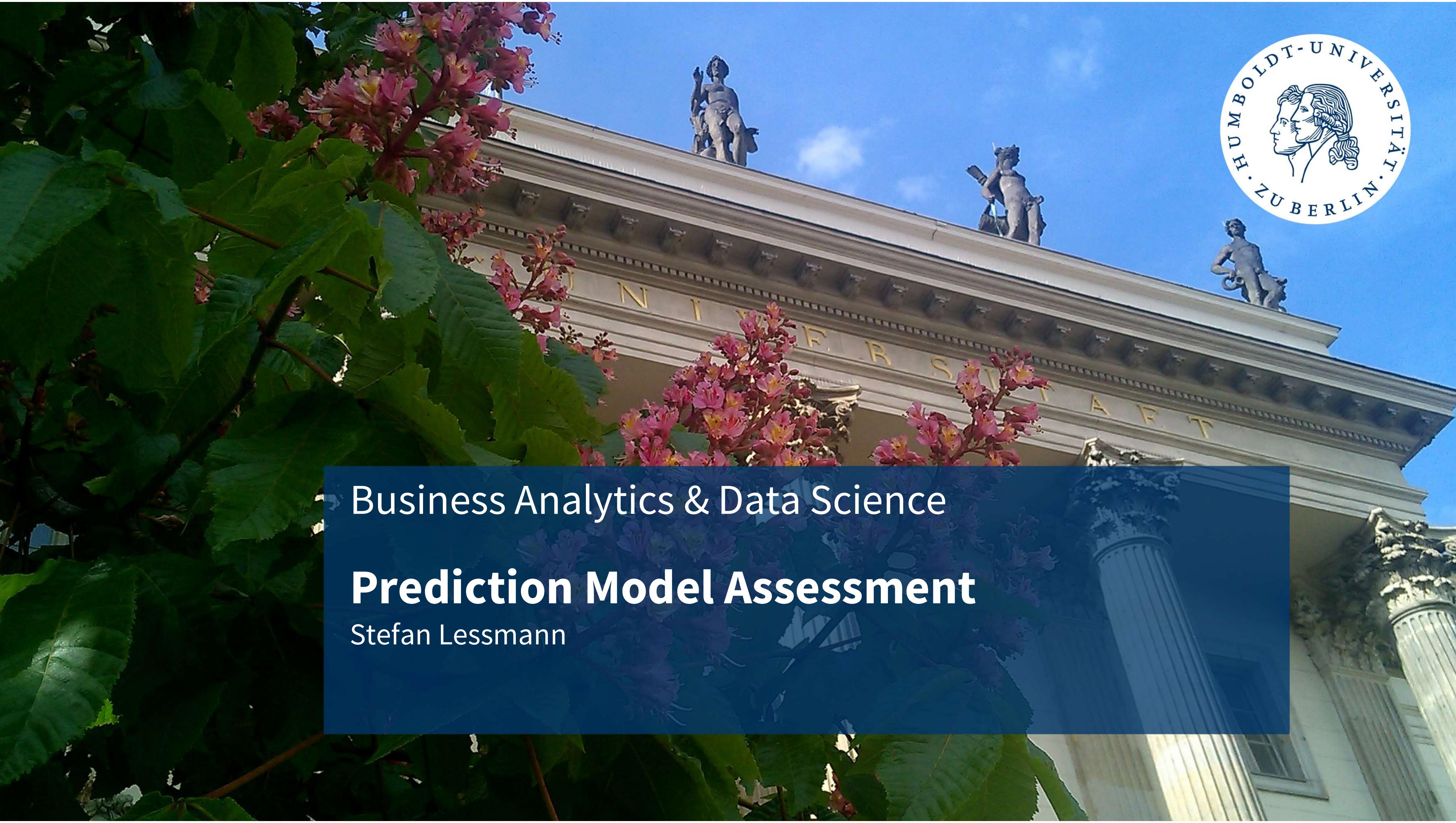


Business Analytics & Data Science

Prediction Model Assessment

Stefan Lessmann

Agenda

Introduction
Motivation and dimensions of model performance

Performance Indicators for Regression and Classification
Error measures, confusion matrix, and ROC analysis

Simulation of prediction model application
Resubstitution estimate, split sampling, and cross-validation

Summary

Introduction

Motivation and dimensions of model performance

Relevance of Model Assessment

- **Machine learning paradigm**
  - Inductive approach toward problem solving
  - Empirical evaluation is instrumental to that approach
- **Make informed modeling decisions**
  - Theory support often unavailable
    - Which learning algorithm is most suitable?
    - What is the best way to impute missing values?
    - Should we truncate outliers?
  - Expert judgement highly useful but expertise is scarce and costly
- **Accountability and replicability**

Dimensions of Model Performance

Many factors determine the value of a machine learning model

Accuracy

How well does the model predict? For example, is it able to distinguish good and bad risks with high accuracy?

Scalability

How much time is needed to build and to apply the model? Does it scale to large data sets?

Robustness

Can the model cope with noise and missing values? How about irrelevant and correlated attributes?

Comprehensibility

Can we understand the model? Is it clear how it transforms attribute values into predictions of the response variable?

Justifiability

Is the use of attributes within the model in line with business rules/ understanding?

Calibration

For probability forecasts! Out of 100 events predicted to have 90% chance, about 90 should have occurred. True?

Assessing Predictive Performance – Intuition and Ingredients
Comparing model-based forecasts to actual outcomes

- **The more forecasts agree with true values of the target better the model**
- **Question 1: How measures agreement between forecasts & actuals?**
  - Standard error measures for regression and classification
  - Does an accuracy indicator reflect business performance?
- **Question 2: How to know the true values of the target variable?**
  - The point of developing a predictive model is to forecast future values of the target
  - We never know actual target values a priori
  - How to assess a model prior to deployment?
- **Two core ingredients of forecast accuracy evaluation**
  - Measures for predictive performance
  - Practice to organize the available data

Y	$\hat{Y}$
…	…
…	…
…	…
…	…
…	…
…	…
…	…
…	…
…	…

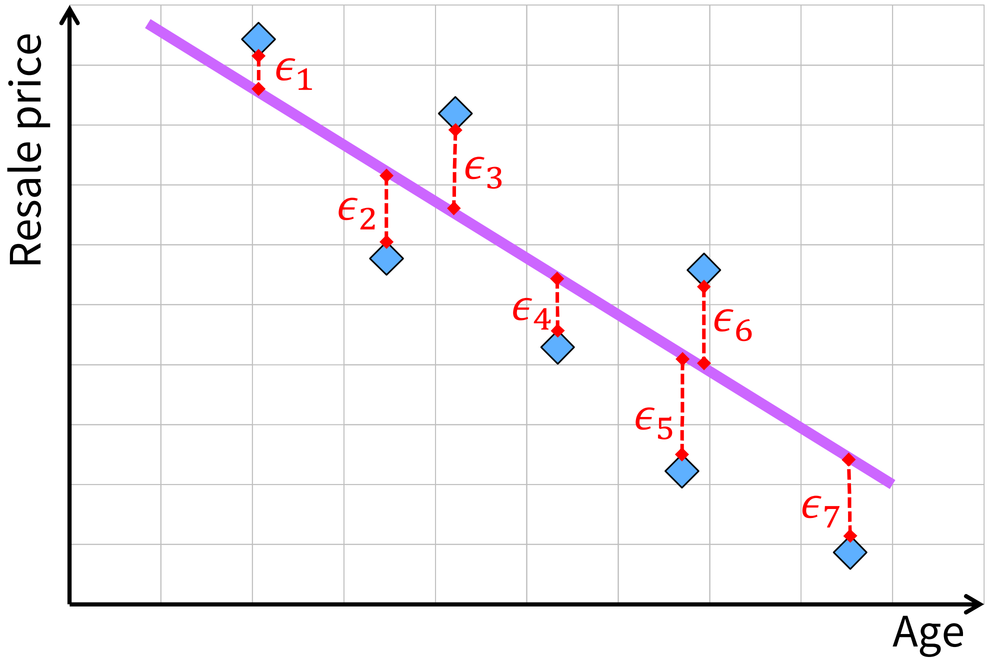
Performance Indicators for Regression and Classification

Error measures, confusion matrix, and ROC analysis

Measuring Forecast Accuracy in Regression

Compare model-based forecasts to true realizations of the target variable

- **Model residuals capture the difference between a true outcome and a forecast**
- **Error measures aggregate residuals into an overall measure of forecast error**
- **Forecast error and accuracy are just two sides of one coin**



$$\begin{bmatrix} \epsilon_1 = y_1 - \hat{y}_1 \\ \epsilon_2 = y_2 - \hat{y}_2 \\ \epsilon_3 = y_3 - \hat{y}_3 \\ \epsilon_4 = y_4 - \hat{y}_4 \\ \epsilon_5 = y_5 - \hat{y}_5 \\ \epsilon_6 = y_6 - \hat{y}_6 \\ \epsilon_7 = y_7 - \hat{y}_7 \end{bmatrix}$$

$$TE = \sum_{i=1}^{n=7} \epsilon_i = \sum_{i=1}^{n=7} (y_i - \hat{y}_i)$$

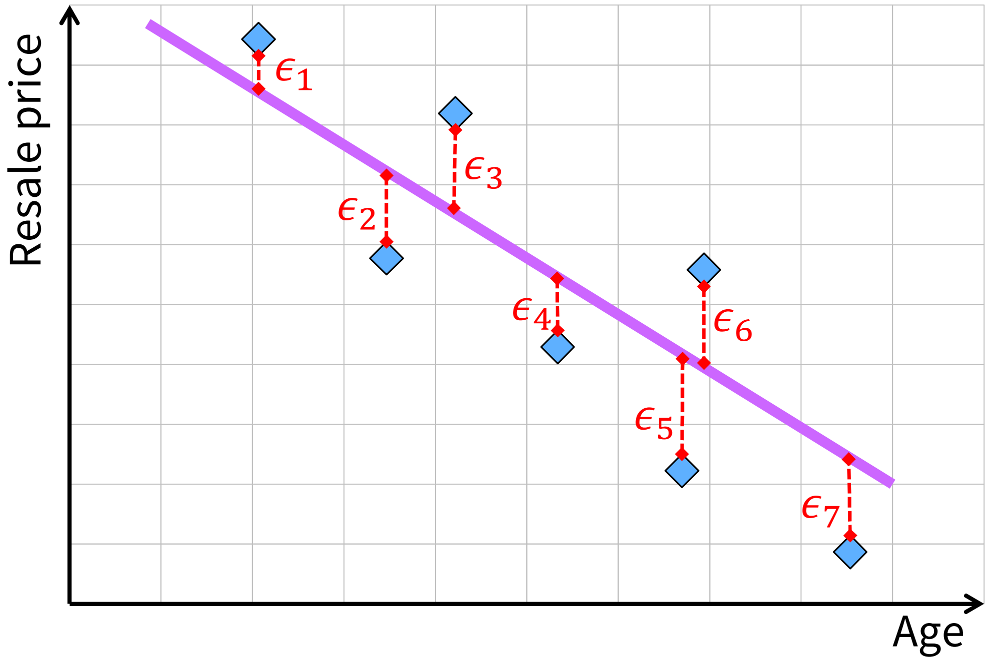
Total error (TE)

- Positive and negative residuals even out
  - Can be used as a measure of model bias (see later)
  - Less useful for error/accuracy measures
- Magnitude depends on the number of data points

Common Error Measures for Regression

Squared error measures

- **Measures of squared errors emphasizes large residuals**
- **Note that RMSE is of the same scale as the target variable**
  - For example, resale price is measured in USD
  - MSE is measured in USD^2 whereas RMSE is measures in USD



Squared error (SE)

$$SE = \sum_{i=1}^{n=7} \epsilon_i^2 = \sum_{i=1}^{n=7} (y_i - \hat{y}_i)^2$$

Mean squared-error (MSE)

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

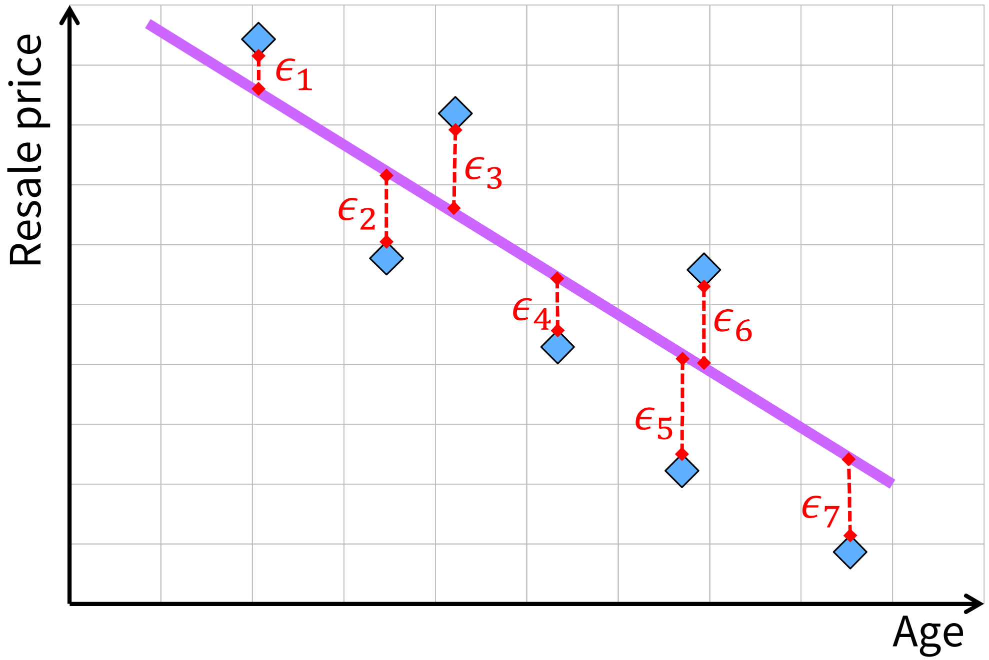
Root-mean squared-error (RMSE)

$$RMSE = \sqrt{MSE}$$

Common Error Measures for Regression

Absolute error measures

- **Measures of absolute errors are perhaps easiest to understand**
- **Mathematically, they are less convenient to work with**
  - No easy derivative c.f. squared error
  - Matters if we use a measure for both, model training and model evaluation



Absolute error (AE)

$$AE = \sum_{i=1}^{n} |y_i - \hat{y}_i|$$

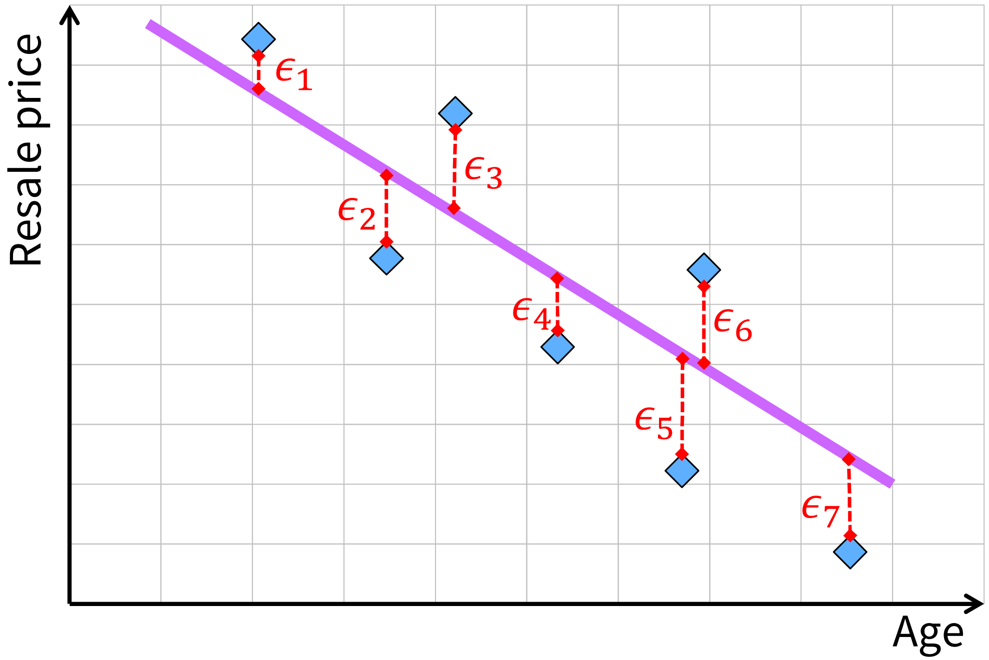
Mean absolute error (MAE)

$$MAE = \frac{1}{n} \sum_{i=1}^{n} |y_i - \hat{y}_i|$$

Common Error Measures for Regression

Percentage error measures

- **Consider ration of the error to actual value**
- **Supports comparing models for different outcomes**
  - Resale price forecasting model with actual prices in USD
  - Sales forecasting model with outcome in units sold
  - But always be careful with comparisons of different models



Mean percentage error

$$MPE = \frac{100\%}{n} \sum_{i=1}^{n} \frac{y_i - \hat{y}_i}{y_i}$$

Mean absolute percentage error

$$MAPE = \frac{100\%}{n} \sum_{i=1}^{n} \left| \frac{y_i - \hat{y}_i}{y_i} \right|$$

Symmetric MAPE

$$sMAPE = \frac{100\%}{n} \sum_{i=1}^{n} \frac{|y_i - \hat{y}_i|}{|y_i| + |\hat{y}_i|}$$

Common Performance Indicators for Classification
Confusion matrix for binary classification problem

		Actual Class	
		Positive $(Y = 1)$	**Negative** $(Y = \mathbf{0})$
Predicted Class	**Positive** $(\hat{Y} = 1)$	True Positive (TP)	False Positive (FP)
	Negative $(\hat{Y} = 0)$	False Negative (FN)	True Negative (TN)

- **Classification accuracy / Percentage correctly classified** $$\frac{TP + TN}{TP + TN + FP + FN}$$
- **Classification error** $$\frac{FP + FN}{TP + TN + FP + FN}$$
- **Specificity** $$\frac{TN}{TN + FP}$$
- **Sensitivity / Recall** $$\frac{TP}{TP + FN}$$
- **Precision** $$\frac{TP}{TP + FP}$$

Common Performance Indicators for Classification

Confusion matrix is a function of the classification cut-off

i	Y	$\hat{p}(Y = 1\|\boldsymbol{X})$
1	1	0.9
2	1	0.7
3	1	0.6
4	0	0.6
5	0	0.2

$\tau = 0.5$

	Positive $(Y = 1)$	**Negative** $(Y = 0)$
Positive $(\hat{Y} = 1)$	3	1
Negative $(\hat{Y} = 0)$	0	1

To obtain a **discrete class prediction**, compare $\hat{p}(Y = 1|\boldsymbol{X})$ to **cut-off** τ:

predict $\hat{Y} = 1$ if $\hat{\boldsymbol{p}}(Y = 1|\boldsymbol{X}) > \tau$,

and $\hat{Y} = 0$ otherwise.

Common Performance Indicators for Classification

Receiver Operating Characteristic (ROC) Curve

- **Generalization of the confusion matrix**
  - One confusion matrix corresponds to one cut-off
  - ROC curve depicts classifier performance across **all cut-offs**
- **Two-dimensional graph of sensitivity (TP rate) vs. 1-specificity (FP rate)**
  - Passes through the points (0,0) where all cases are classified as Positive
  - And the point (1,1) where all cases are classified as Negative
  - Guessing classes at random produces a straight line through (0,0) and (1,1)
    - Naïve benchmark
    - Every classifier's ROC curve should be above the diagonal
  - Optimal point (0,1), classifier makes no errors
  - The more the ROC curve approaches the optimal point, the better the classifier

Construction of the ROC Curve

Visualization of classifier performance across all cut-offs

i	Y	$\hat{p}(Y = 1 \mid X)$
1	1	0.9
2	1	0.7
3	1	0.6
4	0	0.6
5	0	0.2

Compare $\hat{p}(Y = 1|X)$ to **cut-off** τ:
predict $\hat{Y} = 1$ if $\hat{\boldsymbol{p}}(Y = 1|X) > \tau$,
and $\hat{Y} = 0$ otherwise.

$\tau = 0.9$

	Positive $(Y = 1)$	**Negative** $(Y = 0)$
Positive $(\hat{Y} = 1)$	0	0
Negative $(\hat{Y} = 0)$	3	2

$\tau = 0.7$

	Positive $(Y = 1)$	**Negative** $(Y = 0)$
Positive $(\hat{Y} = 1)$	1	0
Negative $(\hat{Y} = 0)$	2	2

$\tau = 0.6$

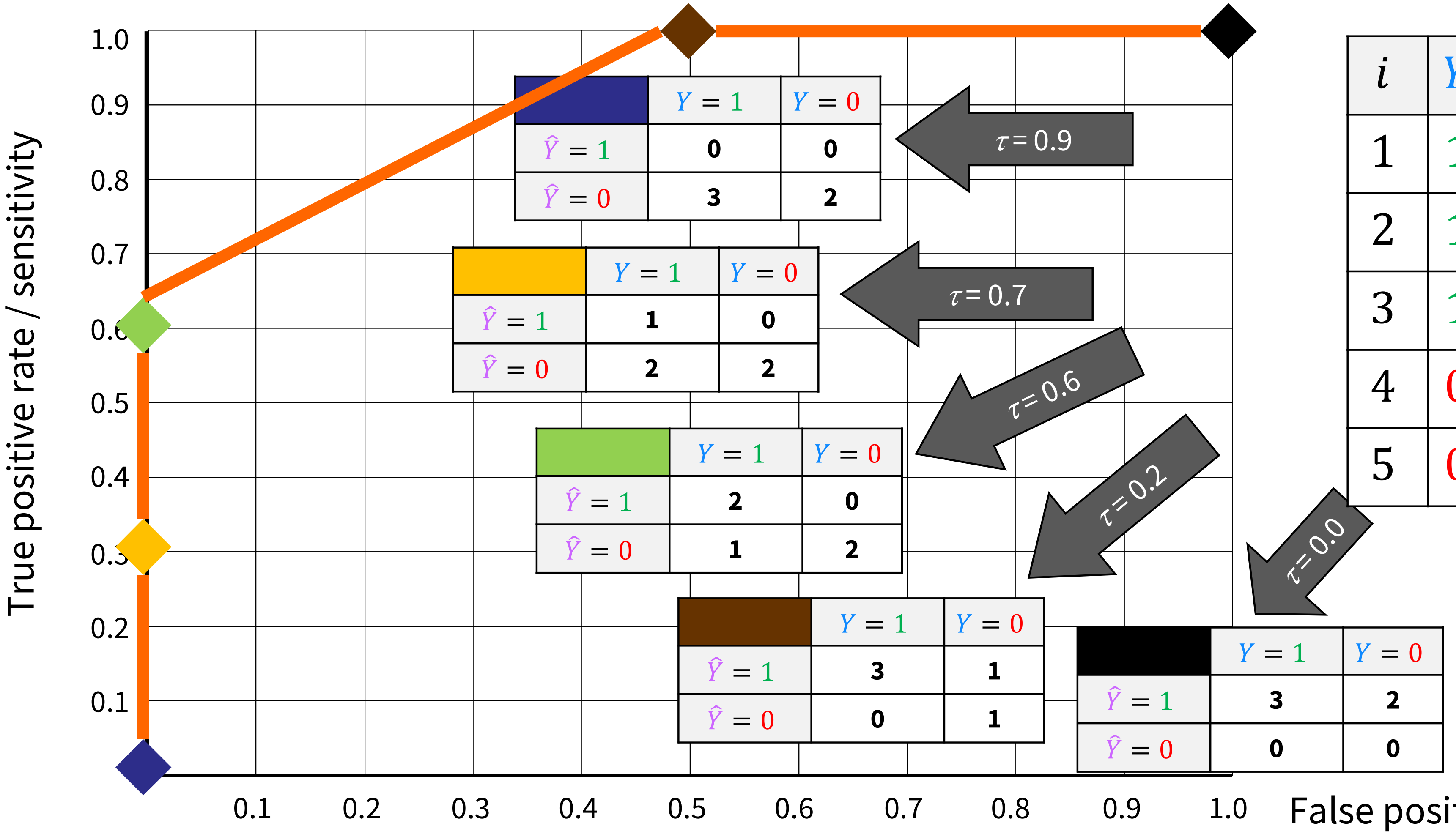
	Positive $(Y = 1)$	**Negative** $(Y = 0)$
Positive $(\hat{Y} = 1)$	2	0
Negative $(\hat{Y} = 0)$	1	2

$\tau = 0.2$ …

$\tau = 0.0$ …

Construction of the ROC Curve

Visualization of classifier performance across all cut-offs



i	Y	$\hat{p}(Y = 1 \mid X)$
1	1	0.9
2	1	0.7
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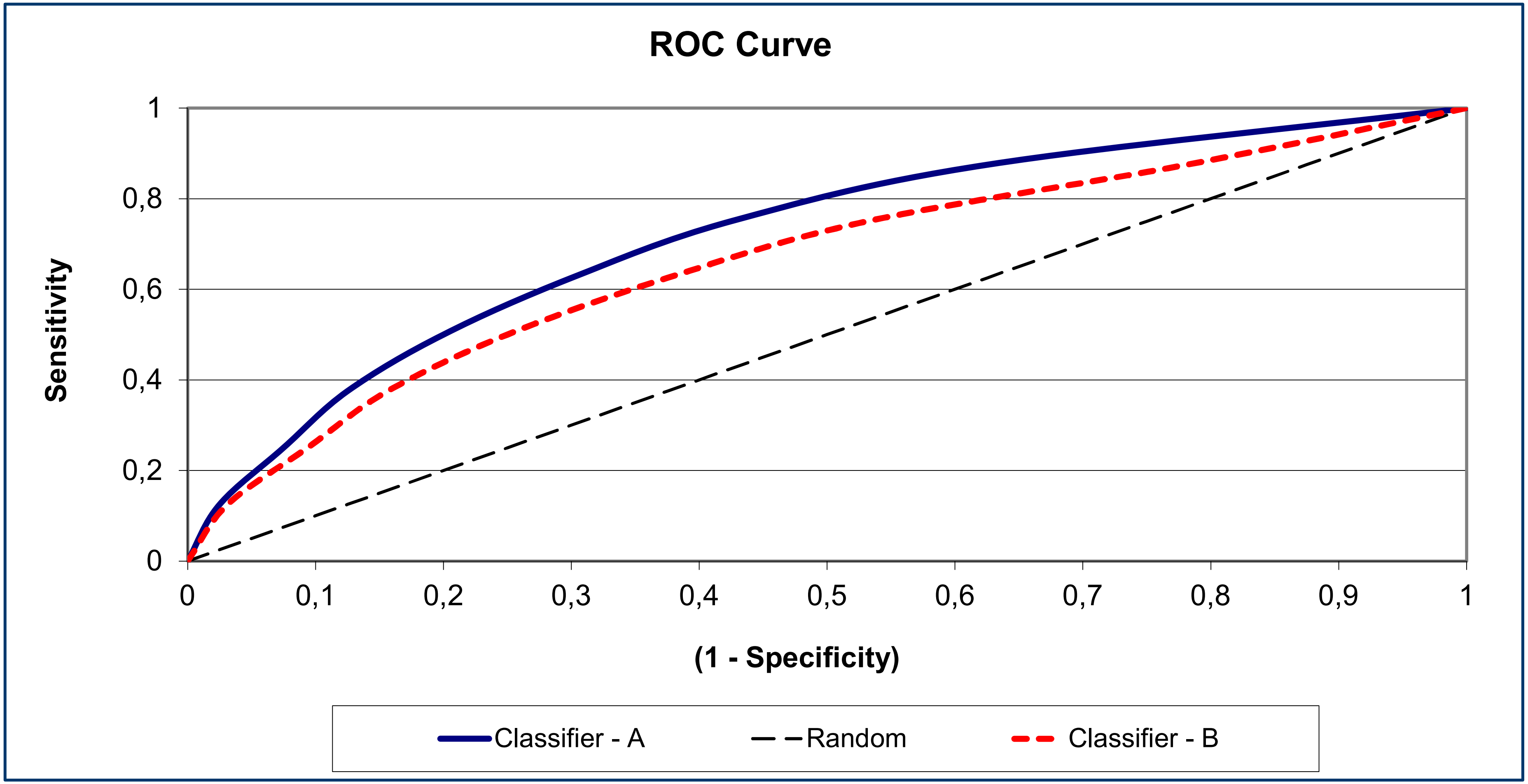
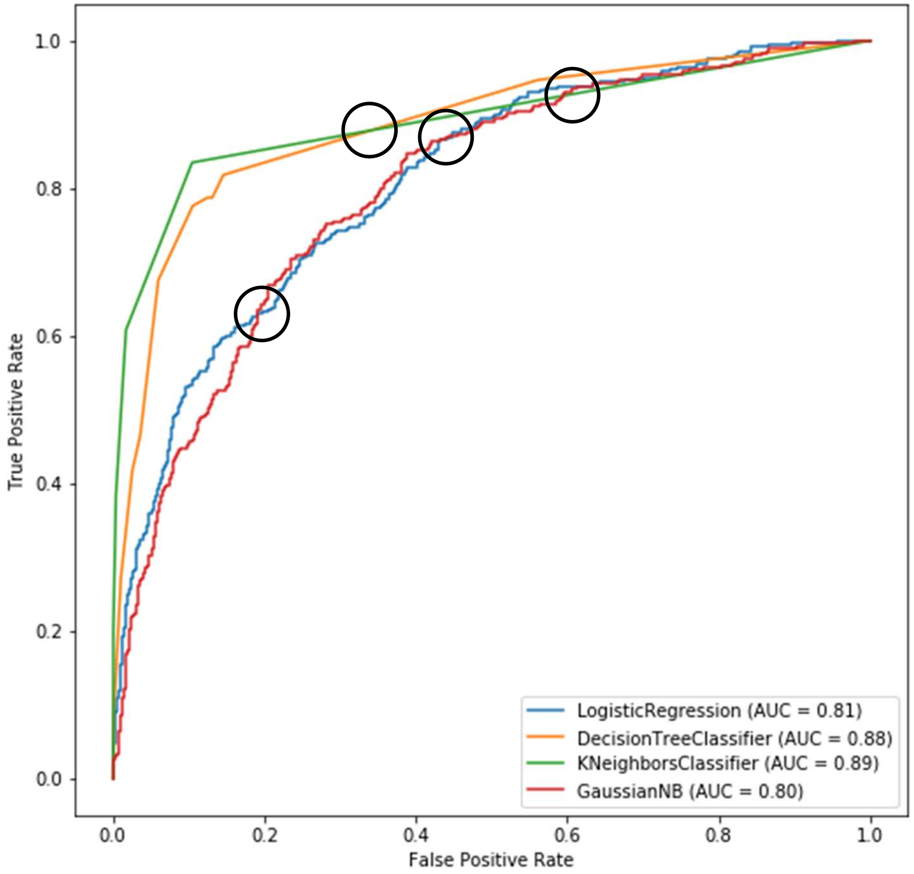
Construction of the ROC Curve

Comparing two classifiers (A and B) in ROC space



The Area Under the ROC Curve
Summarizes the ROC curve in a single number

- **Useful to compare intersecting ROC curves**
- **The higher the better**
  - Classifier is on average closer to the optimum
  - Good classifier: AUC well above 0.5
- **Equivalent to Wilcoxon or Mann-Whitney or U- statistic**
  - The AUC estimates the probability that a randomly chosen positive instance is correctly ranked higher than a randomly chosen negative (Hanley and McNeil, 1982)
  - Assesses classifier's ability to discriminate between positives and negatives?
  - AUC is a **ranking indicator**
  - Ranking based on classifier's **score distribution**
- **See Fawcett (2006) for a good introduction**



Further Indicators of Predictive Accuracy

A vast set of other generic and application-specific measures exist

- **Predictive accuracy of classification models**
  - Precision & recall, precision-recall curve, area under the PR-curve (e.g., Saito & Rehmsmeier 2015)
  - Brier score, log-loss, cross-entropy
  - H-measure (Hand & Anagnostopoulos 2013, 2014; Hand 2009)
  - Cost- and Brier curves (Hernández-Orallo et al. 2011, Drummond & Holte 2006)
- **Predictive accuracy of regression models**
  - Theil's U, MSE decomposition, skill scores (e.g., Nikolopoulos et al. 2007, Wheatcroft 2019)
  - (Asymmetric) error costs (e.g., Dress et al. 2018)
- **Examples of application specific measures**
  - Lift-/Gain analysis, uplift-/qini curves (e.g., Surry & Radcliffe 2011, Devriendt et al. 2021)
  - Expected maximum profit criterion for churn/credit scoring (Verbraken et. al. 2012, 2014)

Simulation of prediction model application

Resubstitution estimate, split sampling, and cross-validation

Data Organization for Assessing Prediction Performance

Remember Question 2 from above?

- **Question 2: How to know the true values of the target variable?**
  - The point of developing a predictive model is to forecast future values of the target
  - We never know actual target values a priori
  - How to assess a model prior to deployment?
- **Requiring us to ‘know’ future outcomes is not practical**
- **Best we can do is to rely on observed outcomes from historical data**
  - Practices to use available historic, labelled data for training and testing
  - Resubstitution estimate, split-sampling and cross-validation, and others

Resubstitution Estimate
(Re-)Use the training data for model assessment

- **Performance =** $f\,(\text{training error, model complexity})$
- **Penalize for complexity**
  - Complexity typically measured as no. of estimated parameters
  - Akaike Information Criterion (AIC) = -2 log L + 2 (no. of parameters)
  - Bayesian Information Criterion (BIC) = -2 log L + (no. of parameters) * log(no. of observations)
- **Resubstitution estimate is well-established for explanatory models**
  - Understand underlying mechanisms of real-world phenomena and test hypotheses
  - Is the effect of X on Y statistically significant? How does Y changes with a 1% increase in X?
- **Resubstitution estimate is inappropriate for predictive models**
  - Need ‘fresh’ data to judge whether a model predicts accurate into unseen data
  - Powerful learning algorithms can easily overfit the training set (e.g., deep decision tree)

Data Organization Intuition

Reserve some of the historical data for model testing

Learning Algorithm

Stage 1: Model Training

Data-driven development of a predictive model using labelled data $\mathcal{D} = \{Y_i, \boldsymbol{X}_i\}_{i=1}^{n}$

Historical data for training incl. Y

i	Y	X_1	X_2	…	X_m
1	…	…	…	…	…
2	…	…	…	…	…
…	…	…	…	…	…
n	…	…	…	…	…

Model

Stage 2: Model Testing

Apply trained model to the hold-out data to obtain prediction and compare to known actuals.

Historical data for testing incl. Y

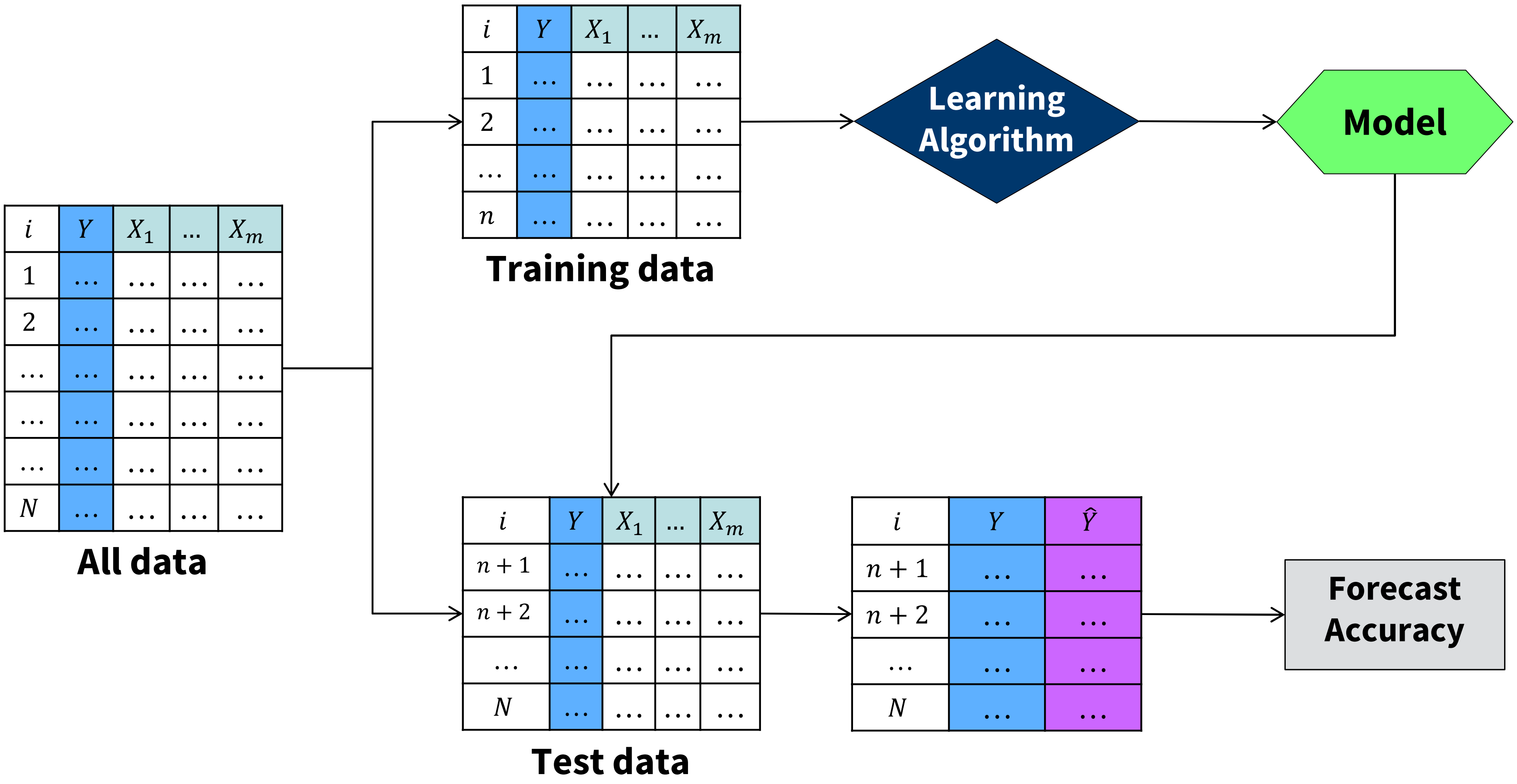
i	Y	X_1	…	X_m
$n+1$	…	…	…	…
$n+2$	…	…	…	…
…	…	…	…	…
N	…	…	…	…

Forecasts of Y

i	Y	$\hat{Y}$
$n+1$	…	…
$n+2$	…	…
…	…	…
N	…	…

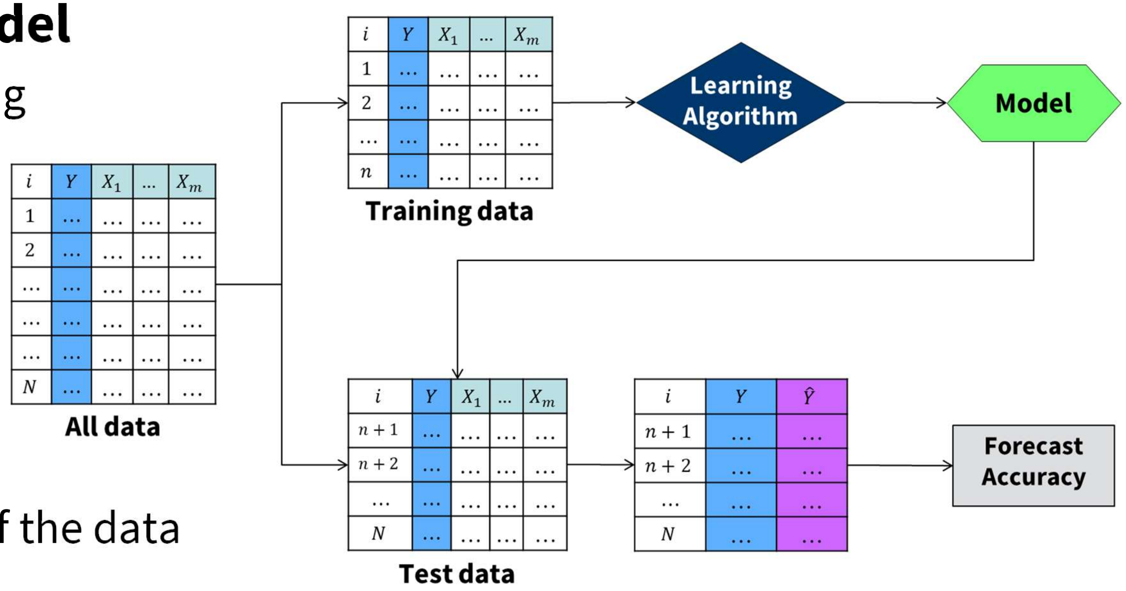
Measuring Forecast Accuracy Needs ‘Fresh’ Data Not Used for Training

Hold-out method: split data in disjoint subsets for training & testing



Hold-Out Method Under the Microscope

- **Simulates real-world application of model**
  - Model is applied to data not used during training
  - Caveat: training and test data stem from same sample
  - Assumes a static environment with stable data generation process
  - Ideally use out-of-time validation
- **Data splitting is wasteful**
  - Train / test set often comprise 70 / 30 percent of the data
  - Much data lost for training; same for testing
- **High variance / risk of drawing a 'lucky' test sample**
- **Many alternatives exist (e.g., cross-validation)**
  - Increase efficiency of data usage
  - Increase robustness of performance estimate



K-Fold Cross Validation

Repeat model training & hold-out evaluation K times on different subsets

- **Say we have a data set with 10 observations and set K=5**
- **We split the data into K=5 partitions of equal size (i.e., two observations)**
- **We use one partition for hold-out validation of a model, which we train on the union of the other partitions**

i	Product	List price [$]	Age [month]	Industry	…	Resale price [$]	
1	Dell XPS 15’	2,500	36	Mining	…	347	Fold 1
2	Dell XPS 15’	2,500	24	Health	…	416	
3	Dell XPS 17’	3,000	36	Manufacturing	…	538	Fold 2
4	HP Envy 17’	1,300	24	Office	…	121	
5	HP EliteBook 850	1,900	36	Manufacturing	…	172	Fold 3
6	Lenovo Yoga 11’	799	12	Office	…	88	
7	Lenovo Yoga 13’	1,100	12	Office	…	266	Fold 4
8	Dell Inspiron 15'	1,499	12	Manufacturing	…	189	
9	HP Envy 15’	2,300	24	Health	…	235	Fold 5
10	MacBook	2,750	12	Office	…	1,125	

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- **We use one partition for hold-out validation of a model, which we train on the union of the other partitions**
- **We repeat this K times each time using a different partition for hold-out validation**

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10	MacBook	2,750	12	Office	…	1,125

Iteration 1

Training data

Validation data

K-Fold Cross Validation

Repeat model training & hold-out evaluation K times on different subsets

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- **We repeat this K times each time using a different partition for hold-out validation**

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8	Dell Inspiron 15'	1,499	12	Manufacturing	…	189
9	HP Envy 15’	2,300	24	Health	…	235
10	MacBook	2,750	12	Office	…	1,125

Iteration 2

Training data

Validation data

K-Fold Cross Validation

Repeat model training & hold-out evaluation K times on different subsets

- Say we have a data set with 10 observations and set K=5
- We split the data into K=5 partitions of equal size (i.e., two observations)
- We use one partition for hold-out validation of a model, which we train on the union of the other partitions
- We repeat this K times each time using a different partition for hold-out validation

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9	HP Envy 15'	2,300	24	Health	…	235
10	MacBook	2,750	12	Office	…	1,125

Iteration 3

Training data

Validation data

K-Fold Cross Validation

Repeat model training & hold-out evaluation K times on different subsets

- Say we have a data set with 10 observations and set K=5
- We split the data into K=5 partitions of equal size (i.e., two observations)
- We use one partition for hold-out validation of a model, which we train on the union of the other partitions
- We repeat this K times each time using a different partition for hold-out validation

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Iteration 4

Training data

Validation data

K-Fold Cross Validation

Repeat model training & hold-out evaluation K times on different subsets

- **Say we have a data set with 10 observations and set K=5**
- **We split the data into K=5 partitions of equal size (i.e., two observations)**
- **We use one partition for hold-out validation of a model, which we train on the union of the other partitions**
- **We repeat this K times each time using a different partition for hold-out validation**

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10	MacBook	2,750	12	Office	…	1,125

Iteration 5

Training data

Validation data

K-Fold Cross Validation

Each (sub-)model gives forecasts for the corresponding validation fold

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6	Lenovo Yoga 11'	799	12	Office	…	88
7	Lenovo Yoga 13'	1,100	12	Office	…	266
8	Dell Inspiron 15'	1,499	12	Manufacturing	…	189
9	HP Envy 15'	2,300	24	Health	…	235
10	MacBook	2,750	12	Office	…	1,125

i	Product	List price [$]	Age [month]	Industry	…	Resale price [$]
1	Dell XPS 15'	2,500	36	Mining	…	347
2	Dell XPS 15'	2,500	24	Health	…	416
3	Dell XPS 17'	3,000	36	Manufacturing	…	538
4	HP Envy 17'	1,300	24	Office	…	121
5	HP EliteBook 850	1,900	36	Manufacturing	…	172
6	Lenovo Yoga 11'	799	12	Office	…	88
7	Lenovo Yoga 13'	1,100	12	Office	…	266
8	Dell Inspiron 15'	1,499	12	Manufacturing	…	189
9	HP Envy 15'	2,300	24	Health	…	235
10	MacBook	2,750	12	Office	…	1,125

Model 1

Model 2

Model 3

Model 4

Model 5

i	Resale price [$]	Forecast
1	347	325
2	416	398

i	Resale price [$]	Forecast
3	538	612
4	121	101

i	Resale price [$]	Forecast
5	172	214
6	88	59

i	Resale price [$]	Forecast
7	266	307
8	189	182

i	Resale price [$]	Forecast
9	235	231
10	1,125	875

K-Fold Cross Validation
Each (sub-)model gives forecasts for the corresponding validation fold

i	Resale price [$]	Forecast
1	347	325
2	416	398

i	Resale price [$]	Forecast
3	538	612
4	121	101

i	Resale price [$]	Forecast
5	172	214
6	88	59

i	Resale price [$]	Forecast
7	266	307
8	189	182

i	Resale price [$]	Forecast
9	235	231
10	1,125	875

Thanks to cross-validation, we obtain hold-out forecasts for the entire data set. We can assess our model based on these hold-out forecast using any forecast accuracy indicator.
Unlike the basic hold-out method, no data is lost for either training **or** validation. Instead, each observations contributes information to both steps, training **and** validation.

i	Resale price [$]	Forecast
1	347	325
2	416	398
3	538	612
4	121	101
5	172	214
6	88	59
7	266	307
8	189	182
9	235	231
10	1,125	875

The disadvantage or ‘cost’ of cross-validation is that we have to train K models. Training an advanced model on a large data set can consume a significant amount of time and computer resources. However, whenever this is feasible, cross-validation will give a more robust estimate of forecast accuracy and model performance.

Summary

Summary

Learning goals

- Experimental designs to assess predictive models
- Accuracy indicators for regression & classification

Findings

- Model performance has facets beyond accuracy
- Accuracy measures contrast actuals vs. forecasts
- Confusion matrix depends on classification cut-off
- ROC analysis generalizes the confusion matrix
- No in-sample evaluation! Hold-out data is crucial
- Pros and cons of cross-validation vs. split sample

What next

- Demo notebook on prediction model evaluation
- Some theory on supervised learning

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Thank you for your attention!

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Photo: Heike Zappe

Appendix

Further dimensions of model performance

Dimensions of Model Performance

Many factors determine the value of an analytical model

Accuracy

How well does the model predict? For example, is it able to distinguish good and bad risks with high accuracy?

Scalability

How much time is needed to build and to apply the model? Does it scale to large data sets?

Robustness

Can the model cope with noise and missing values? How about irrelevant and correlated attributes?

Comprehensibility

Can we understand the model? Is it clear how it transforms attribute values into predictions of the response variable?

Justifiability

Is the use of attributes within the model in line with business rules/ understanding?

Calibration

For probability forecasts! Out of 100 events predicted to have 90% chance, about 90 should have occurred. True?

Dimensions of Model Performance
Scalability

- **Consumption of time resources**
- **Time needed to build model (training time)**
  - Depends on number of cases and attributes
  - Run-time complexity
  - Importance depends on update frequency
- **Time needed to generate predictions**
  - Much less than training time
  - Critical in real-time settings (e.g., E-Commerce)
- **Both time factors differ substantially across algorithms**

- **Consumption of memory resources**
  - During model building
  - When storing final model
  - Big data prohibits keeping all training data in memory
- **Sensitivity with respect to hyperparameters**
  - Building one model is never enough
  - Some models need a lot more tuning than others
- **Parallelization important**
  - Model building
  - Model tuning

Dimensions of Model Performance
Robustness

- **Real-world data is noisy**
  - Missing values
  - Erroneous data entries
  - Wrong labels
  - Irrelevant / correlated attributes
- **Real-world phenomena change over time**
  - Concept drift
  - Model recalibration versus re-estimation
- **How to these factors affect the model?**
  - During model building
  - After model building

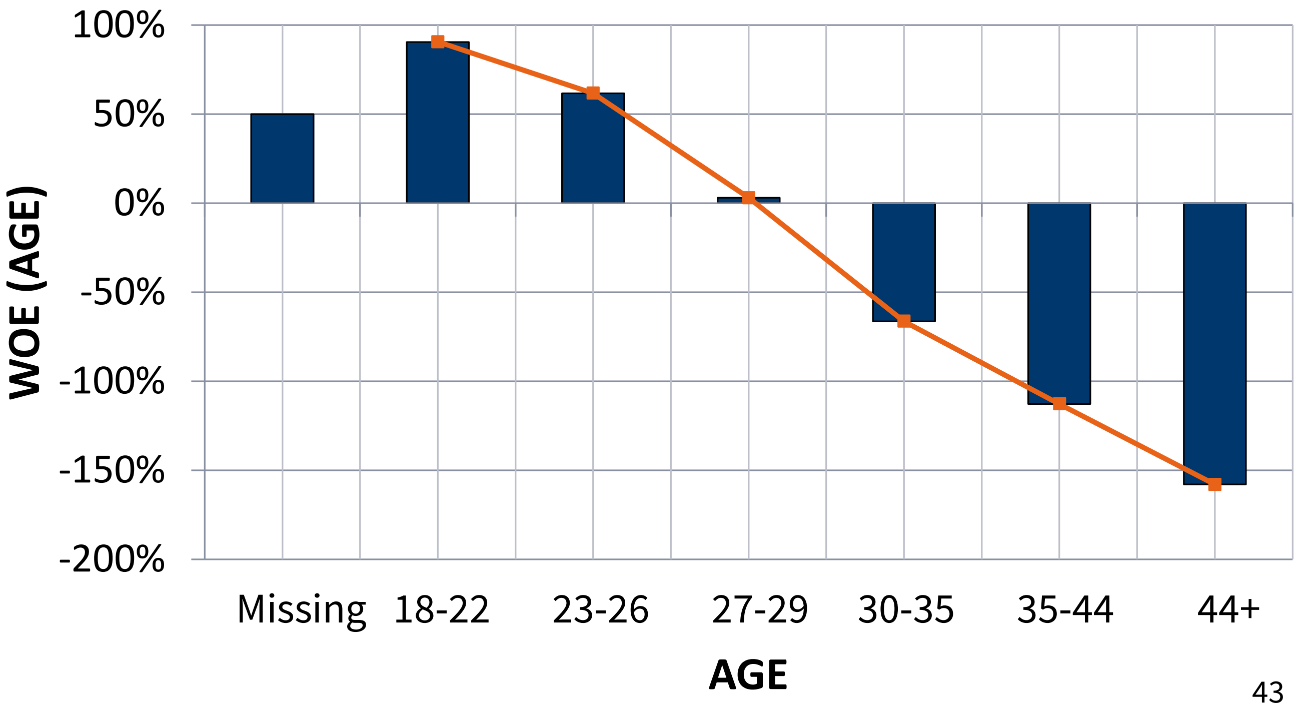
Dimensions of Model Performance
Comprehensibility: crucial and challenging to measure

- **Is it possible to understand how a model translates attribute values into prediction?**
  - Alternative terms: interpretability, transparency, white-box (vs. black-box) model
  - Becoming increasingly relevant with the raising popularity of machine learning
  - “Managers don’t trust black-box models”
- **New research fields on interpretable machine learning (see subsequent sessions)**
  - Global interpretability: equivalent to above point. How do covariates govern predictions
  - Local interpretability: how was the prediction of a specific observation determined by covariate values
- **Prediction versus insight and correlation versus causality**
  - Prediction: “Next month, we sell 100 laptops”
  - Insight: “Sales increase by 2% if we lower prices by €50”
  - Standard machine learning models are correlational

Dimensions of Model Performance

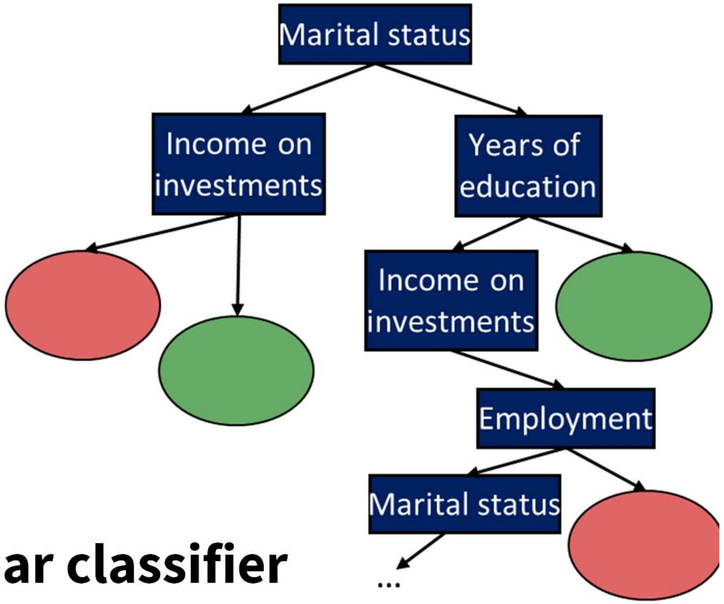
Justifiability: a key driver of model acceptance in industry

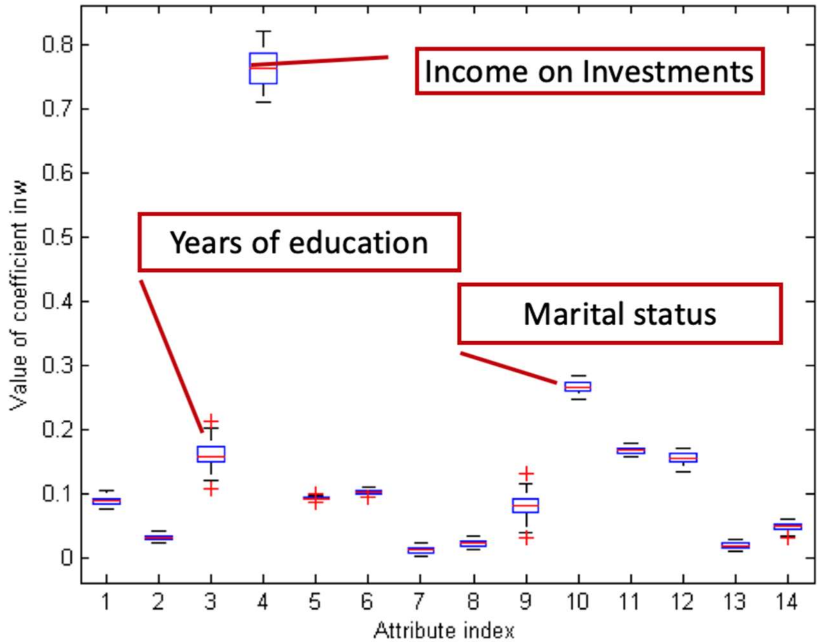
- **Does the way in which attribute values affect predictions agrees with prior beliefs or business rules?**
  - Exemplary business rules: sales decrease with price, long-term customers are more profitable than new customers, etc.
  - Requires interpretability
- **Credit risk example**
  - Business rule: credit risk decreases with age
  - Test: does WOE show this trend



Dimensions of Model Performance
Comprehensibility / Justifiability Example

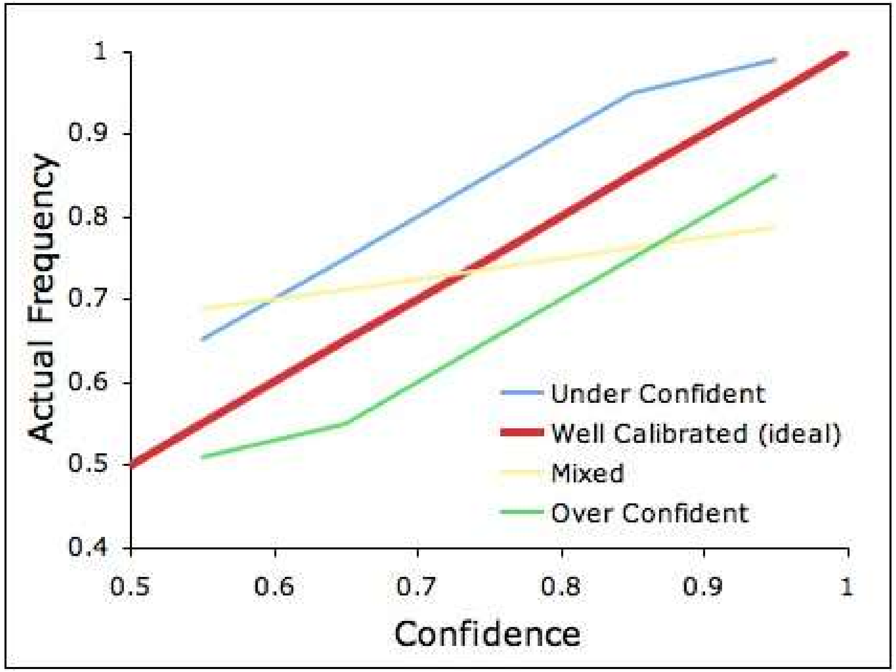
- **US Census data set from UCI library** (https://archive.ics.uci.edu/ml/datasets/Adult)
- **Classification task**
  - Is household income below or above $50,000 p.a.?
  - Fourteen attributes describing a household
    - Marital status
    - Working hours
    - Academic degree
    - Years of education
    - Country of origin
    - Income on investments
    - Employment
    - …
- **Result of tree and linear classifier**





Dimensions of Model Performance
Calibration

- **Feature of probabilistic predictions**
- **Credit Scoring Example**
  - Model makes risk forecasts for 100 credit applications
  - Forecasts are all the same and predict default of 90%
  - Then, we should eventually observe 90 actual defaults
- **For prediction models**
  - Calibration can be poor
  - Special treatment needed
  - See, e.g., Bequé et al. (2017)



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