# Performance measures

Fall 2019

# Reminders/comments

- Hope you had a nice reading week!
- Today: a bit more info about designing experiments, including understanding how to measure generalization
    - for your mini-project
- Assignment 3 due this week
    - We will go over the gradient for NNs
- Initial draft of mini-project due next week

# Goal for your empirical study

- Try to keep the biases in mind when designing your experiment
- You will not be able to obtain a perfect experiment design
- But, you can be careful about
  - introducing really obviously fixable biases
  - picking inappropriate algorithms
  - giving some algorithms an unfair advantage
  - picking inappropriate error measures

# Reminder: Experimental set-up

- Performance measures
- Sampling: How to obtain multiple samples of performance?
- Making conclusions: Statistical significance tests
- Careful statistical work done on executing empirical studies; pros and cons to each
  - for a nice reference, see Evaluating Learning Algorithms: A Classification Perspective (http://www.mohakshah.com/tutorials/icml2012/Tutorial-ICML2012/Tutorial_at_ICML_2012.html); slides in this lecture use some of the material there
  - "Prediction error estimation: a comparison of resampling methods"

# Regression objectives

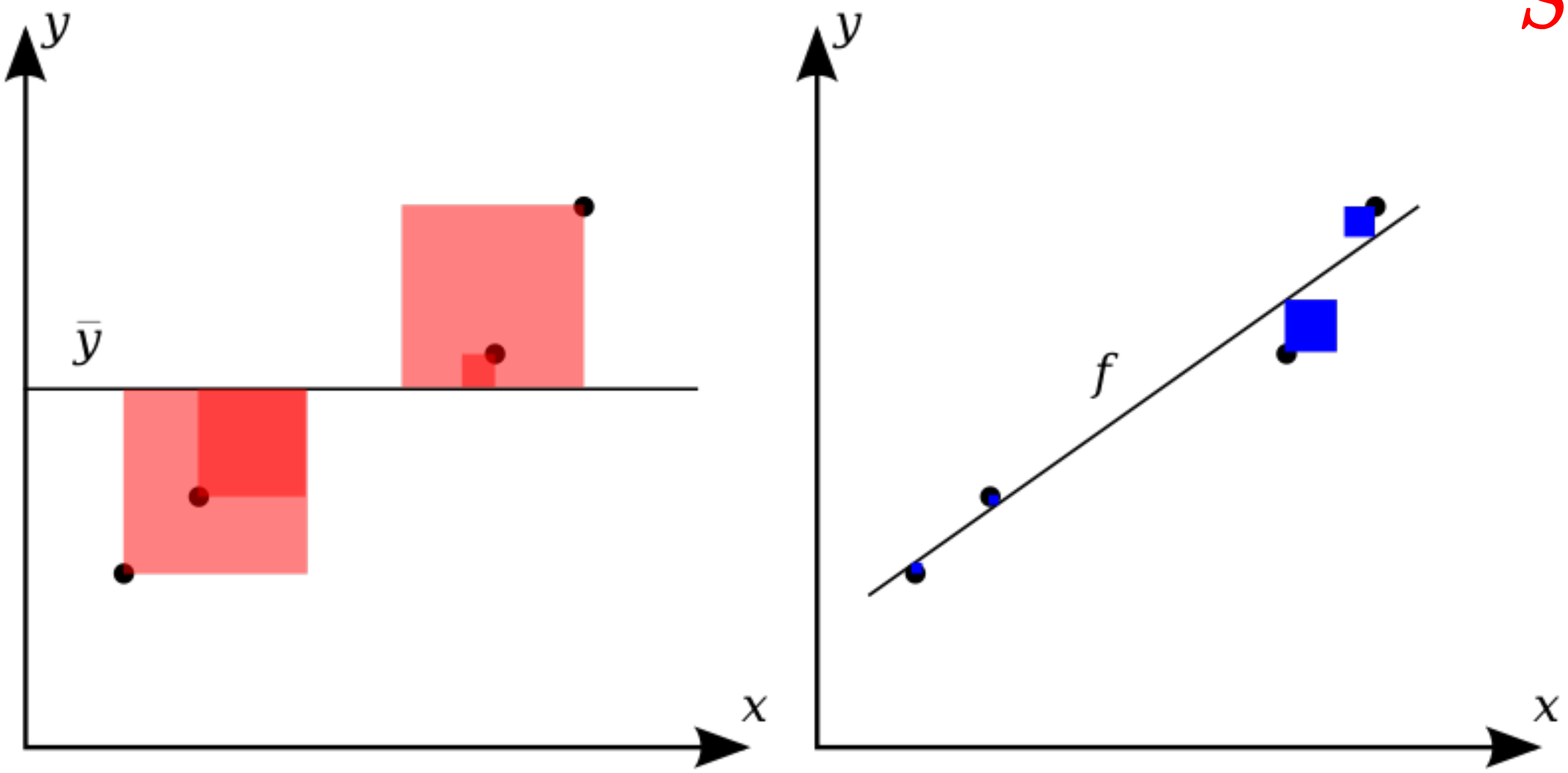
- We have looked at l2 error for estimating parameters (i.e., as an objective) and to measure performance

- Other options:
  - l1 error — can be difficult to optimize, still a useful measure of error
  - smooth l1 — smooth and convex, easier to optimize, not usually used as a measure of error (unless reporting accuracy of optimizer)
  - R-squared — coefficient of determination
  - Variance unexplained
  - Percentage error — rescale by magnitude of values

# R-squared measure

- Also called “coefficient of determination”

$$R^2 = 1 - \frac{SS_{\text{res}}}{SS_{\text{tot}}}$$



- The sum of squares of residuals, also called the residual sum of squares:

$$SS_{\text{res}} = \sum_i (y_i - f_i)^2$$

- The total sum of squares (proportional to the variance of the data):

$$SS_{\text{tot}} = \sum_i (y_i - \bar{y})^2,$$

Larger R-squared is better

# R-squared is monotone in number of features

- As add more features, the R-squared measure cannot decrease. Why?

$$R^2 \equiv 1 - \frac{SS_{\text{res}}}{SS_{\text{tot}}}. \qquad SS_{\text{res}} = \sum_i (y_i - f_i)^2 \qquad SS_{\text{tot}} = \sum_i (y_i - \bar{y})^2,$$

- Is this an issue?

- Alternative: adjusted R-squared — penalize the number of explanatory variables (features)

# Percentage error

- If use error ll val1 - val2 ll, and get 0.1, is this good?
- One option: percentage errors (issues?)
- Mean absolute percentage error (MAPE)

$$\mathrm{M} = \frac{1}{n}\sum_{t=1}^{n}\left|\frac{A_t - F_t}{A_t}\right|,$$

- Symmetric MAPE

$$\mathrm{SMAPE} = \frac{1}{n}\sum_{t=1}^{n}\frac{|F_t - A_t|}{(|A_t| + |F_t|)/2}$$

# Classification terminology

- True positives — samples predicted by classifier to be positive that have true label positive
- False positives — samples predicted by classifier to be positive that have true label negative
- True negatives — samples predicted by classifier to be negative that have true label negative
- False negatives — samples predicted by classifier to be negative that have true label positive

# Confusion Matrix for binary classification

**True class**

**Predicted class**

| | **0** | **1** |
|---|---|---|
| **0** | ***N*₀₀** tn ☺ | ***N*₀₁** fn ☹ |
| **1** | fp ***N*₁₀** ☹ | ***N*₁₁** tp ☺ |

**Number of data points whose true class was 0 but predicted class was 1.**

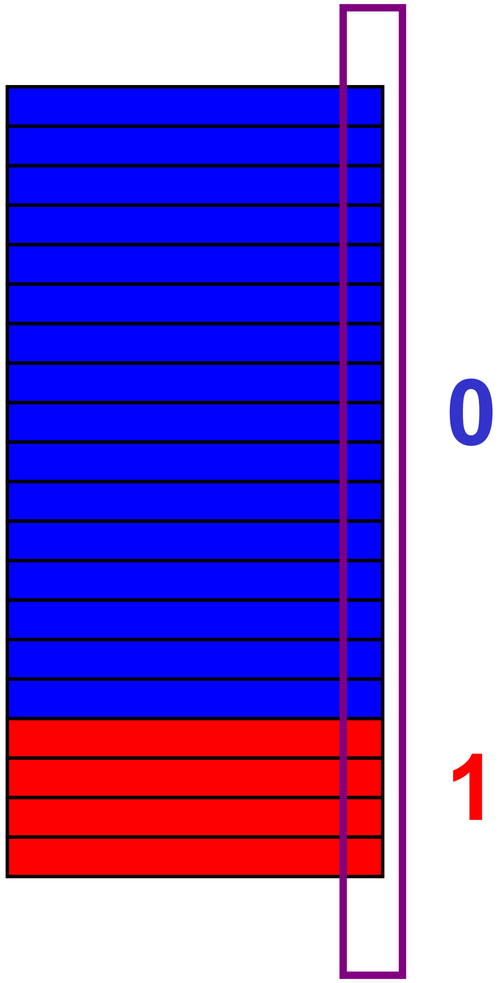
$$Accuracy = \frac{N_{00} + N_{11}}{N_{00} + N_{10} + N_{01} + N_{11}}$$

$$Error = 1 - Accuracy$$

# Why all these values to determine classification accuracy?

- Understanding algorithm performance is multi-faceted; reporting more than one measure is often useful
- This is especially true in classification, where important to measure both false positives and false negatives
  - In some cases, much more hazardous to have a false positive than a false negative (or vice versa)
- Avoid issues with imbalanced datasets

# Example of importance of measures: imbalanced datasets



**16 data points have class 0 (majority class)**

**4 data points have class 1 (minority class)**

**Trivial classifier: always predict majority class**

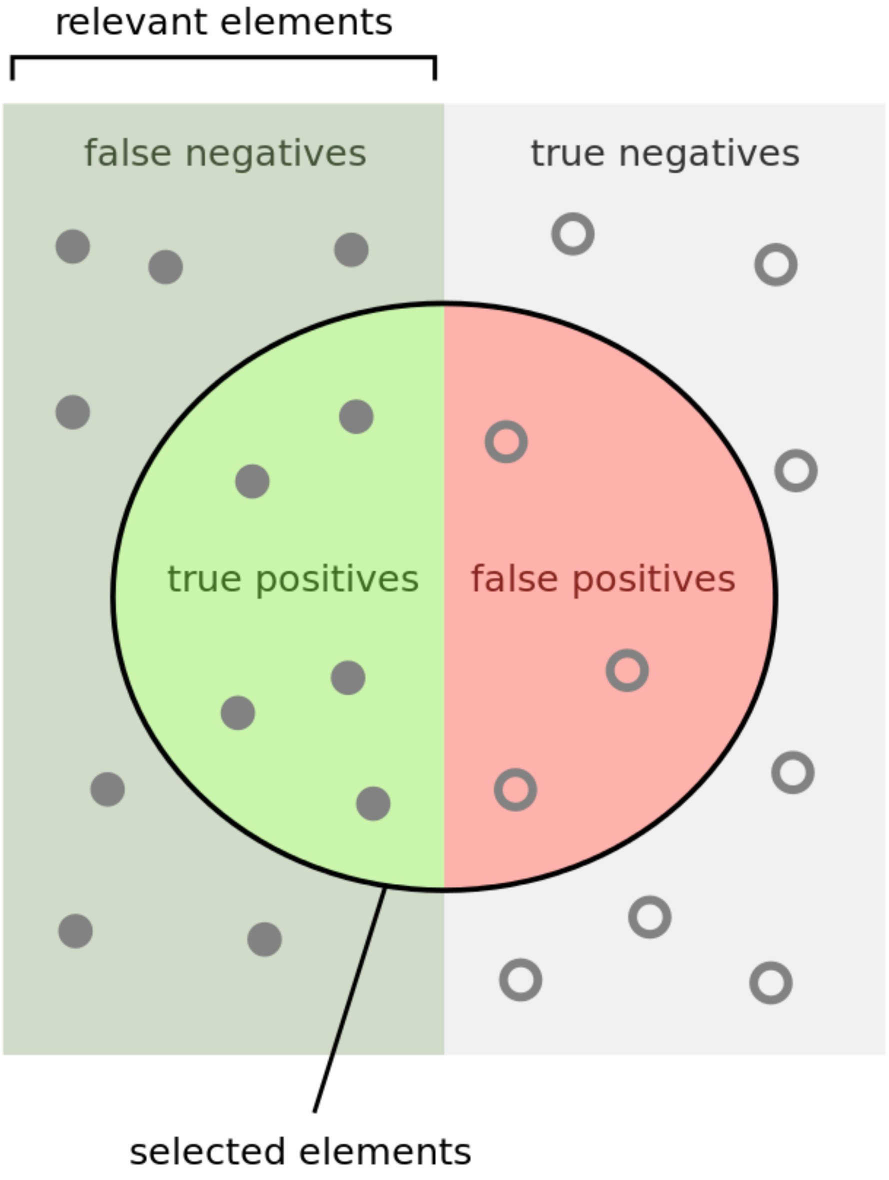
**Accuracy of a trivial classifier is: 16/20 = 80%**

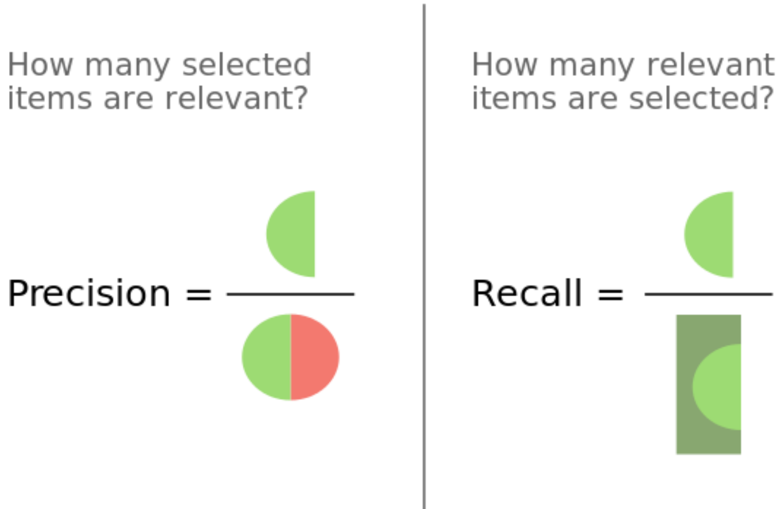
# Precision and recall

- Example: when a search engine returns 30 pages only 20 of which were relevant while failing to return 40 additional relevant pages, its precision is 20/30 = 2/3 while its recall is 20/60 = 1/3.

$$\text{recall} = \frac{\text{tp}}{\text{fn} + \text{tp}}$$

$$\text{precision} = \frac{\text{tp}}{\text{fp} + \text{tp}}$$




How many selected items are relevant?
Precision =
How many relevant items are selected?
Recall =

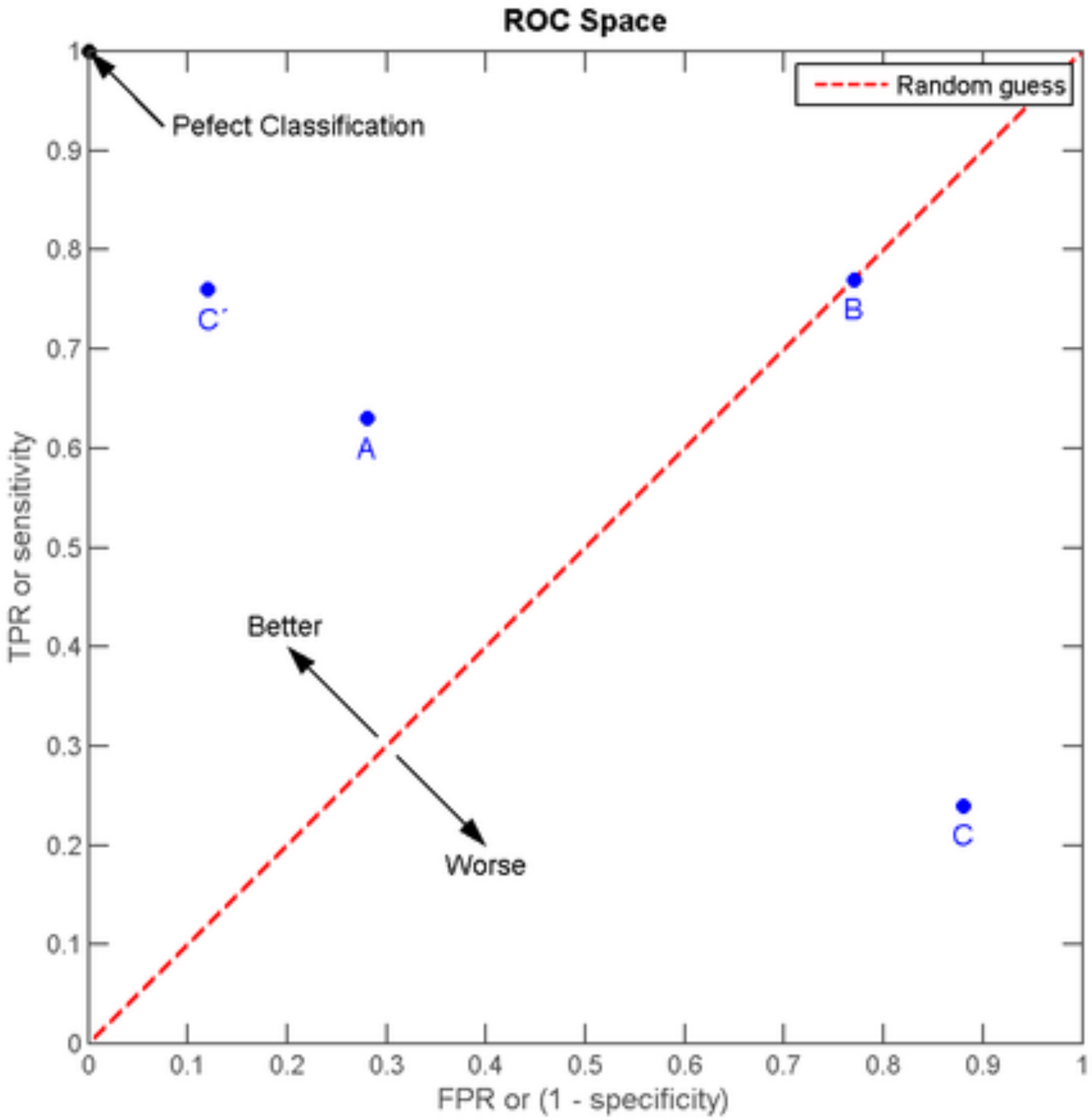
# TPR and FPR

- TPR = Recall = TP/(FN + TP) = TP/NumPositives
  - True Positive Rate

- FPR = Recall = FP/(FP + TN) = FP/NumNegatives
  - False Positive Rate

# ROC space

Predict positive if
p(y=1|x) > threshold

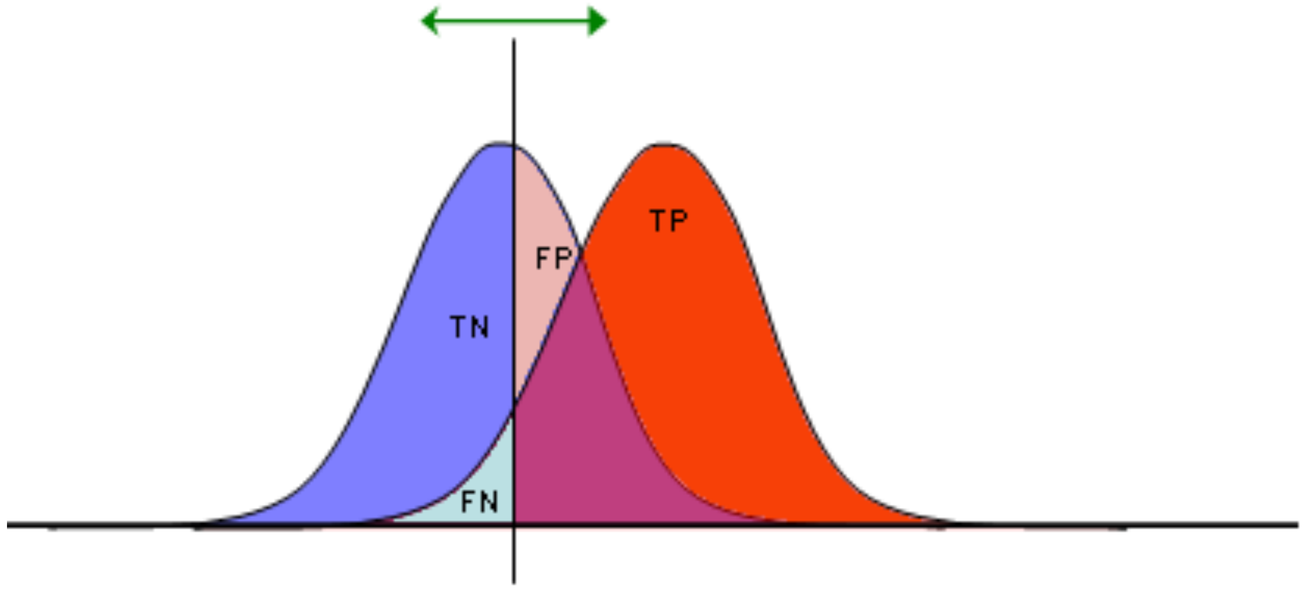


Threshold = 0

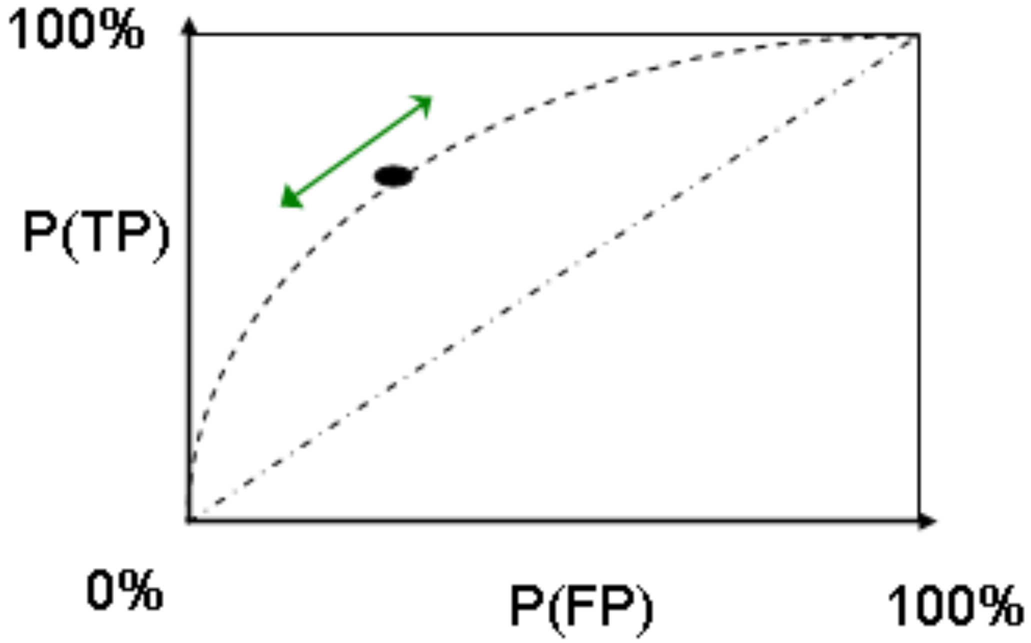
Threshold = 1

# ROC Curve example

e.g., diseased people, healthy people
blood protein levels normally distributed
Parameter that changes: threshold

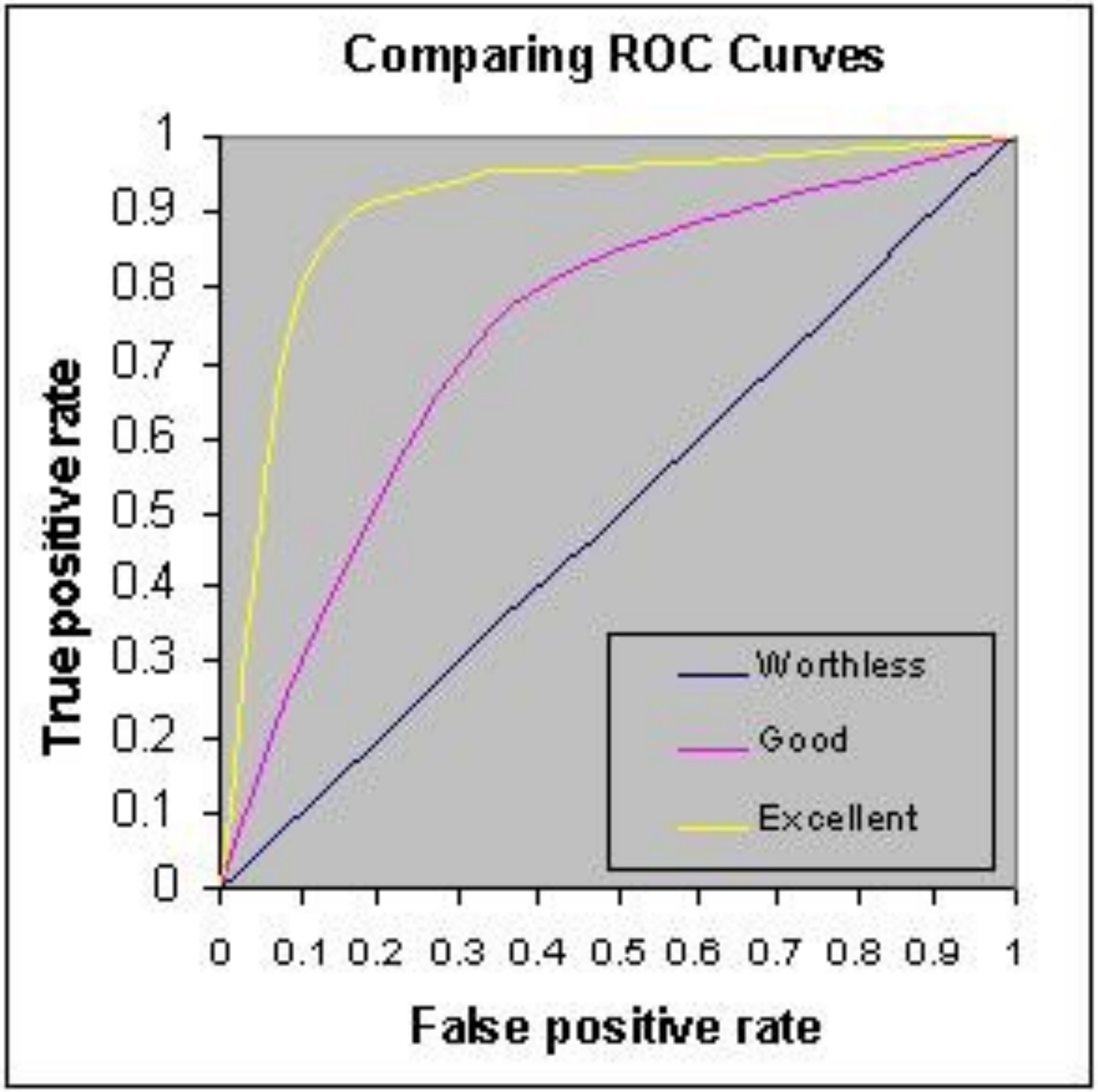


| | |
|---|---|
| TP | FP |
| FN | TN |
| 1 | 1 |



# ROC Curve

Predict positive if
$p(y=1|x) >$ threshold



Threshold = 0

Threshold = 1

# Area under the curve

- AUC or AUCROC gives the area under the ROC curve
- AUC is equal to the probability that a classifier will rank a randomly chosen positive instance higher than a randomly chosen negative one
- Some issues in using AUC to compare classifiers
    - see “Measuring classifier performance: a coherent alternative to the area under the ROC curve”, Hand, JMLR, 2009
    - can give unequal important to a FPR or TPR for different classifiers
    - see also Rob Holte’s nice work on Cost Curves: https://webdocs.cs.ualberta.ca/~holte/CostCurves/

# Statistical significant test

- Can the observed results be attributed to real characteristics of the learner under scrutiny or are they observed by chance?

- Hypothesis testing:
    - State a null hypothesis, e.g., the expected errors of two classifiers is equivalent
    - Choose a statistical significance test to reject the null hypothesis; failing to reject the null hypothesis does not mean we accept it
    - Rejecting the null hypothesis gives us some confidence in the belief that our observations did not occur merely by chance.

# Types of errors

- Type 1 error: rejecting the null hypothesis when it is true
  - could occur if you select alpha too large (e.g., alpha = 0.05)
  - could occur if you violate assumptions, e.g., equal variances
- Type 2 error: failure to reject the null hypothesis when it is false
  - these usually occur if we select a test with insufficient power, e.g., just checking if intervals overlap

# Recall our sampling approaches

- k-fold cross validation
- Monte carlo CV
- For internal validation, common to use a single validation set or use k-fold cross validation

# Monte carlo CV

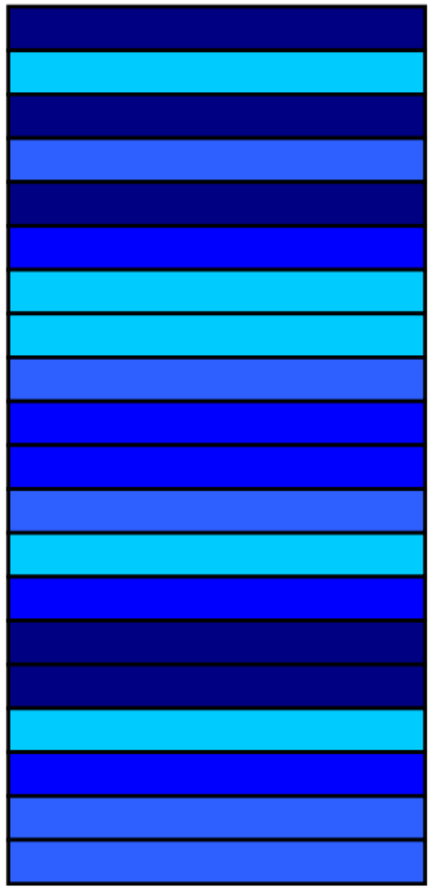
- Also called “repeated learning testing-model” or repeated random subsampling
- Randomly sample without replacement the training set and the test set
    - or for smaller datasets, first sample the training set and use the rest for test
- Repeat this random subsample m times to obtain m training/ test splits

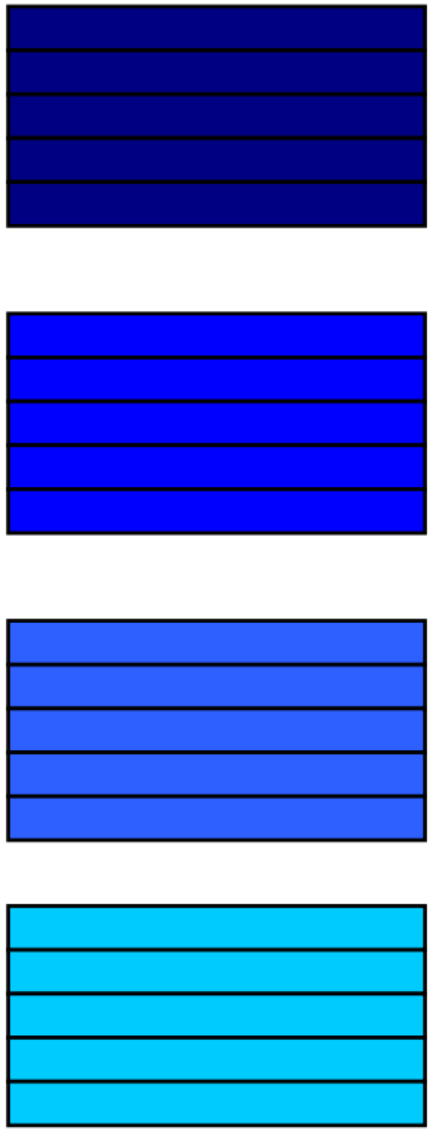
# k-fold CV

**Randomly and evenly split into 4 non-overlapping partitions**

***D***

**20 data points**





**Partition 1.**

**Data points: 1, 3, 5, 15, 16**

**Partition 2.**

**Data points: 6, 10, 11, 14, 17**

**Partition 3.**

**Data points: 4, 9, 12, 19, 20**

**Partition 4.**

**Data points: 2, 7, 8, 13, 17**

- Learn model on k-1 folds and test on the hold-out fold (done k times); average k error estimates

# Bias for k-fold CV

- Train on k-1 folds, test on the other
- Each training set is only (k-1)/k as a big as the original training set; eventually, though, we will train on the entire set
  - wait, why not just remove this bias by training on only k-1 folds?
- Will this bias the estimated prediction error to be higher or lower than the true expected error?
- Bias is minimized when k = n (leave-one-out), but can give a high-variance estimate of error (still a debate on this)
- k = 5 or 10 is an in-between that balances this bias-variance and training time

# What does this tell us about a single train-validation split?

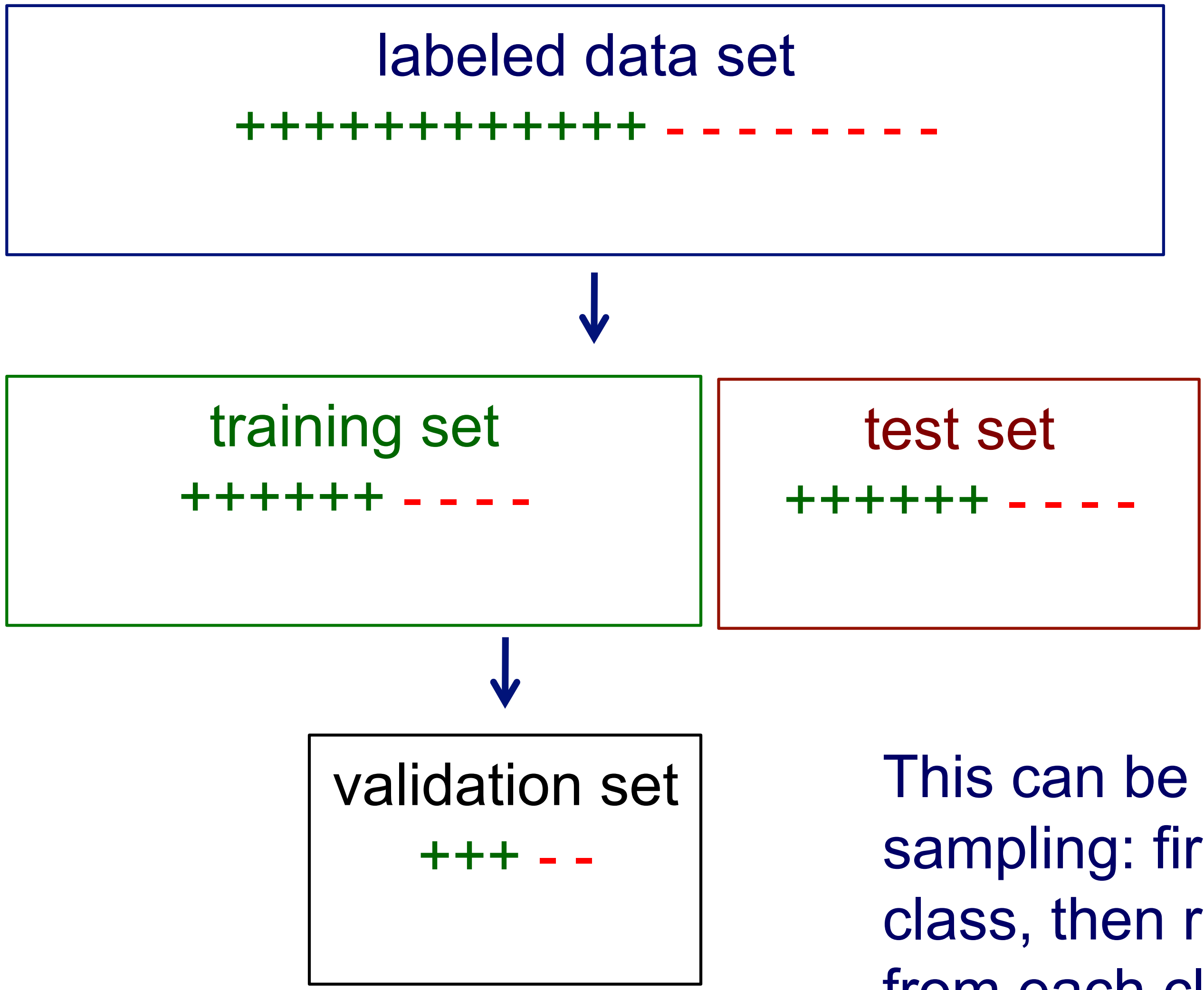
- A single split, to put aside one validation set, is almost like k-fold cross validation with k = 2
  - though, we only actually train on one fold and test on the other
- This is likely to have higher bias, and over-estimate the true expected error (pessimistic bias)

# LOOCV

- Why could this give a high-variance estimate?
    - i.e., if we saw a different training set, the estimate could be quite different
- Its too much like having one training set, and one test set
    - large correlation between k learned models
- Can overfit parameter selection to this one training set, and can find spurious connections to test set
    - find the parameters that are the best for this training set
    - if you had a different training set, maybe different parameters
    - k-fold for smaller k really does learn k models that are more significantly different, picking parameters that are "good" across training sets you could see

# Stratified sampling

- When randomly selecting training or validation sets, we may want to ensure that class proportions are maintained in each selected set



labeled data set

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

training set

++++++ - - - -

test set

++++++ - - - -

validation set

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This can be done via stratified sampling: first stratify instances by class, then randomly select instances from each class proportionally.

# Which sampling approach should I use?

- No definitive answer, mostly empirical support
- For how to select k, bias-variance trade-off
  - for small k, high-bias and low-variance
  - for large k, low bias but high variance (e.g., leave-one-out)
  - Some experiments showing that a reasonable balance is k = 10
  - Also determined by computational resources; large k expensive
- For how to select between sampling methods,
  - repeated CV and Monte Carlo CV shown to have fewer Type 1 errors
- Criteria for internal and external CV may be quite different

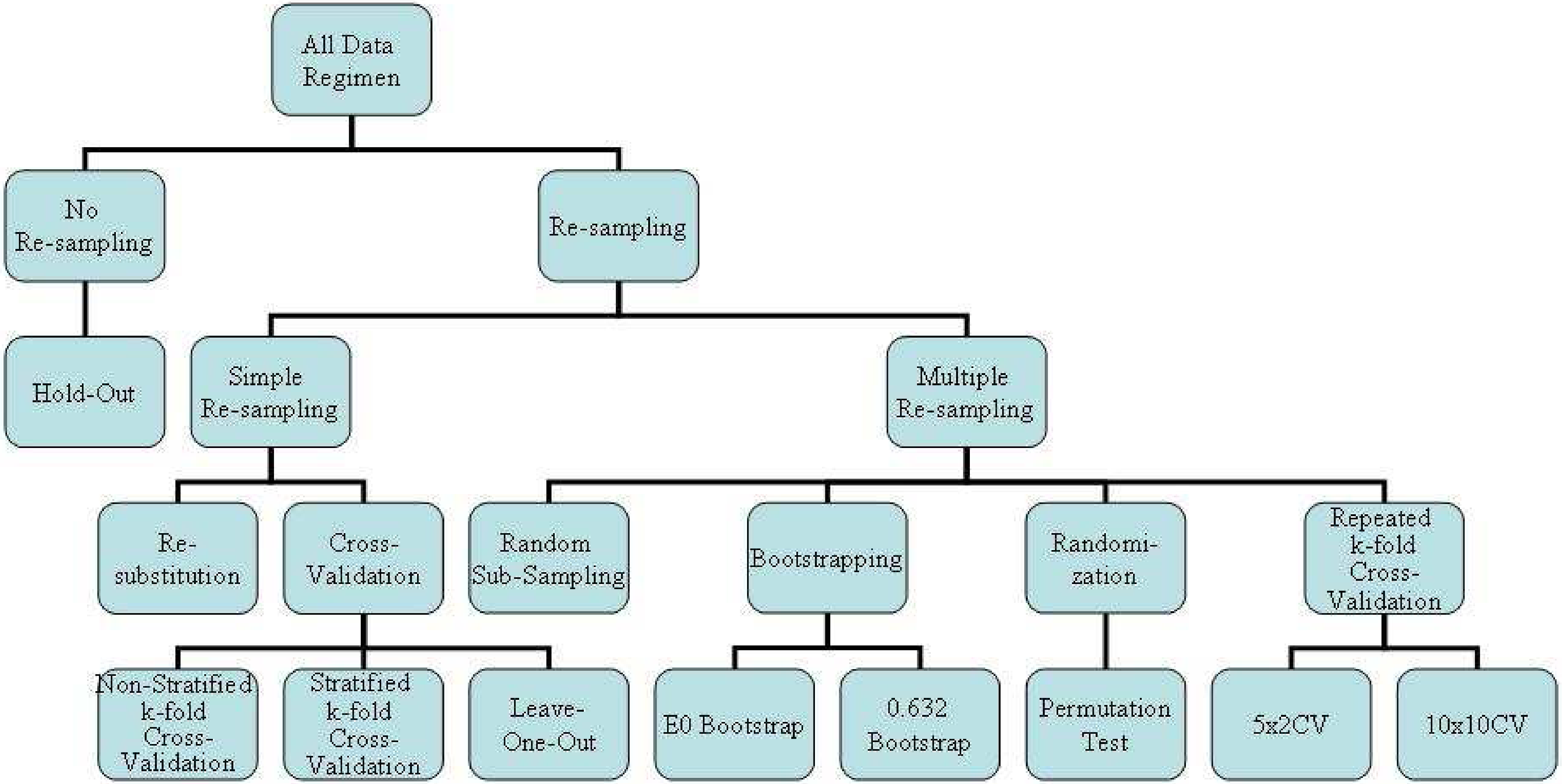
# Internal

- Training k models can be expensive; want smaller k
- k-fold CV a reasonable choice because gives an almost unbiased estimate of accuracy

# External

- Want to use hypothesis testing, e.g., Null Hypothesis is that the means of these two algorithms is the same
- Want a sampling technique that has less Type 1 errors
- Assumptions require independent samples of error, but empirically k-fold is not necessarily better than repeated sampling

# Re-sampling summary



# Experiments

- “What if I cannot find any difference between the algorithms?”
    - If you ran a fair experiment, with lots of repetitions (random splits of training and test) to get a large enough number of samples of the error, then that is a fine result
    - Remember that algorithms have many parameters that can strongly affect their performance
- “How do I select parameter ranges?”
    - the best is to provide a large enough range; this can be slow
- “Do I have to sweep all parameters in the CV?”
    - No, but remember that any choice of parameters affects your conclusion —> it is much less interesting to conclude that linear regression with regularization weight = 0.1 is outperformed by Poisson regression

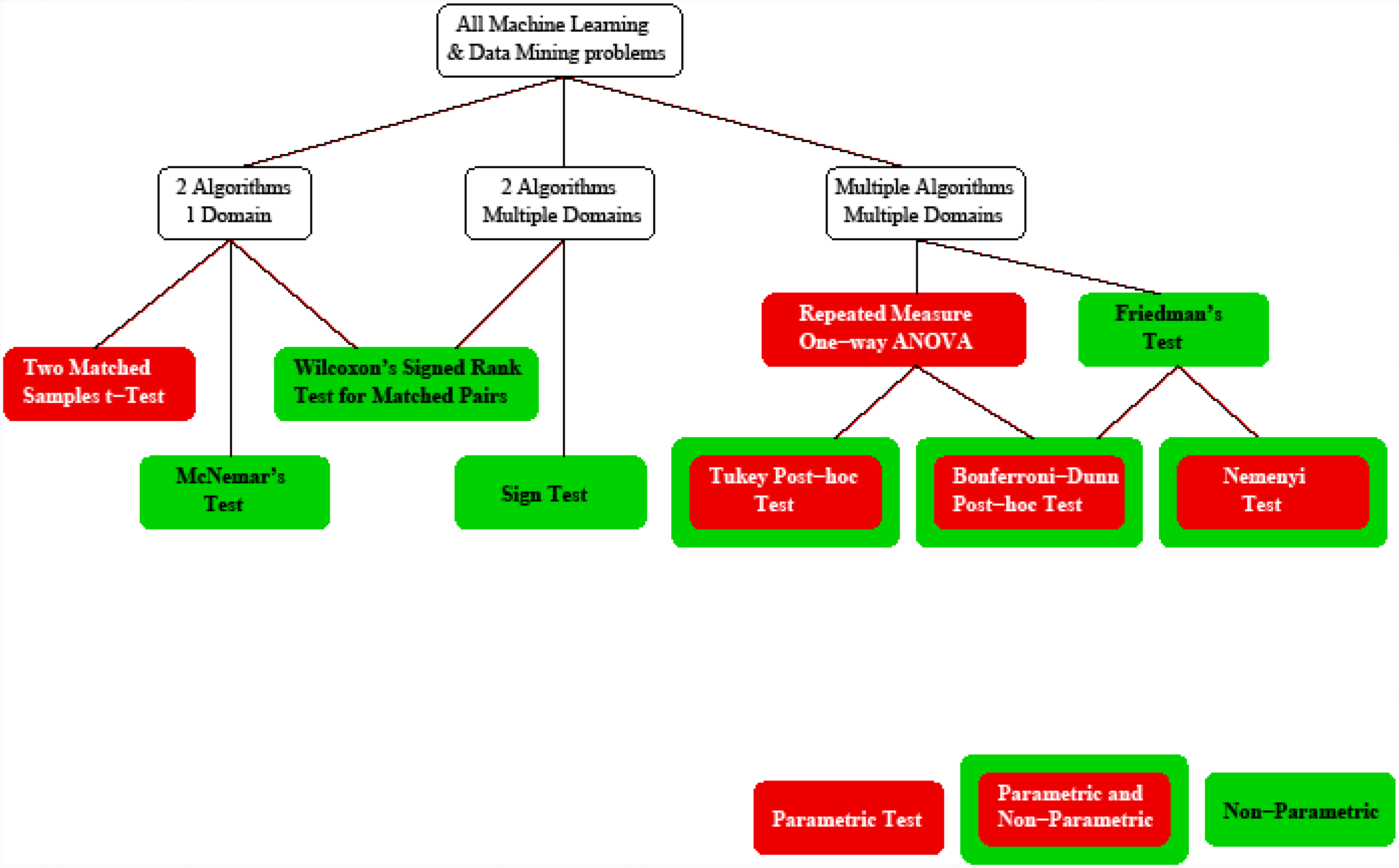
# Avoiding meta-parameters

- Other strategies to select meta-parameters, rather than letting data tell you the choice
- We have mathematical characterizations of generalization
- These allow some development of criteria to adjust training error
  - e.g., AIC criterion

# How to choose significance tests?

- Try to satisfy assumptions and use some rules of thumb
- Parametric statistical tests make stronger assumptions about the distribution of the data
- Non-parametric tests make weaker assumptions, but are less powerful (less able to reject the null hypothesis when it is false)
- Selection based on type of problem
  - comparing 2 algorithms on a single domain
  - comparing 2 algorithms across domains
  - comparing multiple algorithms across domains

# Statistical test summary



All Machine Learning & Data Mining problems

2 Algorithms 1 Domain

2 Algorithms Multiple Domains

Multiple Algorithms Multiple Domains

Two Matched Samples t–Test

McNemar's Test

Wilcoxon's Signed Rank Test for Matched Pairs

Sign Test

Repeated Measure One–way ANOVA

Friedman's Test

Tukey Post–hoc Test

Bonferroni–Dunn Post–hoc Test

Nemenyi Test

Parametric Test

Parametric and Non–Parametric

Non–Parametric

# Assumptions of the t-test

- The Normality or Pseudo-Normality Assumption: samples come from normally distributed population (the sample size of the testing set should be greater than 30, though this does not give a guarantee).

- The Randomness of the Samples: The sample should be representative of the underlying population. Therefore, the instances of the testing set should be randomly chosen from their underlying distribution.

- Equal Variance of the populations: The two samples come from populations with equal variance.

# Example where assumptions of t-test violated

- Equal Variance: variance of C4.5 and NB cannot be considered equal.

- Not warranted to use the t-test to compare C4.5 to NB on the Labour data.

- A better test to use is
  - Welch’s t-test
  - non-parametric alternative, McNemar’s Test

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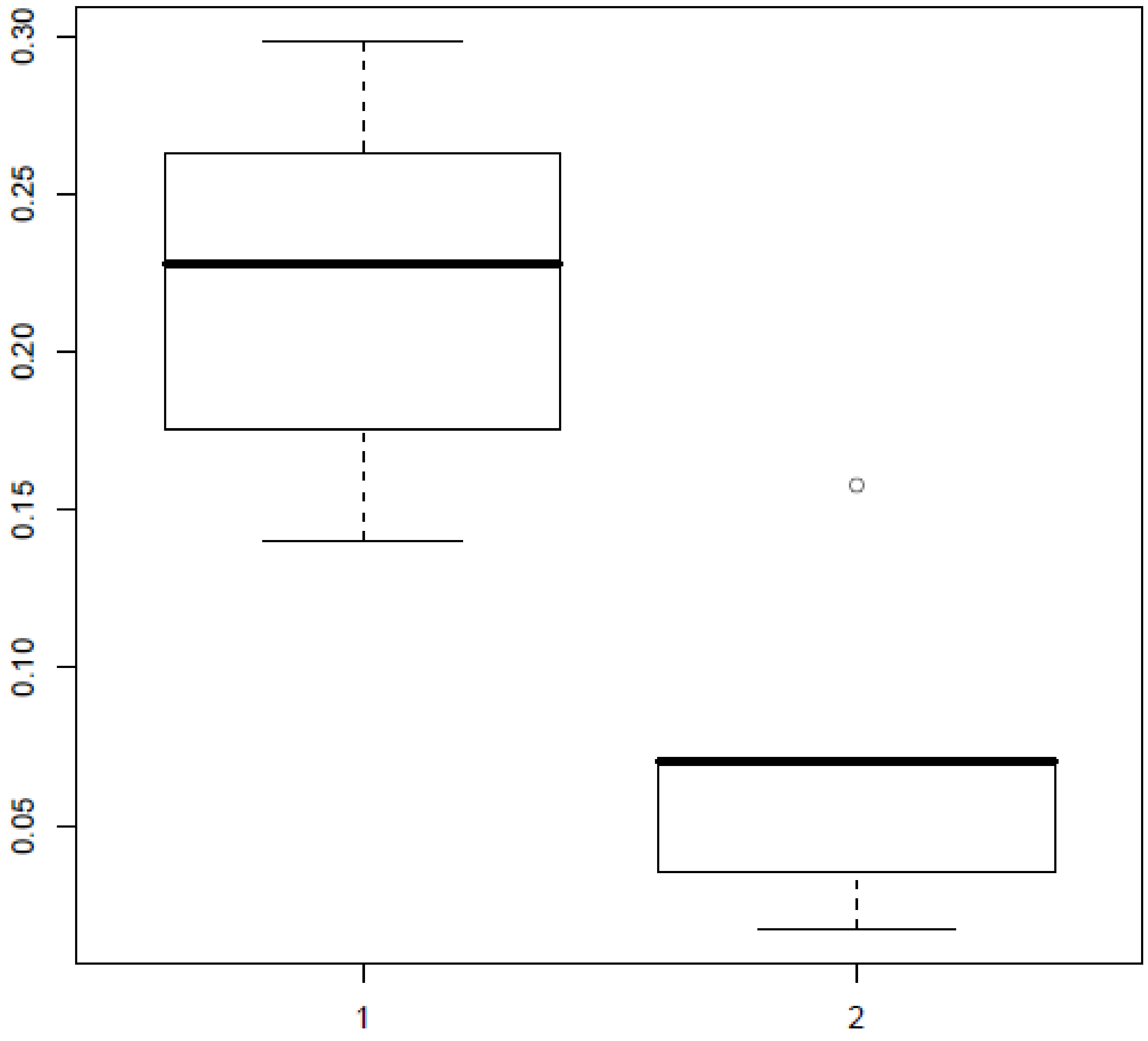

# One-tailed versus two-tailed

- One-sided question: is algorithm 1 better than algorithm 2?
- Two-sided question: are algorithm 1 and 2 two different?
  - i.e., either could be better
- Usually we care about one-sided
  - p = Pr (T > t), where T is a random variable
  - for paired t-test, little t reflects the average difference scaled by variance and samples
  - t = average difference / [ sample std deviation x sqrt(numsamples)]

# Whiteboard

- Statistical significance tests
- Rademacher complexity