Model Evaluation

Data Science Dojo

Limitation of Accuracy

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

Classifier Evaluation

- Metrics for Performance Evaluation

How to evaluate the performance of a model?

- Methods for Performance Evaluation

How to obtain reliable estimates?

- Methods for Model Comparison

How to compare the relative performance among competing models?

Model Evaluation

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Metrics for Performance Evaluation

- Focus on the predictive capability of a model
  - Rather than how fast it takes to classify or build models, scalability, etc.
- Confusion Matrix:

		PREDICTED CLASS	
		Class=Yes	Class=No
ACTUAL CLASS	Class=Yes	a	b
	Class=No	c	d

a: TP (true positive)

b: FN (false negative)

c: FP (false positive)

d: TN (true negative)

Metrics for Performance Evaluation

		PREDICTED CLASS	
		Class=Yes	Class=No
ACTUAL CLASS	Class=Yes	a (TP)	b (FN)
	Class=No	c (FP)	d (TN)

Most widely-used metric:

$$\text{Accuracy} = \frac{a+d}{a+b+c+d} = \frac{TP+TN}{TP+TN+FP+FN}$$

Cost Matrix

	PREDICTED CLASS		
ACTUAL CLASS	C(i|j)	Class=Yes	Class=No
	Class=Yes	C(Yes|Yes)	C(No|Yes)
	Class=No	C(Yes|No)	C(No|No)

C(i|j): Cost of misclassifying class j example as class i

Computing Cost of Classification

Cost Matrix	PREDICTED CLASS		
	C(i|j)	+	-
ACTUAL CLASS	+	-1	100
	-	1	0

Model M_2	PREDICTED CLASS		
		+	-
ACTUAL CLASS	+	250	45
	-	5	200

Accuracy = 90%

Cost = 4255

Model M_1	PREDICTED CLASS		
		+	-
ACTUAL CLASS	+	150	40
	-	60	250

Accuracy = 80%

Cost = 3910

Cost vs Accuracy

Count	PREDICTED CLASS		
		Class=Yes	Class=No
ACTUAL CLASS	Class=Yes	a	b
	Class=No	c	d

Cost	PREDICTED CLASS		
		Class=Yes	Class=No
ACTUAL CLASS	Class=Yes	p	q
	Class=No	q	p

Accuracy is proportional to cost if:

1. C(Yes|No)=C(No|Yes) = q
2. C(Yes|Yes)=C(No|No) = p

$N = a + b + c + d$

$Accuracy = (a + d)/N$

$$\begin{aligned} Cost &= p\,(a + d) + q\,(b + c) \\ &= p\,(a + d) + q\,(N - a - d) \\ &= q\,N - (q - p)(a + d) \\ &= N\,[q - (q-p) \times Accuracy] \end{aligned}$$

Cost-Sensitive Measures

$$\text{Precision (p)} = \frac{a}{a+c}$$

$$\text{Recall (r)} = \frac{a}{a+b}$$

$$\text{F - measure (F)} = \frac{2rp}{r+p} = \frac{2a}{2a+b+c}$$

- Precision is biased towards C(Yes|Yes) & C(Yes|No)
- Recall is biased towards C(Yes|Yes) & C(No|Yes)
- F-measure is biased towards all except C(No|No)

$$\text{Weighted Accuracy} = \frac{w_1 a + w_4 d}{w_1 a + w_2 b + w_3 c + w_4 d}$$

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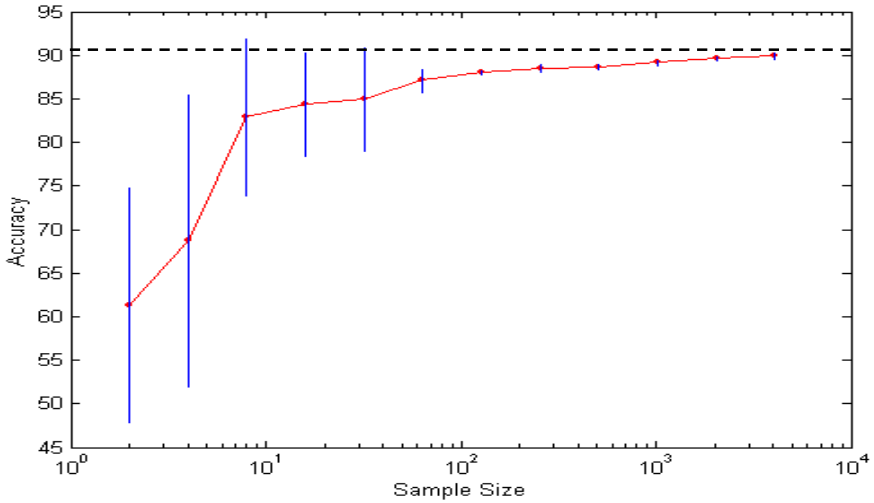
Methods for Performance Evaluation

- How to obtain a reliable estimate of performance?
- Performance of a model may depend on other factors besides the learning algorithm:
  - Class distribution
  - Cost of misclassification
  - Size of training and test sets

Learning Curve



- Learning curve shows how accuracy changes with varying sample size
- Requires a sampling schedule for creating a learning curve:
  - Arithmetic sampling (Langley, et al)
  - Geometric sampling (Provost et al)
- Effect of small sample size:
  - Bias in the estimate
  - Variance of estimate

Methods of Estimation

- Holdout
  - Reserve 2/3 for training and 1/3 for testing
- Cross validation
  - Partition data into k disjoint subsets
  - k-fold: train on k-1 partitions, test on the remaining one
  - Leave-one-out: k = n
- Random subsampling
  - Repeated holdout
- Stratified sampling
  - Oversampling vs undersampling
- Bootstrap
  - Sampling with replacement

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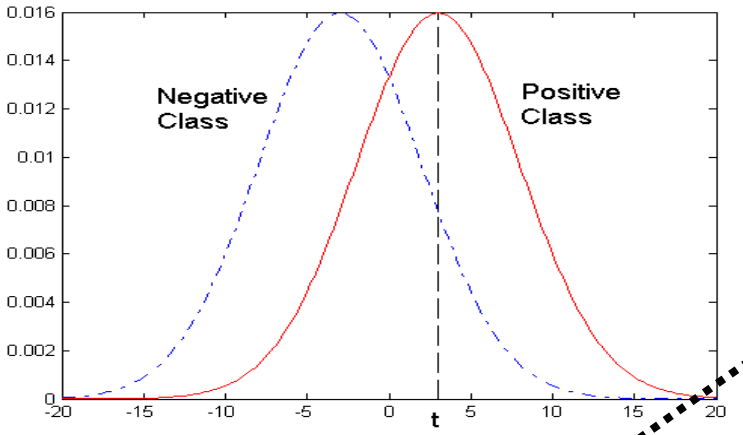
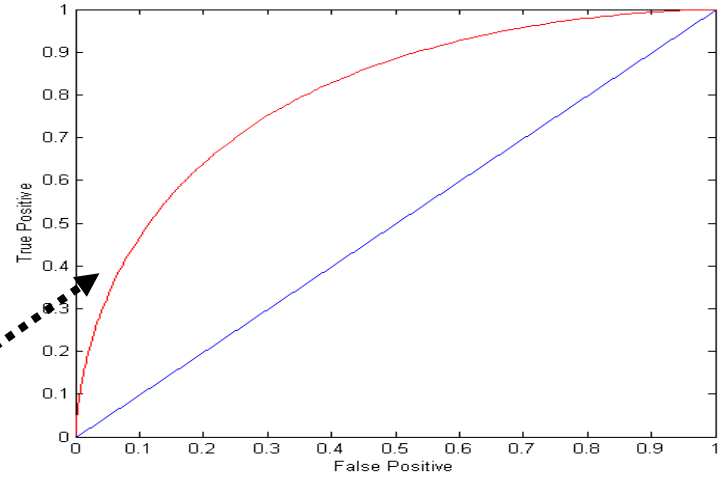
ROC (Receiver Operating Characteristic)

- Developed in 1950s for signal detection theory to analyze noisy signals
  - Characterize the trade-off between positive hits and false alarms
- ROC curve plots TP (on the y-axis) against FP (on the x-axis)
- Performance of each classifier represented as a point on the ROC curve
  - Changing the threshold of the algorithm, sample distribution, or cost matrix changes the location of the point

ROC Curve

- 1-dimensional data set containing 2 classes (positive and negative)
- Any points located at x > t are classified as positive





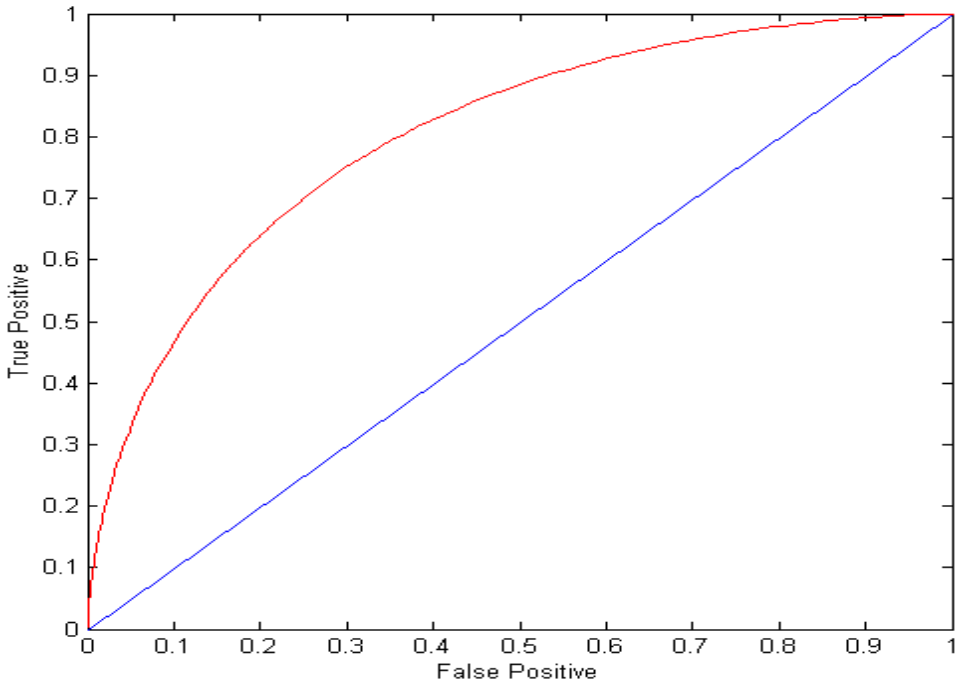
At threshold t:

TP=0.5, FN=0.5, FP=0.12, FN=0.88

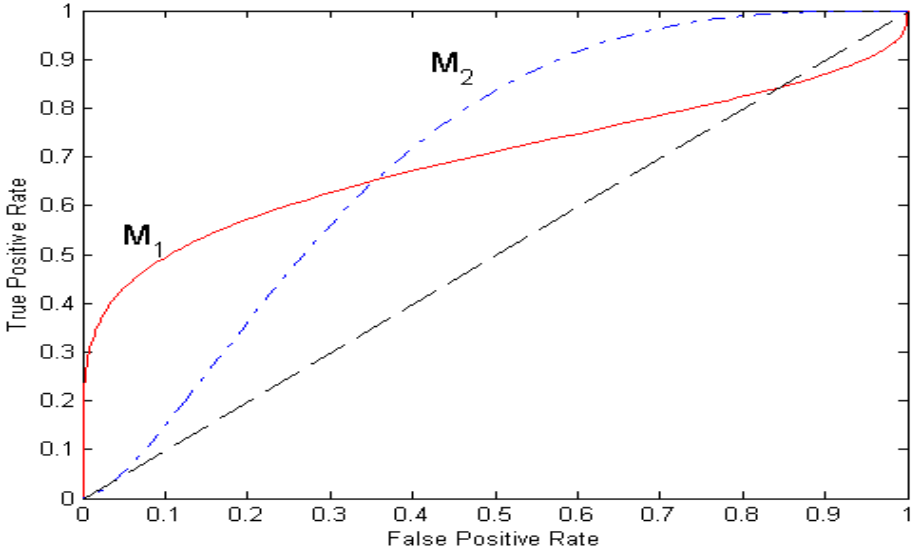
ROC Curve

- (TP,FP):
- (0,0): declare everything to be negative class
- (1,1): declare everything to be positive class
- (1,0): ideal

- Diagonal line:
  - Random guessing
  - Below diagonal line:
    - Prediction is opposite of the



Using ROC for Model Comparison



- No model consistently outperforms the other
  - M_1 is better for small FPR
  - M_2 is better for large FPR
- Area under the ROC curve
  - Ideal:
    - Area = 1
  - Random guess:
    - Area = 0.5

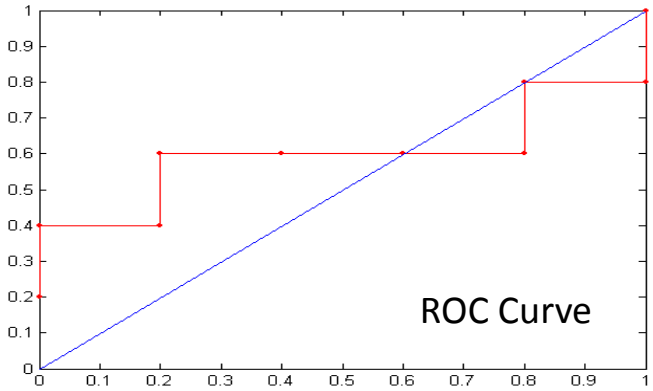
How to Construct a ROC Curve

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

- Use classifier that produces posterior probability for each test instance P(+|A)
- Sort the instances according to P(+|A) in decreasing order
- Apply threshold at each unique value of P(+|A)
- Count the number of TP, FP, TN, FN at each threshold
- TP rate, TPR = TP/(TP+FN)
- FP rate, FPR = FP/(FP + TN)

How to Construct a ROC Curve

	Class	+	-	+	-	-	-	+	-	+	+	
Threshold >=		0.25	0.43	0.53	0.76	0.85	0.85	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
→	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



Test of Significance

- Given two models:
  - Model M1: accuracy = 85%, tested on 30 instances
  - Model M2: accuracy = 75%, tested on 5000 instances
- Can we say M1 is better than M2?
  - How much confidence can we place on accuracy of M1 and M2?
  - Can the difference in performance measure be explained as a result of random fluctuations in the test set?

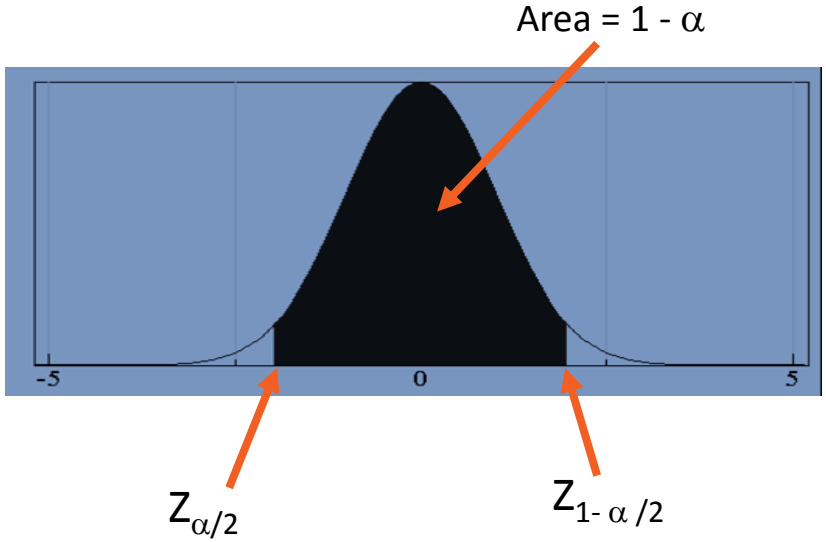
Confidence Interval for Accuracy

- Prediction can be regarded as a Bernoulli trial
  - A Bernoulli trial has 2 possible outcomes
  - Possible outcomes for prediction: correct or incorrect
  - Collection of Bernoulli trials has a Binomial distribution:
    - $x \sim Bin(N, p)$ x: number of correct predictions
    - e.g.: Toss a fair coin 50 times, how many heads would turn up?
      Expected number of heads = $N \times p = 50 \times 0.5 = 25$
- Given x (# of correct predictions) or equivalently, acc=x/N, and N (# of test instances), can we predict p (true accuracy of model)?

Confidence Interval for Accuracy

- For large test sets (N > 30),
  - acc has a normal distribution with mean p
  - and variance p(1-p)/N

$$P(Z_{\alpha/2} < \frac{acc - p}{\sqrt{p(1-p)/N}} < Z_{1-\alpha/2}) = 1-\alpha$$



- Confidence Interval for p:

$$p = \frac{2 \times N \times acc + Z_{\alpha/2}^2 \pm \sqrt{Z_{\alpha/2}^2 + 4 \times N \times acc - 4 \times N \times acc^2}}{2(N + Z_{\alpha/2}^2)}$$

Confidence Interval for Accuracy

- Consider a model that produces an accuracy of 80% when evaluated on 100 test instances:
  - N=100, acc = 0.8
  - Let 1-α = 0.95 (95% confidence)
  - From probability table, Zα/2=1.96

N	50	100	500	1000	5000
p(lower)	0.670	0.711	0.763	0.774	0.789
p(upper)	0.888	0.866	0.833	0.824	0.811

1-α	Z
0.99	2.58
0.98	2.33
0.95	1.96
0.90	1.65

QUESTIONS