EPL448: Data Mining on the Web – Labs 8

University of Cyprus
Department of
Computer Science

Παύλος Αντωνίου

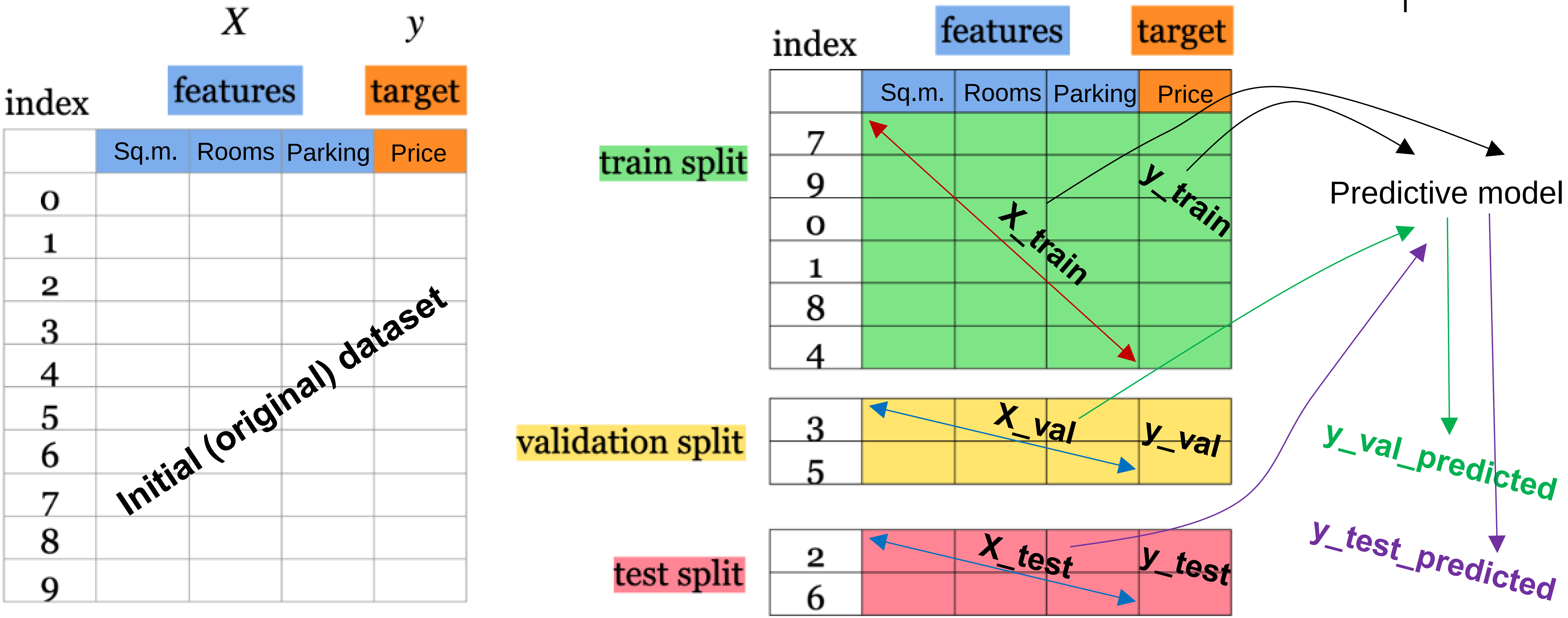
Γραφείο: B109, ΘΕΕ01

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. The model ***sees*** and ***learns*** from this data.
  - **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.
  - **Test dataset**: Used to provide unbiased **evaluation of a final model**. Only used once a model is completely trained (using training & validation datasets)

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

Training / validation / test datasets



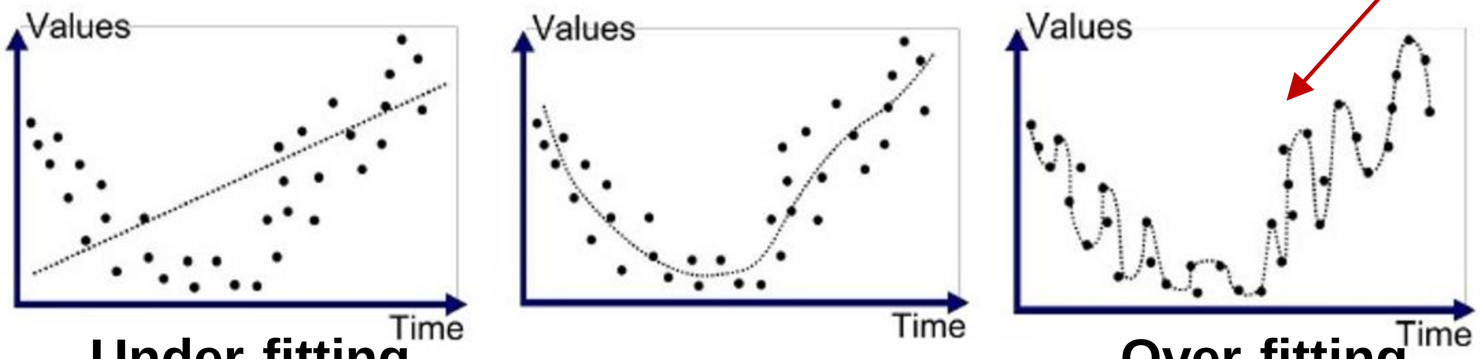
- During testing phase, predictive modelling technique sees both features (X_train) and the target (y_train) values
- During validation and testing phases, only features (X_val, X_test respectively) are given as input to predictive technique so as to predict the target values. Predictive model is evaluated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

Over-fitting

Underfitting: model fails to capture underlying pattern in training data



Under-fitting **Over-fitting**

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

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
    - 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 basic exploratory data analysis (EDA) to understand the structure of the dataset
  - This includes checking for missing values, understanding data types and feature distributions, and getting an initial sense of the data
- Splitting 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)
- Preprocessing and Transformation
  - After splitting, perform all preprocessing steps (such as scaling, normalization, encoding, and imputation) separately on the training set
    - We can keep different versions of the training dataset: original & with transformations
  - 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 and Selection
  - 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

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**: A classification problem is when the output variable (y) is a category, such as “disease” or “no disease” (binary classification) and “red” or “blue” or “green” (multiclass classification)
    - Popular techniques: Logistic Regression (binary classification), 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**: A regression problem is when the output variable (y) is a 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 (or target variable) y which takes 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}, …) equations
  - Support Vector Regression
  - Ensemble Regression (e.g. Random Forest Regressor, Ada Boost 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):

$$y = \beta_0 + \sum_{j=1}^{p} \beta_j * X_j = \beta_0 + \beta_1 * X_1 + \beta_2 * X_2 + \cdots$$

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

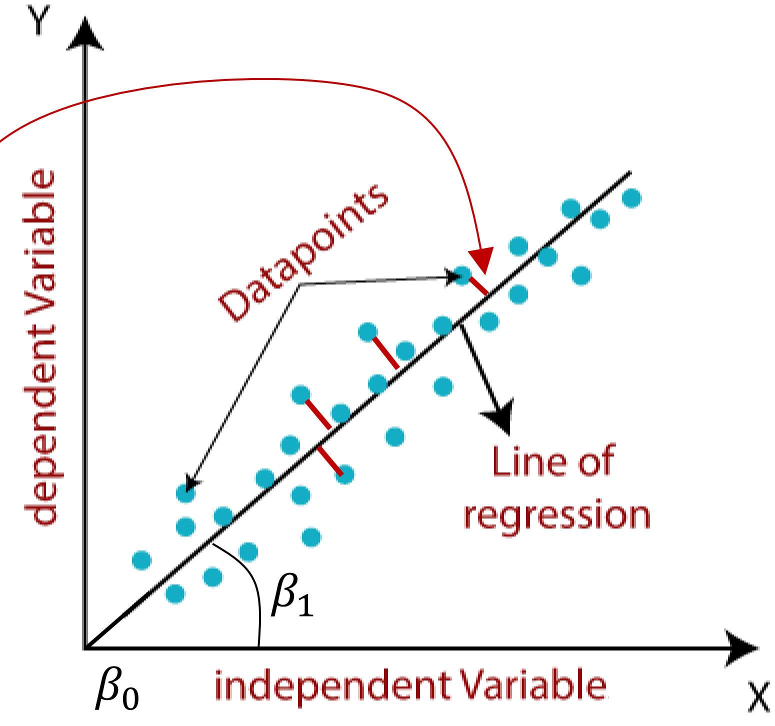
Simple Linear Regression

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

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

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

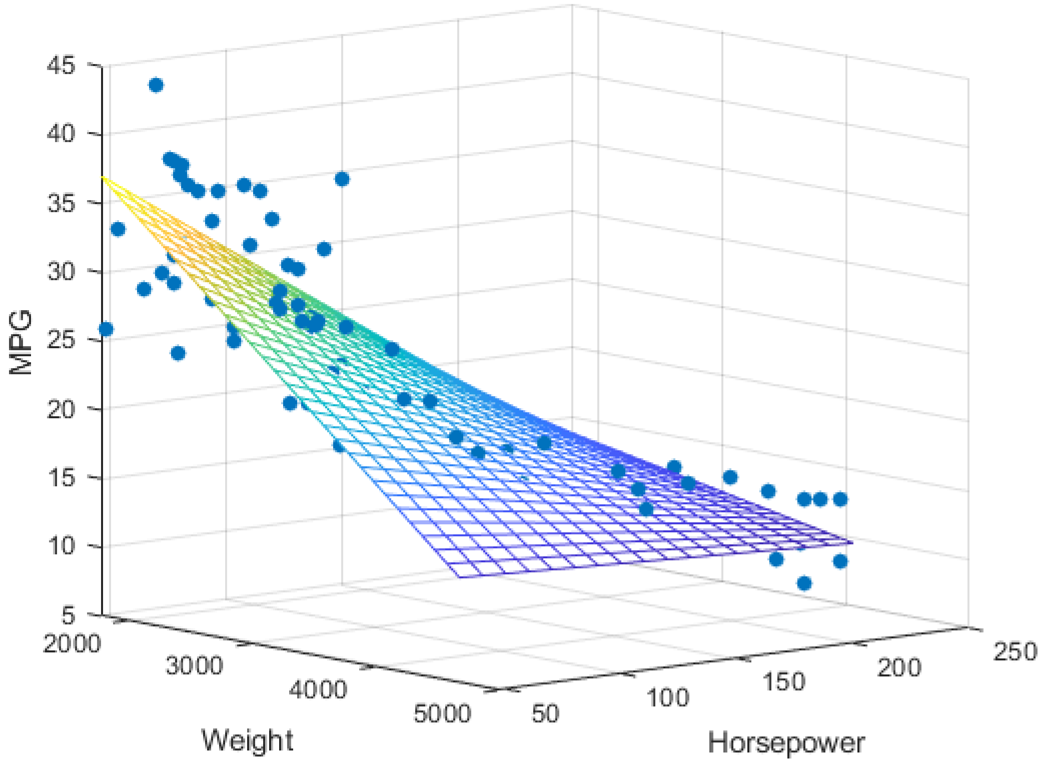
  - **Goal: Fit the best intercept line (evaluate β_0 and β_1) that passes between all data points that minimizes the error**
  - y : Dependent variable (target variable)
  - X : Independent variable (feature)
  - β_0 : Intercept (the target value when X = 0)
  - β_1 : Slope. Explains the change in Y when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

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



In this image n=2
Two independent variables:
- Weight
- Horsepower

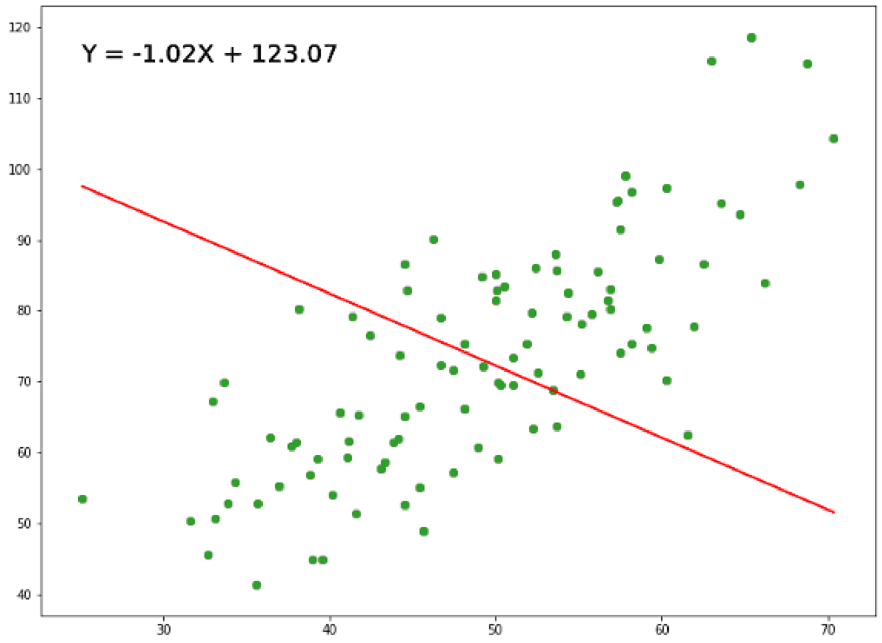
Dependent variable:
- MPG (miles per gallon)

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) such that the sum of squared error is minimized.

2. **Gradient descent** finds the linear model 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, or simply leave them in and note that multicollinearity is present.
    - There are some techniques to remove multicollinearity such as centering each correlated variable (remove mean value from all observed values of each variable) -- StandardScaler
- 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

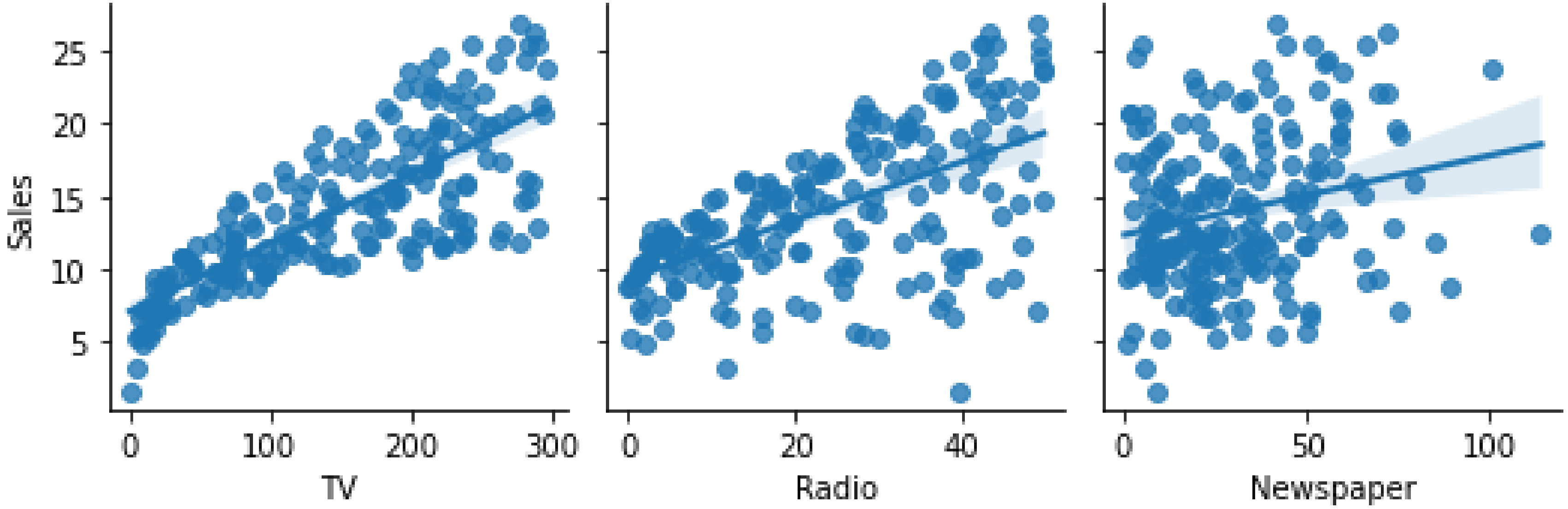
Independent variables (features) — TV, Radio, Newspaper; target variable — Sales

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.

Linear Regression: Testing assumptions

- Linearity

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

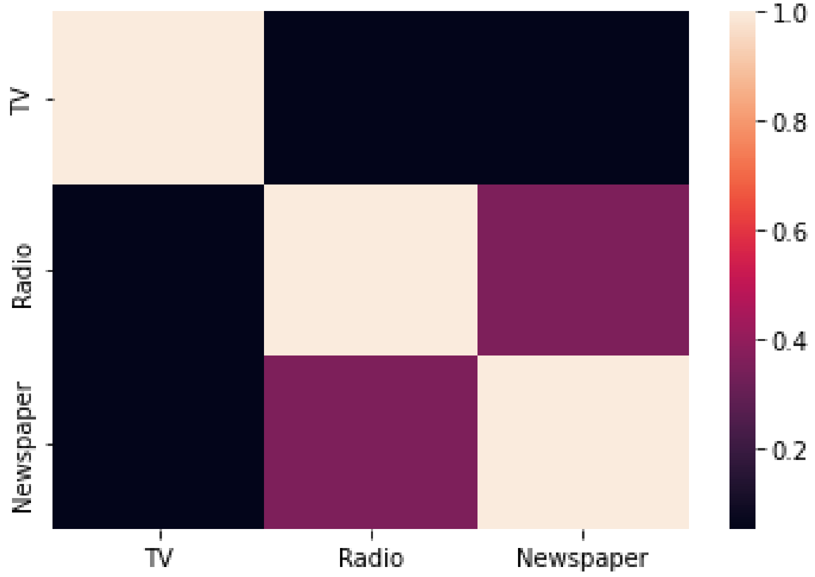


By looking at the plots we can see that none of the independent variables has an accurately linear relationship with Sales but TV and Radio do still better than Newspaper which seems to hardly have any specific shape. So, it shows that a linear regression fitting might not be the best model for it. A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

Non standardized independent values

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.

Non standardized independent values

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%

X_train

```
[[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. ]
```

X_2

```
 [ 57.5   32.8   23.5]
 [120.2   19.6   11.6]
 [  8.6    2.1    1. ]
 [199.8    2.6   21.2]]
```

y_train

```
[22.1
 10.4
  9.3
 18.5
 12.9
  7.2
```

y_2

```
 11.8
 13.2
  4.8
 10.6]
```

-

Non standardized independent values

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

X_train

```
[[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. ]
```

X_val

```
 [ 57.5  32.8  23.5]
 [120.2  19.6  11.6]
```

X_test

```
 [  8.6   2.1   1. ]
 [199.8   2.6  21.2]]
```

y_train

```
[22.1
 10.4
  9.3
 18.5
 12.9
  7.2
```

y_val

```
 11.8
 13.2
```

y_test

```
  4.8
 10.6]
```

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: $y = 2.99 + 0.044*x_1 + 0.196*x_2 - 0.0027*x_3$

Non standardized independent values

Linear Regression: Making prediction

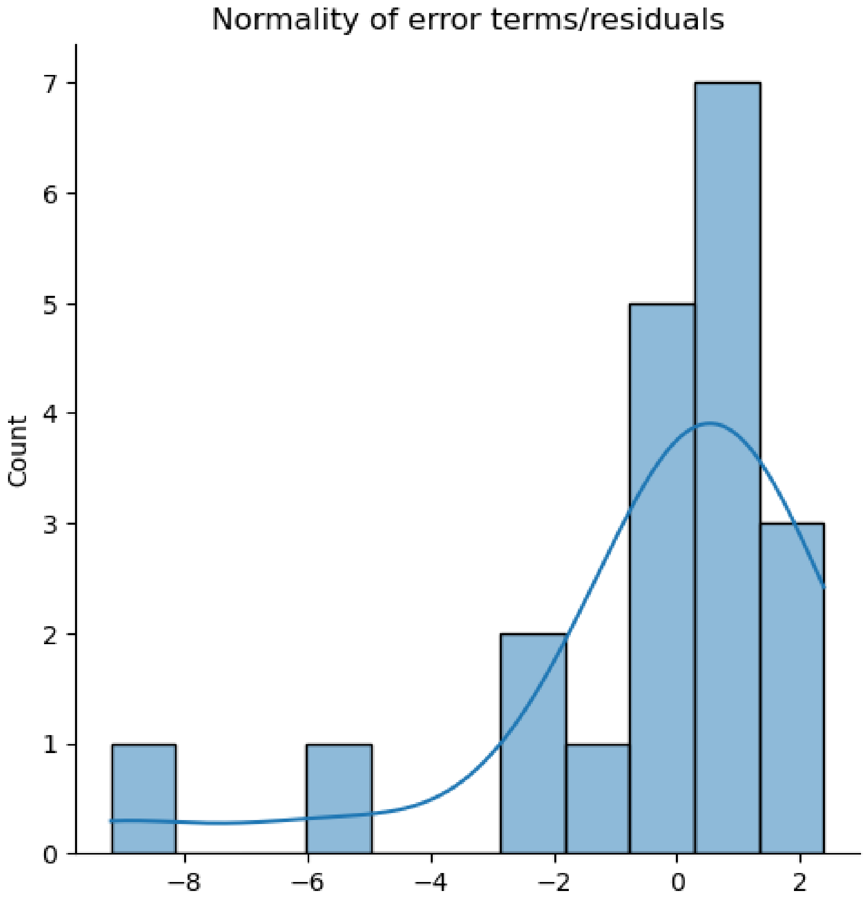
```
from sklearn.linear_model import LinearRegression
lregr = LinearRegression()

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]
```

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) # => 3.463801353587156e-10, residuals
deviate from normal distrib.
```



Data rescaling/standardization

- The values of β coefficients represent the influence of each input feature on the target variable: $y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_3 + \cdots \beta_n X_n + \epsilon$
  - 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 rescaling/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 rescale input features using MaxMinScaler, StandardScaler, RobustScaler shown in Lab 4

Data rescaling/standardization

- Min-max scaler rescales each feature individually into a given range, e.g. [0, 1]
- Standard scaler rescales each feature individually to make values have zero mean ($\mu = 0$) and unit variance ($\sigma^2 = 1$)
  - Assumes that feature fits a Gaussian distribution (bell curve) with a well-behaved mean and standard deviation
  - Centers data around zero
- Robust scaler rescales 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 to rescale/standardize features?

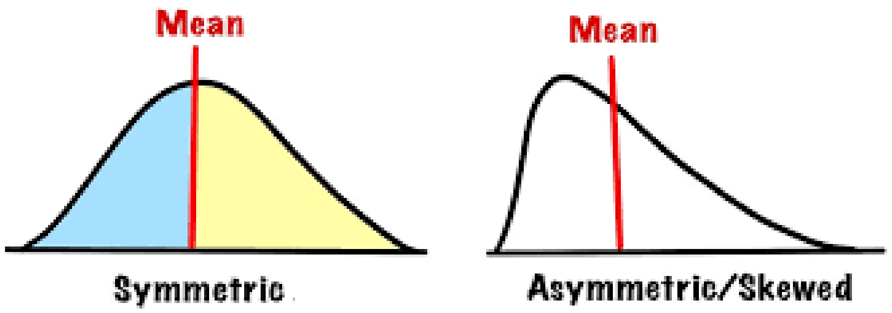
- When regression is used for making β coefficients directly comparable to one another and reveal the influence of each feature on target thus making it easy to present effects to non-statisticians

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

When to unskew features/target variable?

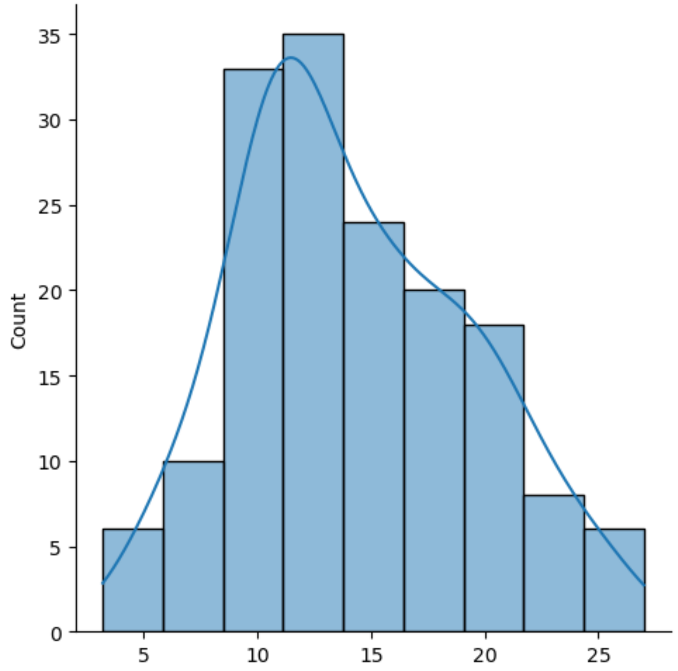
- Unskewing transformations attempt to make long-tail distribution of a variable symmetric as Gaussian/normal (bell-shaped) distribution
  – Unskewing transformations: BoxCox, Yeo-Johnson, Sqrt, Log

- 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 under the peak where the majority of values lay



Linear Regression: Target variable distribution

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




```
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) # => 0.039750209255936864, not normal distrib.
```

Distribution is skewed (not symmetrical) -- that it has a higher number of data points having low values, i.e., products with less Sales. So, when we train our model on this data, it will perform better at predicting the Sales of products with lower Sales as compared to those with higher Sales ➔ Solution: Unskew target variable (See 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

Linear Regression

Standardized independent values

```
# 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.
- 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 machine learning 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:
  - MSE: Mean Squared Error $MSE = \frac{1}{n}\sum_{i=1}^{n}(\hat{y}_i - y_i)^2$
    - Error is squared: Large prediction errors are penalized
  - MAE: Mean Absolute Error $MAE = \frac{1}{n}\sum_{i=1}^{n}|\hat{y}_i - y_i|$
    - Does not penalize large prediction errors
  - RMSE: Root Mean Squared Error $RMSE = \sqrt{\frac{1}{n}\sum_{i=1}^{n}(\hat{y}_i - y_i)^2}$
  - 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)

minimize (MSE, MAE, RMSE)

maximize (R-squared)

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

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
```

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: 1.038652835763308 5 ,
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)
```

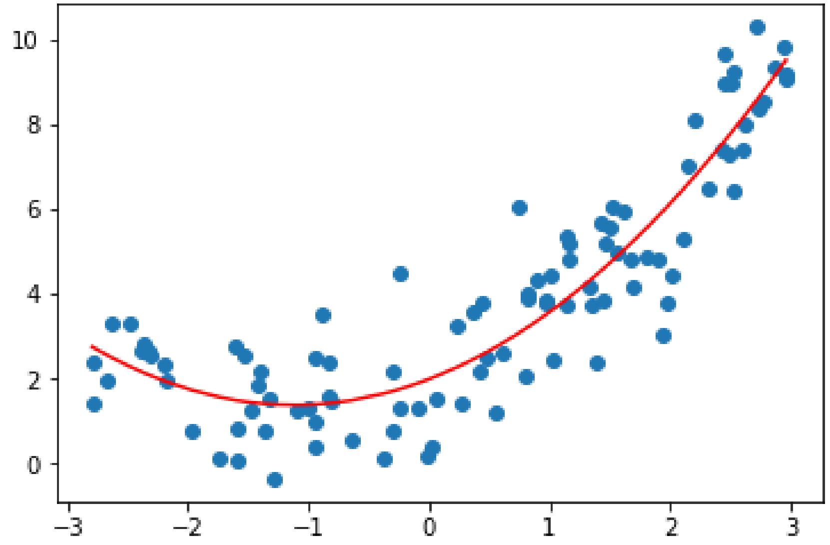
```
MSE_unscaled = mean_squared_error(y_val, y_pred_unscaled)
RMSE_unscaled = np.sqrt(MSE_unscaled)
r2 = r2_score(y_val, y_pred_unscaled)
```

```
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

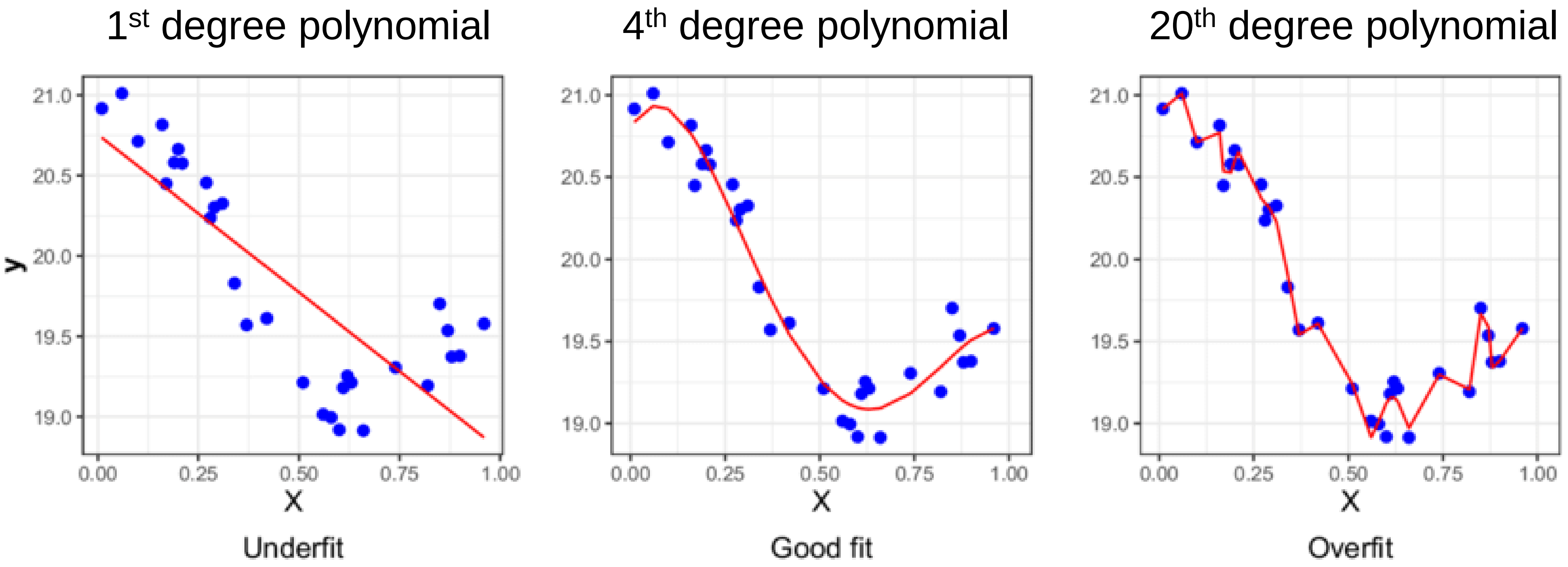
- Relationships between the independent variable(s) x and the dependent variable y are modelled as an n^{th} degree polynomial in x

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

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

Polynomial regression: of which degree?

- Increasing the degrees of the model also increases the risk of over-fitting the data



- The degree of the polynomial to fit is a hyperparameter that cannot be inferred while fitting the machine to the training set because it needs to be set prior the learning phase

How to find the right degree of the equation?

- In order to find the right degree for the model to prevent over-fitting or under-fitting, we can use any of the two approaches below:
  - Forward Degree Selection:
    - Start with a model of degree=1 and at each step gradually increase the model's degree until the best possible model (e.g. that minimizes MSE, RMSE) is reached
  - Backward Degree Selection:
    - Start with model of a large degree and at each step gradually decrease the model's degree until the best possible model is reached
  - At each step:
    - **Train** the model using the ***training dataset***
    - **Predict** the target value using the ***validation dataset***
    - Evaluate the performance of the model using any evaluation measure (MSE, RMSE, R2)
  - At the end, when the best model is chosen, evaluate its **final performance** by predicting the target value using the **testing dataset**.

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. beyond 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 $\beta_0, \beta_1, \beta_2, \beta_3$
- In a two-feature dataset X_1, X_2

  Interaction term
  - 2nd degree polynomial model : $y = \beta_0 + \beta_1 X_1 + \beta_2 X_2 + \beta_3 X_1^2 + \beta_4 X_1 X_2 + \beta_5 X_2^2$
    - 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 $\beta_0, \beta_1, \beta_2, \beta_3, \beta_4, \beta_5$

Is rescaling/unskewing needed?

- While creating power terms (e.g. X_1^2 , X_1^3), if X_1 is not centered first (using StandardScaler or RobustScaler), the squared and cubic terms will be highly correlated with X_1
- 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
- Both situations can negatively affect the estimation of the β coefficients, therefore centering can be applied on all input features prior creating power and interaction terms (see here)
- Feature and target variable distributions are not required to be Gaussian, but unskewing transformation is generally recommended if distributions are heavily skewed

Polynomial Regression: Boston Housing Dataset

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

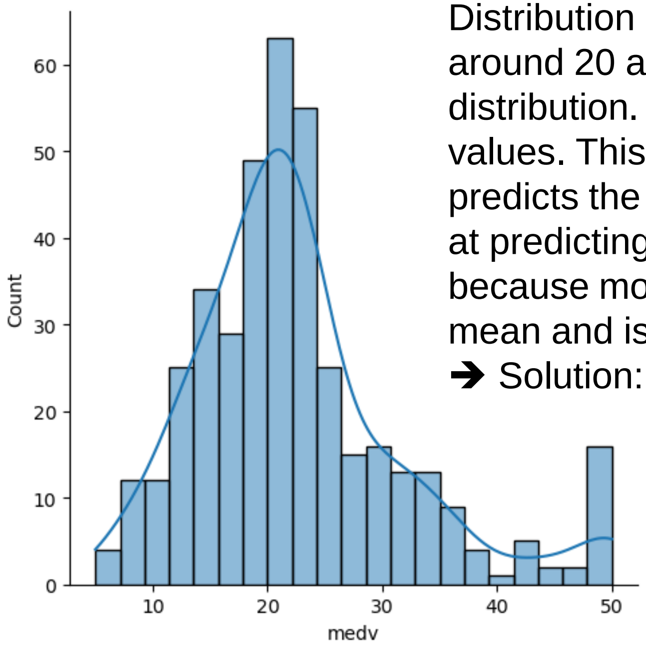
```
import numpy as np
import matplotlib.pyplot as plt

import pandas as pd
import seaborn as sns

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

# 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)
```

	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

Data transformation

- Feature standardization and rescaling do not improve the predictive power of the model when using linear regressors
- 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
```



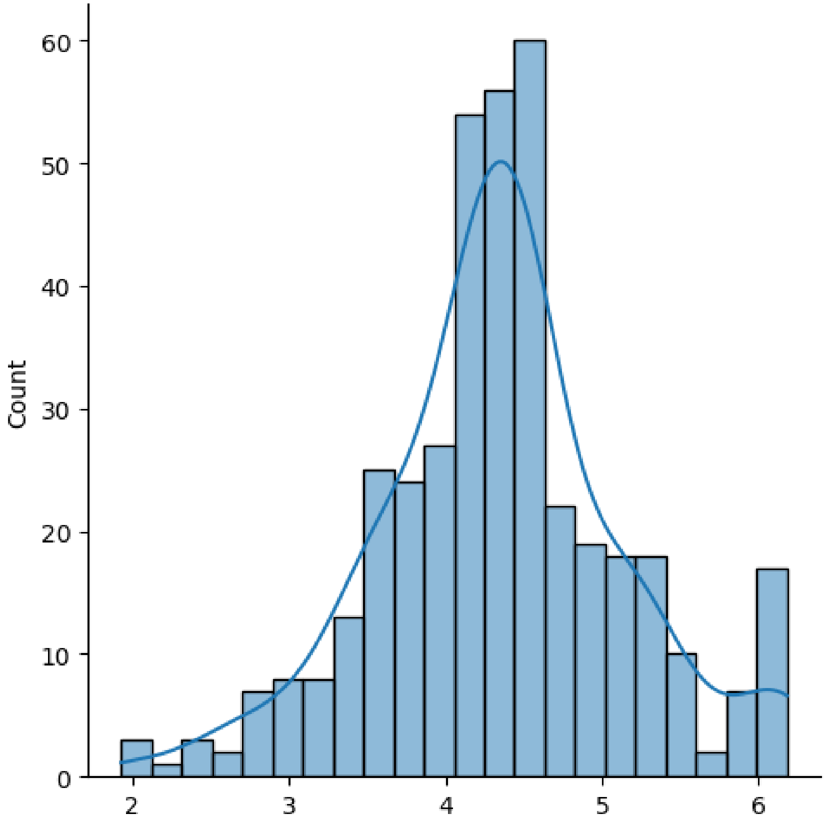
Distribution is skewed (not symmetrical): The mean is around 20 and the first part already looks quite like a normal distribution. But there is a large right tail of higher MEDV values. This could lead to the problem, that the model better predicts the MEDV values around the mean but is quite bad at predicting the MEDV values from the right tail. This is because most of the time the model sees values around the mean and is therefore biased towards these MEDV values.
➔ Solution: Unskew target variable (See Appendix)

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) # => 0.13691571809545577
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

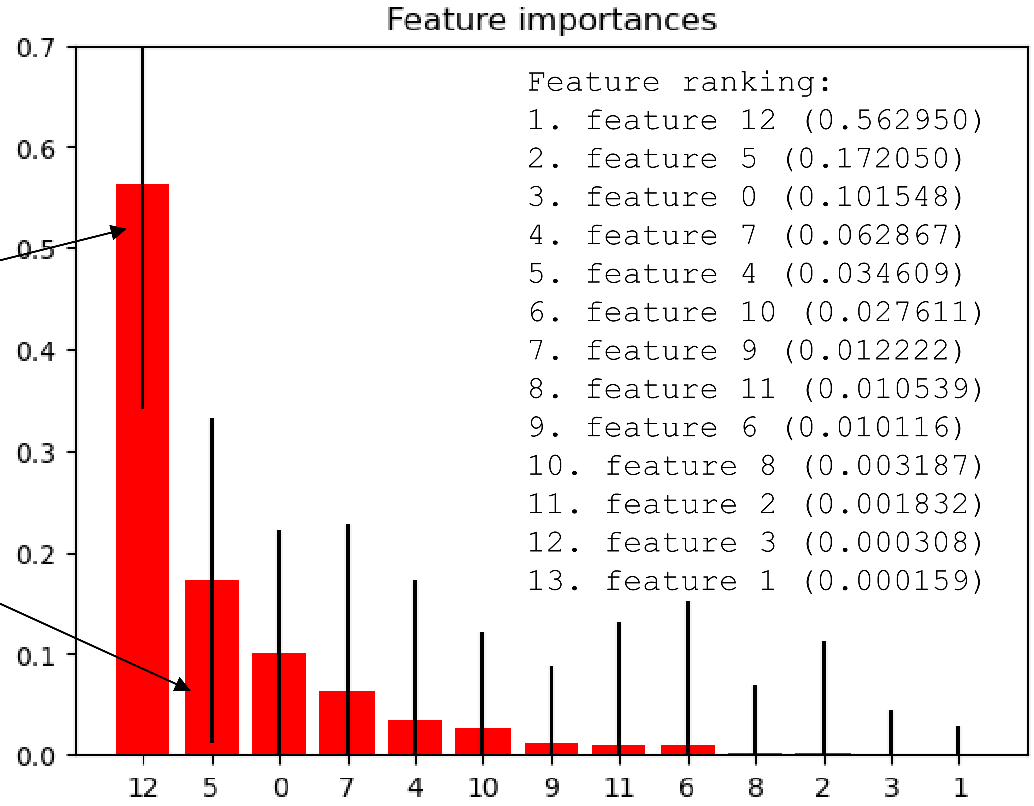
Feature Selection – Correlation matrix

- 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

	crim	zn	indus	chas	nox	rm	age	dis	rad	tax	ptratio	black	lstat	medv
crim	1	-0.2	0.42	-0.048	0.43	-0.18	0.34	-0.39	0.61	0.58	0.28	-0.32	0.46	-0.39
zn	-0.2	1	-0.54	-0.035	-0.53	0.34	-0.57	0.66	-0.32	-0.32	-0.42	0.17	-0.42	0.39
indus	0.42	-0.54	1	0.098	0.78	-0.37	0.62	-0.71	0.63	0.74	0.4	-0.35	0.59	-0.48
chas	-0.048	-0.035	0.098	1	0.13	0.065	0.1	-0.12	-0.00093	-0.018	-0.12	0.033	-0.045	0.16
nox	0.43	-0.53	0.78	0.13	1	-0.29	0.72	-0.78	0.64	0.69	0.21	-0.37	0.61	-0.43
rm	-0.18	0.34	-0.37	0.065	-0.29	1	-0.24	0.2	-0.2	-0.26	-0.36	0.071	-0.58	0.66
age	0.34	-0.57	0.62	0.1	0.72	-0.24	1	-0.74	0.46	0.49	0.26	-0.25	0.6	-0.38
dis	-0.39	0.66	-0.71	-0.12	-0.78	0.2	-0.74	1	-0.51	-0.55	-0.23	0.29	-0.49	0.25
rad	0.61	-0.32	0.63	-0.00093	0.64	-0.2	0.46	-0.51	1	0.92	0.47	-0.44	0.5	-0.38
tax	0.58	-0.32	0.74	-0.018	0.69	-0.26	0.49	-0.55	0.92	1	0.46	-0.43	0.54	-0.45
ptratio	0.28	-0.42	0.4	-0.12	0.21	-0.36	0.26	-0.23	0.47	0.46	1	-0.18	0.37	-0.51
black	-0.32	0.17	-0.35	0.033	-0.37	0.071	-0.25	0.29	-0.44	-0.43	-0.18	1	-0.34	0.32
lstat	0.46	-0.42	0.59	-0.045	0.61	-0.58	0.6	-0.49	0.5	0.54	0.37	-0.34	1	-0.74
medv	-0.39	0.39	-0.48	0.16	-0.43	0.66	-0.38	0.25	-0.38	-0.45	-0.51	0.32	-0.74	1

Feature Selection – Importance

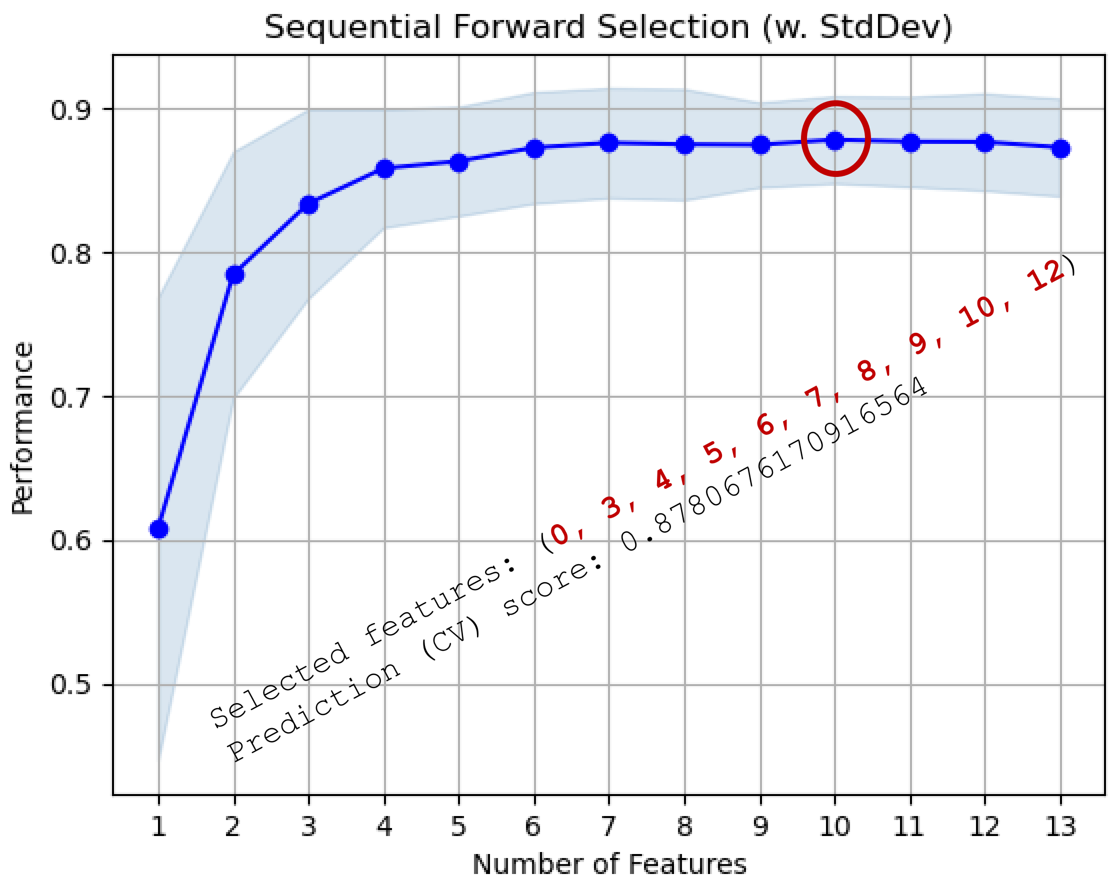
```
# Feature Importance using ExtraTreeClassifier
from sklearn.ensemble import GradientBoostingRegressor
# Build an estimator and compute the feature importances
estimator = GradientBoostingRegressor(n_estimators=100, random_state=0)

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

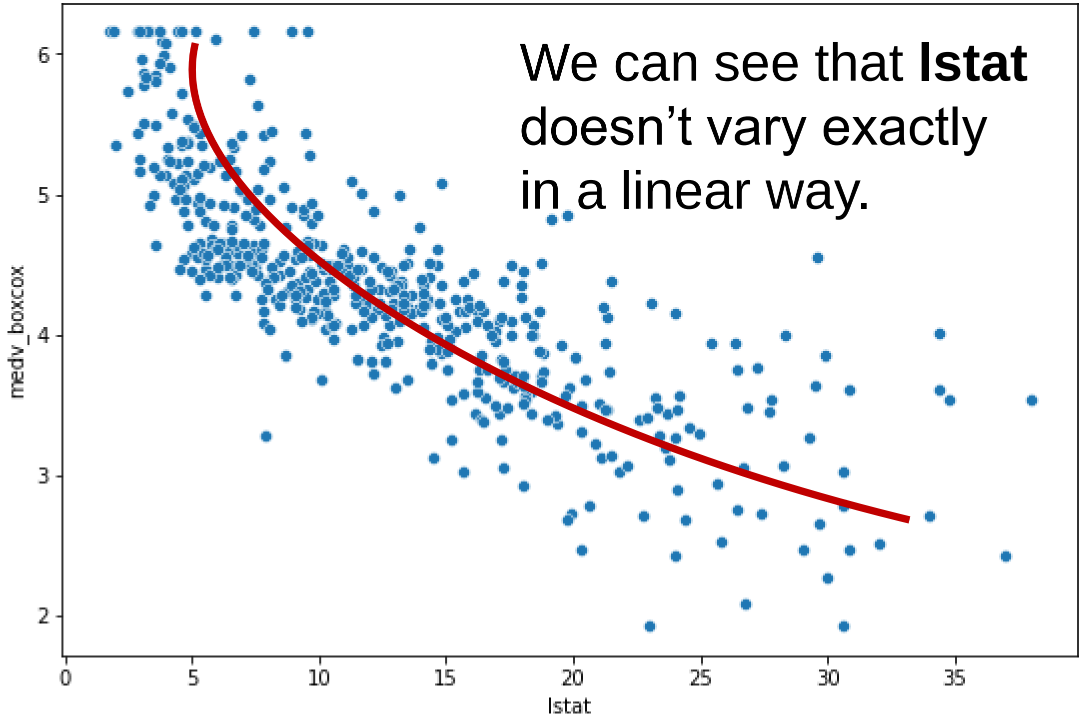
```
from mlxtend.feature_selection import SequentialFeatureSelector as SFS
from mlxtend.plotting import plot_sequential_feature_selection as plot_sfs

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_)
```

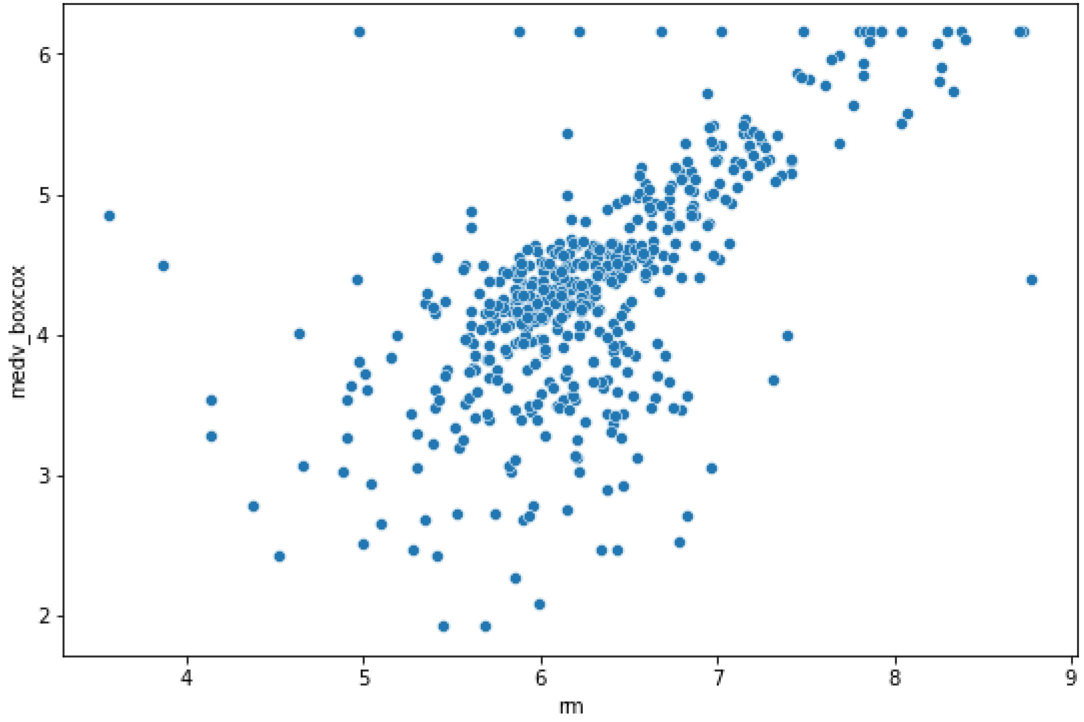


Feature Selection

```
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 use both Linear and Polynomial regression to build a predictive model for predicting the target variable





Linear Regression on Boston dataset

- Results using the initial dataset without transformations

```
Model performance on validation dataset
--------------------------------------
RMSE is 5.203457199881524
R2 score is 0.6312661056498 37
```

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

```
Model performance on validation dataset
--------------------------------------
RMSE is 4.770472127125568
R2 score is 0.6900784237549225
```

- Better performance is experienced when target variable is unskewed

Linear Regression (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 mean value of Y when all X=0
  - Default value is true: 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)


# 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)
```

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	$lstat^2$	lstat * rm	rm^2
[[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.

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 (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 (validation) data, we cannot determine if it is underfitting, overfitting, or "well-generalized"

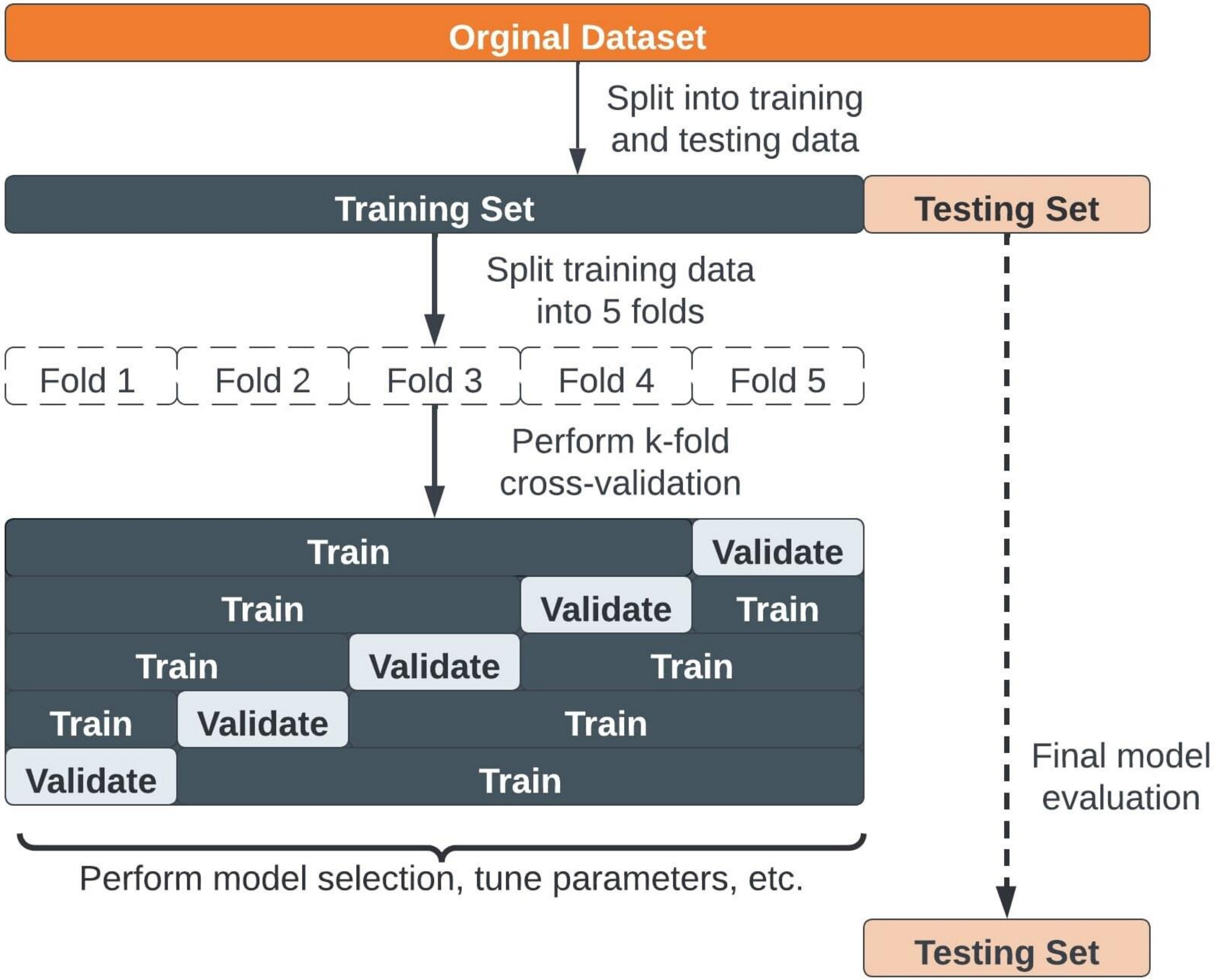
- Solution: Repeat the process of randomly splitting data into subsets and average results => **Cross Validation (CV)**

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
- 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

Cross validation

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
  - Run linear regression

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

- A 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)
```

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 estimator across ALL searched params:\n", search.best_estimator_)
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 3.2201573383614345
R2 score is 0.8675577863835
```

Pipelines

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

```
im = SimpleImputer(strategy="mean")
sc = StandardScaler()
preprocessing_pipeline = Pipeline([("imputer", im), ("scaler", sc)])
```

```
pf = PolynomialFeatures()
lr = LinearRegression()
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 feature set
- We can apply different transformations per column using `ColumnTransformer`. Example:
  - 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([
    ('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')
    ))
])
```

'yeo-johnson': works with positive and negative values

'boxcox': works with strictly positive values

- 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.

Pipelines with TranformedTargetRegressor

- `TranformedTargetRegressor` with log transformation

Pipeline **without** target transformation

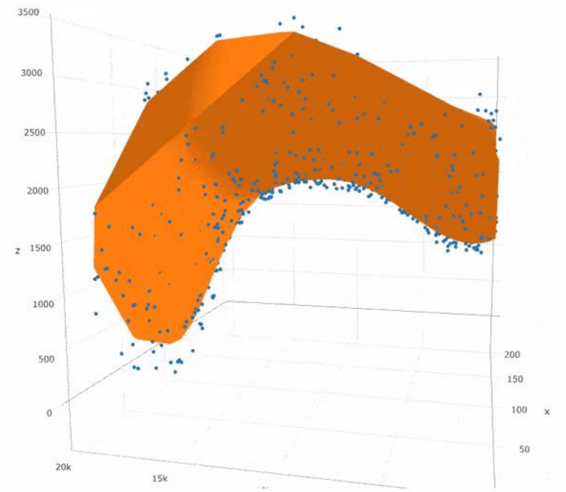
```
training_pipeline = Pipeline([
    ("poly", PolynomialFeatures()),
    ("linear", LinearRegression())
])
```

Pipeline **with** target transformation

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

Support Vector Regression (SVR)

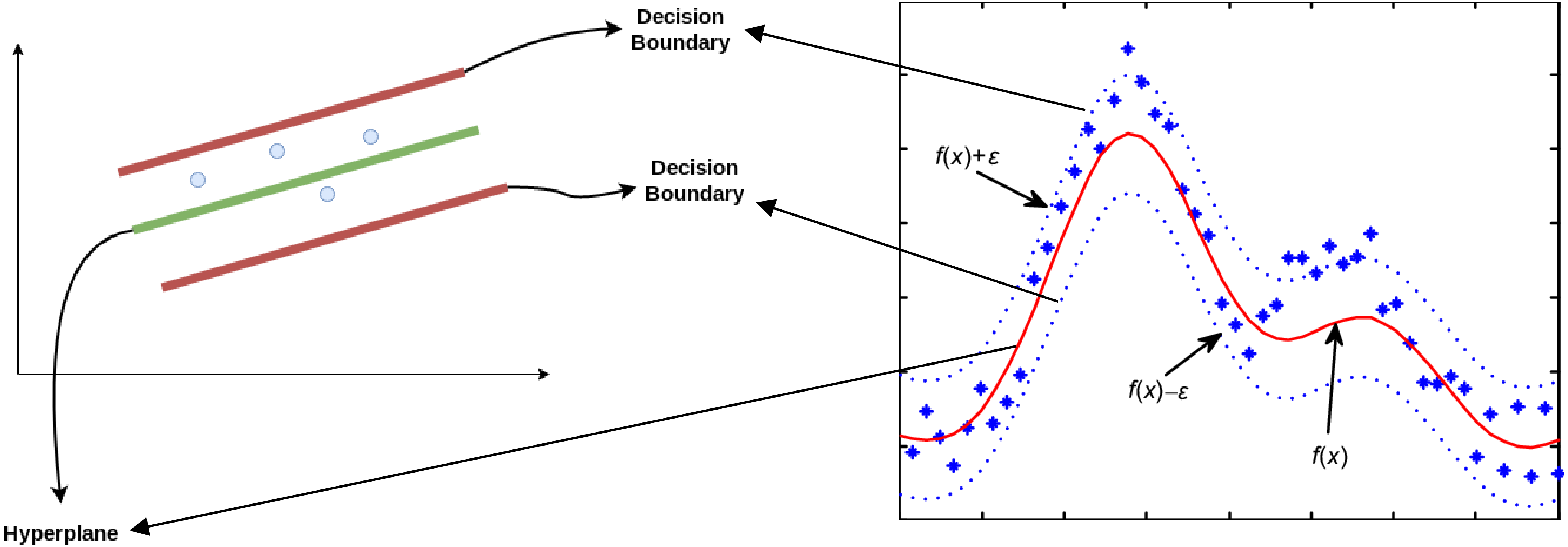
- Basic idea of support vector regression
  – Find optimal hyperplane that approximates the relationship between the input features and the target variable.



- Hyperplane: A hyperplane is a decision surface that is used to predict the continuous output and fits the data points. Each data point is a row of the dataset. The data points on either side of the hyperplane that are closest to the hyperplane are called Support Vectors. These are used to plot the required surface that shows the predicted output of the algorithm.

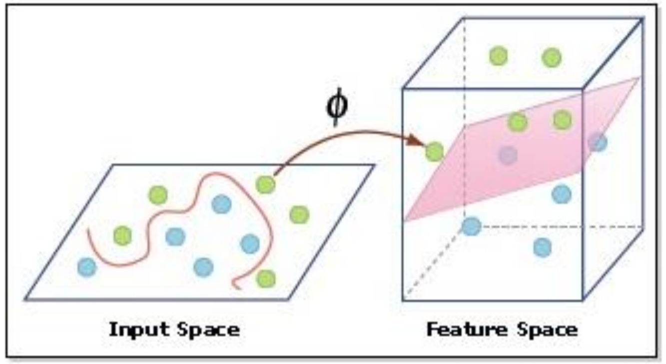
Support Vector Regression (SVR)

- Decision Boundaries: These are the two surfaces that are drawn around the hyperplane at a distance of ε (epsilon).
  - SVR basically considers the points that are within the decision boundaries
  - Best fit: the hyperplane that fits a maximum number of points.



Support Vector Regression (SVR)

- 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.



Support Vector Regression (SVR)

- SVR important hyperparameters:
  - kernel: default value is rbf
  - C: Regularization parameter. The strength of the regularization is inversely proportional to C. Must be strictly positive. Default value is 1.0
  - epsilon: boundary threshold (ε), default value is 0.1
  - gamma: kernel coefficient for rbf, poly and sigmoid, default value is 'scale'
  - degree: degree of the polynomial kernel (poly)
- In distance-based regression algorithms (such as Support Vector Regressor - SVR) that use (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. $\mathrm{D}istance(X_1, X_2) = \sqrt{(3-1027)^2 + (4-2123)^2}$ 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 rescaling/unskewing needed?

- Ensemble methods (Random Forest, XGBoost, AdaBoost) do not require feature rescaling to be performed as they are not sensitive to the variance in the data
- A skewed dependent 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.

Appendix

University of Cyprus
Department of
Computer Science

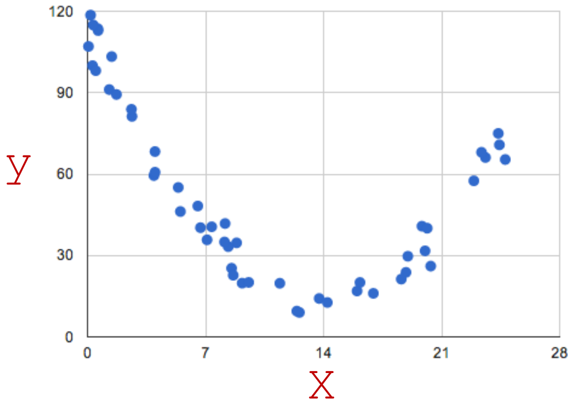
Is validation dataset needed?

- While it is possible to split your dataset into just training and testing sets, incorporating a validation set or using cross-validation is generally recommended for model tuning and selection.
- **Use Direct Train-Test Split**
  - When you have a large enough dataset that ensures the training and test sets are sufficiently representative of the entire dataset.
  - When you are primarily interested in a quick evaluation and you are not performing hyperparameter tuning
- **Use Train-Validation-Test Split**
  - When you want to tune hyperparameters and select the best model configuration before evaluating the final performance on a test set.
  - This approach provides a dedicated validation set for model selection and tuning, while keeping the test set strictly for final evaluation.

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)

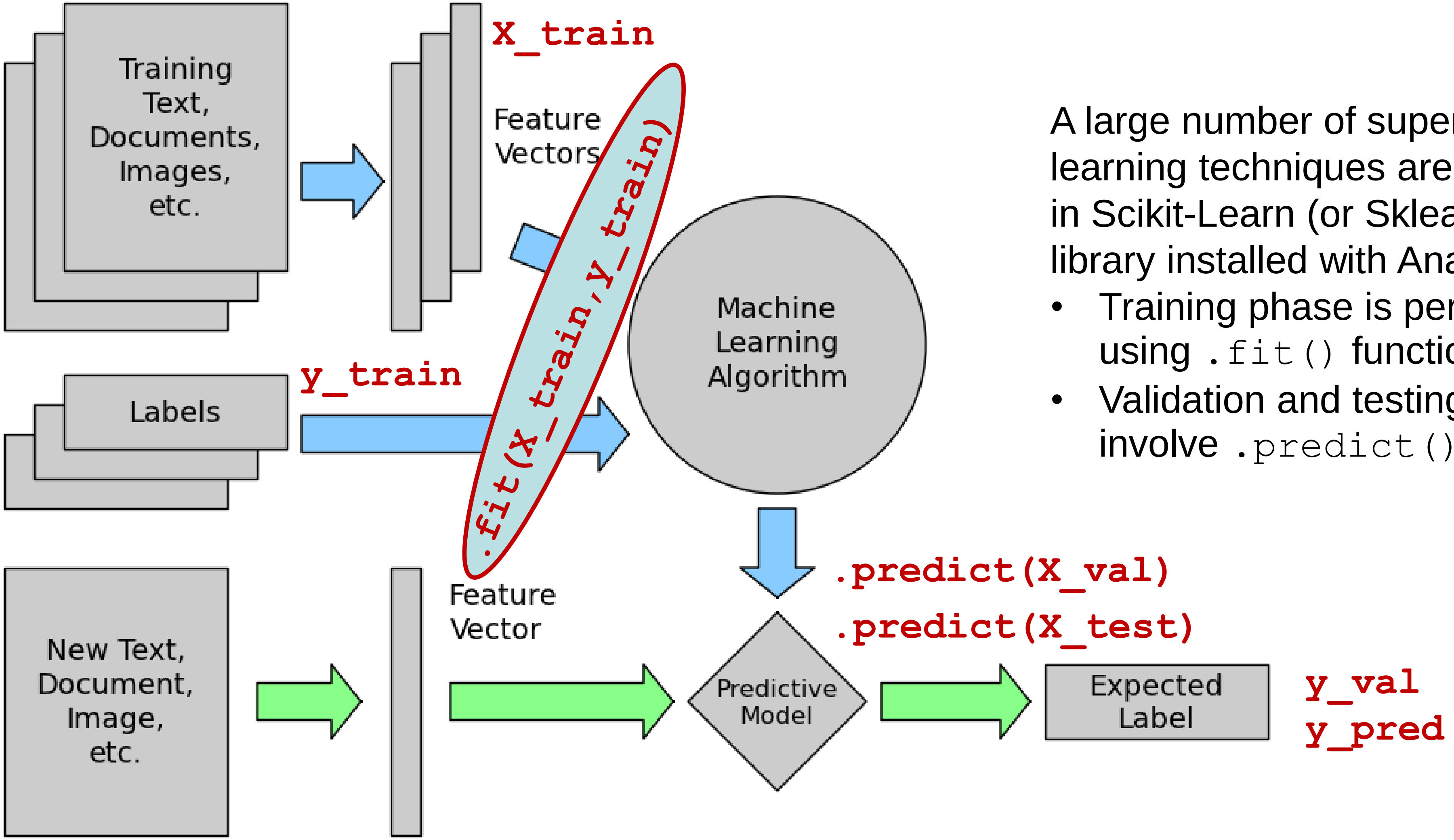
– The outcome of training phase can be the model e.g.: $y = 0.45 + 0.7X + 1.2X^2$

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 (2nd degree) model, change the degree of the polynomial equation e.g. to 3, re-run on training (phase) data to create a new cubic (3rd 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

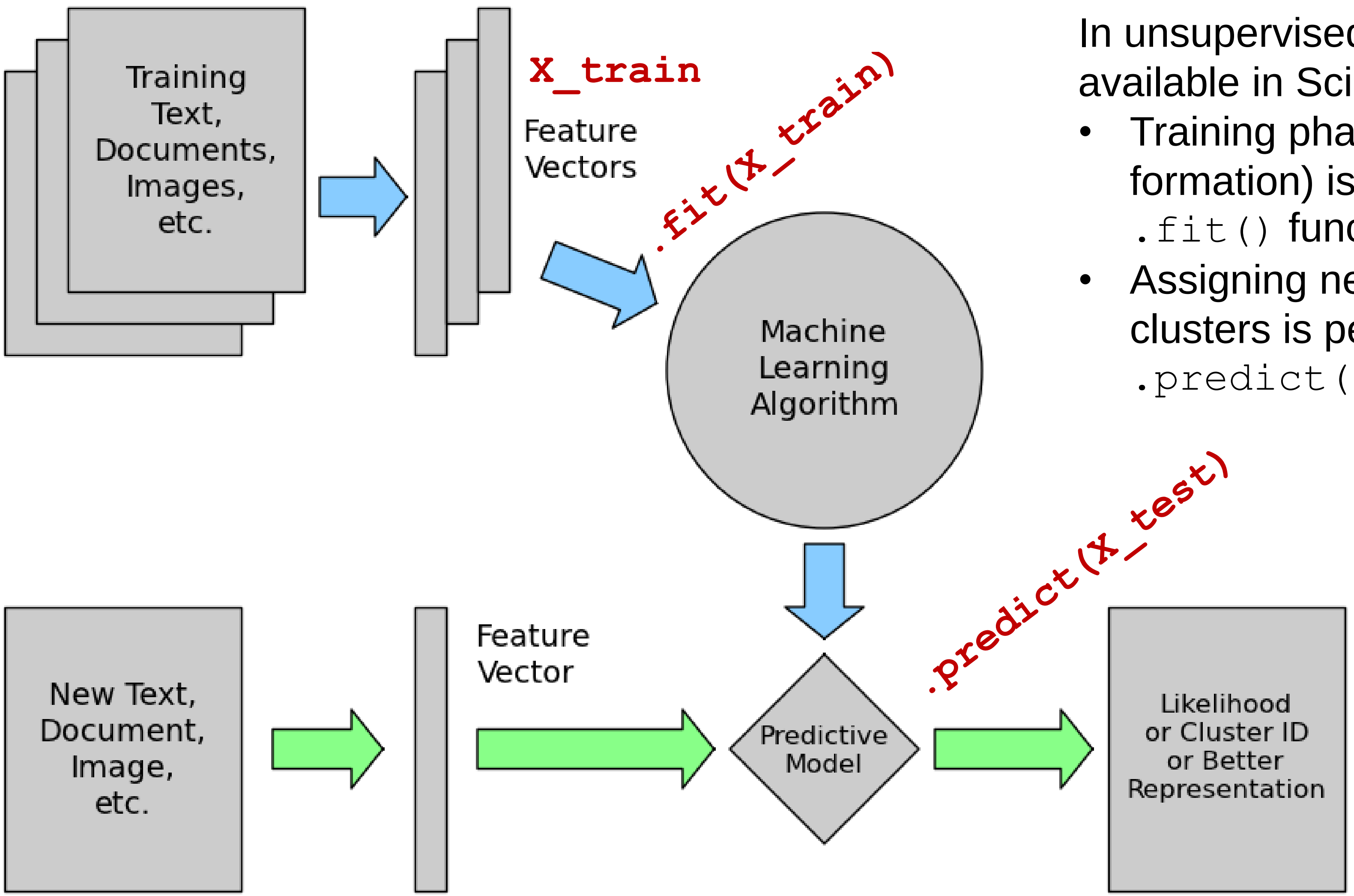
Predictive techniques: Supervised learning



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

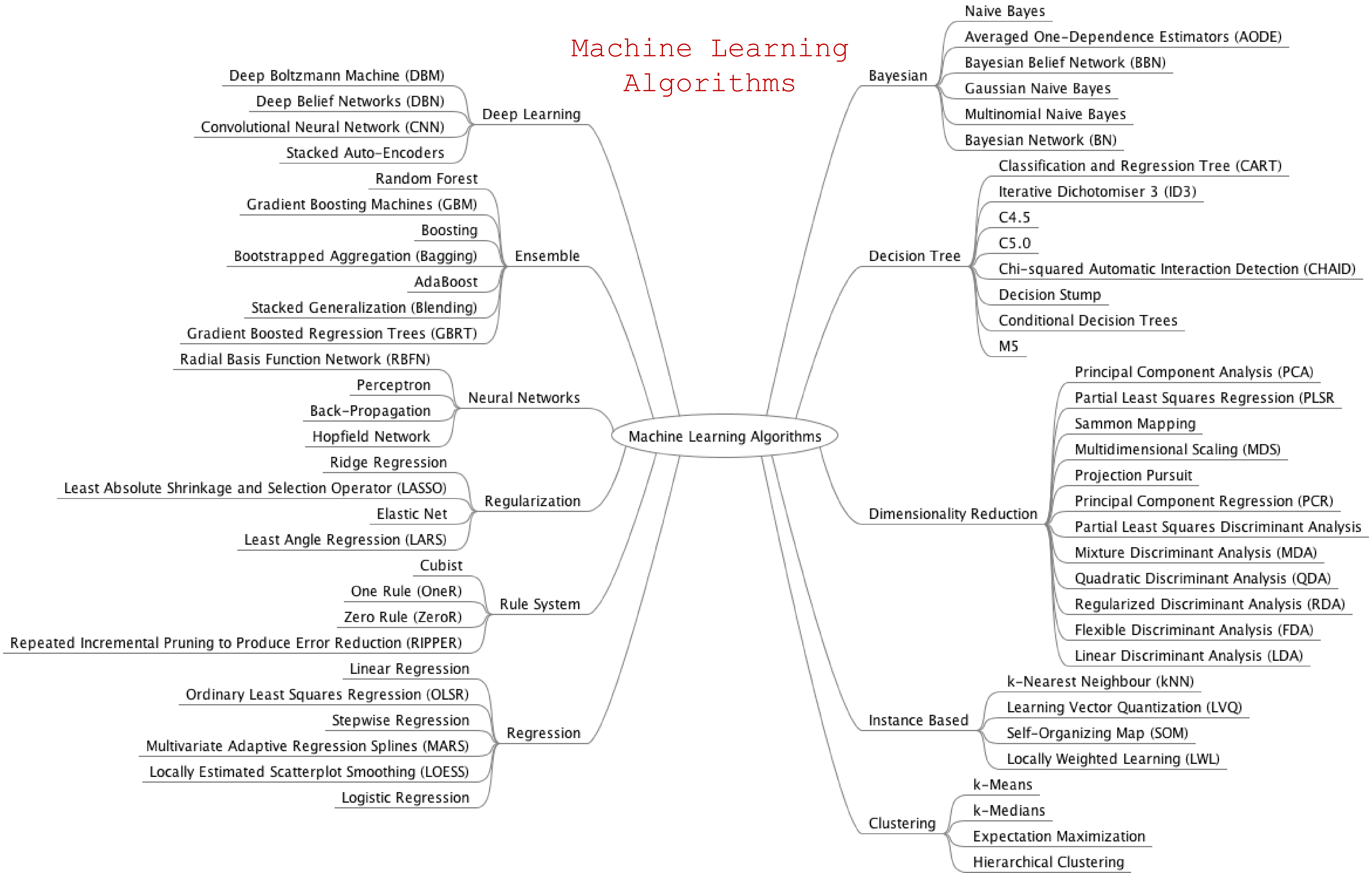
Predictive techniques: Unsupervised learning



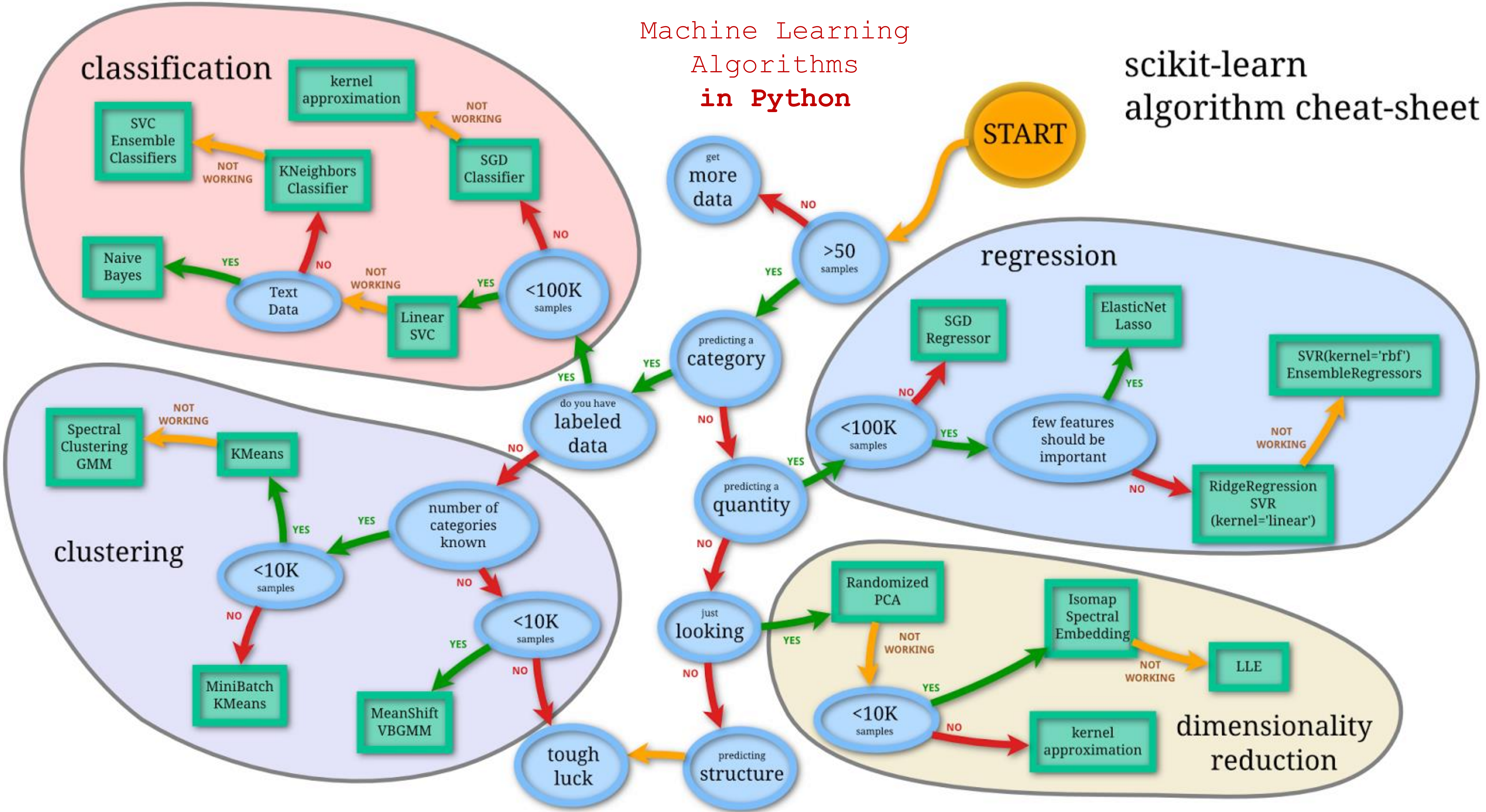
In unsupervised learning techniques available in Scikit-Learn (or Sklearn)

- 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



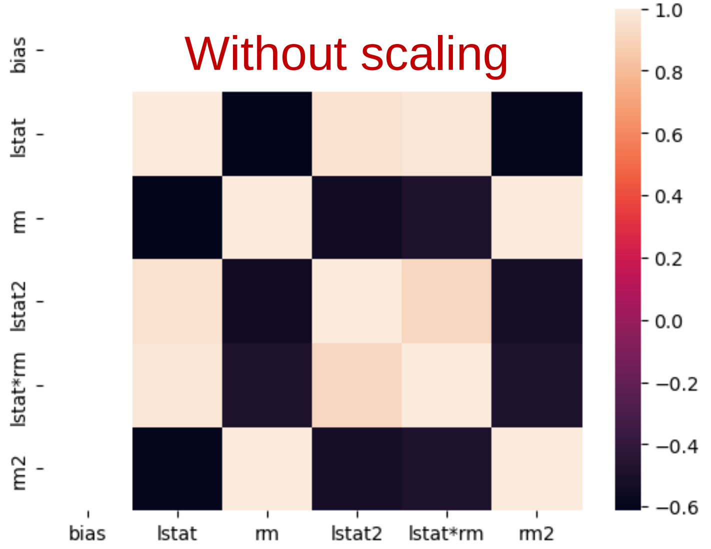
https://scikit-learn.org/stable/tutorial/machine_learning_map/index.html

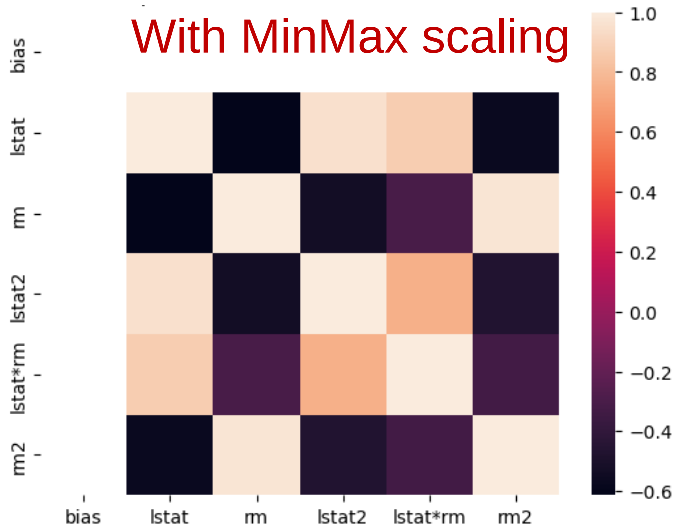
Evaluation metrics discussion

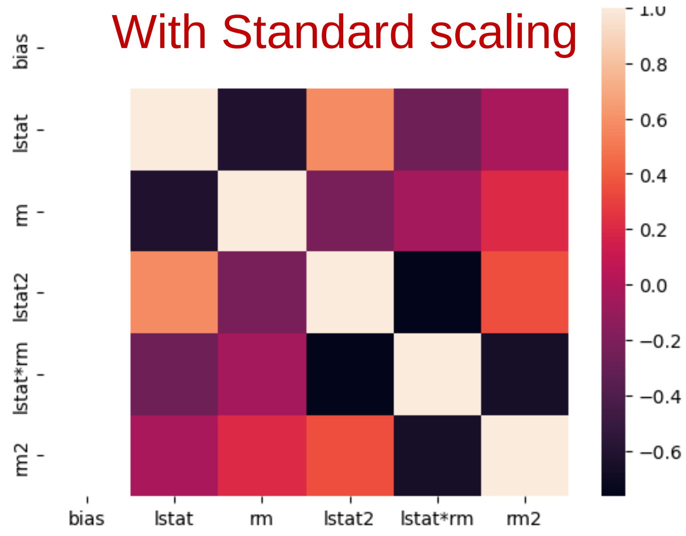
- The idea behind the squared (MSE) and the absolute error (MAE) is to avoid mutual cancellation of the positive and negative errors
  - MSE and MAE have only non-negative values
- In MSE, error is squared => prediction error is being heavily penalized
  - In case of data outliers, MSE will become much 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

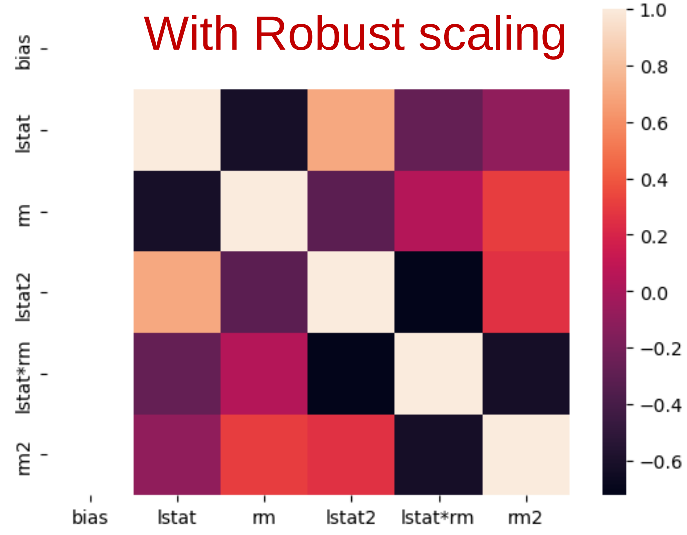
Scaling vs correlation

- Correlation among original features, power and interaction terms





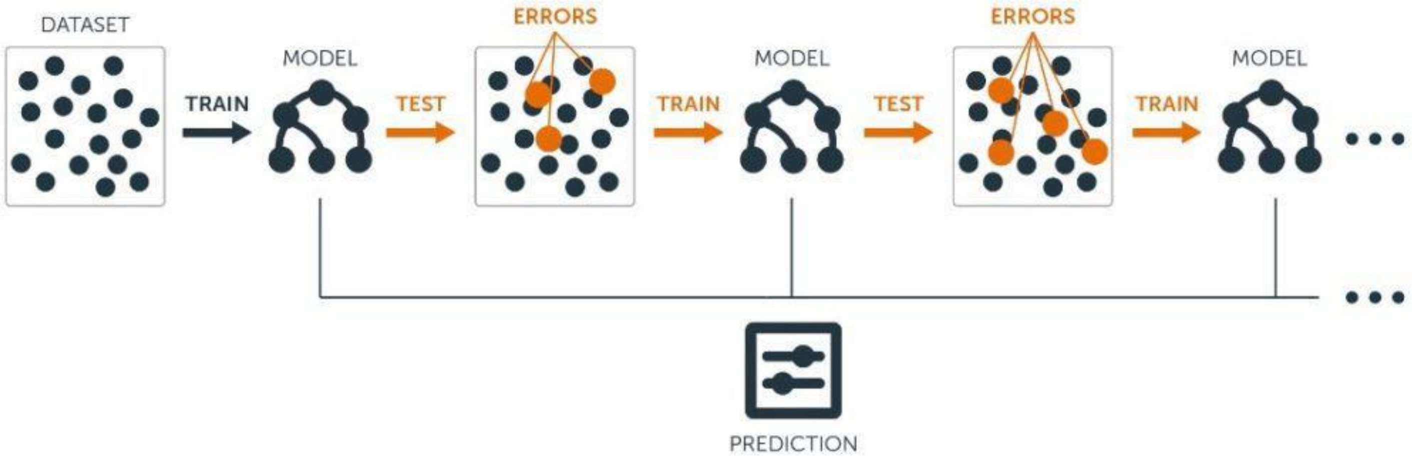




- There is minimal correlation when centering-based scalers (Standard, Robust) are applied
- Source code is found here

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

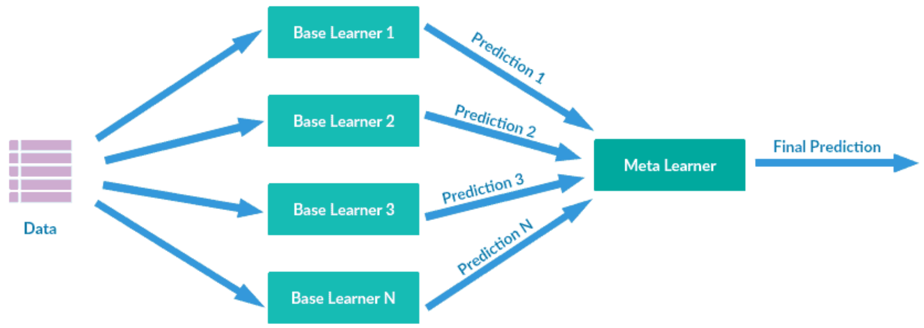


Basic Types of Ensemble Learning

- 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]()

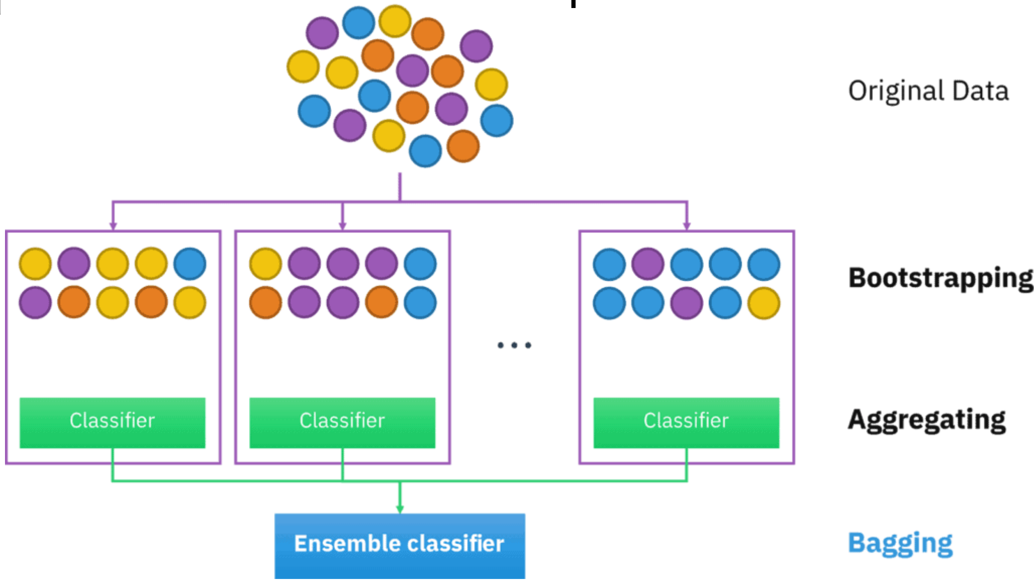
Random Forest Regression

- 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

Training dataset: D
N samples



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.