*** * * Artificial Intelligence and Machine Learning * * ***

Evaluation of Machine Learning Models

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Find all slides on GitHub (DaWe1992/Applied_ML_Fundamentals)

Lecture Overview

Agenda for this Unit

Section:

Evaluation Methods and Data Splits

Introduction
Out-of-Sample Testing and Data Splits
Cross-Validation / LOO-Validation

Evaluation of trained Models

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

Out-of-Sample Testing

- The performance cannot be measured on the training data **(why?)**
- 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
- **Stratified splits**
  - **Random splits may be suboptimal** if the class distribution is imbalanced
  - A stratified split ensures that the proportion of each class in the original dataset is preserved in both the training and test sets

Three Splits: Train, Dev/Validation, Test

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

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

Issues with fixed Splits

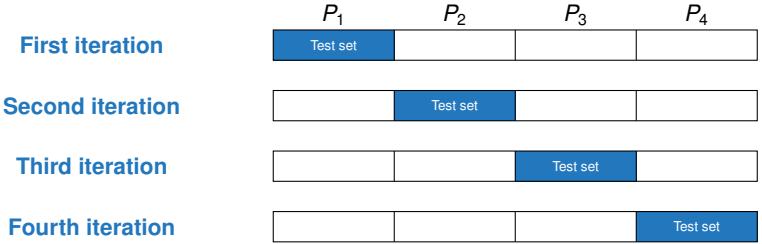
Problems:

1. **Training data is wasted for testing**
2. **Labeling additional training examples may be expensive *(with respect to time and money)***

Solution: Use the cross-validation (X-Val) technique

Cross-Validation

- Also referred to as K-fold X-Val
- Split the dataset into K equally sized partitions $\boldsymbol{P} := \{P_1, P_2, \ldots, P_K\}$
- For each partition P_k: Use $\boldsymbol{P} \backslash \{P_k\}$ for training and P_k for testing
- Average the resulting errors



Cross-Validation (Ctd.)

We get K trained models when using K-fold X-Val

Question: Which of these models is used in production?

Answer:

- None of these models is used
- X-Val is only used for error estimation
- The final model is trained on the whole dataset

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

LOO X-Val is equal to N-fold X-Val

- We use $N - 1$ examples for training
- We use one example for testing

Advantage: LOO X-Val makes best use of the available data

Disadvantage: This technique is very expensive for large datasets

Section:

Evaluation Metrics for Classifiers

Confusion Matrices
Drawback of Accuracy
Precision, Recall and F_1-Score
ROC and AUC

Types of Errors

False positive (type I error):

A $\ominus$ example is classified as $\oplus$, e. g. a non-spam e-mail is classified as spam

False negative (type II error):

An instance labeled as $\oplus$ is classified as $\ominus$, e. g. a spam e-mail is not detected

Please note: The costs of false negatives and false positives can be different depending on the context!

Confusion Matrices (two Classes)

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

Legend:

tp	true positive
fn	false negative
fp	false positive
tn	true negative

		Classified	
		$\oplus$	$\ominus$
Is	$\oplus$	**#tp**	#fn
	$\ominus$	#fp	**#tn**

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

$$\text{error} = 1 - \text{accuracy}$$

Confusion Matrices (multiple Classes)

		Classified			
		A	**B**	**C**	Σ
Is	**A**	$N_{A,A}$	$N_{B,A}$	$N_{C,A}$	N_A
	B	$N_{A,B}$	$N_{B,B}$	$N_{C,B}$	N_B
	C	$N_{A,C}$	$N_{B,C}$	$N_{C,C}$	N_C
	Σ	$\overline{N_A}$	$\overline{N_B}$	$\overline{N_C}$	N

$$accuracy = \frac{N_{A,A} + N_{B,B} + N_{C,C}}{N}$$

Drawback of Accuracy

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

Conclusion: We need some more sophisticated evaluation metrics!

Precision and Recall

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

$$P := \frac{\#\text{tp}}{\#\text{tp} + \#\text{fp}} \tag{1}$$

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

$$R := \frac{\#\text{tp}}{\#\text{tp} + \#\text{fn}} \tag{2}$$

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:

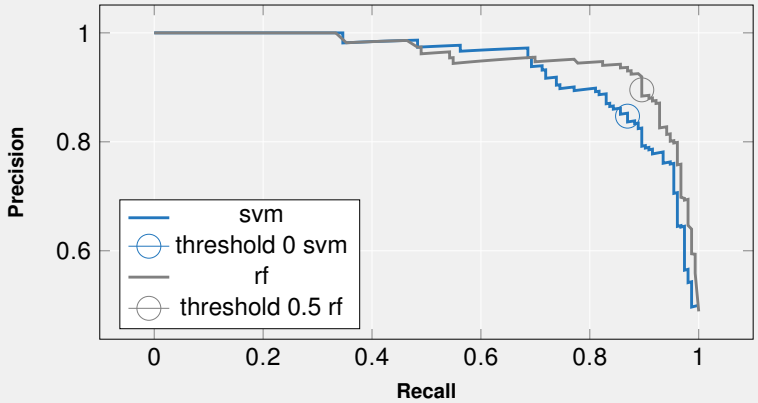
- Classify all instances as $\oplus$
- But precision is bad... *(many $\ominus$ instances are classified as $\oplus$)*

Precision-Recall Curves / P-R Curves

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

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

Example: Precision-Recall Curves / P-R-Curves



Precision or Recall?

Question: When to use precision, when to use recall?

Answer: This depends on the cost of fp and fn

- If fp are expensive $\Rightarrow$ **use precision (why?)**
- If fn are expensive $\Rightarrow$ **use recall (why?)**

Often we combine both metrics, precision and recall, to define a new metric

Combining Precision and Recall: F_1-Score

We define the **F_1-score**:

$$F_1 := \frac{2 \cdot P \cdot R}{P + R} \tag{3}$$

$$F_\beta := (1 + \beta^2) \cdot \frac{P \cdot R}{(\beta^2 \cdot P) + R} \qquad (\beta \in \mathbb{R}^+) \tag{4}$$

- The F_1-score is the harmonic mean of precision and recall
- Large values of β emphasize recall

Calculation for multiple Classes (Example Precision)

- Precision must be calculated for each class separately
- For K classes we get K results: **How to combine these results?**
  - **Macro average:** Calculate P for each class and average the results

$$P_{\text{macro}} := \frac{1}{K} \sum_{k=1}^{K} P_k \tag{5}$$

  - **Micro average:** Sum the number of tp and fp for all classes and calculate P

$$P_{\text{micro}} := \sum_{k=1}^{K} \#\text{tp}_k \Big/ \sum_{k=1}^{K} (\#\text{tp}_k + \#\text{fp}_k) \tag{6}$$

Calculation for multiple Classes (Example Precision, Ctd.)

		Classified				
		A	**B**	**C**	**D**	Σ
Is	**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

Calculation for multiple Classes (Example Precision, Ctd.)

$$P_A = \frac{40}{40 + 48} = 0.45 \qquad P_B = \frac{51}{51 + 33} = 0.61$$

$$P_C = \frac{27}{27 + 21} = 0.56 \qquad P_D = \frac{8}{8 + 19} = 0.30$$

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

$$P_{micro} = \frac{40 + 51 + 27 + 8}{(40 + 51 + 27 + 8) + (48 + 33 + 21 + 19)} = 0.51$$

ROC-Curves

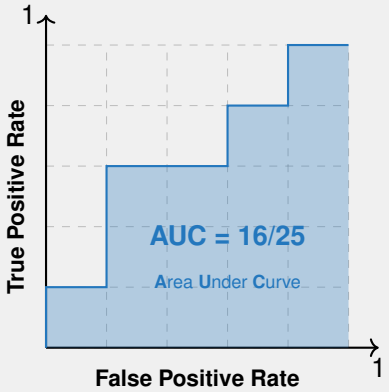
- ROC is short for **R**eceiver **O**perating **C**haracteristic
- Borrowed from signal theory *(hence the name...)*
- Uses *true positive rate* (recall) and *false positive rate* $:= \frac{\#\text{fp}}{\#\text{fp}+\#\text{tn}}$

General procedure:

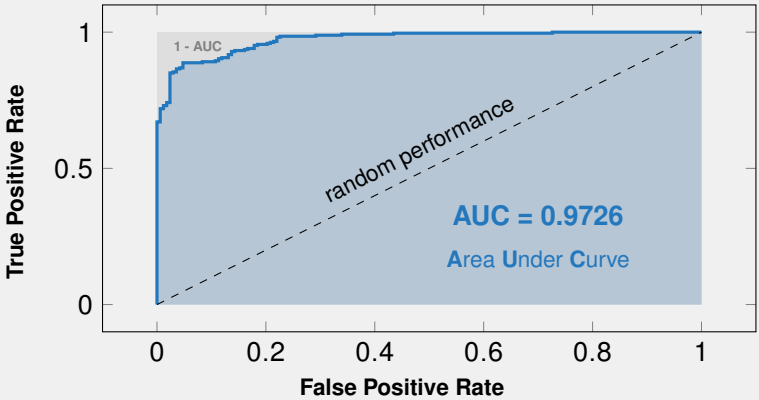
- Rank test instances by decreasing certainty of the positive class $\oplus$
- Start at the origin $(0, 0)$
- If the next instance in the ranking is $\oplus$: move $1/|\oplus|$ up
- If the next instance in the ranking is $\ominus$: move $1/|\ominus|$ right

Sample ROC-Curve (Example 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 (Example II)



ROC-Curve Interpretation

- The AUC can be interpreted as **the probability of a positive example always being listed before a negative example**
- A high AUC value implies a good class separation:
  - **AUC = 1.0:** All $\oplus$ listed before all $\ominus$ **(desiderata)**
  - **AUC = 0.5:** Random ordering **(worst case)**
  - **AUC = 0.0:** All $\ominus$ listed before all $\oplus$ **(not the worst case $\Rightarrow$ invert classification)**

Please note: ROC-curves are only defined for binary classification problems *(however, generalizations for multi-class problems exist)*

Section:

Evaluation Metrics for Regressors

Coefficient of Determination, RMSE and MAE
An Example

Coefficient of Determination

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

$$R^2 := \frac{\sum_{n=1}^{N} \left(h_{\boldsymbol{\theta}}(\boldsymbol{x}^n) - \overline{y} \right)^2}{\sum_{n=1}^{N} \left(y_n - \overline{y} \right)^2}, \qquad R^2 \in [0, 1] \tag{7}$$

- The numerator represents the variance explained by the model
- The denominator represents the total variance in the dataset

RMSE and MAE

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

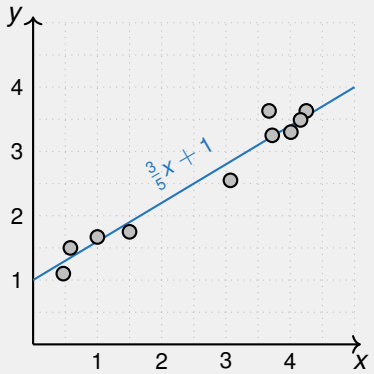
$$\text{RMSE} := \sqrt{\frac{1}{N}\sum_{n=1}^{N}\left(h_{\boldsymbol{\theta}}(\boldsymbol{x}^n) - y_n\right)^2} \tag{8}$$

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

$$\text{MAE} := \frac{1}{N}\sum_{n=1}^{N}\left|h_{\boldsymbol{\theta}}(\boldsymbol{x}^n) - y_n\right| \tag{9}$$

Example: Evaluation of Regressors

$\boldsymbol{x}^n$	y_n	$h_{\boldsymbol{\theta}}(\boldsymbol{x}^n)$
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
$\overline{y} = 2.59$		



Example: Evaluation of Regressors (Ctd.)

- Coefficient of determination:

$$R^2 = \frac{(1.28 - 2.59)^2 + \ldots + (3.55 - 2.59)^2}{(1.10 - 2.59)^2 + \ldots + (3.63 - 2.59)^2}$$

$$= \frac{7.97}{8.89} = \mathbf{0.90}$$

Example: Evaluation of Regressors (Ctd.)

- Root mean square error:

$$\text{RMSE} = \sqrt{\frac{1}{10}\left[(1.28 - 1.10)^2 + \ldots + (3.55 - 3.63)^2\right]} = \mathbf{0.19}$$

- Mean absolute error:

$$\text{MAE} = \frac{1}{10}\left(|1.28 - 1.10| + \ldots + |3.55 - 3.63|\right) = \mathbf{0.15}$$

Section:

Model Selection and Model Complexity

Hyperparameter Tuning: Grid Search and Random Search

Bias and Variance / Bias-Variance Decomposition

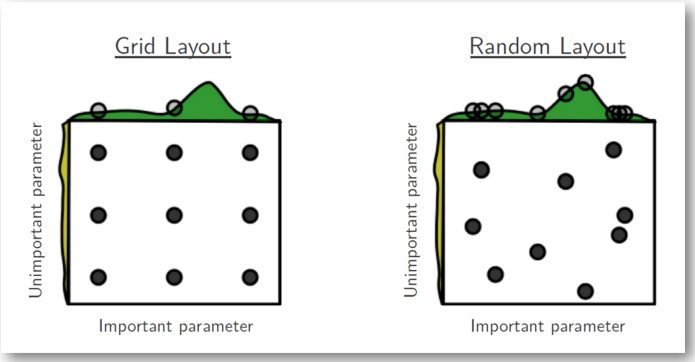
Hyperparameter Tuning with Grid Search

- **Grid search** is applied to find **optimal hyperparameter settings**
- Hyperparameter tuning should be done on the `dev` set
- We have to specify the search space / ranges of hyperparameter values
- Grid search will try **all combinations** to find the best model

Disadvantages of grid search:

1. It is **computationally very expensive** ⇒ `Scikit-learn` provides parameters to parallelize the search: `n_jobs=-1` to use all cores
2. It may not find the optimal setting ⇒ **Use random search!**

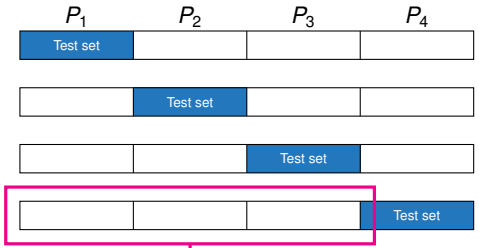
Grid Search vs. random Search



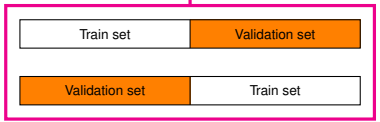
cf. BERGSTRA/BENGIO.2012, https://www.jmlr.org/papers/volume13/bergstra12a/bergstra12a.pdf, page 284

Nested Cross-Validation

Outer Loop
(Average test scores)



Inner Loop
(Hyperparameter tuning)



Bias-Variance Decomposition for MSE

- Suppose that we have a training set $\mathcal{D} := \left\{(x_1, y_1), \ldots, (x_N, y_N)\right\}$
- There is an **unknown** function $f(x)$ such that

$$y = f(x) + \varepsilon \tag{10}$$

- The noise term ε has zero mean and variance σ_ε^2, i. e. $\mathbb{E}\{\varepsilon\} = 0$ and $\mathbb{V}\{\varepsilon\} = \sigma_\varepsilon^2$
- Based on the dataset $\mathcal{D}$ we want to find a function $\widehat{f}(x; \mathcal{D})$ which approximates $f(x)$ as well as possible
- For this we try to minimize the mean squared error $\mathbb{E}_{\mathcal{D},\varepsilon}\left\{\left(y - \widehat{f}(x; \mathcal{D})\right)^2\right\}$

Bias-Variance Decomposition for MSE (Ctd.)

- We can decompose the **expected error** of $\widehat{f}(x, \mathcal{D})$ into bias and variance
- We use $\mathbb{B}_{\mathcal{D}}$ to denote the **bias** *(expected deviation of the model from the true function)*, and $\mathbb{V}_{\mathcal{D}}$ to denote the **variance** of the model $\widehat{f}$
- The variance of the noise term σ_ε^2 is **irreducible**

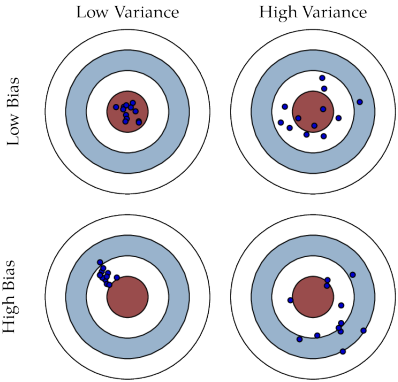
Bias-Variance decomposition of the mean squared error:

$$\mathbb{E}_{\mathcal{D},\varepsilon}\left\{\left(y - \widehat{f}(x;\mathcal{D})\right)^2\right\} = \mathbb{B}_{\mathcal{D}}^2\left\{\widehat{f}(x;\mathcal{D})\right\} + \mathbb{V}_{\mathcal{D}}\left\{\widehat{f}(x;\mathcal{D})\right\} + \sigma_\varepsilon^2 \qquad (11)$$

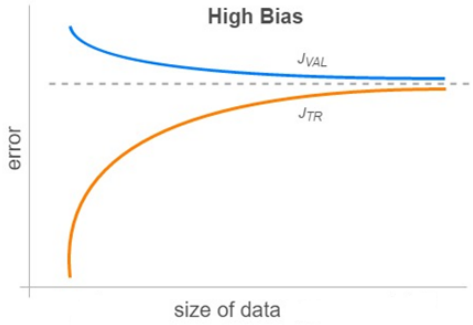
Bias and Variance

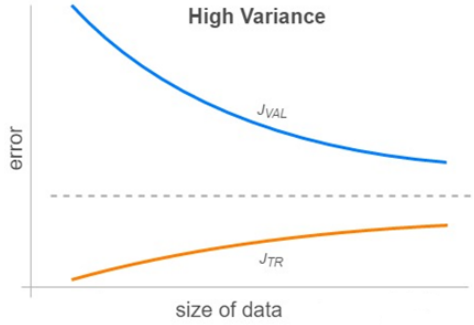
The **bias** results from erroneous assumptions in the learning algorithm. High bias can cause an algorithm to miss the relevant relations between features and target outputs **(underfitting)**.

The **variance** is an error from sensitivity to small fluctuations in the training set. High variance may result from an algorithm modeling the random noise in the training data **(overfitting)**.



Bias and Variance (Ctd.)





Recall: Expectation and Variance

- Let $\mathcal{X}$ be a random variable. $\Omega(\mathcal{X})$ is the domain of $\mathcal{X}$ *(i. e. the set of possible values $\mathcal{X}$ can take)*
- Definition of **expectation** *(discrete case)*:

$$\mathbb{E}\{\mathcal{X}\} := \sum_{k \in \Omega(\mathcal{X})} k \cdot p(\mathcal{X} = k) \tag{12}$$

- Definition of **variance** *(discrete case)*:

$$\mathbb{V}\{\mathcal{X}\} := \sum_{k \in \Omega(\mathcal{X})} \left(k - \mathbb{E}\{\mathcal{X}\}\right)^2 \cdot p(\mathcal{X} = k) \tag{13}$$

Recall: Expectation and Variance (Ctd.)

Let $\mathcal{X}$ and $\mathcal{Y}$ be random variables and $a, b \in \mathbb{R}$:

- **Linearity** of $\mathbb{E}$: **(very important!)**

$$\mathbb{E}\{a\mathcal{X} + b\mathcal{Y}\} = a\mathbb{E}\{\mathcal{X}\} + b\mathbb{E}\{\mathcal{Y}\} \tag{14}$$

- If $\mathcal{X}$ and $\mathcal{Y}$ are independent: $\mathbb{E}\{\mathcal{X}\mathcal{Y}\} = \mathbb{E}\{\mathcal{X}\}\mathbb{E}\{\mathcal{Y}\}$
- $\mathbb{V}\{\mathcal{X}\} = \mathbb{E}\{\mathcal{X} - \mathbb{E}^2\{\mathcal{X}\}\} = \mathbb{E}\{\mathcal{X}^2\} - \mathbb{E}^2\{\mathcal{X}\}$
- $\mathbb{V}$ is **not** linear: $\mathbb{V}\{a + b\mathcal{X}\} = b^2\mathbb{V}\{\mathcal{X}\}$
- However, if $\mathcal{X}$ and $\mathcal{Y}$ are uncorrelated: $\mathbb{V}\{\mathcal{X} + \mathcal{Y}\} = \mathbb{V}\{\mathcal{X}\} + \mathbb{V}\{\mathcal{Y}\}$

Derivation of the Bias-Variance Decomposition for MSE

- **Notation:** In the following we will drop the dependence on the dataset to simplify the notation, i. e. we write $\widehat{f}$ instead of $\widehat{f}(x; \mathcal{D})$
- The MSE is given by

$$\begin{aligned} \text{MSE} &:= \mathbb{E}\left\{(y - \widehat{f})^2\right\} = \mathbb{E}\left\{y^2 - 2y\widehat{f} + \widehat{f}^2\right\} \\ &= \underbrace{\mathbb{E}\left\{y^2\right\}}_{❶} - 2\underbrace{\mathbb{E}\left\{y\widehat{f}\right\}}_{❷} + \underbrace{\mathbb{E}\left\{\widehat{f}^2\right\}}_{❸} \end{aligned} \tag{15}$$

Derivation of the Bias-Variance Decomposition for MSE (Ctd.)

We rewrite term ❶:

$$
\begin{aligned}
\mathbb{E}\left\{y^2\right\} &= \mathbb{E}\left\{(f+\varepsilon)^2\right\} && \text{Definition of } y \\
&= \mathbb{E}\left\{f^2\right\} + 2\mathbb{E}\left\{f\varepsilon\right\} + \mathbb{E}\left\{\varepsilon^2\right\} && \text{Linearity of } \mathbb{E} \\
&= f^2 + 2f\mathbb{E}\left\{\varepsilon\right\} + \mathbb{E}\left\{\varepsilon^2\right\} && f \text{ does not depend on } \mathcal{D} \\
&= f^2 + \sigma_\varepsilon^2 && \mathbb{E}\left\{\varepsilon\right\} = 0 \qquad (16)
\end{aligned}
$$

Derivation of the Bias-Variance Decomposition for MSE (Ctd.)

We rewrite term ❷:

$$
\begin{aligned}
\mathbb{E}\{y\widehat{f}\} &= \mathbb{E}\{(f+\varepsilon)\widehat{f}\} && \text{Definition of } y \\
&= f\mathbb{E}\{\widehat{f}\} + \mathbb{E}\{\varepsilon\widehat{f}\} && \text{Linearity of } \mathbb{E} \\
&= f\mathbb{E}\{\widehat{f}\} + \mathbb{E}\{\varepsilon\}\mathbb{E}\{\widehat{f}\} && \widehat{f} \text{ and } \varepsilon \text{ are independent} \\
&= f\mathbb{E}\{\widehat{f}\} && \mathbb{E}\{\varepsilon\} = 0 \qquad (17)
\end{aligned}
$$

Derivation of the Bias-Variance Decomposition for MSE (Ctd.)

Term ❸ is straight-forward:

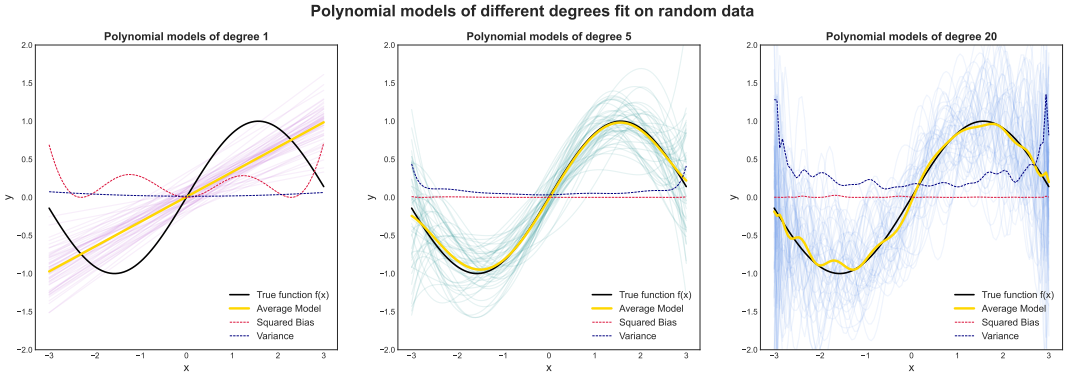
$$\begin{aligned}\mathbb{E}\left\{\widehat{f}^2\right\} &= \mathbb{E}\left\{\widehat{f}^2\right\} - \mathbb{E}^2\left\{\widehat{f}\right\} + \mathbb{E}^2\left\{\widehat{f}\right\} \\ &= \mathbb{V}\left\{\widehat{f}\right\} + \mathbb{E}^2\left\{\widehat{f}\right\} \end{aligned} \tag{18}$$

Derivation of the Bias-Variance Decomposition for MSE (Ctd.)

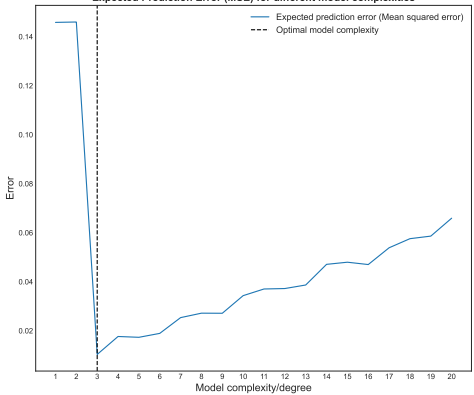
- Let us now plug these results into our MSE definition:

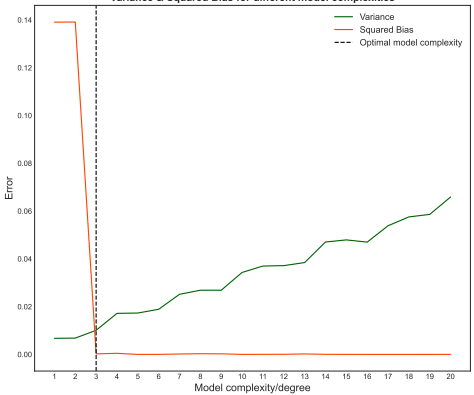
$$
\begin{aligned}
\text{MSE} &= \mathbb{E}\left\{y^2\right\} - 2\mathbb{E}\left\{y\widehat{f}\right\} + \mathbb{E}\left\{\widehat{f}^2\right\} \\
&= f^2 + \sigma_\varepsilon^2 - 2f\mathbb{E}\left\{\widehat{f}\right\} + \mathbb{V}\left\{\widehat{f}\right\} + \mathbb{E}^2\left\{\widehat{f}\right\} \\
&= \left(f - \mathbb{E}\left\{\widehat{f}\right\}\right)^2 + \mathbb{V}\left\{\widehat{f}\right\} + \sigma_\varepsilon^2 \\
&= \mathbb{E}^2\left\{\left(f - \widehat{f}\right)\right\} + \mathbb{V}\left\{\widehat{f}\right\} + \sigma_\varepsilon^2 \\
&= \mathbb{B}^2\left\{\widehat{f}\right\} + \mathbb{V}\left\{\widehat{f}\right\} + \sigma_\varepsilon^2
\end{aligned}
\tag{19}
$$

Visualization: Bias-Variance Decomposition

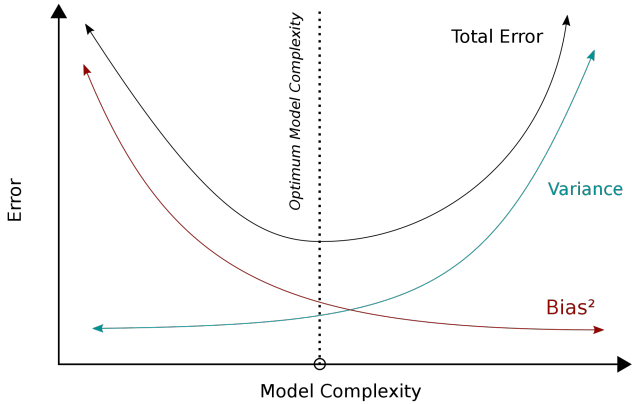


Visualization: Bias-Variance Decomposition (Ctd.)

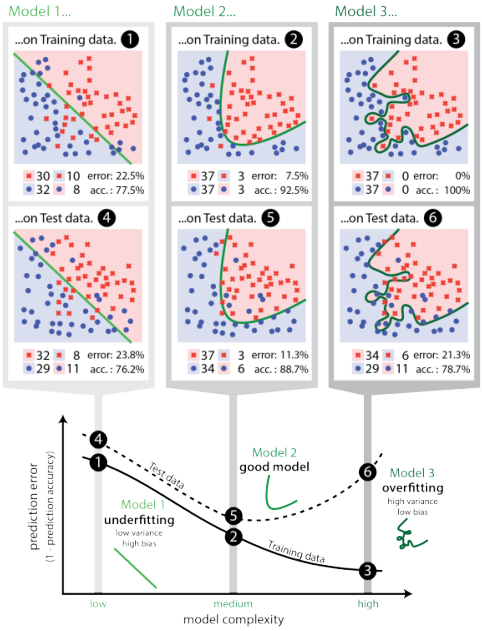




Bias, Variance, and Model Complexity



Use early stopping!



Section:

Wrap-Up

Summary
Recommended Literature
Self-Test Questions
Lecture Outlook

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 F_1-score are **more robust w. r. t. imbalanced datasets**
- ROC curves are used for the evaluation of rankers
- Hyperparameters are optimized using **grid search** or **random search**
- Keep the **bias-variance trade-off** in mind! We can decompose the error into bias and variance

Recommended Literature

1. **Evaluation metrics**
   - [MURPHY.2012], chapter 5.7.2, pages 182 – 186
2. **Bias-Variance decomposition**
   - [BISHOP.2006], chapter 3.2, pages 147 – 152

(For free PDF versions, see list in GitHub readme!)

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 F_1-score?
5. Your model produces an AUC value of 0. What does this mean?
6. Random search is usually preferred to optimize hyperparameters. Why?
7. Your model does not perform well due to its high bias. Your boss suggests adding more training examples. How would you respond?

What's next...?

I	Machine Learning Introduction
II	Optimization Techniques
III	Bayesian Decision Theory
IV	Non-parametric Density Estimation
V	Probabilistic Graphical Models
VI	Linear Regression
VII	Logistic Regression
VIII	Deep Learning
IX	Evaluation
• **X**	Decision Trees
XI	Support Vector Machines
XII	Clustering
XIII	Principal Component Analysis
XIV	Reinforcement Learning
XV	Advanced Regression

Thank you very much for the attention!

*** * * Artificial Intelligence and Machine Learning * * ***

Topic: Evaluation of Machine Learning Models

Term: Summer term 2025

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Do you have any questions?