*** Applied Machine Learning Fundamentals ***
Evaluation of ML Models

Daniel Wehner, M.Sc.

SAP SE / DHBW Mannheim

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Lecture Overview

Unit I	Machine Learning Introduction
Unit II	Mathematical Foundations
Unit III	Bayesian Decision Theory
Unit IV	Probability Density Estimation
Unit V	Regression
Unit VI	Classification I
Unit VII	**Evaluation**
Unit VIII	Classification II
Unit IX	Clustering
Unit X	Dimensionality Reduction

Agenda for this Unit

Section:

Evaluation Methods and Data Splits

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Evaluation of trained Models

1. **Validation through experts**: A domain expert checks plausibility
   - Subjective, time-intensive, costly
   - Often the only option
2. **Validation on data**: Evaluate performance on a **separate (!)** test set
   - Labeled data is scarce, could be better used for training
   - Fast and simple, no domain knowledge needed
3. **On-line validation**: Test model in a fielded application
   - Bad models may be costly
   - Gives the best estimate for the overall utility

Important

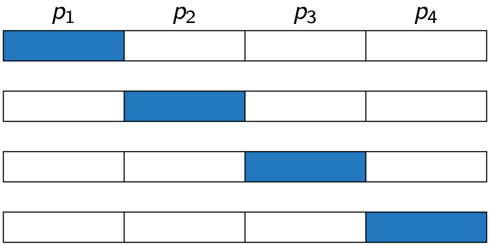
Out-of-Sample Testing

- The performance cannot be measured on the training data ($\Rightarrow$ overfitting!)
- Usually, a portion of the available data is reserved for testing
  - $^2/_3$ for training, $^1/_3$ for testing (evaluation)
  - The model is trained on the training set and evaluated on the test set
- **Problems**:
  - Waste of data
  - Labeling may be expensive
- **Solution**: Cross-Validation (X-Val)

Important

Cross-Validation (X-Val)

- Split the data set into k equally sized partitions $P = \{p_1, p_2, \ldots, p_k\}$
- `For each` partition p_i `do:` use p_i for testing and $P \setminus \{p_i\}$ for training
- Average the results; e. g. 4-fold X-Val:



Leave-One-Out Cross-Validation (LOO X-Val)

- n-fold X-Val
  - n is the number of examples
  - Use $n-1$ examples for training, one example for testing
- Properties
  - Makes best use of the data
  - Very expensive for large data sets (large n)

If k-fold X-Val is performed, we get k trained models!

- **Which model is used in production?**
- **Answer:** None. X-Val is only used for error estimation. The final model is trained on the entire data set

Three Splits: Train, Dev/Validation, Test

In practice it is common to split the data into three portions:

Stratified splits have the same class dist. as the entire data set

1. **Training set** (used for training as before)
2. **Dev/Validation set**
    - Used for hyper-parameter tuning of the model
    - Using the test set for that would be cheating
3. **Test set**
    - The final model is tested on the test set
    - Test set is used to estimate the **generalization error**

Section:

Evaluation Metrics

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Types of Errors

- **Type I Error**: False negatives
  - An instance which is labeled $\oplus$ is classified as $\ominus$
  - E. g. a spam e-mail is not detected
- **Type II Error**: False positives
  - An instance which is labeled $\ominus$ is classified as $\oplus$
  - E. g. a non-spam (ham) e-mail is classified as spam

a. k. a. α/β error

Depending on the context the costs of false negatives and false positives can be different!

Confusion Matrices (two Classes)

- How often is class $\mathcal{C}_i$ confused with class $\mathcal{C}_j$?
- Calculate **accuracy**:

	Classified $\oplus$	**Classified** $\ominus$
Is $\oplus$	true positives (tp)	false negatives (fn)
Is $\ominus$	false positives (fp)	true negatives (tn)

$$accuracy = \frac{tp + tn}{tp + tn + fp + fn}$$

$$error = 1 - accuracy$$

Confusion Matrices (multiple Classes)

	A	B	C	D	Σ
A	$n_{A,A}$	$n_{B,A}$	$n_{C,A}$	$n_{D,A}$	n_A
B	$n_{A,B}$	$n_{B,B}$	$n_{C,B}$	$n_{D,B}$	n_B
C	$n_{A,C}$	$n_{B,C}$	$n_{C,C}$	$n_{D,C}$	n_C
D	$n_{A,D}$	$n_{B,D}$	$n_{C,D}$	$n_{D,D}$	n_D
Σ	$\overline{n_A}$	$\overline{n_B}$	$\overline{n_C}$	$\overline{n_D}$	n

$$accuracy = \frac{n_{A,A} + n_{B,B} + n_{C,C} + n_{D,D}}{n}$$

Drawback of Accuracy

- Real-world data sets are usually **imbalanced**, i. e. some classes appear more frequently than others
- **Example**:
  - A data set $\mathcal{D}$ contains two classes $\mathcal{C}_1$ and $\mathcal{C}_2$
  - $\mathcal{C}_1$ appears 99 % of the time, $\mathcal{C}_2$ 1 % of the time
  - It is easy to reach 99 % accuracy by always predicting the majority class
  - **Is this useful?** *Probably not...*

We need some more sophisticated evaluation metrics!

Precision and Recall

Precision: Ratio of *tp* to all instances predicted as $\oplus$

$$Precision\ (P) = \frac{tp}{tp + fp} \tag{1}$$

Recall (Sensitivity): Ratio of *tp* to all instances actually labeled as $\oplus$

$$Recall\ (R) = \frac{tp}{tp + fn} \tag{2}$$

Precision-Recall-Trade-Off

There is a trade-off between precision and recall:

It is very easy to get 100 % precision:

- Simply classify one instance as $\oplus$ where you are absolutely sure
- But recall is bad... *(many $\oplus$-instances are not detected)*

It is also quite easy to achieve 100 % recall:

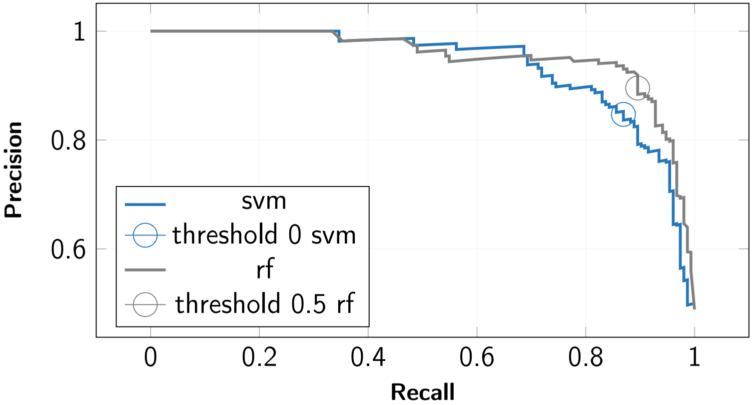
- Classify all instances as $\oplus$
- But precision is bad... *(many $\ominus$-instances are detected)*

Precision-Recall Curves / P-R-Curves

- Visualization of the Precision-Recall-trade-off
- Influence precision and recall by changing thresholds
- **Example**:
  - Consider a ranker, e. g. a logistic regression classifier
  - It outputs probabilities for each class
  - The threshold when to predict $\oplus$ can be changed
  - This has an influence on precision and recall

A P-R-curve plots precision and recall for all possible thresholds.

Precision-Recall Curves / P-R-Curves (Ctd.)



Combining Precision and Recall: F1-Score

- When to use precision, when recall?
- This depends on the cost of *fp* and *fn*
  - If *fp* are expensive $\Rightarrow$ **use precision!**
  - If *fn* are expensive $\Rightarrow$ **use recall!**
- **F1-score** *(harmonic mean of precision and recall)*

Why the harmonic mean?

$$F_1 = \frac{2 \cdot P \cdot R}{P + R} \qquad F_\beta = (1 + \beta^2) \cdot \frac{P \cdot R}{(\beta^2 \cdot P) + R} \quad (\beta \in \mathbb{R}^+) \tag{3}$$

- Large β emphasizes recall

Calculation for multiple Classes (Example Precision)

- Precision must be calculated for each class separately
- For $|\mathcal{C}|$ classes we get $|\mathcal{C}|$ results. **How to combine?**
  - Macro average: Calculate P for each class and average the result

$$P_{macro} = \frac{P_A + P_B + P_C + P_D}{|\mathcal{C}|} \tag{4}$$

  - Micro average: Sum all tp and fp for all classes and calculate P

$$P_{micro} = \frac{tp_A + tp_B + tp_C + tp_D}{(tp_A + tp_B + tp_C + tp_D) + (fp_A + fp_B + fp_C + fp_D)} \tag{5}$$

Calculation for multiple Classes (Example Precision)

	A	B	C	D	Σ
A	40	12	4	8	64
B	7	51	2	0	60
C	2	17	27	11	57
D	39	4	15	8	66
Σ	88	84	48	27	247

Cols: Prediction
Rows: Gold label

$$P_A = \frac{40}{40 + 48} = 0.45$$

$$P_B = 0.61$$

$$P_C = 0.56$$

$$P_D = 0.30$$

$$P_{macro} = \frac{0.45 + 0.61 + 0.56 + 0.30}{4} = 0.48$$

$$P_{micro} = \frac{40 + \ldots + 8}{(40 + \ldots + 8) + (48 + \ldots + 19)} = 0.51$$

ROC-Curves

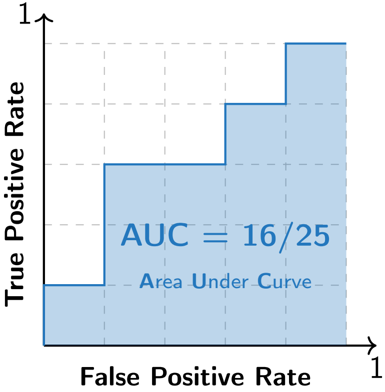
- ROC = **R**eceiver **O**perating **C**haracteristic
- Borrowed from signal theory *(hence the name)*
- Uses *true positive rate* (recall) and *false positive rate* $= \frac{fp}{fp+tn}$

General procedure:

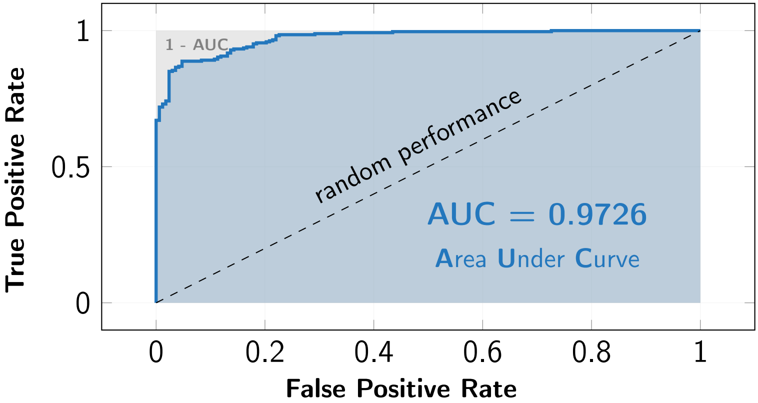
- Rank test instances by decreasing certainty of class $\oplus$
- Start at the origin $(0, 0)$
- If the next instance in the ranking is $\oplus$: move $1/|\oplus|$ up
- If the next instance in the ranking is $\ominus$: move $1/|\ominus|$ right

Sample ROC-Curve I

Rank	Prob.	True class
1	0.95	$\oplus$
2	0.85	$\ominus$
3	0.78	$\oplus$
4	0.75	$\oplus$
5	0.62	$\ominus$
6	0.41	$\ominus$
7	0.37	$\oplus$
8	0.22	$\ominus$
9	0.15	$\oplus$
10	0.05	$\ominus$



Sample ROC-Curve II



ROC-Curve Interpretation

- AUC can be interpreted as the probability of a positive example always being listed before a negative example
- A high AUC value entails a good class separation:

AUC = 1.0: All $\oplus$ listed before all $\ominus$ (desiderata)
AUC = 0.5: Random ordering
AUC = 0.0: All $\ominus$ listed before all $\oplus$ (not the worst case $\Rightarrow$ Invert classification)

Analogy: It is like a quiz. But you can answer those questions first where you feel the most certain (ranking). If you answer the first questions wrong, you don't perform well $\Rightarrow$ **small AUC**.

Section:

Cost-sensitive Evaluation

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Cost-Sensitive Evaluation

- Predicting class $\mathcal{C}_i$ instead of the correct class $\mathcal{C}_j$ is associated with a cost-factor $c(\mathcal{C}_i|\mathcal{C}_j)$
- Usually, there are only costs for wrong predictions

- 0/1-Loss:

$$c(\mathcal{C}_i|\mathcal{C}_j) = \begin{cases} 0 & \text{if } i = j \\ 1 & \text{if } i \neq j \end{cases}$$

- General case (two class problems):

	Classified $\oplus$	Classified $\ominus$
Is $\oplus$	$c(\oplus\|\oplus)$	$c(\ominus\|\oplus)$
Is $\ominus$	$c(\oplus\|\ominus)$	$c(\ominus\|\ominus)$

Cost-Sensitive Evaluation Examples

- **Loan applications**

  Rejecting applicants who will not pay back $\rightarrow$ **no costs**
  Accepting applicants who will pay back $\rightarrow$ **gain**
  Accepting applicants who will not pay back $\rightarrow$ **big loss**
  Rejecting applicants who would pay back $\rightarrow$ **loss**
- **Spam-mail filtering**
- **Medical diagnosis**
- ...

Expected Costs / Loss and Cost Ratio

- Expected loss $\mathcal{L}$:

$$\mathcal{L} = tpr \cdot c(\oplus|\oplus) + fpr \cdot c(\oplus|\ominus) + fnr \cdot c(\ominus|\oplus) + tnr \cdot c(\ominus|\ominus) \tag{6}$$

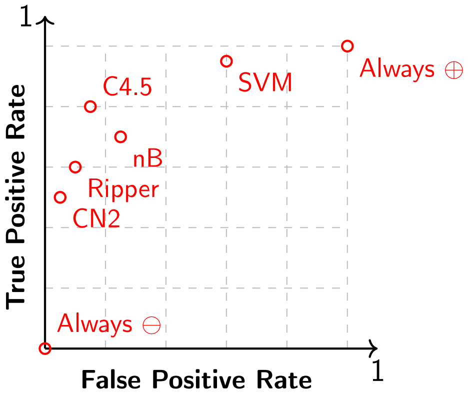
- If there are no costs for a correct classification:

$$\mathcal{L} = fpr \cdot c(\oplus|\ominus) + fnr \cdot c(\ominus|\oplus) \tag{7}$$

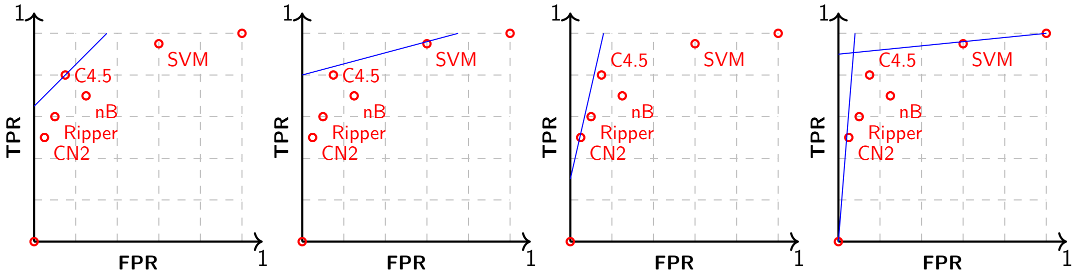
- **Cost ratio** *(false positives are r times as expensive as false negatives)*

$$r = \frac{c(\oplus|\ominus)}{c(\ominus|\oplus)} = \frac{c_{fp}}{c_{fn}} \tag{8}$$

Classifiers in ROC-Space – Example



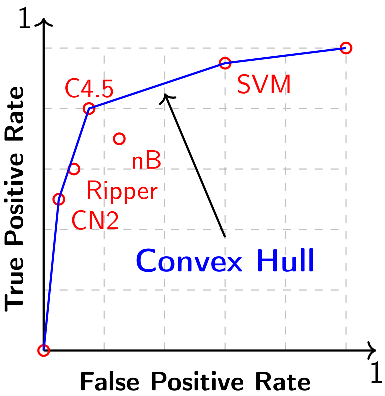
Classifiers in ROC-Space – Example (Ctd.)



$r = 1$ | $r = 1/4$ | $r = 4$ | $r < 1/4; r > 4$

Classifiers in ROC-Space – Example (Ctd.)

Classifiers on the convex hull minimize costs for some cost ratio. **Classifiers below the convex hull are always suboptimal.**



Classifiers in ROC-Space (Ctd.)

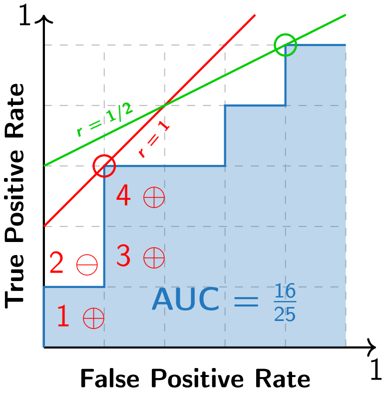
- It is possible to reach any point on the convex hull
- **Interpolation of two adjacent classifiers in ROC-space:**
  - `Classifier 1`: tpr_1 and fpr_1
  - `Classifier 2`: tpr_2 and fpr_2
  - If `classifier 1` is used to predict $q \cdot 100\,\%$ and `classifier 2` for the rest:

$$tpr_{inter} = q \cdot tpr_1 + (1 - q) \cdot tpr_2$$

$$fpr_{inter} = q \cdot fpr_1 + (1 - q) \cdot fpr_2$$

Calibrating Thresholds

Rank	Prob.	True class
1	0.95	⊕
2	0.85	⊖
3	0.78	⊕
4	0.75	⊕
5	0.62	⊖
6	0.41	⊖
7	0.37	⊕
8	0.22	⊖
9	0.15	⊕
10	0.05	⊖



Section:

Miscellaneous

Evaluation of Regressors

- **Coefficient of determination R^2:**

$$R^2 = \frac{\sum_{i=1}^{n}(h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}) - \overline{y})^2}{\sum_{i=1}^{n}(y^{(i)} - \overline{y})^2} = \frac{\text{Variance explained by model}}{\text{Total variance}} \qquad R^2 \in [0, 1] \tag{9}$$

- **Root mean square error (RMSE):**

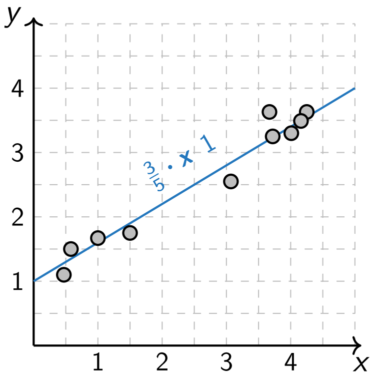
$$RMSE = \left(\frac{1}{n} \cdot \sum_{i=1}^{n} \left(h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}) - y^{(i)}\right)^2\right)^{1/2} \tag{10}$$

- **Mean absolute error (MAE):**

$$MAE = \frac{1}{n} \cdot \sum_{i=1}^{n} |h_{\boldsymbol{\theta}}(\boldsymbol{x}^{(i)}) - y^{(i)}| \tag{11}$$

Evaluation of Regressors (Ctd.)

$x^{(i)}$	$y^{(i)}$	$h_\theta(x^{(i)})$
0.47	1.10	1.28
0.58	1.50	1.35
1.00	1.67	1.60
1.50	1.75	1.90
3.07	2.55	2.84
3.67	3.63	3.20
3.72	3.25	3.23
4.01	3.30	3.41
4.16	3.49	3.50
4.25	3.63	3.55
$\bar{y} = 2.59$		



Evaluation of Regressors (Ctd.)

- Coefficient of determination:

$$R^2 = \frac{(1.28 - 2.59)^2 + \cdots + (3.55 - 2.59)^2}{(1.10 - 2.59)^2 + \cdots + (3.63 - 2.59)^2} = \frac{7.97}{8.89} = 0.90 \tag{12}$$

- Root mean square error:

$$RMSE = \left(\frac{1}{10} \cdot [(1.28 - 1.10)^2 + \cdots + (3.55 - 3.63)^2] \right)^{1/2} = 0.19 \tag{13}$$

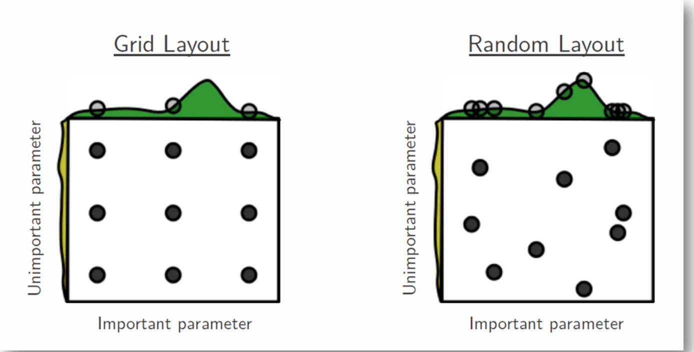
- Mean absolute error:

$$MAE = \frac{1}{10} \cdot (|1.28 - 1.10| + \cdots + |3.55 - 3.63|) = 0.15 \tag{14}$$

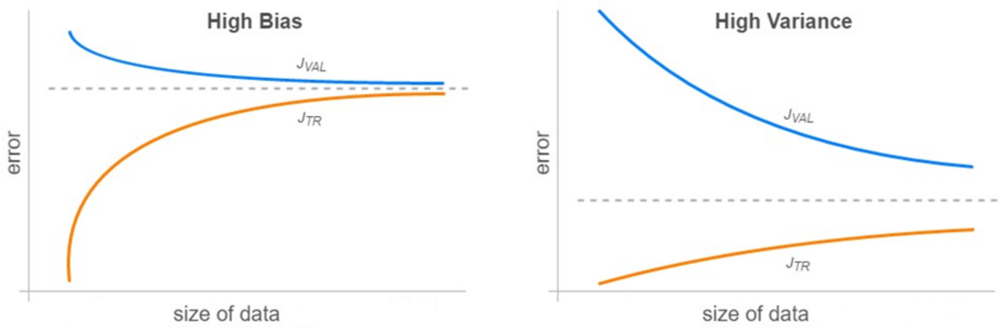
Grid Search

- Grid search is applied to find **optimal parameter settings**
- For the optimization the **dev** data set is used
- We have to specify the search space / ranges of parameter values
- Grid search will try **all parameter combinations** to find the best model
  - Computationally very expensive
  - Scikit-learn provides parameters to parallelize the search (`n_jobs=-1` $\Rightarrow$ use all cores available)
  - May not find the optimal setting $\Rightarrow$ random search

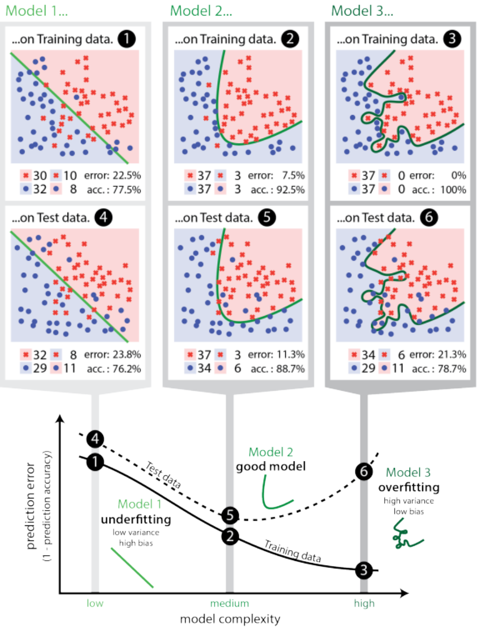
Grid Search vs. random Search



Bias and Variance



Use early stopping!



Section:

Wrap-Up

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Summary

- **Out-of-sample testing:** Split data into `train`, `dev` and `test` sets
- Cross-validation makes **maximum use of the data**
- Confusion matrices reveal **which classes are frequently confused**
- Precision, recall and F1 are **more robust w. r. t. imbalanced data sets**
- ROC curves are used for the evaluation of rankers
- Different classifiers can be optimal assuming a different cost model
- Hyper-parameters are optimized using **grid search** or **random search**
- Keep the **bias-variance trade-off** in mind!

Self-Test Questions

1. Why should you split the data into `train`, `dev` and `test` sets?
2. You perform 10-fold cross validation. How many models do you have to learn? Which one do you use in production?
3. What is the problem with accuracy?
4. Why do we apply the harmonic mean to compute the F1 score?
5. Your model gets an AUC value of 0. What does this mean?
6. Random search is usually preferred to optimize hyper-parameters. Why?
7. Your model does not perform well due to its high bias. Your boss suggests adding more training data. How would you respond?

What's next...?

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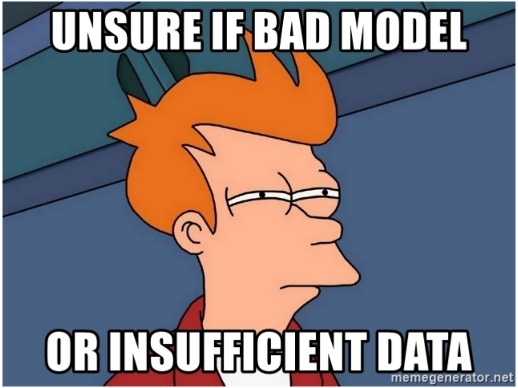
Unit VIII	**Classification II**
Unit IX	Clustering
Unit X	Dimensionality Reduction

Recommended Literature and further Reading I

[1] Machine Learning
Tom Mitchell. McGraw-Hill Science. 1997.
→ Link, cf. chapter 5

Meme of the Day



Thank you very much for the attention!

Topic: *** Applied Machine Learning Fundamentals *** Evaluation of ML Models
Term: Winter term 2020/2021

Contact:

Daniel Wehner, M.Sc.
SAP SE / DHBW Mannheim
daniel.wehner@sap.com

Do you have any questions?