Evaluating a Classification Model

ROC, AUC, confusion matrix, and metrics

Topics

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This tutorial is derived from Data School's Machine Learning with scikit-learn tutorial. I added my own notes so anyone, including myself, can refer to this tutorial without watching the videos.

1. Review of model evaluation

- Need a way to choose between models: different model types, tuning parameters, and features
- Use a **model evaluation procedure** to estimate how well a model will generalize to out-of-sample data
- Requires a **model evaluation metric** to quantify the model performance

2. Model evaluation procedures

1. **Training and testing on the same data**
    - Rewards overly complex models that "overfit" the training data and won't necessarily generalize
2. **Train/test split**
    - Split the dataset into two pieces, so that the model can be trained and tested on different data

- Better estimate of out-of-sample performance, but still a "high variance" estimate
- Useful due to its speed, simplicity, and flexibility

3. **K-fold cross-validation**
    - Systematically create "K" train/test splits and average the results together
    - Even better estimate of out-of-sample performance

3. Model evaluation metrics

- **Regression problems:** Mean Absolute Error, Mean Squared Error, Root Mean Squared Error
- **Classification problems:** Classification accuracy
    - There are many more metrics, and we will discuss them today

4. Classification accuracy

Pima Indian Diabetes dataset from the UCI Machine Learning Repository

In [1]:
```
# read the data into a Pandas DataFrame
import pandas as pd

url = 'https://archive.ics.uci.edu/ml/machine-learning-databases/pima-
```

```
indians-diabetes/pima-indians-diabetes.data'

col_names = ['pregnant', 'glucose', 'bp', 'skin', 'insulin', 'bmi', 'p
edigree', 'age','label']

pima = pd.read_csv(url, header=None, names=col_names)
```

In [2]:

```
# print the first 5 rows of data from the dataframe
pima.head()
```

Out[2]:

	pregnant	glucose	bp	skin	insulin	bmi	pedigree	age	label
0	6	148	72	35	0	33.6	0.627	50	1
1	1	85	66	29	0	26.6	0.351	31	0
2	8	183	64	0	0	23.3	0.672	32	1
3	1	89	66	23	94	28.1	0.167	21	0
4	0	137	40	35	168	43.1	2.288	33	1

- label
  - 1: diabetes
  - 0: no diabetes
- pregnant
  - number of times pregnant

Question: Can we predict the diabetes status of a patient given their health measurements?

In [3]:

```
# define X and y
feature_cols = ['pregnant', 'insulin', 'bmi', 'age']
```

```
# X is a matrix, hence we use [] to access the features we want in fea
ture_cols
X = pima[feature_cols]

# y is a vector, hence we use dot to access 'label'
y = pima.label
```

In [4]:
```
# split X and y into training and testing sets
from sklearn.cross_validation import train_test_split
X_train, X_test, y_train, y_test = train_test_split(X, y,
random_state=0)
```

In [5]:
```
# train a logistic regression model on the training set
from sklearn.linear_model import LogisticRegression

# instantiate model
logreg = LogisticRegression()

# fit model
logreg.fit(X_train, y_train)
```

Out[5]:
```
LogisticRegression(C=1.0, class_weight=None, dual=False, fit_interce
pt=True,
          intercept_scaling=1, max_iter=100, multi_class='ovr', n_jo
bs=1,
          penalty='l2', random_state=None, solver='liblinear', tol=
0.0001,
          verbose=0, warm_start=False)
```

In [6]:
```
# make class predictions for the testing set
y_pred_class = logreg.predict(X_test)
```

Classification accuracy: percentage of correct predictions

In [7]:
```
# calculate accuracy
from sklearn import metrics
```

```
print(metrics.accuracy_score(y_test, y_pred_class))
```

```
0.692708333333
```

Classification accuracy is 69%

Null accuracy: accuracy that could be achieved by always predicting the most frequent class

- We must always compare with this

In [8]:
```
# examine the class distribution of the testing set (using a Pandas Se
ries method)
y_test.value_counts()
```

Out[8]:
```
0    130
1     62
Name: label, dtype: int64
```

In [9]:
```
# calculate the percentage of ones
# because y_test only contains ones and zeros, we can simply calculate
 the mean = percentage of ones
y_test.mean()
```

Out[9]:
```
0.3229166666666667
```

32% of the

In [10]:
```
# calculate the percentage of zeros
1 - y_test.mean()
```

Out[10]:
```
0.6770833333333333
```

In [11]:
```
# calculate null accuracy in a single line of code
# only for binary classification problems coded as 0/1
max(y_test.mean(), 1 - y_test.mean())
```

Out[11]: 0.6770833333333333

This means that a dumb model that always predicts 0 would be right 68% of the time

- This shows how classification accuracy is not that good as it's close to a dumb model
- It's a good way to know the minimum we should achieve with our models

In [12]:
```
# calculate null accuracy (for multi-class classification problems)
y_test.value_counts().head(1) / len(y_test)
```

Out[12]:
```
0    0.677083
Name: label, dtype: float64
```

Comparing the **true** and **predicted** response values

In [13]:
```
# print the first 25 true and predicted responses
print('True:', y_test.values[0:25])
print('False:', y_pred_class[0:25])
```

```
True: [1 0 0 1 0 0 1 1 0 0 1 1 0 0 0 0 1 0 0 0 1 1 0 0 0]
False: [0 0 0 0 0 0 0 1 0 1 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0]
```

Conclusion:

- Classification accuracy is the **easiest classification metric to understand**
- But, it does not tell you the **underlying distribution** of response values
    - We examine by calculating the null accuracy
- And, it does not tell you what **"types" of errors** your classifier is making

5. Confusion matrix

Table that describes the performance of a classification model

In [14]:

```python
# IMPORTANT: first argument is true values, second argument is predict
ed values
# this produces a 2x2 numpy array (matrix)
print(metrics.confusion_matrix(y_test, y_pred_class))
```

```
[[118  12]
 [ 47  15]]
```

n=192	**Predicted: 0**	**Predicted: 1**
Actual: 0	118	12
Actual: 1	47	15

- Every observation in the testing set is represented in **exactly one box**
- It's a 2x2 matrix because there are **2 response classes**
- The format shown here is **not** universal
  - Take attention to the format when interpreting a confusion matrix

Basic terminology

- **True Positives (TP):** we *correctly* predicted that they *do* have diabetes
    - 15
- **True Negatives (TN):** we *correctly* predicted that they *don't* have diabetes
    - 118
- **False Positives (FP):** we *incorrectly* predicted that they *do* have diabetes (a "Type I error")
    - 12
    - Falsely predict positive
    - Type I error
- **False Negatives (FN):** we *incorrectly* predicted that they *don't* have diabetes (a "Type II error")
    - 47
    - Falsely predict negative
    - Type II error

- 0: negative class
- 1: positive class

In [15]:

```
# print the first 25 true and predicted responses
print('True', y_test.values[0:25])
print('Pred', y_pred_class[0:25])
```

```
True [1 0 0 1 0 0 1 1 0 0 1 1 0 0 0 0 1 0 0 0 1 1 0 0 0]
Pred [0 0 0 0 0 0 0 1 0 1 0 1 0 0 0 0 0 0 0 0 0 0 0 0 0]
```

In [16]:
```
# save confusion matrix and slice into four pieces
confusion = metrics.confusion_matrix(y_test, y_pred_class)
print(confusion)
#[row, column]
TP = confusion[1, 1]
TN = confusion[0, 0]
FP = confusion[0, 1]
FN = confusion[1, 0]
```

```
[[118  12]
 [ 47  15]]
```

n=192	**Predicted: 0**	**Predicted: 1**	
Actual: 0	TN = 118	FP = 12	130
Actual: 1	FN = 47	TP = 15	62
	165	27	

6. Metrics computed from a confusion matrix

Classification Accuracy: Overall, how often is the classifier correct?

In [17]:
```
# use float to perform true division, not integer division
print((TP + TN) / float(TP + TN + FP + FN))
print(metrics.accuracy_score(y_test, y_pred_class))
```

```
0.692708333333
0.692708333333
```

Classification Error: Overall, how often is the classifier incorrect?

- Also known as "Misclassification Rate"

In [18]:
```
classification_error = (FP + FN) / float(TP + TN + FP + FN)

print(classification_error)
print(1 - metrics.accuracy_score(y_test, y_pred_class))
```

```
0.307291666667
0.307291666667
```

Sensitivity: When the actual value is positive, how often is the prediction correct?

- Something we want to maximize
- How "sensitive" is the classifier to detecting positive instances?
- Also known as "True Positive Rate" or "Recall"
- TP / all positive
    - all positive = TP + FN

In [19]:
```
sensitivity = TP / float(FN + TP)

print(sensitivity)
print(metrics.recall_score(y_test, y_pred_class))
```

```
0.241935483871
0.241935483871
```

Specificity: When the actual value is negative, how often is the prediction correct?

- Something we want to maximize
- How "specific" (or "selective") is the classifier in predicting positive instances?
- TN / all negative
    - all negative = TN + FP

In [20]:
```python
specificity = TN / (TN + FP)

print(specificity)
```

```
0.907692307692
```

Our classifier

- Highly specific
- Not sensitive

False Positive Rate: When the actual value is negative, how often is the prediction incorrect?

In [21]:
```python
false_positive_rate = FP / float(TN + FP)

print(false_positive_rate)
print(1 - specificity)
```

```
0.0923076923077
0.0923076923077
```

Precision: When a positive value is predicted, how often is the prediction correct?

- How "precise" is the classifier when predicting positive instances?

In [22]:
```
precision = TP / float(TP + FP)

print(precision)
print(metrics.precision_score(y_test, y_pred_class))
```

```
0.555555555556
0.555555555556
```

Many other metrics can be computed: F1 score, Matthews correlation coefficient, etc.

Conclusion:

- Confusion matrix gives you a **more complete picture** of how your classifier is performing
- Also allows you to compute various **classification metrics**, and these metrics can guide your model selection

Which metrics should you focus on?

- Choice of metric depends on your **business objective**
  - Identify if FP or FN is more important to reduce
  - Choose metric with relevant variable (FP or FN in the equation)
- **Spam filter** (positive class is "spam"):
  - Optimize for **precision or specificity**
    - precision
      - false positive as variable
    - specificity

- false positive as variable
- Because false negatives (spam goes to the inbox) are more acceptable than false positives (non-spam is caught by the spam filter)

- **Fraudulent transaction detector** (positive class is "fraud"):
  - Optimize for **sensitivity**
    - FN as a variable
  - Because false positives (normal transactions that are flagged as possible fraud) are more acceptable than false negatives (fraudulent transactions that are not detected)

7. Adjusting the classification threshold

In [23]:
```
# print the first 10 predicted responses
# 1D array (vector) of binary values (0, 1)
logreg.predict(X_test)[0:10]
```

Out[23]:
```
array([0, 0, 0, 0, 0, 0, 0, 1, 0, 1])
```

In [24]:
```
# print the first 10 predicted probabilities of class membership
logreg.predict_proba(X_test)[0:10]
```

Out[24]:
```
array([[ 0.63247571,  0.36752429],
       [ 0.71643656,  0.28356344],
       [ 0.71104114,  0.28895886],
       [ 0.5858938 ,  0.4141062 ],
       [ 0.84103973,  0.15896027],
       [ 0.82934844,  0.17065156],
       [ 0.50110974,  0.49889026],
```

```
[ 0.48658459,  0.51341541],
[ 0.72321388,  0.27678612],
[ 0.32810562,  0.67189438]])
```

- Row: observation
  - Each row, numbers sum to 1
- Column: class
  - 2 response classes there 2 columns
    - column 0: predicted probability that each observation is a member of class 0
    - column 1: predicted probability that each observation is a member of class 1
- Importance of predicted probabilities
  - We can rank observations by probability of diabetes
    - Prioritize contacting those with a higher probability
- predict_proba process
  1. Predicts the probabilities
  2. Choose the class with the highest probability
- There is a 0.5 classification threshold
  - Class 1 is predicted if probability > 0.5
  - Class 0 is predicted if probability < 0.5

In [25]:

```
# print the first 10 predicted probabilities for class 1
logreg.predict_proba(X_test)[0:10, 1]
```

Out[25]:

```
array([ 0.36752429,  0.28356344,  0.28895886,  0.4141062 ,  0.15896
```

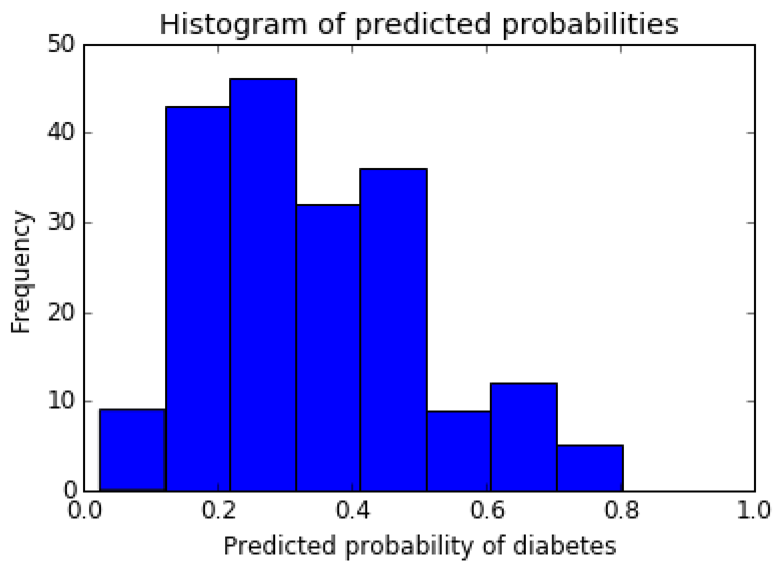
```
027,
        0.17065156,  0.49889026,  0.51341541,  0.27678612,  0.67189
438])
```

In [26]:
```
# store the predicted probabilities for class 1
y_pred_prob = logreg.predict_proba(X_test)[:, 1]
```

In [57]:
```
# allow plots to appear in the notebook
%matplotlib inline
import matplotlib.pyplot as plt

# adjust the font size
plt.rcParams['font.size'] = 12
```

In [58]:
```
# histogram of predicted probabilities

# 8 bins
plt.hist(y_pred_prob, bins=8)

# x-axis limit from 0 to 1
plt.xlim(0,1)
plt.title('Histogram of predicted probabilities')
plt.xlabel('Predicted probability of diabetes')
plt.ylabel('Frequency')
```

Out[58]:
```
<matplotlib.text.Text at 0x11c2b1128>
```



- We can see from the third bar
    - About 45% of observations have probability from 0.2 to 0.3
    - Small number of observations with probability > 0.5
    - This is below the threshold of 0.5
    - Most would be predicted "no diabetes" in this case
- Solution
    - **Decrease the threshold** for predicting diabetes
        - **Increase the sensitivity** of the classifier
            - This would increase the number of TP
                - More sensitive to positive instances
                - Example of metal detector

- Threshold set to set off alarm for large object but not tiny objects
- YES: metal, NO: no metal
- We lower the threshold amount of metal to set it off
- It is now more sensitive to metal
- It will then predict YES more often

In [29]:
```
# predict diabetes if the predicted probability is greater than 0.3
from sklearn.preprocessing import binarize
# it will return 1 for all values above 0.3 and 0 otherwise
# results are 2D so we slice out the first column
y_pred_class = binarize(y_pred_prob, 0.3)[0]
```

```
/Users/ritchieng/anaconda3/envs/py3k/lib/python3.5/site-packages/skl
earn/utils/validation.py:386: DeprecationWarning: Passing 1d arrays
 as data is deprecated in 0.17 and willraise ValueError in 0.19. Res
hape your data either using X.reshape(-1, 1) if your data has a sing
le feature or X.reshape(1, -1) if it contains a single sample.
  DeprecationWarning)
```

In [30]:
```
# print the first 10 predicted probabilities
y_pred_prob[0:10]
```

Out[30]:
```
array([ 0.36752429,  0.28356344,  0.28895886,  0.4141062 ,  0.158960
27,
        0.17065156,  0.49889026,  0.51341541,  0.27678612,  0.671894
38])
```

In [40]:
```
# print the first 10 predicted classes with the lower threshold
y_pred_class[0:10]
```

Out[40]:
```
array([ 1.,  0.,  0.,  1.,  0.,  0.,  1.,  1.,  0.,  1.])
```

In [41]:
```
# previous confusion matrix (default threshold of 0.5)
print(confusion)
```

```
[[118  12]
 [ 47  15]]
```

In [42]:
```
# new confusion matrix (threshold of 0.3)
print(metrics.confusion_matrix(y_test, y_pred_class))
```

```
[[80 50]
 [16 46]]
```

- The row totals are the same
- The rows represent actual response values
  - 130 values top row
  - 62 values bottom row
- Observations from the left column moving to the right column because we will have more TP and FP

In [46]:
```
# sensitivity has increased (used to be 0.24)
print (46 / float(46 + 16))
```

```
0.7419354838709677
```

In [44]:
```
# specificity has decreased (used to be 0.91)
print(80 / float(80 + 50))
```

```
0.6153846153846154
```

Conclusion:

- **Threshold of 0.5** is used by default (for binary problems) to convert predicted probabilities into class predictions

- Threshold can be **adjusted** to increase sensitivity or specificity
- Sensitivity and specificity have an **inverse relationship**
    - Increasing one would always decrease the other
- Adjusting the threshold should be one of the last step you do in the model-building process
    - The most important steps are
        - Building the models
        - Selecting the best model

8. Receiver Operating Characteristic (ROC) Curves

Question: Wouldn't it be nice if we could see how sensitivity and specificity are affected by various thresholds, without actually changing the threshold?

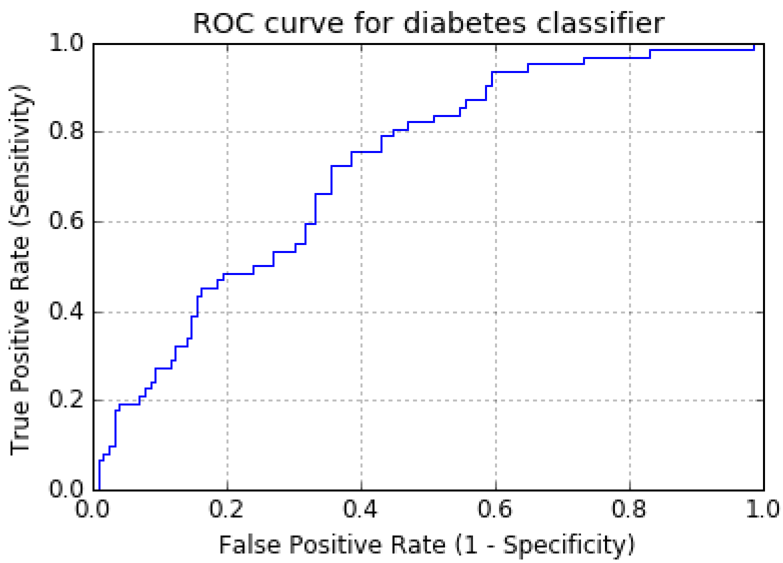
Answer: Plot the ROC curve.

- Receiver Operating Characteristic (ROC)

In [59]:

```
# IMPORTANT: first argument is true values, second argument is predict
ed probabilities

# we pass y_test and y_pred_prob
# we do not use y_pred_class, because it will give incorrect results w
ithout generating an error
# roc_curve returns 3 objects fpr, tpr, thresholds
# fpr: false positive rate
```

```
# tpr: true positive rate
fpr, tpr, thresholds = metrics.roc_curve(y_test, y_pred_prob)

plt.plot(fpr, tpr)
plt.xlim([0.0, 1.0])
plt.ylim([0.0, 1.0])
plt.rcParams['font.size'] = 12
plt.title('ROC curve for diabetes classifier')
plt.xlabel('False Positive Rate (1 - Specificity)')
plt.ylabel('True Positive Rate (Sensitivity)')
plt.grid(True)
```



- ROC curve can help you to **choose a threshold** that balances sensitivity and specificity in a way that makes sense for your particular context
- You can't actually **see the thresholds** used to generate the curve on the ROC curve itself

In [63]:
```
# define a function that accepts a threshold and prints sensitivity an
```

```python
d specificity
def evaluate_threshold(threshold):
    print('Sensitivity:', tpr[thresholds > threshold][-1])
    print('Specificity:', 1 - fpr[thresholds > threshold][-1])
```

In [64]:
```python
evaluate_threshold(0.5)
```

```
Sensitivity: 0.241935483871
Specificity: 0.907692307692
```

In [65]:
```python
evaluate_threshold(0.3)
```

```
Sensitivity: 0.725806451613
Specificity: 0.615384615385
```

9. AUC

AUC is the **percentage** of the ROC plot that is **underneath the curve**:

In [67]:
```python
# IMPORTANT: first argument is true values, second argument is predict
ed probabilities
print(metrics.roc_auc_score(y_test, y_pred_prob))
```

```
0.724565756824
```

- AUC is useful as a **single number summary** of classifier performance
- Higher value = better classifier
- If you randomly chose one positive and one negative observation, AUC represents the likelihood that your classifier will assign a **higher predicted probability** to the positive observation

- AUC is useful even when there is **high class imbalance** (unlike classification accuracy)
    - Fraud case
        - Null accuracy almost 99%
        - AUC is useful here

In [68]:
```
# calculate cross-validated AUC
from sklearn.cross_validation import cross_val_score
cross_val_score(logreg, X, y, cv=10, scoring='roc_auc').mean()
```

Out[68]:
```
0.73782336182336183
```

Use both of these whenever possible

1. **Confusion matrix advantages:**
    - Allows you to calculate a **variety of metrics**
    - Useful for **multi-class problems** (more than two response classes)
2. **ROC/AUC advantages:**
    - Does not require you to **set a classification threshold**
    - Still useful when there is **high class imbalance**

10. Confusion Matrix Resources

- Blog post: [Simple guide to confusion matrix terminology]() by me

- Videos: Intuitive sensitivity and specificity (9 minutes) and The tradeoff between sensitivity and specificity (13 minutes) by Rahul Patwari
- Notebook: How to calculate "expected value" from a confusion matrix by treating it as a cost-benefit matrix (by Ed Podojil)
- Graphic: How classification threshold affects different evaluation metrics (from a blog post about Amazon Machine Learning)

11. ROC and AUC Resources

- Lesson notes: ROC Curves (from the University of Georgia)
- Video: ROC Curves and Area Under the Curve (14 minutes) by me, including transcript and screenshots and a visualization
- Video: ROC Curves (12 minutes) by Rahul Patwari
- Paper: An introduction to ROC analysis by Tom Fawcett
- Usage examples: Comparing different feature sets for detecting fraudulent Skype users, and comparing different classifiers on a number of popular datasets

12. Other Resources ¶

- scikit-learn documentation: Model evaluation
- Guide: Comparing model evaluation procedures and metrics by me
- Video: Counterfactual evaluation of machine learning models (45 minutes) about how Stripe evaluates its fraud detection model, including slides