Accuracy, Cross-Validation, Overfitting, and ROC

Slides adopted from Data Mining for Business Analytics

Stern School of Business
New York University
Spring 2014

Evaluation

How do we measure generalization performance?

Evaluating Classifiers: Plain Accuracy

$$\text{Accuracy} = \frac{\text{Number of correct decisions made}}{\text{Total number of decisions made}}$$

$$= 1 - \text{error rate}$$

- *Too* simplistic..

Evaluating Classifiers: The Confusion Matrix

- A confusion matrix for a problem involving n classes is an $n \times n$ matrix,
  - with the columns labeled with actual classes and the rows labeled with predicted classes
- It separates out the decisions made by the classifier,
  - making explicit how one class is being confused for another

Actual class

Predicted class

	p	n
Y	True Positives	False Positives
N	False Negatives	True Negatives

$FPR = FP/(FP+TN)$.

- The errors of the classifier are the false positives and false negatives

Building a Confusion Matrix

1: Default
0: No Default

Actual Class	Predicted Class
0	0
1	1
0	1
0	1
0	0
1	1
0	0
0	0
1	1
1	0

Actual class

Predicted class

	Default (1)	No Default(0)	Total
Default (1)	3	2	5
No Default (0)	1	4	5
Total	4	6	10

Other Evaluation Metrics

- Precision $= \frac{TP}{TP+FP}$: out of all *reported* positives, how many percent were true positives.
- FPR = FP/(FP+TN): out of all ground-truth negatives, how many percent were false positives
- Recall $= \frac{TP}{TP+FN}$: out of all ground-truth positives, how many percent were true positives
- TPR = TP/(TP+FN)=Recall
- F_1−measure (F_1-score) $= 2\times\frac{\text{precision}\times\text{recall}}{\text{precision}+\text{recall}}$

F_β [edit]

A more general F score, F_β, that uses a positive real factor β, where β is chosen such that recall is considered β times as important as precision, is:

$$F_\beta = (1+\beta^2)\cdot\frac{\text{precision}\cdot\text{recall}}{(\beta^2\cdot\text{precision})+\text{recall}}.$$

Over-fitting the data

- Finding chance occurrences in data that look like interesting patterns, but which do not generalize, is called over-fitting the data

- We want models to apply not just to the exact training set but to the general population from which the training data came
  - Generalization

Over-fitting

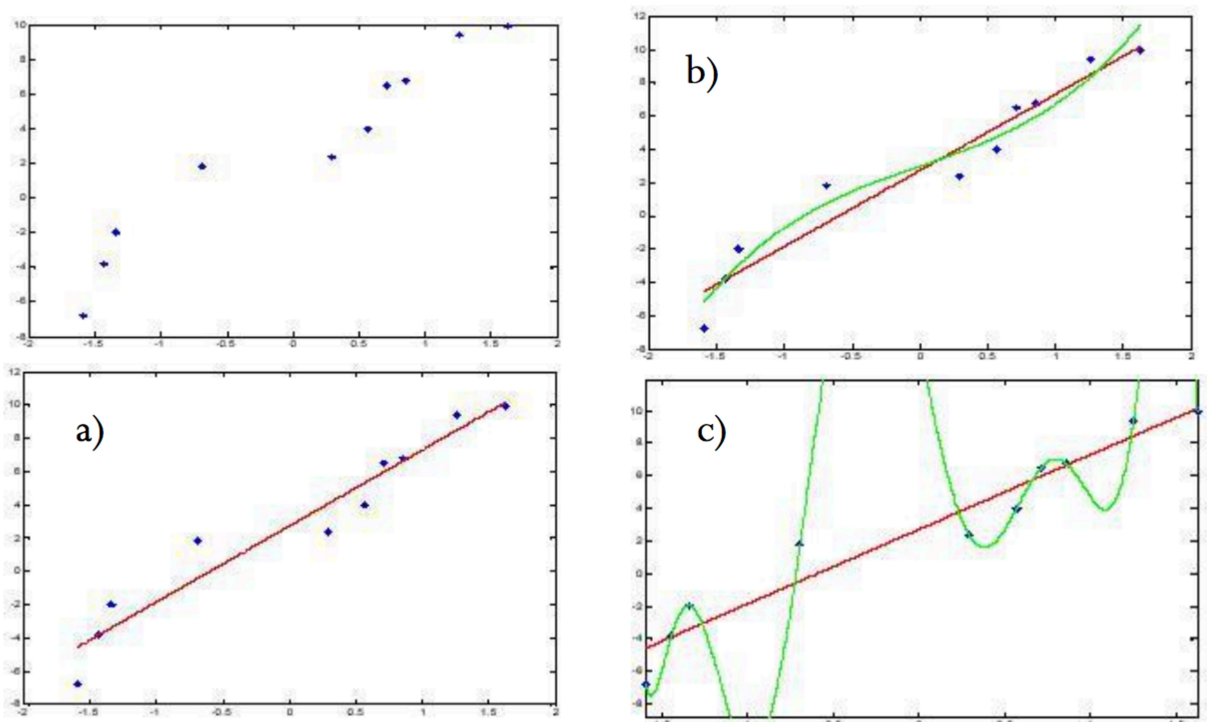
- The tendency of DM procedures to tailor models to the training data, *at the expense of generalization* to previously unseen data points.

- All data mining procedures have the tendency to over-fit to some extent
  - Some more than others.

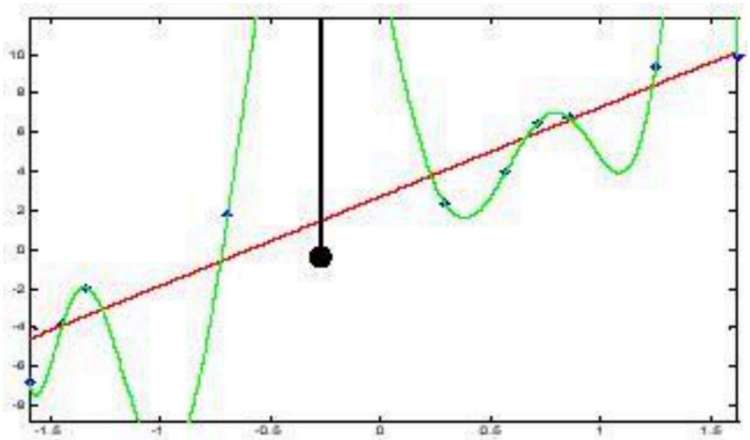
- "If you torture the data long enough, it will confess"

- There is no single choice or procedure that will eliminate over-fitting
  - recognize over-fitting and manage complexity in a principled way.

What's over-fitting ?



What's over-fitting ?



- $h \in H$ overfits training data if there's an alternative $h' \in H$ such that:

  $err_{train}(h) < err_{train}(h')$

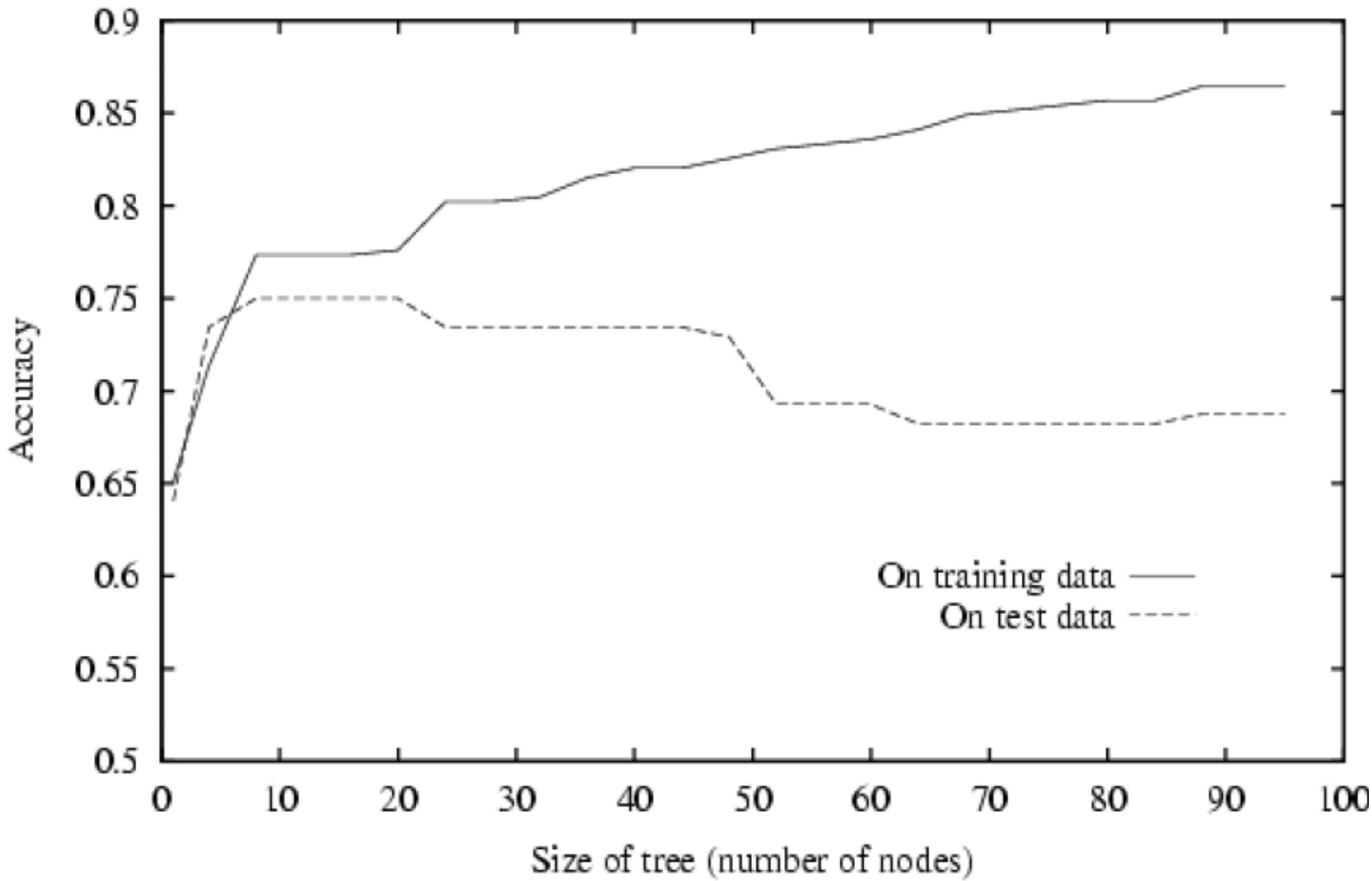
  AND

  $err_{test}(h) > err_{test}(h')$

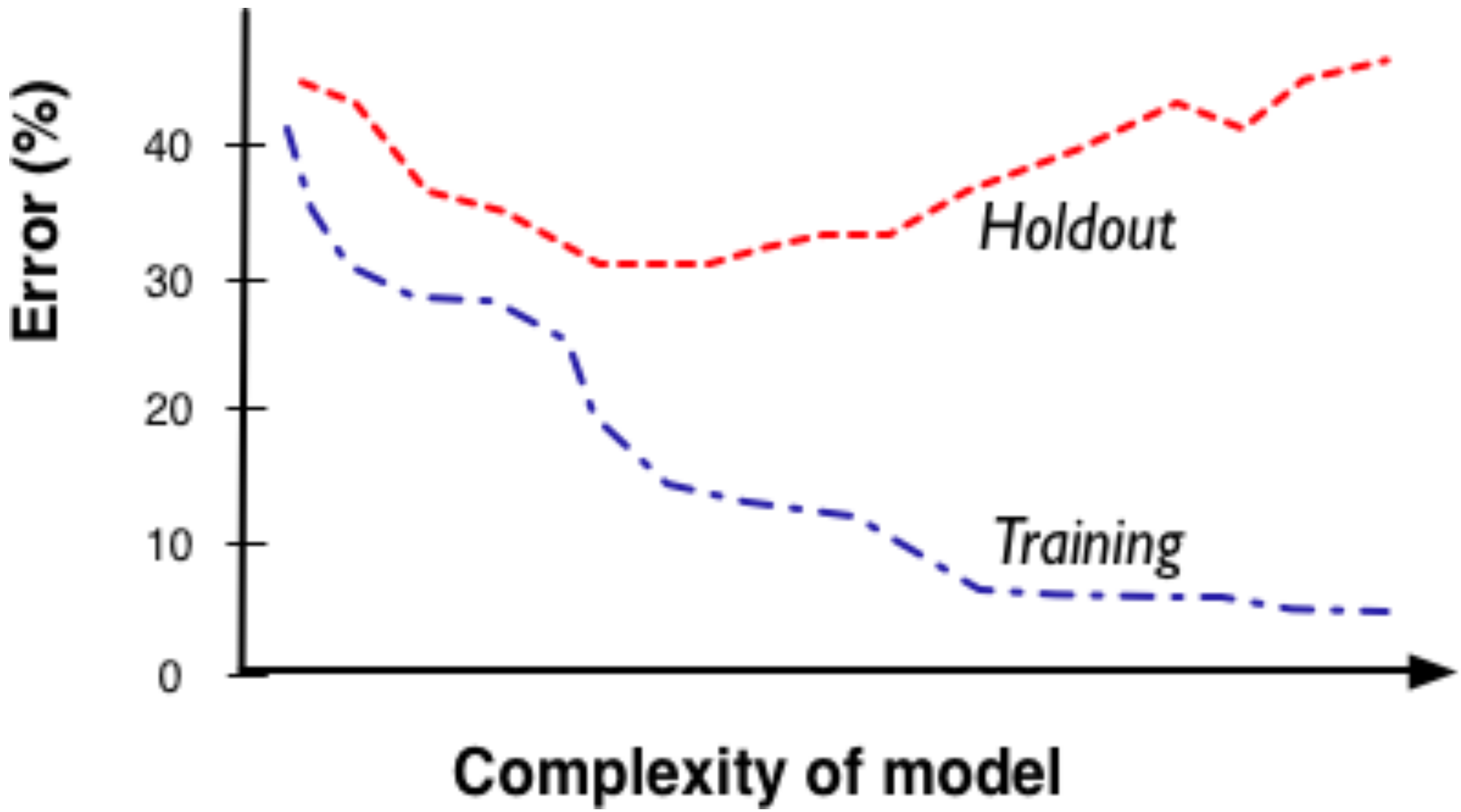
An example of over-fitting in DTree

- Each leaf corresponds to a single training point and the full tree is merely a convenient implementation of a lookup table

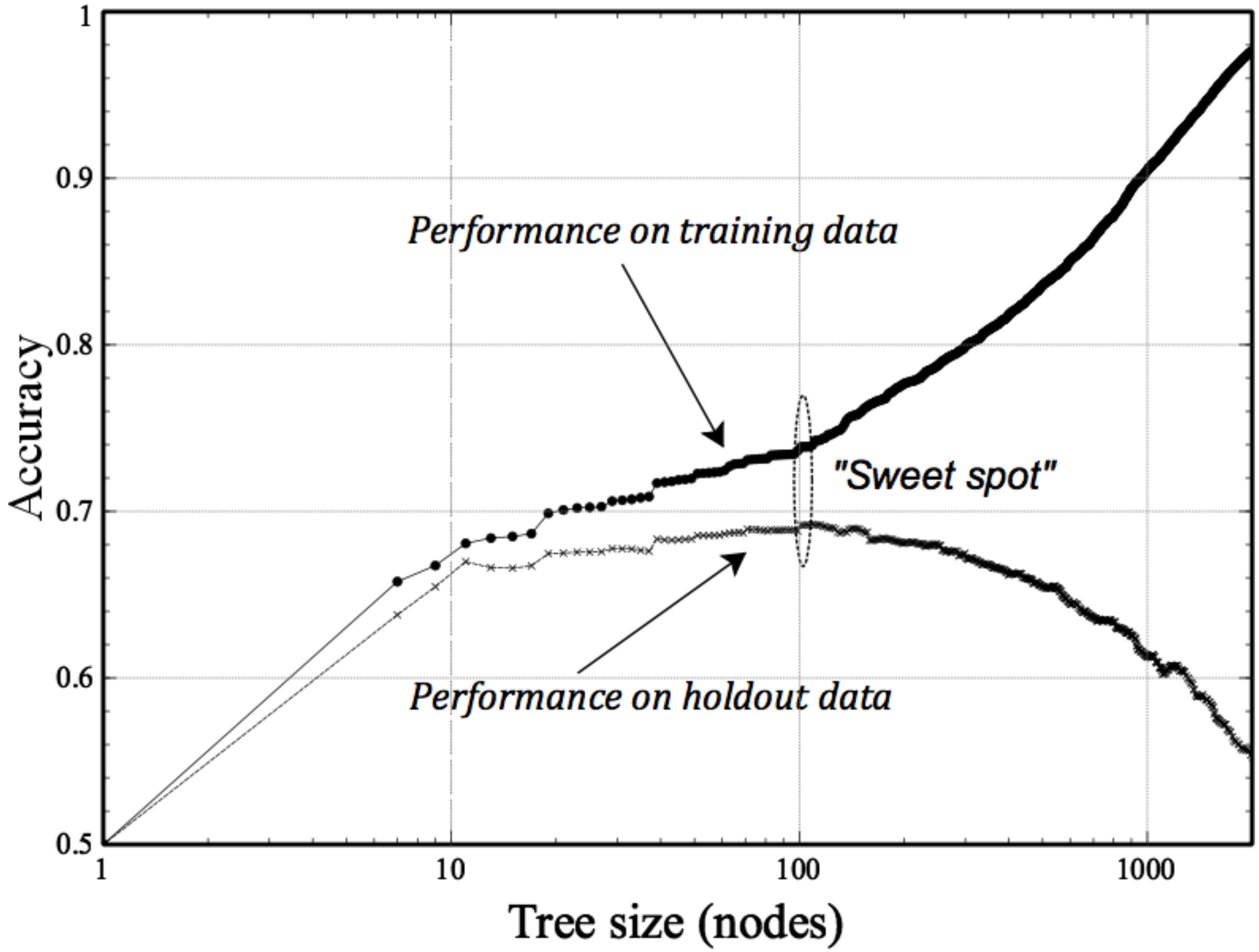
Tree Complexity and Over-fitting



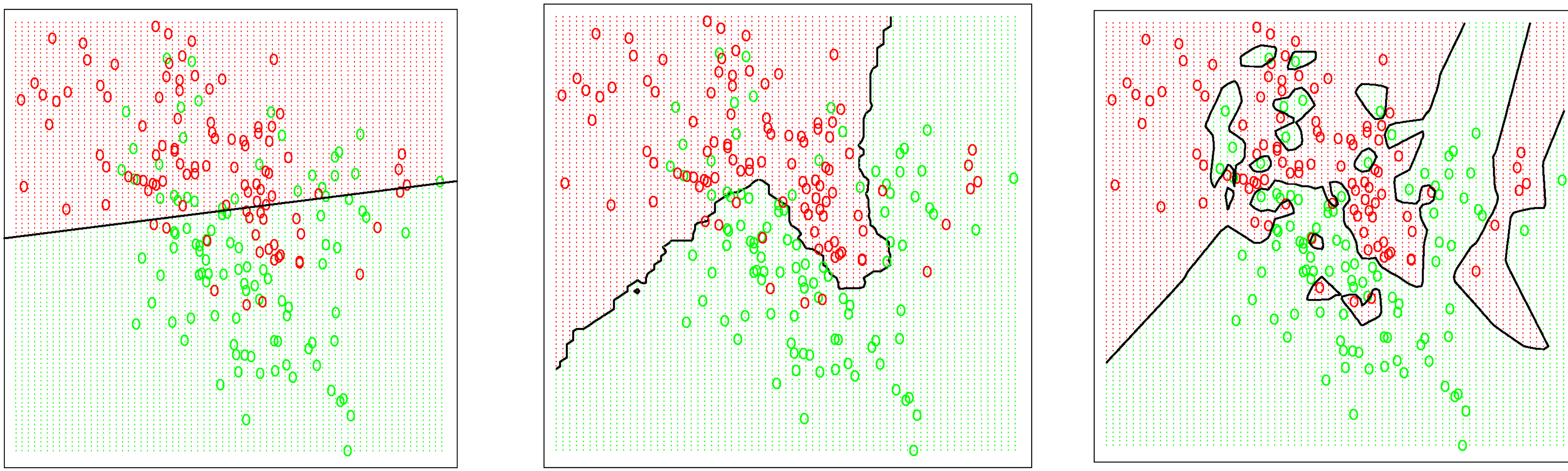
Fitting Graph



Over-fitting in tree induction



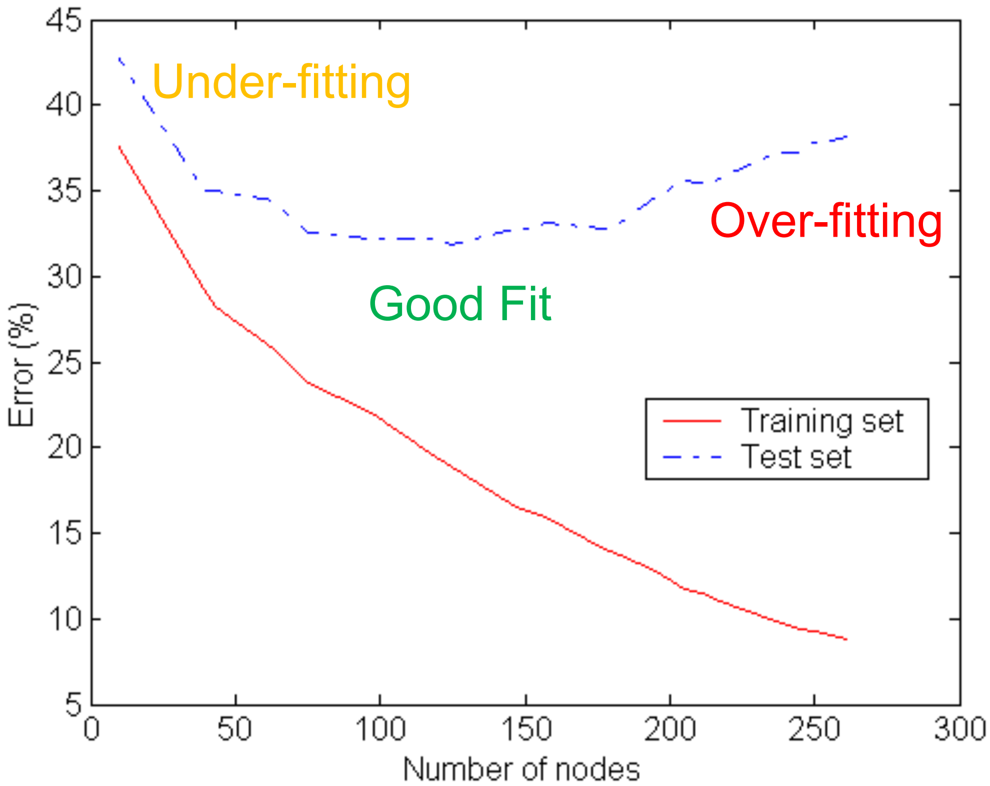
Need for holdout evaluation



Under-fitting Good Over-fitting

- In sample evaluation is in favor or “memorizing”
- On the *training data* the right model would be best
- But on *new data* it would be bad

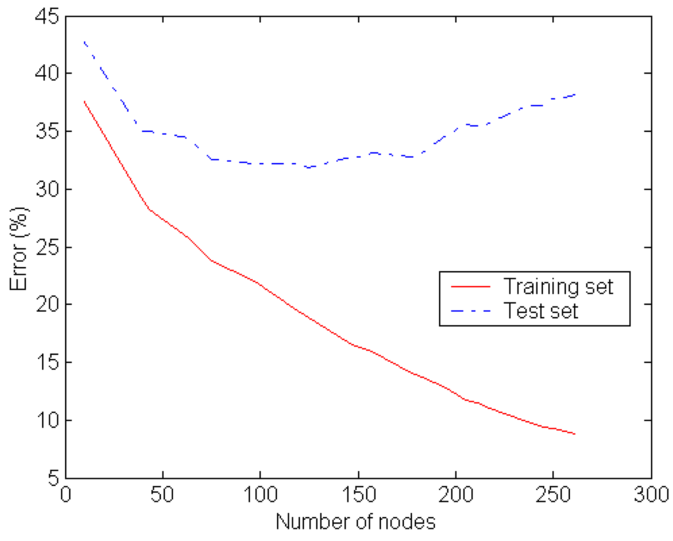
Over-fitting



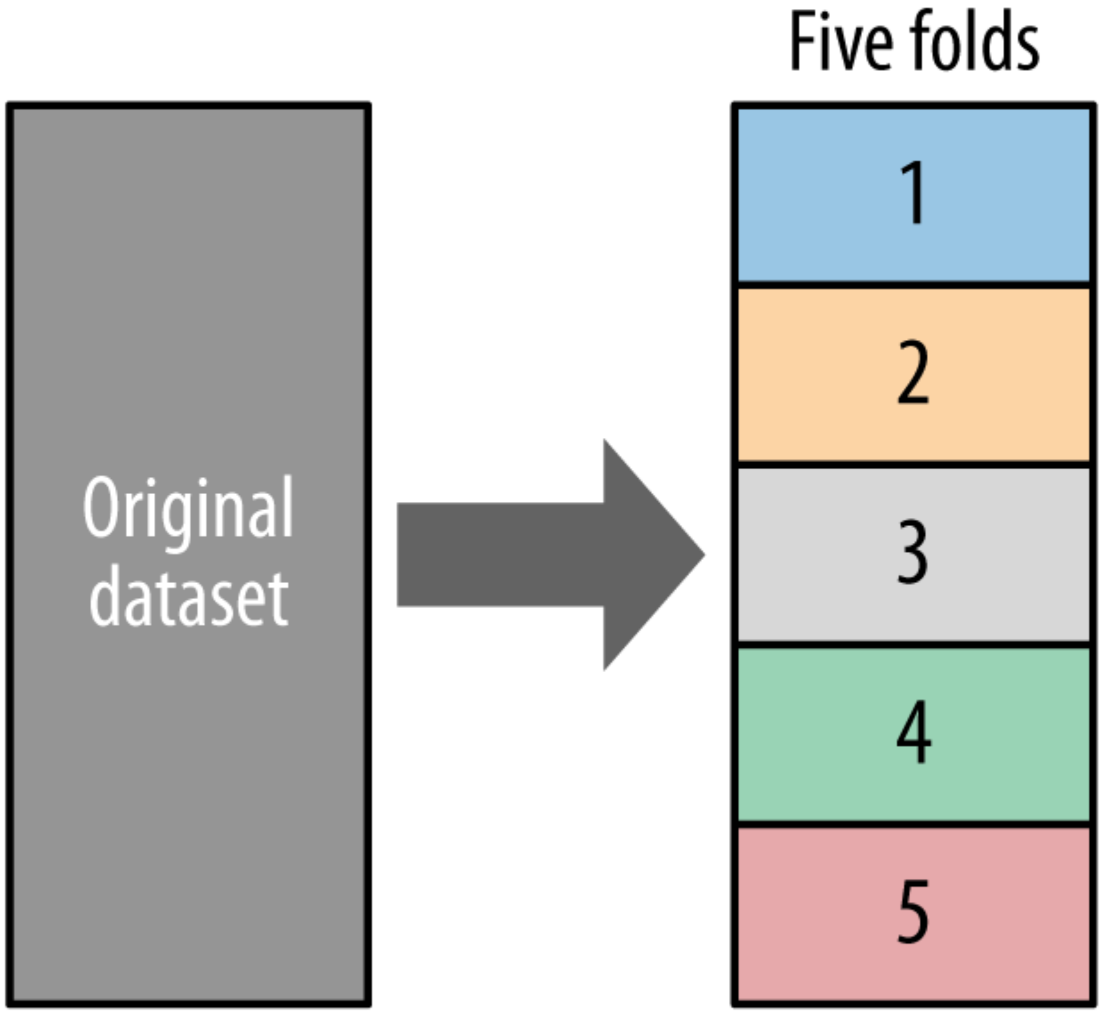
- Over-fitting: Model “memorizes” the properties of the particular training set rather than learning the underlying concept or phenomenon

Holdout validation

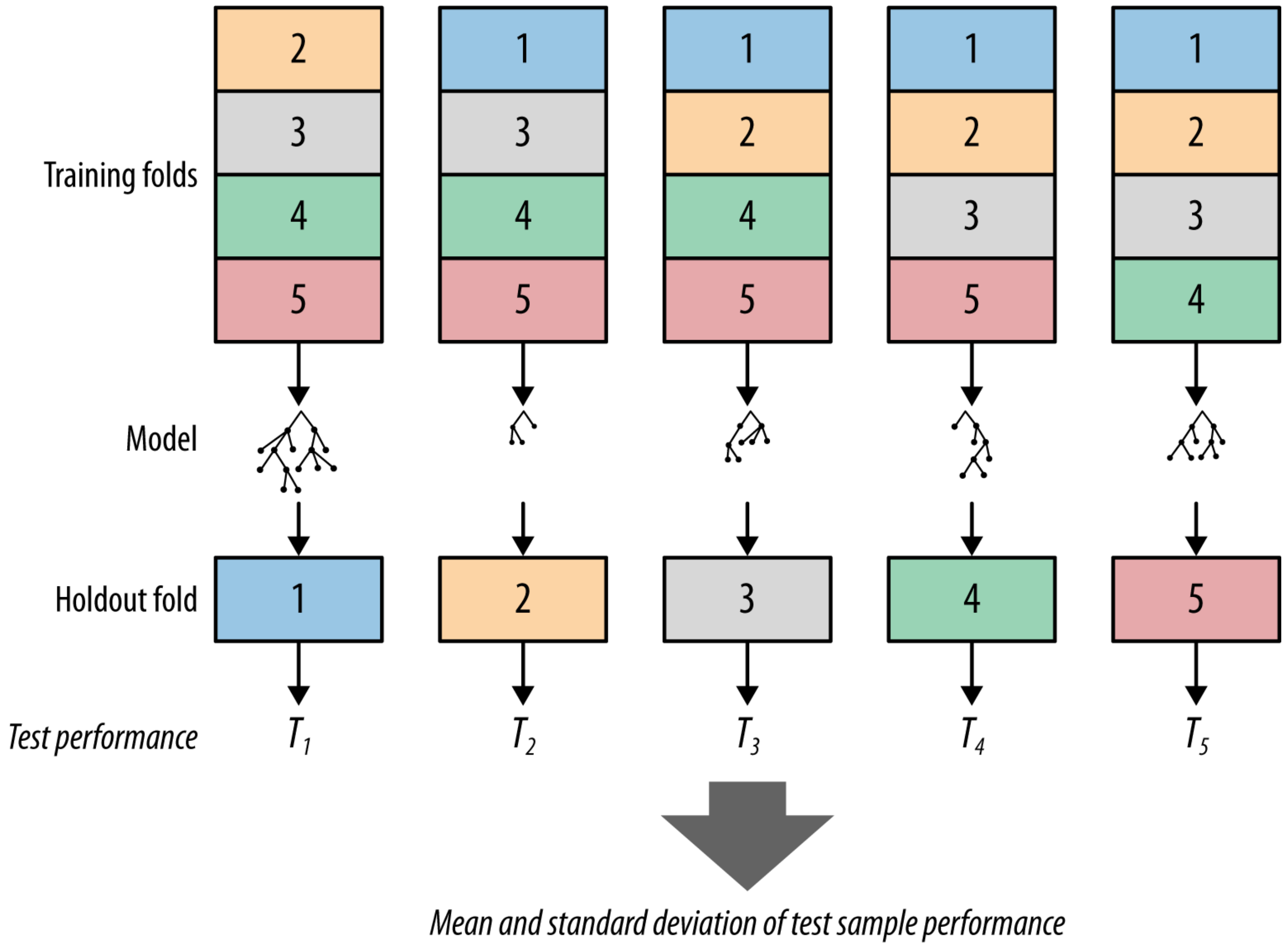
- We are interested in generalization
  - The performance on data not used for training
- Given only one data set, we hold out some data for evaluation
  - Holdout set for final evaluation is called the test set
- Accuracy on training data is sometimes called **“in-sample” accuracy**, vs. **“out-of-sample” accuracy** on test data



Cross-Validation



Cross-Validation



From Holdout Evaluation to Cross-Validation

- Not only a simple estimate of the generalization performance, but also some statistics on the estimated performance,
  - such as the mean and variance
- Better use of a limited dataset
  - Cross-validation computes its estimates over *all* the data
- Used for comparing different learning procedure
  - e.g. Decision Trees vs Logistic Regression
- Used for comparing hyper-parameters in a specific procedure
  - e.g. the maximum depth (minimum amount of data in the leaf node) of the decision tree.

Avoid over-fitting

- Two ways of avoid over-fitting for DTree
  I. Stop growing when data split not statistically significant (pre-pruning)
  II. Grow full tree, then post-pruning

For Option I:

Hard to estimate the size of the tree

Pre-Pruning: When to stop splitting (I) Number of instances

- Frequently, a node is not split further if
  - The number of training instances reaching a node is smaller than a certain percentage of the training set
    - (e.g. 5%)
  - Regardless the impurity or error.
  - Any decision based on too few instances causes variance and thus generalization error.

Pre-Pruning: When to stop splitting (2) Threshold of information gain value

- Set a small threshold value, splitting is stopped if

  $\Delta i(s) \leq \beta$

- Benefits: Use all the training data. Leaf nodes can lie in different levels of the tree.
- Drawback: Difficult to set a good threshold

Avoid over-fitting

- Two ways of avoid over-fitting for D-Tree

  I. Stop growing when data split not statistically significant (pre-pruning)

  II. Grow full tree, then post-pruning

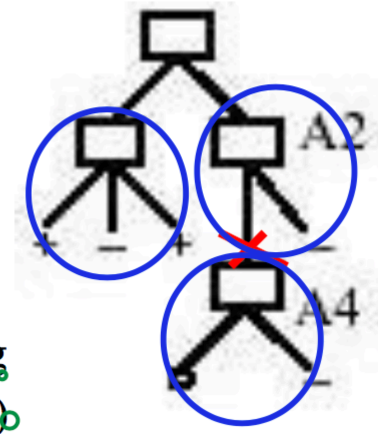
For option II:

- How to select "best" tree?
  - Measure performance over training data (statistical pruning)
    - Confidence level (will be introduced later)
  - Measure performance over separate validation data set
- MDL (Minimize Description Length 最小描述长度):

  minimize (*size*(tree) + *size*(misclassifications(tree)))

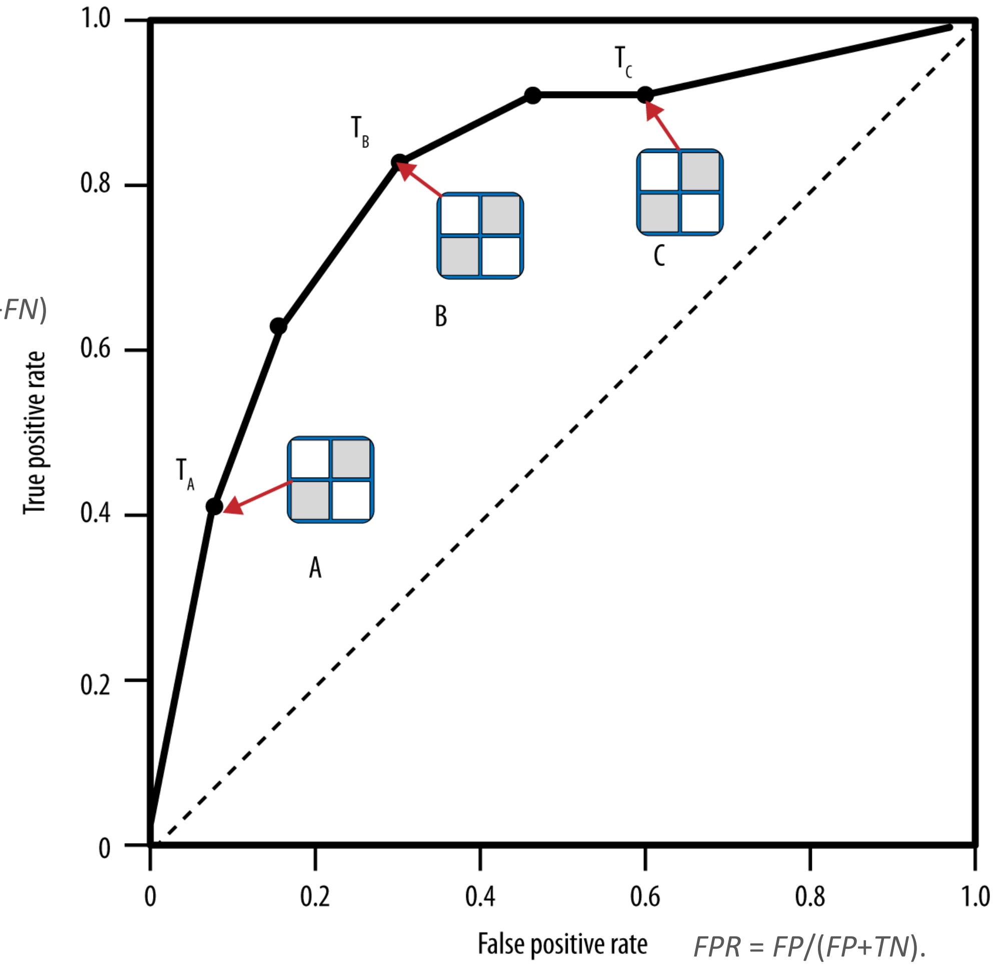
Post-pruning (1). Reduced-Error pruning

- Split data into training set and validation set
  - Validation set:
    - Known label
    - Test performance
    - No model updates during this test!
- Do until further pruning is harmful:
  - Evaluate impact on validation set of pruning each possible node (plus the subtree it roots)
  - Greedily remove the one that most improves validation set accuracy



How to assign the label of the new leaf node?

ROC Graphs and Curves



TPR = *TP*/(*TP*+*FN*)

FPR = *FP*/(*FP*+*TN*).

Generating ROC curve: Algorithm

- For each test, count the number of true positives TP (positives with prediction above the cutoff) and false positives FP (negatives above the cutoff)

- Calculate TP rate (TP/P) and FP (FP/N) rate

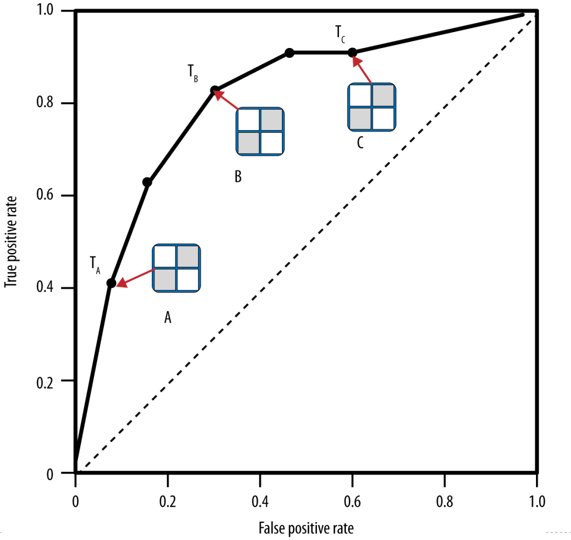
- Plot current number of TP/P as a function of current FP/N

ROC Graphs and Curves

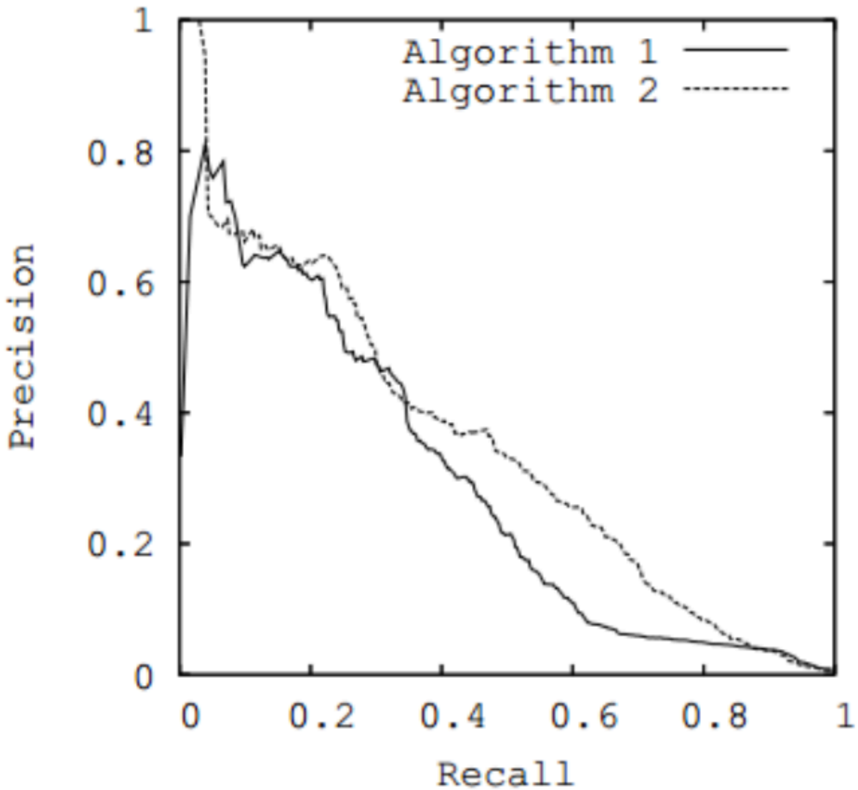
- ROC graphs decouple classifier performance from the conditions under which the classifiers will be used
- Not the most intuitive visualization for many business stakeholders

Area Under the ROC Curve (AUC)

- The area under a classifier's curve expressed as a fraction of the unit square
  - Its value ranges from zero to one
- The AUC is useful when a single number is needed to summarize performance, or when nothing is known about the operating conditions
  - A ROC curve provides more information than its area



P-R Curve: Tradeoff between Precision and Recall



- Precision $= \frac{TP}{TP+FP}$
- Recall $= \frac{TP}{TP+FN}$

AUPRC: Area under P-R Curve

Thanks!

Questions?