Classification Metrics

Rob McCulloch

1. Classification Metrics

To examine the *fit* of a model we need a metric to measure our success or, conversely, a loss to measure our failure.

For numeric outcomes, the industry standard is RMSE (root mean squared error) or just MSE.

For classification, there are a few different metrics that are used that we need to be aware of.

We will look at

- cross entropy
- the confusion matrix and miss-classification
- the lift curve
- ROC and AUC

We have already used the second one in text classification with Naive Bayes.

2. Cross Entropy

For categorical outcomes cross entropy is just another name for the (- log likelihood loss).

For a binary out come if $y \in \{0, 1\}$ and $\hat{p}$ is the probability of y=1 from a model then we often write

$$L(y, \hat{p}) = -[y \ \log(\hat{p}) + (1 - y) \ \log(1 - \hat{p})].$$

Which is the same as $-\log(\hat{p})$ if $y = 1$ and $\log(1 - \hat{p})$ if $y = 0$ which is minus the log of the probability of what happened.

For data (train or test) $\{x_i, y_i\}$, with $\hat{p}_i$ the estimated prob $Y = 1$ given x_i and a model, then we sum (or average) the loss:

$$L(y, \hat{p}) = \frac{1}{n} \sum_{i=1}^{n} -[y_i \ \log(\hat{p}_i) + (1 - y_i) \ \log(1 - \hat{p}_i))].$$

In sklearn.metrics this is simply called the log loss.

```
In [5]: #from sklearn.metrics import log_loss
   ...: y_true = [0, 0, 1, 1]
   ...: y_pred = [[.9, .1], [.8, .2], [.3, .7], [.01, .99]]
   ...: print(log_loss(y_true, y_pred))
   ...: temp = -np.log(.9) -np.log(.8) - np.log(.7) - np.log(.99)
   ...: print(temp/4.0)
0.1738073366910675
0.1738073366910675
```

For a multinomial outcome with $y \in \{1, 2, \ldots, K\}$.

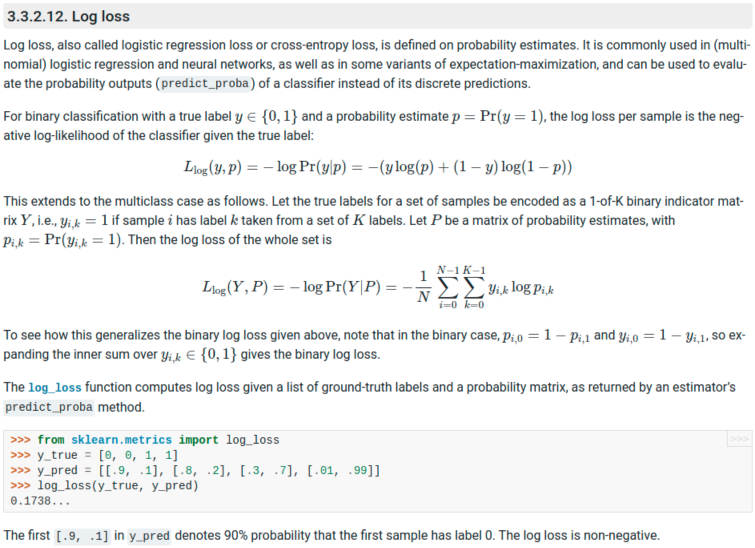
Given $x_i, \; i = 1, 2, \ldots, n$, let $p_{ij} = P(Y = j \mid x_i)$.

Let $y_{ij} = 1$ if $Y_i = j$ and 0 otherwise.

Then the loss is (average of - log lik) is

$$L = -\frac{1}{n} \sum_{i=1}^{n} \sum_{j=1}^{K} y_{ij} \, \log(p_{ij}).$$

in sklearn.metrics



3.3.2.12. Log loss

Log loss, also called logistic regression loss or cross-entropy loss, is defined on probability estimates. It is commonly used in (multinomial) logistic regression and neural networks, as well as in some variants of expectation-maximization, and can be used to evaluate the probability outputs (`predict_proba`) of a classifier instead of its discrete predictions.

For binary classification with a true label $y \in \{0, 1\}$ and a probability estimate $p = \operatorname{Pr}(y = 1)$, the log loss per sample is the negative log-likelihood of the classifier given the true label:

$$L_{\log}(y, p) = -\log \operatorname{Pr}(y|p) = -(y \log(p) + (1 - y) \log(1 - p))$$

This extends to the multiclass case as follows. Let the true labels for a set of samples be encoded as a 1-of-K binary indicator matrix Y, i.e., $y_{i,k} = 1$ if sample i has label k taken from a set of K labels. Let P be a matrix of probability estimates, with $p_{i,k} = \operatorname{Pr}(y_{i,k} = 1)$. Then the log loss of the whole set is

$$L_{\log}(Y, P) = -\log \operatorname{Pr}(Y|P) = -\frac{1}{N} \sum_{i=0}^{N-1} \sum_{k=0}^{K-1} y_{i,k} \log p_{i,k}$$

To see how this generalizes the binary log loss given above, note that in the binary case, $p_{i,0} = 1 - p_{i,1}$ and $y_{i,0} = 1 - y_{i,1}$, so expanding the inner sum over $y_{i,k} \in \{0, 1\}$ gives the binary log loss.

The `log_loss` function computes log loss given a list of ground-truth labels and a probability matrix, as returned by an estimator's `predict_proba` method.

```
>>> from sklearn.metrics import log_loss
>>> y_true = [0, 0, 1, 1]
>>> y_pred = [[.9, .1], [.8, .2], [.3, .7], [.01, .99]]
>>> log_loss(y_true, y_pred)
0.1738...
```

The first `[.9, .1]` in `y_pred` denotes 90% probability that the first sample has label 0. The log loss is non-negative.

3. Confusion and Miss-classification

Let's use the forensic glass data.

Glass has been shattered and you are trying to guess the type of glass which is one of the three categores WinF, WinNF, Other, from three features obtained from the glass shards.

summary(ddf)

```
   type          RI               Al               Na        
 WinF :70   Min.   :0.0000   Min.   :0.0000   Min.   :0.0000  
 WinNF:76   1st Qu.:0.2358   1st Qu.:0.2804   1st Qu.:0.3274  
 Other:68   Median :0.2867   Median :0.3333   Median :0.3865  
            Mean   :0.3167   Mean   :0.3598   Mean   :0.4027  
            3rd Qu.:0.3515   3rd Qu.:0.4174   3rd Qu.:0.4654  
            Max.   :1.0000   Max.   :1.0000   Max.   :1.0000  
```

Note that the three x's are already standardized.

Let's use KNN in R.

```
near = kknn(type~.,ddf,ddf,k=10,kernel = "rectangular")
```

Note that I am looking at the *in-sample* "fit".
I only have 214 observations.

`near$fitted[1:50]:`

```
 [1] WinF  WinNF WinNF WinF  WinF  WinNF WinF  WinF  WinF  WinF  WinNF WinF
[13] WinNF WinF  WinF  WinF  WinF  WinF  WinF  WinNF WinNF WinF  WinF  WinF
[25] WinF  WinF  WinF  WinF  WinF  WinF  WinF  WinF  WinF  WinF  WinF  Other
[37] WinF  WinF  WinF  WinF  WinF  WinF  WinF  WinF  WinF  WinNF WinNF WinF
[49] WinF  WinF
Levels: WinF WinNF Other
```

`near$prob[1:5,]`

```
     WinF WinNF Other
[1,]  0.6   0.3   0.1
[2,]  0.4   0.4   0.2
[3,]  0.1   0.9   0.0
[4,]  0.7   0.3   0.0
[5,]  0.8   0.2   0.0
```

The two-way table relating the observed Y with the predicted (or fitted) Y is called the *confusion matrix*.

Data label on columns, “fitted” label on rows.

So, there are 58+11+1 observations with Y =WinF.
Of those 11 were predicted to be WinNF.

```
knnfit  WinF WinNF Other
  WinF    58    13    14
  WinNF   11    57    12
  Other    1     6    42
```

We like the diagonals big!
Missclassification rate: (214-(58+57+42))/214 = 0.27

Here is the confusion matrix from the multinomial logit fit:

```
logitfit WinF WinNF Other
   WinF    45    19    15
   WinNF   21    45    13
   Other    4    12    40
```

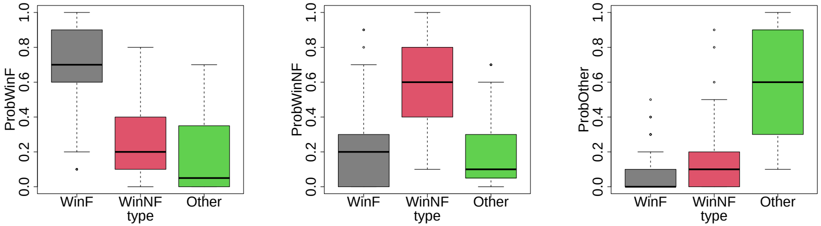
```
> (214-(45+45+40))/214
[1] 0.3925234
```

Not as good as from KNN.

But this is in-sample !!!!!

How good are the probabilities ??

The first plot is $P(Y = WinF \mid x)$ vs. y=glass type.
The second plot is $P(Y = WinNF \mid x)$ vs. y=glass type.
The third plot is $P(Y = Other \mid x)$ vs. y=glass type.



pretty good !!

4. Lift

The *lift curve* is a popular method for graphically displaying the effectiveness of an estimate of $\hat{p} = P(Y = 1 \mid x)$ for a binary Y.

You have a vector of y and a corresponding vector of $\hat{p}$.

Each of the y is either a 0 or a 1.

You get to choose observations, and the faster you find all the 1's the better!!

If you believe $\hat{p}$, your first choice will be the one with the biggest $\hat{p}$ your second choice will be the one with the second biggest $\hat{p}$ and so on.

That is, you would sort so that we go from biggest $\hat{p}$ to smallest and then take the observations in that order.

We then plot (% observations taken) vs. (% 1's found).

Let's use the tabloid data and logistic regression.

y=purchase which is whether a customer makes a purchase when mailed a "tabloid".

Our features are engineered from past purchases. E.g. nTab is number of past orders tiggered by a tabloid.

10,000 train observations.

```
purchase      nTab           moCbook          iRecMer1           llDol
0:9742   Min.   : 0.000   Min.   : 1.248   Min.   :0.01961   Min.   :-2.303
1: 258   1st Qu.: 0.000   1st Qu.:50.000   1st Qu.:0.01961   1st Qu.:-2.303
         Median : 0.000   Median :50.000   Median :0.01961   Median :-2.303
         Mean   : 1.857   Mean   :47.597   Mean   :0.09362   Mean   :-1.387
         3rd Qu.: 2.000   3rd Qu.:50.000   3rd Qu.:0.07398   3rd Qu.:-2.303
         Max.   :81.000   Max.   :50.000   Max.   :0.96819   Max.   : 7.310
   nTablog
Min.   :0.0000
1st Qu.:0.0000
Median :0.0000
Mean   :0.6255
3rd Qu.:1.0986
Max.   :4.4067
```

nTablog is log(nTab+1).

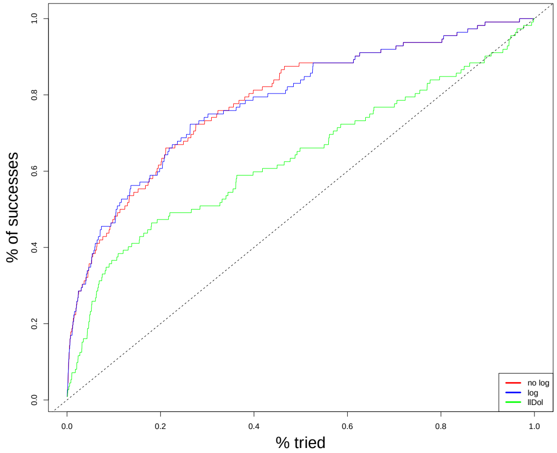
$258/10000 = 0.0258$

5,000 test observations.

```
purchase      nTab           moCbook          iRecMer1           llDol
0:4888   Min.   : 0.000   Min.   : 1.183   Min.   :0.01961   Min.   :-2.303
1: 112   1st Qu.: 0.000   1st Qu.:50.000   1st Qu.:0.01961   1st Qu.:-2.303
         Median : 0.000   Median :50.000   Median :0.01961   Median :-2.303
         Mean   : 1.775   Mean   :47.745   Mean   :0.09848   Mean   :-1.421
         3rd Qu.: 2.000   3rd Qu.:50.000   3rd Qu.:0.07965   3rd Qu.:-2.303
         Max.   :47.000   Max.   :50.000   Max.   :0.96819   Max.   : 6.948
   nTablog
Min.   :0.0000
1st Qu.:0.0000
Median :0.0000
Mean   :0.6005
3rd Qu.:1.0986
Max.   :3.8712
```

$112/4888 = 0.02291326$

Out of sample lift curves with and without the log in nTab and with just IIDol.



From 20% of the data you get 60% of the good ones!!!

Note:

Suppose you were just guessing which case to try (as opposed to picking one with a big $\hat{p}$).

That is, you randomly pick an observation and see if you get a 1. Repeat.

After 30% of the observations *on average* you would have 30% of the 1's.

After p% of the observations *on average* you would have p% of the 1's.

Thus, the "y=x" line in the lift plot is the average performance you would get by being ignorant and just guessing.

5. ROC and AUC

ROC and AUC are two popular methods for assessing the quality of a classifier for a binary y.

ROC stands for the incomprehensible term “receiver operator characteristics”.

We look at missclassification rates for various values of s using the rule: classify $Y = 1$ if $P(Y = 1 \mid x) \approx \hat{p} > s$.

In particular, we consider probability cutoffs s other than .5.

The ROC curve summarizes the 2x2 confusion matrix given $\hat{y} = 1$ if $\hat{p} > s$ and 0 otherwise as s varies.

Given an s value we have the confusion matrix:

```
        y=0  y=1
yhat=0  TN   FN
yhat=1  FP   TP
```

where:

TN: correctly classified 0
FP: incorrectly classified 1
FN: incorrectly classified 0
TP: correctly classified 1

```
         y=0  y=1
yhat=0   TN   FN
yhat=1   FP   TP
```

The Sensitivity is

$$\frac{TP}{TP + FN}$$

out of the $y = 1$ *observations, what fraction do we get right*

The Specificity is

$$\frac{TN}{TN + FP}$$

out of the $y = 0$ *observations, what fraction do we get right*

Using the log(nTab+1) model and the test data we classify $Y = 1$ if $P(Y = 1 \mid x) \approx \hat{p} > .02$ we get this confusion matrix.

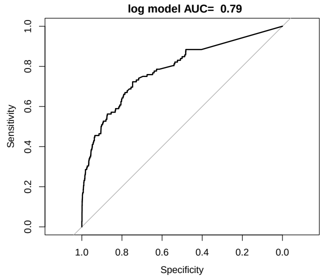
```
    y
yhat    0    1
   0 3616   31
   1 1272   81
```

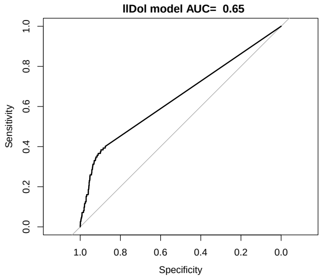
ROC looks at:

- Sensitivity: % of y=1 correctly classified: $81/(81+31) = 0.72$
- Specificity: % of y=0 correctly classified: $3616/(1272+3616) = 0.74$

We want Sensitivity and Specificity big.

For each value of the cutoff s you will get a pair of Sensitivity and Specificity values.
The ROC curve plots the Specificity vs. the Sensitivity as you vary the cutoff s.
AUC is the area under the ROC curve.





As we go from left to right, s goes from 1 to 0.

At $s = 1$, $\hat{y} = 0$ for all the observations so, we get all the 0's right but none of the 1's. (Specificity,Sensitivity) = (1,0).

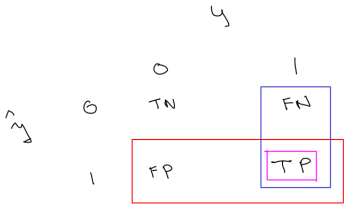
At $s = 0$, $\hat{y} = 1$ for all the observations so, we get all the 1's but none of the 0's. (Specificity,Sensitivity) = (0,1).

There are many measures based on these same quantities!!!

Precision is TP/(TP + FP).

Recall (same as Sensitivity) is TP/(TP + FN).

F1 score is harmonic mean of Precision and recall.



y
0
1
ŷ
0
TN
FN
1
FP
TP