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

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SAP SE

October 30, 2019

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Agenda October 30, 2019

Section:

Evaluation Methods and Data Splits

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Evaluation of trained Models

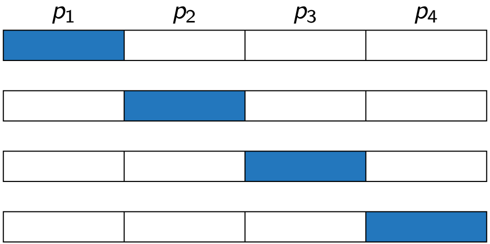
1. **Validation through experts**: A domain expert checks plausibility
   - Subjective, time-intensive, costly
   - Often the only option
2. **Validation on data**: Evaluate performance on a **separate (!)** test set
   - Labeled data is scarce, could be better used for training
   - Fast and simple, 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

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)

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!

Important

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:

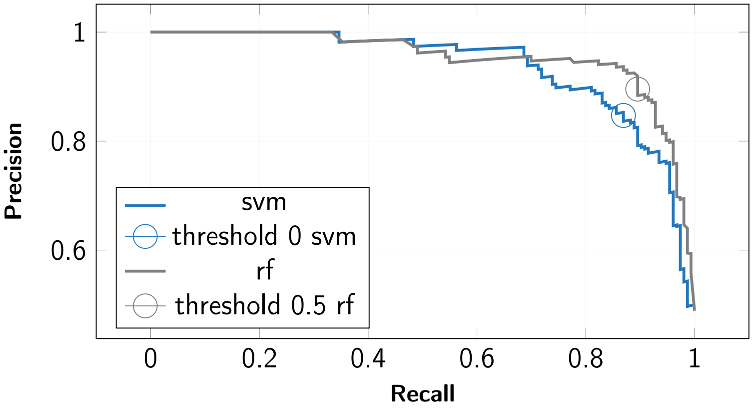
- Classify all instances as $\oplus$
- But precision is bad... *(many $\ominus$-instances are detected)*

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)*

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

- Large β emphasizes recall

Why the harmonic mean?

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

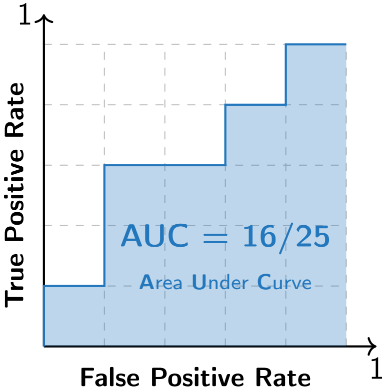
- ROC = **R**eceiver **O**perating **C**haracteristic
- Borrowed from signal theory *(hence the name)*
- Uses *true positive rate* (recall) and *false positive rate* $= \frac{fp}{fp+tn}$

General procedure:

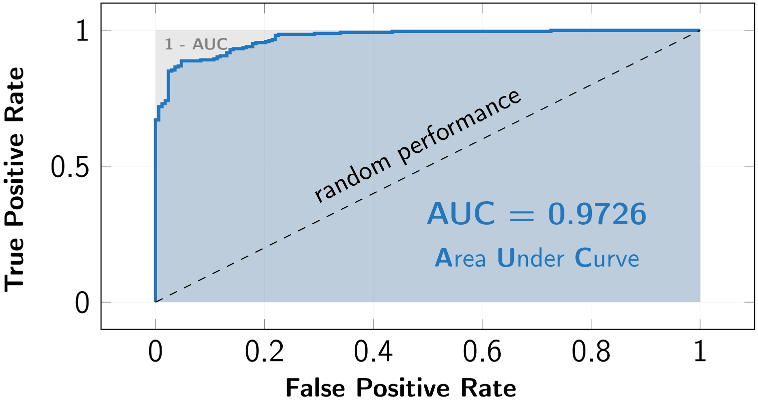
- Rank test instances by decreasing certainty of class $\oplus$
- Start at the origin $(0, 0)$
- If the next instance in the ranking is $\oplus$: move $^1/_{|\oplus|}$ up
- If the next instance in the ranking is $\ominus$: move $^1/_{|\ominus|}$ right

Sample ROC-Curve I

Rank	Prob.	True class
1	0.95	⊕
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	⊖



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 $\mathcal{L}$:

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

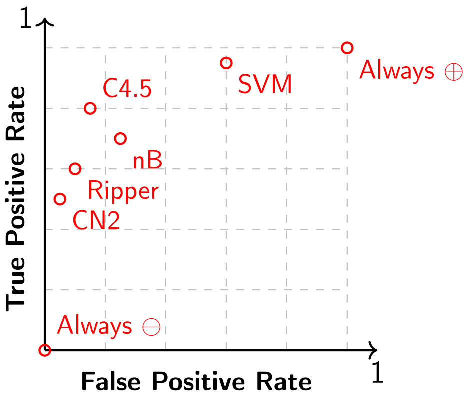
- If there are no costs for a correct classification:

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

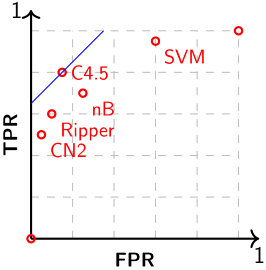
- **Cost ratio** *(false positives are r times as expensive as false negatives)*

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

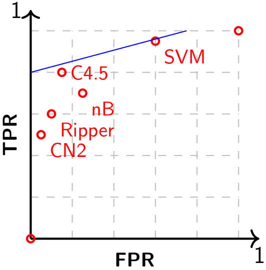
Classifiers in ROC-Space – Example



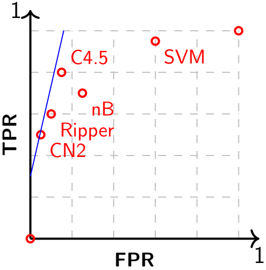
Classifiers in ROC-Space – Example (Ctd.)



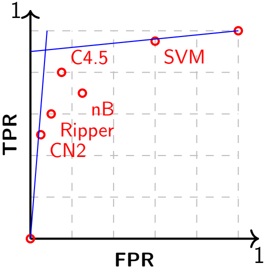
$r = 1$



$r = 1/4$



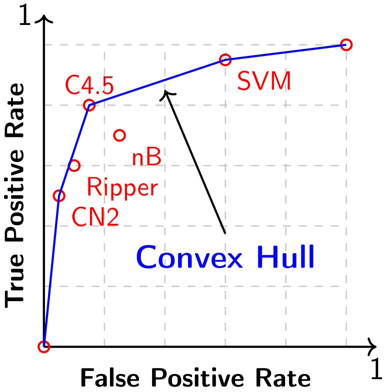
$r = 4$



$r < 1/4; r > 4$

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	⊖
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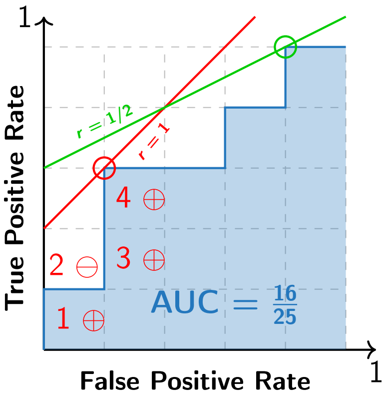

Section:

Miscellaneous

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Evaluation of Regressors

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

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

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

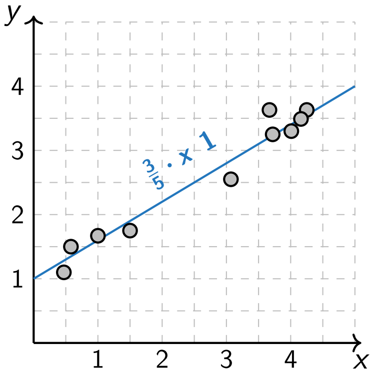
$$RMSE = \left(\frac{1}{n} \cdot \sum_{i=1}^{n} \left(h_{\boldsymbol{\theta}}(\mathbf{x}^{(i)}) - y^{(i)}\right)^2\right)^{1/2} \tag{10}$$

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

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

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:

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

- Root mean square error:

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

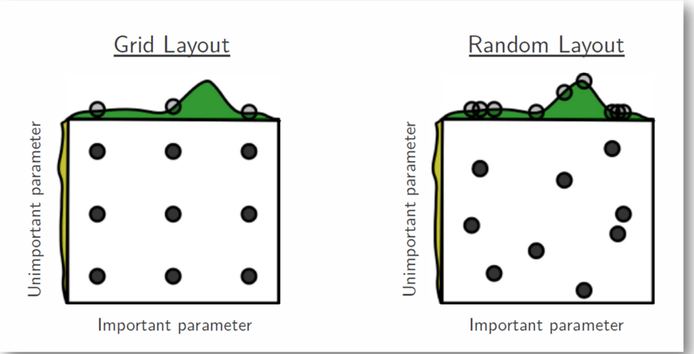
- Mean absolute error:

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

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` ⇒ use all cores available)
  - May not find the optimal setting ⇒ random search

Grid Search vs. random Search



Section:

Wrap-Up

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Summary

Lecture Overview

Unit I: Machine Learning Introduction

Self-Test Questions

Recommended Literature and further Reading

Thank you very much for the attention!

Topic: *** Applied Machine Learning Fundamentals *** Evaluation of ML Models
Date: October 30, 2019

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Do you have any questions?