# Practical ML Advice
& Evaluation.

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Based on slides from Jude Shavlik and Tom Dietterich

## Proper Experimental Methodology Can Have a Huge Impact:

A 2002 paper in *Nature* (a major journal) needed to be corrected due to "training on the testing set"

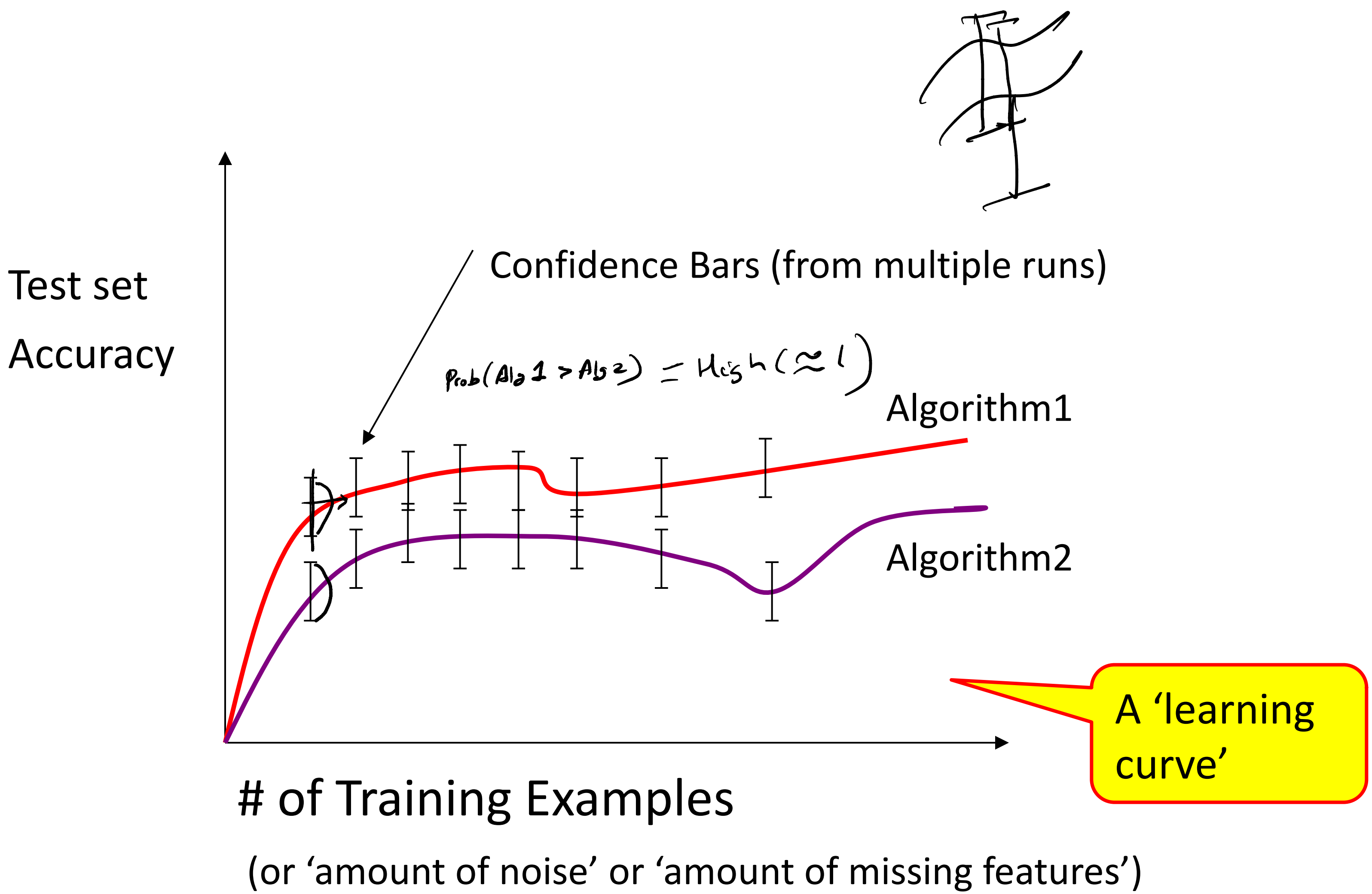
Original report : 95% accuracy (5% error rate)

Corrected report (which still is buggy):

73% accuracy (27% error rate)

Error rate increased over 400%!!!

# Some Typical ML Experiments



# Typical Experiments

Ablation Experiments

Regression

Comp A = Extra Featurg
Comp B = Poly Features

| | Test Set Performance |
|---|---|
| Full System (A + B) | 80% |
| Without Module A | 75% |
| Without Module B | 62% |
| | |

5%

18%

# Experimental Methodology

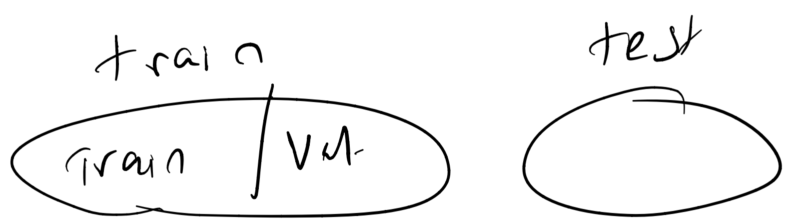
1) Start with a dataset of labeled examples
2) Randomly partition into *N* groups
3a) *N* times, combine *N* -1 groups into a train set
3b) Provide training set to learning system
3c) Measure accuracy on "left out" group (the test set)

| | | | |
|---|---|---|---|
| train | test | train | train |

Called *N*-fold cross validation

# Validation Sets

- Often, an ML system has to choose when to stop learning, select among alternative answers, etc.
- One wants the model that produces the highest accuracy on **future** examples (“overfitting avoidance”)
- It is a **“cheat”** to look at the **test** set while still learning
- Better method
  - Set aside part of the training set
  - Measure performance on this validation data to estimate future performance for a given set of hyperparameters
  - Use best hyperparameter settings, train with **all** training data (except **test** set) to estimate future performance on **new** examples



# Tune Hyper-parameters

$(w, b) = \text{Train}(\text{Data}, \lambda)$

Hyperparams $= \lambda$ (E.g: Regularizn, Depth of tree, ..)

Loop over $\lambda$:

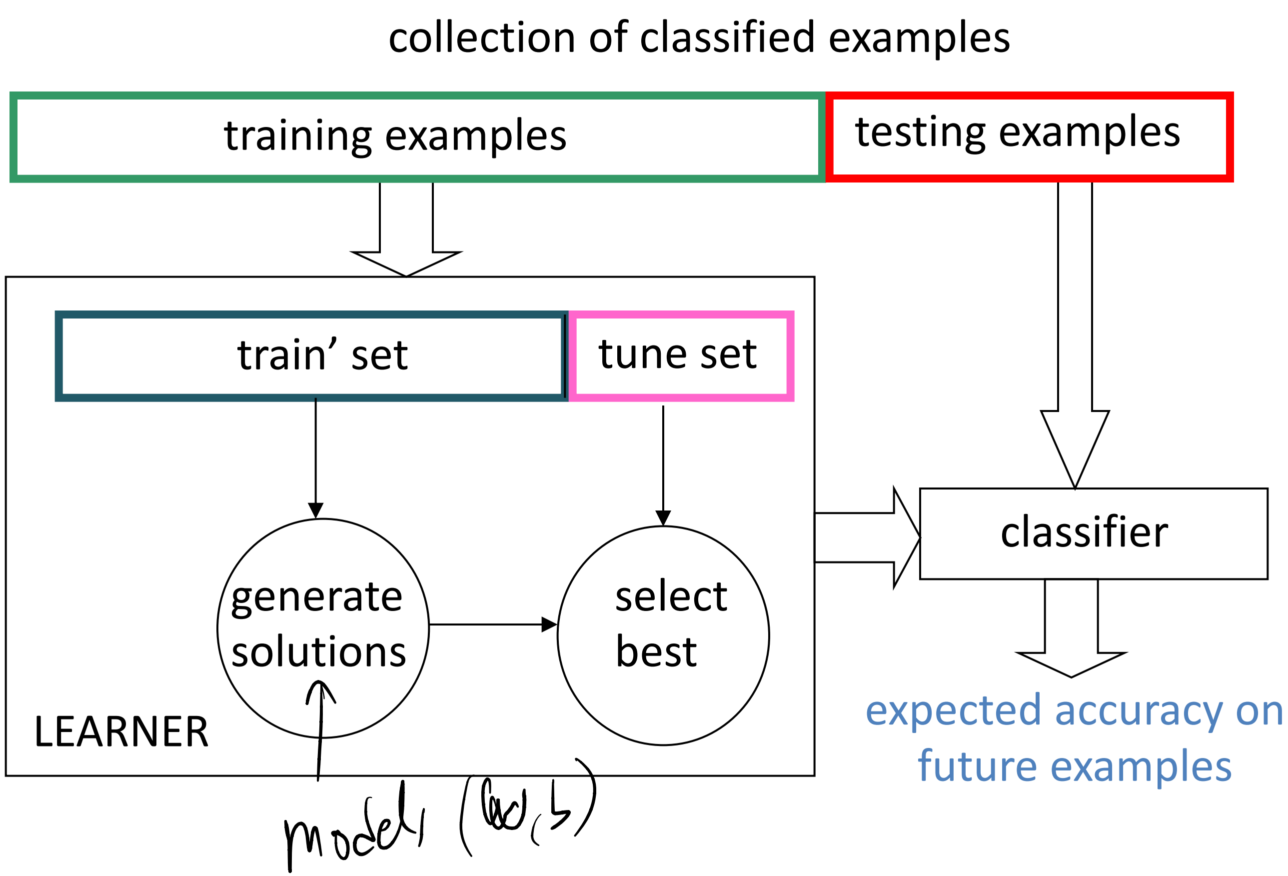
$\quad (w_\lambda, b_\lambda) = \text{Train}(\text{Data}, \lambda)$

$\quad \text{Val}_\lambda = \text{Val}(w_\lambda, b_\lambda)$ ← Test on Val Data.

$\lambda^* = \max_\lambda \text{Val}_\lambda$

$\text{Test}(w_{\lambda^*}, b_{\lambda^*})$ & Deploy $(w_{\lambda^*}, b_{\lambda^*})$

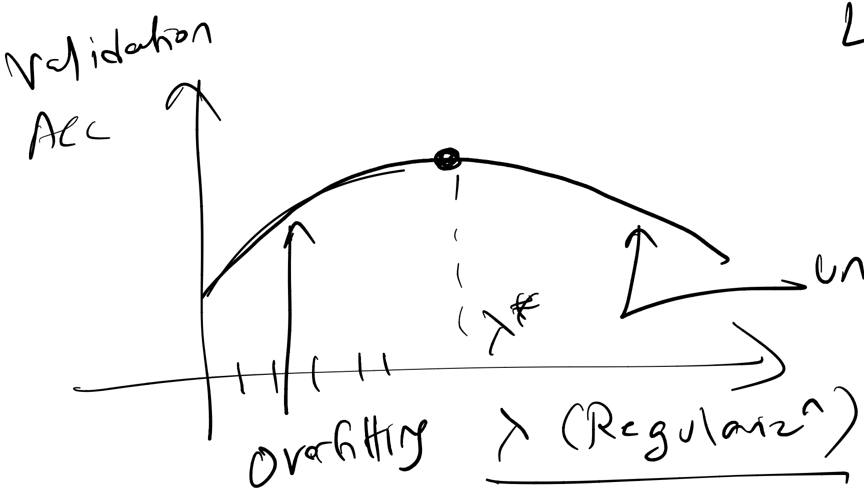
# A typical Learning system



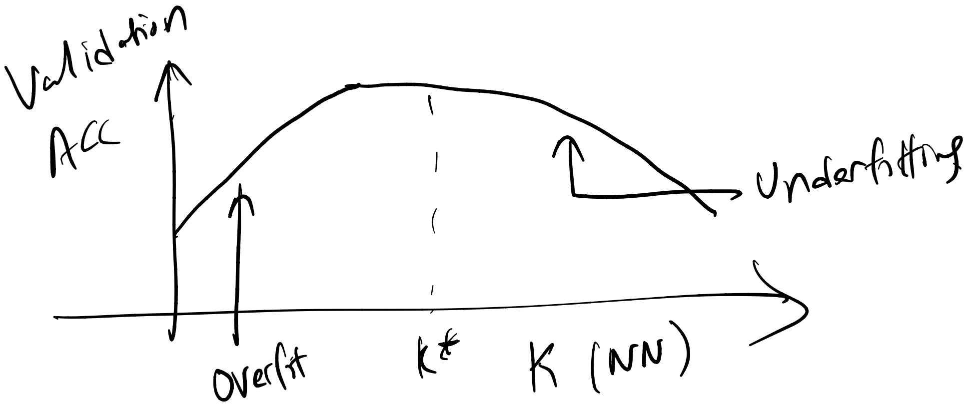

Statistical techniques such as 10-fold cross validation and *t*-tests are used to get meaningful results

# Typical Hyper-Parameter Tuning

$$L(w) + \lambda \|w\|^2$$




← Linear Regression



# Multiple Tuning sets

- Using a **single** tuning set can be unreliable predictor, plus some data “wasted”

  1) For each possible set of hyperparameters

     a) Divide training data into **train** and **valid.** sets, using ***N*-fold cross validation**

     b) Score this set of hyperparameter values: average **valid.** set accuracy over the *N* folds

  2) Use **best** set of hyperparameter settings and **all** (train + valid.) examples

  3) Apply resulting model to **test** set

# EVALUATING ML MODELS

[ classification ]

# Contingency Tables

(special case of 'confusion matrices')

G.T Label

**True Answer**

| Algorithm Answer / Prediction | True Answer: + | True Answer: - |
|---|---|---|
| + | n(1,1) [true pos] | n(1,0) [false pos] |
| - | n(0,1) [false neg] | n(0,0) [true neg] |

Counts of occurrences

# TPR and FPR

**True Positive Rate** $= \; n(1{,}1) \,/\, (\, n(1{,}1) + n(0{,}1)\,)$

(TPR) $=$ correctly categorized +'s / total positives

$\sim$ P(algo outputs + | + is correct) ← $\frac{\# TP}{\# Pos}$

**False Positive Rate** $= \; n(1{,}0) \,/\, (\, n(1{,}0) + n(0{,}0)\,)$

(FPR) $=$ incorrectly categorized –'s / total neg's

$\sim$ P(algo outputs + | - is correct) ← $\frac{\# FP}{\# Neg}$

Can similarly define False Negative Rate and True Negative Rate

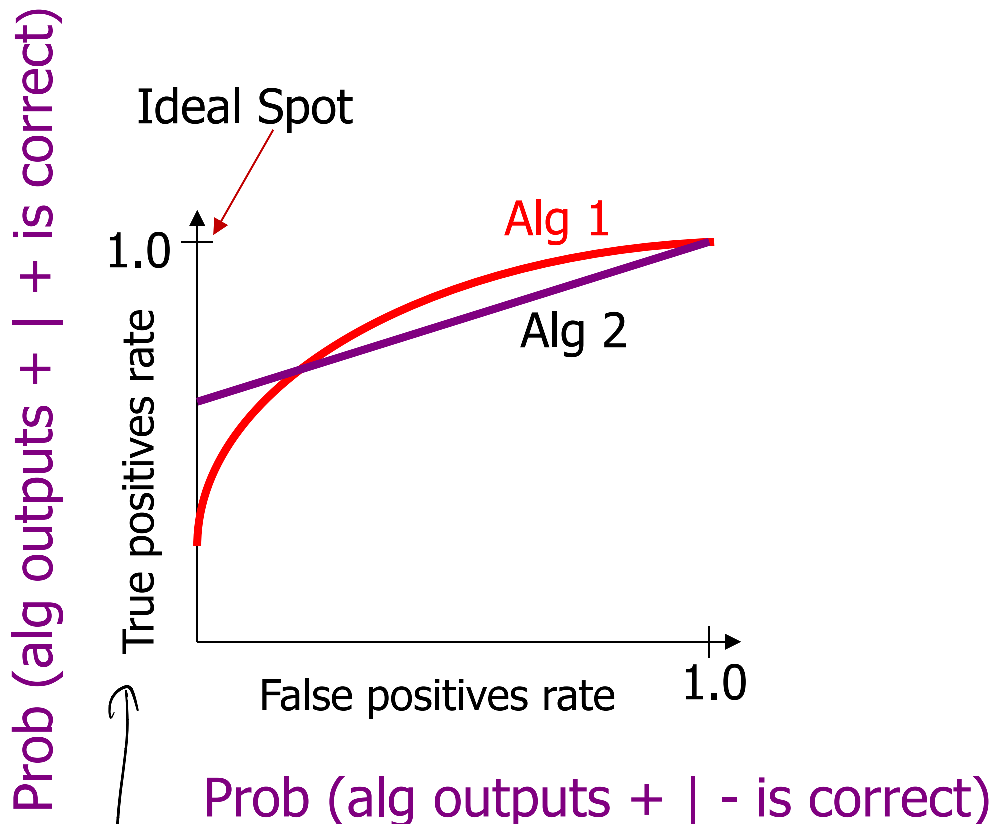
$\frac{\# FN}{\# Pos}$ $\frac{\# TN}{\# Neg}$

# ROC Curves

- ROC: *Receiver Operating Characteristics*
- Started for radar research during WWII
- Judging algorithms on accuracy alone may not be good enough when **getting a positive wrong** costs more than **getting a negative wrong** (or vice versa)
  - e.g., medical tests for serious diseases
  - e.g., a movie-recommender system

e.g Autonomous Driving System

# ROC Curves Graphically




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

$\frac{\#TP}{\#Pos}$

$\frac{\#FP}{\#Neg}$

# Creating an ROC Curve

**The Standard Approach:**

- You need an ML algorithm that outputs NUMERIC results such as prob(example is +) $p(y=1|x)$
- You can use ensemble methods to get this from a model that only provides Boolean outputs
  - e.g., have 100 models vote & count votes

# Alg. for Creating ROC Curves

Step 1: Sort predictions on test set ← $p(y=1|x)$

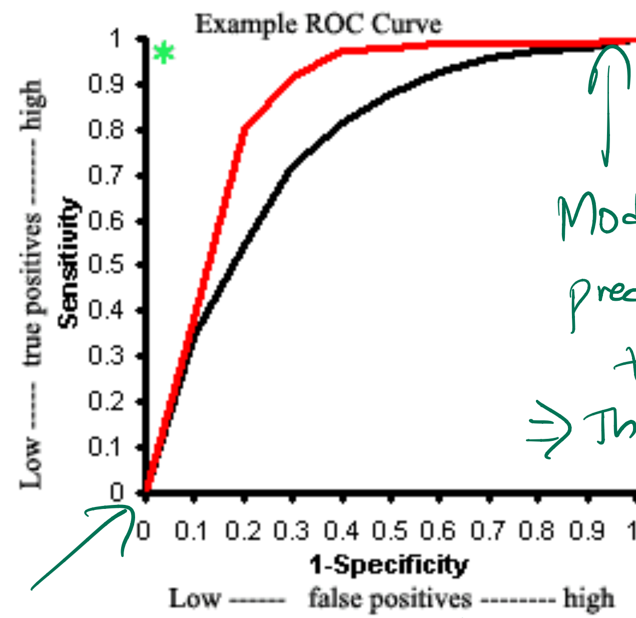
-ive | Low = Conf of being -

true | High = Conf of being +

Step 2: Locate a *threshold* between examples with opposite categories

Step 3: Compute TPR & FPR for each threshold of Step 2

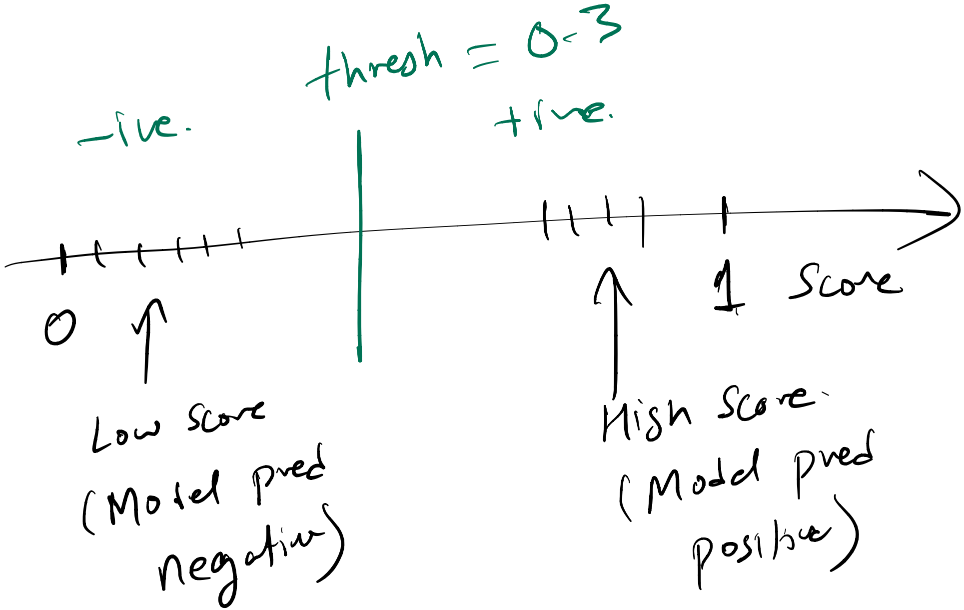
Step 4: Connect the dots




Model pred everything true ⇒ Thresh = 0

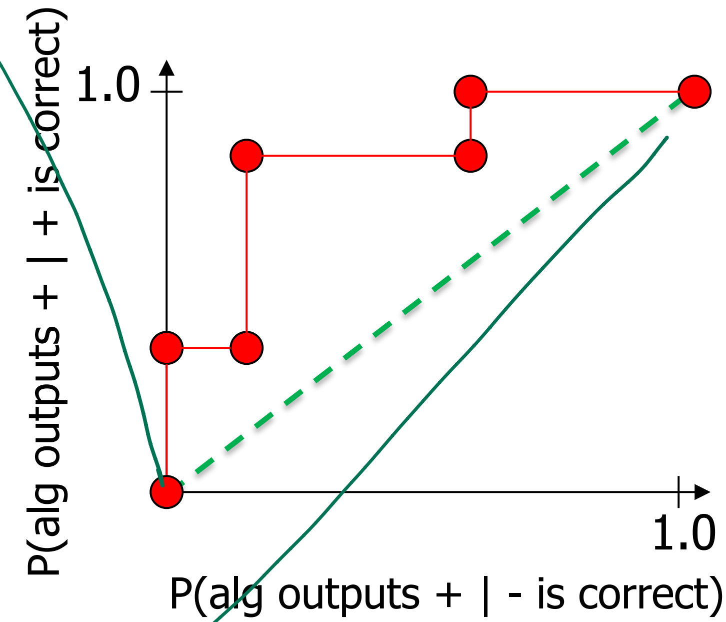
Model predicts -ives everything ⇒ Thresh = 1

Model pred.


thresh = 0.3
-ive.
+ive.
0
1
Score
Low score
(Model pred negative)
High score.
(Model pred positive)

# Plotting ROC Curves - Example

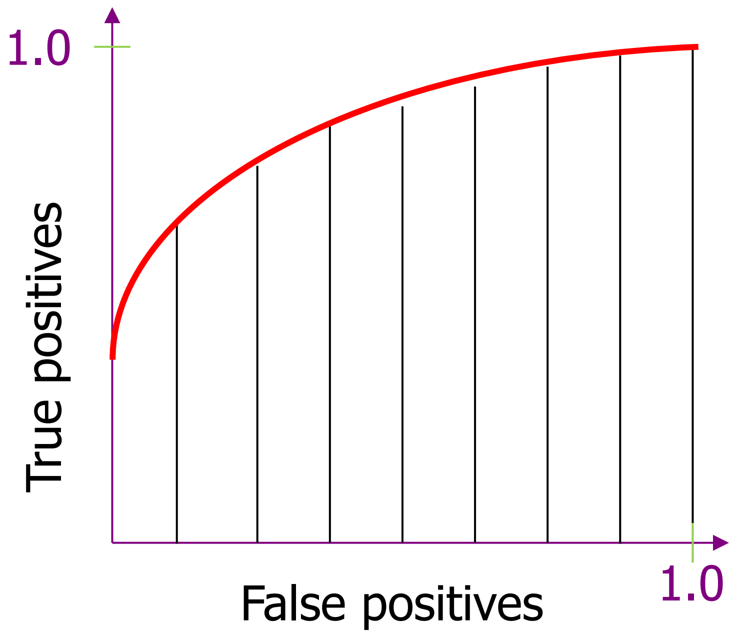
| ML Algo Output (Sorted) | | | Correct Category |
|---|---|---|---|
| Ex 9 | .99 | | + |
| Ex 7 | .98 | TPR=(2/5), FPR=(0/5) | + |
| Ex 1 | .72 | TPR=(2/5), FPR=(1/5) | - |
| Ex 2 | .70 | | + |
| Ex 6 | .65 | TPR=(4/5), FPR=(1/5) | + |
| Ex 10 | .51 | | - |
| Ex 3 | .39 | TPR=(4/5), FPR=(3/5) | - |
| Ex 5 | .24 | TPR=(5/5), FPR=(3/5) | + |
| Ex 4 | .11 | | - |
| Ex 8 | .01 | TPR=(5/5), FPR=(5/5) | - |




Algorithm predicts + if its output is $\geq 0$

# Area Under ROC Curve

- A common metric for experiments is to numerically integrate the ROC Curve
  - Usually called AUC
  - Probability that ML alg. will "rank" a randomly chosen positive instance higher than a randomly chosen negative one
  - Can summarize the curve **too much** in practice



# Why Accuracy is Bad Choice for Imbalanced problems

Spam = 10%

Not spam = 90%

Model 1 & 2

Acc = 90%

Model 1

| | | Actual + | Actual − |
|---|---|---|---|
| Pred | + | 5 | 5 |
| | − | 5 | 85 |

Model 2

| | | Actual + | Actual − |
|---|---|---|---|
| Pred | + | 0 | 0 |
| | − | 10 | 90 |

# Asymmetric Error Costs

- Assume that cost(FP) ≠ cost(FN)
- You would like to pick a threshold that minimizes

$$E(total\ cost) = \ cost(FP) \times \mathrm{pr}(FP) \times (\#\ of\ neg\ ex's)$$
$$cost(FN) \times \mathrm{pr}(FN) \times (\#\ of\ pos\ ex's)$$

- You could also have (maybe negative) costs for TP and TN (assumed zero in above)

# ROC's & Skewed Data

- One strength of ROC curves is that they are a good way to deal with skewed data (|+| >> |-|) since the axes are fractions (rates) independent of the # of examples

- You must be careful though!
  - Low FPR * (many negative ex) = sizable number of FP
  - Possibly more than # of TP

# Precision vs. Recall

- Think about search engines...

- **Precision** = (# of relevant items retrieved)
  / (total # of items retrieved)
  = n(1,1) / ( n(1,1) + n(1,0) )
  $\cong$ P(is pos | called pos)

$$\frac{\#TP}{\underbrace{\#TP + \#FP}_{\#(\text{Pred Pos})}}$$

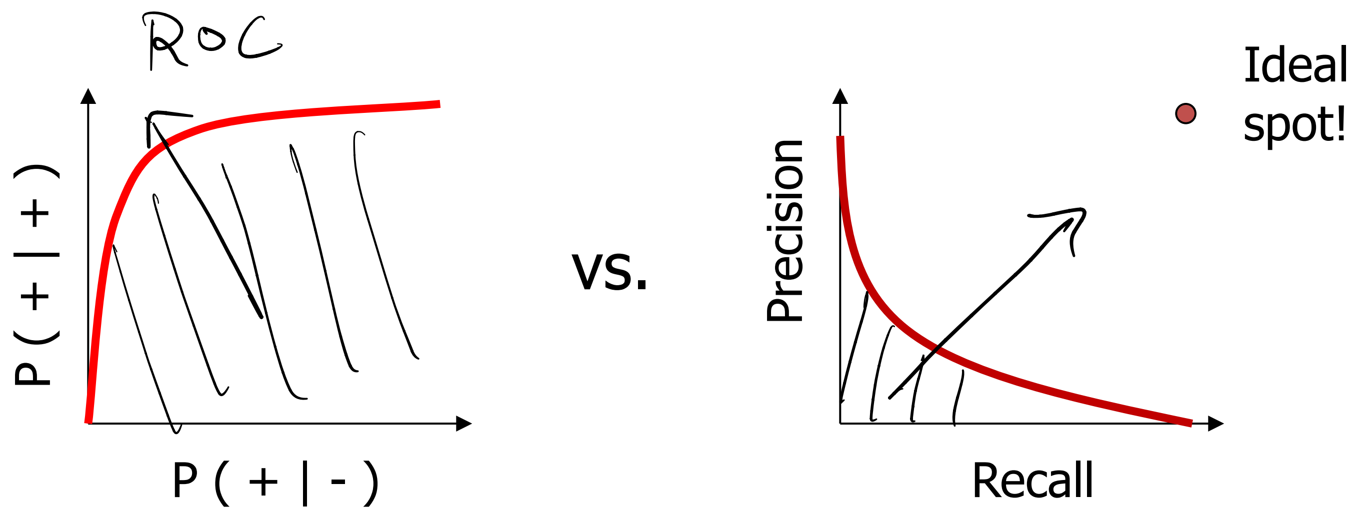
- **Recall** = (# of relevant items retrieved)
  / (# of relevant items that exist)
  = n(1,1) / ( n(1,1) + n(0,1) ) = <u>TPR</u>
  $\cong$ P(called pos | is pos)

$$\frac{\#TP}{\#Pos}$$

- Notice that n(0,0) is not used in either formula
  Therefore you get <u>no</u> credit for filtering out <u>ir</u>relevant items

# ROC vs. Precision-Recall

You can get very different visual results on the same data!



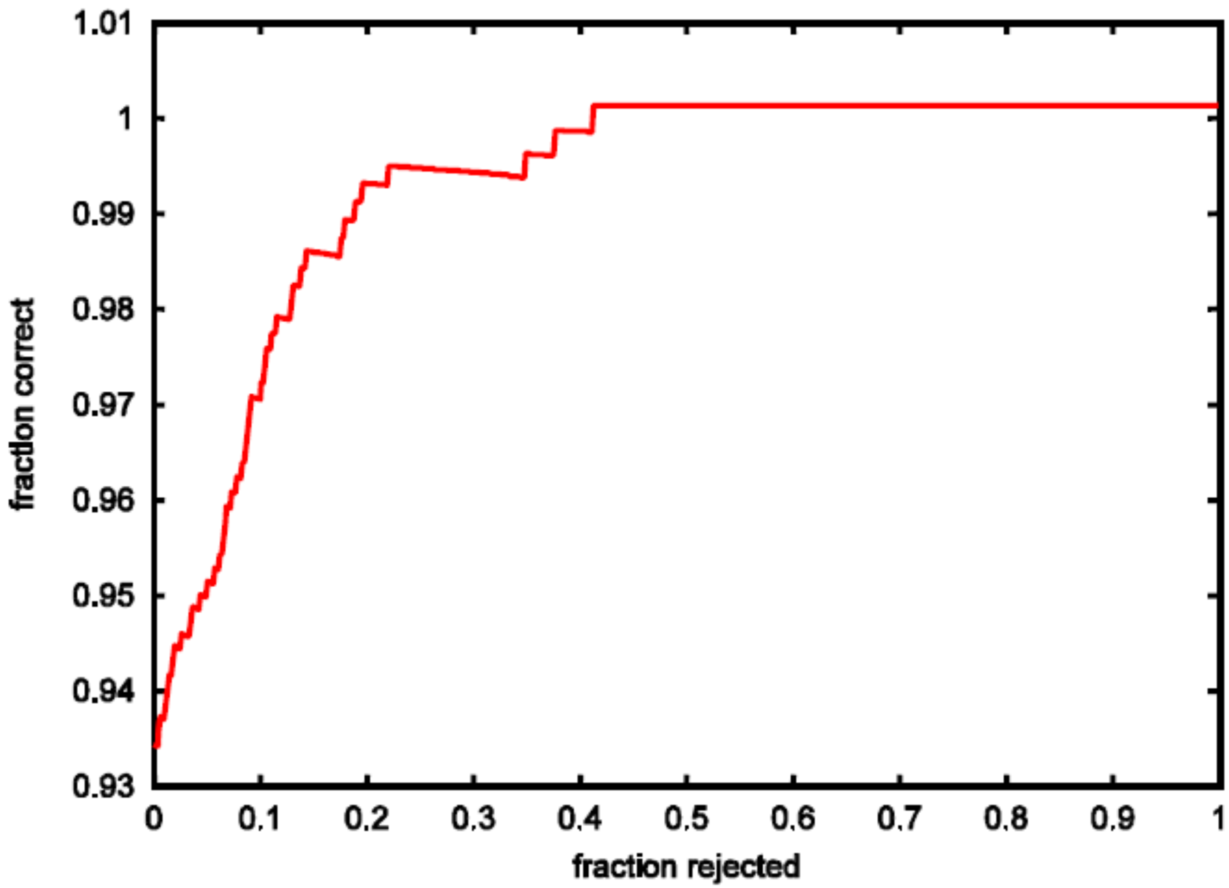

The reason for this is that there may be lots of – ex's
(e.g., might need to include 100 neg's to get 1 more pos)

# Rejection Curves

- In most learning algorithms, we can specify a threshold for making a rejection decision
  - Probabilistic classifiers: adjust cost of rejecting versus cost of FP and FN
  - Decision-boundary method: if a test point $\boldsymbol{x}$ is within $\theta$ of the decision boundary, then reject
    - Equivalent to requiring that the "activation" of the best class is larger than the second-best class by at least $\theta$

# Rejection Curves

- Vary θ and plot fraction correct versus fraction rejected



# The F1 Measure

- Figure of merit that combines precision and recall

$$F_1 = 2 \cdot \frac{P \cdot R}{P + R} = \frac{2}{\frac{1}{P} + \frac{1}{R}}$$

where $P$ = precision; $R$ = recall. This is twice the harmonic mean of $P$ and $R$.

- We can plot $F1$ as a function of the classification threshold $\theta$