DSC510: Introduction to Data Science and Analytics
Lab 6: Regression

University of Cyprus
Department of
Computer Science

Pavlos Antoniou

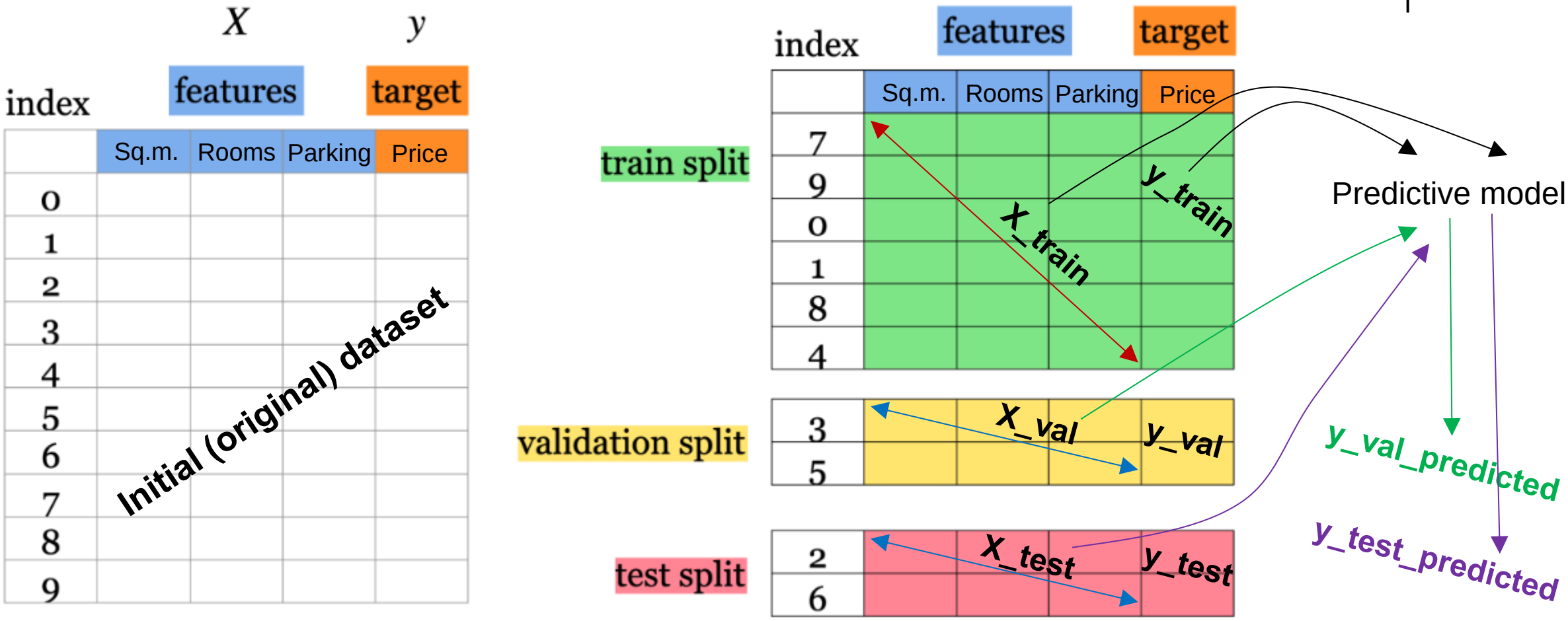
Office: B109, FST01

Predictive modeling techniques

- Predictive modeling techniques help translate raw data into value
  - Machine learning predictive techniques such as Support Vector Machines (SVMs), Decision trees, boosting methods, learn from data and build models
- Data + Predictive Modeling Technique → Predictive Model
  - 3 phases to prepare a predictive model: Training – Validation – Test
- Split initial dataset into 3 smaller datasets
  - **Training dataset**: The actual dataset used to train the model and evaluate **parameters**. The model ***sees*** and ***learns*** from this data | 70-80%
  - **Validation dataset**: Used to provide unbiased **evaluation of model** fit on testing dataset and ***fine-tune*** the model ***hyperparameters****. The model occasionally sees this data, but never "learns" from this | 10-15%
  - **Test dataset**: Used to provide unbiased **evaluation of the final model**. Only used once model is completely trained and validated | 10-15%

* Cannot be learned from data, during the training process.

Training / validation / test datasets

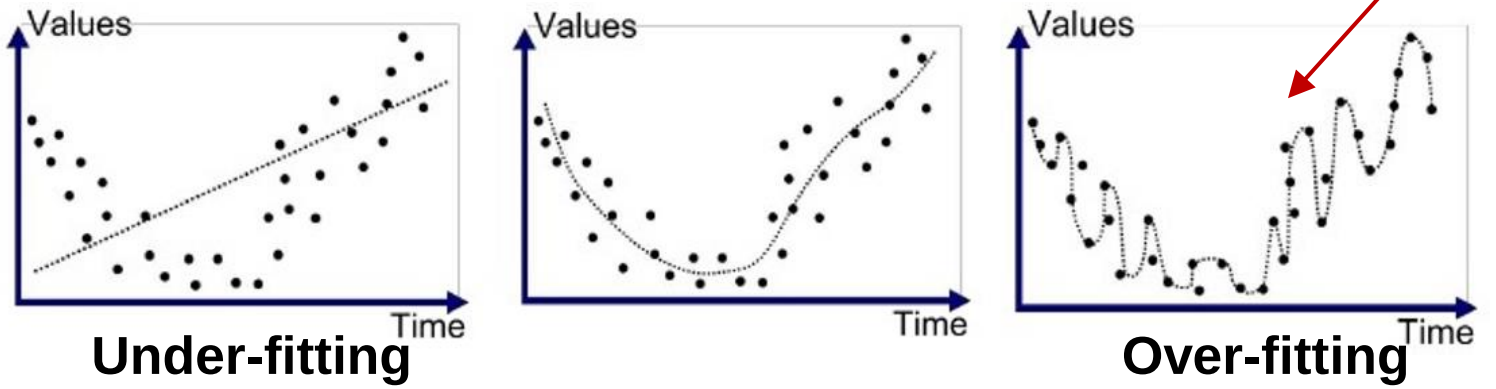


- During testing phase, predictive modelling technique sees both features (X_train) and the target (y_train) values
- During validation and testing phases, only features (X_val, X_test respectively) are given as input to predictive technique so as to predict the target values. Predictive model is evaluated on its effectiveness to correctly predict the target values by comparing the predicted with the original target values.

Splitting datasets against overfitting

- Training a predictive modelling technique and evaluating its performance on the same data a methodological mistake because may lead to:
  - High accuracy on seen data
  - Low accuracy (fail to predict / classify) on unseen data

Underfitting: model fails to capture underlying pattern in training data



Over-fitting: model learns training data too well but fails to generalize to new data

- Splitting dataset into 3 parts (training, validation and testing datasets) can prevent overfitting:
  - ensures that model generalize well on unseen data

When to split a dataset? Why?

- Splitting the dataset into training, validation and test datasets should typically be one of the first steps in a data science project, **before** performing any data preprocessing and transformations
- Why split the dataset early?
  - Avoid data leakage: avoid passing information from test set to validation / training sets
    - Example: Scaling features using information from the entire dataset may lead towards modifying data (rows) that will end up in the training dataset from data that will end up in the “unseen” (test) set
  - Realistic evaluation: **test dataset should simulate new, truly unseen data**
    - Performing data imputing, data encoding, data transformation (scaling, standardizing, unskewing) and feature selection based on the training set alone ensures that test data are truly unseen and not involved as happens in a real-world scenario

Best practices in a data science project

- Initial data exploration
  - **Before splitting** the data, perform exploratory data analysis (EDA) to understand the structure of the dataset
  - This includes understanding data types, basic statistics (e.g. mean, std, median), feature/target distributions, checking for missing values and data inconsistencies, getting an initial sense of the data
- Split the data
  - Split the data into training (,validation) and test sets
    - validation not needed if Cross Validation process will be used (we discuss it later)
- Data preprocessing
  - After splitting, perform all preprocessing steps (such as missing values imputation, scaling, encoding) separately on the training set
  - Fit (train) the preprocessing tools (like scalers and encoders) on the training data and then apply these fitted tools to the validation and test sets.

Best practices in a data science project

- Feature Engineering (Selection, Extraction)
  - Conduct feature engineering (feature selection / extraction) based solely on the training data
  - Apply the same feature transformations to the validation and test sets
- Model Training and Tuning
  - Train your models using the training set
  - Use the validation set to tune hyperparameters and select the best model
  - Finally, evaluate the model on the test set to get an unbiased estimate of its performance

Best practices in a data science project

- Beneficial to keep the various versions of dataset at each stage, as it gives you the flexibility to try different approaches without redoing pre-processing steps. Here's a breakdown of why retaining each version could be helpful:
  - **Original Dataset**: Keeping the raw data allows you to revisit it if you need to apply new techniques (e.g. imputing, scaling, encoding) in the future.
  - **Cleaned Data**: Keeping a dataset with just the basic cleaning (imputation, drop useless columns or rows with large number of missing values) lets you experiment with different scaling (min-max, standard, robust) and encoding (label, one hot, cyclical) techniques without starting over.
  - **Scaled and Encoded Data**: Keeping different datasets with various scaling or encoding techniques lets you be compatible with different ML techniques e.g. linear models perform better with scaled data.
  - **Feature-Selected Data**: Retaining a version of your dataset after feature selection can be helpful to evaluate if selected features improve model performance compared to using all features.
  - **PCA or Other Extracted Features**: Keeping a transformed dataset with dimensionality reduction techniques allows you to compare models trained on reduced feature sets versus the full feature set.
- **Why Try Different Versions?**
  - **Model Flexibility**: Some models benefit from standardized scaling, while others don't, and models like tree-based algorithms may perform better with the original features.
  - **Experimentation**: Comparing the results from different versions helps identify the most effective feature engineering and transformation steps for each algorithm.
  - **Efficient Experimentation**: You can re-use pre-processed datasets for quicker experimentation, avoiding the time required to apply transformations again.

Predictive techniques: Supervised learning

- You have input features (X) and an output target variable (y) available and use a predictive modelling technique to build a model that captures the relationship between input and output data
  - Majority of predictive techniques are supervised learning techniques
- Supervised learning problems can be further grouped into:
  - **Classification problems**: the output variable (y) is a category, such as "disease" or "no disease", 0 or 1 (binary classification) and "red" or "blue" or "green" (multiclass classification). Values can be strings or discrete integers
    - Popular techniques: Logistic Regression, Linear Discriminant Analysis (LDA), K-Nearest Neighbors (KNN), Decision Trees (Random Forest), Support Vector Machine (SVM), Naïve Bayes, Gaussian Naïve Bayes, XGBoost, AdaBoost
  - **Regression problems**: the output variable (y) is a continuous numerical value, such as "price" or "weight"
    - Popular techniques: Linear Regression, Polynomial Regression, Support Vector Regression (SVR), Random Forest Regression, XGBoost Regression, AdaBoost Regression

Predictive techniques: Unsupervised learning

- You only have input vars (X) and no corresponding output variable (y)
  - no mapping from input to output data
- Goal: model the underlying structure or distribution in the data in order to learn more about the data, extract insights
- Unsupervised learning problems can be further grouped into:
  - **Clustering problems**: A clustering problem is where you want to discover the inherent groupings in the data, such as grouping customers by purchasing behavior.
    - Popular techniques: k-means
  - **Association problems**: An association rule learning problem is where you want to discover rules that describe large portions of your data, such as people that buy X1 also tend to buy X2
    - Popular techniques: Apriori algorithm

Regression

- The process of estimating the relationships between a dependent variable (target variable) y which takes continuous numerical values and one or more independent (or input) variables (called features) X
  - Example: Estimate the relationship between the house price (dependent var) and the house area in square meters (independent var)
  - House area is independent variable because we cannot mathematically determine it. But, we can determine / predict house price value based on the house area.
- Some regression algorithms:
  - Linear Regression (simple, multiple) – first degree equation
  - Polynomial Regression – higher degree (2^{nd}, 3^{rd}, …) polynomial equations
  - Support Vector Regression
  - Ensemble Regression (e.g. Random Forest Regressor, Ada Boost Regressor, XGBoost Regressor)

Linear Regression (LR)

- Linear regression assumes that the relationships between the dependent (target) variable and the independent variables are linear
- Therefore, the dependent variable y can be calculated from a linear combination of the independent variables (X):

$$y = \beta_0 + \sum_{j=1}^{p} \beta_j * X_j = \beta_0 + \beta_1 * \mathrm{X}_1 + \beta_2 * \mathrm{X}_2 + \cdots$$

- Vector β involves initially unknown coefficients (parameters), which will be evaluated using a training dataset with values for target variable and features

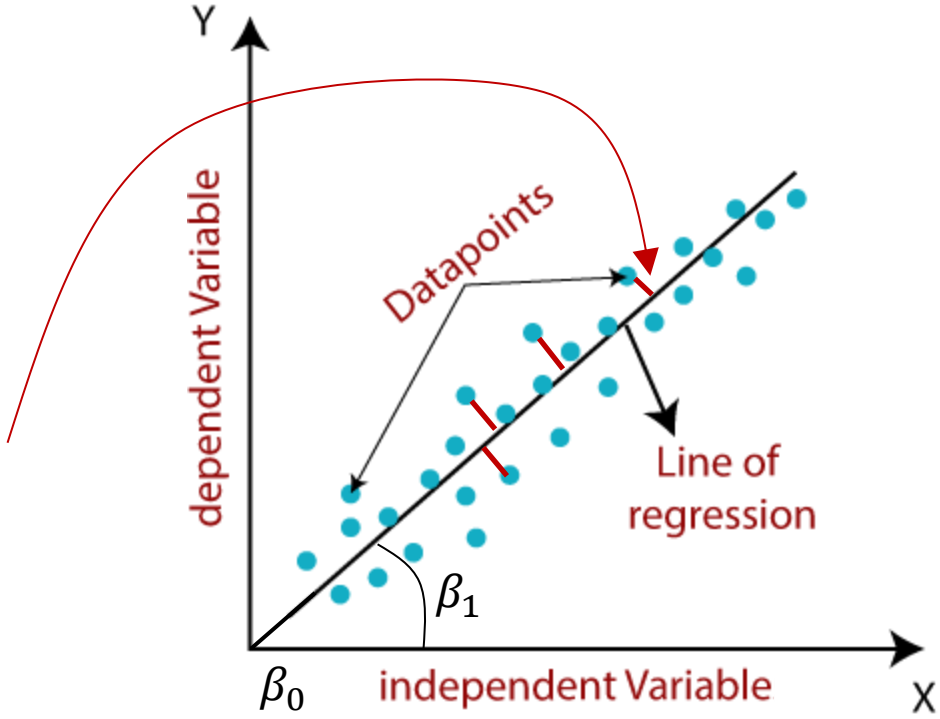
Simple Linear Regression

- **Simple Linear regression**: one independent input variable X:

$$y = \beta_0 + \beta_1 X + \in$$

X	y
0.10	1.51
0.15	0.92
0.17	1.96
0.22	0.53
0.27	0.38

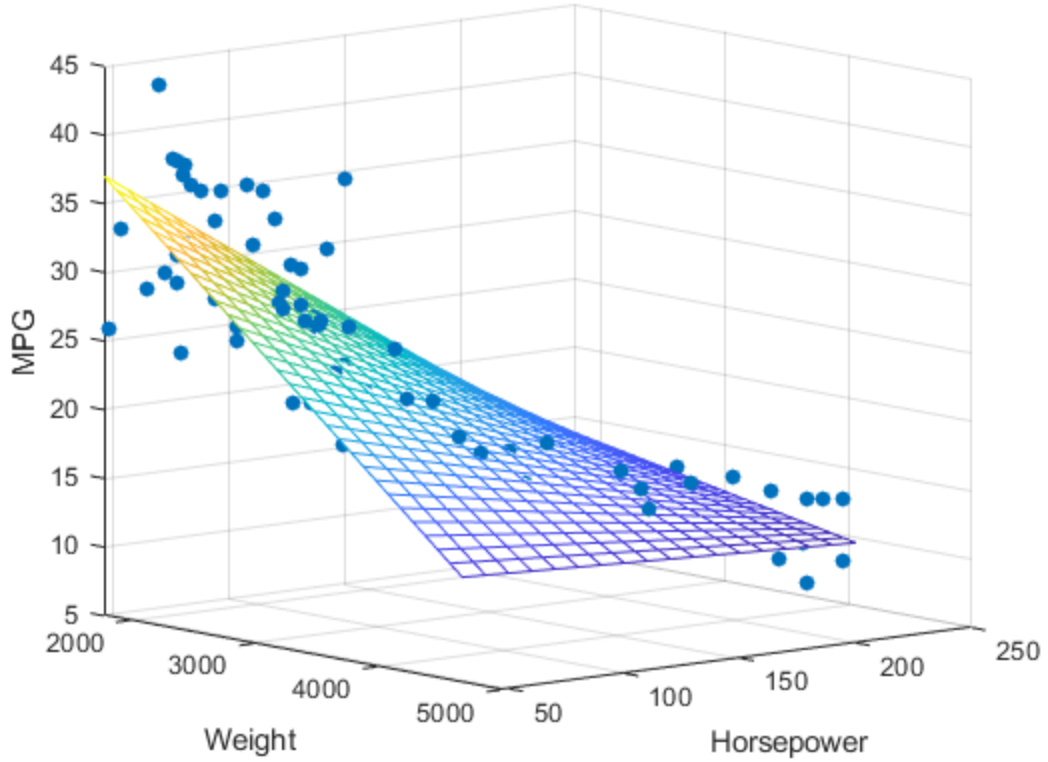
  - **Goal: Fit the best intercept line (evaluate β_0 and β_1) that passes between all data points that minimizes the error**
  - y : Dependent variable (target variable)
  - X : Independent variable (feature)
  - β_0 : Intercept (the target value when X = 0)
  - β_1 : Slope. Explains the change in Y when X changes by 1 unit = $\Delta y/\Delta X$
  - $\in$: Error. This represents the residual value, i.e. the difference between the observed and the fitted (predicted) value



Multiple Linear Regression

- **Multiple Linear regression**: more than one independent variables Xi in the linear function:

$$y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \cdots \beta_n X_n + \in$$



In this image n=2
Two independent variables:

- Weight
- Horsepower

Dependent variable:

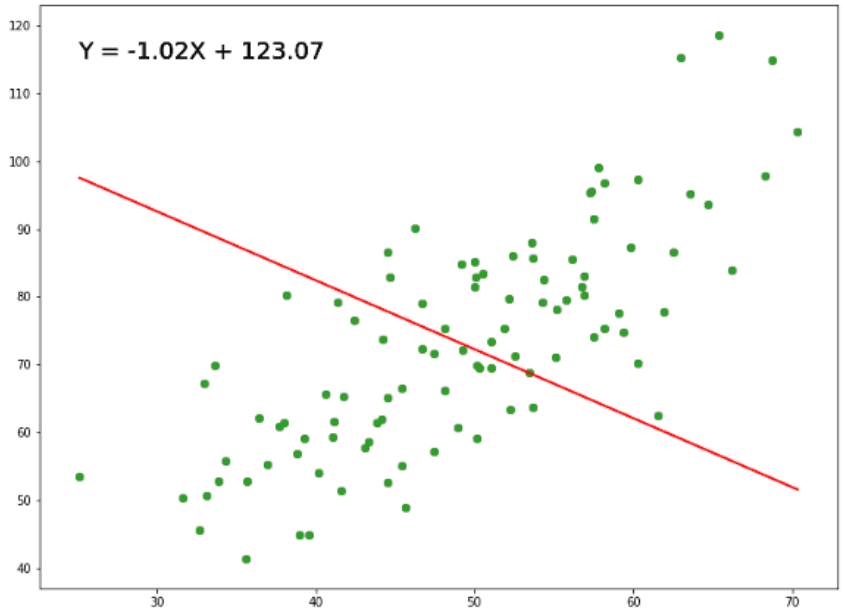
- MPG (miles per gallon)

Regression finds the best-fitting plane that passes through all points minimizing the error

Linear Regression Methods

1. **Ordinary least squares** (OLS) is a non-iterative method that fits a model (line or plane) and finds the β coefficients such that the sum of squared error is minimized.

2. **Gradient descent** finds the linear model β coefficients iteratively



- When the β coefficients are estimated, the equation can be used to predict the target value y given an input X vector

Main assumptions for using Linear Regression

- Linear relationships
  - between each independent variable and the dependent variable
    - can best be tested with scatter plots / pair plots
- No or little multicollinearity
  - Low correlation between two or more independent variables – can be checked with correlation matrix (visualized by heat map)
    - If multicollinearity is discovered, the analyst may drop one of the two variables that are highly correlated
    - PCA can also be used to reduce multicollinearity new features are uncorrelated
- Normality of residuals
  - LR requires the residuals (error terms) of the model to be normally distributed, with mean equal to 0 – can best be checked with a histogram of the residuals; normality test functions are also available

Linear Regression: Get to know data

```
import pandas as pd
import numpy as np
df = pd.read_csv('Advertising.csv')
df.head()
```

	Unnamed: 0	TV	Radio	Newspaper	Sales
0	1	230.1	37.8	69.2	22.1
1	2	44.5	39.3	45.1	10.4
2	3	17.2	45.9	69.3	9.3
3	4	151.5	41.3	58.5	18.5
4	5	180.8	10.8	58.4	12.9

```
df.describe()
```

	Unnamed: 0	TV	Radio	Newspaper	Sales
count	200.000000	200.000000	200.000000	200.000000	200.000000
mean	100.500000	147.042500	23.264000	30.554000	14.022500
std	57.879185	85.854236	14.846809	21.778621	5.217457
min	1.000000	0.700000	0.000000	0.300000	1.600000
25%	50.750000	74.375000	9.975000	12.750000	10.375000
50%	100.500000	149.750000	22.900000	25.750000	12.900000
75%	150.250000	218.825000	36.525000	45.100000	17.400000
max	200.000000	296.400000	49.600000	114.000000	27.000000

Independent variables (features)

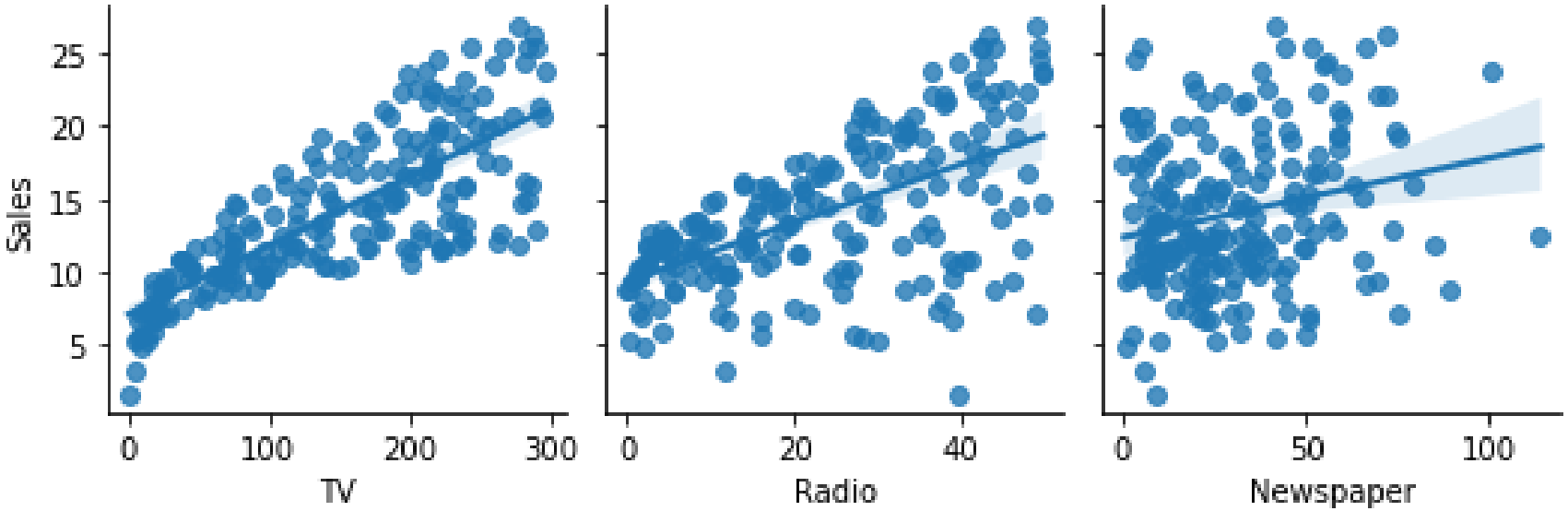
target variable

Dataset description: Sales (in thousands of units) for a particular product based on the advertising budgets (in thousands of dollars) for TV, radio, and newspaper media.
Dataset is clean, without missing and erroneous values

Linear Regression: Testing assumptions

- Linearity

```
sns.pairplot(df,x_vars=["TV","Radio","Newspaper"],y_vars= "Sales",kind="reg")
```

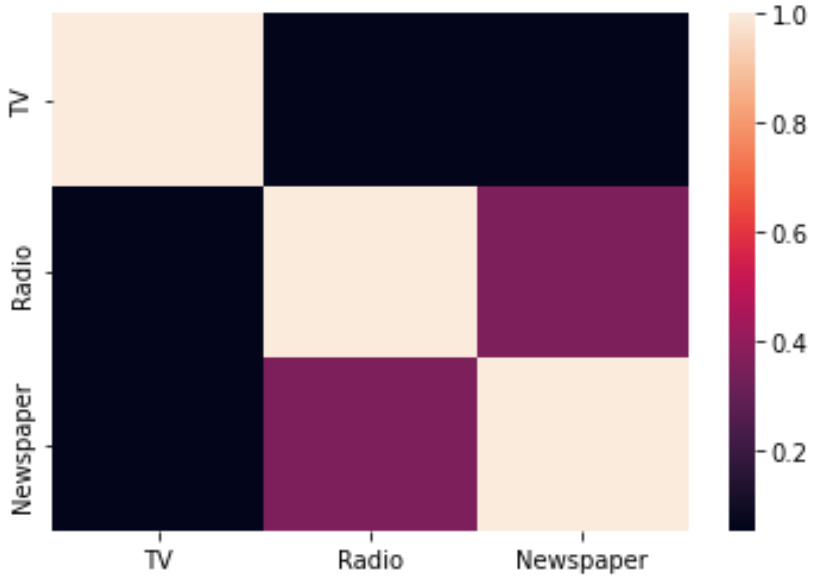


By looking at the plots we can see that none of the independent variables has an accurately linear relationship with Sales but TV and Radio do still better than Newspaper which seems to hardly have any specific shape. So, it shows that a linear regression fitting might not be the best model for it. A linear model might not be able to *efficiently* explain the data in terms of variability, prediction accuracy etc.

Linear Regression: Testing assumptions

- Multicollinearity
  - Independent variables seem to be uncorrelated (there is no correlation between independent variables > 0.75)

```
df_features = df[["TV", "Radio", "Newspaper"]]
sns.heatmap(data=df_features.corr())
plt.show()
```



Linear Regression: Prepare variable vectors

- Normality of residuals require us to perform the regression and calculate the residuals (error terms)

```
# get the values of the dataframe that will be used in the regression model
dataset = df.values

# extract the features (independent variables)
X = dataset[:,1:4]
print(X[0:10])

# extract the dependent (target) variable
y = dataset[:,4]
print(y[0:10])
```

```
[[230.1  37.8  69.2]
 [ 44.5  39.3  45.1]
 [ 17.2  45.9  69.3]
 [151.5  41.3  58.5]
 [180.8  10.8  58.4]
 [  8.7  48.9  75. ]
 [ 57.5  32.8  23.5]
 [120.2  19.6  11.6]
 [  8.6   2.1   1. ]
 [199.8   2.6  21.2]]
```

```
[22.1 10.4  9.3 18.5 12.9  7.2 11.8 13.2  4.8 10.6]
```

Linear Regression: Linear Regressors

```
from sklearn.linear_model import LinearRegression
lregr = LinearRegression()

# ALTERNATIVE REGRESSOR
from sklearn.linear_model import SGDRegressor
sgdr = SGDRegressor()
```

LinearRegression() class uses Ordinary Least Squares (OLS) solver from scipy

SGDRegression object uses stochastic gradient descent method

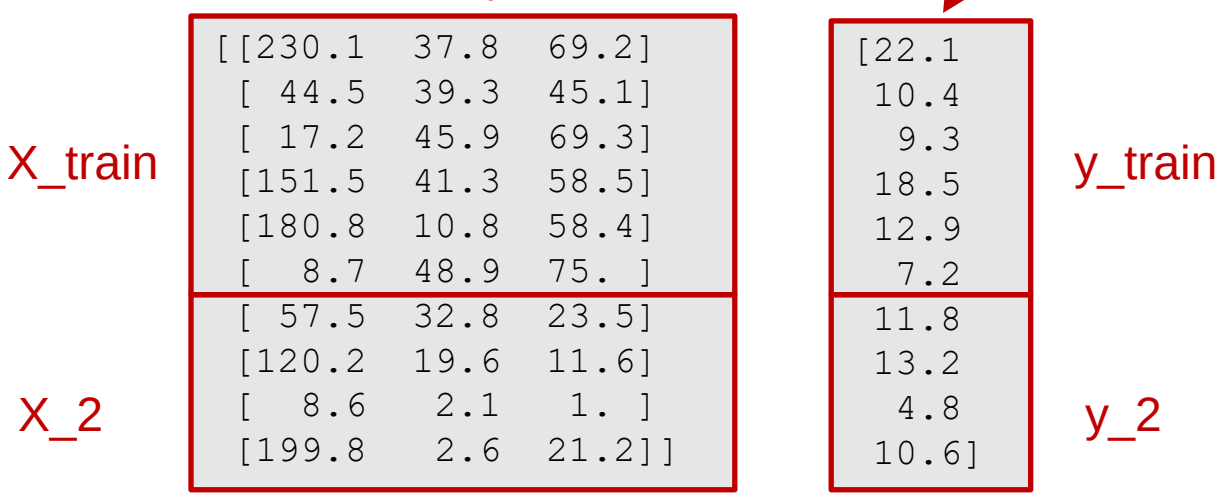
- SGDRegressor uses the iterative method gradient descent to estimate the coefficients
- The main reason why gradient descent could be preferred for linear regression instead of the LinearRegressor is the computational complexity: it's computationally cheaper (faster) to find the solution using the gradient descent in datasets with large number of features.

Linear Regression

```
from sklearn.linear_model import LinearRegression
lregr = LinearRegression()
```

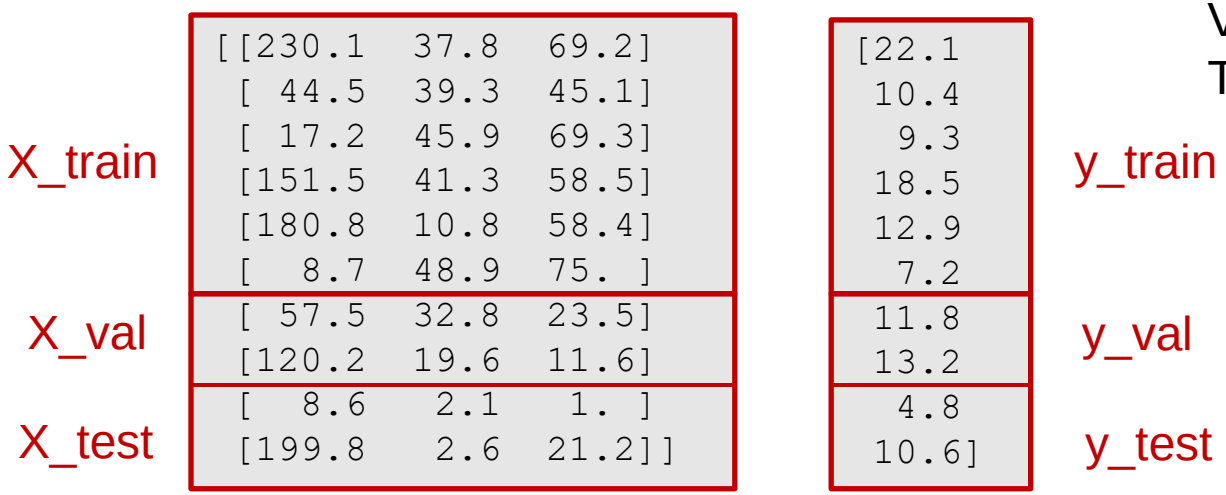
```
from sklearn.model_selection import train_test_split
X_train, X_2, y_train, y_2 = train_test_split(X, y, train_size=0.80)
```

Training data size: 80%
Remaining data (X_2, y_2) size: 20%



Linear Regression: Splitting datasets

```
from sklearn.linear_model import LinearRegression
lregr = LinearRegression()

from sklearn.model_selection import train_test_split
X_train, X_2, y_train, y_2 = train_test_split(X, y, train_size=0.80)
X_val, X_test, y_val, y_test = train_test_split(X_2, y_2, train_size=0.50)
```



Validation data size: 50% of remaining
Testing data size: 50% of remaining

Training data size: 80%
Validation data size: 10%
Testing data size: 10%

Non standardized independent values

Linear Regression: Model training

```
from sklearn.linear_model import LinearRegression
lregr = LinearRegression()

from sklearn.model_selection import train_test_split
X_train, X_2, y_train, y_2 = train_test_split(X, y, train_size=0.80)
X_val, X_test, y_val, y_test = train_test_split(X_2, y_2, train_size=0.50)

# train model (Fit linear model) and evaluate model β coefficients
model = legr.fit(X_train, y_train)
# print model intercept (β0)
print("β0 =", model.intercept_)
# print model coefficients
print("[β1,β2,β3] =", model.coef_)
```

```
β0 = 2.99489303049533
[β1,β2,β3] = [ 0.04458402  0.19649703 -0.00278146]
```

Model after training: $y = 2.9948 + 0.04458*x_1 + 0.19649*x_2 - 0.00278*x_3$

The coefficient 0.04458 for the first feature (TV ads) means that for each additional 1 thousand dollars spent, the sales increase by 0.04458 thousands units, holding the rest features constant.

Non standardized independent values

Linear Regression: Making prediction

```
from sklearn.linear_model import LinearRegression
lregr = LinearRegression()

from sklearn.model_selection import train_test_split
X_train, X_2, y_train, y_2 = train_test_split(X, y, train_size=0.80)
X_val, X_test, y_val, y_test = train_test_split(X_2, y_2, train_size=0.50)

# train model (Fit linear model) and evaluate model β coefficients
model = legr.fit(X_train, y_train)
# print model intercept (β0)
print("β0 =", model.intercept_)
# print model coefficients
print("[β1,β2,β3] =", model.coef_)

# estimate residuals
# predict
y_pred = model.predict(X_val)
# residuals is the differences between real y values (y_val) and predicted y values
residuals = y_val - y_pred
print("Residuals:", residuals[:10])
```

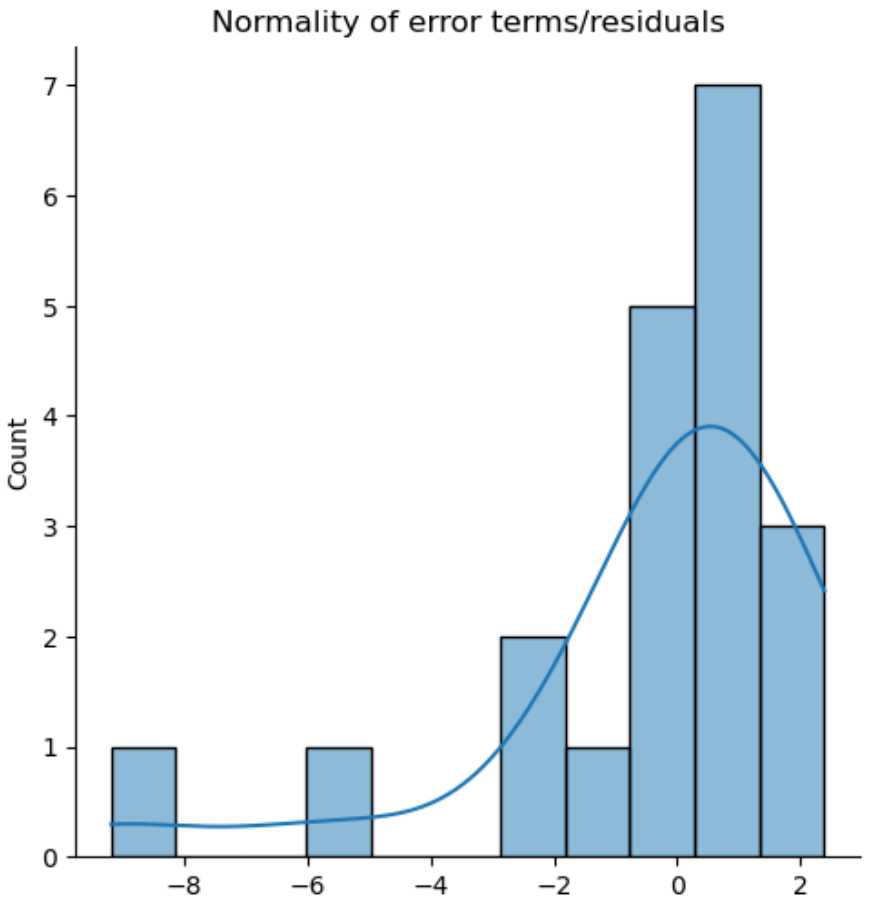
```
Residuals: [0.11256448  2.16206142 -9.18318566
0.21444367  0.62679197 -1.90974587
 -2.03802209  0.9477193   0.30597666  0.03544328]
```

Non standardized independent values

Linear Regression: Testing assumptions

- Normality of residuals
  - Residuals (error terms) of unstandardized input does not seem to be normally distributed
  - Run normality check to test whether the residuals differ from a normal distribution

```
# computing the p-value for the null-hypothesis
that this distribution is a normal distribution
from scipy import stats
_, p = stats.normaltest(residuals)
# p-value of 0.05 or greater means that the
distribution is a normal distribution
print(p) # => 3.4638013535871560e-10, residuals
deviate from normal distribution
```



Data scaling/standardization

- The values of β coefficients represent the influence of each input feature on the target variable: $y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \cdots \beta_n X_n + \in$
  - When regression is used for explaining a phenomenon, i.e. how input features influence the output y, the values of β coefficients can shed light
    - E.g. if β1 > β2 one might say X1 has higher impact than X2 on y since a small change in X1 results in a comparably large effect on y
  - BUT we cannot directly compare the size of the various β coefficients if the input variables are measured on different scales
- By scaling/standardizing variables, coefficients become directly comparable to one another, with the largest coefficient indicating which independent variable has the greatest influence on the dependent variable
  - We can scale input features using MaxMinScaler, StandardScaler, RobustScaler shown in Lab 4

Data scaling/standardization

- Min-max scaler scales each feature individually into a given range, e.g. [0, 1]
- Standard scaler scales each feature individually to make values have zero mean ($\mu = 0$) and unit variance ($\sigma^2 = 1$)
  - It is preferred that the feature to be scaled is close to normal distribution (bell curve) – standard scaler does not perform optimally on highly skewed features
  - Centers data around zero
- Robust scaler scales each feature individually to make values have zero median (median=0) and unit interquartile range (IQR=1)
  - Center data around zero
  - Robust to outliers
- None of these techniques changes the distribution of features, nor have an impact on p-value (used in the normality test)

When is feature scaling needed in LR?

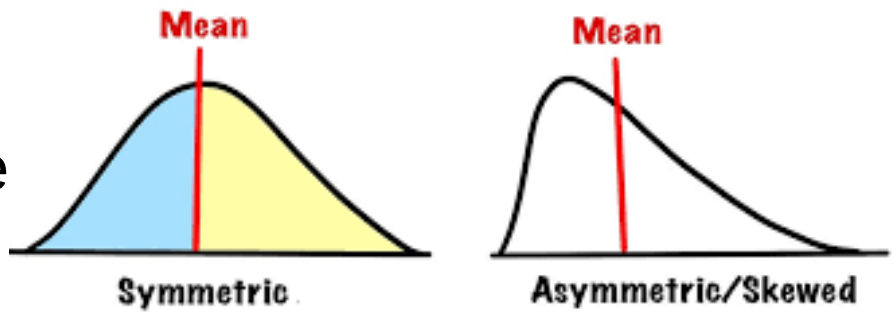
- When linear regression is used for making β coefficients directly comparable to one another and reveal the influence of each feature on target thus making it easy to present effects to non-statisticians

- Technically, feature scaling does not make a difference in linear regression, however, when gradient descent-based algorithms (such as SGDRegressor) are used for Linear Regression, feature scaling is needed to speed up the process of convergence (see more details here)

When is feature/target unskewing needed in LR?

- Unskewing transformations attempt to make long-tail distribution more symmetric, ideally resembling a Gaussian (bell-shaped) distribution
  - Unskewing transformations: BoxCox, Yeo-Johnson, Sqrt, Log

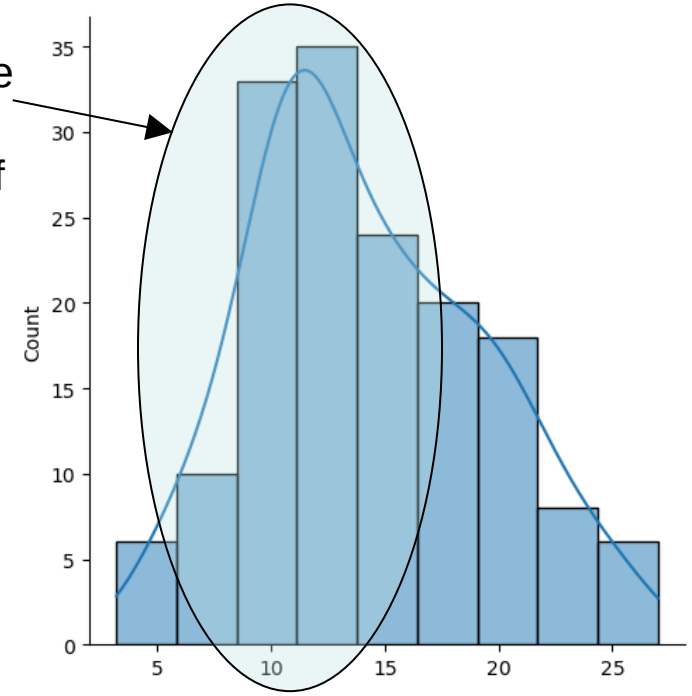
- Linear regression (OLS method) does not require feature and target variable distributions to be normal but requires normality of residuals
  - But, in the presence of highly **skewed target variable**, the trained predictive model tends to underestimate values under the long-tail area and to overestimate values near the peak where the majority of values lay (EXPLANATION). This occurs because the **model is "biased" towards the majority of data**.



Linear Regression: Target variable distribution

- We prefer target variable distribution be more symmetric (unskewed) => predictive algorithm will learn all sales values without bias
- Distribution plot of target (Sales): right skewed (long tail to the right)

We have more products with low number of sales




```
import seaborn as sns
# distribution plot of the target variable
sns.displot(y_train, kde=True)

# computing the p-value for the null-hypothesis that
this distribution is a normal distribution
from scipy import stats
_, p = stats.normaltest(y_train)
# p-value of 0.05 or greater means that the distribution
is a normal distribution
print(p) # => 0.03975020925593686 4, not normal distrib.
```

- Solution: Unskew target variable using techniques of Lab4

Linear Regression: Standardize X / unskew y

```
from sklearn.preprocessing import StandardScaler
sc = StandardScaler()

# train scaler & apply transf on training set
X_train_scaled = sc.fit_transform(X_train)
print(X_train_scaled[0:10])
# apply scaler on validation and test sets
X_val_scaled = sc.transform(X_val)
X_test_scaled = sc.transform(X_test)
# Unskew the target variable values
# Apply box-cox on training dataset to
# estimate λ parameter
y_train_scaled, lambda_bc = boxcox(y_train)
print(y_train_scaled[0:10])
# apply transformation on y validation
y_val_scaled = boxcox(y_val, lambda_bc)
y_test_scaled = boxcox(y_test, lambda_bc)
```

```
[[-1.34155345  1.0355176   1.65941078]
 [-1.4053143   0.08249594 -1.30629738]
 [-0.08995151  0.40243892 -0.81980897]
 [ 0.69761311 -0.18979597 -0.90868666]
 [ 0.76609699  0.01442296  1.28518893]
 [-0.56461564  0.42286082 -1.01627544]
 [-1.67570755 -1.44914602 -1.36243065]
 [-1.57770476  1.38268978  2.77272078]
 [-0.29304164  0.91979354  2.29558792]
 [-0.54218127 -1.20408331  0.19994556]]
```

```
[4.79407796 4.35326964 6.0707102  6.32143636
6.64564903 5.78373694 2.45296201 4.06788525
6.32143636 4.66122092]
```

Transformed vector

Evaluated lambda (λ) value

Estimate the parameter λ on the training data set, then use the estimated value to apply the transformation to the training and test data set to avoid data leakage

λ parameter will also used in reverse BoxCox transformation

Standardized independent values

Linear Regression

```
# create a new model to be trained on scaled data
lregr_scaled = LinearRegression()

# train model (Fit linear model) and evaluate model β coefficients
model_scaled = lregr_scaled.fit(X_train_scaled, y_train_scaled)
# print model intercept
print("β0 =", model_scaled.intercept_)
# print model coefficients
print("[β1,β2,β3] =", model_scaled.coef_)

# estimate residuals
# predict and estimate residuals
y_pred_scaled = model_scaled.predict(X_val_scaled)
```

```
β0 = 5.719657352358076
[β1,β2,β3] = [1.1333148   0.80643841 -0.01058377]
```

"TV", "Radio", "Newspaper"

- Standardization changes the interpretation of coefficients (at the same scale).
- Reveals the “importance” (influence) of each independent variable in predicting the dependent variable.
- TV has the highest coefficient, thus can be inferred that it is the most important factor for increasing sales.

Linear Regression: Model evaluation

- Model evaluation is a core part of building an effective ML model
- Evaluation metrics provide a measure of how good a model performs and how well it approximates the relationship between the dependent variable and the independent variables
- Some regression evaluation metrics:

n = number of data points
y_i = observed value i
$\hat{y}_i$ = predicted value i

minimize

  - MAE: Mean Absolute Error $MAE = \frac{1}{n}\sum_{i=1}^{n}|\hat{y}_i - y_i|$
    - clear, interpretable sense of how far off, on average, predictions are from actual values
    - Does not penalize large prediction errors (caused by outliers)
  - MSE: Mean Squared Error $MSE = \frac{1}{n}\sum_{i=1}^{n}(\hat{y}_i - y_i)^2$
    - Average of squared differences: Large prediction errors are penalized (sensitive to outliers)
  - RMSE: Root Mean Squared Error $RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(\hat{y}_i - y_i)^2}$
    - error in the same units as the target variable, making it more interpretable than MSE

maximize

  - R-squared (R2): a statistical measure of how close the data are to the fitted regression line on a convenient 0-1.0 scale (0: poor fitting, 1: perfect fitting)

Non standardized independent values

Linear Regression: Evaluate model

```
from sklearn.metrics import mean_squared_error
from sklearn.metrics import r2_score

# prediction on validation data
# Model trained on unstandardized features and non-transformed target values
y_pred = model.predict(X_val)
print(y_pred[0:10])

# Mean Squared Error (MSE)
MSE = mean_squared_error(y_val, y_pred)
# Root Mean Squared Error (RMSE)
RMSE = np.sqrt(MSE)
r2 = r2_score(y_val, y_pred)
print("MSE:", MSE, ", RMSE:", RMSE , ", R2:", r2)
```

```
[15.48743552  6.53793858 10.78318566 11.58555633 21.17320803
15.10974587  18.13802209  7.4522807  12.29402334 10.46455672]
MSE: 7.289025693003447 , RMSE: 2.699819566749498 , R2:
0.7703057423991149
```

77% of the variance in the target variable (Sales) is explained by the features in model.
77% fitting of the model on data points

Standardized independent values Unskewed target values

Linear Regression: Evaluate model

```
# prediction on validation data
# Model trained on standardized features and (box-cox) transformed target values
y_pred_scaled = model_scaled.predict(X_val_scaled)
```

```
MSE_scaled = mean_squared_error(y_val_scaled, y_pred_scaled)
RMSE_scaled = np.sqrt(MSE_scaled)
r2 = r2_score(y_val_scaled, y_pred_scaled)
```

```
MSE: 1.0787997132391625 , RMSE: 1.0386528357633085 ,
R2: 0.6630640925730389
```

- Model performance in terms of R2 seems worse than without scaling but predicted values for Sales (y_pred_scaled) and validation values for Sales (y_val_scaled) are box-cox transformed; not directly comparable with original values
- Revert to original scale using inverse box-cox and measure error

```
y_pred_unscaled = inv_boxcox(y_pred_scaled, lambda_bc)
```

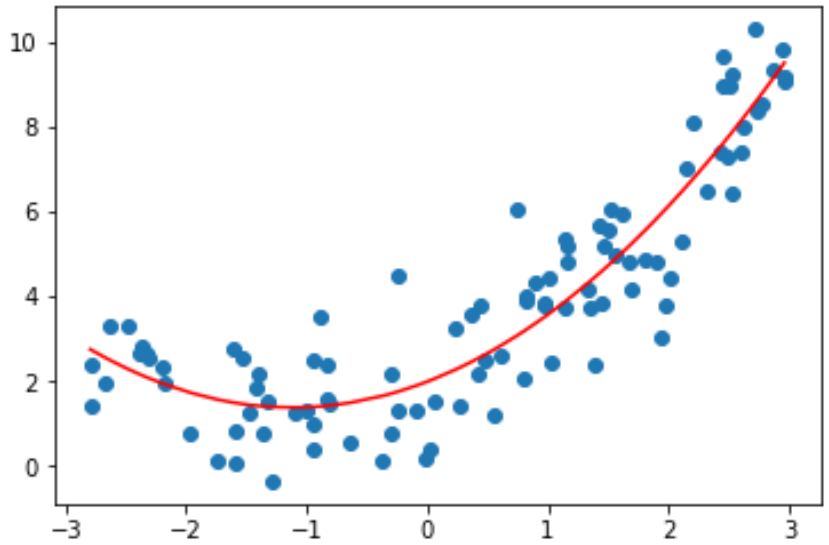
```
MSE_unscaled = mean_squared_error(y_val, y_pred_unscaled)
RMSE_unscaled = np.sqrt(MSE_unscaled)
r2 = r2_score(y_val, y_pred_unscaled)
```

```
MSE: 6.010514707137693 , RMSE: 2.451635108889105 ,
R2: 0.8105946155766224
```

- R2 score is higher than before we had a model trained on non-transformed data – better performance with scaling and unskewing

Polynomial (or non-linear) regression

- When non-linear relationship (curve) is observed between dependent and independent variables
- Polynomial Regression comes to the play which predicts the best fit that follows the pattern (curve) of the data, as shown in the pic below:



Polynomial regression

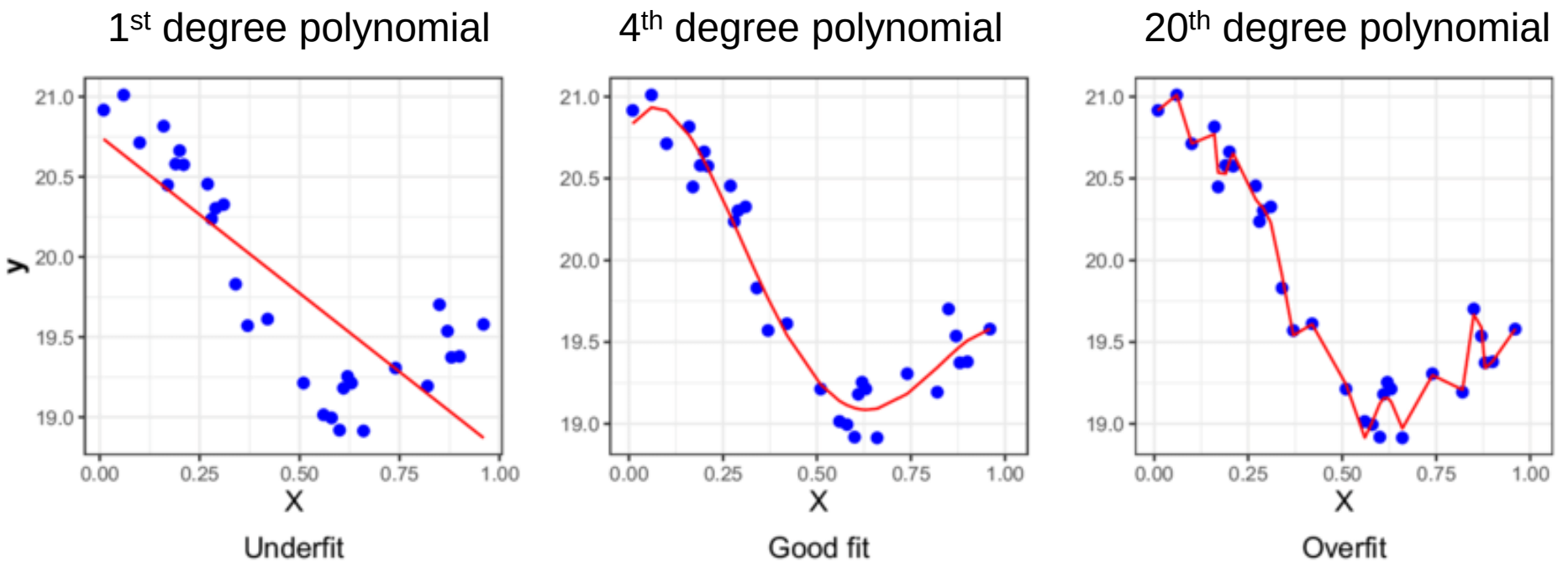
- Relationships between the independent variable(s) x and the dependent variable y are modelled as an n^{th} degree polynomial in x

- Example (for one independent variable X):
  - quadratic model (2^{nd} degree) : $y = \beta_0 + \beta_1 X + \beta_2 X^2 + \in$
  - cubic model (3^{rd} degree) : $y = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3 + \in$

- Predictive performance of the model generally tends to increase (i.e. prediction error is getting lower) as we increase the degree of the model, but …

Polynomial regression: of which degree?

- Increasing the degrees of the model also increases the risk of over-fitting the data (high accuracy on training data, not well generalization on unseen data)



Overfitting occurs when the model fits the “noise” in the data rather than the underlying trend.

- The degree of the polynomial to fit is a hyperparameter that cannot be inferred while fitting (training) model to the training set because it needs to be set in advance (before training)

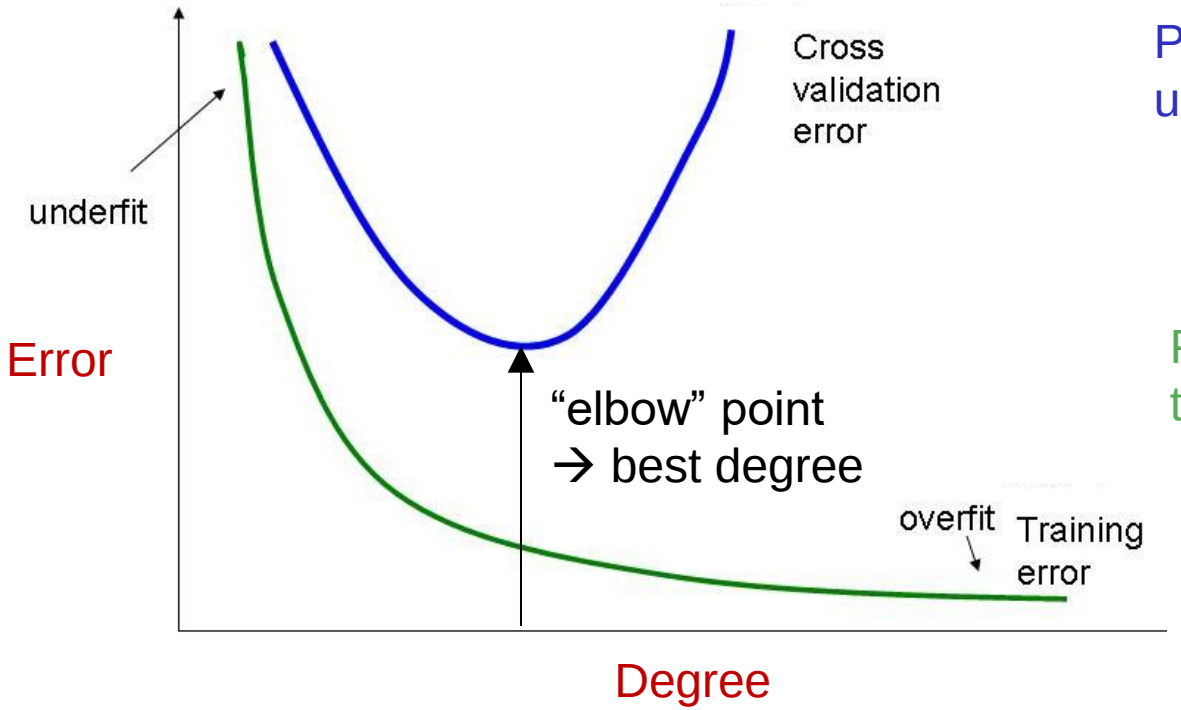
How to find the right degree of the equation?

- One approach to find the right degree while preventing over-fitting or under-fitting, is to start with a model of degree=1 and then gradually increase the model's degree until the performance (e.g. MSE, RMSE, R2) on unseen data stops getting better significantly → as increasing the degree beyond this point leads to overfitting
  - At each step:
    - **Train** the model using the ***training dataset***
    - **Predict** the target value using the ***validation dataset***
    - Evaluate model performance using any measure (e.g. MSE, RMSE, R2)

    It is strongly recommended to use Cross Validation (explained later)
  - At the end, when the best model is chosen, evaluate its **final performance** by predicting the target value using the **test dataset**.
- The whole process can be automated using GridSearchCV (see later)

How to find the right degree of the equation?

- One approach to find the right degree while preventing over-fitting or under-fitting, is to start with a model of degree=1 and then gradually increase the model's degree until the performance (e.g. MSE, RMSE, R2) on unseen data stops getting better significantly → as increasing the degree beyond this point leads to overfitting



Performance (error) on unseen data using CV

Performance (error) on training data

Training Polynomial regression model using Linear Regressor

- Let's say we have dataset of one input feature, and we need to build a polynomial regression model of 3rd degree (cubic model)
  - $y = \beta_0 + \beta_1 X + \beta_2 X^2 + \beta_3 X^3$
- Polynomial regression model can be trained using linear regressor (LR) since LR doesn't know that X^2 and X^3 are the square of X and the cube of X respectively, it just thinks they are another features
  - Prior running LR we expand the dataset, i.e. using the column X of the dataset, we create the extra columns X^2 and X^3
    - The unknown parameters to be estimated after training are β_0, β_1, β_2, β_3
- When having more than one features, interaction terms appear
  - 2nd degree polynomial model : $y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1^2 + \beta_4 X_1 X_2 + \beta_5 X_2^2$ (Interaction term)
    - You apply linear regression for five inputs: x_1, x_2, x_1^2, $x_1 x_2$, and x_2^2
    - Result of regression: the values of six parameters β_0, β_1, β_2, β_3, β_4, β_5

When is scaling/unskewing needed in PR?

- Feature scaling is often needed in polynomial regression, and it can significantly impact the stability of the model:
  - Scaling facilitates faster convergence when gradient descent algorithms (e.g. SGDRegressor) will be used
  - Scaling makes beta coefficients comparable: When features are scaled, the coefficients reflect the relative importance more accurately and the influence of each feature on target variable, making it easier to interpret the model
  - Scaling removes multicollinearity (high correlation among features)
    - While creating power terms (e.g. X_1^2 , X_1^3), if X_1 is not centered first i.e. to have zero mean (using StandardScaler or RobustScaler), the squared and cubic terms will be correlated with X_1 (see here)
    - While creating interaction terms (e.g. X_1X_2), if both X_1 and X_2 are not centered first, some amount of collinearity will be induced, i.e. X_1X_2 will be correlated with X_1 and X_2

  leading to stable coefficient estimates ➔ model insensitive to small changes in data

Polynomial Regression: Boston Housing Dataset

- Dataset: 506 houses by 13 features
- Objective: predict house prices

```
import numpy as np
import matplotlib.pyplot as plt

import pandas as pd
import seaborn as sns

boston = pd.read_csv('Boston.csv')
boston.head()
```

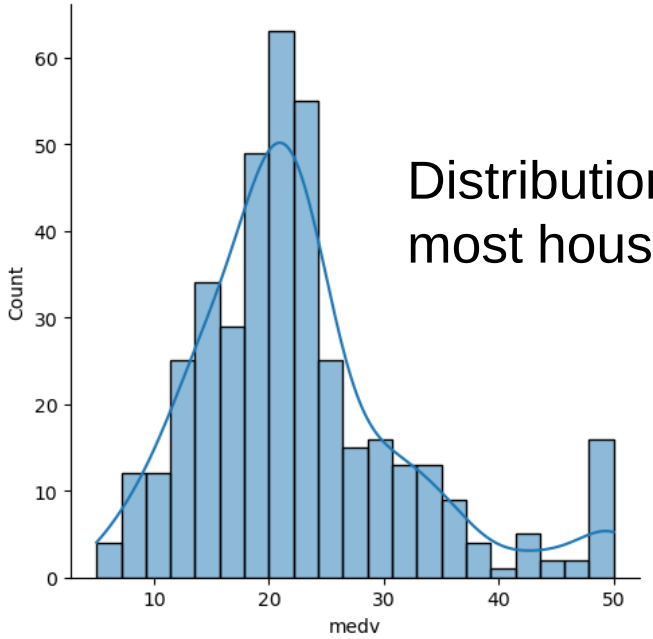
	crim	zn	indus	chas	nox	rm	age	dis	rad	tax	ptratio	black	lstat	medv
0	0.00632	18.0	2.31	0	0.538	6.575	65.2	4.0900	1	296	15.3	396.90	4.98	24.0
1	0.02731	0.0	7.07	0	0.469	6.421	78.9	4.9671	2	242	17.8	396.90	9.14	21.6
2	0.02729	0.0	7.07	0	0.469	7.185	61.1	4.9671	2	242	17.8	392.83	4.03	34.7
3	0.03237	0.0	2.18	0	0.458	6.998	45.8	6.0622	3	222	18.7	394.63	2.94	33.4
4	0.06905	0.0	2.18	0	0.458	7.147	54.2	6.0622	3	222	18.7	396.90	5.33	36.2

```
# extract features and target variables
X = boston.drop(columns=['medv'])
y = boston['medv']

# split to training, validation and test dataset (80% / 10% / 10%)
X_train, X_2, y_train, y_2 = train_test_split(X, y, random_state = 5, train_size = 0.8)
X_val, X_test, y_val, y_test = train_test_split(X_2, y_2, random_state = 5, train_size = 0.5)
```

Data transformation

- Feature scaling do not improve the predictive power of the model when using linear regressors; however useful when performing polynomial regression for the stability of the model
- Target variable transformations (such as Box Cox, Yeo-Johnson when skewness is apparent) can improve the model predictive power

```
# distribution of the target values
sns.displot(y_train, kde=True)
plt.show()

# statistical test
# p-value >= 0.05 means that the
distribution is a normal distribution
from scipy import stats
_, p = stats.normaltest(y_train)
print(p) # => 1.76 e-20
```



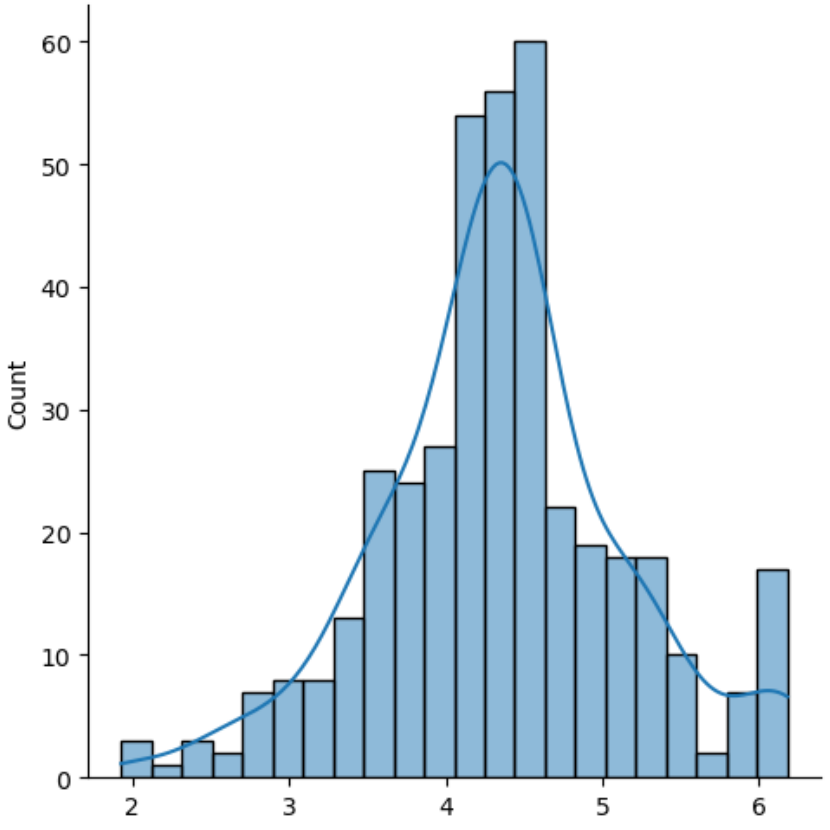
Distribution is skewed (not symmetrical): most houses have low prices

Data transformation

- Here, we use boxcox transformation

```
# y - transformation (box cox)
from scipy.stats import boxcox
y_train_bc, lambda_bc = boxcox(y_train)
_, p = stats.normaltest(y_train_bc)
print(p) # => 0.1369157180954557 7
sns.displot(y_train_bc, kde=True)
```

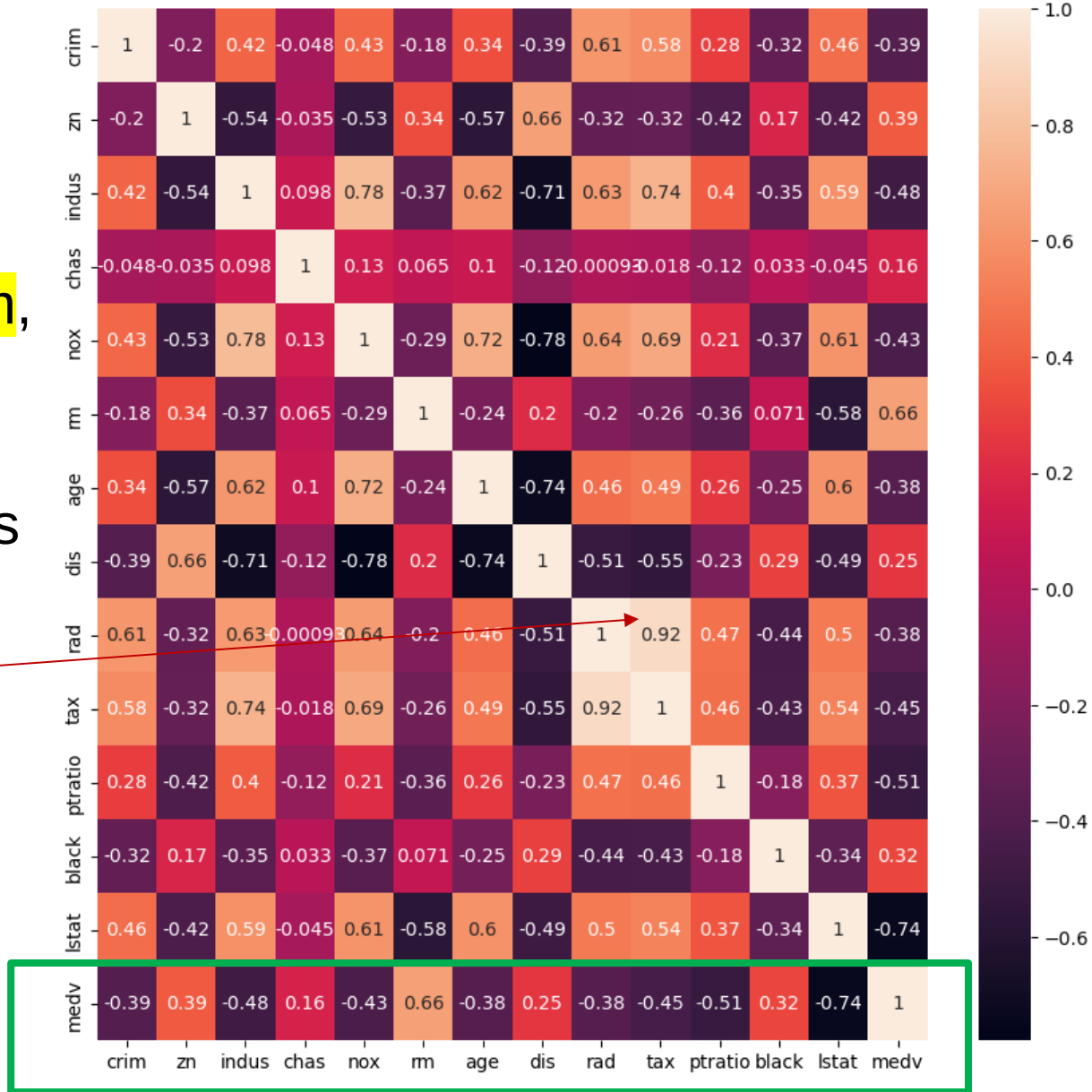
Transformed vector
Selected lambda (λ) value (λ value can be used in reverse Box Cox transf.)



- Distribution of the transformed target variable
  - This distribution already looks quite similar to a normal distribution and achieves a p-value of 0.13, which is larger than 0.05. Therefore, we can say that the distribution approaches a normal distribution

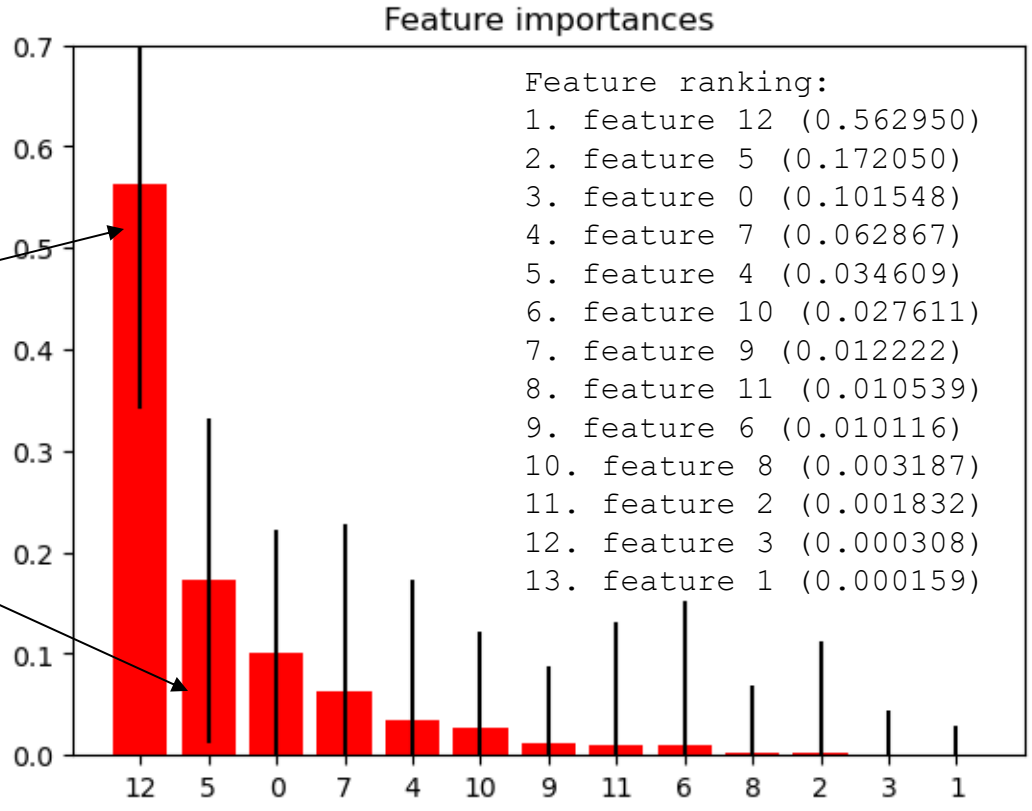
Feature Selection – Correlation matrix

- Create correlation matrix on the training dataset
- Observations:
  - As we can see, only the features rm, and lstat are highly correlated with the output variable medv_boxcox
  - Avoid using high correlated features together to avoid multi-collinearity
    - rad / tax are strongly correlated
    - dis / indus / age are strongly correlated



Feature Selection – Importance

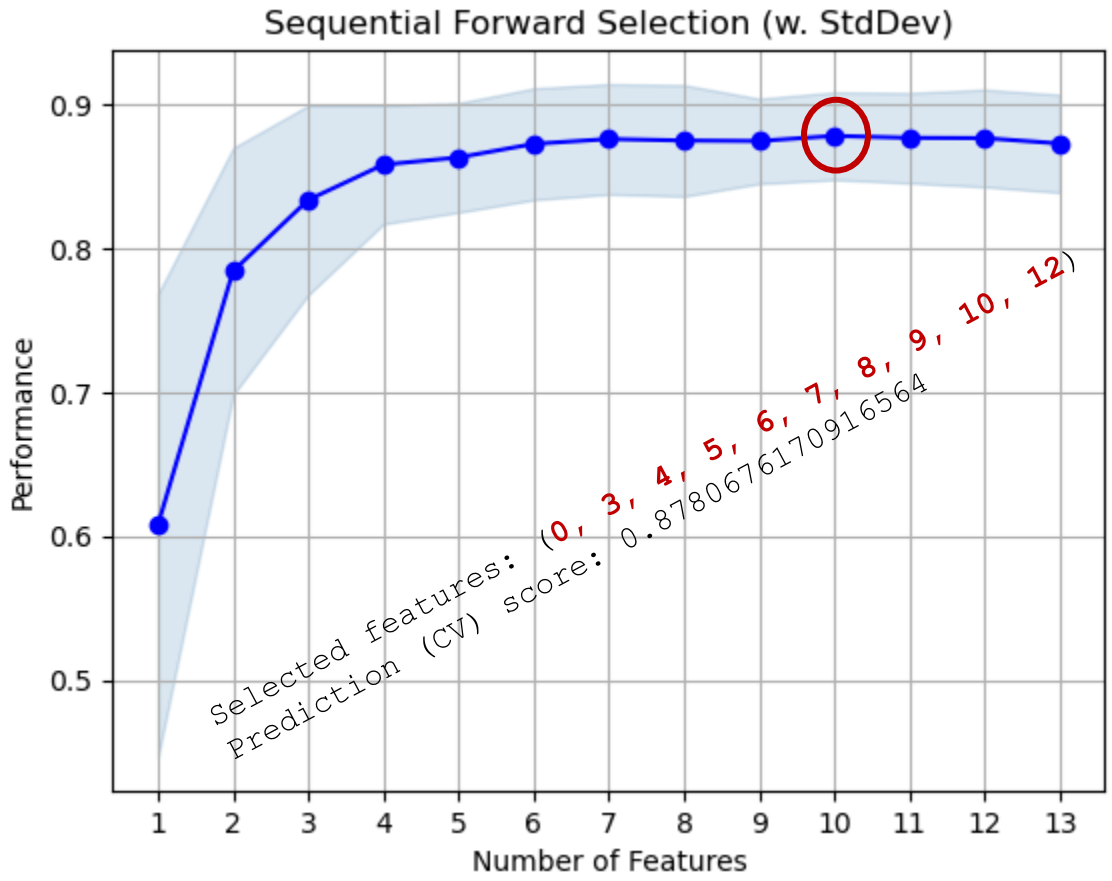
```
# Feature Importance using ExtraTreeClassifier
from sklearn.ensemble import GradientBoostingRegressor
# Build an estimator and compute the feature importances
estimator = GradientBoostingRegressor(n_estimators=100, random_state=0)

estimator.fit(X_train, y_train_bc)
# Lets get the feature importances.
# Features with high importance score higher.
importances = estimator.feature_importances_
```



As we can see, the features lstat, and rm achieve the highest importance among all features for predicting the transformed target variable

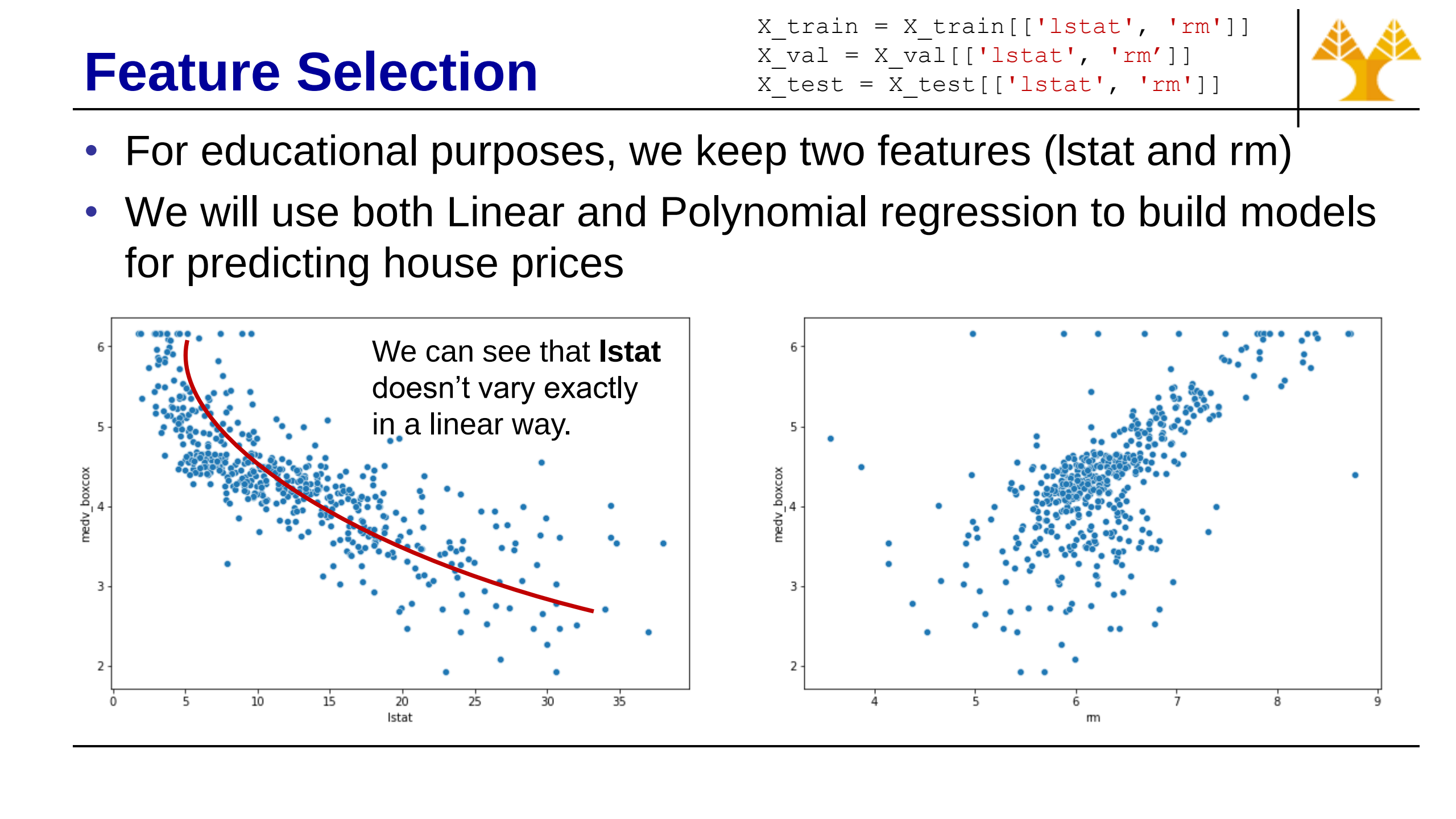
Feature Selection – Sequential Forward Selec

```
from mlxtend.feature_selection import SequentialFeatureSelector as SFS
from mlxtend.plotting import plot_sequential_feature_selection as plot_sfs

sfs = SFS(estimator,
          k_features=(2,13),
          forward=True,
          floating=False,
          scoring='r2',
          cv=10)

sfs = sfs.fit(X_train, y_train_bc)

plot_sfs(sfs.get_metric_dict(), kind='std_dev')

plt.title('Sequential Forward Selection')
plt.grid()
plt.show()
print('Selected features:',sfs.k_feature_idx_)
print('Prediction (CV) score:',sfs.k_score_)
```



Feature Selection

```
X_train = X_train[['lstat', 'rm']]
X_val = X_val[['lstat', 'rm']]
X_test = X_test[['lstat', 'rm']]
```



- For educational purposes, we keep two features (lstat and rm)
- We will use both Linear and Polynomial regression to build models for predicting house prices

Linear Regression on Boston dataset

- Results using the initial dataset without transformations (feature scaling, target unskewing)

```
Model performance on validation dataset
----------------------------------------
RMSE is 5.203457199881524
R2 score is 0.631266105649837
```

- Results (on original scale) using Box Cox transformation on target variable

```
Model performance on validation dataset
----------------------------------------
RMSE is 4.770472127125568
R2 score is 0.690078423754922 5
```

- Better performance is experienced when unskewing transformation is applied on the target variable

Linear Regression (playing with hyperparameters)

- No hyperparameters used thus far: `lr = LinearRegression()`
- If hyperparameters are to be used, they need to be set prior training
- Linear regression can set the `fit_intercept` hyperparameter
  - The intercept term (often labeled the constant β_0) is the expected value of Y when all X=0
  - Default value of fit_intercept hyperparameter is true, i.e. β_0 is part of the model
- Set `lr = LinearRegression(`**`fit_intercept=False`**`)` and follow the process (training, prediction on validation dataset, model evaluation) using the transformed target variable
  - Significant improvement of the model

```
Model performance on validation dataset (without intercept term)
--------------------------------------------------------------------
RMSE is 3.8402695055646077
R2 score is 0.7991589449167994
```

Polynomial Regression (degree = 2)

```
from sklearn.preprocessing import PolynomialFeatures

poly_features = PolynomialFeatures(degree=2)

# transform training set features to higher degree features
X_train_poly = poly_features.fit_transform(X_train)
print(X_train[0:5])
print(X_train_poly[0:5])


# fit the transformed features to Linear Regression
poly_model = LinearRegression()
# train the model
poly_model.fit(X_train_poly, y_train_bc)
```

convert the original features (X_train) into their higher order terms (X_train_poly) via the PolynomialFeatures class

```
      lstat     rm
33    18.35  5.701
283    3.16  7.923
418   20.62  5.957
502    9.08  6.120
402   20.31  6.404
```

	lstat	rm	lstat²	lstat * rm	rm²
[[1.	18.35	5.701	336.7225	104.61335	32.501401]
[1.	3.16	7.923	9.9856	25.03668	62.773929]
[1.	20.62	5.957	425.1844	122.83334	35.485849]
[1.	9.08	6.12	82.4464	55.5696	37.4544]
[1.	20.31	6.404	412.4961	130.06524	41.011216]]

Bias column: Feature in which all polynomial powers are zero. Acts as an intercept term in a linear model.

```
# transform validation set features to higher degree features
X_val_poly = poly_features.fit_transform(X_val)

# predicting on validation dataset
y_val_predict = poly_model.predict(X_val_poly)

# revert to original scale
y_val_predict_orig = inv_boxcox(y_val_predict, lambda_bc)
```

Polynomial Regression (degree = 2)

```
# evaluating the model on validation dataset
rmse_val_orig = np.sqrt(mean_squared_error(y_val, y_val_predict_orig))
r2_val_orig = r2_score(y_val, y_val_predict_orig)

print("Model performance on validation dataset (original scale")
print("----------------------------------------")
print("RMSE is {}".format(rmse_val_orig))
print("R2 score is {}".format(r2_val_orig))
```

```
The model performance for the validation set
----------------------------------------
RMSE of training set is 4.177886288872826
R2 score of training set is 0.7622928102676387
```

We can observe that the RMSE error is lower (thus better) when using polynomial regression as compared to linear regression with default hyperparameters but higher (thus worse) when compared to linear regression with `fit_intercept=False`. However, hyperparameter tuning needs to be performed to:

- **explore different polynomial degrees beyond 2**
- **keep interaction_only features (e.g. remove $lstat^2$ and rm^2), default is False**
- **try without include_bias, default is True**

Problem with dataset splitting

- Results shown thus far (in terms of RMSE, R2) depend on a particular choice (split) for testing and validation datasets to train and evaluate the model
  - Based on the model's performance on unknown/unseen (validation) data for a single split, we cannot determine if it is underfitting, overfitting, or "well-generalized"

- Solution: Repeat the process of randomly splitting data into subsets (training and validation) and average results from all iterations => **Cross Validation (CV)**

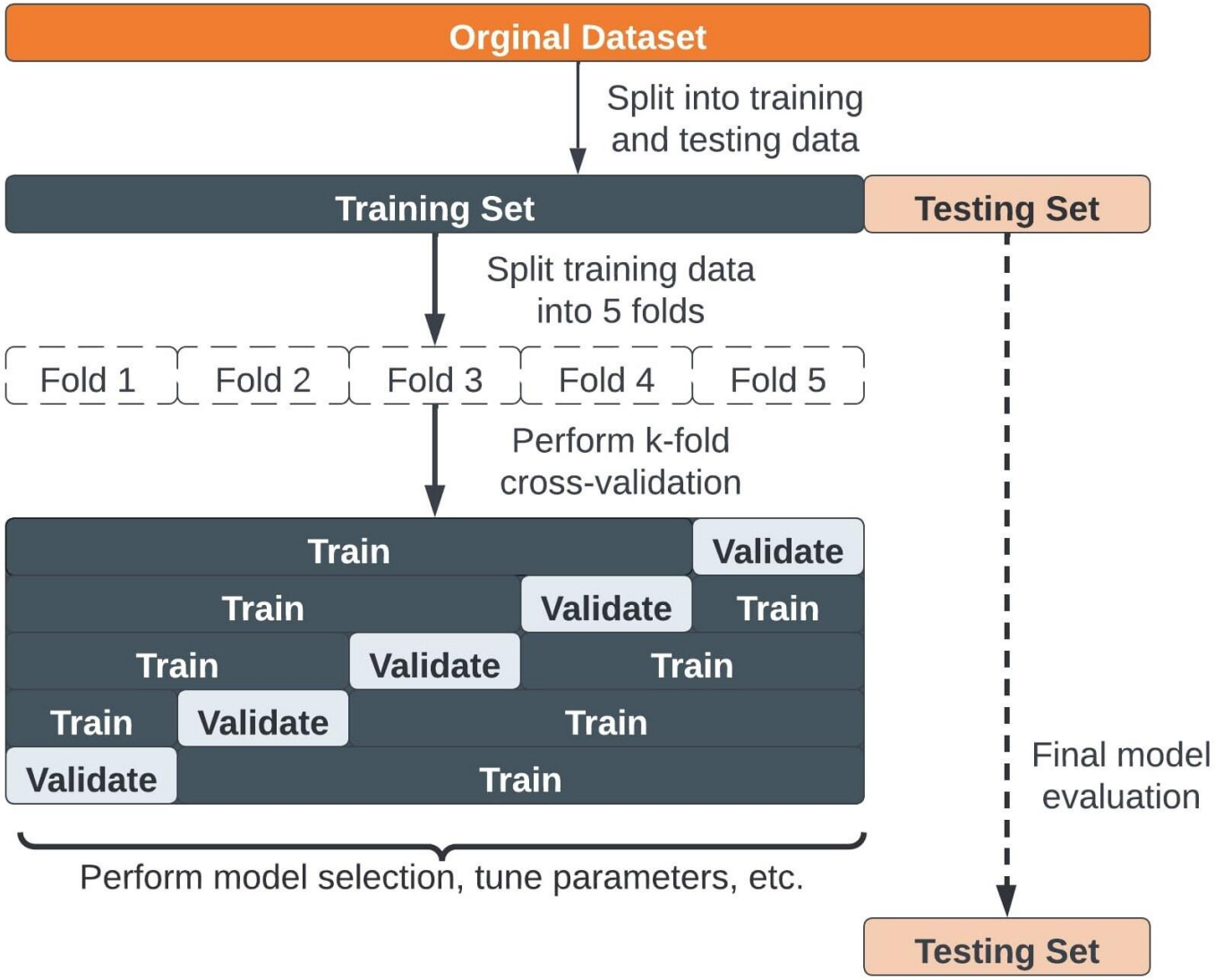
K-folds Cross Validation

- Prior running Cross-Validation, split initial dataset into train/test
- Split train dataset randomly into k subsets called folds
- Repeat:
  - Train model on k-1 folds
  - Use k^{th} fold as validation dataset to measure model performance
    - Measure score (e.g. RMSE, R2 for regression, accuracy, f1-score for classification)
- Until each of k folds has served as validation fold
- Combine (average) k recorded scores to estimate the error/accuracy of the model: cross-validation score

Cross validation

- Modify model hyperparameters and re-run cross validation to find the best hyperparameter values
- Test dataset is used for the unbiased final evaluation of the model with the best model parameters and hyperparameters

k-folds Cross Validation



GridSearchCV

- Cross validation (CV) process creates a series of train and validation splits to train and measure the predictive power of the model
- During training (within CV process), best values for **model parameters are determined**
- Model **hyper-parameters cannot be directly learnt from the training phase**; thus, they need to be set before the CV process
  - When modifying a hyper-parameter, full CV process needs to be repeated
  - When multiple hyper-parameters are involved in a model, finding the best combination of hyper-parameter values is a hard job
- Data encoding, transformation should be performed right after dataset splitting, within the CV process to avoid data leakage
- Best strategy to implement all these steps: **GridSearchCV**

Exhaustive param search: GridSearchCV

- **GridSearchCV**: Exhaustive search over a specified hyper parameter combination for an estimator (classifier / regressor)
- Grid of hyper-parameter values is specified with the param_grid list
  - For example, for Polynomial Features estimator with `degree`, `interaction_only` and `include_bias` hyperparameters:

```
param_grid = [
    { "degree": [1, 2, 3, 4], "interaction_only": [True, False] },
    { "degree": [1, 2, 3], "include_bias ": [True, False] }
]
```

  - specifies that two grids will be explored:
    - combination of degree values [1, 2, 3, 4] and interaction_only True/False,
    - combination of degree values [1, 2, 3, 4] and include_bias True/False
- Evaluates model for each combination using CV for a scoring metric

```
grid = GridSearchCV(estimator, param_grid, cv=10, scoring = 'r2', n_jobs=-1)
grid.fit(X_train, y_train)
```

n_jobs parameter is provided by many sklearn estimators (e.g. in RandomForest, GridsearchCV, etc.). It accepts number of cores to use for parallelization. If value of -1 is given then it uses all cores. Therefore, I would like to recommend to you to use **n_jobs=-1** where applicable to speed-up your computations.

Pipeline

- Recall that polynomial regression process involves 2 sequential steps:
  - Create polynomial features
  - Apply linear regression

  } 2-step estimator

- It is possible to create a pipeline combining these two steps (PolynomialFeatures and LinearRegression)

- The pipeline is used as estimator in GridSearchCV

Polynomial regression: Pipeline with GridSearchCV

```
from sklearn.pipeline import Pipeline
from sklearn.model_selection import GridSearchCV

# split dataset to train/test 80% / 20%
X_train, X_test, y_train, y_test = train_test_split(X, y, random_state = 5, train_size = 0.8)

# Define a pipeline involving PolynomialFeatures
# and LinearRegression steps
pf = PolynomialFeatures()
lr = LinearRegression()

# name each step
pipe = Pipeline(steps=[("poly", pf), ("linear", lr)])

# Parameters of pipelines can be set using '__' separated parameter names:
param_grid = [
    { "poly__degree": [1, 2, 3, 4, 5], "poly__interaction_only": [True, False], "poly__include_bias": [True, False] },
    { "poly__degree": [1, 2, 3, 4], "poly__interaction_only": [True, False], "poly__include_bias": [True, False], "linear__fit_intercept": [True, False] }
]

# make grid object for GridSearchCV and fit the dataset
search = GridSearchCV(pipe, param_grid, scoring = 'r2', cv=10, n_jobs=-1)
search.fit(X_train, y_train)
```

Two-step pipeline (create polynomial features + apply regression) is the estimator.
We name each step ("poly" and "linear") so as to refer to its hyper-parameters, e.g. linear__fit_intercept is the fit_intercept thyperparameter of the linear regressor

The sklearn scoring API always maximizes the score, so metrics which need to be minimized like RMSE are negated (`"neg_root_mean_squared_error"`)

Polynomial regression: Pipeline with GridSearchCV

```
# print results
print(" Results from Grid Search " )
print("\n The best score across ALL searched params:\n", search.best_score_)
print("\n The best parameters across ALL searched params:\n", search.best_params_)

# Evaluate on the test set
best_model = search.best_estimator_
y_pred = best_model.predict(X_test)

# root mean square error of the model
rmse = (np.sqrt(mean_squared_error(y_test, y_pred)))

# r-squared score of the model
r2 = r2_score(y_test, y_pred)

print("\nModel performance on validation dataset")
print("------------------------------------")
print('RMSE is {}'.format(rmse))
print('R2 score is {}'.format(r2))
```

```
 Results from Grid Search

 The best score across ALL searched params:
 0.8239040045809777

 The best parameters across ALL searched params:
 {'linear__fit_intercept': False, 'poly__degree': 2,
'poly__include_bias': True, 'poly__interaction_only': True}

Model performance on testing dataset
------------------------------------
RMSE is 3.220157338361434
R2 score is 0.8675577863835
```

Best performance achieved with Polynomial regression thus far

Pipelines

- A pipeline accepts a list of estimators not only predictors but also data imputers, encoders, transformers to be applied prior training a predictor

```
im = SimpleImputer(strategy="mean")      # fill missing values
sc = StandardScaler()                    # scale features
preprocessing_pipeline = Pipeline([("imputer", im), ("scaler", sc)])
```

```
pf = PolynomialFeatures()                # create polynomial features
lr = LinearRegression()                  # linear regressor
training_pipeline = Pipeline([("poly", pf), ("linear", lr)])
```

```
# Pipelines can be attached to one another!
full_pipeline = Pipeline([("preprocessing", preprocessing_pipeline),
("training", training_pipeline)])
```

```
param_grid = [
    { "training__poly__degree": [1, 2, 3, 4, 5], "training__poly__interaction_only": [True, False],
"training__poly__include_bias": [True, False] },
    { "training__poly__degree": [1, 2, 3, 4], "training__poly__interaction_only": [True, False], "training__poly__include_bias":
[True, False], "training__linear__fit_intercept": [True, False] }
]
```

Pipelines with ColumnTransformer

- By default, transformations are applied to all columns of the dataset
- We can apply different transformations per column using `ColumnTransformer`. Example for applying different imputation strategy:
  - For int-based features (e.g. `chas` & `rad`) we will apply most_frequent imputation strategy
  - For `rm` and `age` we will apply mean imputation strategy followed by standard scaling
  - For the remainder features do nothing

```
from sklearn.compose import ColumnTransformer
from sklearn.preprocessing import StandardScaler
from sklearn.impute import SimpleImputer
pipeline1 = Pipeline([('freq_imputer', SimpleImputer(strategy='most_frequent'))])
pipeline2 = Pipeline([('mean_imputer', SimpleImputer(strategy='mean')), ('scaler',
StandardScaler())])
preprocessing_pipeline = ColumnTransformer(transformers = [
    ('pipeline1', pipeline1, ['chas', 'rad']),
    ('pipeline2', pipeline2, ['rm', 'age']),
    # set remainder to passthrough to pass along all
    # the un-specified columns untouched to the next steps
], remainder='passthrough')
```

Pipelines with TranformedTargetRegressor

- Imputers, encoders and transformations are applied on input features
- Transformations (e.g. boxcox) on target variable can be applied using `TranformedTargetRegressor`

Pipeline **without** target transformation

```
training_pipeline = Pipeline([
    ("poly", PolynomialFeatures()),
    ("linear", LinearRegression())
])
```

Pipeline **with** target transformation

```
training_pipeline = Pipeline([
    ('poly', PolynomialFeatures()),
    ('linear', TransformedTargetRegressor(
        regressor=LinearRegression(),
        transformer=PowerTransformer(method='yeo-johnson')
    ))
])
```

- TransformedTargetRegressor is a meta-estimator that performs regression on a transformed target variable
- **Regressor** and **Transformer** are given as input
- PowerTransformer can be used to apply either boxcox or yeo-johnson transformations.

`'yeo-johnson'` → works with positive and negative values

`'boxcox'` → works with strictly positive values

Pipelines with TranformedTargetRegressor

- `TranformedTargetRegressor` with log transformation

Pipeline **without** target transformation

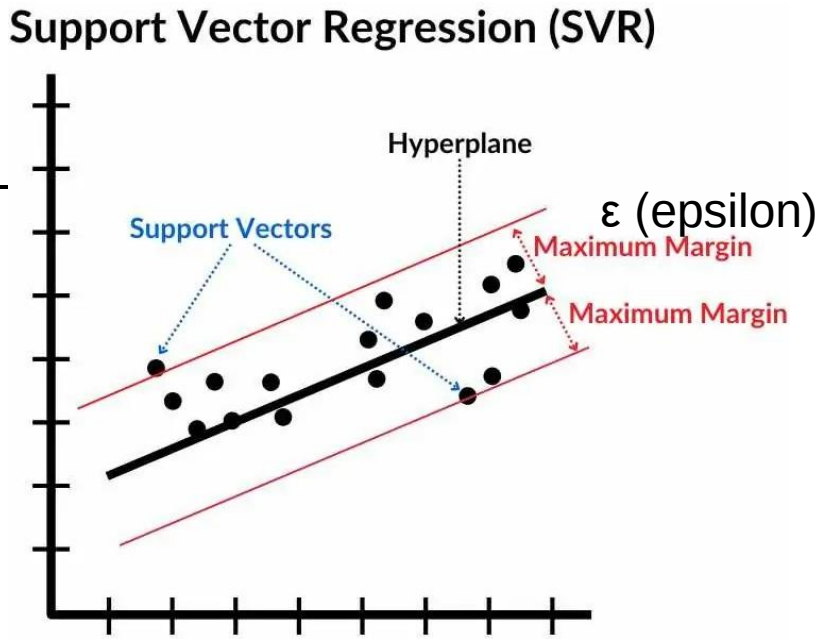
```
training_pipeline = Pipeline([
    ("poly", PolynomialFeatures()),
    ("linear", LinearRegression())
])
```

Pipeline **with** target transformation

```
training_pipeline = Pipeline([
    ('poly', PolynomialFeatures()),
    ('linear', TransformedTargetRegressor(
        regressor=LinearRegression(),
        func=np.log, inverse_func=np.exp
    ))
])
```

We can apply a transformer by setting the **func** parameter (transformation function) and **inverse_func** (reverse transformation function) instead of using the transformer parameter (see previous slide)

Support Vector Regression (SVR)



- Basic idea of support vector regression
  - Find optimal hyperplane that approximates the relationship between input features (X) and the target variable (y).
- **Hyperplane**: In the context of SVR, the hyperplane is a function (a line in 2D, or a plane in higher dimensions) that predicts the continuous output for a given set of input features
- **Epsilon (ε) Margin**: SVR introduces a margin of tolerance (ε) around the hyperplane.
  - Data points within this margin are considered "correctly predicted“ (no penalty is given to errors)
  - Data points that fall outside the margin or are on its boundary (called **support vectors**) contribute to the error term, and the goal is to minimize these errors

Support Vector Regression

- The objective of SVR is to minimize the following two key things:
  - **Prediction Error**: For points outside the epsilon margin, the error is proportional to how far the points deviate from the margin. The goal is to **minimize this error for points outside the margin**.
  - **Model Complexity**: SVR also tries to minimize the norm of the weights (w), which controls the flatness of the hyperplane. A **flatter hyperplane** is preferable because it helps generalize better (low error on unseen data).

Support Vector Regression hyperparameters

- Epsilon: defines a margin of tolerance around the hyperplane
  - Low epsilon → overfitting, High epsilon → underfitting | default value: 0.1
- C is a penalty parameter that controls the trade-off between the complexity of the model (flatness of the hyperplane) and the amount of allowed deviations (points falling outside the epsilon margin)
  - Low C → underfitting, High C → overfitting | default value: 1.0
- Kernel: a mathematical function that transforms data into a higher dimensional space (generally used for finding a better hyperplane)
  - The most widely used kernels include linear, polynomial (poly), radial basis function (rbf) and sigmoid | default value: RBF
- More details can be found in Appendix

Choosing the right values for hyperparams

- Epsilon:
  - Start Small: A smaller ϵ (e.g., 0.01) allows for a more sensitive model, capturing more details of the training data
  - Grid Search: Use a grid search to test different values for ϵ. Common ranges are between 0 and 1, depending on the scale of your data
- C:
  - Start with Defaults: Common default values are 1 or 10.
  - Logarithmic Scale in Grid Search: Use a logarithmic scale (e.g., 0.1, 1, 10, 100) to cover a wide range of values effectively
- Kernel:
  - Data Distribution: Start with a linear kernel if you suspect a linear relationship. For more complex relationships, consider the RBF kernel.
  - Experimentation in Grid Search: Try different kernels and see how they perform on your data
    - Hyperparameter Tuning: Each kernel may have specific hyperparameters (like σ for the RBF kernel, or degree for polynomial kernel) that also need tuning.

Scaling in Support Vector Regression (SVR)

- Support Vector Regressor is a distance-based regression algorithms that uses (Euclidean or Manhattan) distances between data points ➔ feature scaling is needed so that all the features contribute equally to the distance otherwise distance may be dominated by features with larger scales
  - E.g. $Distance(X_1, X_2) = \sqrt{(3-1027)^2 + (4-2123)^2}$ distance is dominated by X_2 values

SVR with GridSearchCV

- Exhaustive search over specified parameter values for an estimator

```
from sklearn.model_selection import GridSearchCV
# Define a pipeline involving Robust Scaler and SVR
pipe_svr = Pipeline(steps=[
        ("scaler", RobustScaler()),
        ("svr", TransformedTargetRegressor(regressor=SVR(),
         transformer=PowerTransformer(method='yeo-johnson')))
])
# parameter grid
parameter_grid = [
 {'svr__regressor__C': [1, 10, 100, 1000], 'svr__regressor__ kernel': ['linear']},
 {'svr__ regressor__ C': [1, 10, 100, 1000], 'svr__regressor__gamma': [0.001, 0.0001], 'svr__regressor__kernel': ['rbf']},
 {'svr__ regressor__C': [1, 10, 100, 1000], 'svr__regressor__degree': [1, 2, 3, 4, 5, 6], 'svr__regressor__ kernel':
['poly']}]

# make grid_SVC object for GridSearchCV and fit the dataset
grid_SVR = GridSearchCV(pipe_svr, parameter_grid, scoring = 'neg_root_mean_squared_error', n_jobs=-1)
grid_SVR.fit(X_train, y_train)

# print results
print(" Results from Grid Search " )
print("\n The best estimator across ALL searched params:\n", grid_SVR.best_estimator_)
print("\n The best score across ALL searched params:\n", -grid_SVR.best_score_)
print("\n The best parameters across ALL searched params:\n", grid_SVR.best_params_)
```

```
The best estimator across ALL searched params:
 Pipeline(steps=[('scaler', RobustScaler()), ('svr',
SVR(C=1000, gamma=0.001))])

 The best score across ALL searched params:
 0.7649632977483316

Model performance on validation dataset
--------------------------------------
RMSE is 2.9887655163221054
R2 score is 0.8859078053060818
```

SVR model does not outperform the polynomial model. It achieves slightly lower R2 score.

Ensemble learning

- Ensemble learning: train multiple ML algorithms (learners) and combine their predictions in some way
- Ensemble model is a model that consists of many base (weak) models which tends to make more accurate predictions than individual (weak) base models
- We have three kinds of ensemble methods using:
  - Sequential Homogeneous Learners (Boosting), e.g. AdaBoostRegressor, GradientBoostingRegressor, LightGBM (installation) XGBoost (installation), CatBoost (installation)
  - Parallel Homogeneous Learners (Bagging), e.g. BaggingRegressor, RandomForestRegressor
  - Parallel Heterogeneous Learners (Stacking), e.g. StackingRegressor

For more info please see the Appendix

Is scaling/unskewing needed?

- Ensemble methods (Random Forest, XGBoost, AdaBoost) do not require feature scaling to be performed as they are not sensitive to the variance in the data
- A skewed dependent (target) variable is not necessarily a problem for ensemble methods per se – there are no assumptions as for example the normality of residuals (errors) that need to be met like in the linear model

RandomForestRegressor with GridSearchCV

Warning: This may run several minutes!!

```
from sklearn.ensemble import RandomForestRegressor
# Number of trees in random forest
n_estimators = [int(x) for x in np.linspace(start = 200, stop = 1000, num = 10)]
# Maximum number of levels in tree
max_depth = [int(x) for x in np.linspace(10, 110, num = 11)]
max_depth.append(None)
# Minimum number of samples required to split a node
min_samples_split = [2, 5, 10]
# Minimum number of samples required at each leaf node
min_samples_leaf = [1, 2, 4]
# Method of selecting samples for training each tree
bootstrap = [True, False]

# Create the random grid
parameter_grid = {'rf__regressor__n_estimators': n_estimators,
                  'rf__regressor__max_features': max_features,
                  'rf__regressor__max_depth': max_depth,
                  'rf__regressor__min_samples_split': min_samples_split,
                  'rf__regressor__min_samples_leaf': min_samples_leaf,
                  'rf__regressor__bootstrap': bootstrap}
pipe = Pipeline([("rf", TransformedTargetRegressor(regressor=RandomForestRegressor(),
transformer=PowerTransformer(method='yeo-johnson')))])

# make grid_RF object for GridSearchCV and fit the dataset
grid_RF = GridSearchCV(pipe, parameter_grid, scoring = 'r2', n_jobs=-1)
grid_RF.fit(X_train, y_train)
# print results
print(" Results from Grid Search " )
print("\n The best estimator across ALL searched params:\n", grid_RF.best_estimator_)
print("\n The best score across ALL searched params:\n", grid_RF.best_score_)
print("\n The best parameters across ALL searched params:\n", grid_SVR.best_params_)
```

```
The best parameters across ALL searched params:
 {'rf__regressor__bootstrap': False,
'rf__regressor__max_depth': 60,
'rf__regressor__max_features': 'sqrt',
'rf__regressor__min_samples_leaf': 1,
'rf__regressor__min_samples_split': 2,
'rf__regressor__n_estimators': 377}

Model performance on testing dataset
------------------------------------
RMSE is 2.8937476393967922
R2 score is 0.8930468561703625
```

Slightly better results than SVR model but slightly worse than the polynomial model.

Tuning hyperparameters

- It is crucial to systematically study each model's hyperparameters and carefully select a range of values for each one.
- This helps ensure that you avoid excessive training times during the grid search process while still capturing the model's performance characteristics. Here's a step-by-step approach:
  1. Understand the Hyperparameters: Familiarize yourself with the hyperparameters of the specific ensemble models you are using (e.g., Random Forest, Gradient Boosting, etc.). Research their effects on model performance and interpretability.
  2. Identify Important Hyperparameters: Focus on the hyperparameters that most significantly impact model performance. For example:
     - For Random Forest: Number of trees (n_estimators), maximum depth of trees (max_depth), minimum samples per leaf (min_samples_leaf).
     - For Gradient Boosting: Learning rate (learning_rate), number of boosting stages (n_estimators), and maximum depth of individual trees (max_depth).

Tuning hyperparameters

3. Define Value Ranges: Based on your understanding of the model and the dataset, choose reasonable ranges for the hyperparameters. Start with broader ranges to explore their influence, then narrow them down as you gain insights after performing GridSearch. For instance:
   - n_estimators: 50, 100, 150, 200
   - max_depth: 3, 5, 7, 10
   - min_samples_leaf: 1, 2, 5
4. Utilize Logarithmic Scaling: For parameters that can vary widely, such as the learning rate in Gradient Boosting, consider using a logarithmic scale to cover a broader range more effectively. For example, you might test values like 0.01, 0.1, 1, and 10.
5. Start with Coarse Search: Begin with a coarser grid to get an overview of how the hyperparameters interact. This will help you identify promising regions in the hyperparameter space without extensive computation.
6. Implement Grid Search CV

Tuning hyperparameters

7. Analyze Results: After the grid search, review the results to identify the best-performing hyperparameter combinations. Use validation metrics to evaluate how well the model generalizes to unseen data.
8. Refine and Iterate: If needed, refine the hyperparameter ranges based on the results of the initial grid search. You can perform a second round of tuning with more focused ranges around the best parameters identified.

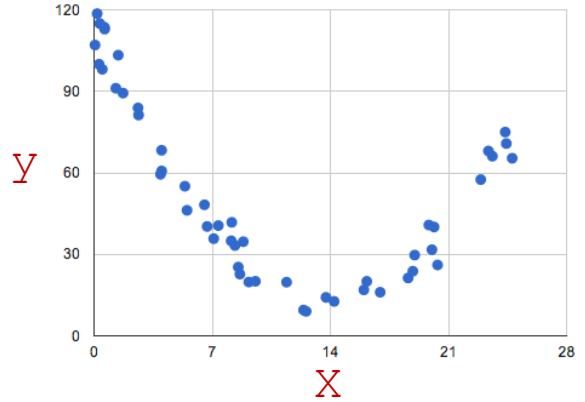
Appendix

University of Cyprus
Department of
Computer Science

Predictive modeling techniques

1. Learning/training phase:
   - Train data used to train a predictive modelling technique & create a model
     - model represents what was learned by a machine learning algorithm
   - Example:
     - Dataset: given input variable X we want to evaluate the output y

X	y
0.10	1.51
0.15	0.92
0.17	1.96
0.22	0.53
0.27	0.38



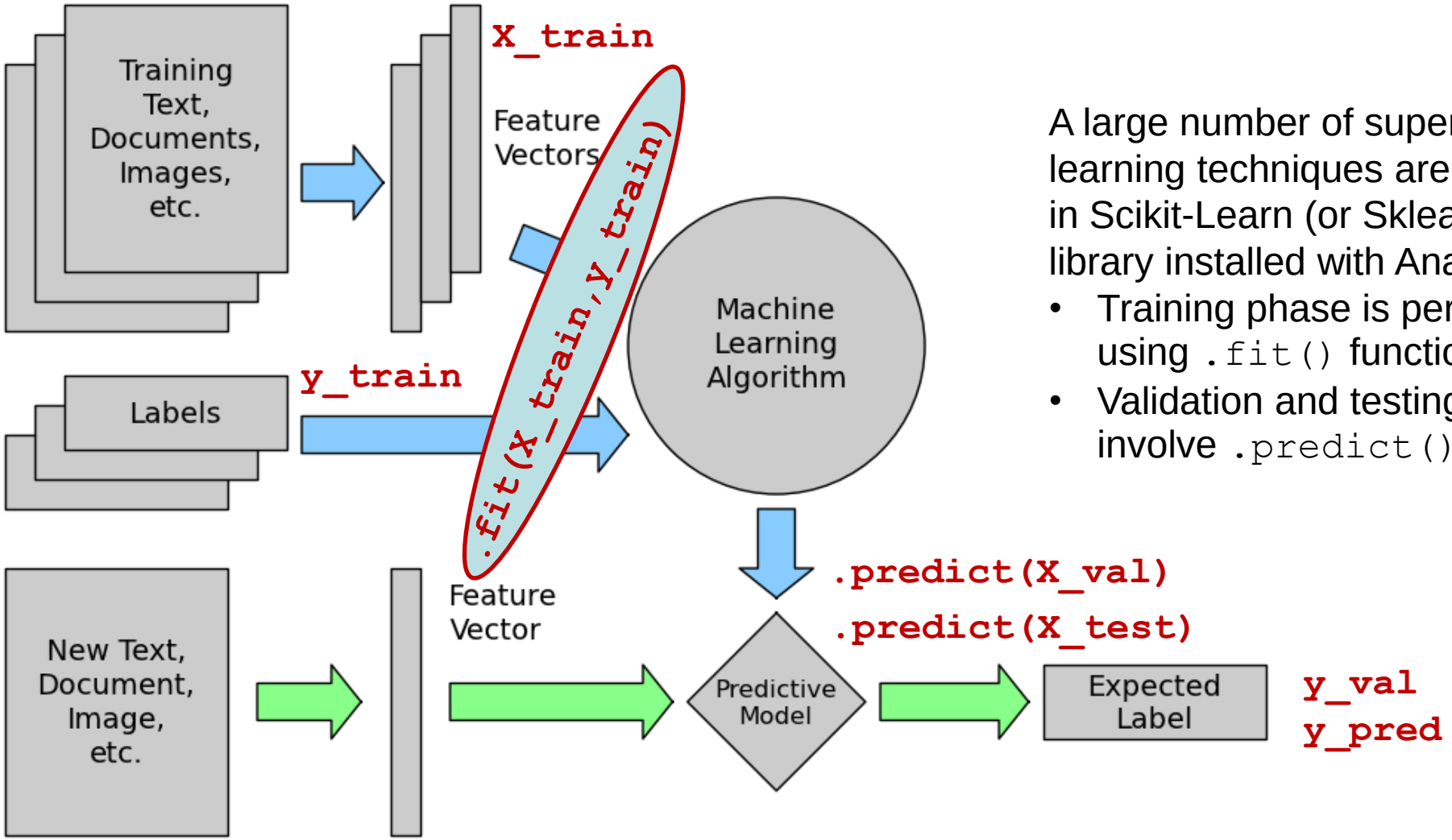
     - Predictive modelling technique to train: use a Polynomial equation and try to fit data (find the "best curve" that passes between points): $y = \beta_0 + \beta_1 X + \beta_2 X^2$
       - » Equation parameters: β_0, β_1, β_2 will be estimated during training
       - » Equation hyperparameter: degree of the polynomial function (configured prior training)
     - The outcome of training phase can be the model e.g.: $y = 0.45 + 0.7X + 1.2X^2$

Predictive modeling techniques

2. Validation phase
   - Validation data used to make predictions and measure the performance (e.g. error between real and predicted target values) of the model and to tune hyperparameters
   - Example:
     – After measuring the performance of the quadratic (2^{nd} degree) model, change the degree of the polynomial equation e.g. to 3, re-run on training (phase) data to create a new cubic (3^{rd} degree) model and measure the performance of the new model on validation data – repeat by changing the degree until the best model (with best performance, e.g. lower error) is achieved
3. Testing phase
   - Estimate the performance of the final model (with "best" parameters and hyperparameters) using test data (not seen during training and validation phases)
   - This is the final performance of the model

– Application phase:
   - Apply the final model e.g.: $y = 0.65 + 0.13X + 1.9X^2 + 0.77X^3$ to real-world input data (a new value of X not in the initial dataset) and predict output y

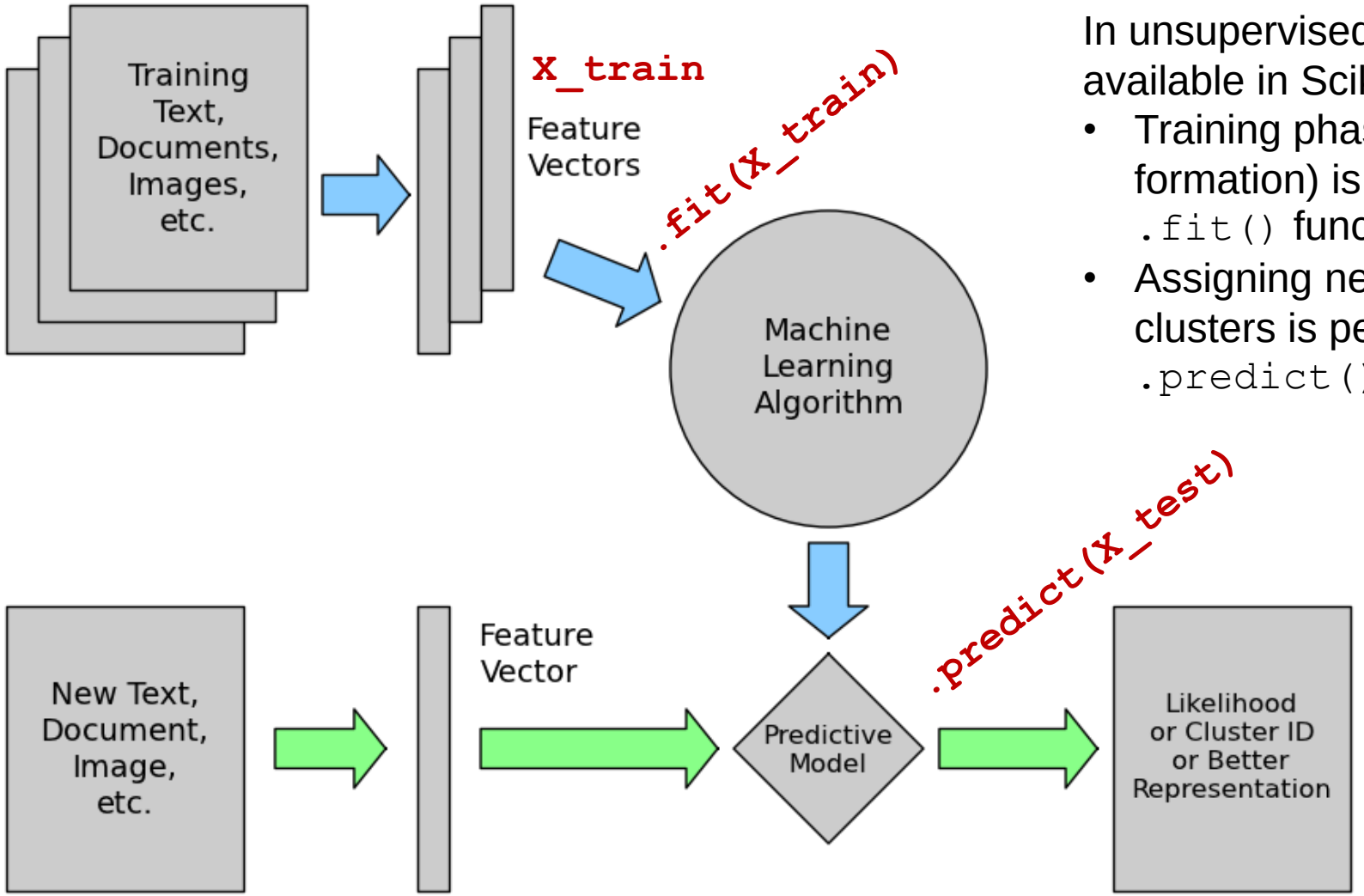
Predictive techniques: Supervised learning



A large number of supervised learning techniques are available in Scikit-Learn (or Sklearn) library installed with Anaconda

- Training phase is performed using `.fit()` function
- Validation and testing phase involve `.predict()` function

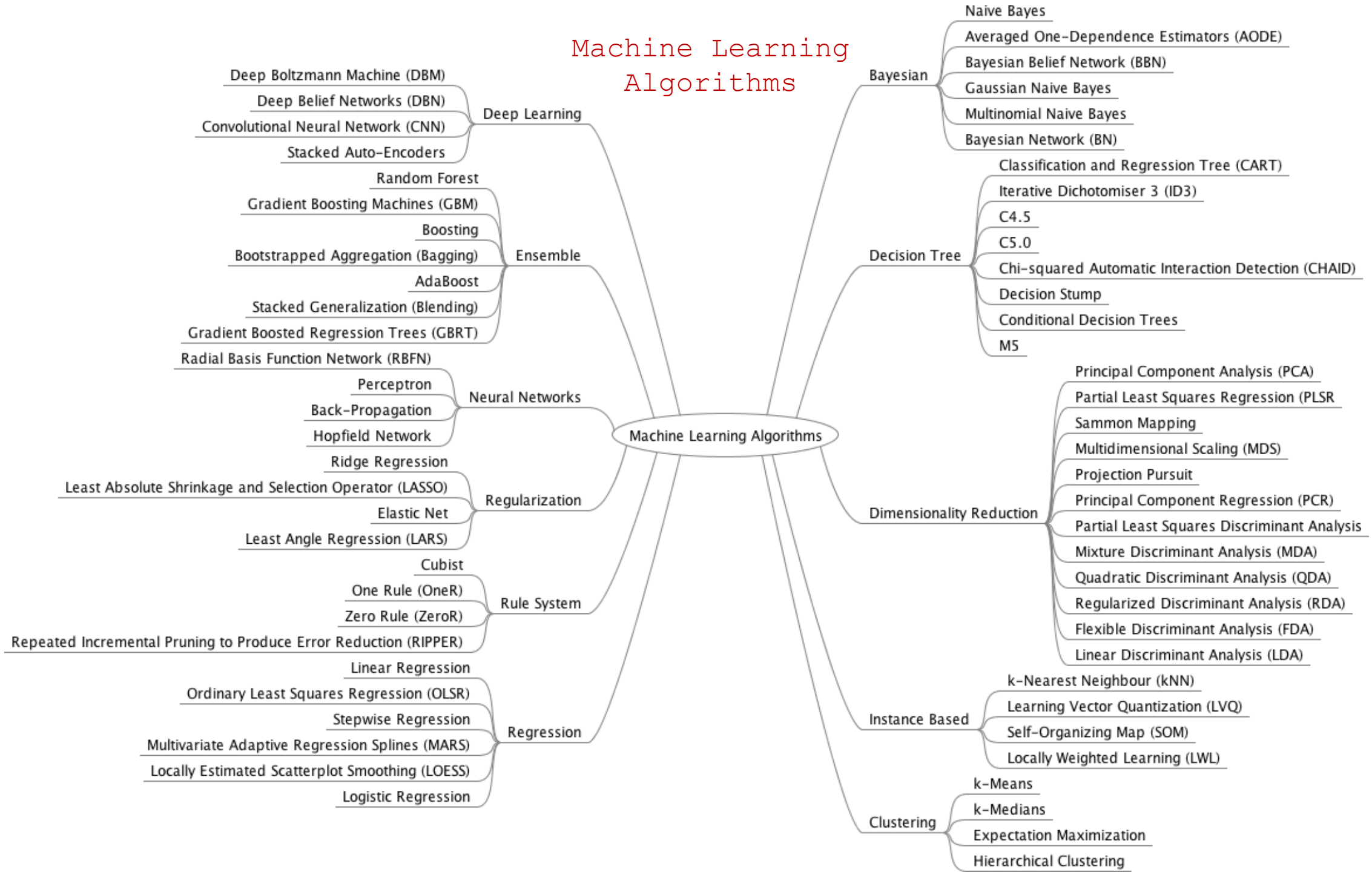
Predictive techniques: Unsupervised learning



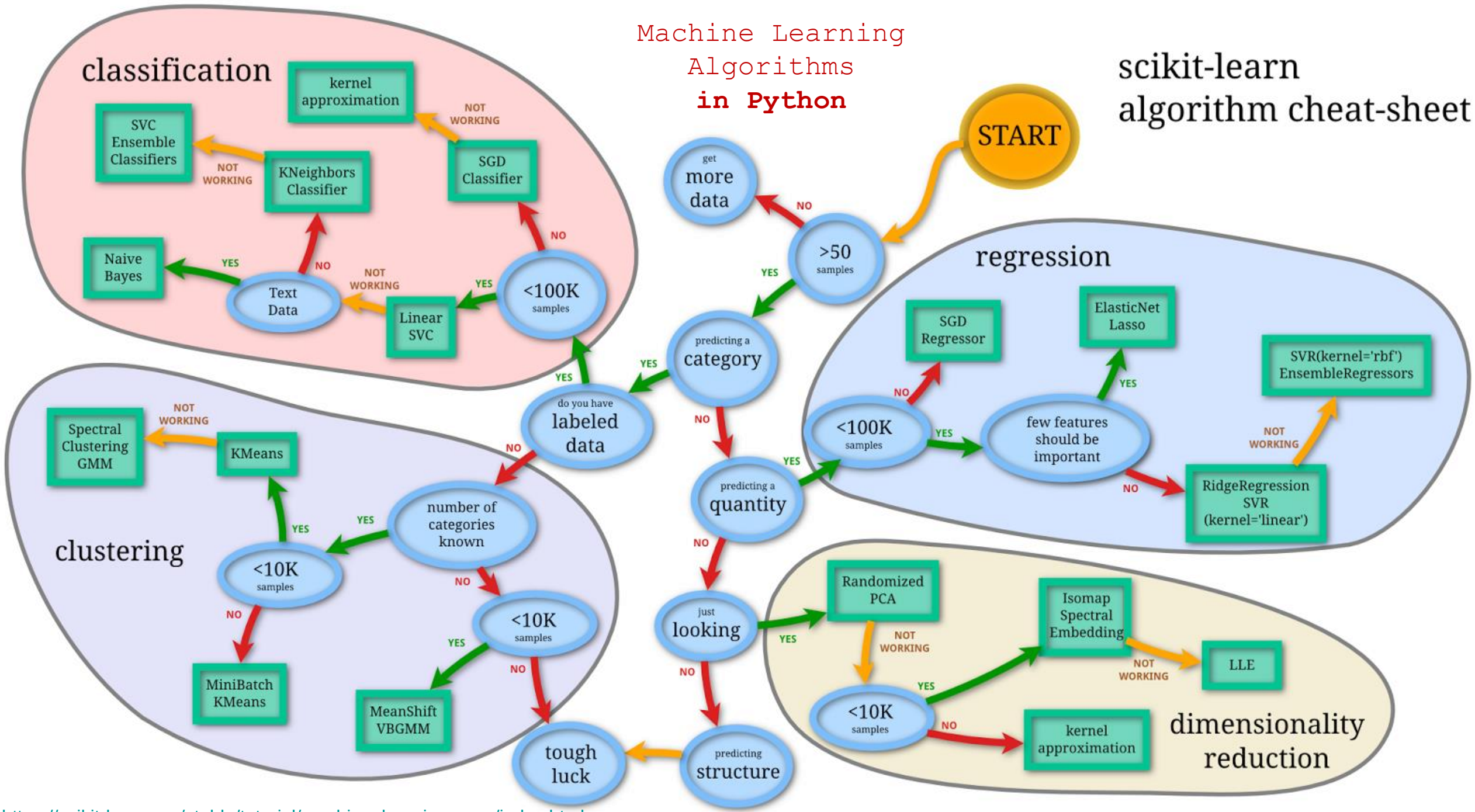
In unsupervised learning techniques available in Scikit-Learn (or Sklearn)

- Training phase (e.g. cluster formation) is performed using `.fit()` function
- Assigning new data into existing clusters is performed by `.predict()` function

Machine Learning Algorithms



Machine Learning Algorithms in Python



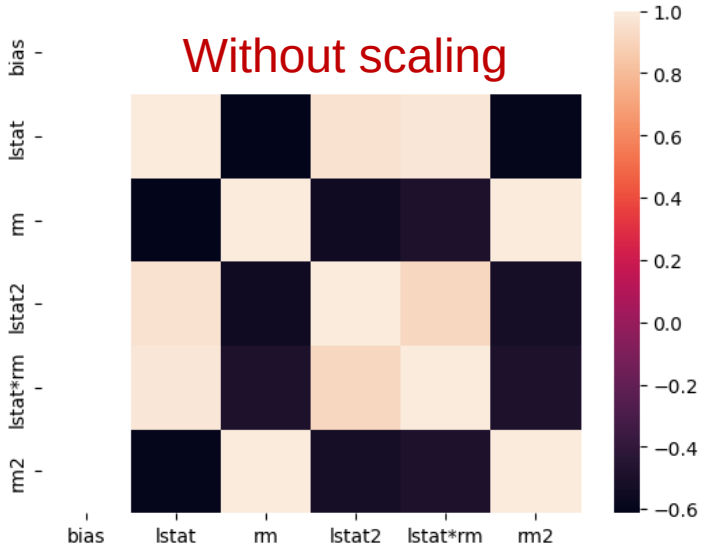
https://scikit-learn.org/stable/tutorial/machine_learning_map/index.html

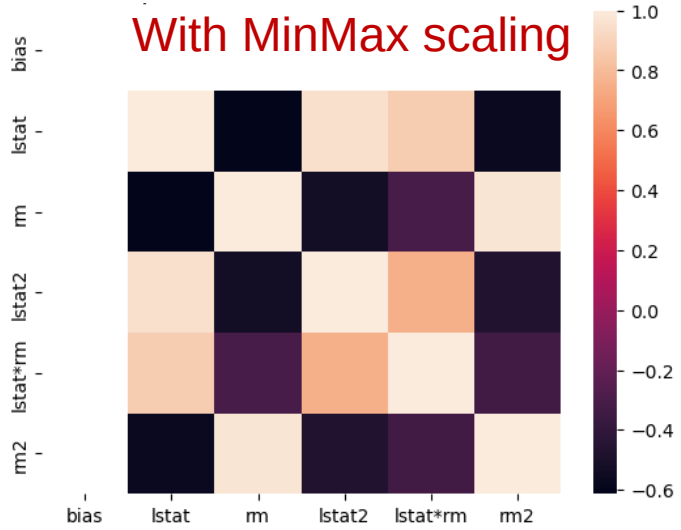
Evaluation metrics discussion

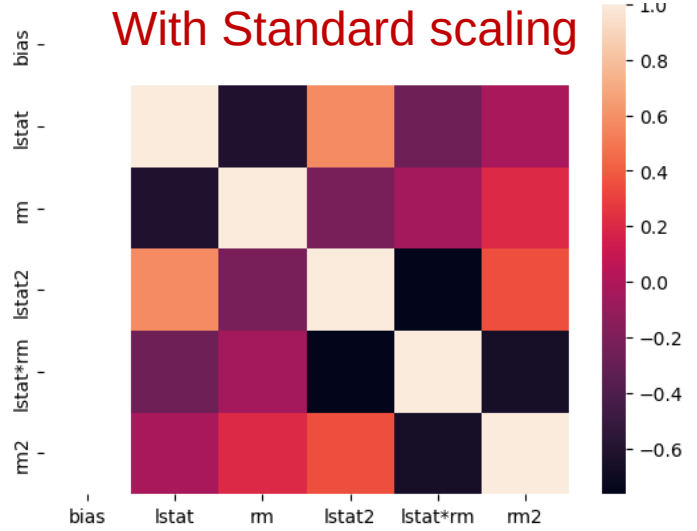
- The idea behind the squared (MSE) and the absolute error (MAE) is to avoid mutual cancellation of the positive and negative errors
  - MSE and MAE have only non-negative values
- In MSE, error is squared => prediction error is being heavily penalized
  - In case of data outliers, MSE will become much larger compared to MAE
  - Based on the application, this property may be considered positive or negative:
    - For example, emphasizing large errors may be a desirable discriminating measure when evaluating models
- MAE preserves the same units of measurement
- In MSE, the unit of measurement is squared
- **RMSE** is used then to return the MSE error to the original unit by taking the square root of it, while maintaining the property of penalizing higher errors

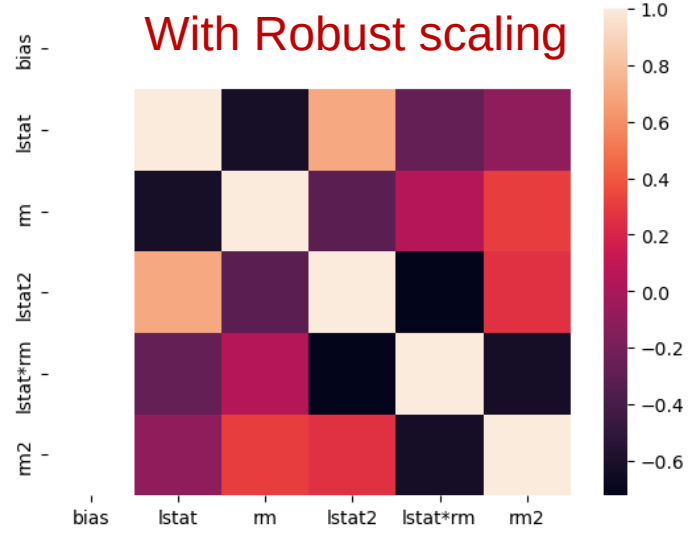
Scaling vs correlation

- Correlation among original features, power and interaction terms









- There is minimal correlation when centering-based scalers (Standard, Robust) are applied
- Source code is found here

Support Vector Regression hyperparameters

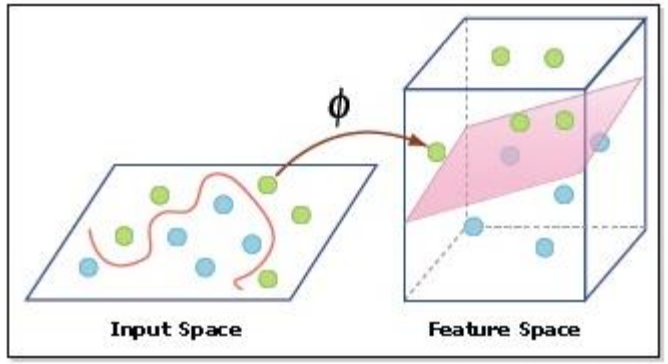
- Epsilon: defines a margin of tolerance around the hyperplane
  - **Low ε**: A smaller epsilon results in narrow margin, making model strict, as it tries to fit points closely within the margin. This can lead to **overfitting**, because the model tries to reduce the error even for data points that are at close distance (but fall outside the margin).
  - **High ε**: A larger epsilon margin allows the model to tolerate more error (accepting more data points within margin without being penalized), resulting in a smoother fit. The model becomes less sensitive to individual data points (since many data points are inside the margin), which can help avoid overfitting but risks **underfitting**.

Support Vector Regression hyperparameters

- C is a **penalty** parameter that controls the trade-off between the complexity of the model (flatness of the hyperplane) and the amount of allowed deviations (points falling outside the epsilon margin).
  - **Low C**: A smaller value of C makes the model more tolerant to errors, allowing a wider margin with more points lying outside the epsilon tube. This results in a simpler model that may **underfit** the data, ignoring small errors to generalize better.
  - **High C**: A larger C forces the model to minimize error, resulting in a tighter fit to the training data. The model will be less tolerant of deviations, trying to fit as many points as possible within the epsilon margin. This can lead to **overfitting** as the model tries too hard to fit the training data.

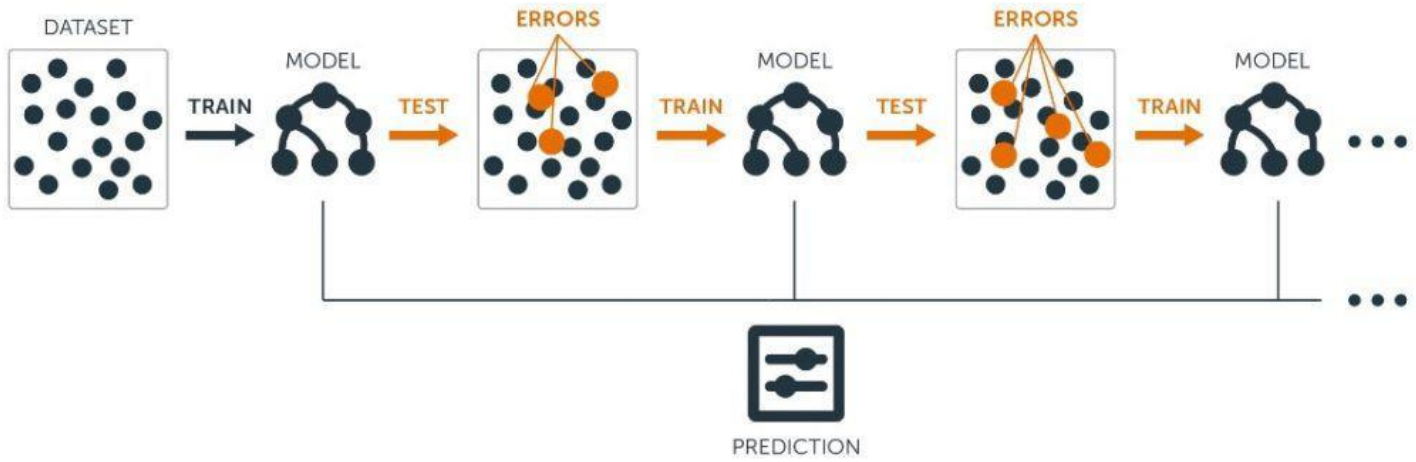
Support Vector Regression hyperparameters

- Kernel: A kernel is a set of mathematical functions that takes data as input and transform it into the required form. These are generally used for finding a better hyperplane in a higher dimensional space
  - The most widely used kernels include linear, polynomial (poly), radial basis function (rbf) and sigmoid. By default, RBF is used as the kernel. Each of these kernels are used depending on the dataset.



Basic Types of Ensemble Learning

- Sequential Ensemble Learning (boosting)
  - Key ideas:
    - base learners are dependent on the results from previous base learners
    - every subsequent base model corrects the prediction made by its predecessor fixing the errors in it
    - overall performance can be gradually increased
  - Cons: tends to overfit the training data
  - Examples: AdaBoost, Stochastic Gradient Boosting, XGBoost, CatBoost

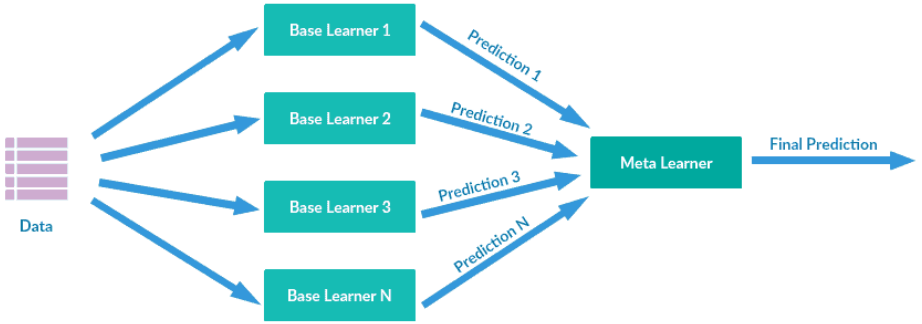


Basic Types of Ensemble Learning

- Parallel ensemble learning using homogeneous learners (also called bagging)
  - all base learners are homogeneous (same machine learning algorithm) and execute in parallel on different random subsets of the original dataset
  - no dependency between the base learners
  - results of all base models are combined in the end (using averaging for regression and voting for classification problems)
    - Averaging: every learner make a prediction (predicted value) for each data point, and the final predicted value for that point is the average of all predicted values
    - Voting: every learner makes a prediction (votes) for each data point (row in dataset) to which category should be assigned to and the final output prediction for that point is the category that receives more than half (or the majority) of the votes
  - See more here
  - Examples: sklearn.ensemble.BaggingRegressor, sklearn.ensemble.RandomForestRegressor

Basic Types of Ensemble Learning

- Parallel ensemble learning using heterogeneous learners (also called stacking)
  - all base learners are heterogeneous (different machine learning algorithm) and execute in parallel
    - Base Learners are trained using the available data
  - meta learner combines predictions of base learners
    - Meta Learner is trained to make a final prediction using the Base Learners' predictions on the input data – base models' predictions are used as input features to meta learner
  - stacking obtains better performance results than any of the individual weak learners



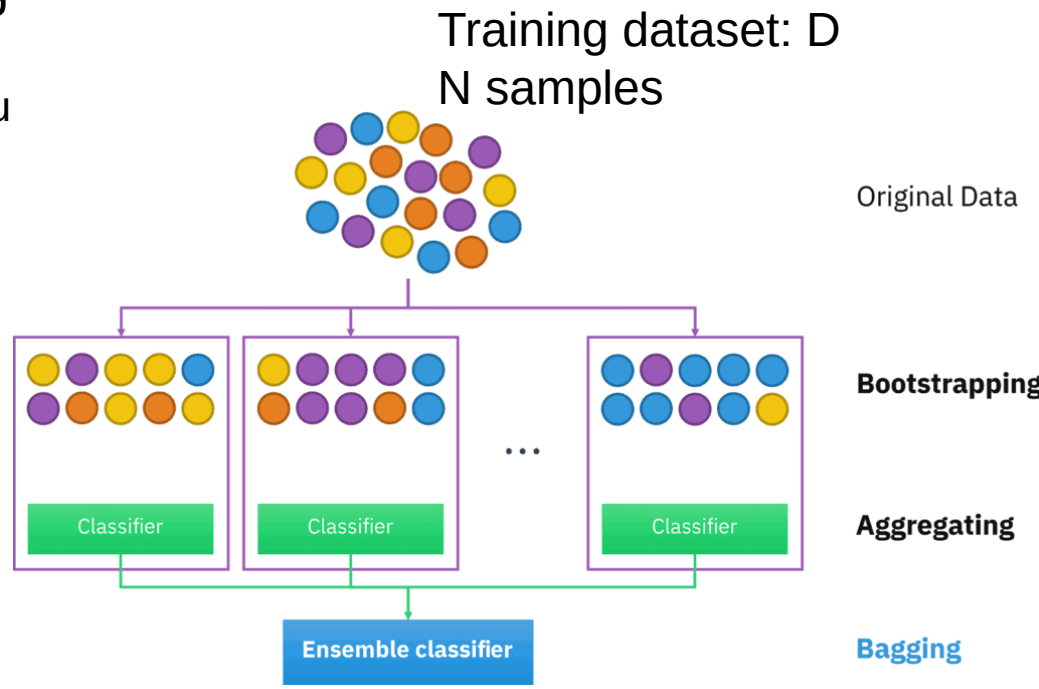
  - Example: sklearn.ensemble.StackingRegressor

Random Forest Regression

- A Random Forest is a bagging ensemble technique
- Performs both regression and classification tasks with the use of multiple decision trees as base models
- The name “Random Forest” comes from the bootstrapping idea of data randomization (training datasets for each tree taken from random subsets of the initial training dataset) and building multiple Decision Trees (Forest)
- RandomForestRegressor class
  - sklearn.ensemble.RandomForestRegressor
  - More info here

Bagging in detail

- Parallel Ensemble Learning of homogeneous learners: Bootstrapping (resampling) => Aggregating => Bagging
  1. To start with, let's assume you have some original data that you want to use as your training set (dataset D with N samples). You want to have K base models in our ensemble.
  2. In order to promote model variance, Bagging requires training each model in the ensemble on a randomly drawn subset of the training set. The number of samples in each subset is usually equal to the original dataset (N), although it can be smaller.
  3. To create each subset, you need to use a bootstrapping technique:
     a) First, randomly pull a sample from your original dataset D and put it to your subset
     b) Second, return the sample to D (this technique is called sampling with replacement)
     c) Third, perform steps (a) and (b) N (or less) times to fill your subset
     d) Then perform steps (a), (b), and (c) K – 1 time to have K subsets for each of your K base models
  4. Train each of K base models on its subset, make predictions using test (unseen) dataset
  5. Combine (aggregate) the prediction of each sample (row) from the test dataset and evaluate the final result for each sample



If you are solving a Classification problem, you should use a voting process to determine the final result. The result is usually the most frequent class among K model predictions. In the case of Regression, you should just take the average of the K model predictions.

Bagging in detail (sampling with replacement)

Training datasets (with 10 samples/rows each)

Original dataset	1	2	3	4	5	6	7	8	9	10
Base Model 1 dataset	7	8	10	8	2	5	10	10	5	9
Base Model 2 dataset	1	4	9	1	2	3	2	7	3	2
Base Model 3 dataset	1	8	5	10	5	5	9	6	3	7

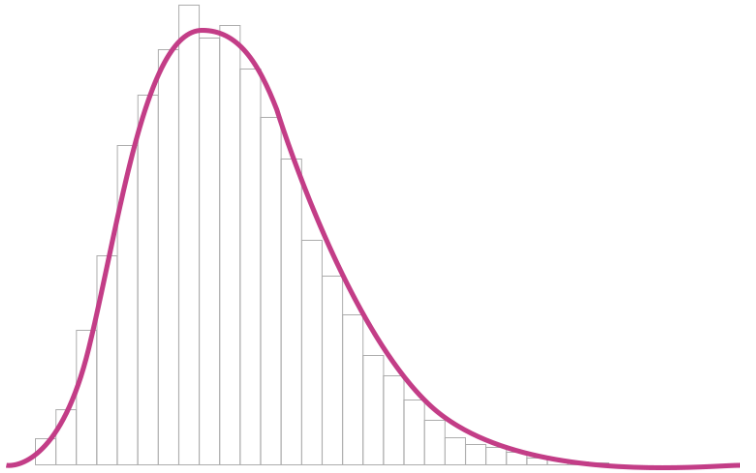
- Boostrapping process creates a new training dataset for each base model
- Some samples (rows) of the initial training dataset can be selected multiple times within a base model's training dataset
- Build multiple base models – each one trained on its own dataset
- Use each base model to make a prediction using the test dataset
- Combine (average) predictions to provide the final ensemble algorithm prediction

Feature scaling in gradient descent algorithms

- The algorithms work by iteratively updating the model parameters in small steps, nudging them in the direction that minimizes the prediction error.
- Sometimes your model won’t converge at all if you don’t scale your features.
- This is because the gradient descent algorithm will be jumping around the parameter space, heavily influenced by the features with the largest ranges.
- In cases where the features are already on a similar scale or when using optimization algorithms that do not rely on gradients, feature scaling might not have a significant impact on performance.

Problem of skewness explained

- You're building a **regression model** to predict the **sales** of products based on certain features (like price, category, etc.). Here's how the distribution of sales looks in your dataset:
  - **Most products** have low sales (near 100 units sold), which means the data is concentrated here. These products are under the **peak** of the distribution.
  - **Fewer products** have very high sales (like 10,000 units sold), meaning they fall in the **long tail**.



- The dataset is **right-skewed**, meaning the majority of products have low sales, while a few products have very high sales
  - If you train a typical **linear regression** or a basic ML model without addressing skewness, model will tend to focus more on **predicting well** for the **majority class** (products with low sales). Since the majority of the training examples represent low-sales products, the model will learn patterns that help it predict values closer to those lower sales.

How Does the Model Perform in the Peak?

- **Overestimation in Low-Sales Region**
- Since there are many products with sales close to 100 units (for example), the model might generalize poorly and predict values slightly **above** 100 for most of the products in this region.
  - Let's say the actual sales for a product is **90**, but the model predicts **105**. This is an overestimation because the model is biased towards a slightly higher average in this region.
- Why? The model has learned to favor a more general prediction, often based on the **mean** or **median** of the majority class (low-sales products), and might miss the nuances of individual low-sales products, predicting higher than the actual values.

How Does the Model Perform in the Long Tail?

- **Underestimation in High-Sales Region**
- For products in the long tail (those with very high sales), the model is **less trained** to handle them because there are far fewer examples of such products in the training data.
  - If the actual sales for a product is **10,000** units, the model might predict only **7,500** units, significantly **underestimating** the sales.
- Why? The model has learned patterns from mostly low-sales products. Since there are fewer high-sales examples to learn from, the model struggles to extrapolate and generalize to these higher values. It tends to predict closer to the central tendency of the distribution (closer to the mean), which lies somewhere in the lower-sales region where the products with lower sales exist.

Why Does This Happen? (The Role of Bias)

- This behavior happens because the model is learning from a dataset where **low-sales products dominate**. The model tends to focus on minimizing errors for the majority class (low-sales products), causing it to become biased toward the patterns in that region. Consequently:
  1. **For products with low sales**: The model has many examples to learn from, but its generalization may slightly shift predictions **upward** (overestimation) due to bias towards the majority class.
  2. **For products with high sales**: The model lacks enough examples and tends to **underestimate** the true sales because it's biased toward the values seen more frequently in training (low sales).