Sapienza University of Rome

Master in Artificial Intelligence and Robotics
Master in Engineering in Computer Science

Machine Learning

A.Y. 2020/2021

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2. Classification Evaluation

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Overview

- Statistical evaluation
- Performance metrics

References
T. Mitchell. Machine Learning. Chapter 5

Statistical methods for estimating accuracy

Performance evaluation in classification based on *accuracy* or *error rate*.

Questions:

- How to estimate accuracy of a hypothesis h?
- Given accuracy of h over a limited sample of data, how well does this estimate its accuracy over additional examples?
- Given that h outperforms h' over some sample of data, how probable is it that h is more accurate in general?
- When data is limited what is the best way to use data to both learn h and estimate its accuracy?
- Is accuracy the unique performance metric to evaluate classification methods?

Example

Consider a typical classification problem:

$f : X \to Y$

$\mathcal{D}$: probability distribution over X

S : sample of n instances drawn from X (according to distribution $\mathcal{D}$) and for which we know $f(x)$

Consider a hypothesis h, solution of a learning algorithm obtained from S.

What is the best estimate of the accuracy of h over future instances drawn from the same distribution?

What is the probable error in this accuracy estimate?

Two Definitions of Error/Accuracy

The **true error** of hypothesis h with respect to target function f and distribution $\mathcal{D}$ is the probability that h will misclassify an instance drawn at random according to $\mathcal{D}$.

$$error_{\mathcal{D}}(h) \equiv \Pr_{x \in \mathcal{D}}[f(x) \neq h(x)]$$

The **sample error** of h with respect to target function f and data sample S is the proportion of examples h misclassifies

$$error_S(h) \equiv \frac{1}{n} \sum_{x \in S} \delta(f(x) \neq h(x))$$

where $\delta(f(x) \neq h(x))$ is 1 if $f(x) \neq h(x)$, and 0 otherwise.

Note: $accuracy(h) \equiv 1 - error(h)$

Two Definitions of Error

The **true error** cannot be computed, the **sample error** is computed only on a small data sample.

How well does $error_S(h)$ estimate $error_{\mathcal{D}}(h)$?

Note: the goal of a learning system is to be accurate in $h(x), \forall x \notin S$

If $accuracy_S(h)$ is very high, but $accuracy_{\mathcal{D}}(h)$ is poor, then our system would not be very useful.

Problems in Estimating the True Error

Estimation bias

$$bias \equiv E[error_S(h)] - error_{\mathcal{D}}(h)$$

1. If S is the training set used to compute h, $error_S(h)$ is optimistically biased
2. For unbiased estimate, h and S must be chosen independently $E[error_S(h)] = error_{\mathcal{D}}(h)$
3. Even with unbiased S, $error_S(h)$ may still *vary* from $error_{\mathcal{D}}(h)$. The smaller the set S, the greater the expected variance.

Confidence Intervals

If

- S contains n examples, drawn independently of h and each other
- $n \geq 30$

Then

- With approximately N% probability, $error_{\mathcal{D}}(h)$ lies in interval

$$error_S(h) \pm z_N \sqrt{\frac{error_S(h)(1 - error_S(h))}{n}}$$

where

$N\%$:	50%	68%	80%	90%	95%	98%	99%
z_N:	0.67	1.00	1.28	1.64	1.96	2.33	2.58

Estimators

How to compute $error_S(h)$

1. Partition the data set D ($D = T \cup S$, $T \cap S = \emptyset$, $|T| = 2/3|D|$)
2. Compute a hypothesis h using training set T
3. Evaluate $error_S(h) = \frac{1}{n} \sum_{x \in S} \delta(f(x) \neq h(x))$

$error_S(h)$ is a random variable (i.e., result of an experiment)

$error_S(h)$ is an unbiased *estimator* for $error_{\mathcal{D}}(h)$

NOTE:

- $error_{\mathcal{D}}(h)$ is needed to evaluate hypothesis h, but *cannot be computed!*
- We must use an estimate
- The best we can do is to use $error_S(h)$ (suitably computed)

Trade off between training and testing

In general

- Having more samples for training and less for testing improves performance of the model:
  potentially better model, but $error_S(h)$ does not approximate well $error_{\mathcal{D}}(h)$
- Having more samples for evaluation and less for training reduces variance of estimation:
  $error_S(h)$ approximates well $error_{\mathcal{D}}(h)$, but this value may be not satisfactory.

Trade off for medium sized datasets: 2/3 for training, 1/3 for testing.

Comparing two hypotheses

Given two hypotheses h_1, h_2, the true comparison is

$$d \equiv error_{\mathcal{D}}(h_1) - error_{\mathcal{D}}(h_2)$$

and its estimator is

$$\hat{d} \equiv error_{S_1}(h_1) - error_{S_2}(h_2)$$

$\hat{d}$ is an *unbiased estimator* for d, iff h_1, h_2, S_1 and S_2 are independent from each other.

$$E[\hat{d}] = d$$

Note: still valid if $S_1 = S_2 = S$.

Overfitting

Consider error of hypothesis h over

- training data: $error_S(h)$
- entire distribution $\mathcal{D}$ of data: $error_{\mathcal{D}}(h)$

Hypothesis $h \in H$ **overfits** training data if there is an alternative hypothesis $h' \in H$ such that

$$error_S(h) < error_S(h')$$

and

$$error_{\mathcal{D}}(h) > error_{\mathcal{D}}(h')$$

Evaluation of a learning algorithm

How can we evaluate the performance of a learning algorithm?

h is the solution of learning algorithm L when using a training set T
$h = L(T)$

$error_S(h)$ is the result of only one experiment and the confidence interval can be large.

We can perform many experiments and compute $error_{S_i}(h)$ for different independent sample data S_i.

$\Rightarrow$ **K-Fold Cross Validation** method

K-Fold Cross Validation

1. Partition data set D into k disjoint sets $S_1, S_2, \dots, S_k$ ($|S_i| > 30$)
2. For $i = 1, \dots, k$ do

   use S_i as test set, and the remaining data as training set T_i
   - $T_i \leftarrow \{D - S_i\}$
   - $h_i \leftarrow L(T_i)$
   - $\delta_i \leftarrow error_{S_i}(h_i)$
3. Return

$$error_{L,D} \equiv \frac{1}{k} \sum_{i=1}^{k} \delta_i$$

Note: $accuracy_{L,D} = 1 - error_{L,D}$

Comparing learning algorithms L_A and L_B

Which algorithm is better?

We would like to estimate:

$$E_{S \subset \mathcal{D}}[error_{\mathcal{D}}(L_A(S)) - error_{\mathcal{D}}(L_B(S))]$$

where $L(S)$ is the hypothesis output by learner L using training set S

i.e., the expected difference in true error between hypotheses output by learners L_A and L_B, when trained using randomly selected training sets S drawn according to distribution $\mathcal{D}$.

This measure can be again approximated by a K-Fold Cross Validation.

Comparing learning algorithms L_A and L_B

Use K-Fold Cross Validation to compare algorithms L_A and L_B.

1. Partition data set D into k disjoint sets $S_1, S_2, \dots, S_k$ ($|S_i| > 30$)
2. For i from 1 to k, do

   use S_i as test set, and the remaining data as training set T_i
   - $T_i \leftarrow \{D - S_i\}$
   - $h_A \leftarrow L_A(T_i)$
   - $h_B \leftarrow L_B(T_i)$
   - $\delta_i \leftarrow error_{S_i}(h_A) - error_{S_i}(h_B)$
3. Return

$$\bar{\delta} \equiv \frac{1}{k} \sum_{i=1}^{k} \delta_i$$

Note: if $\bar{\delta} < 0$ we can estimate that L_A is better than L_B.

Performance metrics in classification

Is accuracy always a good performance metric?

Example:
Binary classification $f : X \rightarrow \{-,+\}$, with training set D containing 90% of negative samples.

$h_1(x)$ has 90% of accuracy, $h_2(x)$ has 85% of accuracy.

Which one is better?

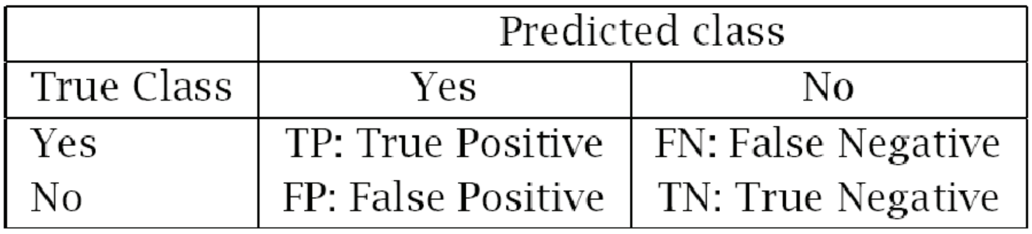
Performance metrics in classification

$h_1(x) = -$ (most common value of Y in D)
$h_2(x)$ is the result of a classification algorithm

In some cases, accuracy only is not enough to assess the performance of a classification method.

Unbalanced data sets are very common in problems related to anomaly detection (e.g, malware analysis, fraud detection, medical tests, etc.)

Performance metrics in classification



	Predicted class	
True Class	Yes	No
Yes	TP: True Positive	FN: False Negative
No	FP: False Positive	TN: True Negative

Error rate = | errors | / | instances | = (FN + FP) / (TP + TN + FP + FN)
Accuracy = 1 - Error rate = (TP + TN) / (TP + TN + FP + FN)

Problems when datasets are unbalanced.

Other performance metrics in classification

	Predicted class	
True Class	Yes	No
Yes	TP: True Positive	FN: False Negative
No	FP: False Positive	TN: True Negative

Recall = | true positives | / | real positives | = TP / (TP + FN)
ability to avoid false negatives (1 if FN = 0)

Precision = | true positives | / | predicted positives | = TP / (TP + FP)
ability to avoid false positives (1 if FP = 0)

Impact of false negatives and false positives depend on the application.

F1-score $= 2(Precision \cdot Recall)/(Precision + Recall)$

Confusion Matrix

In a classification problem with many classes, we can compute how many times an instance of class C_i is classified in class C_j.

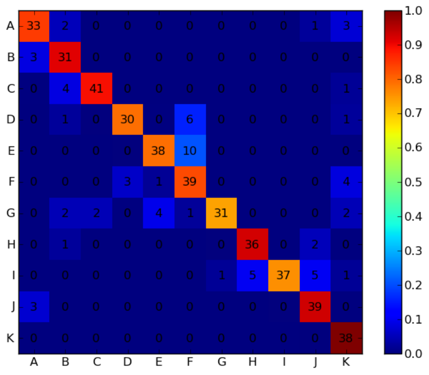
	C_1	C_2	C_3	C_4	C_5
C_1					
C_2					
C_3					
C_4					
C_5					

Main diagonal contains accuracy for each class.

Outside the diagonal, the errors. It is possible to see which classes are more often confused.

Confusion Matrix

Often represented with color-maps



	A	B	C	D	E	F	G	H	I	J	K
A	33	2	0	0	0	0	0	0	0	1	3
B	3	31	0	0	0	0	0	0	0	0	0
C	0	4	41	0	0	0	0	0	0	0	1
D	0	1	0	30	0	6	0	0	0	0	1
E	0	0	0	0	38	10	0	0	0	0	0
F	0	0	0	3	1	39	0	0	0	0	4
G	0	2	2	0	4	1	31	0	0	0	2
H	0	1	0	0	0	0	0	36	0	2	0
I	0	0	0	0	0	0	1	5	37	5	1
J	3	0	0	0	0	0	0	0	0	39	0
K	0	0	0	0	0	0	0	0	0	0	38

Other performance measures

- Recall, Sensitivity, True Positive Rate
  $TPR = TP/P = TP/(TP + FN)$
- Specificity, True Negative Rate
  $TNR = TN/N = TN/(TN + FP)$
- False Positive Rate
  $FPR = FP/N = TP/(TN + FP)$
- False Negative Rate
  $FNR = FN/P = FN/(TP + FN)$
- ROC curve: plot TPR vs FPR varying classification threshold
- AUC (Area Under the Curve)

Summary

- Performance evaluation of machine learning methods is important and tricky.
- k-Fold Cross Validation is a general prototype method to evaluate classification methods.
- Several performance metrics can be considered and in some cases best metrics to use depend on the application.
- Performance estimation is very useful also during the execution of an algorithm.