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

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 ε_i is mean independent of X_i that is $E\left[\varepsilon_i \middle| X_i\right] = 0$

(ii) and therefore ε_i is uncorrelated with any function of X_i

6.1. Key Concepts

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 dependent variable is a discrete variable (dummy variable, “label“ , “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)

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
  - Is the best predictor when the underlying function is indeed linear
  - 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

The Loss Function and Mean Squared Error

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

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

- 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 are often considered (sometimes at the expense of interpretability)

The Loss Function and Mean Squared Error

- To assess the quality of the prediction in a regression problem (i.e. with a continuous outcome), we thus often use the **mean squared error (MSE)**
- We use the data set (or part of it) to compute the MSE

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

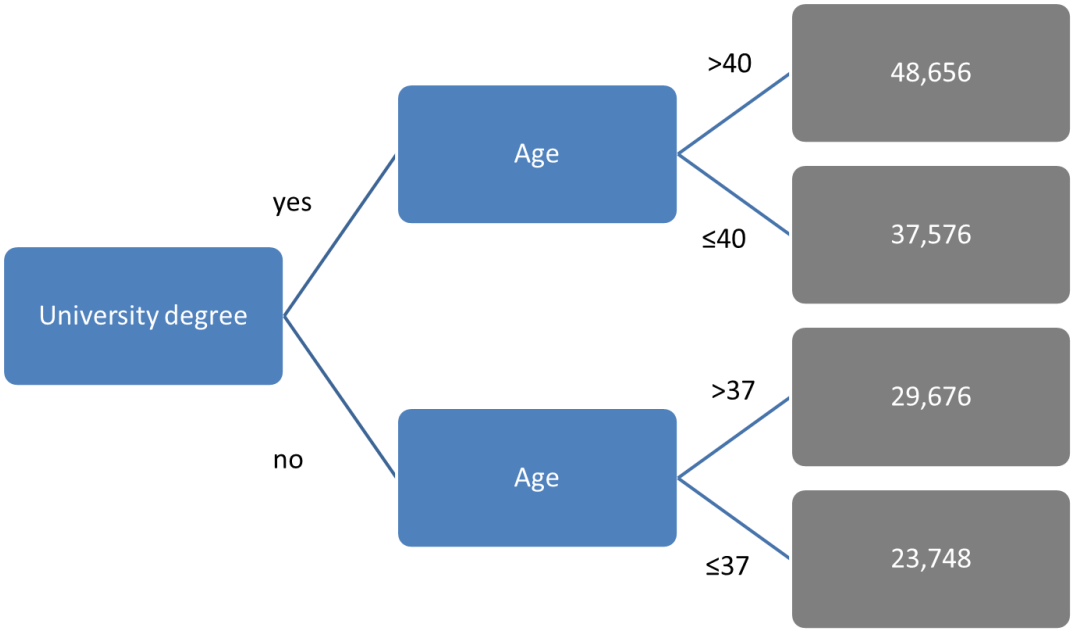
Recall from Chapter 2: The Mean Squared Error is directly connected to R^2

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

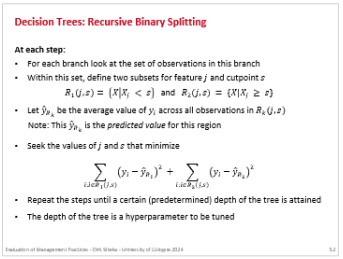
- Minimizing the MSE corresponds to maximizing the R^2 (as $V[y_i]$ is given)
- The R^2 has a more accessible interpretation than the MSE: *The share of the variance in the outcome that is predictable based on the features*
- A prediction yielding $R^2 = 1$ would be perfect, one with $R^2 = 0$ useless

6.2 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



Trees are contructed as follows: ("Recursive Binary Splitting")

- Begin at the top of the tree & successively split the predictor space
- Each split generates two new branches
- To perform the split
  - select feature j and cutpoint s **such that the** split into two "regions" (for instance, age<45 and age>=45) **leads to the smallest loss** (MSE)
  - 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
  - …
- Repeat up to a specific maximal depth of the tree (which you have to set as a hyperparameter)

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()
  - and columns with df = dfp.dropna(axis=1)

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
from sklearn.metrics import mean_squared_error, r2_score
```

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

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

  - X is the (two dimensional) feature matrix
  - y is the (one dimensional) dependent variable to be predicted
- We can then use the results to make predictions

  lreg.predict([[50]]) predicts the y for $X = 50$
- We obtain the R^2 with r2_score(y, lreg(X))

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, y)
```

- Where max_depth specifies the maximal depth of the tree (the number of layers)
- You can also set min_samples_leaf specifying a minimal number of observations 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
import matplotlib.pyplot as plt
```

- 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 Engagement

- We again work with the Linked Personnel Panel (LPP) data
- Your task now is to train an algorithm that predicts job engagement
- To save some time download a notebook LPPEngaDataCleaning
  - This notebook already performs data cleaning (dropping NaN values, generating scales for personality traits etc.)
  - Note: in general be careful in the data cleaning process and check your steps (when you for instance drop all rows where there is missing data for at least some variables you may loose large parts of the data quickly)
- Save a copy as EngagementPred & work with this copy
- Recall: you can find a variable description here: https://github.com/dsliwka/EEMP2024/blob/main/Data/VariablesLabelsLPP.pdf
- And a documentation (unfortunately only in German) here: https://github.com/dsliwka/EEMP2024/blob/main/Data/Lpp_CampusFileDocumentation.pdf

Your Task

Predicting Engagement

- First prepare the data for the prediction task:
  - Define your y vector y=..
  - Define your feature matrix X=..
    Note: Here keep all variables except the outcome variable (engagement)
- Now train a decision tree with a maximum depth of 3
- Plot the tree and interpet your findings
- Compute the mean squared error and the R^2 of this prediction
- Save the notebook

Hyperparameters

- **Parameters** are learned by the algorithm during training (like regression coefficients, or cutpoints in a decision tree)
- **Hyperparameters** refers to something that is passed to the algorithm, i.e. is set by the user and determines how the algorithm works
  - The depth of a tree 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 (→ tuning of 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**

6.3 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

Key element of ML:

- Assess the prediction quality **out-of-sample**!
- To do so: Randomly split the sample D in two parts D_{train} and D_{test}
  - Use only a subset D_{train} of the data to train the algorithm
  - Use the remainder D_{test} 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}

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

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

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

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=156)
```

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=156

Python

Training and Test R^2

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

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

- Print the training R^2:

```
print(r2_score(y_train, dtree.predict(X_train)))
```

- Print the test R^2 :

```
print(r2_score(y_test,  dtree.predict(X_test)))
```

- It can be convenient to print rounded numbers (here with two digits):

```
print(round(r2_score(y_test,  dtree.predict(X_test)),2))
```

Your Task — Predicting Engagement

- Open again your notebook EngagementPred
- 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=156
- Create a notebook cell in which you
  - Train the a decision tree on the training set (again with max_depth=3)
  - Print the R^2
    - on the training set and
    - on the test set
- Interpret your findings
- Save the notebook

Your Task

Predicting Engagement

- Generate a cell in which you train the tree and compute the train and test R^2s
  - Copy the cell four time
  - In each cell t a different depth of the tree (vary it from 2 to 5)
  - Run the cells
- Compare the training and test R^2 between the four cells
  - How does the training R^2 change?
  - How does the test R^2 change?

6.4 Optimal Complexity: Bias and Variance

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 decision tree is more flexible when the tree is deeper
  - it then can adapt more flexibly to specific patterns in the data
- …

Note:

- A more flexible model is more likely to be able to come closer 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
  - An algorithm that exhibits little bias can estimate the CEF precisely when we have an extremely large sample

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
  (Note the relationship to the standard error in regressions!)
- It is preferable to have a low variance!
  - Then the predictions are rather stable. 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 an 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

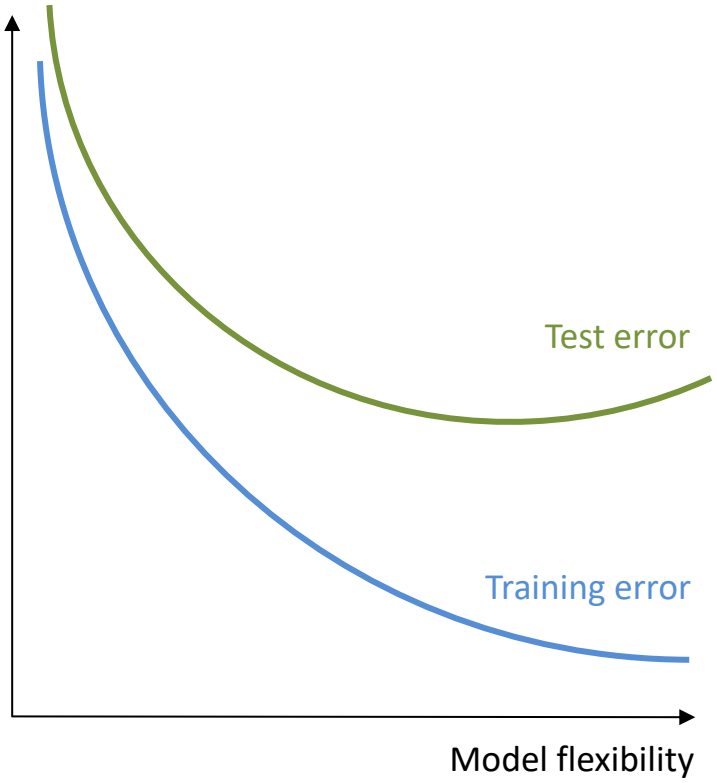
$$V[\epsilon] + \left(E\left[\hat{f}_D(X_0)\right] - f(X_0)\right)^2 + E\left[\left(\hat{f}_D(X_0) - E\left[\hat{f}_D(X_0)\right]\right)^2\right]$$

where

  - $V[\epsilon]$ is the *irreducible error*
  - $E\left[\hat{f}_D(X_0)\right] - f(X_0)$ is the *bias* of the algorithm
  - $E\left[\left(\hat{f}_D(X_0) - E\left[\hat{f}_D(X_0)\right]\right)^2\right]$ 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
  - Model becomes so flexible that it will map random patterns in training data
  - Hence, the **variance** increases
  - A very complex model will "memorize" the training data & thus **overfit**



6.5 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 data into two parts & fitting a tree to both halves, the results could be quite different (if the sampe size is not very large)
  - 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

Important:

- If the different trees are very similar, the improvement will be small as they will make similar predictions
- Hence a *random* forest introduces 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 features** as candidates to use for the next split

Random Forests: Bagging

Bagging:

(James/Witten/Hastie/Tibshirani (2023, pp. 343))

- 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 randomly drawn subset of P of the M features to be used for the next split (P is set as a hyperparameter)
- Idea: “decorrelate” the trees to force them to learn where it is more difficult
- 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=100).
                                      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
  - follow the convention to use the square root of M by specifying max_features='sqrt'
- You may also set further tree hyperparameters such as max_depth or min_samples_leaf

Your Task — Predicting Engagement

- Open again your notebook EngagementPred
- 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 R^2
- Save the notebook

6.6 Interpretation: Feature Importance & Partial Dependence Plots

- We use ML methods to make predictions but often we also want to understand & interpret how these predictions work
- For some methods like linear regressions or (shallow) decision trees that is quite easy
- For others such as random forests and in particular when there are many features it is more difficult, and the algorithm remains a “black box“
- Important tools to open the black box to some extent:
  - Estimate the importance of specific features for the prediction
    → feature importance
  - Graphs showing associations
    → partial dependence plots

Permutation Feature Importance

- Estimate the mean squared error of your prediction $MSE(\hat{f}_D, X_{test})$
- For each feature j: Repeat K times
  1. Generate feature matrix $X_{testPerm,jk}$ by randomly permuting feature j
     - That is: just randomly shuffle the values, for instance by splitting the data set in pairs and exchanging the values of the pairs
     - Then this feature is completely uninformative
  2. Estimate the error based on the predictions of the permuted data, i.e. $MSE(\hat{f}_D, X_{testPerm,jk})$
- Calculate permutation feature importance of feature j as

$$i_j = \frac{1}{K} \sum_{k=1}^{K} MSE\left(\hat{f}_D, X_{testPerm,jk}\right) - MSE(\hat{f}_D, X_{test})$$

- That is: How much does the error increase when I make the feature completely uninformative

Python

Permutation Feature Importance

- Import feature importance class:

```
from sklearn.inspection import permutation_importance
```

- Then perform estimation of feature importance

```
perm_importance = permutation_importance(model,
                  X_test, y_test, n_repeats=30, random_state=0)
```

  - For model insert the name of the fitted estimator
  - n_repeats specifies the number of permutations performed

- We obtain the feature importances from

```
perm_importance.importances_mean
```

- We can plot the feature importances in a bar chart:

```
pd.Series(perm_importance.importances_mean,
     index=X_train.columns).sort_values().plot(kind='barh')
```

  - index=X_train.columns determines that the bars get the names of the columns in the DataFrame X_train

Your Task

Predicting Engagement: Feature Importance

- Open again your notebook EngagementPred
- Estimate & plot the permutation feature importance (set n_repeats=30 and random_state=156)
- Which features are most important for your prediction?

Partial Dependence Plots

- From the feature importance we learn about the importance for the feature for the prediction
- But we do not learn **how** a feature matters, for instance
  - is there a positive, negative, or non-monotonic association?
  - what is the magnitude of the respective slope of the CEF?
- To inspect this, we can use **partial dependence plots**
  - Pick a feature to be inspected
  - For different potential values of the feature make a prediction for y holding all other features constant
  - Plot these predictions
- Note: The plots only has a clean ceteris paribus interpretation if the feature in question is uncorrelated with all other features

Python

Partial Dependence Plots

- Import feature importance class:

  ```
  from sklearn.inspection import PartialDependenceDisplay
  ```

- Then plot the partial dependence

  ```
  PartialDependenceDisplay.from_estimator(model,X,['x1','x2'])
  ```

  where

  - model is the fitted estimator
  - X is the feature matrix
  - ['x1', 'x2'] is a list of the features for which you want to plot the partial dependence

- You can also plot two-dimensional partial dependence

  ```
  PartialDependenceDisplay.from_estimator(model,X,[('x1', 'x2')])
  ```

  (Note the round brackets () around the tuple)

Your Task

Predicting Engagement: Partial Dependence Plots

- Open again your notebook EngagementPred
- Plot partial dependence plots for
  - age (Variable alter) and
  - health status (Variable mgesund_allg)
- Plot also a two-dimensional plot with them both [('alter','mgesund_allg')]

6.7 Lasso Regression

- We have seen in the beginning of the lecture that linear regressions can be powerful also for prediction tasks: when the CEF is linear, OLS regressions provide the best estimate
- But a problem we here often face is the choice of explanatoy variables
  - When we have data with many predictors (like the LPP): how do we choose among the variables to put on the right hand side?
  - When we think about estimating polynomial functions (as we did when we added quadratic terms), what is the right order of the polynomial?
  - When we think about interaction terms: which should we put in?
- We face again a bias-variance trade-off
  - When leaving out variables we may not capture the true CEF well enough
  - When including more variables we have a more complex model and are more likely to overfit the training data

Lasso: How it works

- Regression "punishing" coefficients for deviations from zero (shrinkage)
- In Chapter 2 we have seen that an OLS estimator minimizes

$$E\left[\left(Y_i - b_0 - \sum_{k=1}^{M} b_k X_{ik}\right)^2\right]$$

- A Lasso regression instead minimizes

$$E\left[\left(Y_i - b_0 - \sum_{k=1}^{M} b_k X_{ik}\right)^2\right] + \alpha \cdot \sum_{k=1}^{M} |b_k|$$

The key idea is simple:

- $|b_k|$ is the absolute value of the coefficient, i.e. its distance to zero
- Coefficients are thus penalized for deviating from zero and high values of α **reduce overfitting** (a process also called "regularization")
- The hyperparameter α determines again the trade-off between low bias ($\alpha = 0$) and low variance (large α)

Python

Lasso

- To fit a Lasso regression first import:

```
from sklearn.linear_model import Lasso
```

- And then fit:

```
lasso = Lasso(alpha=0.1).fit(X_train, y_train)
```

- You can print the coefficient names and values for instance with

```
print(pd.Series(lasso.coef_, index=X_train.columns))
```

6.8 Tuning of Hyperparameters

- As we have seen in the above, we have to find the right balance when determining the complexity of an algorithm
- The more complex/flexible an algorithm is,
  - the lower the bias (we get closer to the true CEF)
  - but the higher the variance; we are more likely to have overfitting
- We should aim at finding values of the hyperparameters that yield the best out-of-sample prediction (lowest MSE) when applied to new data
- Here it is very useful to make **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

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_{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 with Cross-Validation

- Often we consider models with hyperparameters such as the depth of a tree, or the shrinkage parameter in lasso
- We train an algorithm for a specific hyperparameter α (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 $\hat{f}_D(X, \alpha)$ be the algorithm trained with hyperparameters α
- 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 α 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

Hyperparameter Tuning & Cross-Validation

- Scikit-Learn provides convenient tools to perform hyperparameter tuning
- You can estimate the cross validation error with cross_val_score
  - Performs k-fold cross validation and gives back estimated generalization errors
- Or you directly tune hyperparameters automatically with GridSearchCV
  - You can specify the parameters (such as alpha in lasso) and ranges for these parameters to be checked
  - Then GridSearchCV finds the combination of parameter values that minimizes the cross validation error
- For some estimators scikit learn has built-in cross-validation capabilities to automatically select the best hyperparameters
  - Then the above steps are performed directly when fitting the estimator

Python

Cross-Validation Lasso

- First import the cross-validation Lasso estimator:

```
from sklearn.linear_model import LassoCV
```

- And then fit the estimator (here using 5-fold cross validation)

```
lasso = LassoCV(cv=5).fit(X_train, y_train)
```

- You can then again access the estimated coefficients and R^2 as in the above
- The optimally tuned value of alpha can be displayed by

```
print("Alpha=",lasso.alpha_)
```

- You can again print the coefficient names and values for instance with

```
print(pd.Series(lasso.coef_, index=X_train.columns))
```

Your Task

Predicting Engagement

- Open again your notebook EngagementPred
- Now try to find the optimal value of alpha for a Lasso regression
- It is convenient to directly use LassoCV
- Compute the test R^2 and optimal value of alpha
- Print the coefficient names & values
- Save the notebook

Conclusion

Aim of the course:

- Familiarize you with different empirical methods
- Let you apply these methods to gain practical skills in using Python to work with data

Key messages:

- Linear regressions are a powerful tool to approximate conditional expectations with easily interpretable linear functions
- Other machine learning methods may provide more flexible functional forms but sometimes at the expense of interpretability
- Important to distinguish between the different key objectives (i) to make predictions and (ii) to estimate causal effects
  - For the former: Importance to test prediction quality *out-of-sample*
  - For the latter: Importance to understand the role of *identifying assumptions* and their plausibility in different contexts

Appendix

Decision Trees: Recursive Binary Splitting

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