Lecture 12

# Model Evaluation 5: Performance Metrics

STAT 451: Machine Learning, Fall 2020 Sebastian Raschka <u>http://stat.wisc.edu/~sraschka/teaching/stat451-fs2020/</u>

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STAT 451: Intro to ML

Lecture 12: Model Evaluation 5

1



- 1. Confusion Matrix
- 2. Precision, Recall, and F1 Score
- 3. Balanced Accuracy
- 4. ROC
- 5. Extending Binary Metrics to Multi-class Settings

# 1. Confusion Matrix

- 2. Precision, Recall, and F1 Score
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## Based on

Raschka & Mirjalili 2019: *Python Machine Learning, 3rd Edition* Chapter 6: Learning Best Practices for Model Evaluation and Hyperparameter Tuning

(no lecture notes)

# 2x2 Confusion Matrix



### Loading the Breast Cancer Wisconsin dataset

- In the Breast Cancer Wisconsin dataset, the firt column in this dataset stores the unique ID numbers of patients
- The second column stores the corresponding cancer diagnoses (M = malignant, B = benign)
- Columns 3-32 contain features that were extracted from digitized images of the nuclei of the cancer cells, which
  can be used to build a model to predict whether a tumor is benign or malignant.
- The Breast Cancer Wisconsin dataset has been deposited in the UCI Machine Learning Repository, and more detailed information about this dataset can be found at https://archive.ics.uci.edu/ml/datasets/Breast+Cancer+Wisconsin+(Diagnostic).

[1]:	<pre>import pandas as pd</pre>															
	<pre>df = pd.read_csv('https://archive.ics.uci.edu/ml/'</pre>															
	df.head()															
[1]:		0	1	2	3	4	5	6	7	8	9	 22	23	24	25	
	0	842302	М	17.99	10.38	122.80	1001.0	0.11840	0.27760	0.3001	0.14710	 25.38	17.33	184.60	2019.0	С
	1	842517	М	20.57	17.77	132.90	1326.0	0.08474	0.07864	0.0869	0.07017	 24.99	23.41	158.80	1956.0	С
	2	84300903	М	19.69	21.25	130.00	1203.0	0.10960	0.15990	0.1974	0.12790	 23.57	25.53	152.50	1709.0	0
	3	84348301	М	11.42	20.38	77.58	386.1	0.14250	0.28390	0.2414	0.10520	 14.91	26.50	98.87	567.7	0
	4	84358402	М	20.29	14.34	135.10	1297.0	0.10030	0.13280	0.1980	0.10430	 22.54	16.67	152.20	1575.0	С
	5 rows × 32 columns															

[2]: df.shape

[2]: (569, 32)

First, we are converting the class labels from a string format into integers

```
[3]: from sklearn.preprocessing import LabelEncoder

X = df.loc[:, 2:].values

y = df.loc[:, 1].values

le = LabelEncoder()

y = le.fit_transform(y)

le.classes_
```

```
[3]: array(['B', 'M'], dtype=object)
```

 Here, class "M" (malignant cancer) will be converted to class 1, and "B" will be converted into class 0 (the order the class labels are mapped depends on the alphabetical order of the string labels)

```
[4]: le.transform(['M', 'B'])
```

[4]: array([1, 0])

Next, we split the data into 80% training data and 20% test data, using a stratified split

### 1) Confusion Matrix

More examples at

- http://rasbt.github.io/mlxtend/user\_guide/evaluate/confusion\_matrix/
- and http://rasbt.github.io/mlxtend/user\_guide/plotting/plot\_confusion\_matrix/

```
[6]: from sklearn.preprocessing import StandardScaler
     from sklearn.neighbors import KNeighborsClassifier
     from sklearn.pipeline import make_pipeline
     from mlxtend.evaluate import confusion_matrix
     #or
     #from sklearn.metrics import confusion_matrix
     pipe_knn = make_pipeline(StandardScaler(),
                              KNeighborsClassifier(n_neighbors=5))
     pipe_knn.fit(X_train, y_train)
     y_pred = pipe_knn.predict(X_test)
     confmat = confusion_matrix(y_test, y_pred)
     print(confmat)
     [[71 1]
      [ 3 39]]
```

### Visualizing a Confusion Matrix

```
[9]: from mlxtend.plotting import plot_confusion_matrix
import matplotlib.pyplot as plt
fig, ax = plot_confusion_matrix(conf_mat=confmat, figsize=(2, 2))
plt.show()
```





plt.show()



### False Positive Rate and False Negative Rate

$$TPR^{*} = \frac{TP}{P} = \frac{TP}{TP + FN} = 1 - FNR$$

$$FPR^{*} = \frac{FP}{N} = \frac{FP}{FP + TN} = 1 - TNR$$

$$FNR = \frac{FN}{P} = \frac{FN}{FN + TP} = 1 - TPR$$

$$TNR = \frac{TN}{N} = \frac{TN}{TN + FP} = 1 - FPR$$

 Think of it in a spam classification problem (what are true positives, and if you had to pick one at the expense of the other: would you rather decrease the FPR or increase the TPR?)

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### **False Positive Rate and False Negative Rate**



# **Confusion Matrix for Multi-Class Settings**

**Predicted Labels** 



Confusions matrices are traditionally for binary class problems but we can be readily generalized it to multi-class settings

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### **Multiclass to Binary**

[7]: y\_target = [1, 1, 1, 0, 0, 2, 0, 3] y\_predicted = [1, 0, 1, 0, 0, 2, 1, 3] cm1 = confusion\_matrix(y\_target=y\_target, y\_predicted=y\_predicted) print(cm1) [[2 1 0 0] [1 2 0 0][0 0 1 0] $[0 \ 0 \ 0 \ 1]]$ [8]: cm2 = confusion\_matrix(y\_target=y\_target, y\_predicted=y\_predicted, binary=True) print(cm2) [[4 1] [1 2]]

1. Confusion Matrix

# 2. Precision, Recall, and F1 Score

- 3. Balanced Accuracy
- 4. ROC
- 5. Extending Binary Metrics to Multi-class Settings

### Precision, Recall, and F1 Score

$$PRE = \frac{TP}{TP + FP}$$
$$REC = TPR = \frac{TP}{P} = \frac{TP}{FN + TP}$$
$$F_1 = 2 \cdot \frac{PRE \cdot REC}{PRE + REC}$$

- Terms that are more popular in Information Technology
- Recall is actually just another term for True Positive Rate (or "sensitivity")

### **Precision and Recall**



https://en.wikipedia.org/wiki/Precision and recall

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### **Sensitivity and Specificity**

$$SEN = TPR = REC = \frac{TP}{P} = \frac{TP}{FN + TP}$$
$$SPC = TNR = \frac{TN}{N} = \frac{TN}{FP + TN}$$

Sensitivity (SEN) measures the recovery rate of the Positives and complimentary, *Specificity* (SPC) measures the recovery rate of the Negatives.

## **Matthew's Correlation Coefficient**

- Matthews correlation coefficient (MCC) was first formulated by Brian W. Matthews [1] in 1975 to assess the performance of protein secondary structure predictions
- The MCC can be understood as a specific case of a linear correlation coefficient (Pearson r) for a binary classification setting
- Considered as especially useful in unbalanced class settings
- The previous metrics take values in the range between 0 (worst) and 1 (best)
- The MCC is bounded between the range 1 (perfect correlation between ground truth and predicted outcome) and -1 (inverse or negative correlation) — a value of 0 denotes a random prediction.

$$MCC = \frac{TP \cdot TN - FP \cdot FN}{\sqrt{(TP + FP)(TP + FN)(TN + FP)(TN + FN)}}$$
(10)

[1] Brian W Matthews. Comparison of the predicted and observed secondary structure of T4 phage lysozyme. Biochimica et Biophysica Acta (BBA)- Protein Structure, 405(2):442–451, 1975.

### 2) Precision, Recall, F1 Score

```
from sklearn.preprocessing import StandardScaler
from sklearn.neighbors import KNeighborsClassifier
from sklearn.pipeline import make_pipeline
from mlxtend.evaluate import confusion matrix
```

pipe\_knn.fit(X\_train, y\_train)

```
y_pred = pipe_knn.predict(X_test)
```

```
confmat = confusion_matrix(y_test, y_pred)
```

print(confmat)

```
[[71 1]
[ 3 39]]
```

```
print('Accuracy: %.3f' % accuracy_score(y_true=y_test, y_pred=y_pred))
print('Precision: %.3f' % precision_score(y_true=y_test, y_pred=y_pred))
print('Recall: %.3f' % recall_score(y_true=y_test, y_pred=y_pred))
print('F1: %.3f' % f1_score(y_true=y_test, y_pred=y_pred))
print('MCC: %.3f' % matthews corrcoef(y true=y test, y pred=y pred))
```

```
Accuracy: 0.965

Precision: 0.975

Recall: 0.929

F1: 0.951

MCC: 0.925 <u>https://github.com/rasbt/stat451-machine-learning-fs20/blob/master/L12/code/12_2_pre-recall-f1.ipynb</u>
```

### 3) Using those Metrics in GridSearch

```
from sklearn.model_selection import GridSearchCV
1:
   param_range = [3, 5, 7, 9, 15, 21, 31]
   pipe_knn = make_pipeline(StandardScaler(),
                            KNeighborsClassifier())
   param_grid = [{'kneighborsclassifier__n_neighbors': param_range}]
   gs = GridSearchCV(estimator=pipe_knn,
                     param_grid=param_grid,
                     scoring='f1',
                     cv=10,
                     n_jobs=-1)
   gs = gs.fit(X_train, y_train)
   print(gs.best_score_)
   print(gs.best_params_)
   0.9564099246736818
```

```
{'kneighborsclassifier__n_neighbors': 5}
```

https://github.com/rasbt/stat451-machine-learning-fs20/blob/master/L12/code/12\_2\_pre-recall-f1.ipynb

```
from sklearn.metrics import make_scorer
from mlxtend.data import iris_data
X_iris, y_iris = iris_data()
# for multiclass:
scorer = make_scorer(f1_score, average='macro')
from sklearn.model_selection import GridSearchCV
param_range = [3, 5, 7, 9, 15, 21, 31]
pipe_knn = make_pipeline(StandardScaler(),
                         KNeighborsClassifier())
param_grid = [{'kneighborsclassifier___n_neighbors': param_range}]
gs = GridSearchCV(estimator=pipe_knn,
                  param_grid=param_grid,
                  scoring=scorer,
                  cv=10,
                  n_jobs=-1)
gs = gs.fit(X_iris, y_iris)
print(gs.best_score_)
print(gs.best_params_)
0.9597306397306398
{'kneighborsclassifier n neighbors': 15}
```

https://github.com/rasbt/stat451-machine-learning-fs20/blob/master/L12/code/12\_2\_pre-recall-f1.ipynb

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## **Balanced Accuracy / Average Per-Class (APC) Accuracy**



**Predicted Labels** 

**Predicted Labels** 

		Class 0	Class 1	Class 2
abels	Class 0	3	0	0
Irue L	Class 1	7	50	12
	Class 2	0	0	18

$$ACC = \frac{T}{n}$$
  $ACC = \frac{3+50+18}{90} \approx 0.79$ 

$$APCACC = \frac{83/90 + 71/90 + 78/90}{3} \approx 0.86$$

10

# **Balanced Accuracy / Average Per-Class Accuracy**

# Predicted LabelsClass 0Neg<br/>ClassClass 030Neg<br/>Class780

Predicted Labels

	Class 1	Neg Class
Class 1	50	19
Neg Class	0	21

**True Labels** 

**True Labels** 

### Predicted Labels

	Class 2	Neg Class
Class 2	18	0
Neg Class	12	60

		Class 0	Class 1	Class 2
abels	Class 0	3	0	0
True L	Class 1	7	50	12
	Class 2	0	0	18



### Predicted Labels

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### Example 2 -- Per-Class Accuracy

The per-class accuracy is the accuracy of one class (defined as the pos\_label) versus all remaining datapoints in the dataset.

```
import numpy as np
from mlxtend.evaluate import accuracy_score

y_targ = [0, 0, 0, 1, 1, 1, 2, 2, 2]
y_pred = [1, 0, 0, 0, 1, 2, 0, 2, 2]

std_acc = accuracy_score(y_targ, y_pred)
bin_acc = accuracy_score(y_targ, y_pred, method='binary', pos_label=1)
print(f'Standard accuracy: {std_acc*100:.2f}%')
print(f'Class 1 accuracy: {bin_acc*100:.2f}%')
```

Standard accuracy: 55.56% Class 1 accuracy: 66.67%

### **Predicted Labels**

	Class 0	Class 1	Class 2
Class 0	3	0	0
Class 1	7	50	12
Class 2	0	0	18

$$ACC = \frac{3 + 50 + 18}{90} \approx 0.79$$

$$APCACC = \frac{83/90 + 71/90 + 78/90}{3} \approx 0.86$$

### **Balanced Accuracy**

from mlxtend.evaluate import confusion\_matrix
from mlxtend.evaluate import accuracy\_score
import numpy as np

```
y_targ = np.array(3*[0] + 69*[1] + 18*[2])
y_pred = np.array(10*[0] + 50*[1] + 30*[2])
```

```
std_acc = accuracy_score(y_targ, y_pred)
bin_acc0 = accuracy_score(y_targ, y_pred, method='binary', pos_label=0)
bin_acc1 = accuracy_score(y_targ, y_pred, method='binary', pos_label=1)
bin_acc2 = accuracy_score(y_targ, y_pred, method='binary', pos_label=2)
avg_acc = accuracy_score(y_targ, y_pred, method='average')
print(f'Standard accuracy: {std_acc*100:.2f}%')
print(f'Class 0 accuracy: {bin_acc0*100:.2f}%')
print(f'Class 1 accuracy: {bin_acc1*100:.2f}%')
print(f'Class 2 accuracy: {bin_acc2*100:.2f}%')
print(f'Class 2 accuracy: {bin_acc2*100:.2f}%')
print(f'Average per-class accuracy: {avg_acc*100:.2f}%')
Standard accuracy: 78.89%
Class 0 accuracy: 78.89%
Class 1 accuracy: 78.89%
Class 2 accuracy: 85.93%
```

https://github.com/rasbt/stat451-machine-learning-fs20/blob/master/L12/code/12 3 balanced-acc-Copy1.jpynb

- 1. Confusion Matrix
- 2. Precision, Recall, and F1 Score
- 3. Balanced Accuracy

# **4. ROC**

5. Extending Binary Metrics to Multi-class Settings

# Receiver Operating Characteristic curve (ROC curve)

- Trade-off between True Positive Rate and False Positive Rate
- ROC can be plotted by changing the prediction threshold
- ROC term comes from "Radar Receiver Operators" (analysis of radar [RAdio Direction And Ranging] images)



# **RECAP: False Positive Rate and False Negative Rate**



# Receiver Operating Characteristic curve (ROC curve)

- ?.? = Perfect Prediction
- ?.? = Random Prediction



# **ROC Area Under the Curve (AUC)**



$$TPR = \frac{TP}{P} = \frac{TP}{TP + FN} = 1 - FNR$$

$$FP = \frac{FP}{N} = \frac{FP}{FP + TN} = 1 - TNR$$

$$P = \frac{FP}{N} = \frac{FP}{FP + TN} = 1 - TNR$$

$$P = \frac{FP}{N} = \frac{FP}{FP + TN} = 1 - TNR$$

$$FPR = \frac{FP}{N} = \frac{FP}{FP + TN} = 1 - TNR$$

$$FPR = \frac{FP}{N} = \frac{FP}{FP + TN} = 1 - TNR$$

$$FPR = \frac{FP}{N} = \frac{FP}{FP + TN} = 1 - TNR$$

Balanced case: 100 100 100 100

> TPR = 100/200 = 0.5FPR = 100/200 = 0.5



Ν

False

negatives

(FN)

True

negatives

(TN)

(FP)

# **ROC and k-Fold Cross-Validation**



https://github.com/rasbt/stat451-machine-learning-fs20/blob/master/L12/code/12\_4\_roc.ipynb







1.0

- 1. Confusion Matrix
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# 5. Extending Binary Metrics to Multi-class Settings

### Binary Classifiers and One-vs-Rest (OvR) / One-vs-All (OvA)



# Then, choose the class with the highest confidence

score

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# Select the class by majority vote (and use confidence score in case of ties)

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# Macro and Micro Averaging

$$PRE_{micro} = \frac{TP_1 + \dots + TP_c}{TP_1 + \dots + TP_c + FP_1 + \dots + FP_c}$$

$$PRE_{macro} = \frac{PRE_1 + \dots + PRE_c}{c}$$

Micro-averaging is useful if we want to weight each instance or prediction equally, whereas macro-averaging weights all classes equally to evaluate the overall performance of a classifier with regard to the most frequent class labels.

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# **Balanced Accuracy / Average Per-Class Accuracy**

# Predicted LabelsClass 0Neg<br/>ClassClass 030Neg<br/>Class780

Predicted Labels

	Class 1	Neg Class
Class 1	50	19
Neg Class	0	21

**True Labels** 

**True Labels** 

### Predicted Labels

	Class 2	Neg Class
Class 2	18	0
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abels	Class 0	3	0	0
True L	Class 1	7	50	12
	Class 2	0	0	18



### Predicted Labels

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### sklearn.metrics.precision\_score

sklearn.metrics.precision\_score(y\_true, y\_pred, \*, labels=None, pos\_label=1, average='binary', sample\_weight=None,
zero\_division='warn')

### Compute the precision

### average : string, [None, 'binary' (default), 'micro', 'macro', 'samples', 'weighted']

This parameter is required for multiclass/multilabel targets. If None, the scores for each class are returned. Otherwise, this determines the type of averaging performed on the data:

#### 'binary':

Only report results for the class specified by pos\_label. This is applicable only if targets (y\_{true,pred}) are binary.

### 'micro':

Calculate metrics globally by counting the total true positives, false negatives and false positives.

#### 'macro':

Calculate metrics for each label, and find their unweighted mean. This does not take label imbalance into account.

### 'weighted':

Calculate metrics for each label, and find their average weighted by support (the number of true instances for each label). This alters 'macro' to account for label imbalance; it can result in an F-score that is not between precision and recall.

### 'samples':

Calculate metrics for each instance, and find their average (only meaningful for multilabel classification where this differs from accuracy\_score).

### sklearn.metrics.roc\_auc\_score

sklearn.metrics.roc\_auc\_score(y\_true, y\_score, \*, average='macro', sample\_weight=None, max\_fpr=None, multi\_class='raise', labels=None)

[source]

Compute Area Under the Receiver Operating Characteristic Curve (ROC AUC) from prediction scores.

Note: this implementation can be used with binary, multiclass and multilabel classification, but some restrictions apply (see Parameters).

Read more in the User Guide.

### Parameters: y\_true : array-like of shape (n\_samples,) or (n\_samples, n\_classes)

True labels or binary label indicators. The binary and multiclass cases expect labels with shape (n\_samples,) while the multilabel case expects binary label indicators with shape (n\_samples, n\_classes).

### y\_score : array-like of shape (n\_samples,) or (n\_samples, n\_classes)

Target scores. In the binary and multilabel cases, these can be either probability estimates or nonthresholded decision values (as returned by decision\_function on some classifiers). In the multiclass case, these must be probability estimates which sum to 1. The binary case expects a shape (n\_samples,), and the scores must be the scores of the class with the greater label. The multiclass and multilabel cases expect a shape (n\_samples, n\_classes). In the multiclass case, the order of the class scores must correspond to the order of labels, if provided, or else to the numerical or lexicographical order of the labels in y\_true.

#### average : {'micro', 'macro', 'samples', 'weighted'} or None, default='macro'

If None, the scores for each class are returned. Otherwise, this determines the type of averaging performed on the data: Note: multiclass ROC AUC currently only handles the 'macro' and 'weighted' averages.

#### 'micro':

Calculate metrics globally by considering each element of the label indicator matrix as a label.

#### 'macro':

Calculate metrics for each label, and find their unweighted mean. This does not take label imbalance into account.

# **Dealing with Class Imbalance**

### User Guide

- 1. Introduction
  - 1.1. API's of imbalanced-learn samplers
  - 1.2. Problem statement regarding imbalanced data sets
- 2. Over-sampling
  - 2.1. A practical guide
    - 2.1.1. Naive random over-sampling
    - 2.1.2. From random over-sampling to SMOTE and ADASYN
    - 2.1.3. Ill-posed examples
    - 2.1.4. SMOTE variants
  - 2.2. Mathematical formulation
    - 2.2.1. Sample generation
    - 2.2.2. Multi-class management
- 3. Under-sampling
  - 3.1. Prototype generation
  - 3.2. Prototype selection
    - 3.2.1. Controlled under-sampling techniques
      - 3.2.1.1. Mathematical formulation
    - 3.2.2. Cleaning under-sampling techniques
      - 3.2.2.1. Tomek's links
      - 3.2.2.2. Edited data set using nearest neighbours
      - 3.2.2.3. Condensed nearest neighbors and derived algorithms
      - 3.2.2.4. Instance hardness threshold
- 4. Combination of over- and under-sampling

### https://imbalanced-learn.readthedocs.io/en/stable/user\_guide.html

