Foundations of Machine Learning

Classifier Evaluation

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ML Problems: Recall

	Supervised Learning	Unsupervised Learning
Discrete	classification or categorization	clustering
Continuous	regression	dimensionality reduction

Classification Methods

- k-Nearest Neighbors
- Decision Trees
- Naïve Bayes
- Support Vector Machines
- Logistic Regression
- Neural Networks
- Ensemble Methods (Boosting, Random Forests)

How to evaluate?

Training vs Generalization Error

- Training Error
  - Not very useful
  - Relatively easy to obtain low error
- Generalization Error
  - How well we do on future data

$$E_{train} = \frac{1}{n}\sum_{\substack{i=1 \\ \text{training} \\ \text{examples}}}^{n} \overbrace{error}^{\text{same? different by how much?}}(\underbrace{f_D(\mathbf{x}_i)}_{\substack{\text{value we} \\ \text{predicted}}}, \underbrace{y_i}_{\substack{\text{true} \\ \text{value}}})$$

$$E_{gen} = \underbrace{\int}_{\substack{\text{over all} \\ \text{possible x,y}}} \underbrace{error(f_D(\mathbf{x}), y)}_{\text{error as before}} \underbrace{p(y, \mathbf{x})}_{\substack{\text{how often we expect} \\ \text{to see such x and y}}} d\mathbf{x}$$

How to compute generalization error?

Estimating Generalization Error

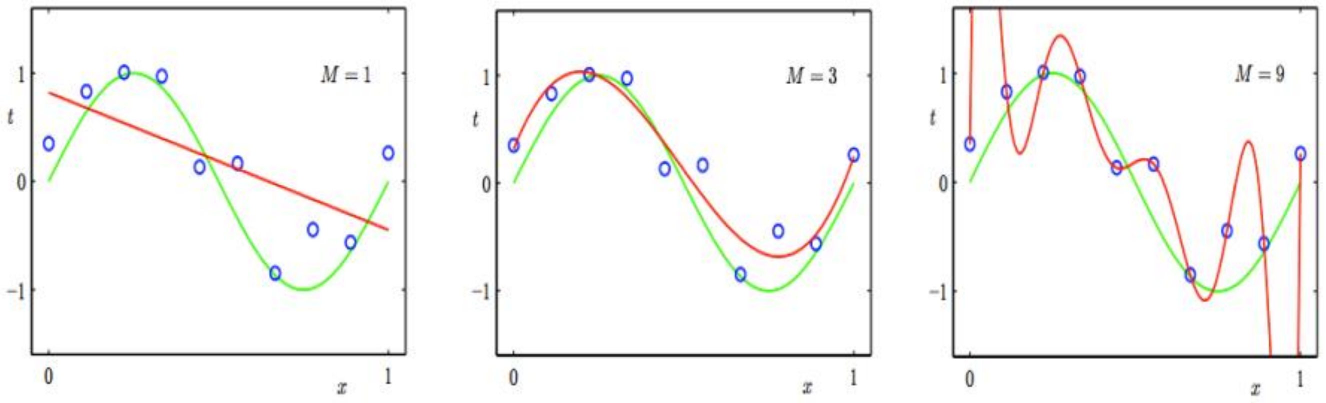
- Testing Error
  - Set aside part of training data (testing set)
  - Learn a predictor without using any of this test data
  - Predict values for testing set, compute error
  - This is an estimate of generalization error

over testing set

$$E_{test} = \frac{1}{n}\sum_{i=1}^{n} error(f_D(\mathbf{x}_i), y_i)$$

Underfitting and Overfitting

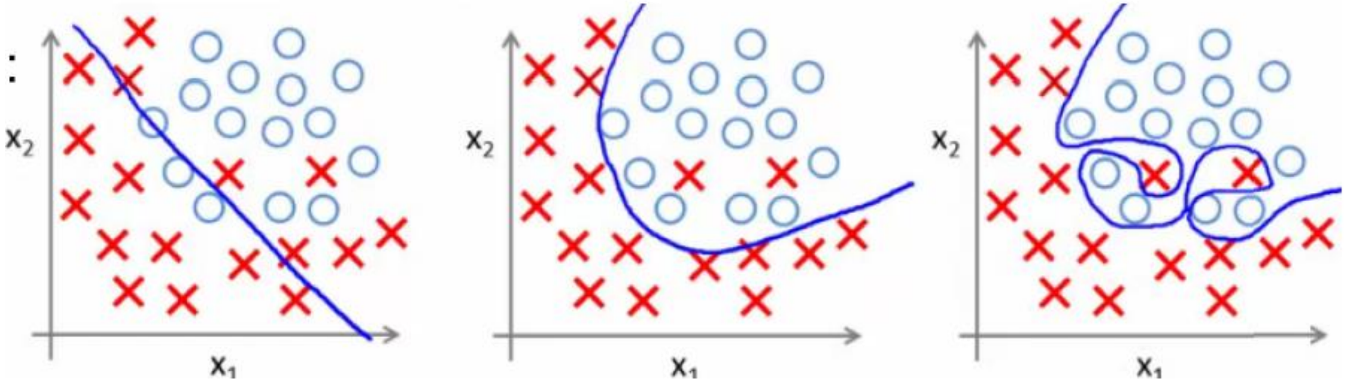
Regression



predictor too inflexible:
cannot capture pattern

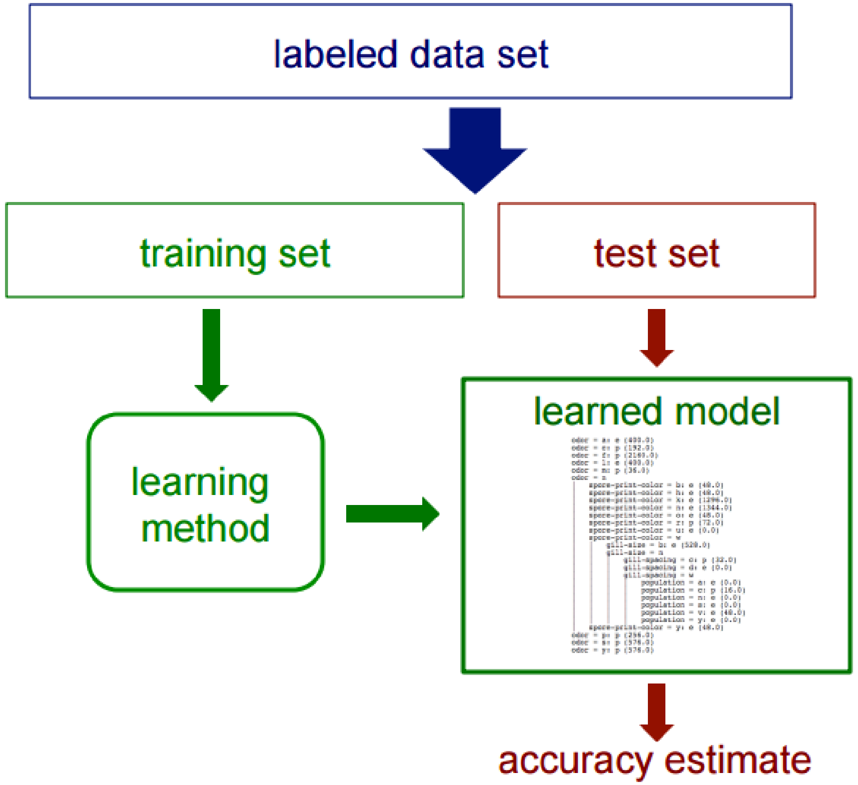
predictor too flexible:
fits noise in the data

Classification



Estimating Generalization Error

- Getting an unbiased estimate of the accuracy of a learned model



```
odor = a: e (400.0)
odor = c: p (192.0)
odor = f: p (2160.0)
odor = l: e (400.0)
odor = m: p (36.0)
odor = n
|   spore-print-color = b: e (48.0)
|   spore-print-color = h: e (48.0)
|   spore-print-color = k: e (1296.0)
|   spore-print-color = n: e (1344.0)
|   spore-print-color = o: e (48.0)
|   spore-print-color = r: p (72.0)
|   spore-print-color = u: e (0.0)
|   spore-print-color = w
|   |   gill-size = b: e (528.0)
|   |   gill-size = n
|   |   |   gill-spacing = c: p (32.0)
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|   |   |   |   population = c: p (16.0)
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odor = p: p (256.0)
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odor = y: p (576.0)
```
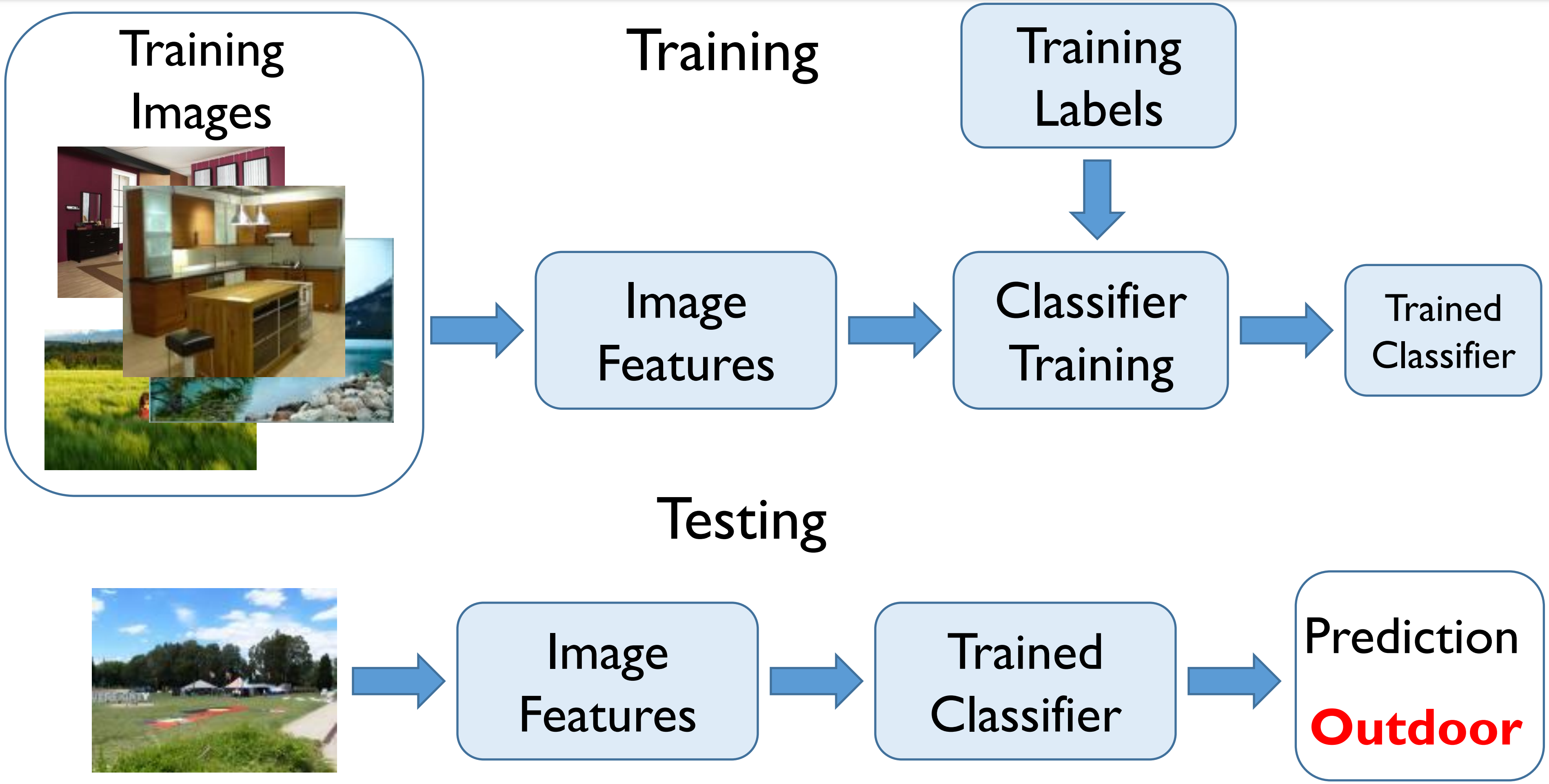

Example: Image Classification



Training

Training Images

Image Features

Training Labels

Classifier Training

Trained Classifier

Testing

Image Features

Trained Classifier

Prediction

Outdoor

Source: Derek Hoiem

Training, Validation, Test Sets

Training set

- NB: Count frequencies, DT: Pick attributes to split on

Validation set

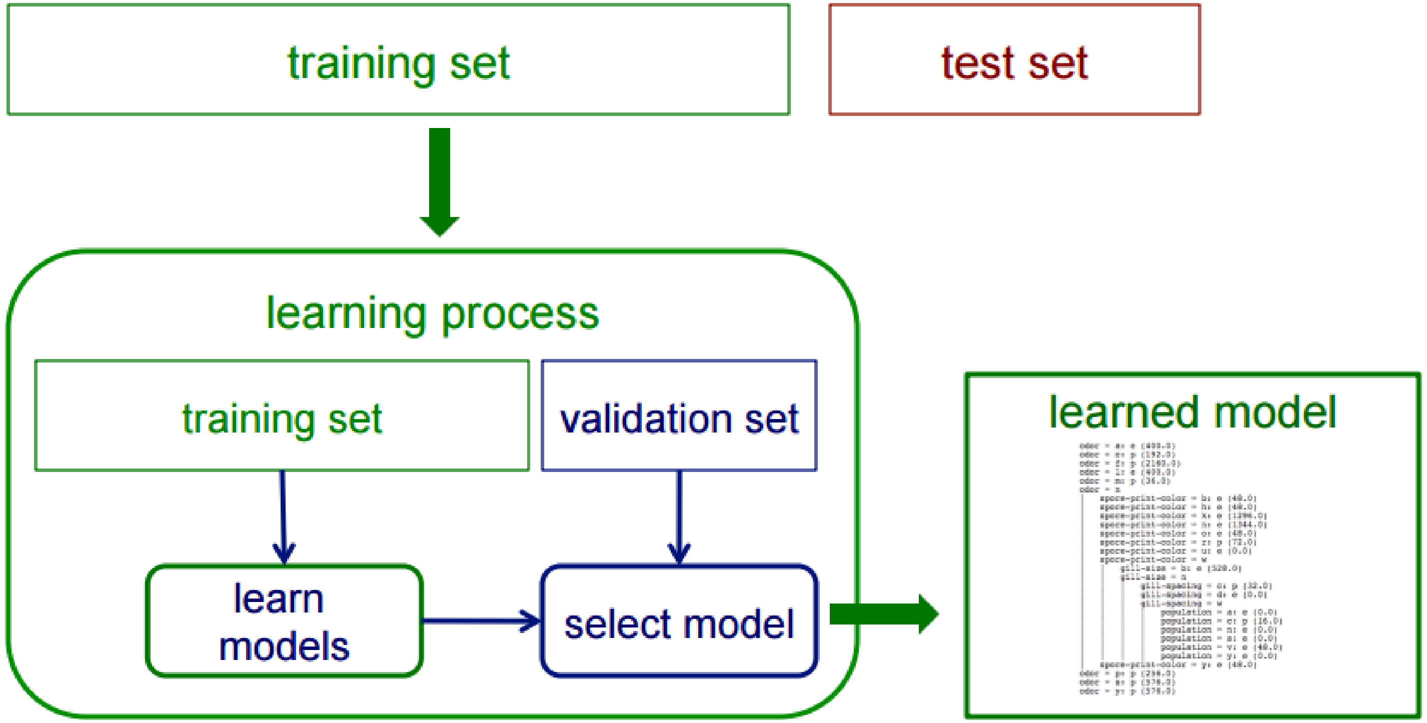
- Pick best-performing algorithm (NB vs DT vs..)
- Fine-tune parameters (Tree depth, k in kNN, c in SVM)

Testing set

- Run multiple trials and average

Use of Validation Sets

- If we want unbiased estimates of accuracy during the learning process:



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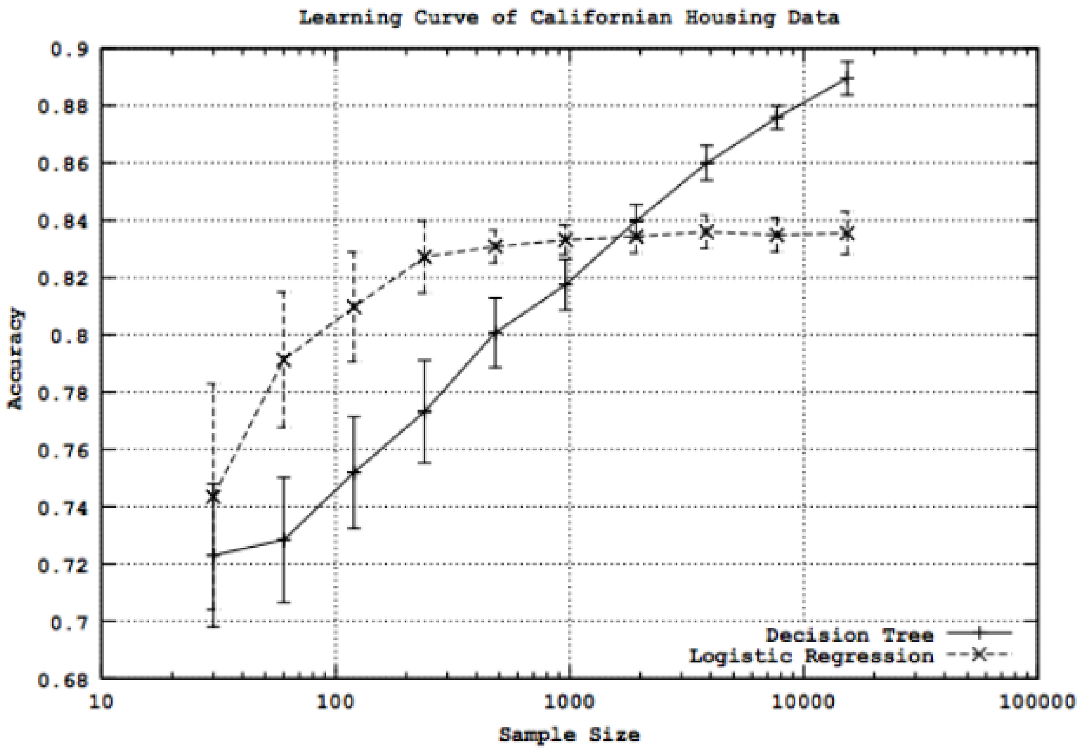
Choosing Training, Validation, Test Sets

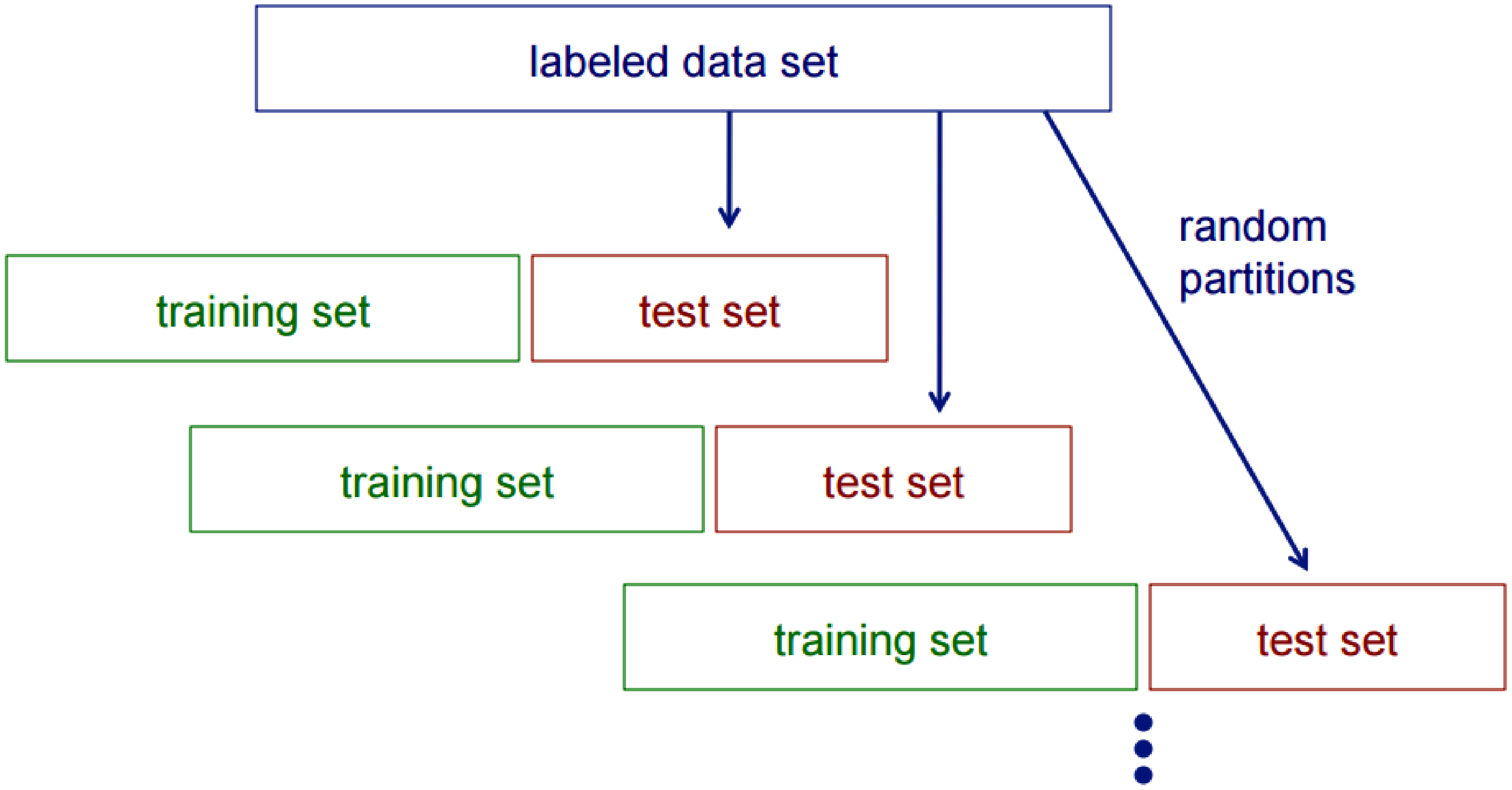
- Split randomly to avoid bias
- Large test set -> estimate future error as accurately as possible (vs) Large training set => better estimates
- How large should a training set be?
  - Study accuracy/error (vs) training set size



Courtesy: Perlich et al. Journal of Machine Learning Research, 2003

Random Resampling

- We can artificially increase training set size using random resampling:



labeled data set

random partitions

training set

test set

training set

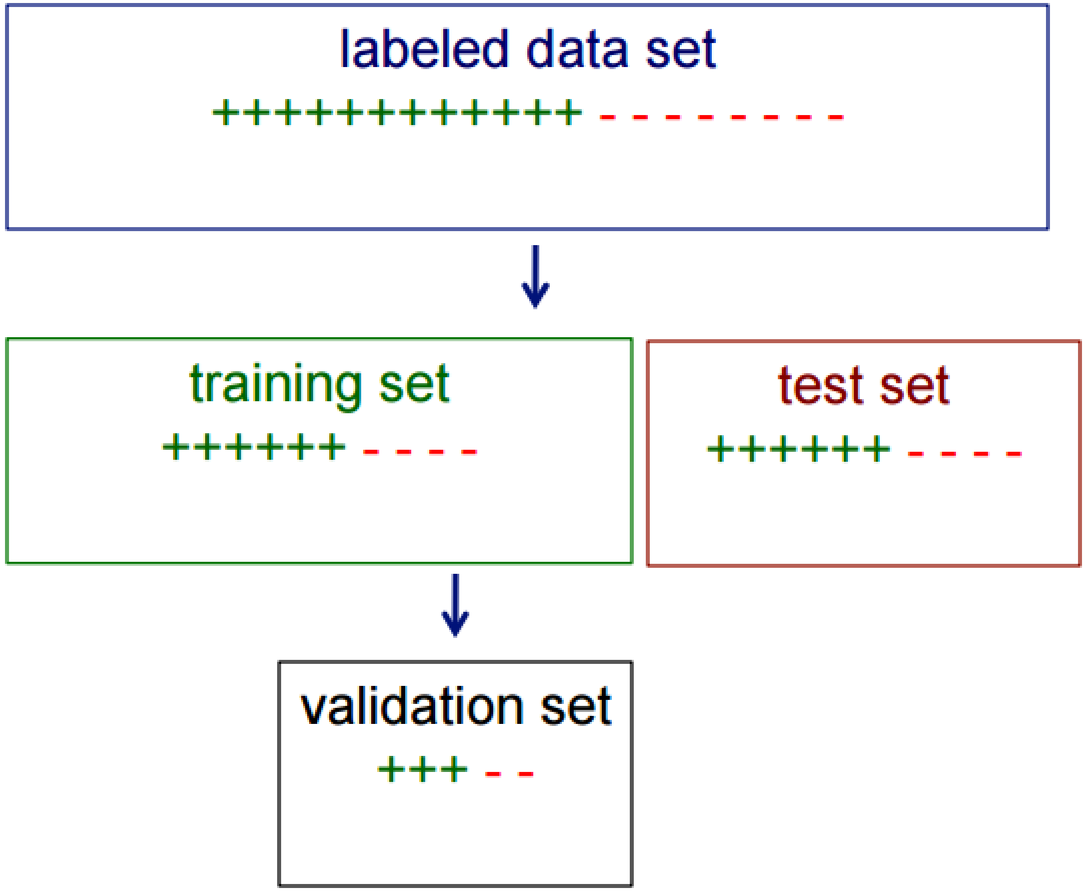
test set

training set

test set

Stratified 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 instances by class, then randomly select instances from each class proportionally.



labeled data set

++++++++++++ - - - - - - - -

training set

++++++ - - - -

test set

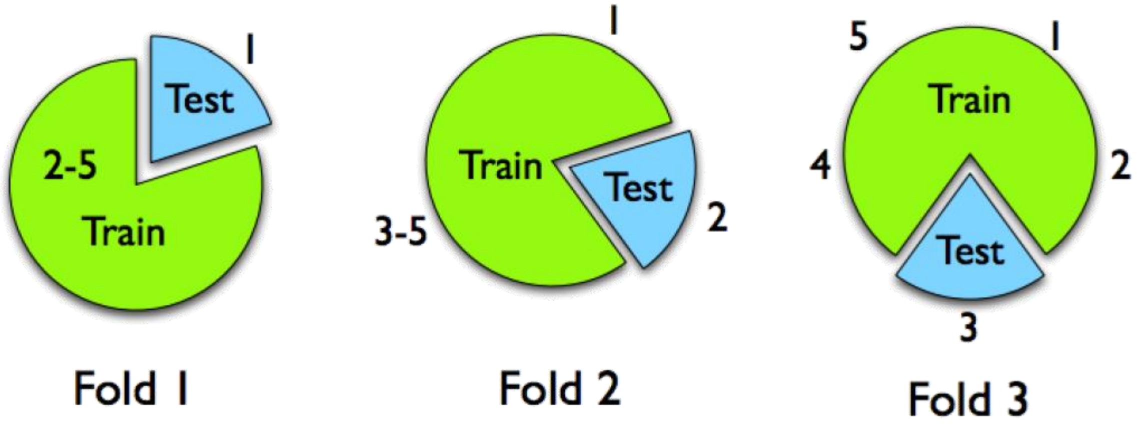
++++++ - - - -

validation set

+++ - -

Model Selection

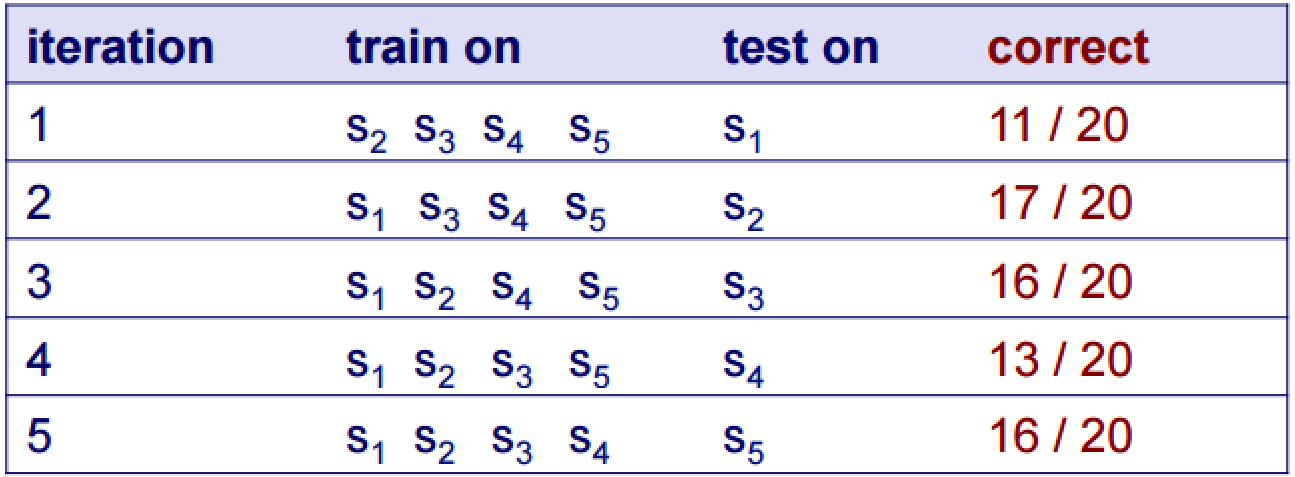
- Resubstitution
- K-fold cross-validation



- Leave-one-out
  - N-fold cross-validation

Cross-Validation: Example

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



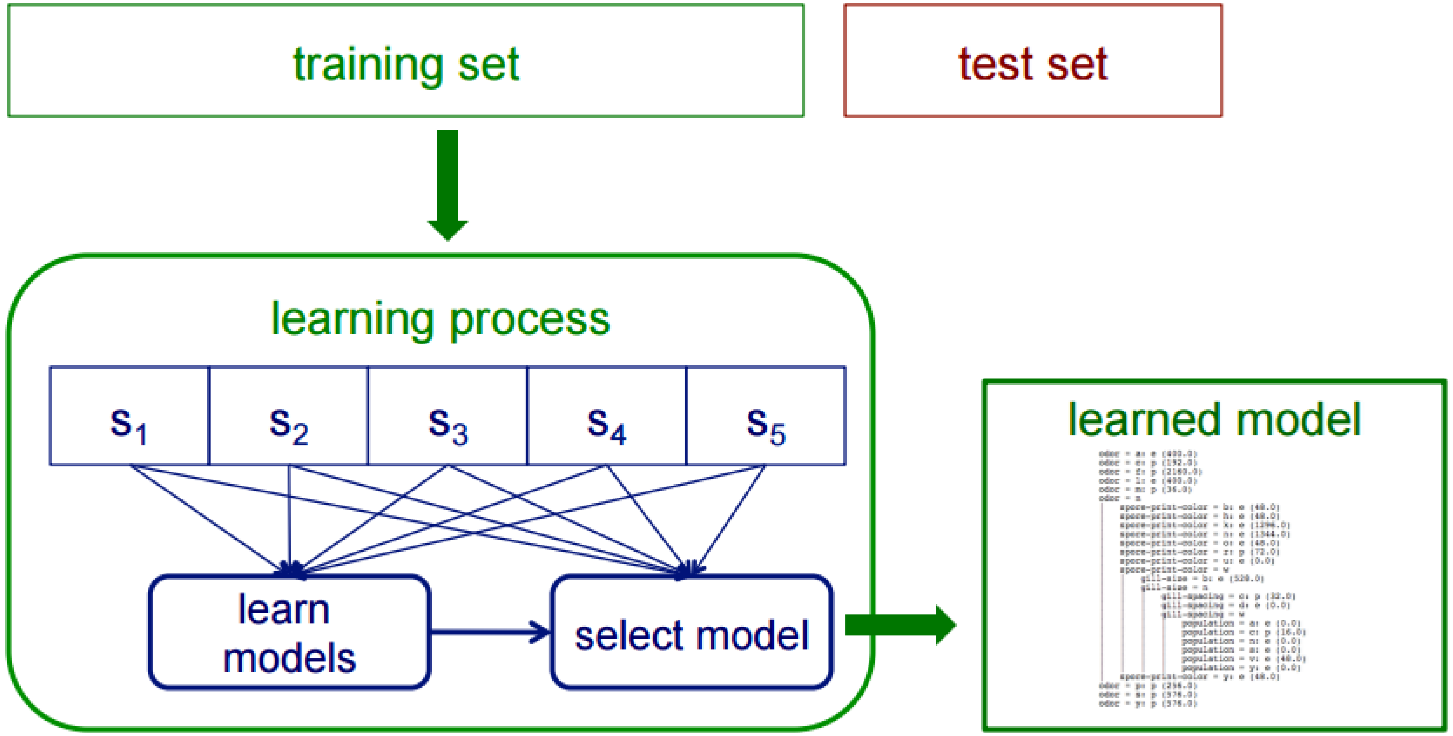
iteration	train on	test on	correct
1	s_2 s_3 s_4 s_5	s_1	11 / 20
2	s_1 s_3 s_4 s_5	s_2	17 / 20
3	s_1 s_2 s_4 s_5	s_3	16 / 20
4	s_1 s_2 s_3 s_5	s_4	13 / 20
5	s_1 s_2 s_3 s_4	s_5	16 / 20

Classification Accuracy = 73/100 = 73%

Note: Whenever we use multiple training sets, as in CV and random resampling, we are evaluating a learning method as opposed to an individual learned model

Cross-Validation: Example

- Instead of a single validation set, we can use cross-validation within a training set to select a model (e.g. to choose the best k in k-NN)



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Evaluation Measures

- Classification
  - How often we classify something right/wrong
- Regression
  - How close are we to what we're trying to predict
- Ranking/Search
  - How correct are the top-k results?
- Clustering
  - How well we describe our data (Not straightforward)

Is accuracy adequate?

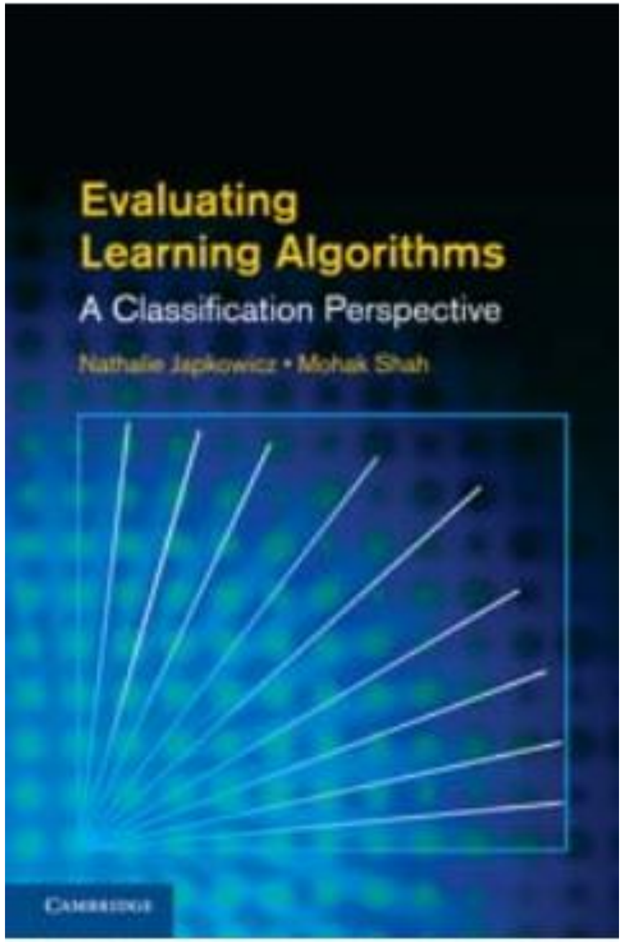
- Accuracy may not be useful in cases where
  - There is a large class skew
    - Is 98% accuracy good if 97% of the instances are negative?
  - There are differential misclassification costs – say, getting a positive wrong costs more than getting a negative wrong
    - Consider a medical domain in which 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

Classification Error: Beyond Accuracy

Evaluating Learning Algorithms: A Classification Perspective

Nathalie Japkowicz & Mohak Shah
Cambridge University Press, 2011

Good tutorial on the topic: http://www.icmla-conference.org/icmla11/PE_Tutorial.pdf


Evaluating Learning Algorithms
A Classification Perspective
Nathalie Japkowicz • Mohak Shah
CAMBRIDGE

Classification Error: Beyond Accuracy

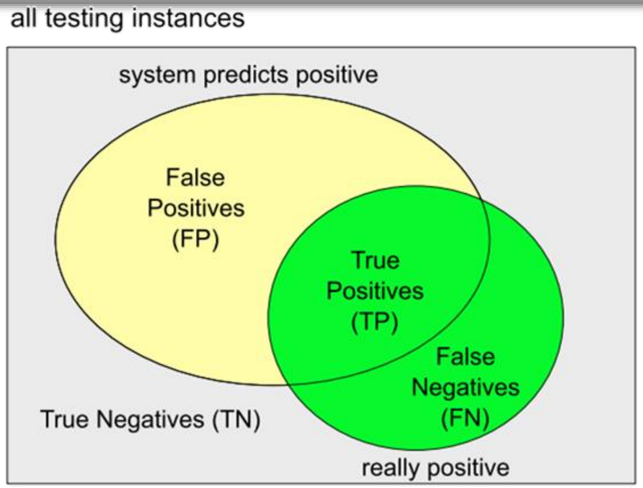
In 2-class problems:

		actual class	
		positive	negative
predicted class	positive	true positives (TP)	false positives (FP)
	negative	false negatives (FN)	true negatives (TN)

$$\text{accuracy} = \frac{\mathrm{TP} + \mathrm{TN}}{\mathrm{TP} + \mathrm{FP} + \mathrm{FN} + \mathrm{TN}}$$

Classification Performance Measures

		Predict positive?	
		Yes	No
Really positive?	Yes	TP	FN
	No	FP	TN



- Classification Error: $\frac{errors}{total} = \frac{FP+FN}{TP+TN+FP+FN}$
- Accuracy = 1-Error: $\frac{correct}{total} = \frac{TP+TN}{TP+TN+FP+FN}$

} meaningless if classes imbalanced

- False Alarm = False Positive rate = FP / (FP+TN)
- Miss = False Negative rate = FN / (TP+FN)
- Recall = True Positive rate = TP / (TP+FN)
- Precision = TP / (TP+FP)

} always report in pairs, e.g.: Miss / FA or Recall / Prec.

- True Positive Rate also called "Sensitivity"
- "Specificity" = 1 – False Alarm

- "Sensitivity" = Probability of a positive test given a patient has the disease
- "Specificity" = Probability of a negative test given a patient is well

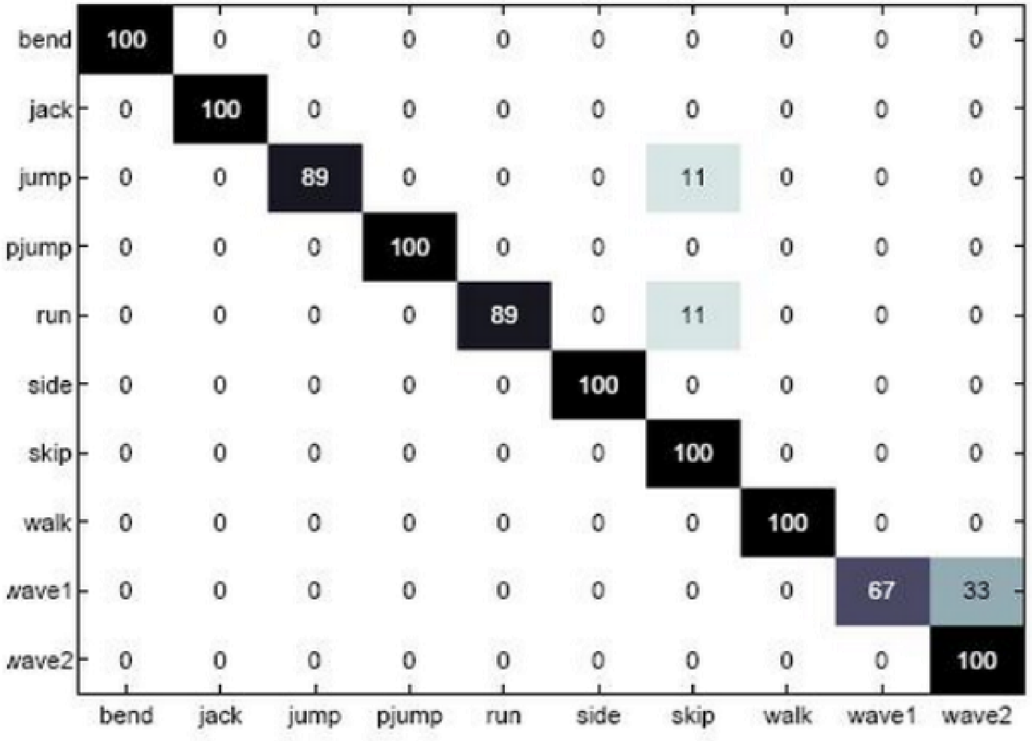
Classification Error: Beyond Accuracy

For multi-class problems?

Confusion Matrix

activity recognition from video

actual class



	bend	jack	jump	pjump	run	side	skip	walk	wave1	wave2
bend	100	0	0	0	0	0	0	0	0	0
jack	0	100	0	0	0	0	0	0	0	0
jump	0	0	89	0	0	0	11	0	0	0
pjump	0	0	0	100	0	0	0	0	0	0
run	0	0	0	0	89	0	11	0	0	0
side	0	0	0	0	0	100	0	0	0	0
skip	0	0	0	0	0	0	100	0	0	0
walk	0	0	0	0	0	0	0	100	0	0
wave1	0	0	0	0	0	0	0	0	67	33
wave2	0	0	0	0	0	0	0	0	0	100

predicted class

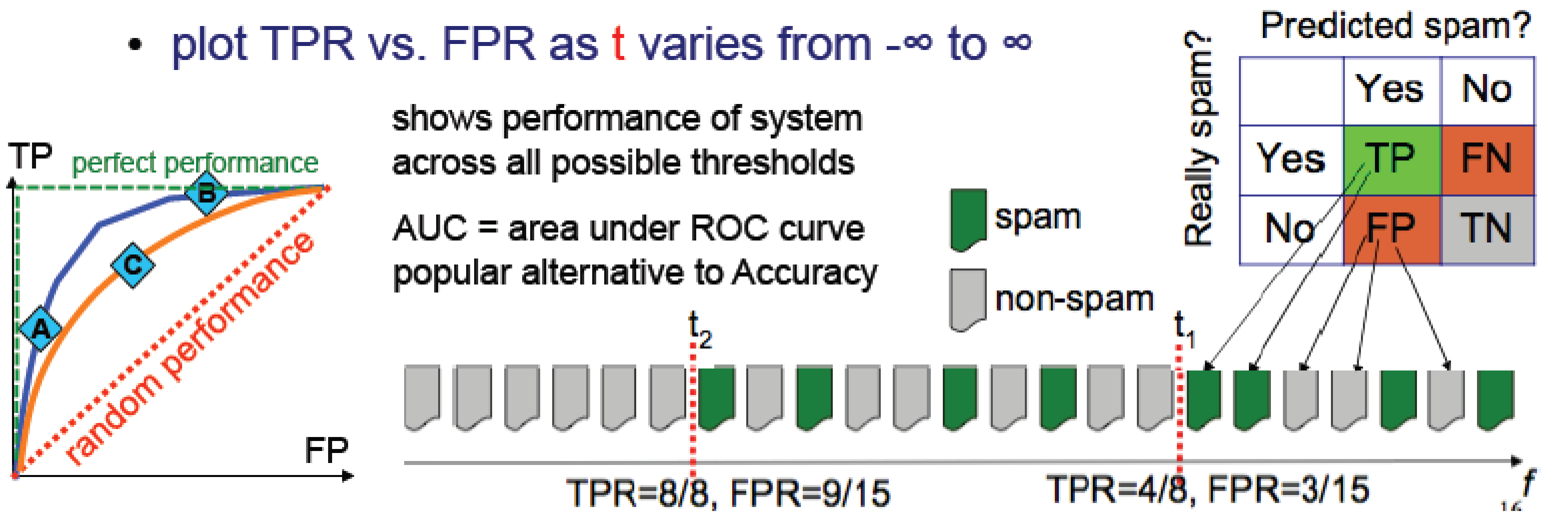
Courtesy: vision.jhu.edu

Utility and Cost

- Sometimes, there is a cost for each error
  - E.g. Earthquake prediction
    - False positive: Cost of preventive measures
    - False negative: Cost of recovery
- Detection Cost (Event detection)
  - Cost = $C_{FP} * FP + C_{FN} * FN$
- F-measure (Information Retrieval)
  - F1 = 2/(1/Recall + 1/Precision)

ROC Curves

- Many algorithms compute "confidence" f(x)
  - Threshold to get decision: spam if f(x) > t, non-spam if f(x) <= t
  - Threshold to determine error rates
- Receiver Operating Characteristic (ROC)



- plot TPR vs. FPR as t varies from -∞ to ∞

shows performance of system across all possible thresholds

AUC = area under ROC curve
popular alternative to Accuracy

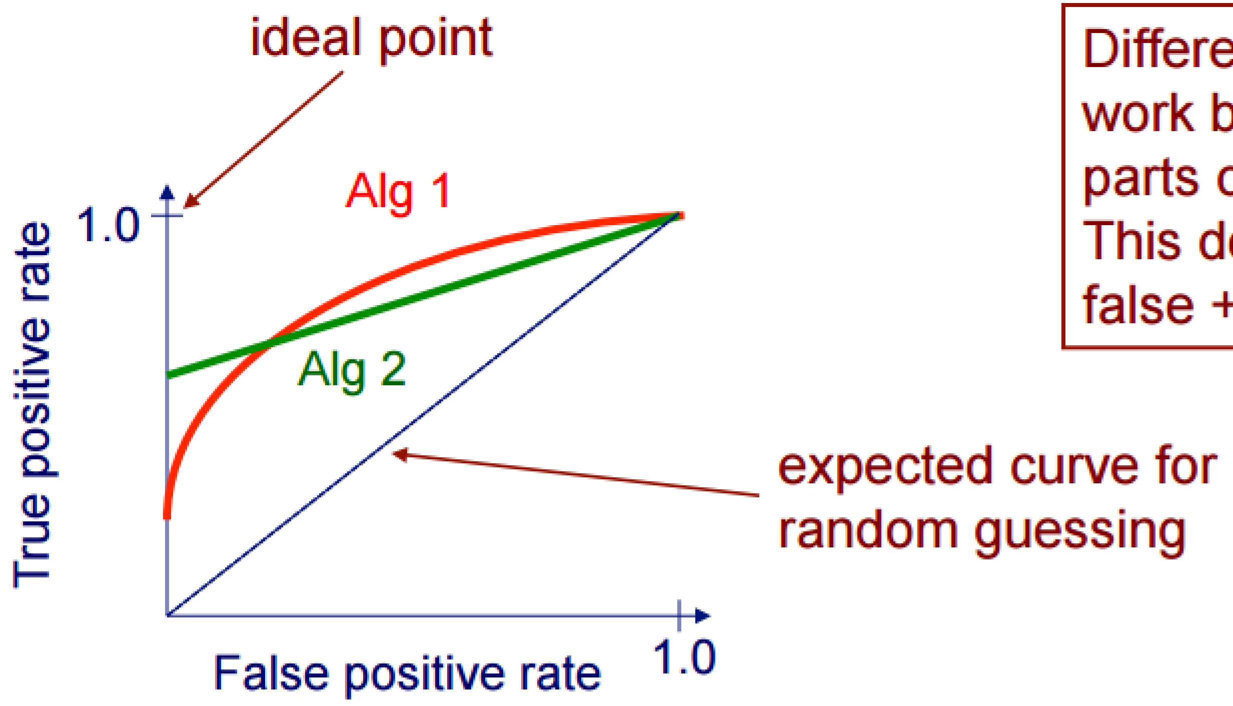
		Predicted spam?	
		Yes	No
Really spam?	Yes	TP	FN
	No	FP	TN

ROC Curve: Algorithm

- 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

ROC Curves

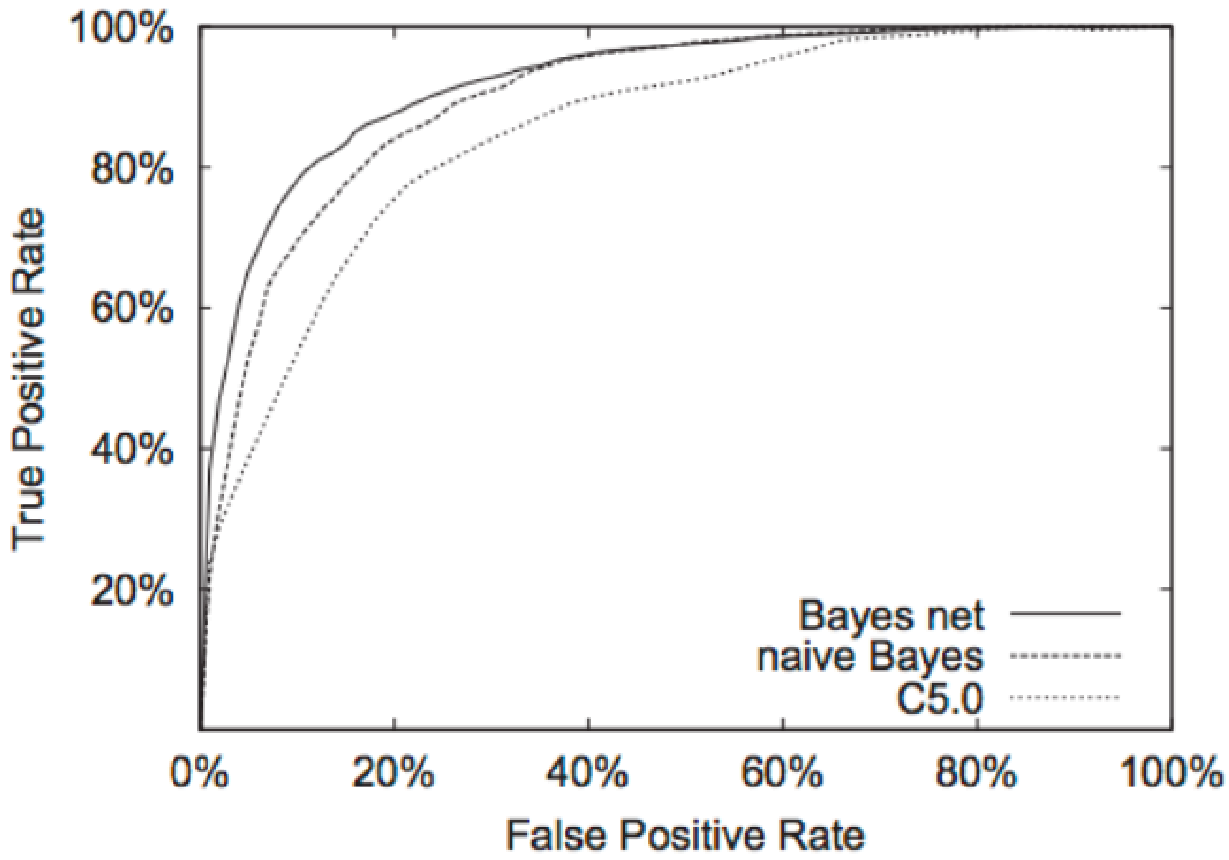
- A Receiver Operating Characteristic (ROC) curve plots the TP-rate vs. the FP-rate as a threshold on the confidence of an instance being positive is varied



expected curve for random guessing

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

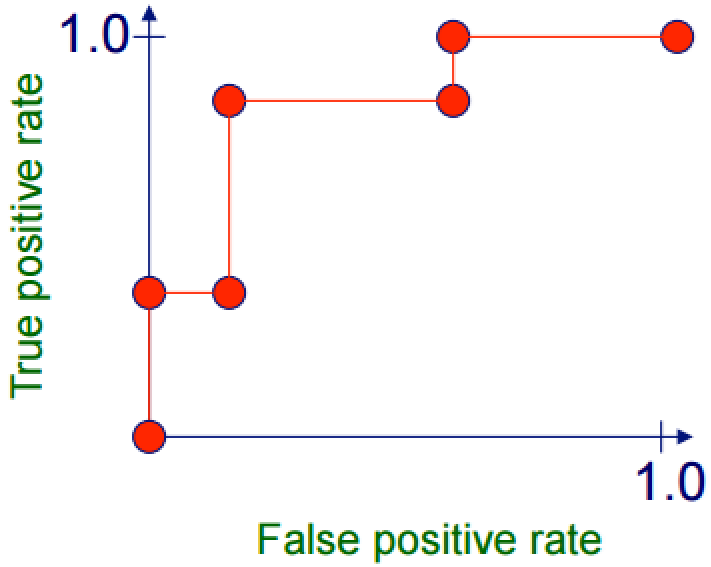
ROC Curve: Example



Courtesy: Bockhorst et al., Bioinformatics 2003

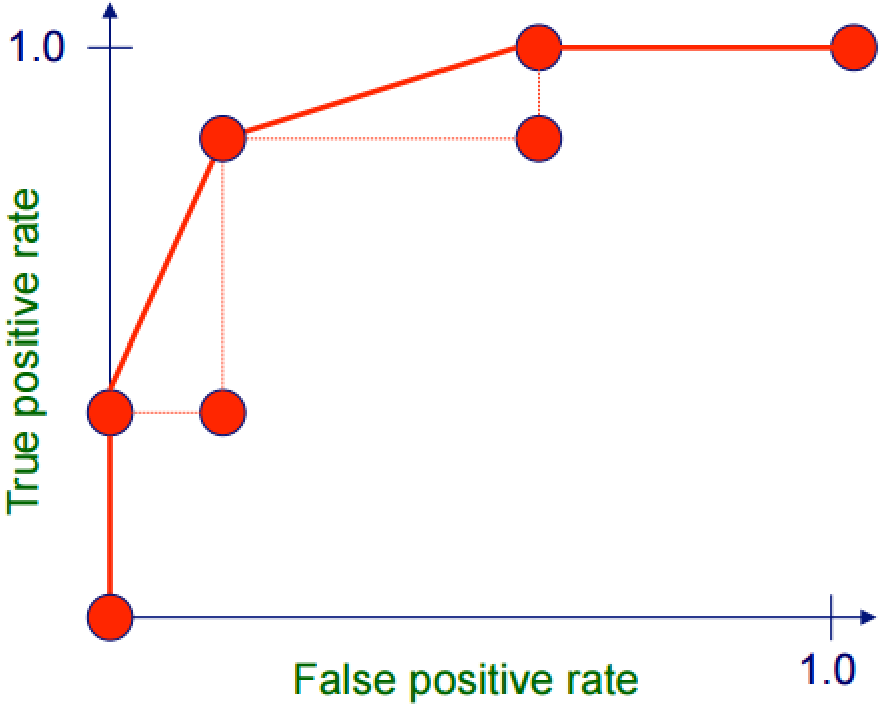
Plotting an ROC Curve

instance	confidence positive		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	-

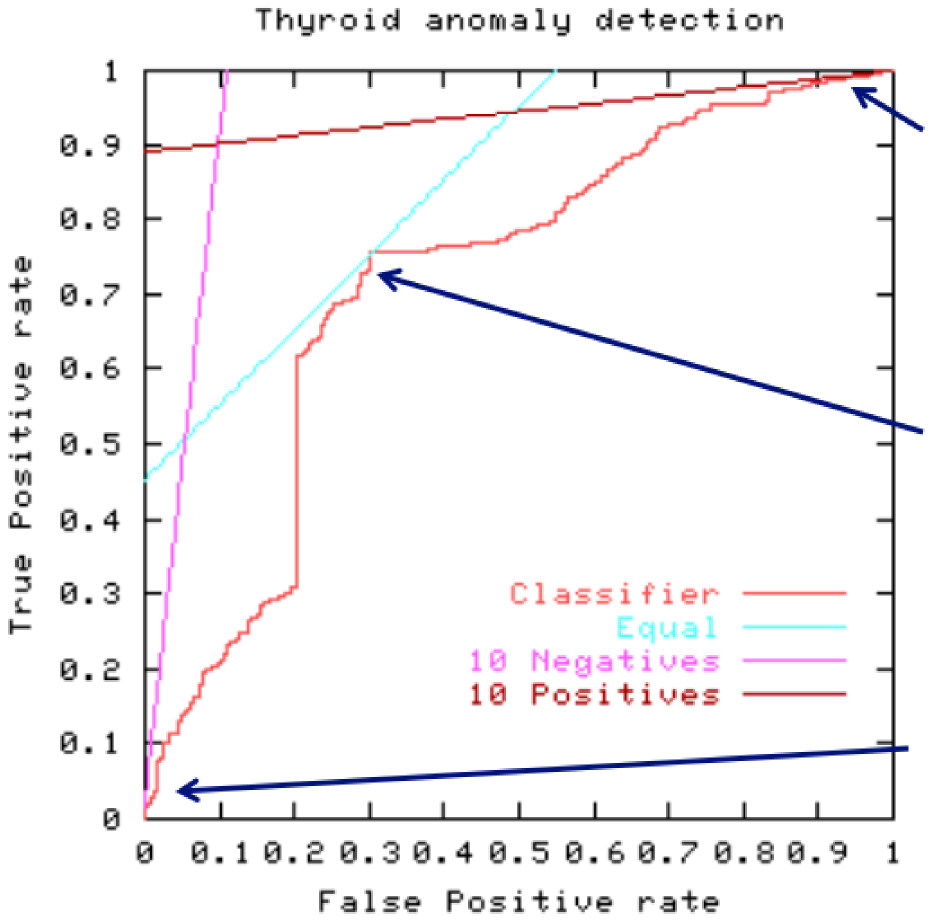


Plotting an ROC Curve

- Can interpolate between points to get convex hull



ROC Curves and Misclassification Costs

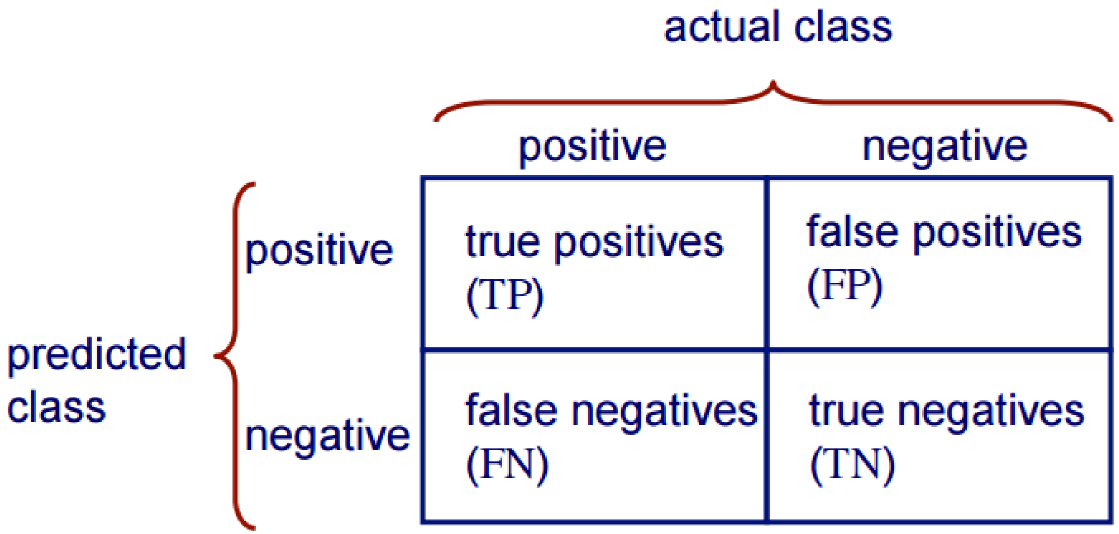


best operating point when FN costs 10× FP

best operating point when cost of misclassifying positives and negatives is equal

best operating point when FP costs 10× FN

Recall: Precision-Recall



		actual class	
		positive	negative
predicted class	positive	true positives (TP)	false positives (FP)
	negative	false negatives (FN)	true negatives (TN)

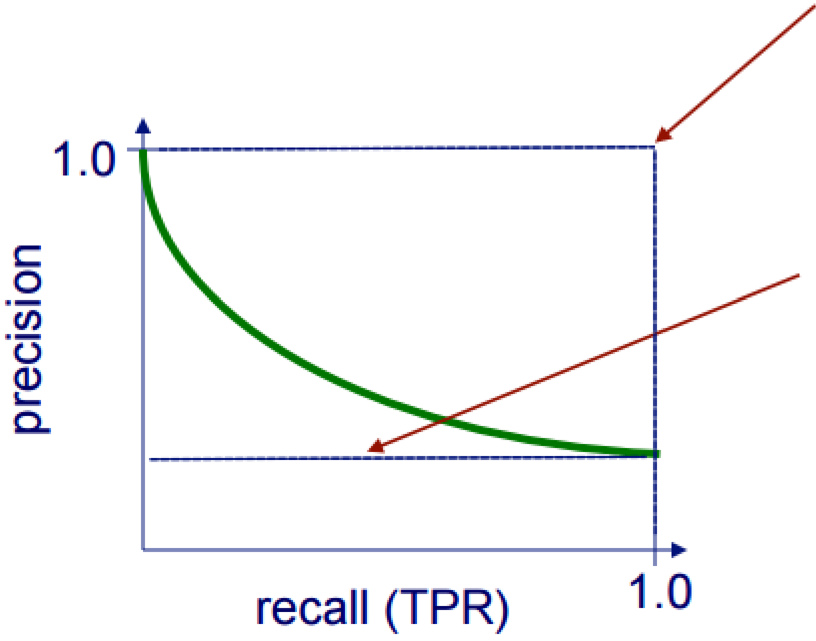
$$\text{recall (TP rate)} = \frac{\text{TP}}{\text{actual pos}} = \frac{\text{TP}}{\text{TP} + \text{FN}}$$

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

Precision/Recall Curves

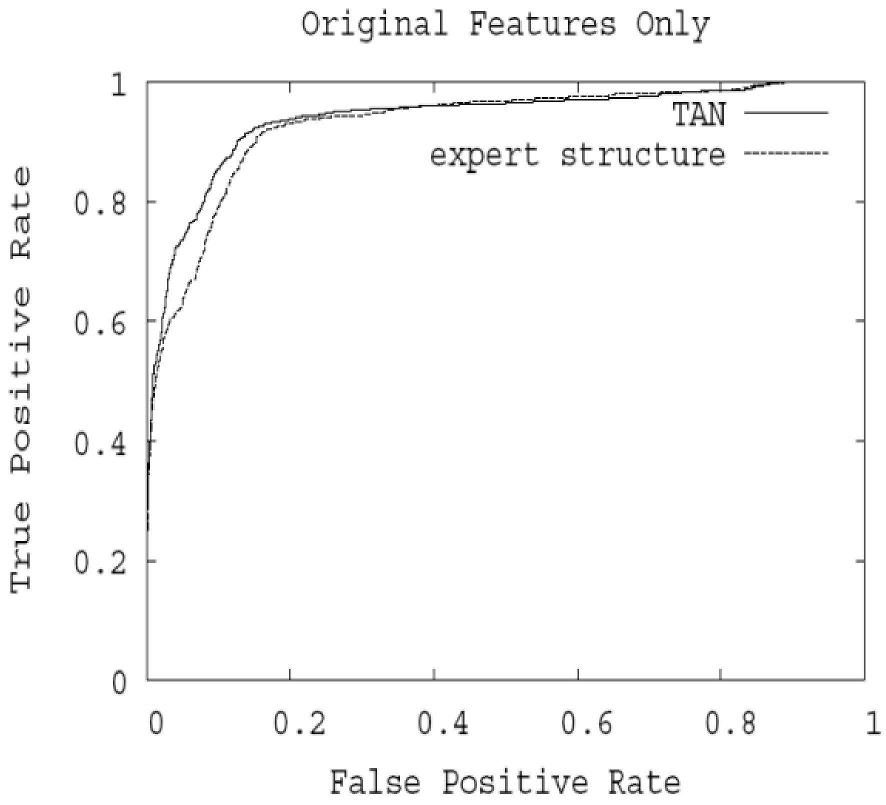
- A precision/recall curve plots the precision vs. recall (TP-rate) as a threshold on the confidence of an instance being positive is varied

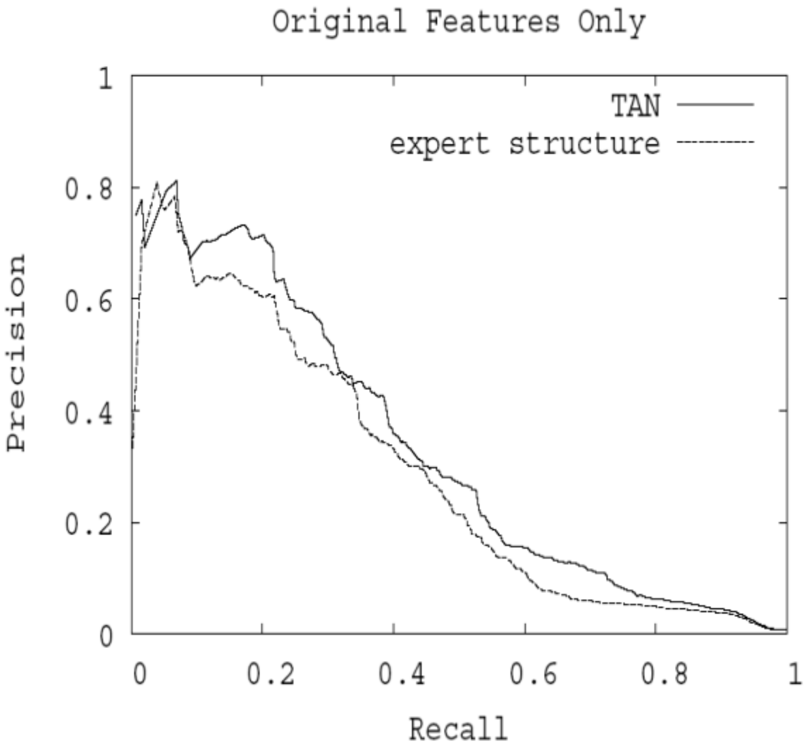
ideal point



default precision determined by the fraction of instances that are positive

ROC + PR Curves: Example



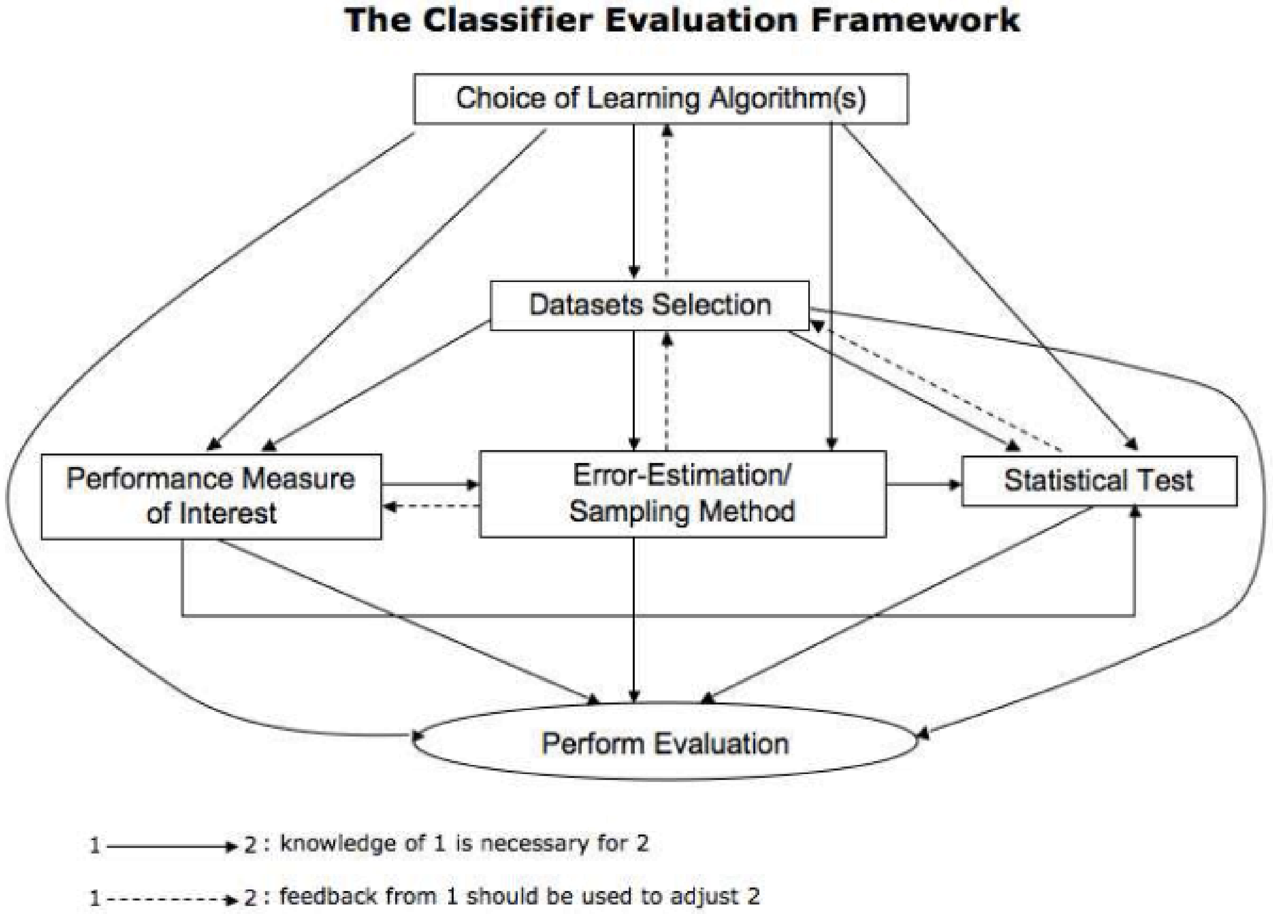


Courtesy: Page, Univ of Wisconsion-Madison

Other Performance Measures

- Kullback-Leibler Divergence: $D_{\mathrm{KL}}(P\|Q) = \sum_i P(i) \log \frac{P(i)}{Q(i)}$
- Gini Statistic:
  - 2 * AUC – 1
- F-score: Harmonic mean of precision and recall
  - (2 * precision * recall)/(precision+recall)
- Akaike Information Criterion:
  - AIC = 2k – 2 ln (L), where L is the max value of the likelihood function for the model, and k is the number of model parameters
  - Used for relative comparison between models

Classifier Evaluation


The Classifier Evaluation Framework
Choice of Learning Algorithm(s)
Datasets Selection
Performance Measure of Interest
Error-Estimation/ Sampling Method
Statistical Test
Perform Evaluation
1 → 2 : knowledge of 1 is necessary for 2
1 - - - → 2 : feedback from 1 should be used to adjust 2

Summarizing: Pitfalls

- Is my held-aside test data really representative of new data?
  - Even if your methodology is fine, someone may have collected features for positive examples differently than for negatives
  - Example: samples from cancer processed by different people or on different days than samples for normal controls
  - Randomization is essential

Pitfalls

- Did I repeat my entire data processing procedure on every fold of cross-validation, using only the training data for that fold?
  - On each fold of cross-validation, did I ever access in any way the label of a test case?
  - Any preprocessing done over entire data set (feature selection, parameter tuning, threshold selection) must not use labels from test set

Pitfalls

- Have I modified my algorithm so many times, or tried so many approaches, on this same data set that I (the human) am overfitting it?
  - Have I continually modified my preprocessing or learning algorithm until I got some improvement on this data set?
  - If so, I really need to get some additional data now to at least test on

Summary

- Rigorous statistical evaluation is extremely important in experimental computer science in general and machine learning in particular
- How good is a learned hypothesis?
- How close is the estimated performance to the true performance?
- Is one hypothesis better than another?
- Is one learning algorithm better than another on a particular learning task?

References

- Key References
  - Chapter 19, EA Introduction to ML, 2nd Edn
  - Chapter 1 (Sec 1.1-1.5), Pattern Recognition and Machine Learning, Bishop
- Other Recommended References
  - http://www.icmla-conference.org/icmla11/PE_Tutorial.pdf (Tutorial on Performance Evaluation of Classifiers)
  - Chapter 5 ('Evaluating Hypotheses'), Machine Learning by Tom Mitchell
    - http://www.cs.cmu.edu/~tom/mlbook.html