# Evaluating Hypothesis and Experimental Design

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Computer Science 367

# Assumptions

- We assume that all datapoints (examples) are drawn independently from a fixed probability distribution defined by the particular problem.
- This is almost never the case!!!

# Evaluating Hypothesis

- Given observed accuracy of a hypothesis over a limited sample of data, how well does this estimate it's accuracy over additional examples?
- Given that one hypothesis outperforms another over some sample of data, how probable is it that this hypothesis is more accurate in general?
- When data is limited what is the best way to use this data to both learn a hypothesis and estimate its accuracy?

# Estimating Hypothesis Accuracy

- Estimating the accuracy with which it will classify future instances - also probable error of this accuracy estimate!!!

- A space of possible instances X.
- Different instances in X may be encountered with different frequencies which is modeled by some unknown probability distribution D.
- Notice D says nothing about whether x is a positive or negative instance.

# Learning Task

- The learning task is to learn the target concept, f, by considering a space H of possible hypothesis.
- Training examples of the target function f are provided to the learner by a trainer who draws each instance independently, according to the distribution D and who then forwards the instance x along with the correct target value f(x) to the learner.
- Are instances ever really drawn independently?

# Sample error

- Sample error - the fraction of instances in some sample S that it misclassifies

$$error_s(h) \equiv \frac{1}{n} \sum_{x \in S} \delta(f(x), h(x))$$

- Where n is the number of samples in S, and $\delta(f(x),h(x))$ is 1 if $f(x) \neq h(x)$ and 0 otherwise

# True Error

- True error - probability it will misclassify a single randomly drawn instance from the distribution D

$$error_D(h) \equiv \Pr_{x \in D}[f(x) \neq h(x)]$$

- Where $\Pr_{x \in D}$ denotes that the probability is taken over the instance distribution D.

# Sample error versus True error

- Really want $error_D(h)$ but can only get $error_S(h)$.
- How good an estimate of $error_D(h)$ is provided by $error_S(h)$?

# Problems with Estimating Accuracy

- Bias in Estimate
- Variance in the Estimate

# Bias in Estimate

- Observed accuracy of the learned hypothesis over the training examples is an optimistically biased estimate of hypothesis accuracy over future examples.
- Especially likely when the learner considers a very rich hypothesis space, enabling it to overfit the training examples.
- Typically we test the hypothesis on some set of test examples chosen independently of the training examples and the hypothesis.

# Variance in Estimate

- Even if the hypothesis accuracy is measured over an unbiased set of test examples, the measured accuracy can still vary from true accuracy, depending on the makeup of the particular set of test examples.

- The smaller the set of test examples, the greater the expected variance.

# Types of Bias

- Machine Learning Bias
- Systematic Error Bias
- "Straight Statistical" Bias

# Machine Learning Bias

- Every inductive learning algorithm must adopt a bias in order to generalize beyond the training data.
- This is good and bad!

# Systematic Error Bias

- If there is systematic error in the training set, the learning algorithm cannot tell the difference between systematic error and real structure in the dataset.

- Therefore systematic error will also create a bias in the estimate.
- Systematic error example - pull-down menus

# Statistical Bias

- Statistical Bias is the systematic error for a given sample size m.

- So this will include “straight statistical bias” and also the ML Bias and the Systematic Error Bias.

- “straight statistical bias”is the notion that as the training set size gets smaller, then the error will go up.

# Statistical Bias Formula

- StatBias(A,m,x) = f´(x) - f(x),

  where A is the learning algorithm, m is the training set size, x is a random example, and f´ is the expected value of f, where the expectation is taken over all possible training sets of fixed size m.

$$f^{'}(x) = \lim_{l \to \infty} \tfrac{i}{l} \sum_{i=1}^{l} f_{s_i}(x)$$

# Variance

- $\text{Variance}(A,m,x) = E[(f_S(x)-f'(x))^2]$, where $f_S$ is a particular hypothesis learned on training set S.

- Variance comes from variation in the training data, random noise in the training data, or random behavior in the learning algorithm itself.

# Error

- So error is just made up of Bias and Variance.

$$\text{Error}(A,m,x)=\text{Bias}(A,m,x)^2+\text{Variance}(A,m,x)$$

- Remember that the Bias includes “straight statistical bias”, Machine Learning Bias, and Systematic Error Bias
- Also Bias is squared only because Variance is already squared

# Four Important Sources of Error

- Random variation in the selection of the test data - got today right
- Random variation in the selection of the training data - stock newsletters
- Randomness in the learning algorithm (e.g., initial weights) - trying 2000 seeds and only one works well
- Random classification error - guys on the line entering data

# Dealing with Error

- Good statistical test should not be fooled by these sources of variation.

- To account for test-data variation and the possibility of random classification error, the statistical procedure must consider the size of the test set and the consequences of changes in the test set.

- To account for training-data variation and internal randomness, the statistical procedure must execute the learning algorithm multiple times and measure the variation in accuracy of the resulting classifiers.

# What is Overfitting

- Given a hypothesis space H, a hypothesis h∈H is said to **overfit** the training data if there exists some alternative hypothesis h´∈H, such that h has a smaller error than h´ over the training examples, but h´ has a smaller error that h over the entire distribution of instances.

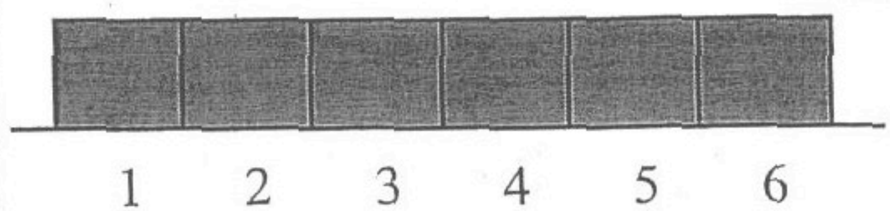
- Not a very useful definition!

# What causes Overfitting?

- Why would complexity cause overfitting???

- What about multiple comparisons?

# Sampling Distributions for 1 die and 10 dice?

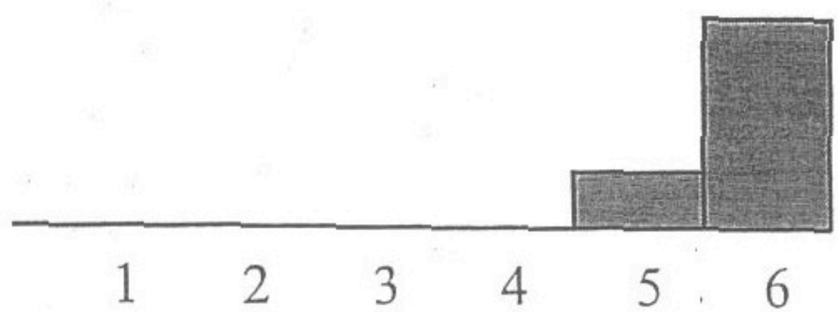



$E(X_i|H_0) = 3.5$

$p(X_i>5|H_0) = 0.167$

(a)

**ampling distributions for one die and ten dice**



# Multiple Comparisons

- Cause overfitting, oversearching, feature selection problems
- Solutions
  - New test data
  - Bonferroni & Sidak (mathematical adjustment, assumes independence)
  - Cross validation - biased if k is to large because then the training sets are virtually the same - leave one out
  - Randomization tests - my favorite - drawback is time complexity - but to estimate p-values between .1 and .01 usually requires no more than 100-1000 trials

# Why does Pruning Decision Trees Work?

- By pruning decision trees we are making the hypothesis space smaller (only small decision trees are allowed) so the effect of the multiple comparison's problem is reduced.

- Do I believe this?

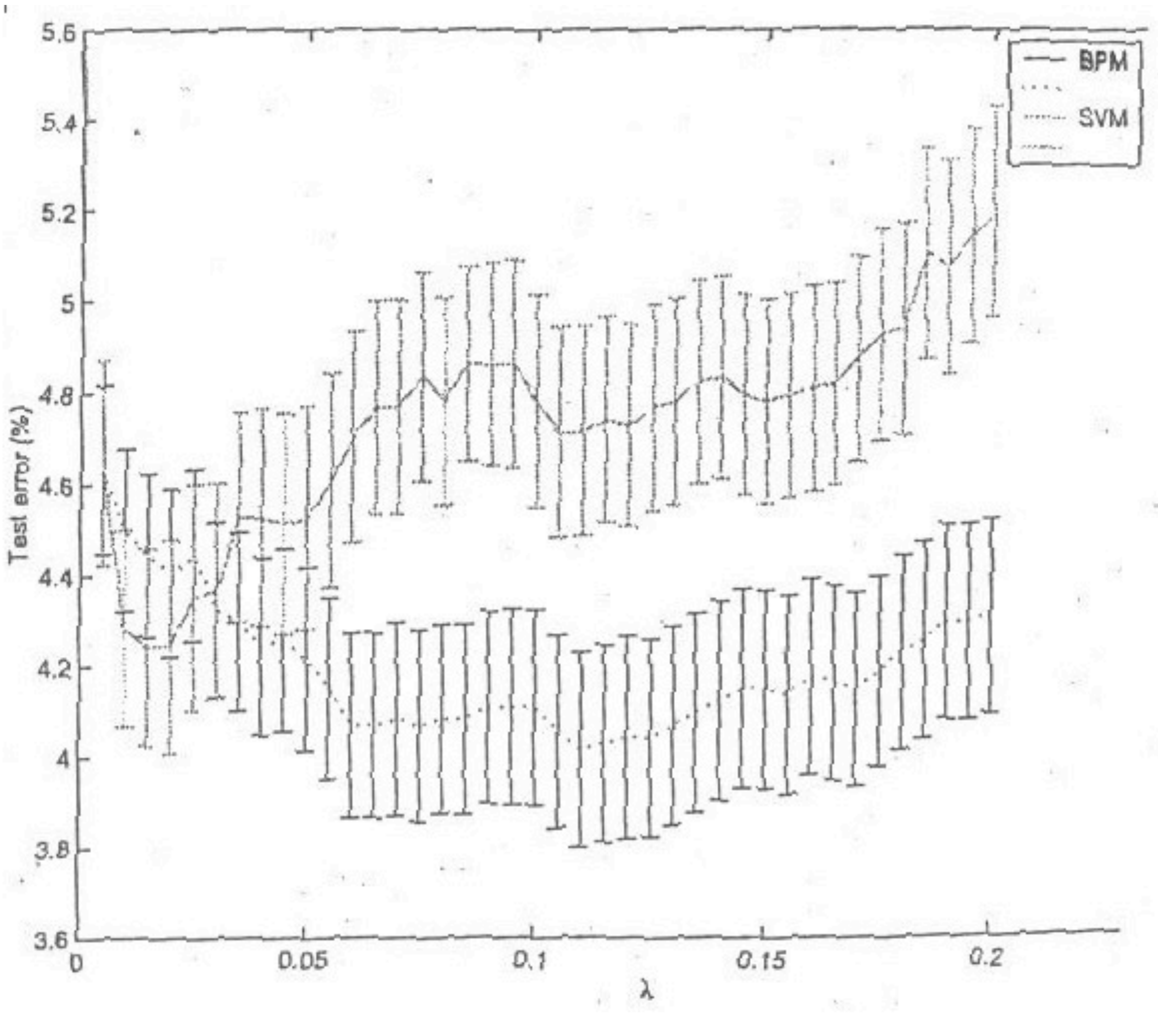
# 10-fold Cross Validation

- Break data into 10 sets of size n/10.
- Train on 9 datasets and test on 1.
- Repeat 10 times and take a mean accuracy.

# Experiments with Standard Deviation

| ex | name | C4.5 | | Randomized C4.5 | | Bagged C4.5 | | Adaboosted C4.5 | |
|---|---|---|---|---|---|---|---|---|---|
| | | P | error rate | P | error rate | P | error rate | P | error rate |
| | sonar | | 0.3257±0.0637 | | 0.2018±0.0545 | * | 0.2752±0.0607 | * | 0.1651±0.0505 |
| | letter | | 0.1225±0.0045 | | 0.0285±0.0023 | | 0.0552±0.0032 | * | 0.0271±0.0023 |
| | splice | * | 0.0575±0.0081 | * | 0.0397±0.0068 | * | 0.0506±0.0076 | | 0.0503±0.0076 |
| | segment | | 0.0328±0.0073 | | 0.0203±0.0058 | | 0.0263±0.0065 | | 0.0151±0.0050 |
| | glass | * | 0.3437±0.0636 | | 0.2277±0.0562 | | 0.2723±0.0596 | * | 0.2277±0.0562 |
| | soybean | | 0.1262±0.0371 | * | 0.0852±0.0312 | * | 0.1009±0.0337 | * | 0.0757±0.0296 |
| | autos | | 0.2326±0.0578 | * | 0.1581±0.0499 | | 0.1814±0.0528 | | 0.1814±0.0528 |
| | satimage | * | 0.1515±0.0157 | | 0.0890±0.0125 | | 0.1020±0.0133 | | 0.0850±0.0122 |
| | annealing | * | 0.0132±0.0075 | | 0.0088±0.0061 | | 0.0099±0.0065 | | 0.0055±0.0048 |
| | krk | | 0.1887±0.0046 | | 0.1309±0.0039 | | 0.1463±0.0041 | * | 0.1026±0.0036 |
| | heart-v | * | 0.2762±0.0620 | * | 0.2429±0.0594 | | 0.2619±0.0609 | * | 0.2810±0.0623 |
| | heart-c | * | 0.2396±0.0481 | * | 0.1853±0.0437 | * | 0.1981±0.0449 | | 0.2045±0.0454 |
| | breast-y | * | 0.2601±0.0508 | * | 0.2500±0.0502 | * | 0.2635±0.0511 | * | 0.3142±0.0538 |
| | phoneme | * | 0.1661±0.0086 | | 0.1437±0.0081 | | 0.1509±0.0082 | * | 0.1464±0.0081 |
| | voting | * | 0.1146±0.0299 | * | 0.0921±0.0272 | * | 0.0966±0.0278 | * | 0.1034±0.0286 |
| | vehicle | | 0.2944±0.0307 | | 0.2477±0.0291 | | 0.2570±0.0294 | | 0.2196±0.0279 |
| | lymph | | 0.1962±0.0640 | | 0.1772±0.0615 | | 0.1835±0.0624 | * | 0.1266±0.0536 |
| | breast-w | * | 0.0494±0.0161 | * | 0.0353±0.0137 | | 0.0367±0.0139 | | 0.0310±0.0128 |
| | credit-g | * | 0.2921±0.0282 | | 0.2416±0.0265 | * | 0.2495±0.0268 | | 0.2347±0.0263 |
| | primary | * | 0.5845±0.0525 | * | 0.5501±0.0530 | | 0.5645±0.0528 | * | 0.5960±0.0522 |
| | shuttle | | 0.0003±0.0003 | | 0.0002±0.0002 | | 0.0002±0.0002 | | 0.0001±0.0002 |
| | heart-s | * | 0.0677±0.0444 | * | 0.0677±0.0444 | * | 0.0677±0.0444 | * | 0.0902±0.0506 |
| | iris | | 0.0563±0.0369 | * | 0.0500±0.0349 | * | 0.0500±0.0349 | * | 0.0688±0.0405 |
| | sick | * | 0.0132±0.0036 | | 0.0137±0.0037 | | 0.0137±0.0037 | * | 0.0095±0.0031 |
| | hepatitis | | 0.1758±0.0599 | | 0.1636±0.0582 | | 0.1636±0.0582 | * | 0.1636±0.0582 |
| | credit-a | * | 0.1614±0.0275 | * | 0.1400±0.0259 | | 0.1371±0.0257 | * | 0.1300±0.0251 |
| | waveform | * | 0.2341±0.0117 | | 0.1784±0.0106 | | 0.1675±0.0104 | | 0.1521±0.0100 |
| | horse-colic | * | 0.1561±0.0371 | | 0.1561±0.0371 | | 0.1481±0.0363 | * | 0.1825±0.0395 |
| | heart-h | * | 0.1645±0.0424 | * | 0.1809±0.0440 | * | 0.1579±0.0417 | | 0.2039±0.0461 |
| | labor | | 0.1493±0.0925 | * | 0.1493±0.0925 | | 0.1194±0.0842 | * | 0.1194±0.0842 |
| | krkp | | 0.0075±0.0030 | | 0.0075±0.0030 | | 0.0056±0.0026 | * | 0.0037±0.0021 |
| | audiology | | 0.2203±0.0540 | * | 0.2458±0.0561 | | 0.1822±0.0503 | * | 0.1525±0.0469 |
| | hypo | | 0.0058±0.0024 | * | 0.0079±0.0028 | | 0.0042±0.0021 | * | 0.0040±0.0020 |

# Experiments with Learning Curves



# Summary

- What questions are we interested in asking?
- 10-fold Cross validation
- Problems to watch out for in experimental design
- Real cause of overfitting.