it to and the range of parameter values which you want to check
- To define the set of parameter values (here 1 to 5) to be checked define a python dictionary (can also be multiple parameters)

```
param_grid = {'n_neighbors' : [1,2,3,4,5]}
```

- Then create a grid search object

```
knn_grid= GridSearchCV(KNeighborsRegressor(),
     param_grid, cv=5, scoring='neg_mean_squared_error')
```

- Now run the fit method of this object like you did before on knn:

```
knn_grid.fit(X_train, y_train)
```

- And then for instance get the value of $k$ that maximizes accuracy

```
print(knn_grid.best_params_)
```

Python

## Grid Search

- The grid search object also has a method that you can use to make predictions based on the optimized set of parameters:

```
knn_grid.predict(X_test)
```

- You can use this to compute the test error and the test $R^2$

```
mean_squared_error(y_test, knn_grid.predict(X_test))
```

```
r2_score(y_test, knn_grid.predict(X_test))
```

Note furthermore:

- The `GridSearchCV` object has an attribute cv_results_ which allows to access the evaluation metrics in more detail
- For instance, `knn_grid.cv_results_['mean_test_score']` is an array containing the mean squared error (when this is the specified scoring method) for all parameter combinations that were checked

## Your Task — Predicting performance

- Open again your notebook `PerformancePrediction`
- Now try to find the optimal number of neighbors in the Knn regression (note: again use the standardized X matrix)
- Perform a grid search defining a parameter grid
  `param_grid={'n_neighbors': np.arange(2,20)}`
  - Note: `np.arange(3,20)` returns an array of values between 3 and 20 with steps of 1
  - (You could also specify larger steps with a third parameter such as `np.arange(2,20,2))`
- What is the optimal number of neighbors?
- Compute the test mean squared error and $R^2$
- Save the notebook

# Validation Set

**Recall:**

- If we use the test data for both model selection and assessment, we will tend to underestimate the true test error of the best model.
- The same holds with cross validation: When we use the whole data set for cross validation (and hyperparameter tuning) there is a risk of overfitting

**To deal with this problem**

- It is advisable to leave out a test set that you do not use in cross validation
- Use this only to estimate the generalization error

**Note:** Useful terminology to distinguish

- *Validation Set*: this data set is used to tune hyperparameters
- *Test Set:* this data set is used to obtain an unbiased estimate for the actual predictive power of the final algorithm

# Model Complexity/Flexibility

A model/algorithm is said to be more **complex** or **flexible** when it has more parameters and thus can more easily adapt to patterns in the data

- A multiple linear regression is, for instance, more complex
  - when it has more explanatory variables and more interaction terms
  - or when it includes polynomial terms
- A knn-regression is more flexible when the number of neighbors is smaller
  - it then can adapt more flexibly to patterns in the near neighboorhood

**Note:**

- A more flexible model is more likely to be able to come close to the true CEF
- But: A more flexible model is also more likely to pick up patterns in the data that are simply due to the specific sampling of the training data
- This consideration leads to an important trade-off between **bias** and **variance**

# Bias

- Recall: When $f(X_0)$ is the true CEF then $Y_0 = f(X_0) + \epsilon$
- Define: An algorithm $\hat{f}$'s **bias** at a specific vector of feature values $X_0$

$$bias\left(\hat{f}(X_0)\right) = E_D\left[\hat{f}_D(X_0)\right] - f(X_0)$$

- Key idea:
  - Suppose we have different training data sets $D$
  - For each training data set we train a specific algorithm to obtain $\hat{f}_D(X_0)$
  - The bias is the difference between the average prediction made by the algorithm across different samples and the true CEF $f(X_0)$
- It is preferable to have a low bias!
- Then there is no systematic difference between our predictions based on certain training data sets and the true CEF

# Variance

- Consider again the use of different training data sets $D$
- Again each training data set yields (in general) a different prediction $\hat{f}_D(X_0)$
- Key question: How much do these estimates vary?
- This estimation **variance** at $X_0$ is

$$variance\left(\hat{f}(X_0)\right) = E\left[\left(\hat{f}_D(X_0) - E\left[\hat{f}_D(X_0)\right]\right)^2\right]$$

- It is the mean squared deviation between predictions made by the same algorithm when trained with different training data sets $D$
- It is preferable to have a low variance!
- Then the predictions are rather consistent, that is if the algorithm is trained on different training data sets, it makes similar predictions for the same feature vector $X_0$

# The Bias-Variance Decomposition

- Suppose now that we draw a observation $(Y_0, X_0)$ from the *test data set*
- Expected mean squared error

$$E\left[\left(Y_0 - \hat{f}_D(X_0)\right)^2\right] = E\left[\left(f(X_0) + \epsilon - \hat{f}_D(X_0)\right)^2\right]$$

- One can show that this is equal to

$$V[\epsilon] + \left(E\left[\hat{f}_D(X_0)\right] - f(X_0)\right)^2 + E\left[\left(\hat{f}_D(X_0) - E\left[\hat{f}_D(X_0)\right]\right)^2\right]$$

where

  - $V[\epsilon]$ is the *irreducible error*
  - $E\left[\hat{f}_D(X_0)\right] - f(X_0)$ is the *bias* of the algorithm
  - $E\left[\hat{f}_D(X_0) - E\left[\hat{f}_D(X_0)\right]\right]$ is the *variance* of the algorithm

# The Bias-Variance Trade-off

- When increasing the flexibility of a model the training error is reduced → a more flexible model can pick up more detailed patterns
- Initially the test/validation error tends to fall as well
  - as otherwise the model is too simple/inflexible
  - here the **bias** is reduced when adding complexity
- But when the complexity increases further, the test error will tend to increase again
  - Here the **variance** increases
  - Model becomes so flexible that it will map random patterns in training data
  - A very complex model will "memorize" the training data & thus **overfit**

# Ensemble Learning and Random Forests

- Decision trees are relatively easy to understand and interpret
- But they tend to suffer from high variance (in particular with high depth):
  - When splitting the training data into two parts & fitting a decision tree to both halves, the results could be quite different
  - In other words, deep trees tend to overfit the data
- But it has turned out that training different trees on the same data set and averaging their predictions improves prediction accuracy
- This is the broader idea of **ensemble** methods in ML: Use multiple learning algorithms and average their predictions to obtain a higher accuracy
- An important and powerful such ensemble method is a **Random Forest**:
  - Train many decision trees & use the average prediction
  - Each single tree will have a high variance, but allows for low bias
  - Averaging across trees will reduce variance

# Ensemble Learning and Random Forests

**Important:**

- If the different trees are very similar, the improvement will be small as they will make similar predictions
- Hence a random forest introduced intentional randomness in the construction of each tree (therefore the name!)

**Random forests introduce two forms of randomness**:

1. For each tree use a different random sample of the data
   - Apply so-called **bootstrap aggregation (bagging)**
   - That is, for each tree draw a sample of the same size as the original data set (with replacement such that an observation can be drawn twice)
   - Train the tree on this sample
2. For each node in a tree consider only a **randomly chosen subset of the fearures** as candidates to use for the next split

# Bootstrap: Example

| Original Sample: | | | Bootstrap Sample: | |
|---|---|---|---|---|
| 1 | Anna | | 5 | Marie |
| 2 | Mehmet | | 2 | Mehmet |
| 3 | Peter | | 3 | Peter |
| 4 | Chloé | | 9 | Herbert |
| 5 | Marie | | 7 | Robert |
| 6 | Huan | | 2 | Mehmet |
| 7 | Robert | | 1 | Anna |
| 8 | Pedro | | 9 | Herbert |
| 9 | Herbert | | 6 | Huan |
| 10 | Rosa | | 3 | Peter |

# Random Forests: Bagging

**Bagging:**

(James/Witten/Hastie/Tibshirani (2022, pp. 340))

- Draw $b = 1, .., B$ different "bootstap samples" of the same size N as the original sample
  - That is, for each sample draw N times an observation from the original sample (with replacement – an observation in the original sample can show up several times in the bootstrap sample!)
  - For each sample $b$ train your algorithm (here: the decision tree) to obtain a predictor $\hat{f}_b(x)$
- Key idea: Data sets are different but they are drawn from the same distribution as the original data so share the underlying characteristics
- The bagging prediction is then simply

$$\hat{f}_{bag}(x) = \frac{1}{B}\sum_{b=1}^{B}\hat{f}_b(x)$$

# Random Forest: Using Subsets of Features at each Split

Underlying reasoning for using only a **subset of the features**:

- Improve the prediction by avoiding that the different trees are too similar
- For instance, when some predictors are very important, the splits at the top of each tree will be very similar (even with bagging)
- But when the trees are similar, their predictions will be highly correlated and then less can be learned from aggregating their results
- Note: splits lower down in the tree have less data and thus are more prone to be affected by noise

**The approach:**

- At each node of the tree allow only a subset of the features to be used for the next split
- This subset is determined by a random draw
- The idea is to “decorrelate” the trees or to force them to learn where it is more difficult to learn

# Random Forest: Using Subsets of Features at each Split

- Subset of features that may be used for a split randomly drawn at each node
- The size of this subset has to be set as a hyperparameter
- If there are $M$ features and this maximal number of features is set to P:
  - At each node the random forest algorithm randomly randomly picks $P$ out of the $M$ features
  - The algoithm then seeks the best split (as usual when estimating a decision tree) but only within this subset of features
- Note:
  - When $P = \mathrm{N}$ then each split can look at all features in the data set and randomness only comes from bootstrapping ("bagging estimator")
  - When $P = 1$ then each split could only use one randomly picked feature
- Recommendation: When there are $M$ features, allow $\mathrm{P} = \sqrt{M}$ features (randomly picked at each node) to be used for the next split

## Python — Random Forest

- To fit a decision tree import:

```
from sklearn.ensemble import RandomForestRegressor
```

- Then we can fit the random forest with:

```
forest =  RandomForestRegressor(n_estimators=10).
                fit(X_train, y_train)
```

  where `n_estimators` sets the number of trees to be estimated

- Another hyperparameter is `max_features` specifying the number of features randomly drawn at each split that can be used for this split, where
  - you can either set a specific number such as `max_features=4`, or
  - do a grid search with `GridSearchCV`, or 
  - follow the convention to use the square root of $M$ by specifying `max_features='sqrt'`
- You may also set (& tune) the tree hyperparameters such as `max_depth`

## Your Task — Predicting performance

- Open again your notebook `PerformancePredictionTree`
- Now train a random forest
  - Set `max_features="sqrt"`
  - Set the number of estimators to 500 and the random state to 181
- Compute the test mean squared error and test $R^2$
- Save the notebook as `PerformancePredictionForest`

# Backup

# Random Forest: Out-of-Bag Error

- There is a very straightforward way to estimate the test error of a bagged model (without the need to perform cross-validation)
- Note: When a **bootstrap sample** is drawn, not all observations in the main sample are used
  - as it is drawn with replacement some observations are drawn several times
  - thus others are not drawn at all in that sample
- It has been shown that on average about 63% of the original observations show up in a bootstrap sample
- Hence, each observation in the data set will not be used in about 37% of the predictions $\hat{f}_b(x)$ and these can be used to estimate the test error
- The **Out-of-bag MSE** is just the average squared distance between the observed values $y_i$ and the average of the predictions $\hat{f}_b(x_i)$ across the samples $b$ that did not include observation $i$