Evaluating Classifiers



and the Class Imbalance Problem

Our First Metrics



•
$$Accuracy = \frac{Number\ of\ correct\ predictions}{Total\ number\ of\ predictions}$$

•
$$Error\ rate = \frac{Number\ of\ wrong\ predictions}{Total\ number\ of\ predictions} = 1 - Accuracy$$

• In a binary classification we use a confusion Matrix:

| | | True condition | | | | |
|---------------------|------------------------------|-------------------------------|------------------------------|--|--|--|
| | Total population | Condition positive | Condition negative | | | |
| Predicted condition | Predicted condition positive | True positive | False positive, Type I error | | | |
| | Predicted condition negative | False negative, Type II error | True negative | | | |

Error and Accuracy

- Error rate = fraction of incorrect predictions on the testing set
 - Probability of misclassification
- Accuracy = fraction of correct predictions on the testing set $(1 error \ rate)$
 - Probability of correct prediction
- Example: A classifier misclassifies 8 out of 30 test cases:
 - Error rate = 8/30 = 0.267
 - Accuracy = 22/30 = 0.733

Class Imbalance Problem

Test set:

| Location | Retailer | Amount | Class |
|----------------------|------------------|--------|-------------------------------|
| Austin | HEB | \$50 | legitimate |
| Austin | UT Co-op | \$300 | legitimate |
| San Antonio | Mi Tierra | \$25 | legitimate |
| Austin | Freebirds | \$7 | legitimate |
| Austin | НЕВ | \$75 | legitimate |
| Austin | Target | \$150 | legitimate |
| Moscow | Tsum | \$5000 | fraudulent |
| Austin | Taco Cabana | \$5 | legitimate |
| San Antonio | Target | \$25 | legitimate |
| Austin | Trader Joe's | \$55 | legitimate |
| Austin | Alamo Drafthouse | \$20 | legitimate |
| | | ••• | |
| (1000 total records) | | | (1 of the 1000 is fraudulent) |

Run it through a classifier that Classifies everything as legitimate...

Accuracy = 999/1000 = 99.9% Error Rate = 1/1000 = 0.1%

Confusion Matrix (Binary Classification)

| | | Predicte | ed Class |
|--------|---|----------|----------|
| | | + | - |
| Actual | + | F++ (TP) | F+- (FN) |
| Class | - | F-+ (FP) | F (TN) |

Error rate: fraction of mistakes $Error \ rate = (FP + FN) / n$

Accuracy: fraction of correct predictions Accuracy = (TP + TN)/n

True positive rate (TPR), or **sensitivity**: fraction of positive examples correctly predicted TPR = TP / (TP + FN)

True negative rate (TNR), or **specificity**: fraction of negative examples correctly predicted TNR = TN / (FP + TN)

False positive rate (FPR): fraction of negative examples predicted as positive FPR = FP / (FP + TN)

False negative rate (FNR): fraction of positive examples predicted as negative FNR = FN / (TP + FN)

| | | Predicte | ed Class |
|--------|---|----------|----------|
| | | + | - |
| Actual | + | 2 | 8 |
| Class | - | 1 | 989 |

Error rate: fraction of mistakes Error rate = (1 + 8) / 1000 = 0.009 = 0.9%

Accuracy: fraction of correct predictions Accuracy = (2 + 989) / 1000 = 0.991 = 99.1%

True positive rate (TPR), or **sensitivity**: fraction of positive examples correctly predicted TPR = 2/10 = 0.2 = 20%

True negative rate (TNR), or **specificity**: fraction of negative examples correctly predicted TNR = 989 / 990 = 0.999 = 99.9%

False positive rate (FPR): fraction of negative examples predicted as positive FPR = 1/990 = 0.001 = 0.1%

False negative rate (FNR): fraction of positive examples predicted as negative FNR = 8 / 10 = 0.8 = 80%

Confusion Matrix with Cross Validation

• Use the SUM

Fold 1: 20 train / 10 test

| | | Predicted Class | |
|--------|---|--------------------|---|
| | | + | - |
| Actual | + | 4 | 2 |
| Class | ı | 1 | 3 |

Fold 2: 20 train / 10 test

| | | | icted ass |
|-----------------|---|---|--------------|
| | | + | - |
| Actual Class | + | 5 | 3 |
| | - | 0 | 2 |

Fold 3: 20 train / 10 test

| | | Predi Cla | |
|--------|---|--------------|---|
| | | + | 1 |
| Actual | + | 1 | 8 |
| Class | - | 0 | 1 |

Final Confusion Matrix: All 30 records

| | | Predi Cla | |
|--------|---|--------------|----|
| | | + | - |
| Actual | + | 10 | 13 |
| Class | - | 1 | 6 |

Precision and Recall

| | | Predicted Class | |
|--------|---|-----------------|-----|
| | | + | - |
| Actual | + | 2 | 8 |
| Class | - | 1 | 989 |

Precision, or Positive Predictive Value (PPV) addresses the question: "Given a positive prediction from the classifier, how likely is it to be correct?"

Recall, or True Positive Rate (TPR) addresses the question: "Given a positive example, will the classifier detect it?"

Class-specific **precision/PPV**: fraction of records that actually are of class C, out of records predicted to be of class C Prec(+) = TP/(TP+FP) = 2/3 = 0.667 = 66.7% Prec(-) = 989/997 = 0.991 = 99.1%

Class-specific **recall/coverage/sensitivity/TPR**: fraction of correct predictions of class C, over all points in class C Rec(+) = TP/(TP+FN) = 2/10 = 0.2 = 20% Rec(-) = 989/990 = 0.999 = 99.9%

Typically, we're only concerned with the precision and recall of the positive (rare) class.

Multi Class Confusion Matrix

| | | | Predicted Class | |
|--------------|-----------------|-------------|-----------------|----------------|
| | | Iris-setosa | Iris-versicolor | Iris-virginica |
| Actual Class | Iris-setosa | 10 | 0 | 0 |
| | Iris-versicolor | 0 | 7 | 5 |
| | Iris-virginica | 0 | 3 | 6 |

Error rate: fraction of mistakes $Error \ rate = 8/31 = 0.258 = 25.8\%$

Accuracy: fraction of correct predictions Accuracy = 23/31 = 0.742 = 74.2%

Class-specific **precision/PPV**: fraction of records that actually are of class \overline{C} , out of records predicted to be of class C

$$Prec(setosa) = 10 / 10 = 1 = 100\%$$

$$Prec(versicolor) = 7/10 = 0.7 = 70\%$$

$$Prec(virginica) = 6 / 11 = 0.545 = 54.5\%$$

Class Confusion

Class-specific **recall/coverage/TPR**: fraction of correct predictions of class C, over all points in class C

$$Rec(setosa) = 10 / 10 = 1 = 100\%$$

$$Rec(versicolor) = 7/12 = 0.583 = 58.83\%$$

$$Rec(virginica) = 6 / 9 = 0.667 = 66.7\%$$

Precision/Recall Tradeoff

| | | Predicte | ed Class |
|--------|---|----------|----------|
| | | + | - |
| Actual | + | 10 | 0 |
| Class | - | 990 | 0 |

Class-specific **precision/PPV**: fraction of records that actually are of class C, out of records predicted to be of class C Prec(+) = 10/1000 = 0.01 = 1%

Class-specific **coverage/recall/TPR**: fraction of correct predictions of class C, over all points in class C Rec(+) = 10/10 = 1 = 100%

Precision/Recall Tradeoff

| | | Predicte | ed Class |
|--------|---|----------|----------|
| | | + | - |
| Actual | + | 1 | 9 |
| Class | - | 0 | 990 |

Class-specific **precision/PPV**: fraction of records that actually are of class C, out of records predicted to be of class C Prec(+) = 1/1 = 1 = 100%

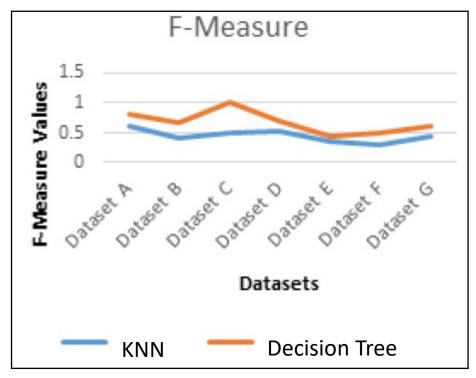
Class-specific **recall/coverage/TPR**: fraction of correct predictions of class C, over all points in class C Rec(+) = 1/10 = 0.1 = 10%

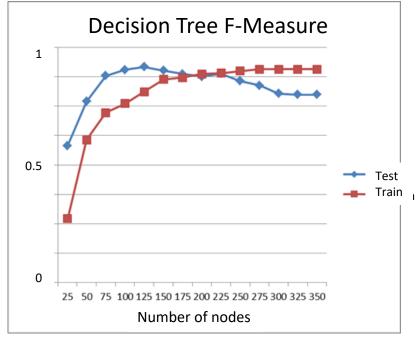
F-measure

 F-measure summarizes both precision and recall into one metric

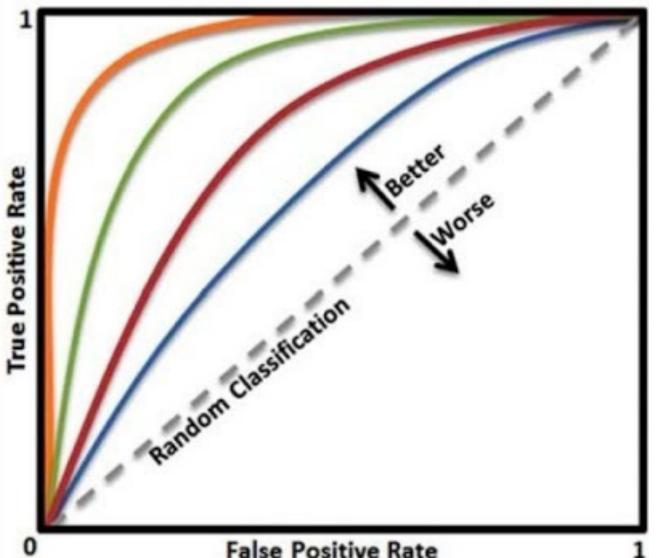
$$F = \frac{2 \times precision \times recall}{precision + recall}$$

- The overall F-measure of the classifier is the mean of the classspecific F-measures
- Or you could consider the F-measure of only the positive class





ROC Curves (Receiver Operating Characteristic)



To draw ROC curve, classifier must produce continuous-valued output

Outputs are used to rank test records, from the most likely positive class record to the least likely positive class record

| ID | Actual Class | Probability YES | Probability NO |
|----|--------------|-----------------|----------------|
| 1 | Υ | 0.35 | 0.65 |
| 2 | N | 0.23 | 0.77 |
| 3 | N | 0.55 | 0.45 |
| 4 | Υ | 0.32 | 0.68 |
| 5 | Υ | 0.54 | 0.46 |
| 6 | N | 0.47 | 0.53 |

| ID | Actual Class | Probability YES | Probability NO |
|----|--------------|-----------------|----------------|
| 1 | Υ | 0.35 | 0.65 |
| 2 | N | 0.23 | 0.77 |
| 3 | Υ | 0.55 | 0.45 |
| 4 | N | 0.32 | 0.68 |
| 5 | Υ | 0.54 | 0.46 |
| 6 | N | 0.47 | 0.53 |

Sort data by Probability YES

| ID | Actual Class | Probability YES | Probability NO |
|----|---------------------|------------------------|----------------|
| 3 | Υ | 0.55 | 0.45 |
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Select a cutoff threshold for the YES class = 0.5

Sort data by Probability YES

| ID | Actual Class | Probability YES | Probability NO |
|----|--------------|-----------------|----------------|
| 3 | Υ | 0.55 | 0.45 |
| 5 | Υ | 0.54 | 0.46 |
| 6 | N | 0.47 | 0.53 |
| 1 | Υ | 0.35 | 0.65 |
| 4 | N | 0.32 | 0.68 |
| 2 | N | 0.23 | 0.77 |

Select a cutoff threshold for the YES class = 0.5

Calculate TPR (sensitivity) and FPR (1-specificity):

| | | Predicte | d Class |
|--------|---|----------|---------|
| | | + | - |
| Actual | + | 2 | 1 |
| Class | - | 0 | 3 |

TPR =
$$2/3 = 0.67$$

FPR = $0/3 = 0$

This becomes a point on our ROC curve

Sort data by Probability YES

| ID | Actual Class | Probability YES | Probability NO |
|----|--------------|-----------------|----------------|
| 3 | Υ | 0.55 | 0.45 |
| 5 | Υ | 0.54 | 0.46 |
| 6 | N | 0.47 | 0.53 |
| 1 | Υ | 0.35 | 0.65 |
| 4 | N | 0.32 | 0.68 |
| 2 | N | 0.23 | 0.77 |

Now adjust the threshold for the YES class = 0.4

Sort data by Probability YES

| ID | Actual Class | Probability YES | Probability NO |
|----|---------------------|-----------------|----------------|
| 3 | Υ | 0.55 | 0.45 |
| 5 | Υ | 0.54 | 0.46 |
| 6 | N | 0.47 | 0.53 |
| 1 | Υ | 0.35 | 0.65 |
| 4 | N | 0.32 | 0.68 |
| 2 | N | 0.23 | 0.77 |

Now adjust the threshold for the YES class = 0.4

Calculate TPR (sensitivity) and FPR (1-specificity):

| | | Predicte | d Class |
|--------|---|----------|---------|
| | | + | - |
| Actual | + | 2 | 1 |
| Class | - | 1 | 2 |

This becomes a point on our ROC curve

How to Construct an ROC curve

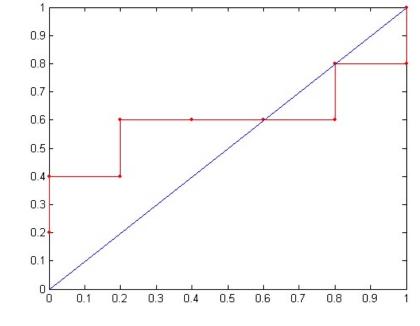
| Instance | Score | True Class |
|----------|--------|------------|
| 1 | 0.95 | + |
| 2 | 0.93 | + |
| 3 | 0.87 | - |
| 4 | 4 0.85 | |
| 5 | 0.85 | - |
| 6 | 0.85 | + |
| 7 | 0.76 | - |
| 8 | 0.53 | + |
| 9 | 0.43 | - |
| 10 | 0.25 | + |

- Use a classifier that produces a continuous-valued score for each instance
 - The more likely it is for the instance to be in the + class, the higher the score
- Sort the instances in decreasing order according to the score
- Apply a threshold at each unique value of the score
- Count the number of TP, FP, TN, FN at each threshold
 - TPR = TP/(TP+FN)
 - FPR = FP/(FP + TN)

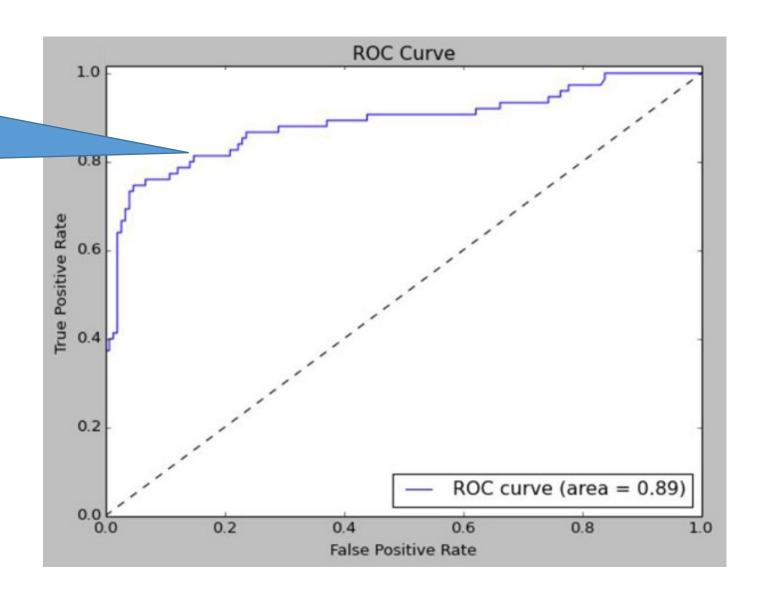
How to construct an ROC curve

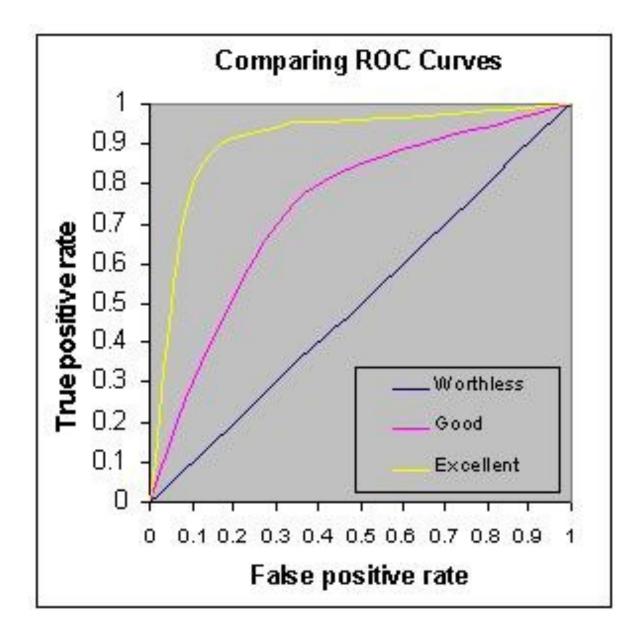
| | Class | + | - | + | - | - | - | + | - | + | + | |
|-------------------|-------|------|------|------|------|-----|------|------|------|------|------|------|
| Threshold >= | | 0.25 | 0.43 | 0.53 | 0.76 | 8.0 | 0.82 | 0.85 | 0.87 | 0.93 | 0.95 | 1.00 |
| | TP | 5 | 4 | 4 | 3 | 3 | 3 | 3 | 2 | 2 | 1 | 0 |
| | FP | 5 | 5 | 4 | 4 | 3 | 2 | 1 | 1 | 0 | 0 | 0 |
| | TN | 0 | 0 | 1 | 1 | 2 | 3 | 4 | 4 | 5 | 5 | 5 |
| | FN | 0 | 1 | 1 | 2 | 2 | 2 | 2 | 3 | 3 | 4 | 5 |
| \longrightarrow | TPR | 1 | 0.8 | 0.8 | 0.6 | 0.6 | 0.6 | 0.6 | 0.4 | 0.4 | 0.2 | 0 |
| → | FPR | 1 | 1 | 0.8 | 0.8 | 0.6 | 0.4 | 0.2 | 0.2 | 0 | 0 | 0 |





Every point on the ROC curve was generated by a single threshold – the threshold selected for run time is called the operating point





Area Under the Curve (AUC) can be used to compare classifiers

1 >= AUC >= 0.9 : excellent (A)

0.9 > AUC >= 0.8 : good (B)

0.8 > AUC >= 0.7 : fair (C)

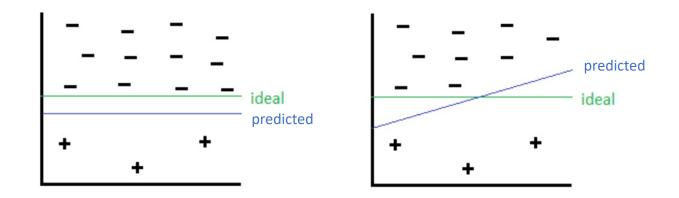
0.7 > AUC >= 0.6 : poor (D)

0.6 > AUC >= 0.5 : fail (F)

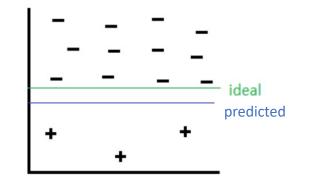
ROC Curves: https://machinelearningmastery.com/assessing-comparing-classifier-performance-roc-curves-2/

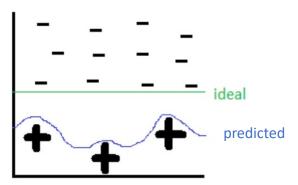
Mitigating Class Imbalances

- Sampling based approaches
 - Undersampling: remove some of the majority class



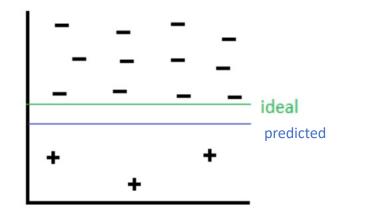
• Oversampling: duplicate the minority class records

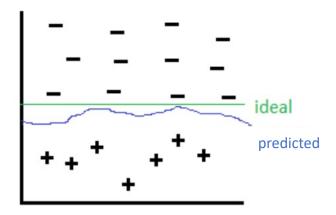




Sampling Algorithms

- SMOTE: Synthetic Minority Over-Sampling Technique
 - For each minority instance C, find it's nearest neighbor N
 - Create a new minority class instance R, using C's features and the difference between C and N's features, multiplied by a random variable
 - R.features = C.features + (C.features N.features) * rand(0,1)





Cost Matrix

A cost matrix can encode a penalty for misclassification errors

| | | Predicted Class | | |
|--------|---|-----------------|-----|--|
| | | + | - | |
| Actual | + | -1 | 100 | |
| Class | 1 | 1 | 0 | |

A negative entry in a cost matrix indicates a reward for making a correct prediction

Can be used for evaluation

| Model 1 | | Predicted Class | |
|-----------------|---|-----------------|-----|
| | | + | - |
| Actual Class | + | 175 | 25 |
| | - | 50 | 250 |

$$F$$
-measure = 0.84

$$Cost = -1(175) + 100(25) + 1(50) + 0(250) = 2375$$

$$Error = 55 / 500 = 0.11$$

$$F$$
-measure = 0.89

$$Cost = -1(170) + 100(30) + 1(25) + 0(275) = 2855$$

Lower error,
Better F-score,
But higher cost

Using Cost Matrix to Evaluate Risk

For a new record, the probability that it is positive is 20% and the probability that it is negative is 80%:

$$P(+) = 0.2$$

$$P(-) = 0.8$$

| Cost Matrix | | Predicted Class | |
|-----------------|---|-----------------|----|
| | | + | - |
| Actual Class | + | -1 | 10 |
| | - | 1 | 0 |

If I classify this record as negative, there is a 20% chance that I'm classifying it wrong and that I'm making a false negative (FN) error. (I would be predicting it as negative, but it is actually positive.) If I'm making that type of error, that is a cost of 10.

There is a 20% chance I'm making an error that costs 10. So the **risk** of classifying this record as negative is: Risk(-) = (0.2)(10) = 2

Similarly, I can calculate the risk of classifying this record as positive. There would be an 80% chance I'm making an error that costs 1:

$$Risk(+) = (0.8)(1) = 0.8$$

Choose to classify as the class that has the lowest risk.