EN3150 Pattern Recognition
Learning from data and related challenges

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What is learning ?

"A computer program is said to learn from experience **E** with respect to some class of tasks **T** and performance measure **P,** if its performance at tasks in **T**, as measured by **P**, improves with experience **E** "[1]

experience **E**

performance measure **P**

tasks **T**

performance at tasks in **T**, as measured by **P**, improves with experience **E**

[1] Mitchell, Tom M. "Machine learning." (1997).

data preparation

Model training

Model Evaluation

Learning from data

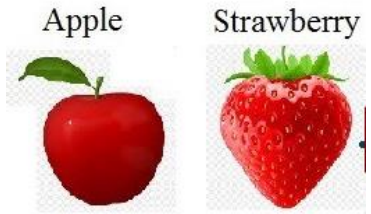
- There are different types of learning from data:
  - Supervised
  - Unsupervised
  - Semi-supervised
  - Reinforcement learning

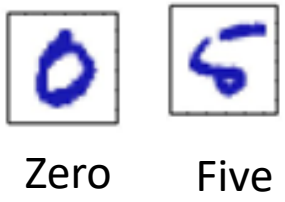
Learning from data: Supervised learning

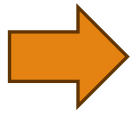
- Supervised learning:
  - The algorithm learns from labeled training data to make predictions or decisions.

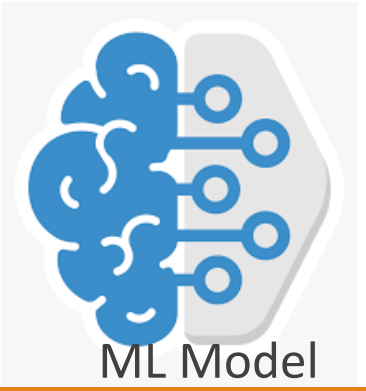
- Labeled training data?
  - The training data consists of input examples (also called features) along with their corresponding output labels (also called targets or ground truth).

- The goal of supervised learning is to learn a mapping function that can predict the correct output label for new, unseen input examples.





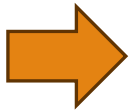


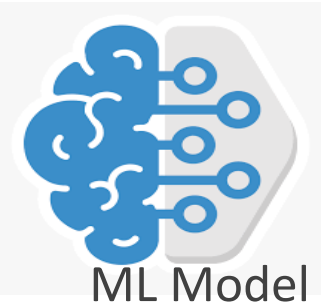


Learning from data: Supervised learning

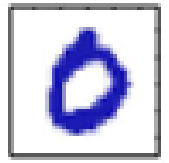
- Labeled training data
  - Handwritten digit - MNIST dataset

Zero Five





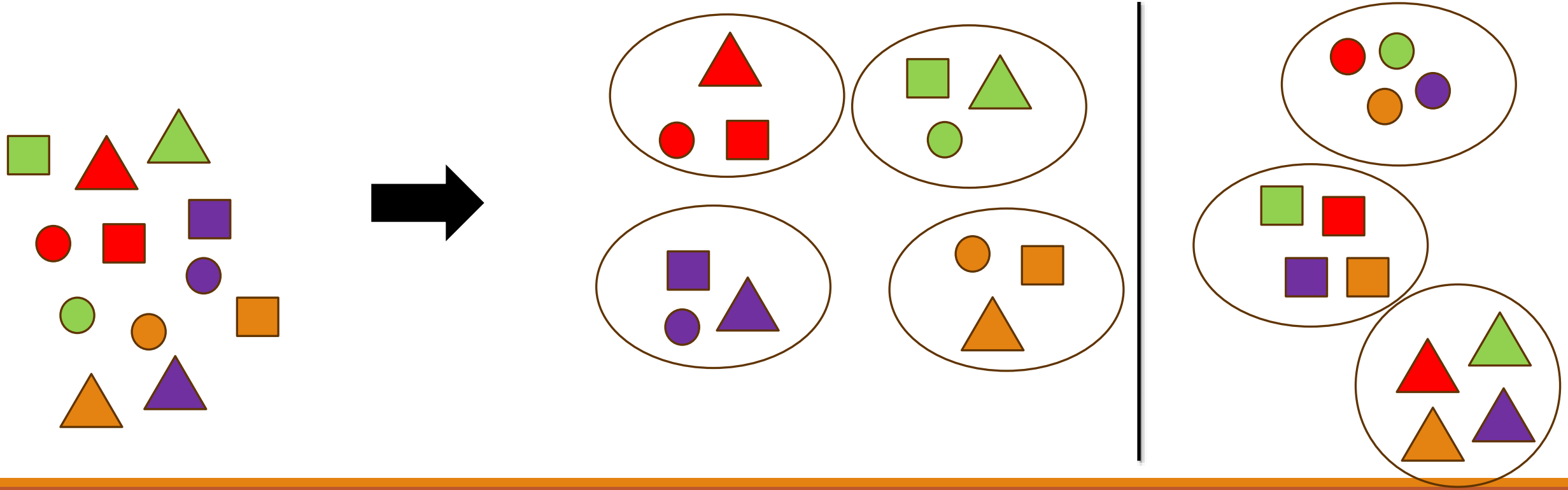
MNIST dataset
28x28 pixel images of handwritten digits (0 to 9) along with their corresponding labels.



0	0	1	...	781	782	783	label
0	0.0	0.0		0.0	0.0	0.0	5
1	0.0	0.0		0.0	0.0	0.0	0
2	0.0	0.0		0.0	0.0	0.0	4
3	0.0	0.0		0.0	0.0	0.0	1
4	0.0	0.0		0.0	0.0	0.0	9

Learning from data: Unsupervised learning

- Unsupervised learning involves training an algorithm on unlabeled data without explicit output labels
  - The algorithm's objective is to find patterns, structures, or relationships within the data.



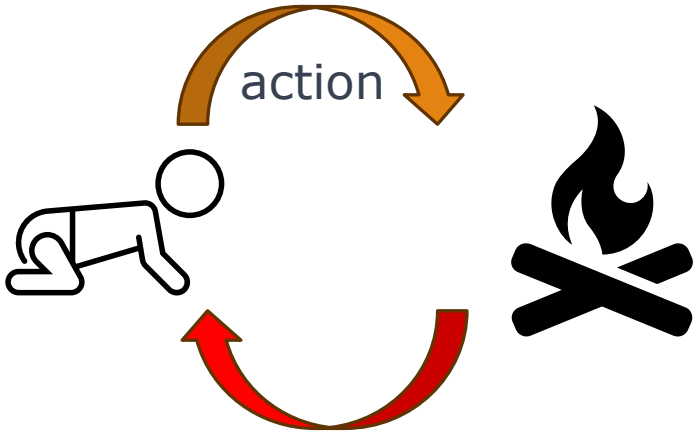
Learning from data: Semi-Supervised Learning

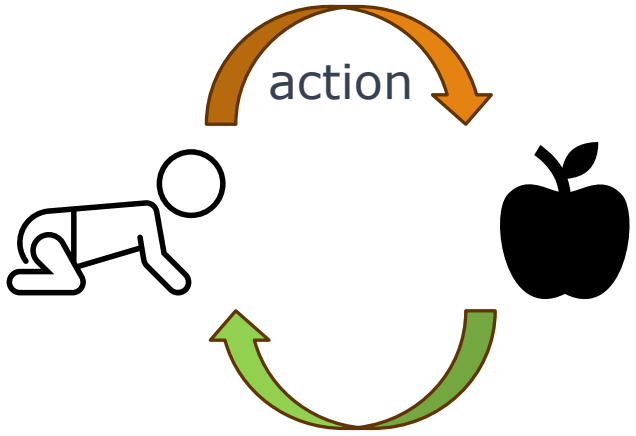
- Semi-supervised learning: supervised + unsupervised learning.

- Training data contains a mixture of labeled and unlabeled examples.

Learning from data: Reinforcement Learning

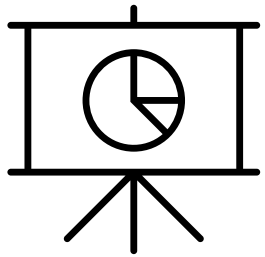
- An agent learns to make decisions by interacting with an environment.
- The agent receives feedback in the form of rewards or penalties based on its actions.
- The goal of the agent is to learn an optimal policy that maximizes the cumulative reward over time.



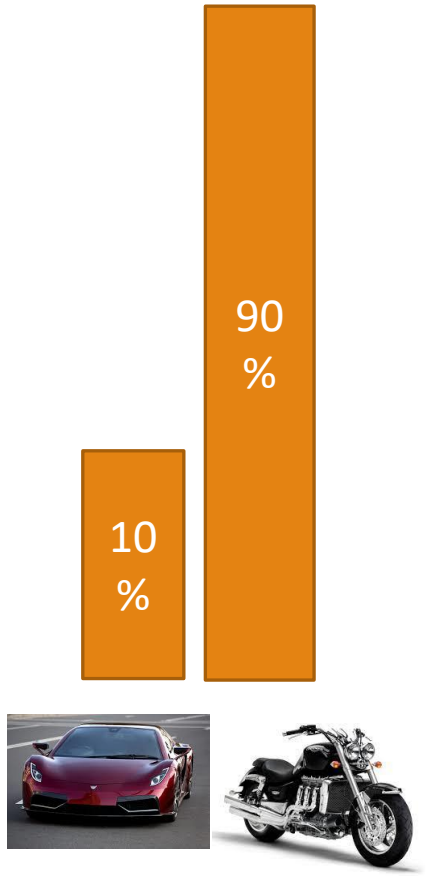


Supervised vs Unsupervised learning

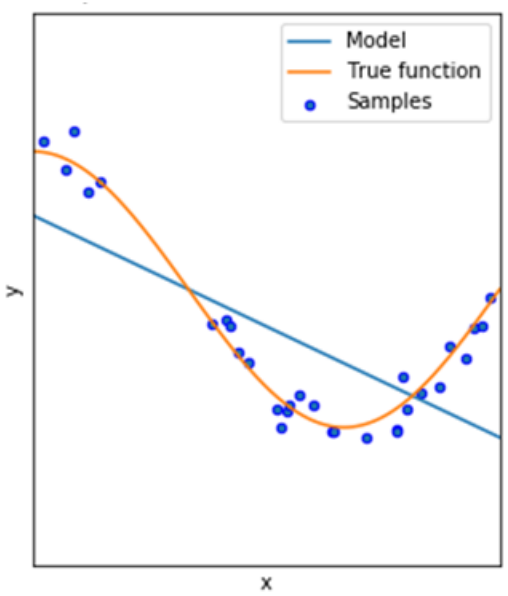
Supervised	Unsupervised
Uses labeled input and output data	Labels are not available
Well-defined objective (As labels are given, so you know possible type of results to expect)	May discover hidden relationships
	Can be used to learn meaningful representations or features from raw data
human intervention is required to label data	
If you have labeled data and a clear target variable to predict, use supervised learning for accurate predictions	If you have large amounts of unlabeled data and want to find patterns or groupings in the data, opt for unsupervised learning
If you have a mix of labeled and unlabeled data, or the cost of labeling data is high, consider using semi-supervised learning to leverage both types of data	



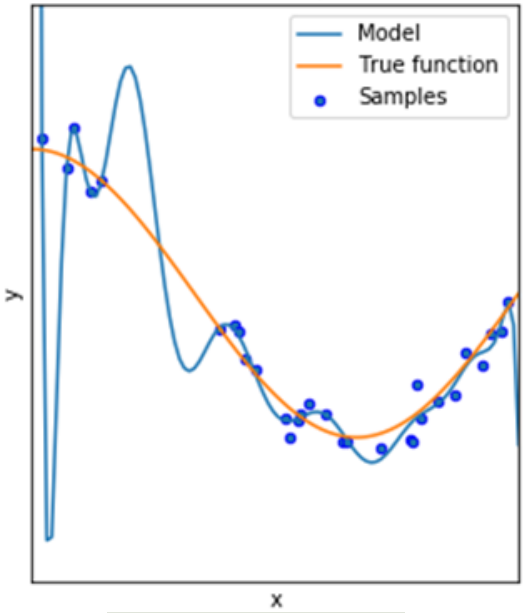
Learning from data and related challenges



- Data Quality and Quantity
  - Noisy, incomplete data can lead to inaccurate and unreliable predictions.
  - Often requires large amount of data
- Data Imbalance:
  - E.g, in classification imbalance classes
    - May lead to poor performance



Underfitting



Overfitting

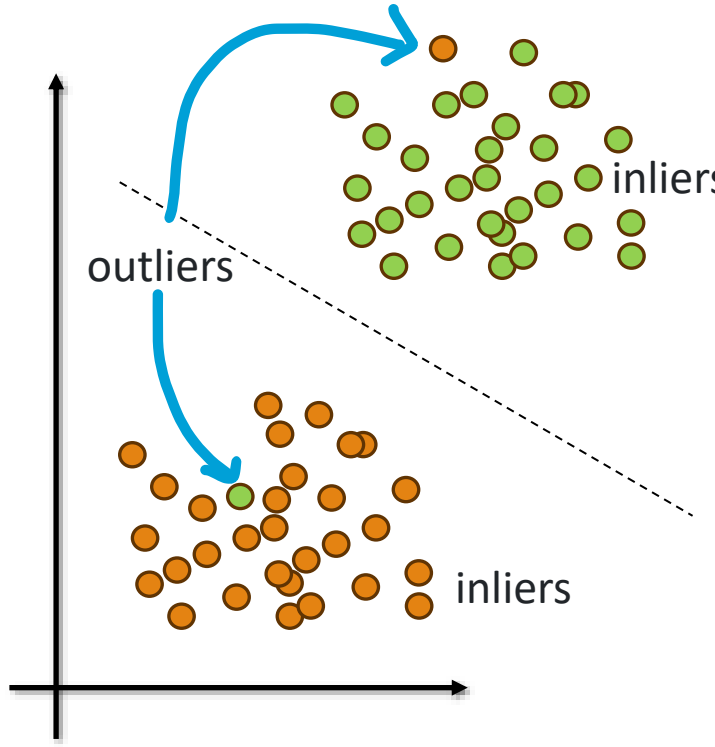
Learning from data and related challenges

- Overfitting: Overfitting occurs when a model performs exceptionally well on the training data but fails to generalize to new, unseen data.
- Underfitting: When a model is too simplistic to capture the underlying patterns in the data.
- Generalization: Ensuring that machine learning models generalize well to new, unseen data.

Data preparation

- Data cleaning: Handle missing or inconsistent data
  - Approaches:
    - Removing them
    - Filling with zeros/mean/median,
    - Interpolation
- Data cleaning: outlier* detection and removing

- Data Preprocessing: Feature scaling (E.g. normalization)
- Data Preprocessing: Dimensionality reduction
  - Principal Component Analysis (PCA)



*An outlier in a dataset refers to a data point that deviates significantly from the majority of the other data points.

Data preparation

- Data Augmentation: Artificially expand the size and diversity of a given dataset.
  - E.g Image rotation, flipping, scaling, cropping ➔ New image

- Imbalanced Data:
  - Undersampling of majority class
  - Generating synthetic samples of the minority class

Data preprocessing example

- https://scikit-learn.org/stable/modules/preprocessing.html

1. Standardization: scale the features of a dataset to have zero mean and unit variance.
2. Scaling features to a range e.g., between 0 and 1
   - Min max scalar ➔ [0, 1]
   - Max Abs Scaler ➔ [-1, 1]

$$\text{Standardization}(x) = \frac{x - \text{mean}(x)}{\text{std}(x)}$$

$$\text{MinMaxScaler}(x) = \frac{x - \min(x)}{\max(x) - \min(x)}$$

$$\text{MaxAbsScaler}(x) = \frac{x}{\max(|x|)}$$

If outliers are there, will it work?

Suggestions?

Data preprocessing example

California Housing Dataset

```
import pandas as pd
from sklearn.datasets import fetch_california_housing
```

Use pandas df.describe() to get followings

	MedInc	AveOccup
count	20640	20640
mean	3.870671	3.070655
std	1.899822	10.386050
min	0.499900	0.692308
25%	2.563400	2.429741
50%	3.534800	2.818116
75%	4.743250	3.282261
max	15.000100	1243.333333

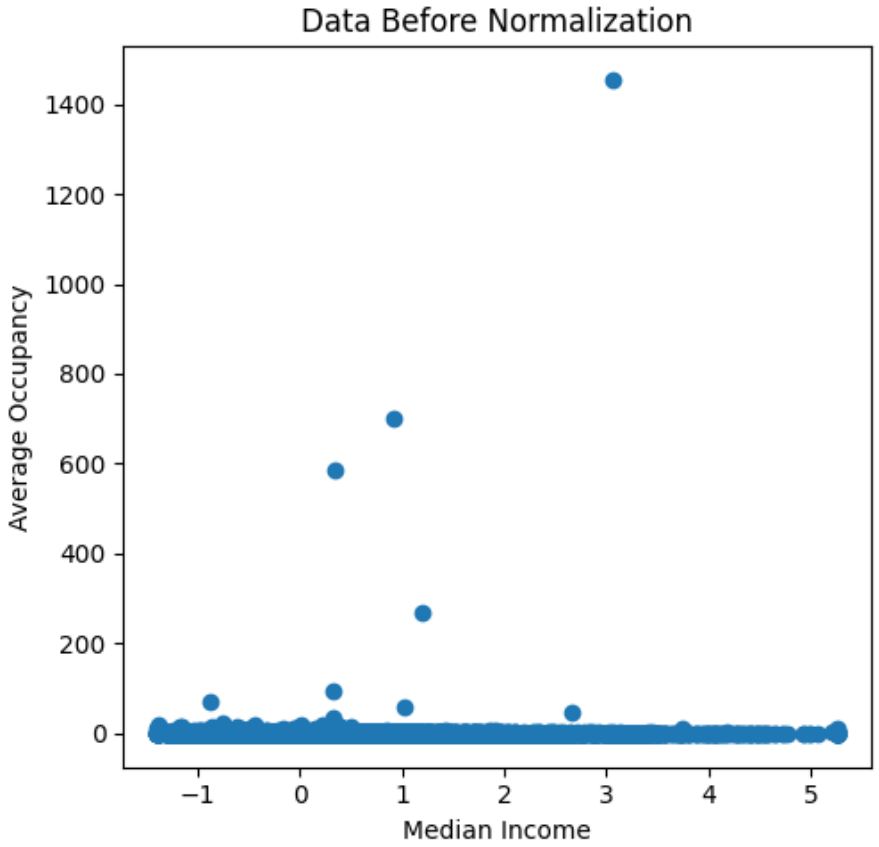
Independent variables

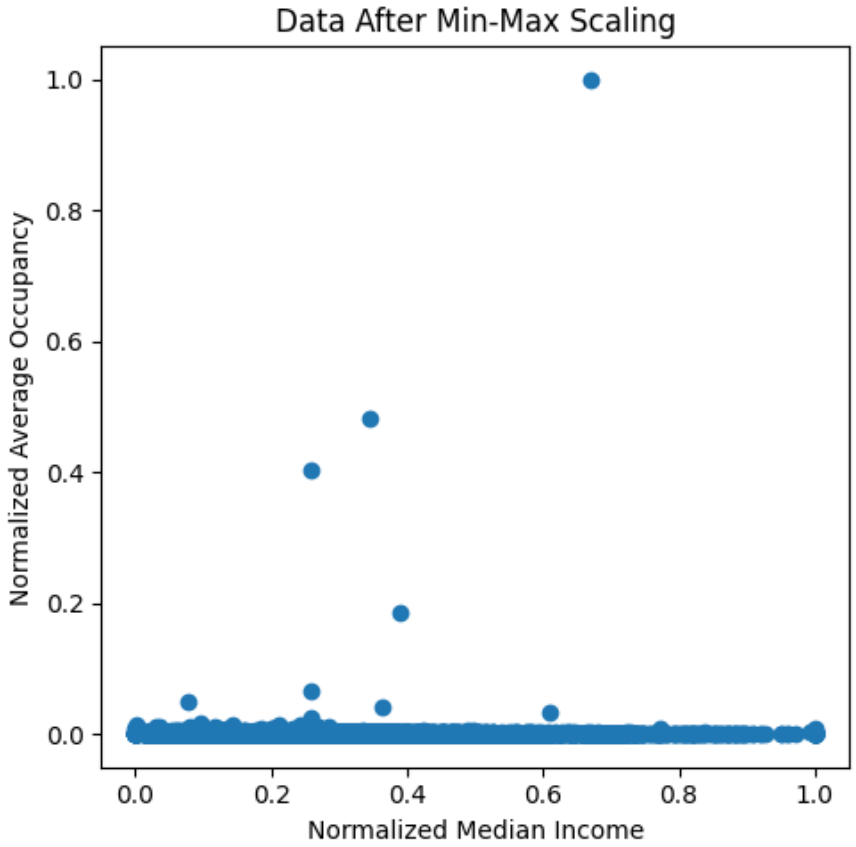
1. MedInc Median income in block group (measured in tens of thousands of US Dollars)
2. HouseAge Median house age in block group (a lower number is a newer building)
3. AveRooms Average number of rooms per household
4. AveBedrms Average number of bedrooms per household
5. Population Block group population
6. AveOccup Average number of household members
7. Latitude Block group latitude (a higher value is farther north)
8. Longitude Block group longitude (a higher value is farther west)

Dependent variable

1. medianHouseValue Median house value for households within a block (measured in US Dollars)

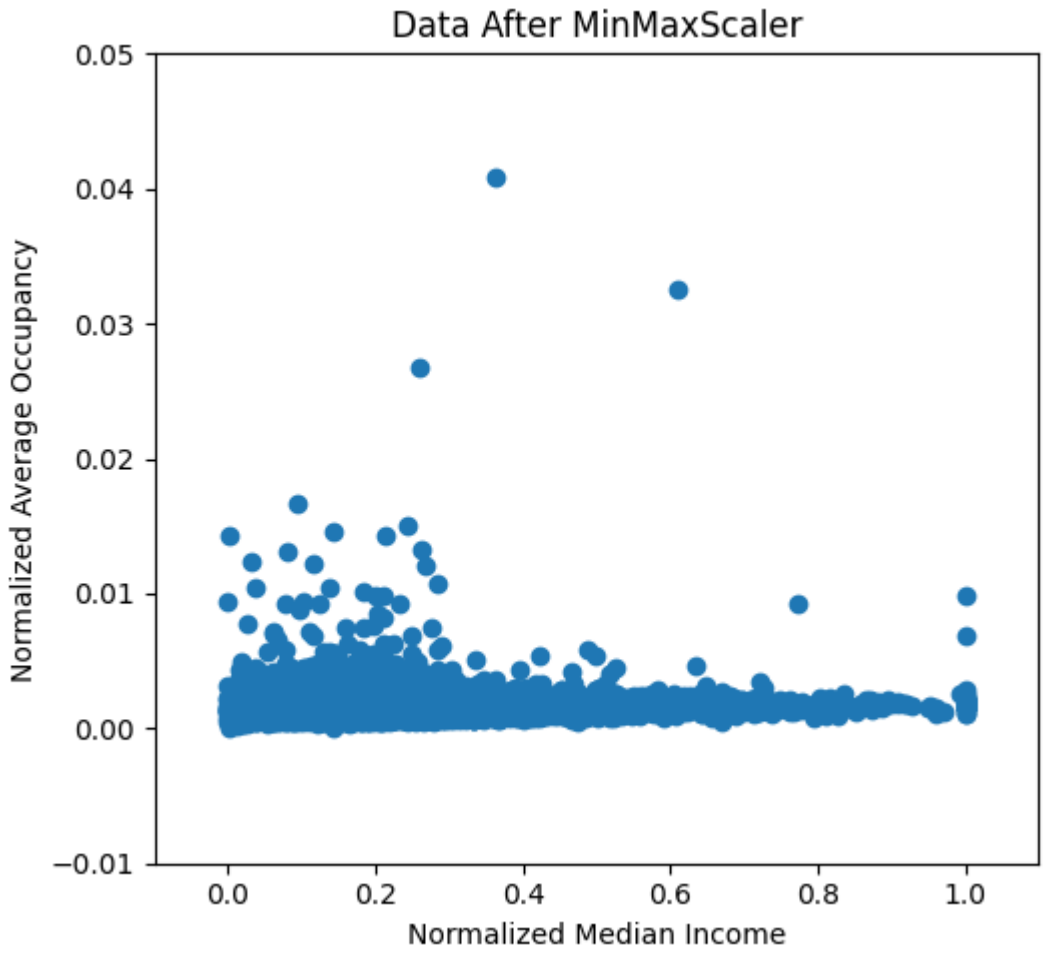
Data preprocessing example: Min-max Scaler





	MedInc	AveOccup
count	20640.000	20640.000
mean	0.232	0.002
std	0.131	0.008
min	0.000	0.000
25%	0.142	0.001
50%	0.209	0.002
75%	0.293	0.002
max	1.000	1.000

Data preprocessing example: Min-max Scaler



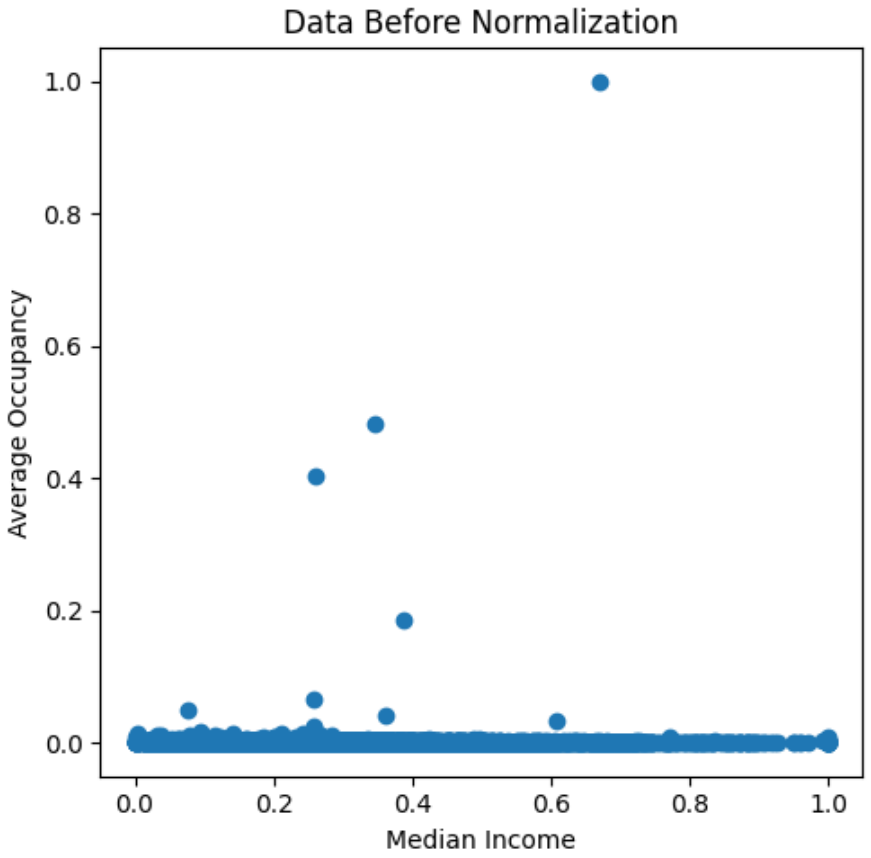
Min-max Scaler

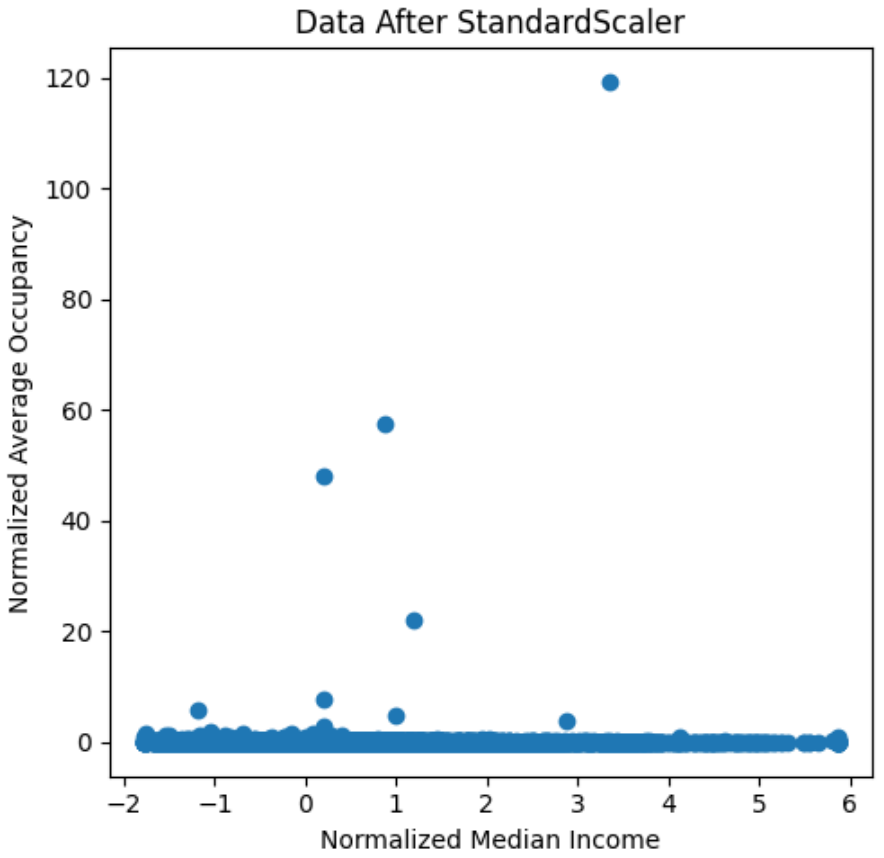
Average Occupancy: Inliers in narrow range [0, 0.005]

Features scales differently

Balanced feature scales cannot be guaranteed with outliers

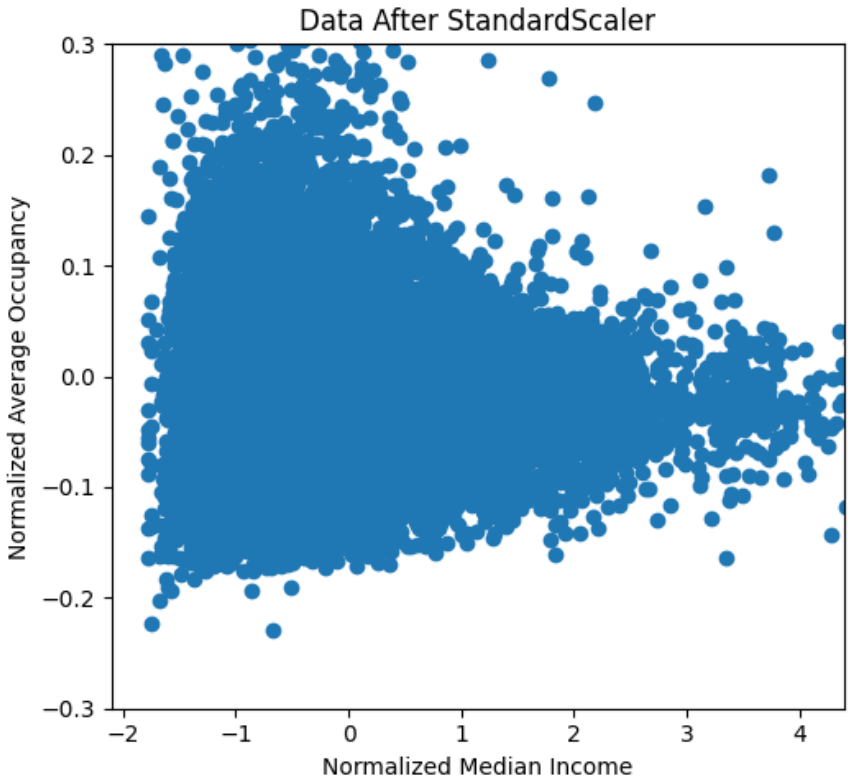
Data preprocessing example: Standard Scaler





	MedInc	AveOccup
count	20640.000	20640.000
mean	0.000	0.000
std	1.000	1.000
min	-1.774	-0.229
25%	-0.688	-0.062
50%	-0.177	-0.024
75%	0.459	0.020
max	5.858	119.419

Data preprocessing example: Standard Scaler

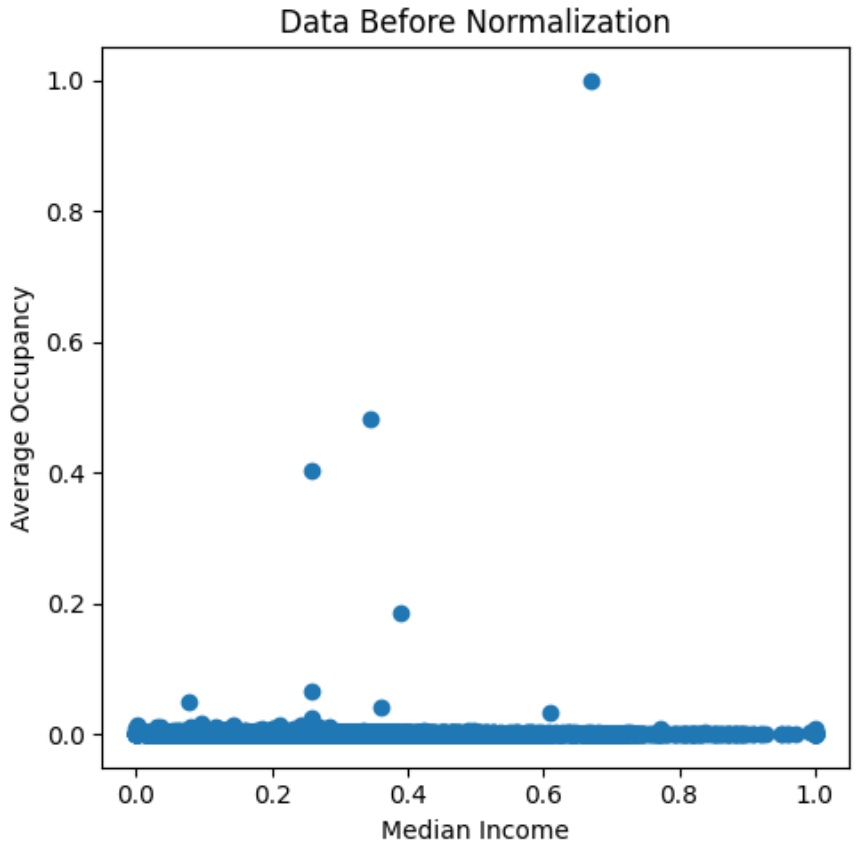


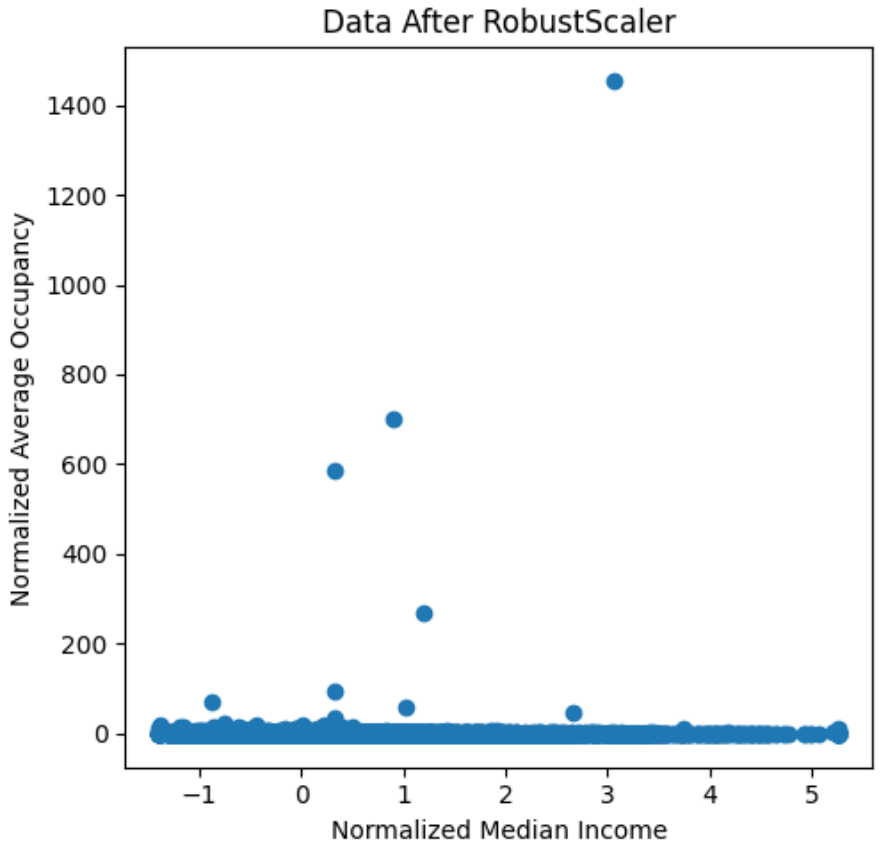
Standard Scaler
Average Occupancy:[-0.2, 0.2]
Median Income [-2, 4]

Features scales differently

Balanced feature scales cannot be guaranteed with outliers

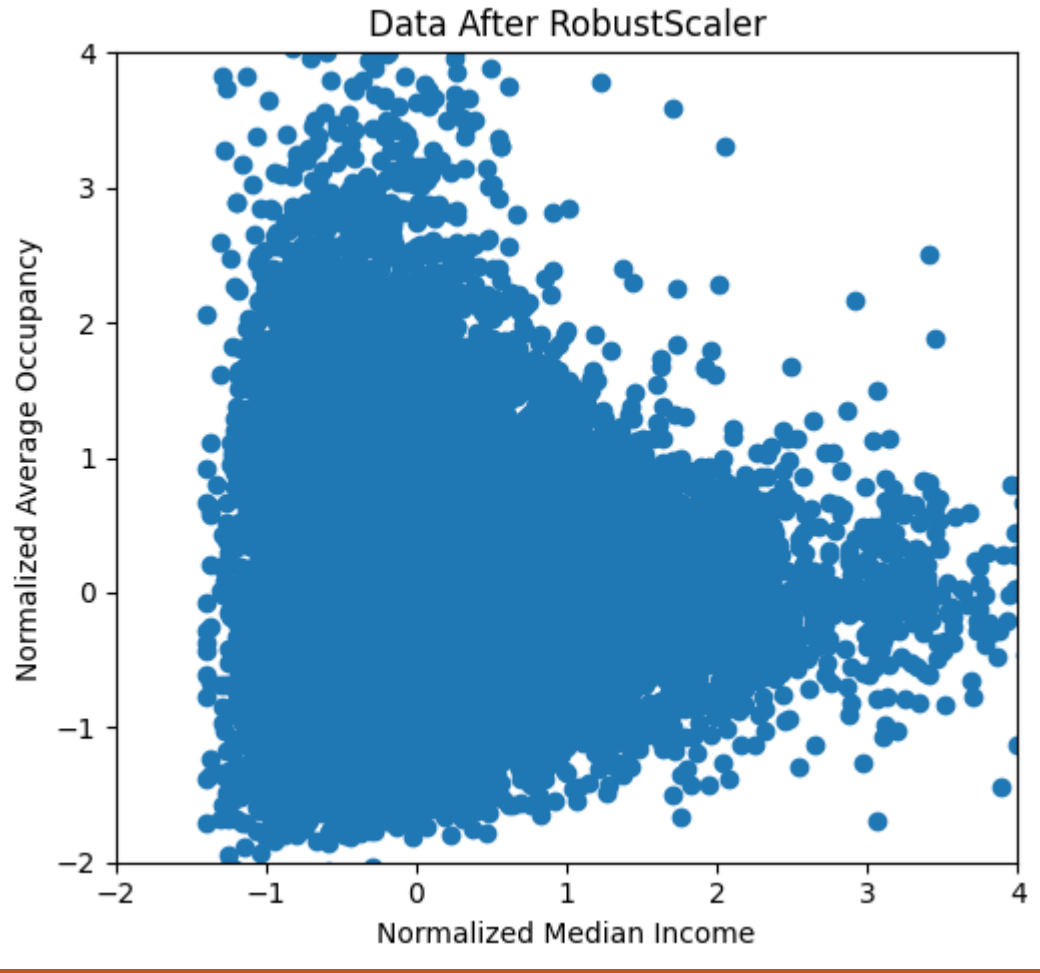
Data preprocessing example: Robust Scalar





	MedInc	AveOccup
count	20640.000	20640.000
mean	0.154	0.296
std	0.872	12.183
min	-1.392	-2.494
25%	-0.446	-0.456
50%	0.000	0.000
75%	0.554	0.544
max	5.260	1455.116

Data preprocessing example: Robust Scalar



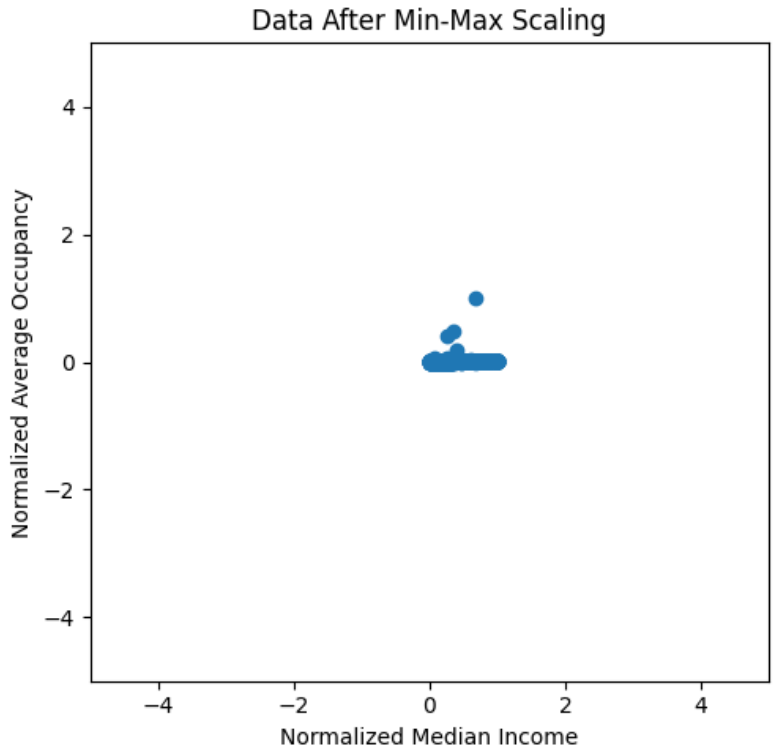
Robust Scaler
Most of data points in both features in range of [-2, 3]

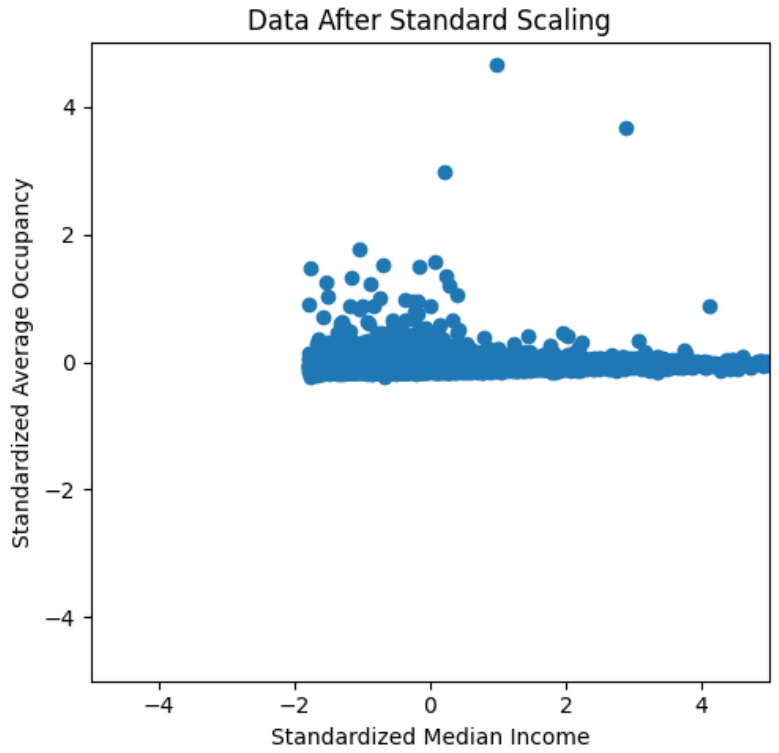
Features scales similarly with outliers as well

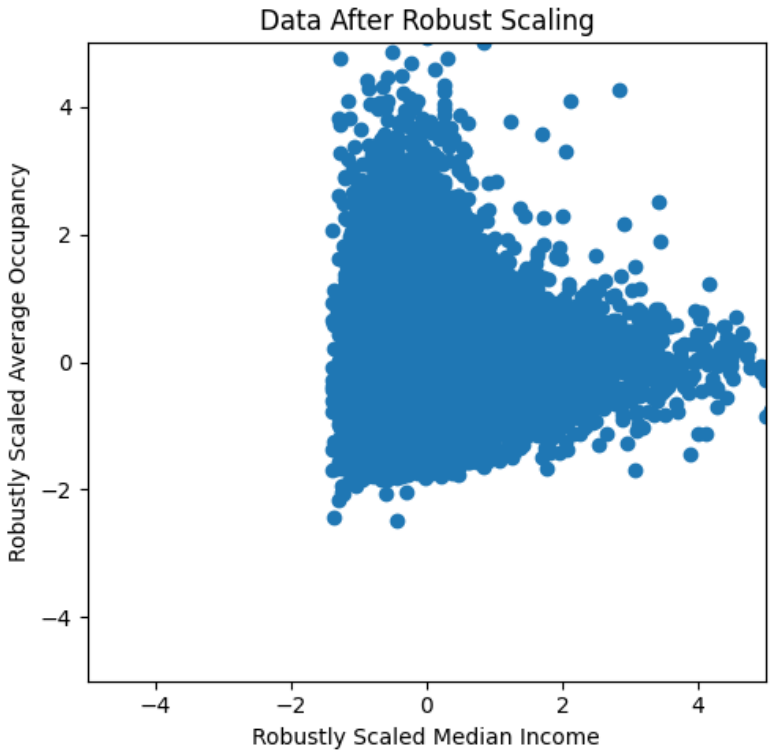
Still outliers are there

[sklearn.preprocessing.RobustScaler — scikit-learn 1.3.0 documentation]

Data preprocessing example: Robust Scalar





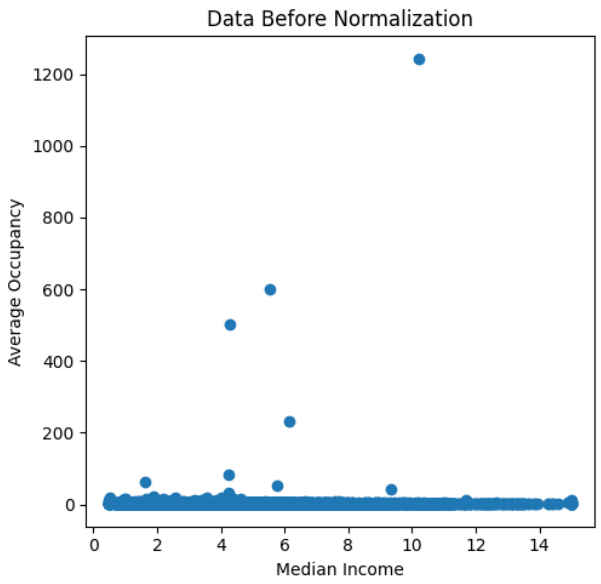


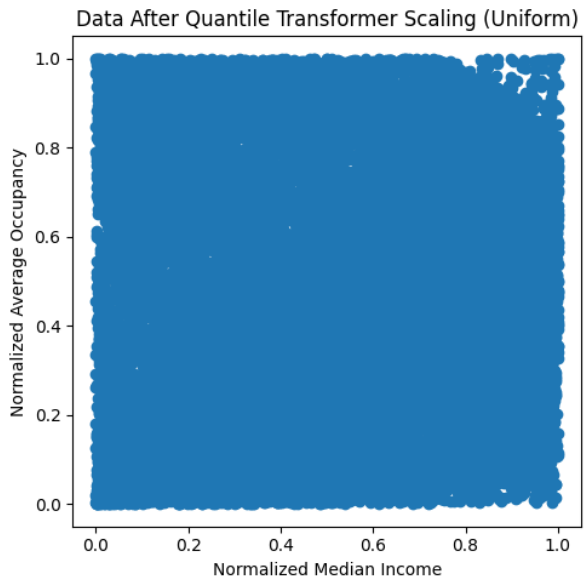
Min-max Scaler
Average Occupancy: Inliers in narrow range [0, 0.005]

Standard Scaler
Average Occupancy:[-0.2, 0.2]
Median Income [-2, 4]

Robust Scaler
Most of data points in both features in range of [-2, 3]

Data preprocessing example: Quantiles information





[sklearn.preprocessing.QuantileTransformer — scikit-learn 1.3.0 documentation]

	MedInc	AveOccup
count	20640.000	20640.000
mean	0.500	0.500
std	0.289	0.289
min	0.000	0.000
25%	0.250	0.250
50%	0.500	0.500
75%	0.750	0.750
max	1.000	1.000

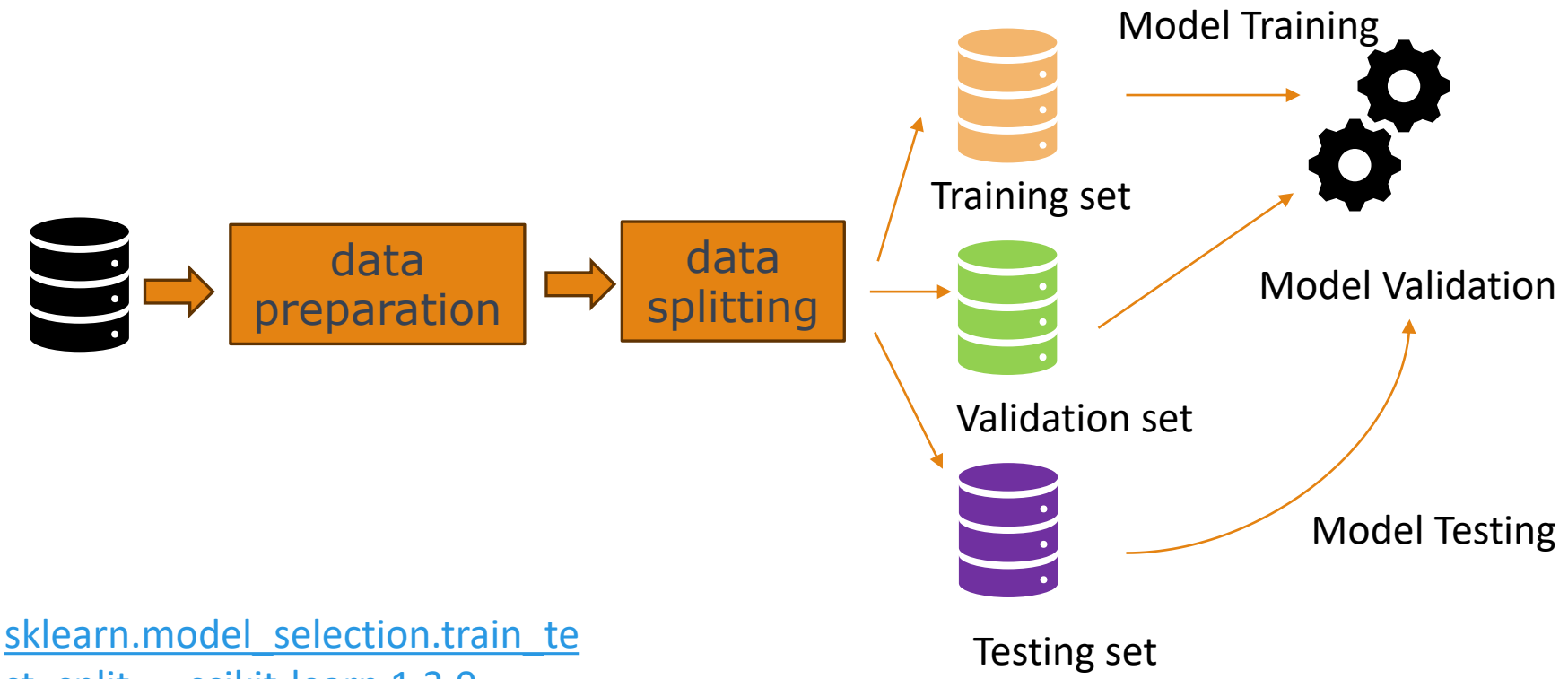
	MedInc	AveOccup
count	20640.000	20640.000
mean	0.004	-0.000
std	1.024	0.999
min	-5.199	-5.199
25%	-0.675	-0.675
50%	-0.000	-0.000
75%	0.674	0.675
max	5.199	5.199

- Non-linear transformation
- spreads out the most frequent values in each feature, aiming to follow a uniform or normal distribution.
- It reduces the impact of outliers, making it a robust preprocessing technique.
- The transformation is applied independently to each feature.
- It estimates the cumulative distribution function of a feature to map original values to a uniform/normal distribution.
- The obtained values are then mapped to the desired output distribution using the associated quantile function.

Homework

- Task: Comparing Data Normalization Methods (See course page in Moodle)

ML Training Process (Supervised Learning)



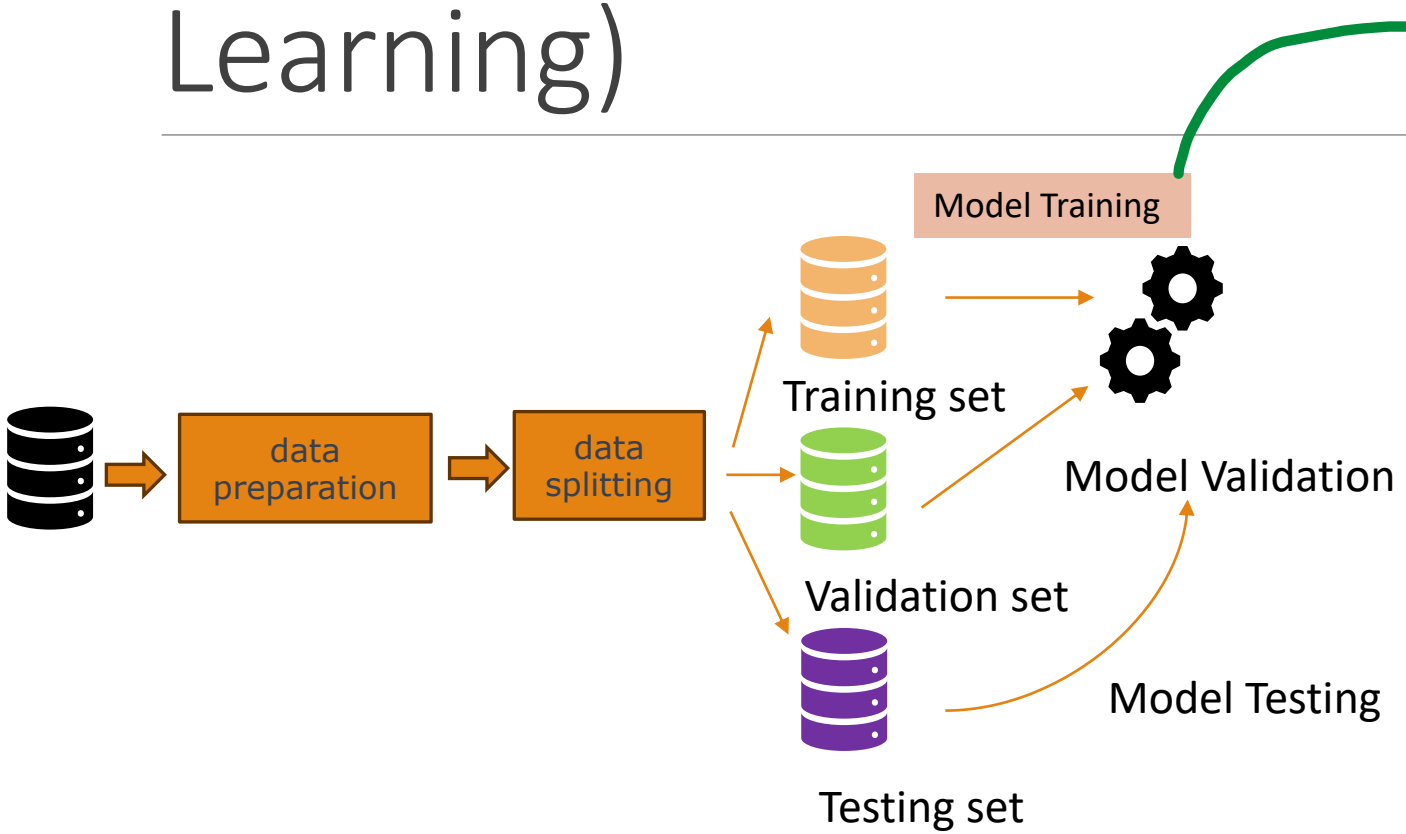
Performance evaluation

- Accuracy
- Precision
- Recall
- F1-Score

- Mean Absolute Error (MAE)
- Mean Squared Error (MSE)
- Root Mean Squared Error (RMSE)

[sklearn.model_selection.train_test_split — scikit-learn 1.3.0 documentation]

ML Training Process (Supervised Learning)



Loss Functions

Used to see how different the guesses made by a machine learning model are from the actual correct answers

- Mean Squared Error (MSE)
- Mean Absolute Error (MAE)
- Binary Cross-Entropy (Log Loss)
- Categorical Cross-Entropy
- Sparse Categorical Cross-Entropy
- Hinge Loss
- Kullback-Leibler Divergence (KL Divergence)
- Huber Loss
- Triplet Loss
- Ranking Losses (e.g., Hinge Rank Loss, RankNet Loss))

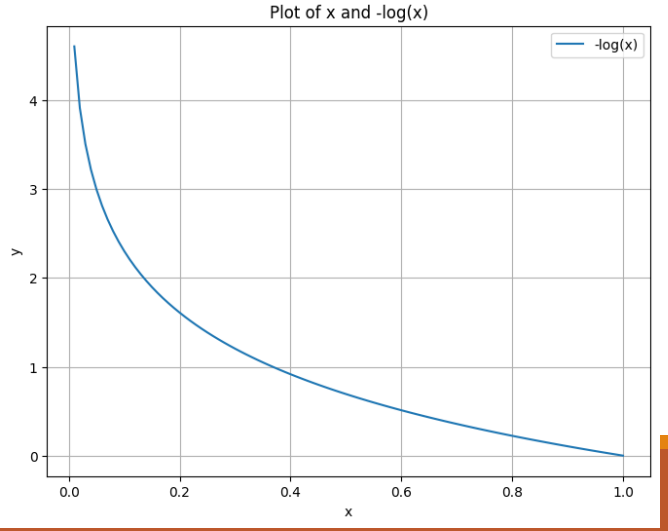
ML Training Process (Supervised Learning)

- Mean Squared Error (MSE)
- Mean Absolute Error (MAE)
- Binary Cross-Entropy (Log Loss) (BCE)
- Categorical Cross-Entropy (CCE)
- Sparse Categorical Cross-Entropy
- Hinge Loss
- Kullback-Leibler Divergence (KL Divergence)
- Huber Loss
- Triplet Loss
- Ranking Losses (e.g., Hinge Rank Loss, RankNet Loss))

$$MSE = \frac{1}{n}\sum_{i=1}^{n}(y_i - \hat{y}_i)^2 \qquad MAE = \frac{1}{n}\sum_{i=1}^{n}|y_i - \hat{y}_i|$$

$$BCE = -\frac{1}{n}\sum_{i=1}^{n}[y_i \log(\hat{y}_i) + (1 - y_i)\log(1 - \hat{y}_i)]$$

$$CCE = -\frac{1}{n}\sum_{i=1}^{n}\sum_{j=1}^{C} y_{i,j}\log(\hat{y}_{i,j})$$



y_i	True target value
$\hat{y}_i$	Predicted value
n	Number of samples in the dataset
C	Number of classes
$y_{i,j}$	One-hot encoded true label for class j
$\hat{y}_{i,j}$	Predicted probability for class j

How to evaluate a model

- Accuracy, Precision, Recall, and F-Score

		Predicted class		
		Positive (+)	Negative (-)	Total
True class	Positive (+)	True Pos. (TP)	False Neg. (FN)	P
	Negative (-)	False Pos. (FP)	True Neg. (TN)	N
Total		P*	N*	

type I error, false alarm

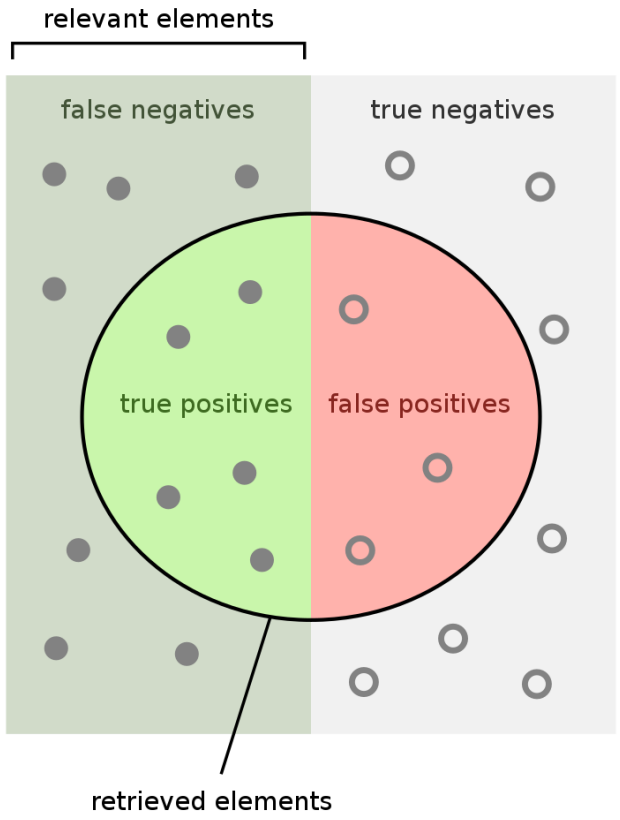
type II error, miss

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

$$\text{Recall} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

$$F_1 = \frac{2}{\left(\frac{1}{\text{Precision}} + \frac{1}{\text{Recall}}\right)}$$

$$\text{Accuracy} = \frac{\text{TP} + TN}{\text{TP} + \text{TN} + \text{FP} + FN}$$



How many retrieved items are relevant?

Precision =

How many relevant items are retrieved?

Recall =

Accuracy can be a misleading metric for imbalanced data sets.

A higher precision indicates a lower rate of false positives, which means the model is making fewer incorrect positive predictions.

A higher recall indicates a lower rate of false negatives, meaning the model is correctly identifying more positive instances

https://en.wikipedia.org/wiki/Precision_and_recall

How to evaluate a model

- Accuracy, Precision, Recall, and F-Score

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

$$\text{Recall} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

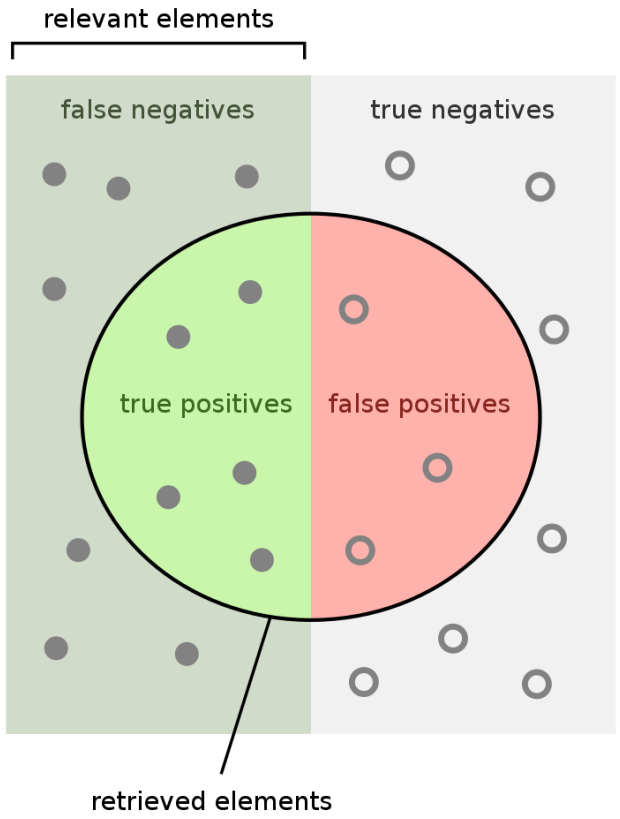
$$F_1 = \frac{2}{\left(\frac{1}{\text{Precision}} + \frac{1}{\text{Recall}}\right)}$$

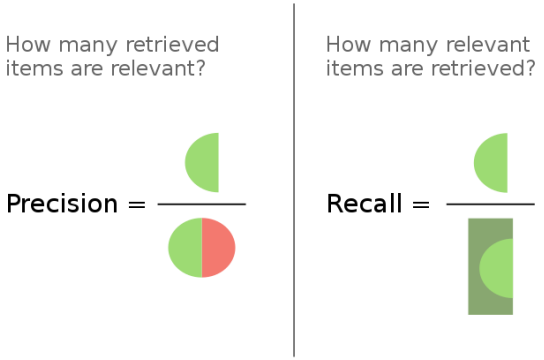
$$\text{Accuracy} = \frac{\text{TP} + TN}{\text{TP} + \text{TN} + \text{FP} + FN}$$

Higher F1-score values indicate a better balance between precision and recall

Higher precision and recall values are generally desired (Application dependent)

- Some scenarios, higher precision (lower rate of false positives (false alarm)) may be more critical (e.g., medical diagnosis)
- Some scenarios, higher recall (lower rate of false negatives (miss)) may be more important (e.g., fraud detection).



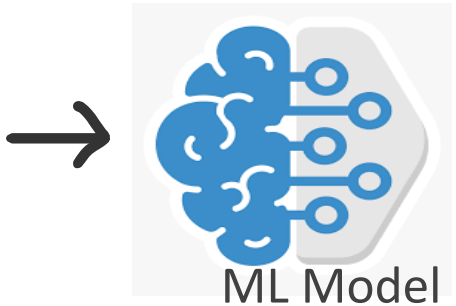


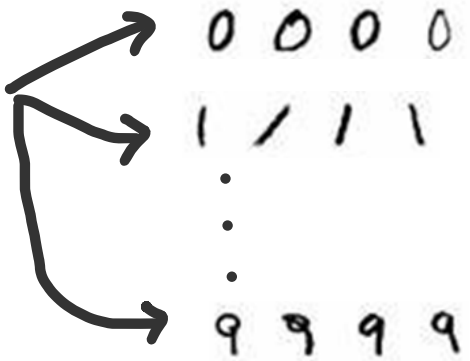
https://en.wikipedia.org/wiki/Precision_and_recall

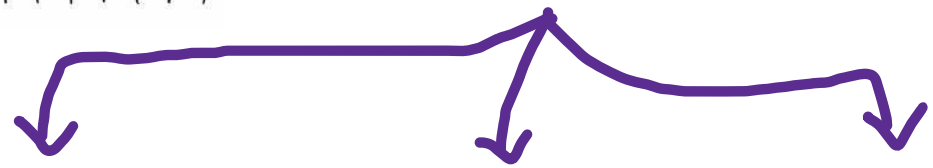
Model selection

- Model selection is the process of choosing the best model from a set of candidate models for a specific task.

Sample of the MNIST dataset of handwritten digits (https://en.wikipedia.org/wiki/MNIST_database)





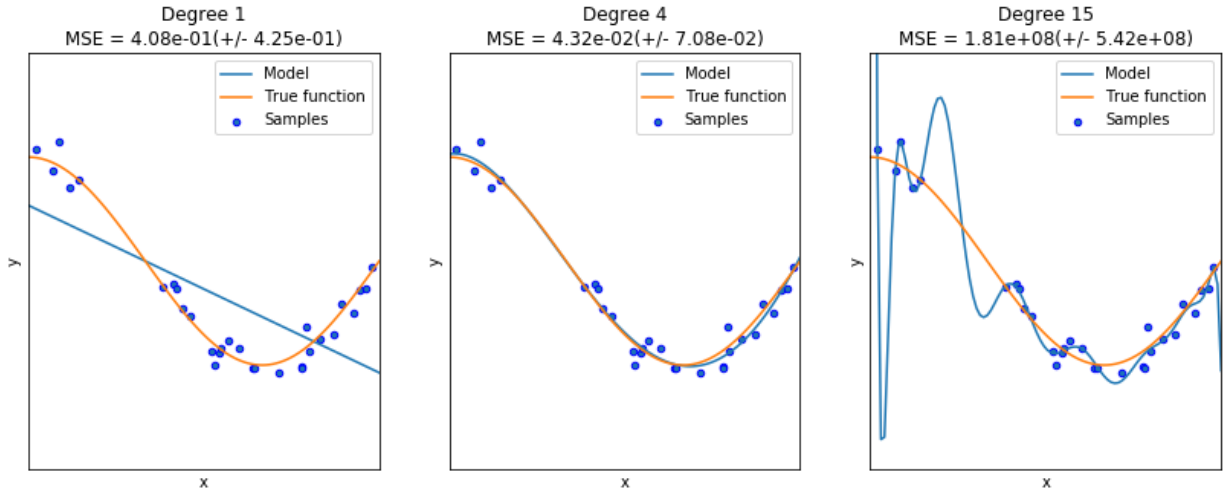


Convolutional Neural Networks (CNNs)

Decision Trees

k-Nearest Neighbors (k-NN)

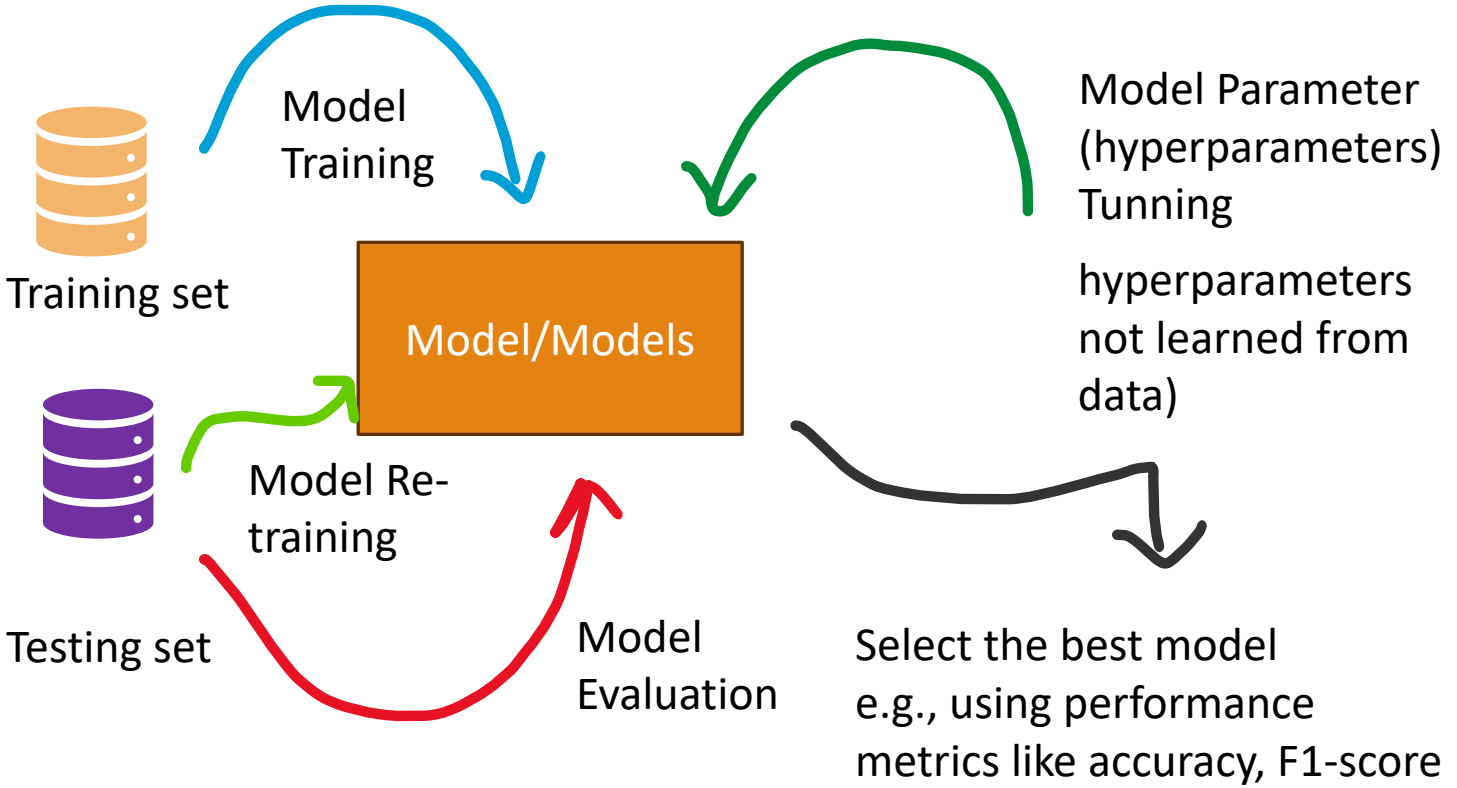
Model selection

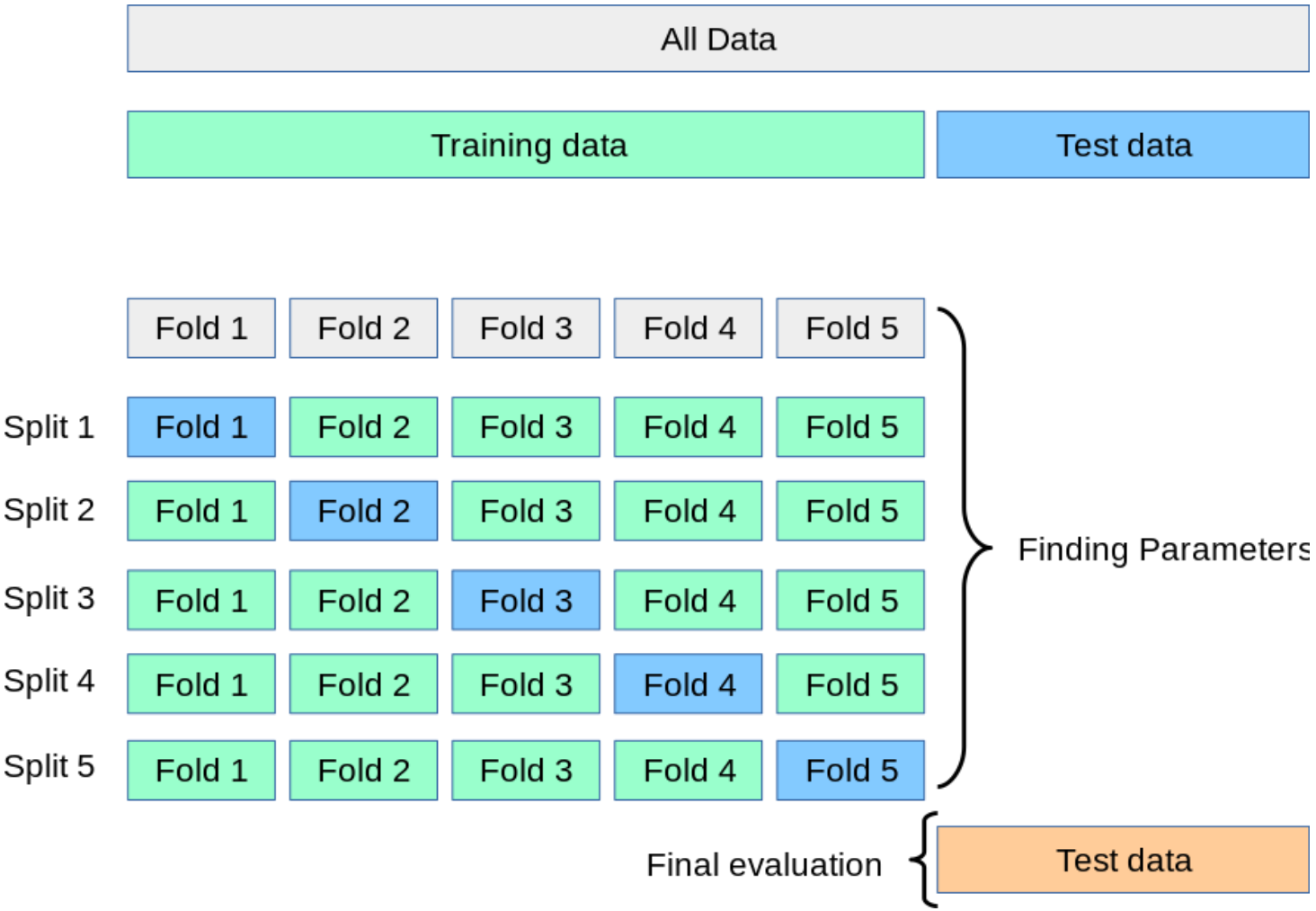


- Hyperparameters (parameters that are set before the training process begins)
  - E.g., Learning Rate
- Hyperparameters not learned from data

Model selection

- Model selection is the process of choosing the best model from a set of candidate models for a specific task.





Model selection

Resampling technique:- k-fold cross validation (k-CV)

- The dataset is divided into k subsets (folds) of approximately equal size.
- The model is trained and evaluated k times, each time using a different fold as the test set and the rest as the training set.
- For each iteration, the model is trained on (k-1) folds and evaluated on the remaining fold.

Image from scikit-learn.org

Model selection:

Resampling technique:- k-fold cross validation (k-CV)

- Reduced Overfitting: Mitigates overfitting by testing the model on unseen data subsets. Ensures better generalization to new data.
- Evaluates model performance for various hyperparameter settings.
- Helps to identify the best hyperparameters for optimal model performance
- Allows fair and consistent evaluation of multiple models
- Maximizes data utilization for both training and testing
- Ensures all available data contributes to model evaluation

Model selection:- Hyper parameter tuning-Grid Search

- Grid Search involves defining a grid of hyperparameter values to explore.
- It systematically evaluates all possible combinations from the grid to identify the best-performing one
- To avoid overfitting during Grid Search, cross-validation is commonly used.
- Grid Search can be computationally expensive when the hyperparameter space is large.

Image from scikit-learn.org

Model Selection: Probabilistic

- Statistical modeling is used to choose the most appropriate model among a set of candidate models.

- Model comparison
  - Akaike Information Criterion (AIC).
  - Bayesian Information Criterion (BIC).
  - Minimum Description Length (MDL).

"Information theory perspective"

Model Selection: Probabilistic

- Akaike Information Criterion (AIC).

$$\ln p(\mathcal{D}|\mathbf{w}_{\mathrm{ML}}) - M$$

Best-fit log likelihood

Number of adjustable parameters of the model

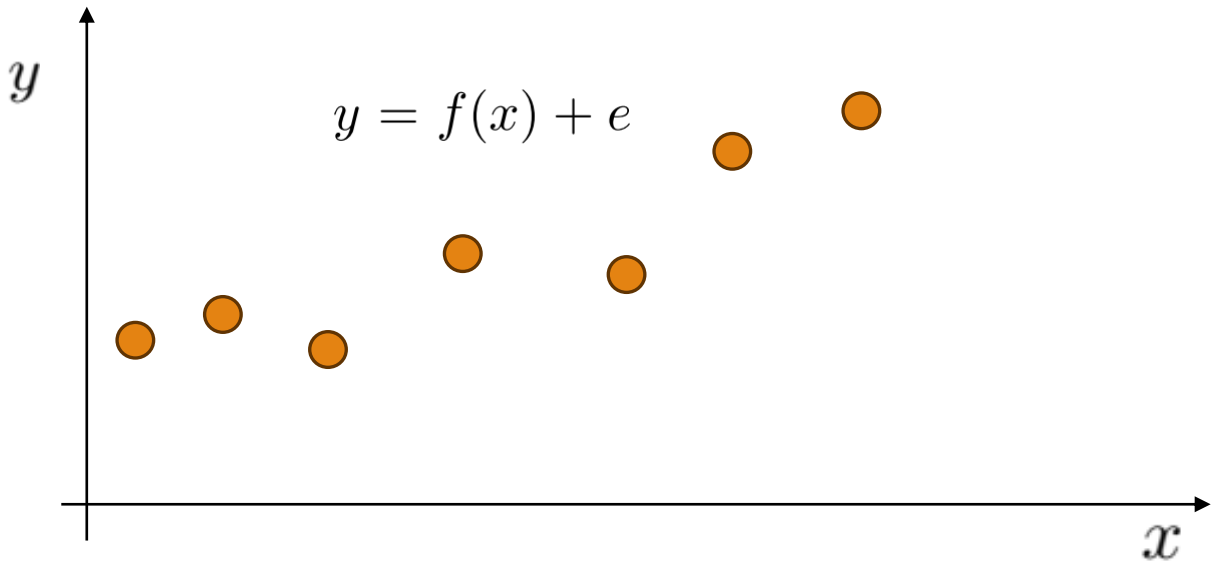
  - ✓ Select the model with the largest value
  - ✓ Both model complexity and model performance is considered

- Bayesian Information Criterion (BIC)- variation of AIC

  - ✓ Generally, more penalize on model complexity than AIC ➔ more complex models less like to select

Bias-variance trade-off.

- Given a dataset with samples denoted as $(x_1, y_1), (x_2, y_2), \ldots, (x_n, y_n)$
- A model $f(x)$ that maps input features x to predicted output y



Mean Squared Error (MSE)

$$\text{MSE} = \frac{1}{n}\sum_{i=1}^{n}(y_{\text{true},i} - y_{\text{pred},i})^2$$

- Learned model $\hat{f}(x)$

Bias-variance trade-off

$$\mathrm{MSE} = \frac{1}{n}\sum_{i=1}^{n}(y_{\mathrm{true},i} - y_{\mathrm{pred},i})^2$$

$$= \left(E[\hat{f}\,(x)] - f(x)\right)^2 + E\left[\left(\hat{f}\,(x) - E[\hat{f}\,(x)]\right)^2\right] + \mathrm{E}((y - f(x))^2)$$

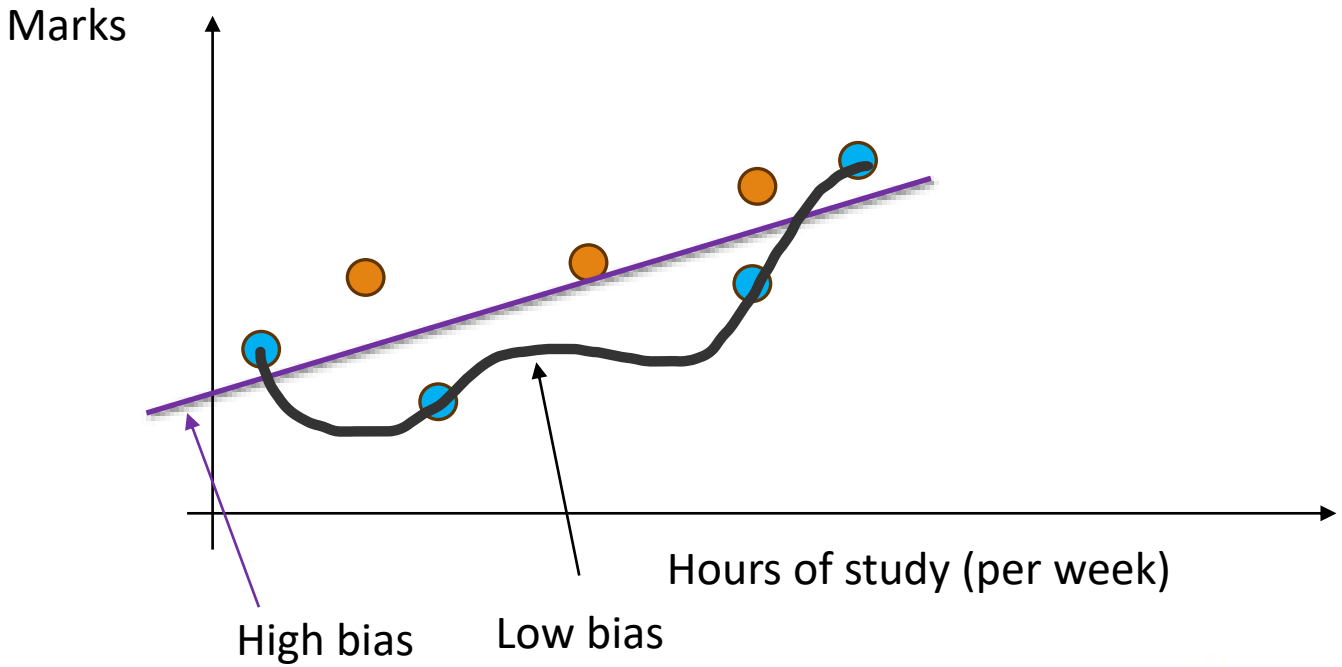
$$= \left(E[\hat{f}\,(x)] - f(x)\right)^2 + E\left[\left(\hat{f}\,(x) - E[\hat{f}\,(x)]\right)^2\right] + \sigma_e^2$$

$$= \mathrm{Bias}^2 + \mathrm{Variance} + \boxed{\mathrm{Irreducible\ Error}}$$

cannot be reduced by any model

Bias-variance trade-off

- High bias: Inability to capture the true relationship between input data and output



Training samples

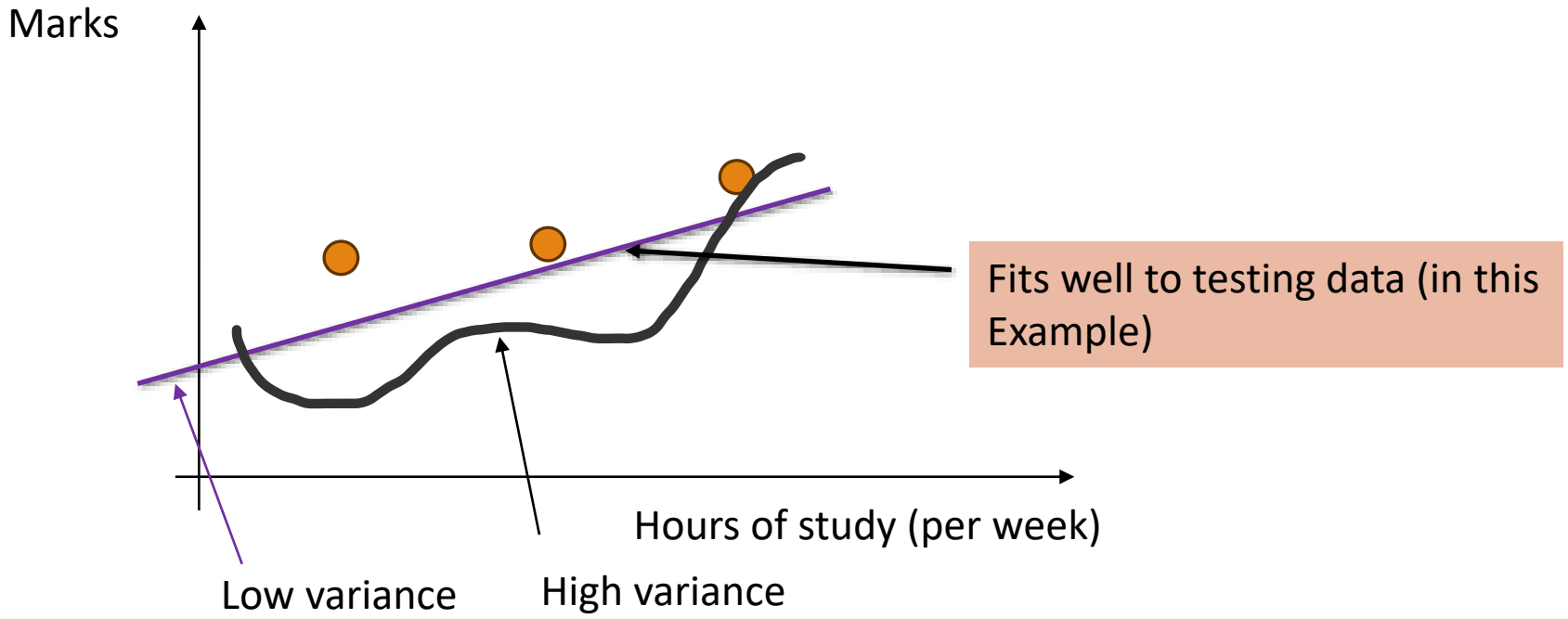
Fits well to training data (in this Example)

$$\left(E[\hat{f}(x)] - f(x)\right)^2 + E\left[\left(\hat{f}(x) - E[\hat{f}(x)]\right)^2\right] + \sigma_e^2$$

$$\text{Bias}^2 + \text{Variance} + \text{Irreducible Error}$$

Bias-variance trade-off

- High variance: Inability to fit different data sets

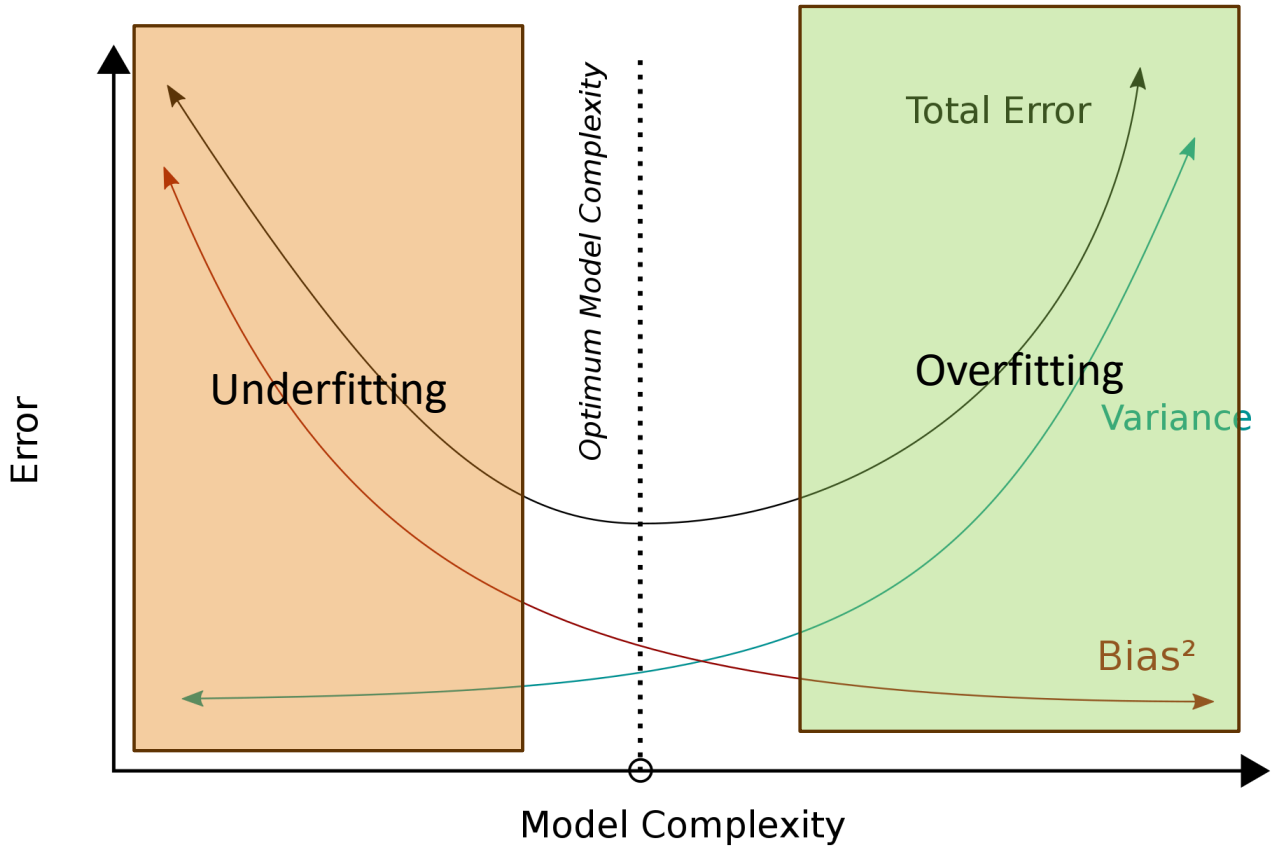


Testing samples

$$\left(E[\hat{f}(x)] - f(x)\right)^2 + E\left[\left(\hat{f}(x) - E[\hat{f}(x)]\right)^2\right] + \sigma_e^2$$

$$\text{Bias}^2 + \text{Variance} + \text{Irreducible Error}$$

Bias-variance trade-off



- Too simple model

  will have high bias but low variance

- A highly complex model

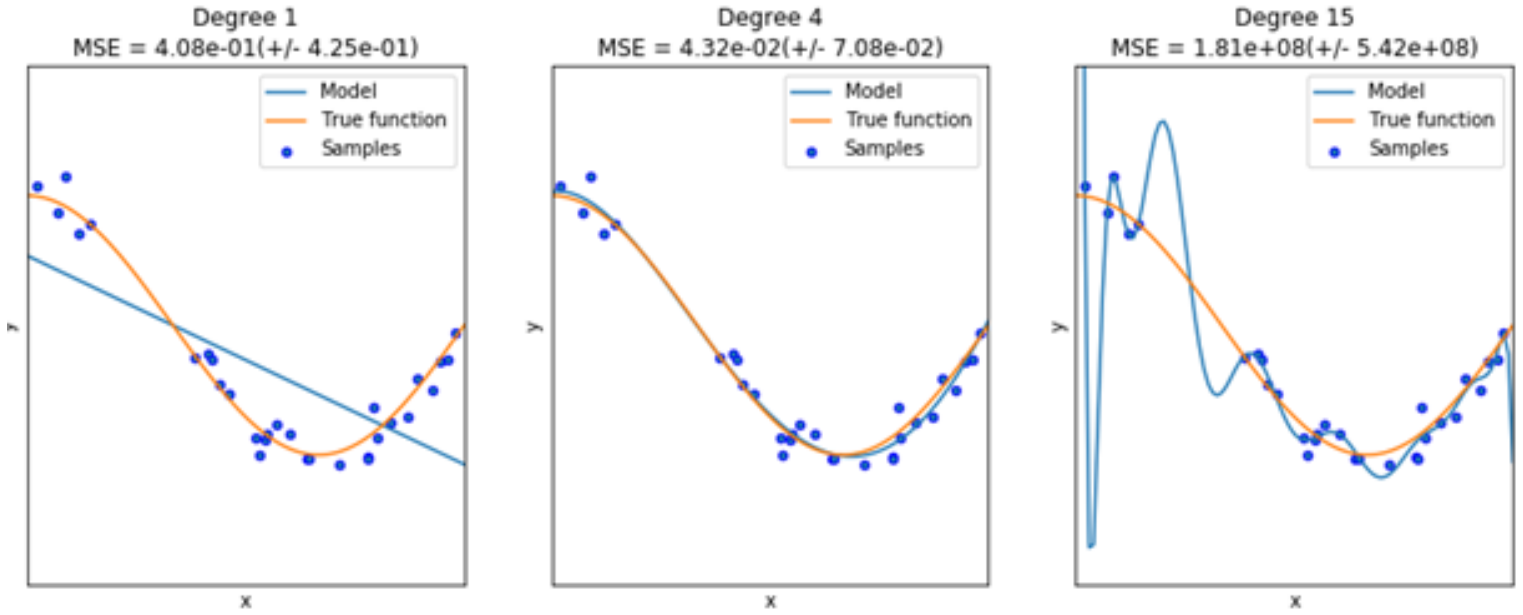
  will have low bias but high variance

$$\left(E[\hat{f}(x)] - f(x)\right)^2 + E\left[\left(\hat{f}(x) - E[\hat{f}(x)]\right)^2\right] + \sigma_e^2$$

$$\text{Bias}^2 + \text{Variance} + \text{Irreducible Error}$$

Image from https://en.wikipedia.org/wiki/Bias%E2%80%93variance_tradeoff

Bias-variance trade-off



Underfitting

high bias but low variance

Overfitting

low bias but high variance

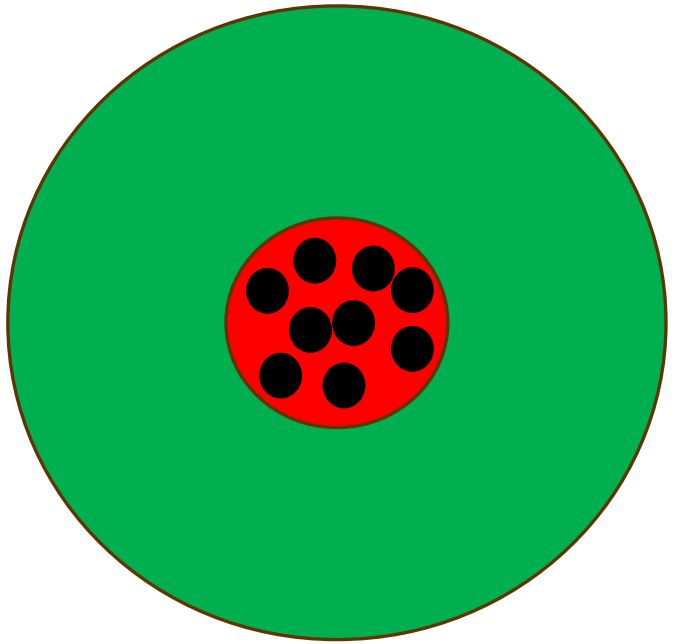
- Too simple model

  will have high bias but low variance

- A highly complex model

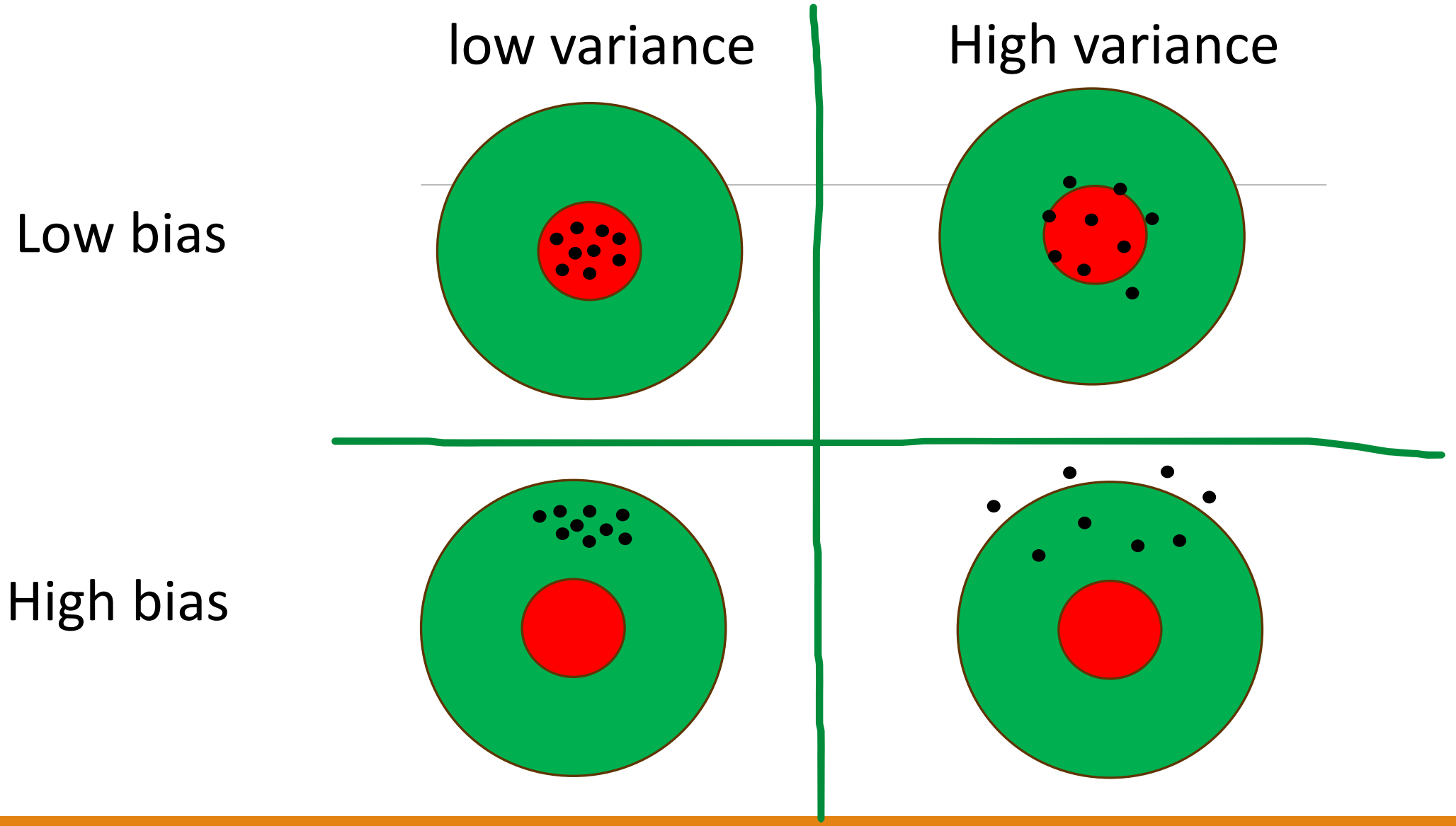
  will have low bias but high variance

Bias-variance trade-off



Low bias and low variance

Bias-variance trade-off



Thank You

Q & A