EVALUATION OF MACHINE LEARNING CLASSIFIERS

Machine Learning



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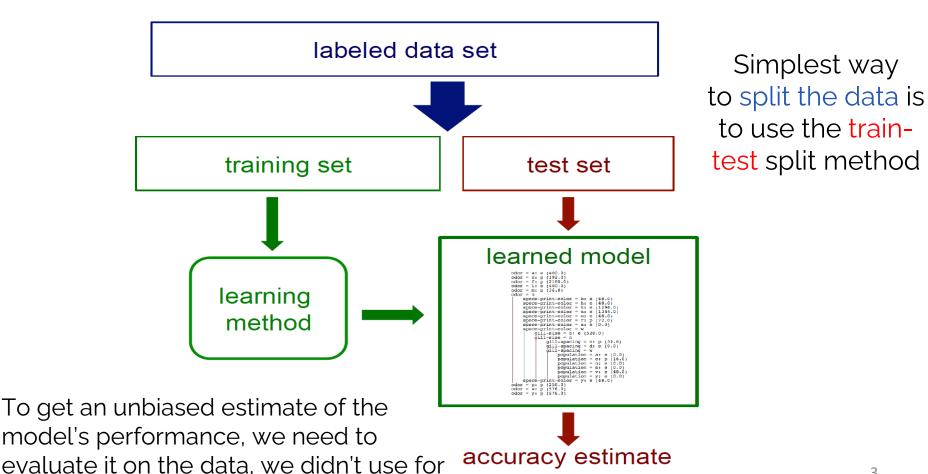
Outline: Evaluation Parameters

- Precision
- Recall
- Accuracy
- F-Measure
- True Positive Rate
- False Positive Rate
- Sensitivity
- ROC

Experiment: Training and Testing

Objective: Unbiased estimate of accuracy

training

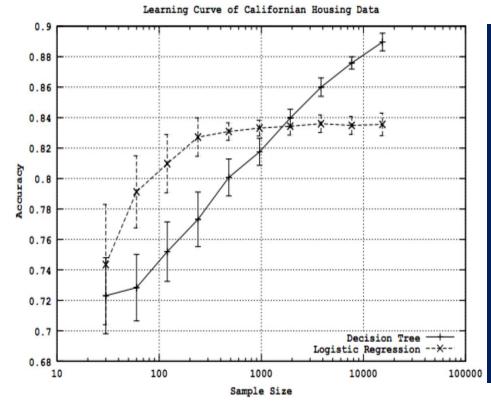


Experiment: Training and Testing...

- How can we get an unbiased estimate of the accuracy of a learned model?
 - ✓ when learning a model, you should pretend that you
 don't have the test data yet (it is "in the mail")*
 - ✓ if the test-set labels influence the learned model in any way, accuracy estimates will be biased
- * In some applications it is reasonable to assume that you have access to the feature vector (i.e. x) but not the y part of each test instance

Learning Curve

- How does the accuracy of a learning method change as a function of the training-set size?
 - ✓ This can be assessed by plotting learning curves.

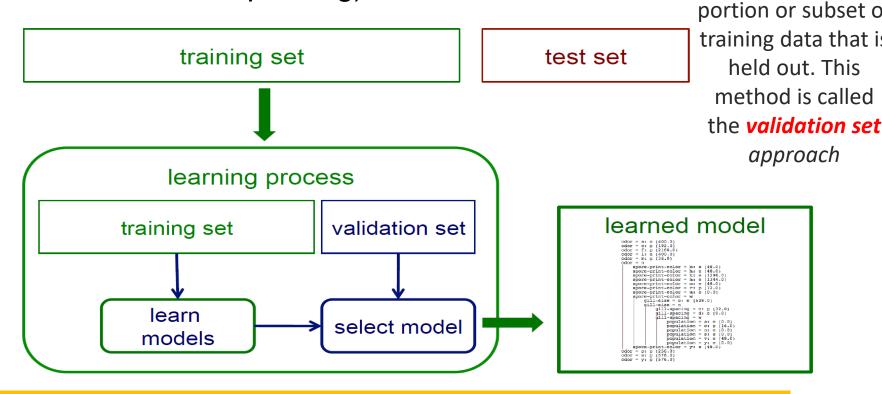


#Given training/test set partition

- for each sample size s on learning curve
- (optionally) repeat n times
- randomly select s instances from training set
 - learn model
- evaluate model on test set to determine accuracy a
- plot (s, a) or (s, avg. accuracy and error bars)

Validation (Tuning) Set

Consider we want unbiased estimates of accuracy during the learning process (e.g. to choose the best level of decision-tree pruning)?

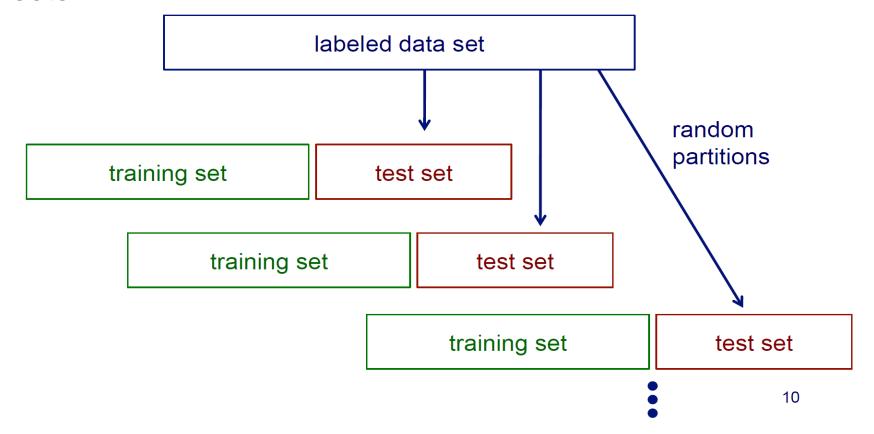


Limitation of Single Training/Test Partition

- We may not have enough data to make sufficiently large
 - ✓ training and test sets a larger test set gives us more reliable estimate of accuracy (i.e. a lower variance estimate)
 - ✓ but... a larger training set will be more representative of how much data we actually have for learning process
- A single training set doesn't tell us how sensitive accuracy is to a particular training sample

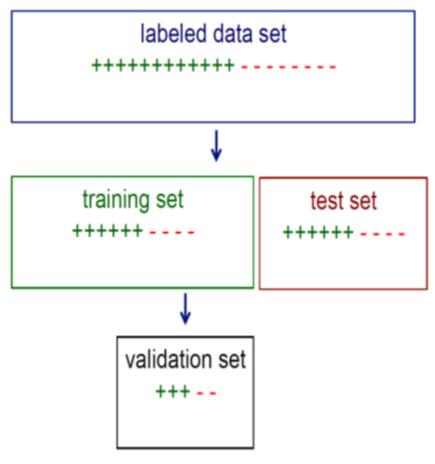
Random Sampling

 It can be addressed the second issue by repeatedly randomly partitioning the available data into training and set sets.



Random Sampling...

- When randomly selecting training or validation sets, we may want to ensure that class proportions are maintained in each selected set.
- This can be done via stratified sampling: first stratify (divider) instances by class, then randomly select instances from each class proportionally.



Cross Validation

- The train and test split has limitations such as the dataset is small, the method is prone to high variance.
- Due to the random partition, the results can be entirely different for different test sets because in some partitions, <u>samples</u> that are easy to classify get into the test set, while in others, the test set receives the 'difficult' ones.
- To deal with this issue, we use <u>cross-validation</u> to evaluate the performance of a machine learning model.

Cross Validation...

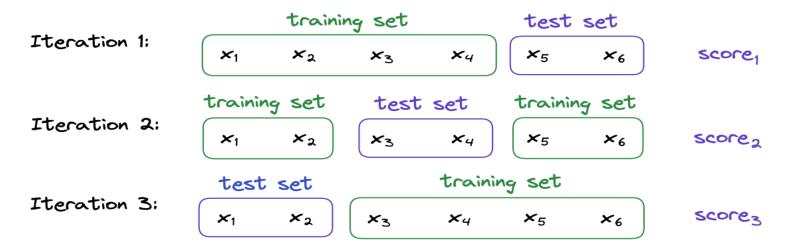
K-Fold Cross Validation

- In k-fold CV, we first divide our dataset into k equally sized subsets. Then, we repeat the train-test method k times such that each time one of the k subsets is used as a test set and the rest k-1 subsets are used together as a training set.
- Finally, we compute the estimate of the model's performance estimate by averaging the scores over the k trials.

K-Fold Cross Validation

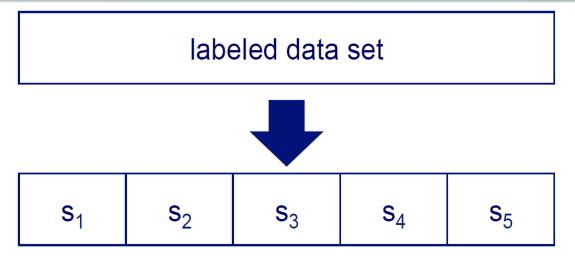
Example of 3-fold

- For example, let's suppose that we have a dataset $S = \{x_1, x_2, x_3, x_4, x_5, x_6\}$,
- First we divide the samples in to 3-fold as $S_1 = \{x_1, x_2\}, S_2 = \{x_3, x_4\}, S_3 = \{x_5, x_6\}$. Then we evaluate the model as



5-fold Cross Validation

Partition
data
into n
subsamples
(S)



Iteratively leave one subsample out for the test set, train on the rest

iteration	train on	test on
1	s ₂ s ₃ s ₄ s ₅	s ₁
2	s ₁ s ₃ s ₄ s ₅	s_2
3	$\mathbf{S}_1 \ \mathbf{S}_2 \ \mathbf{S}_4 \ \mathbf{S}_5$	s ₃
4	$\mathbf{S}_1 \ \mathbf{S}_2 \ \mathbf{S}_3 \ \mathbf{S}_5$	s_4
5	$s_1 s_2 s_3 s_4$	s ₅

5-fold Cross Validation...

Suppose we have 100 instances, and we want to estimate accuracy with cross validation.

iteration	train on	test on	correct
1	$\mathbf{s}_2 \ \mathbf{s}_3 \ \mathbf{s}_4 \ \mathbf{s}_5$	s ₁	11 / 20
2	s ₁ s ₃ s ₄ s ₅	s_2	17 / 20
3	$\mathbf{s}_1 \ \mathbf{s}_2 \ \mathbf{s}_4 \ \mathbf{s}_5$	s ₃	16 / 20
4	s ₁ s ₂ s ₃ s ₅	S ₄	13 / 20
5	s ₁ s ₂ s ₃ s ₄	S ₅	16 / 20

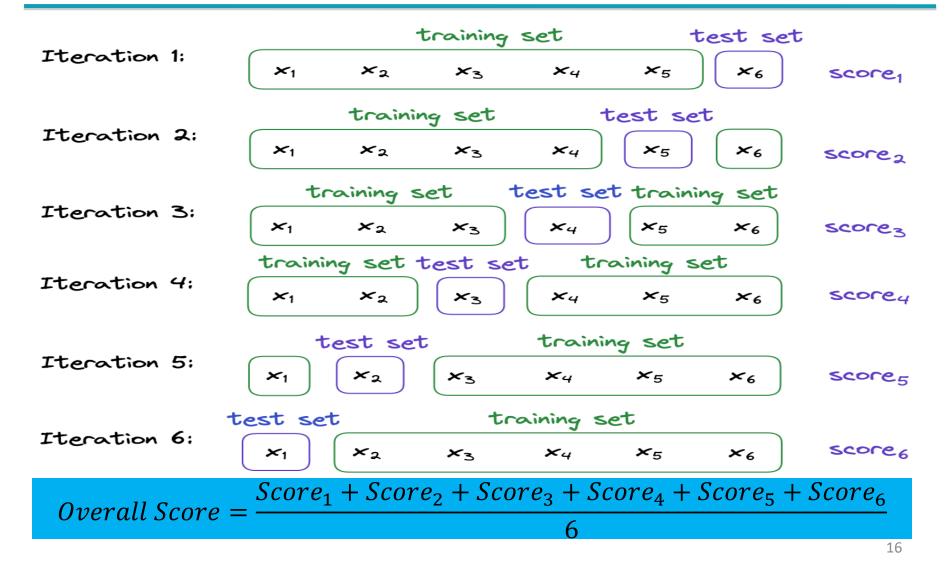
10-fold cross validation is common, but smaller values of n are often accuracy = 73/100 = 73%used when learning takes a lot of time.

Leave-One-Out Cross-Validation

LOOCV

- we train our machine-learning model n times where n is dataset size.
- Each time, only one sample is used as a test set while the rest are used to train our model.
- LOO on previous example $S = \{x_1, x_2, x_3, x_4, x_5, x_6\}$,
- $S_1 = \{x_1\}$
- $S_2 = \{x_2\}$
- $S_3 = \{x_3\}$
- $S_4 = \{x_4\}$
- $S_5 = \{x_5\}$
- $S_6 = \{x_6\}$

LOOCV...



Cross Validation... Summary

- When the size is small, LOOCV is more appropriate since it will use more training samples in each iteration.
- Conversely, we use k-fold cross-validation to train a model on a large dataset, which reduces the training time.
- Using k-Fold Cross-Validation over LOOCV is one of the examples of <u>Bias-Variance Trade-off</u>.
 It reduces the variance shown by LOOCV and introduces some bias by holding out a substantially large validation set

Confusion Matrix

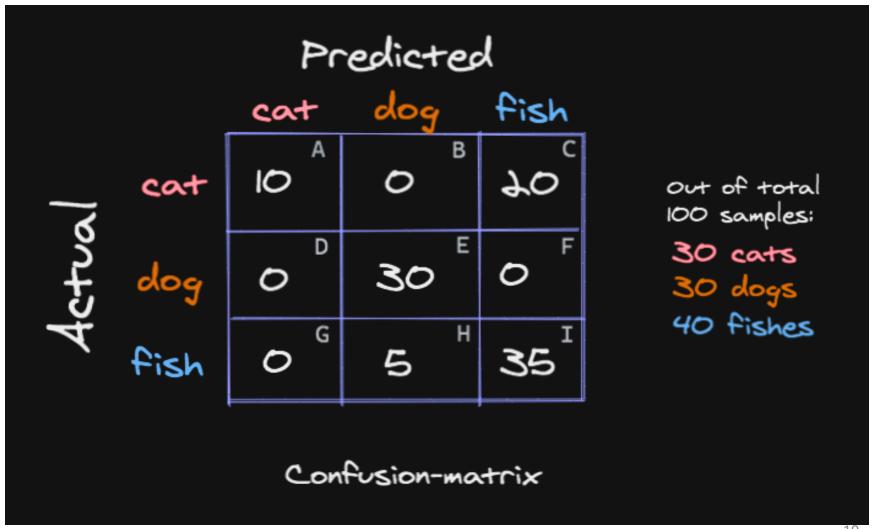
- It is also called as prediction table.
- It is an N×N matrix used for evaluating the performance of a classification model, where N is the number of target classes
- It compares the actual target values with those predicted.
- The columns represent the actual values of the target variable
- The rows represent the predicted values of the target variable.

Actual

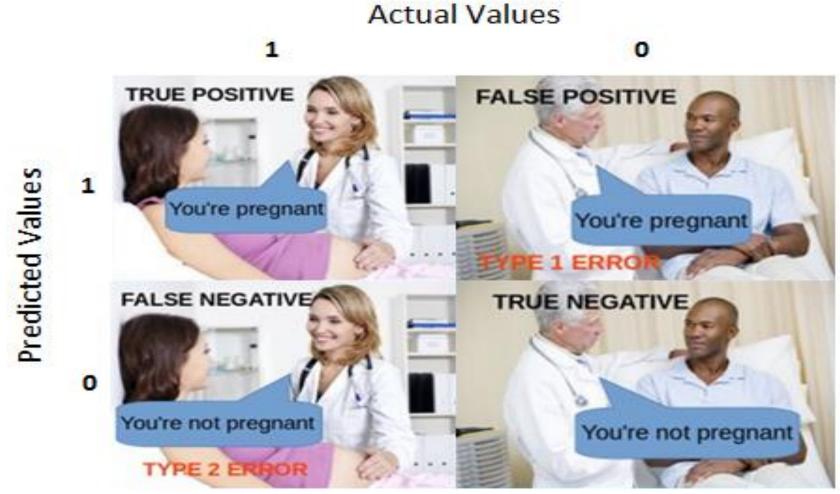
Predicted

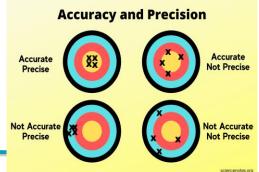
	+ve	-ve
+ve	True Positive	False Positive
-ve	False Negative	True Negative

Confusion Matrix...



Type-I and Type-II Error





Precision

- Precision: measures the correctness achieved in true prediction. Also, tells us how many predictions are actually positive out of all the total positive predicted. Precision should be high(ideally 1)
- "Precision is a useful metric in cases where False Positive is a higher concern than False Negatives"
- Precision/ Positive Prediction Value $P = \frac{t_p}{t_p + f_p}$
- Recall $R = \frac{t_p}{t_p + f_n}$

Issues with "Precision & Recall"

True class →	Pos	Neg
Yes	200 TP	100 FP
No	300 FN	400 TN
	P=500	N=500

True class →	Pos	Neg
Yes	200	100
No	300	0
	P=500	N=100

- Both classifiers gives the same precision and recall values of 66.7% and 40% (Note: the data sets are different)
- They exhibit very different behaviours:
 - ✓ Same positive recognition rate
 - Extremely different negative recognition rate: strong on the left / nil on the right
- Note: Accuracy has no problem catching this!

A combined measure: F

Combined measure that assesses precision/recall tradeoff is F measure (weighted harmonic mean):

$$E = \frac{1}{\alpha \frac{1}{P} + (1 + \alpha) \frac{1}{R}} = \frac{(\beta^2 + 1)PR}{\beta^2 P + R}$$

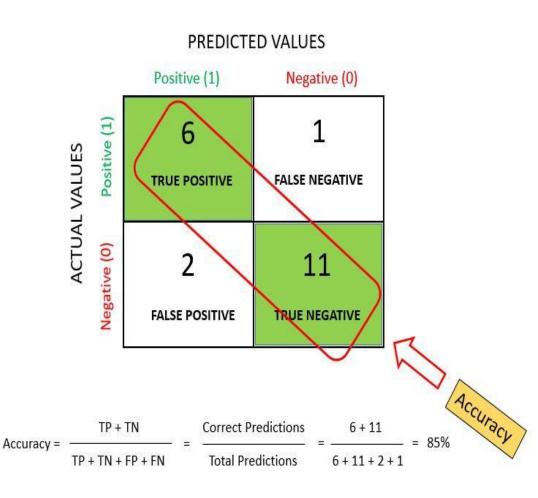
- high F1 score if both Precision and Recall are high
- low F1 score if both Precision and Recall are low
- medium F1 score if one of Precision and Recall is low and the other is high
- People usually use balanced F₁ measure
 - i.e., with $\beta = 1$ or $\alpha = \frac{1}{2}$
- Harmonic mean is a conservative average.

Accuracy

- Measures the correct predictions.
- The accuracy metric is not suited for imbalanced classes.
- Accuracy has its own disadvantages, for imbalanced data, when the model predicts that each point belongs to the majority class label, the accuracy will be high. But, the model is not accurate.
- Accuracy is a valid choice of evaluation for classification problems which are well balanced and not skewed or there is no class imbalance.

Accuracy Measure

- The accuracy of an engine: the fraction of these classifications that are correct.
- $Accuracy(\%) = \frac{(t_p+t_n)}{(t_p+t_n+f_n+f_p)} \times 100$



Accuracy Measure

y labelled Value (0- Negative, 1-Positive)	\widehat{y} predicted value	Output at threshold (0.5)
0	0.3	0
1	0.4	0
0	0.7	1
1	0.8	1
0	0.4	0
1	0.7	1

Confusion Matrix

TP=2	FP=1
FN=1	TN=2

$$Accuracy = \frac{4}{6} = .666$$

$$Precision = \frac{2}{3} = .666$$

$$Recall = \frac{TP}{TP + FN} = \frac{2}{3} = .666$$

Issues with Accuracy

- Consider a 2-class problem
 - Number of Class 0 examples = 9990
 - Number of Class 1 examples = 10
- If model predicts everything to be class 0, accuracy is 9990/10000 = 99.9 %
 - Accuracy is misleading because model does not detect any class 1 example

Issues with Accuracy...

True class →	Pos	Neg
Yes	200	100
No	300	400
	P=500	N=500

True class →	Pos	Neg
Yes	400	300
No	100	200
	P=500	N=500

- Both classifiers gives 60% accuracy.
- They exhibit very different behaviors:
 - ✓ On the left: weak positive recognition rate/strong negative recognition rate
 - ✓ On the right: strong positive recognition rate/weak negative recognition rate

Is accuracy adequate measure?

- Accuracy may not be useful measure in cases where
 - there is a large class skew
 - ✓ Is 98% accuracy good if 97% of the instances are negative?
 - there are differential misclassification costs say, getting a positive wrong costs more than getting a negative wrong.
 - ✓ Consider a medical domain in which a false positive results in an extraneous test but a false negative results in a failure to treat a disease
 - we are most interested in a subset of high-confidence predictions

Miss Classification Error

- Recognition rate=accuracy=success rate
- Miss classification rate= failure rate

	Predicted:	Predicted:
n=165	NO	YES
Actual:		
NO	50	10
Actual:		
YES	5	100

• *Miss Classification Error* =
$$\frac{5+10}{50+10+5+100} = 0.09$$

• Error in percentage=
$$\frac{FN+FP}{TP+FP+TN+FN} * 100$$

Sensitivity & Specificity

- Sensitivity is the metric that evaluates a model's ability to predict true positives of each available category.
- Specificity is the metric that evaluates a model's ability to predict true negatives of each available category.

$$Sensitivity = \frac{True\ Positives}{True\ Positives + False\ Negatives}$$

$$Specificity = \frac{True\ Negatives}{True\ Negatives + False\ Positives}$$

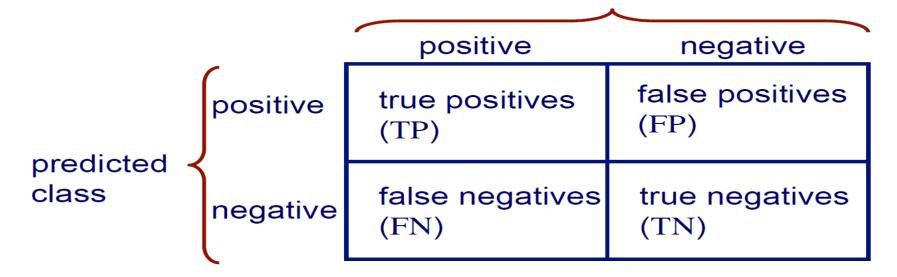
Find Sensitivity and Specificity

Table 2.2 A confusion matrix of a model

	Predicted +1	Predicted -1
Actual +1	95	7
Actual -1	4	94

Other form of Accuracy Metrics

actual class

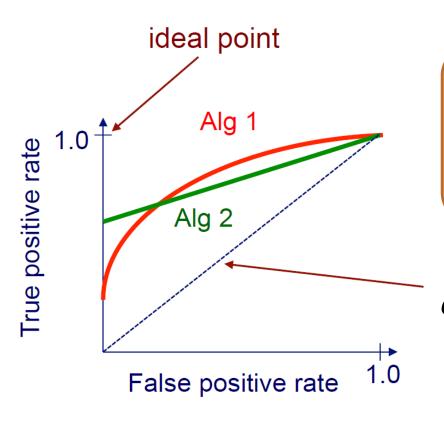


true positive rate (recall) =
$$\frac{TP}{\text{actual pos}}$$
 = $\frac{TP}{TP + FN}$
FP FP

false positive rate =
$$\frac{TT}{\text{actual neg}}$$
 = $\frac{TT}{TN + FP}$

ROC/AUC

 A Receiver Operating Characteristic (ROC)/Area Under Curve plots the TP-rate vs. the FP-rate as a threshold on the confidence of an instance being positive is varied.

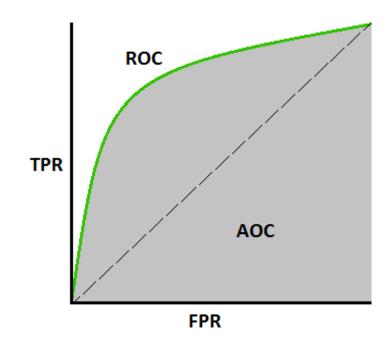


Different methods can work better in different parts of ROC space.
This depends on cost of false + vs. false -

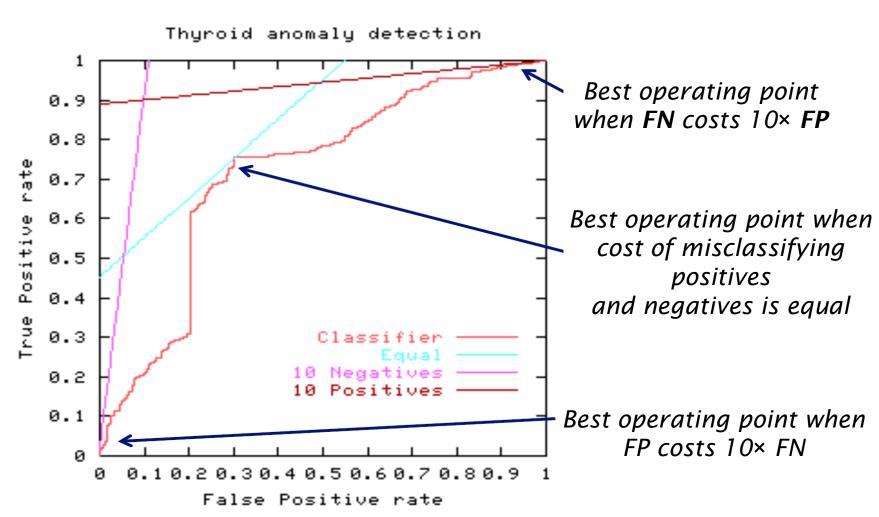
expected curve for random guessing

Area Under the Receiver Operating Characteristics

- AUC-ROC curve measure the performance at various threshold settings.
- ROC is a probability curve and AUC represents the degree or measure of separability.
- AUC tells the model capability of distinguishing between classes.
- Higher AUC, the better the model is at predicting 0 classes as 0 and 1 classes as 1.
- The ROC curve is plotted between TPR & FPR, where TPR is on the y-axis and FPR is on the x-axis.



ROC curves & Misclassification costs



Create ROC of a model

Consider a prediction table at different threshold setting

y labelled Value (0- Negative, 1- Positive)	\hat{y} predicted value	Output at threshold (0.5)	Output at threshold (0.6)	Output at threshold (0.72)	Output at threshold (0.8)
0	0.3	0	0	0	0
1	0.55	1	0	0	0
0	0.75	1	1	1	0
1	0.8	1	1	1	1
0	0.4	0	0	0	0
1	0.7	1	1	0	0

Threshold Setting (0.5)	TP=3	FP=1	TN=2	FN=0	TPR=3/(3+0)=1	FPR=1/(2+1)=.33
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Create ROC of a model...

Threshold setting (0.6)

y labelled Value (0- Negative, 1- Positive)	\hat{y} predicted value	Output at threshold (0.5)	Output at threshold (0.6)	Output at threshold (0.72)	Output at threshold (0.8)
0	0.3	0	0	0	0
1	0.55	1	0	0	0
0	0.75	1	1	1	0
1	0.8	1	1	1	1
0	0.4	0	0	0	0
1	0.7	1	1	0	0

	TP=2	FP=1	TN=2	FN=1	TPR=2/(2+1)=.66	FPR=1/(1+2)=.33
Setting (0.6)						

Create ROC of a model....

Threshold setting (0.72)

y labelled Value (0- Negative, 1- Positive)	\hat{y} predicted value	Output at threshold (0.5)	Output at threshold (0.6)	Output at threshold (0.72)	Output at threshold (0.8)
0	0.3	0	0	0	0
1	0.55	1	0	0	0
0	0.75	1	1	1	0
1	0.8	1	1	1	1
0	0.4	0	0	0	0
1	0.7	1	1	0	0

Threshold Setting (0.72)	TP=1	FP=1	TN=2	FN=2	TPR=1/(1+2)=.33	FPR=1/(1+2)=.33
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Create ROC of a model....

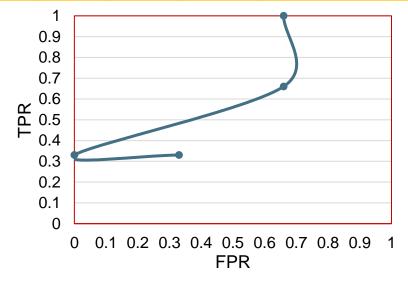
Threshold setting (0.80)

y labelled Value (0- Negative, 1- Positive)	\hat{y} predicted value	Output at threshold (0.5)	Output at threshold (0.6)	Output at threshold (0.72)	Output at threshold (0.8)
0	0.3	0	0	0	0
1	0.55	1	0	0	0
0	0.75	1	1	1	0
1	0.8	1	1	1	1
0	0.4	0	0	0	0
1	0.7	1	1	0	0

Threshold Setting (0.80	TP=1	FP=0	TN=3	FN=2	TPR=1/(1+2)=.33	FPR=0
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Plot of ROC

Threshold Setting (0.5)	TP=3	FP=1	TN=2	FN=0	TPR=3/(3+0)=1	FPR=1/(2+1)=.33
Threshold Setting (0.6)	TP=2	FP=1	TN=2	FN=1	TPR=2/(2+1)=.66	FPR=1/(1+2)=.33
Threshold Setting (0.72)	TP=1	FP=1	TN=2	FN=2	TPR=1/(1+2)=.33	FPR=1/(1+2)=.33
Threshold Setting (0.80	TP=1	FP=0	TN=3	FN=2	TPR=1/(1+2)=.33	FPR=0

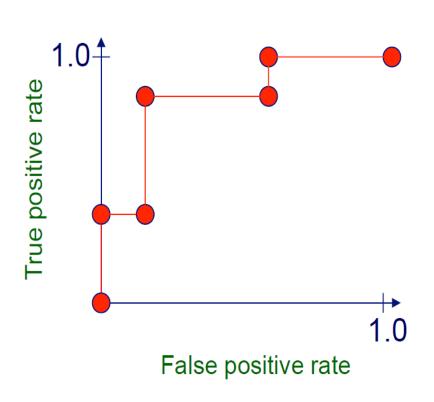


Step to create ROC

- Sort test-set predictions according to confidence that each instance is positive.
- Step through sorted list from high to low confidence
 - ✓ locate a *threshold* between instances with opposite classes (keeping instances with the same confidence value on the same side of threshold)
 - ✓ compute TPR, FPR for instances above threshold
 - ✓ output (FPR, TPR) coordinate

Example of ROC Plot

instance	confider positive	nce	correct class
Ex 9	.99		+
Ex 7	.98	TPR= 2/5, FPR= 0/5	+
Ex 1	.72	TPR= 2/5, FPR= 1/5	_
Ex 2	.70		+
Ex 6	.65	TPR= 4/5, FPR= 1/5	+
Ex 10	.51		-
Ex 3	.39	TPR= 4/5, FPR= 3/5	_
Ex 5	.24	TPR= 5/5, FPR= 3/5	+
Ex 4	.11		-
Ex 8	.01	TPR= 5/5, FPR= 5/5	



Example of ROC Plot ...

Rearrange the samples according to class

Correct class	Instance	Confidence Pos	sitive
+	Ex 9	0.99	
+	Ex 7	0.98	Positive
+	Ex 2	0.70	Class
+	Ex 6	0.65	
+	Ex 5	0.24	
_	Ex 1	0.72	
_	Ex10	0.51	Negative
-	Ex 3	0.39	Negative Class
-	Ex 4	0.11	
-	Ex 8	0.01	

Example of ROC Plot ...

For Threshold 0.72

Correct class	Instance	confidence positive	predicted class
+	Ex 9	0.99	+
+	Ex 7	0.98	+
+	Ex 2	0.70	_
+	Ex 6	0.65	-
+	Ex 5	0.24	-
-	Ex 1	0.72	+
_	Ex10	0.51	_
-	Ex 3	0.39	-
-	Ex 4	0.11	-
-	Ex 8	0.01	-

Confidence > threshold
Positive class
Else
Negative class

TP=2
FP=1
TN=4
FN=3
TPR=TP/TP+FN=2/5
FPR=FP/FP+TN=1/5

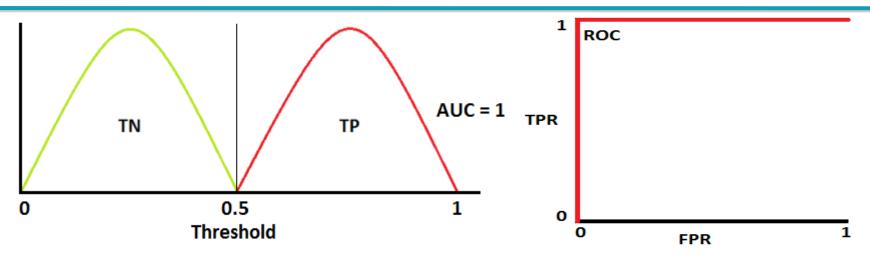
Example of ROC Plot ...

For Threshold 0.65

Correct class	Instance	confidence positive	predicted class
+	Ex 9	0.99	+
+	Ex 7	0.98	+
+	Ex 2	0.70	+
+	Ex 6	0.65	+
+	Ex 5	0.24	-
-	Ex 1	0.72	+
-	Ex10	0.51	-
-	Ex 3	0.39	-
-	Ex 4	0.11	-
-	Ex 8	0.01	-

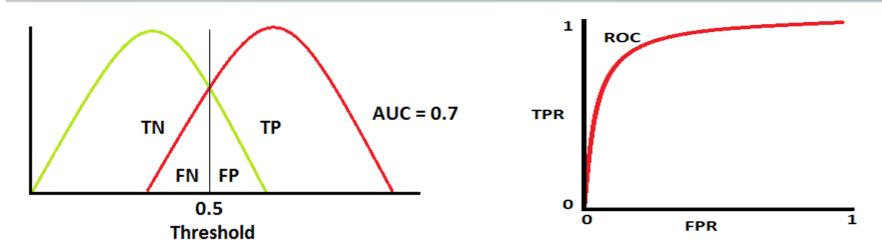
Confidence > threshold
Positive class
Else
Negative class

Significance of ROC



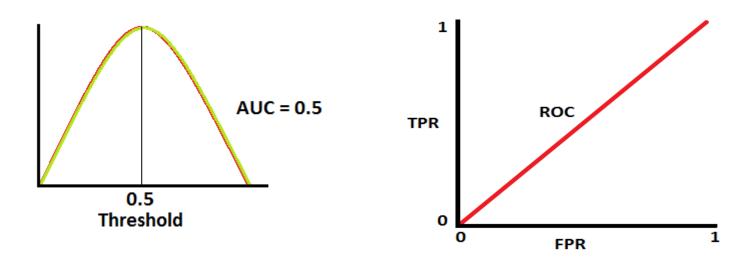
- This is an ideal situation, when two curves don't overlap at all, means model has an ideal measure of separability.
- It is perfectly able to distinguish between positive class and negative class.

Significance of ROC...



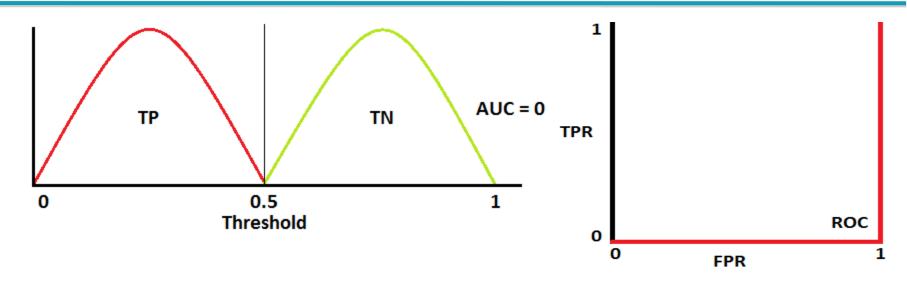
- When two distributions overlap, then type 1 and type 2 errors are introduced.
- Depending upon the threshold, it can be minimized or maximized. When AUC is 0.7, it means there is a 70% chance that the model will be able to distinguish between positive class and negative class.

Significance of ROC...



- This is the worst situation.
- When AUC is approximately 0.5, the model has no discrimination capacity to distinguish between positive class and negative class.

Significance of ROC...



 When AUC is approximately 0, the model is actually reciprocating the classes. It means the model is predicting a negative class as a positive class and vice versa.

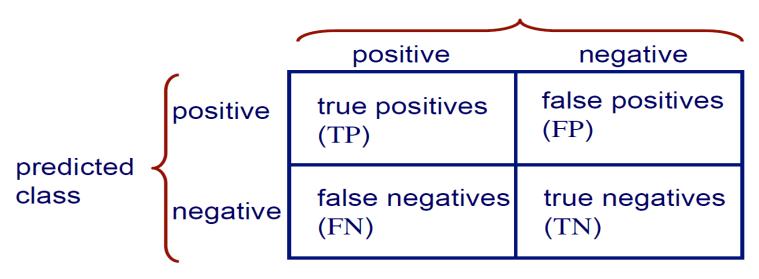


Issues with ROC/AUC

- AUC/ROC has adopted as replacement of accuracy but it has also some criticism such as:
 - The ROC curves on which the AUCs of different classifiers are based may cross, thus not giving an accurate picture of what is really happening.
 - The misclassification cost distributions used by the AUC are different for different classifiers.
 - Therefore, we may be comparing "apples and oranges" as the AUC may give more weight to misclassifying a point by classifier A than it does by classifier B. Ans: H-Measure

Other Accuracy Metrics

actual class

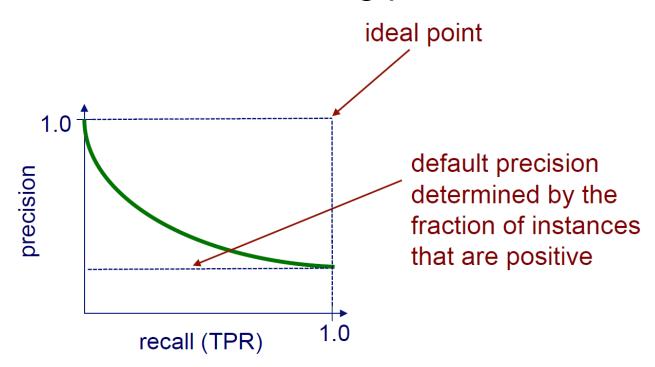


recall (TP rate) =
$$\frac{TP}{\text{actual pos}}$$
 = $\frac{TP}{TP + FN}$

precision =
$$\frac{TP}{\text{predicted pos}} = \frac{TP}{TP + FP}$$

Precision/recall curves

 A precision/recall curve plots the precision vs. recall (TP-rate) as a threshold on the confidence of an instance being positive is varied.



Comment on ROC/PR Curve

Both

- ✓ allow predictive performance to be assessed at various levels of confidence
- assume binary classification tasks
- sometimes summarized by calculating area under the curve

ROC curves

- ✓ insensitive to changes in class distribution (ROC curve does not change if the proportion of positive and negative instances in the test set are varied)
- can identify optimal classification thresholds for tasks with differential misclassification costs

Precision/Recall curves

- ✓ show the fraction of predictions that are false positives
- ✓ well suited for tasks with lots of negative instances

Loss Function

Mean Square Error Loss Function

- ✓ It is used for regression problem
- ✓ Mean square error loss for m-data point is defined as $L_{SE} = \frac{1}{m} \sum_{i=1}^{m} (y_i \widehat{y}_i)^2$
- \checkmark For single point $L_{SE}1 = (y \hat{y})^2$.

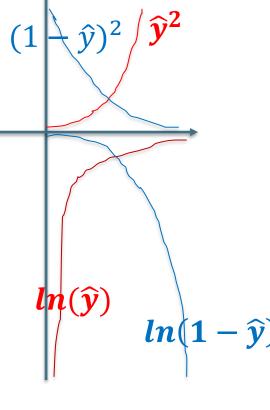
Binary Cross Entropy Loss Function

- ✓ It is used for classification problem
- ✓ BCELF is defined $L_{CE} = -\frac{1}{m} \sum_{i=1}^{m} [y_i \ln(\hat{y}_i) + (1 y_i) \ln(1 \hat{y}_i)]$
- ✓ For single point $L_{CE}1 = y \ln(\hat{y}) + (1 y) \ln(1 \hat{y})$, negative sign ignored, because we interested more in shape.

Example

- Consider a 2-class problem, where ground truth is y = 0. then $L_{SE} \mathbf{1} = \hat{y}^2$ and, y = 1. $L_{SE} \mathbf{1} = (1 \hat{y})^2$.
- Similarly $L_{CE}1 = ln(1 \hat{y})$ and $ln(\hat{y})$
- Consider example,
- $y = 0.8 \hat{y} = 0.9, L_{SE} = 0.81$
- Similarly $L_{CE} = 2.3$
- Gradient $\frac{\partial L_{SE}}{\partial \hat{y}} = 1.8$ and $\frac{\partial L_{CE}}{\partial \hat{y}} = 10.0$

Cross entropy loss penalizes model more



Q1. Suppose a computer program for recognizing dogs in photographs identifies eight dogs in a picture containing 12 dogs and some cats. Of the eight dogs identified, five actually are dogs while the rest are cats. Compute the Precision and recall of the computer program.

Solution:

		Actual dogs		Actual cats
Predicted dogs	TP	5	FP	3
Predicted cats	FN	7	TN	

$$P = \frac{TP}{TP + FP}$$

$$P = \frac{5}{5+3}$$
$$P = \frac{5}{8}$$

$$P = \frac{5}{8}$$

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

$$R = \frac{5}{5+7}$$
$$R = \frac{5}{12}$$

$$R = \frac{5}{12}$$

Q2. A database contains 80 records on a particular topic of which 55 are relevant to a certain investigation. A search was conducted on that topic and 50 records were retrieved. Of the 50 records retrieved, 40 were relevant. Construct the confusion matrix for the search and calculate the precision and recall scores for the search. Each record may be assigned a class label "relevant" or "not relevant".

Solution: All the 80 records were tested for relevance. The test classified 50 records as "relevant". But only 40 of them were actually relevant.

	Actual relevant	Actual not relevant
Predicted relevant	40	10
Predicted not relevant	15	25

- TP = 40
- FP = 10
- FN = 15

The precision P is
$$P = TP/(TP + FP)$$

= $40/(40 + 10) = 4/5$

The recall R is
$$R = TP/(TP + FN)$$

= $40/(40 + 15) = 40/55$

- Using the data in the confusion matrix of a classifier of two-class dataset, several measures of performance can be calculated as well.
- Accuracy = (TP + TN)/(TP + TN + FP + FN) = $\frac{65}{90}$
- Error rate = 1- Accuracy = $1 \frac{65}{90} = \frac{25}{90}$
- Sensitivity = TP/(TP + FN) = $\frac{40}{55}$
- Specificity = TN /(TN + FP) = $\frac{25}{35}$
- F-measure = $(2 \times TP)/(2 \times TP + FP + FN) = \frac{80}{105}$

Q3. Let there be 10 balls (6 white and 4 red balls) in a box and let it be required to pick up the red balls from them. Suppose we pick up 7 balls as the red balls of which only 2 are actually red balls. What are the values of precision and recall in picking red ball?

Solution:

- \blacksquare TP = 2
- FP = 7 2 = 5
- FN = 4 2 = 2

The precision P is P = TP/(TP + FP)= 2/(2+5) = 2/7

The recall R is
$$R = TP/(TP + FN)$$

= $2/(2 + 2) = 1/2$