# Accuracy, Cross-Validation, Overfitting, and ROC

Slides adopted from Data Mining for Business Analytics

Stern School of Business
New York University
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# 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

| Default Truth | Model Prediction |
|---|---|
| 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 | No Default | Total |
|---|---|---|---|
| Default | 3 | 2 | 5 |
| No Default | 1 | 4 | 5 |
| Total | 4 | 6 | 10 |

# Other Evaluation Metrics

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

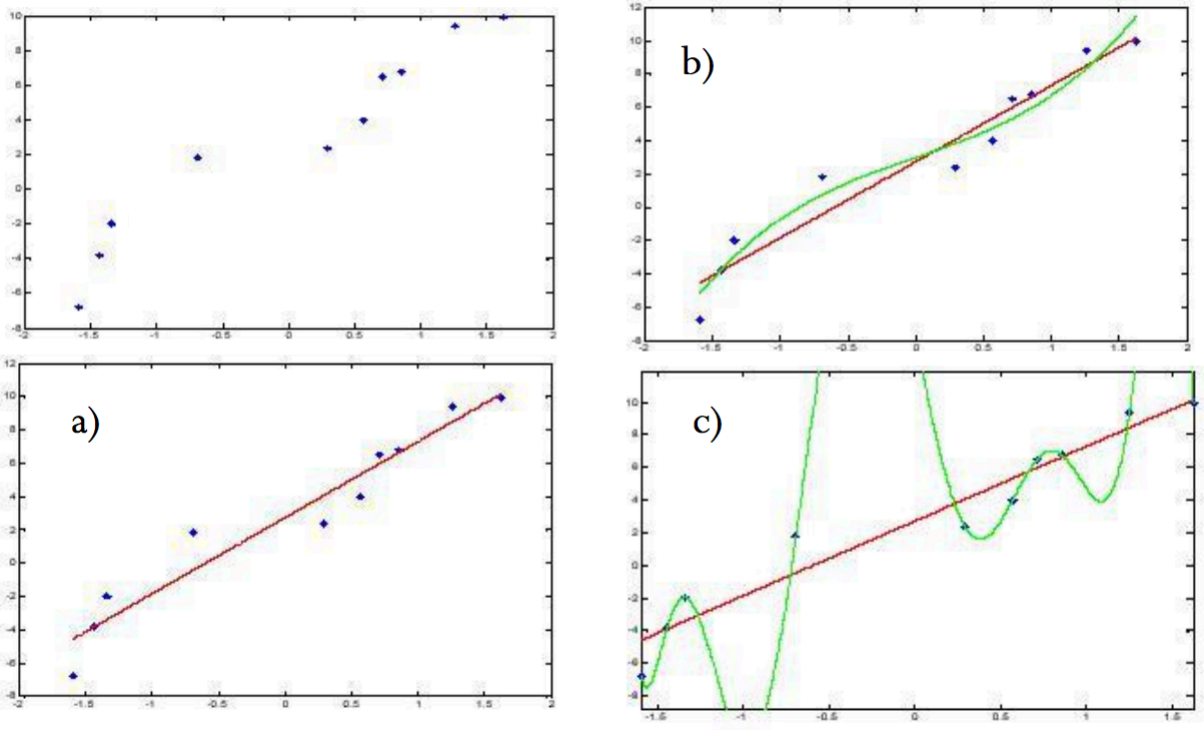
# Over-fitting the data

- 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

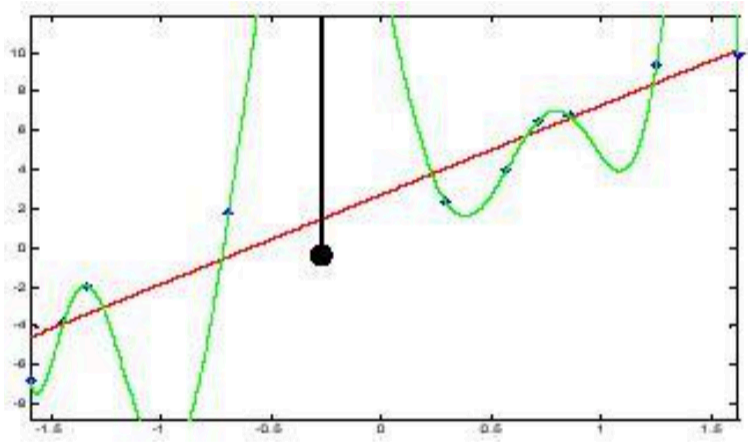
# Over-fitting

- 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:

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

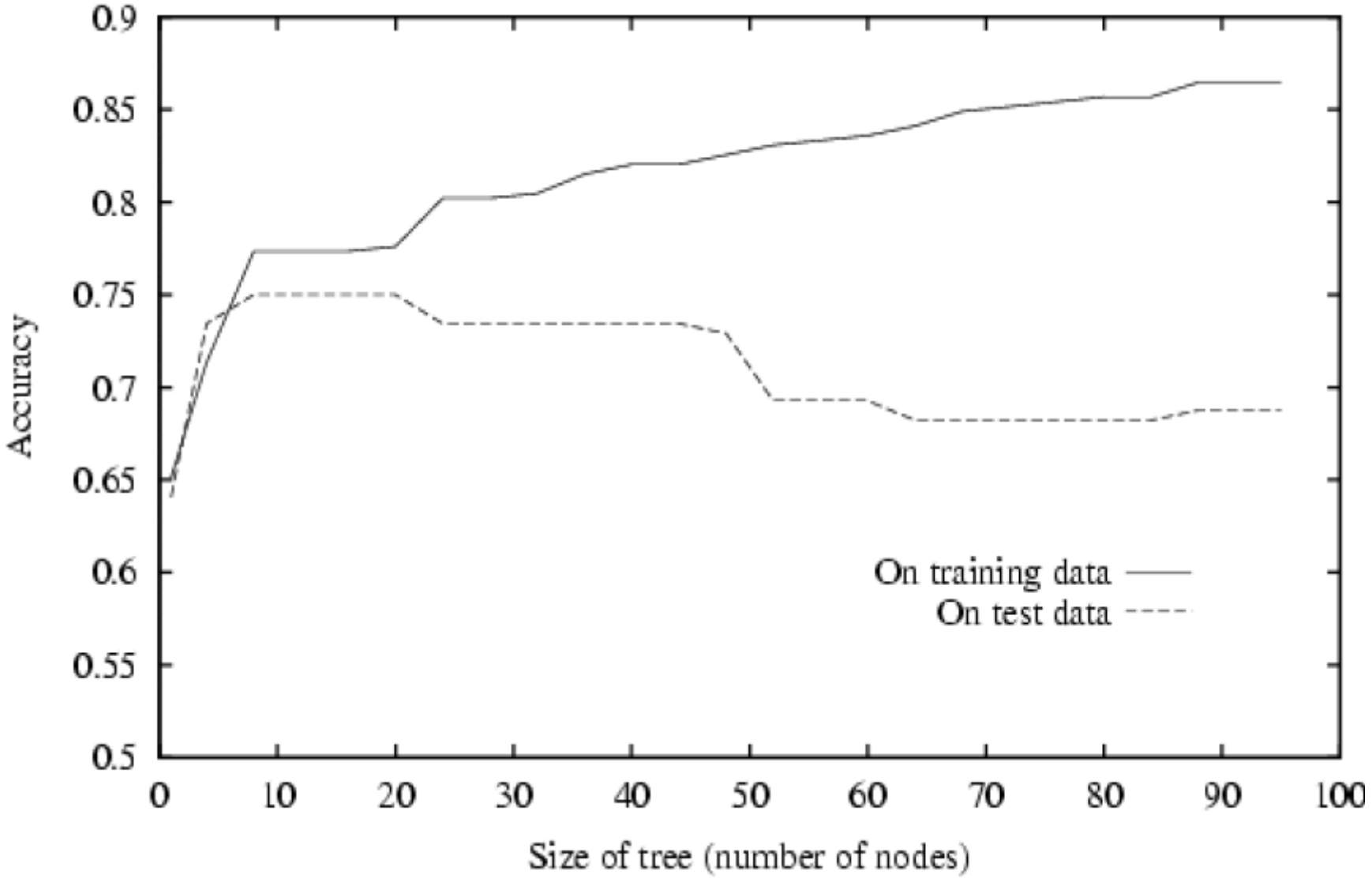
AND

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

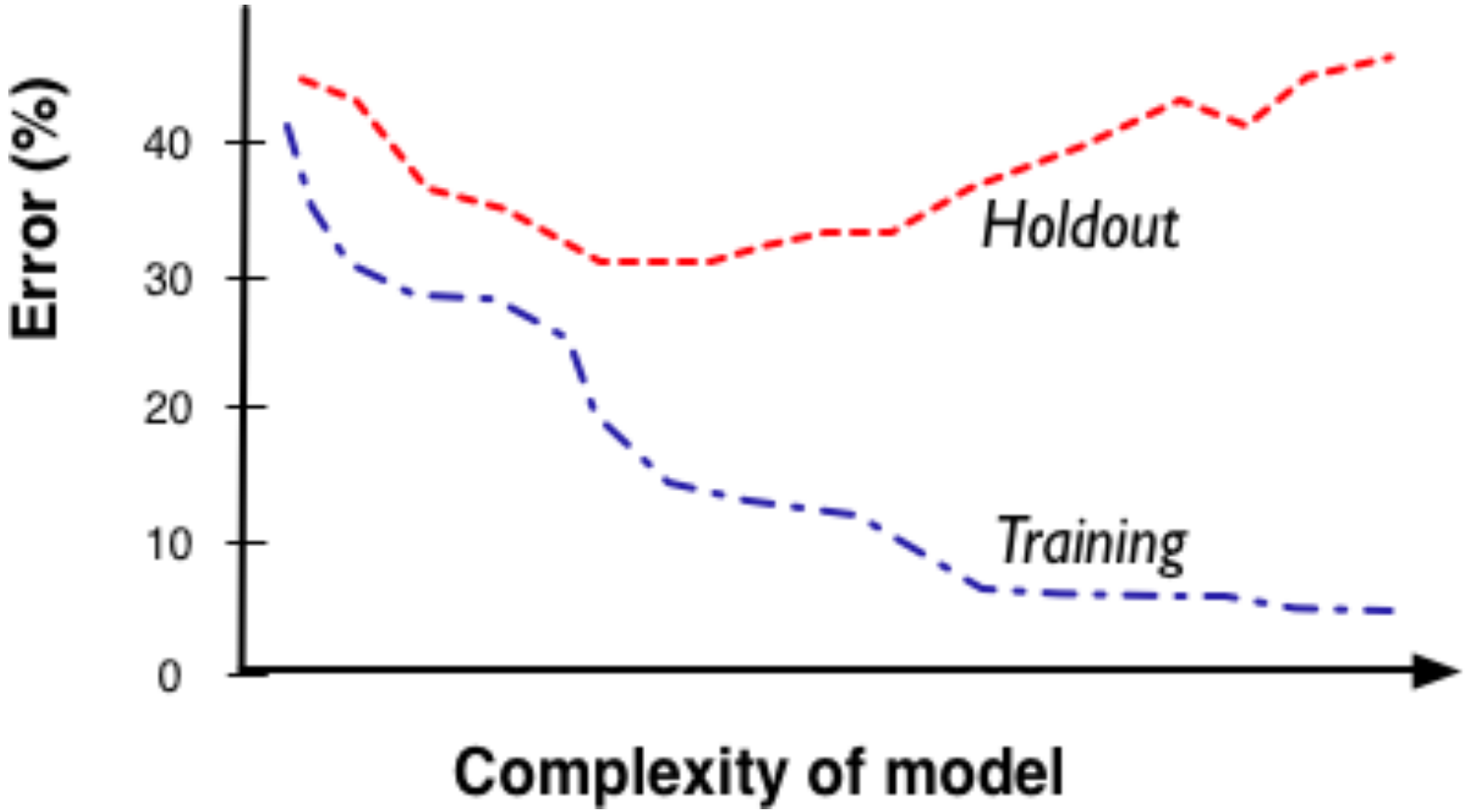
An example of over-fitting in DTree

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

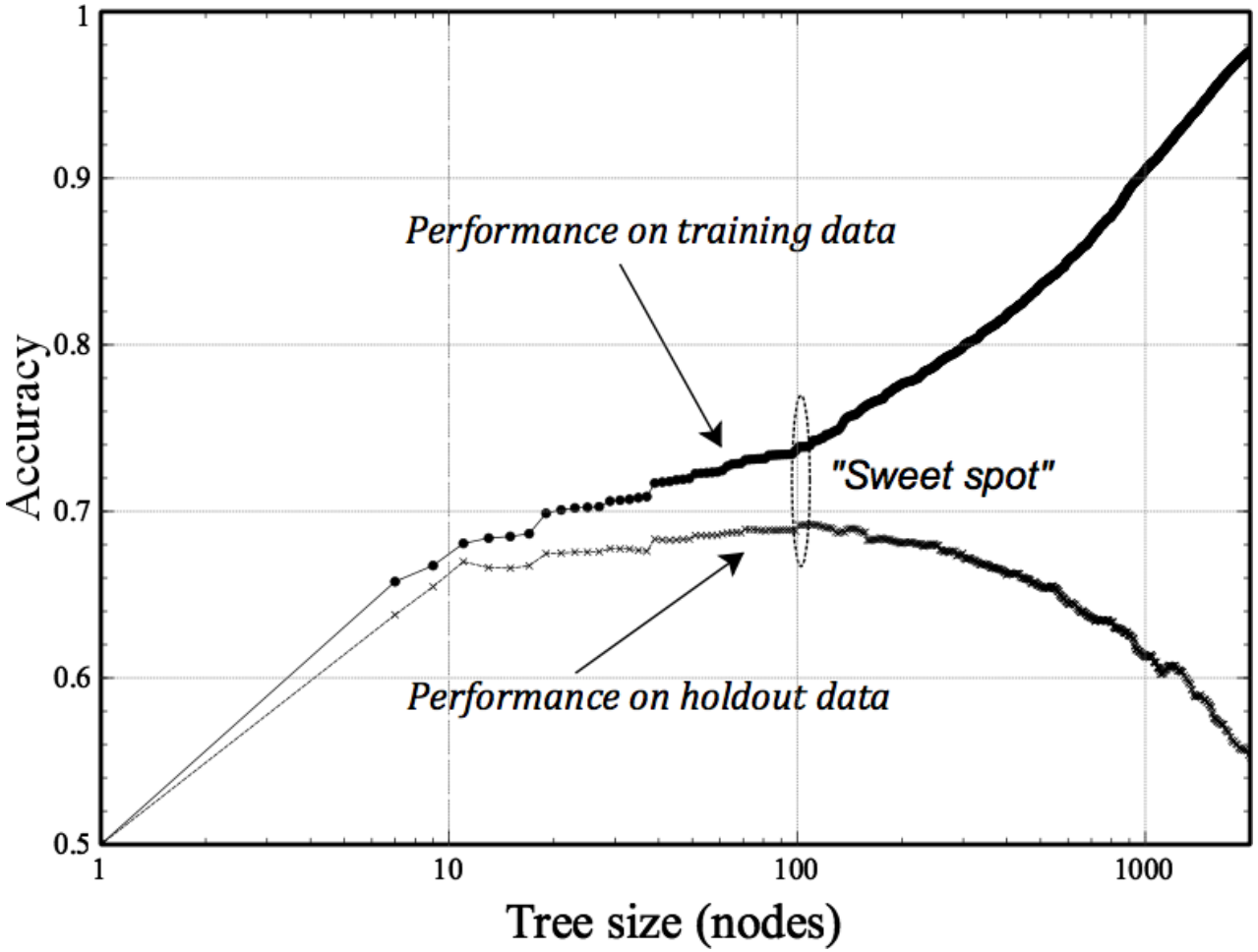
# Tree Complexity and Over-fitting



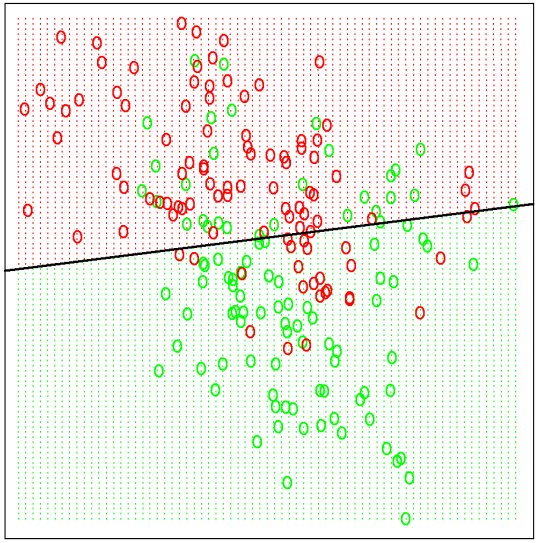
# Fitting Graph

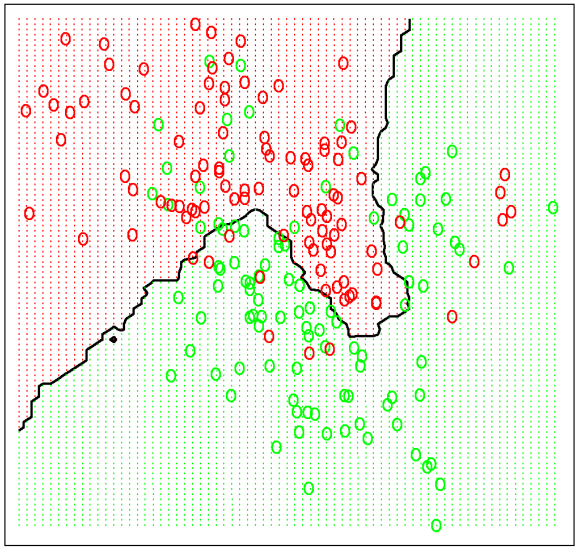


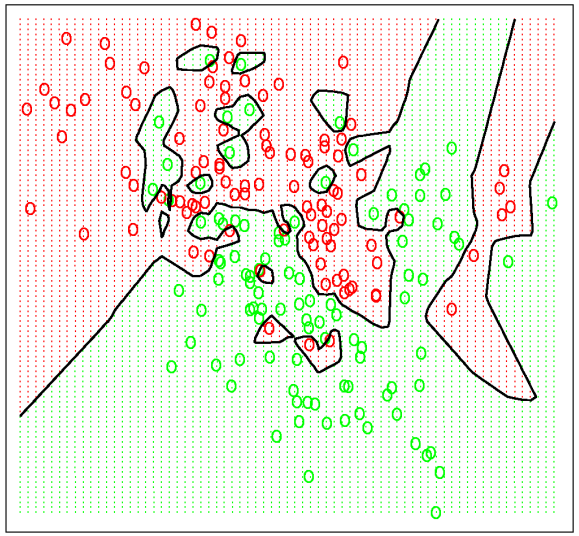
# Over-fitting in tree induction



# Need for holdout evaluation







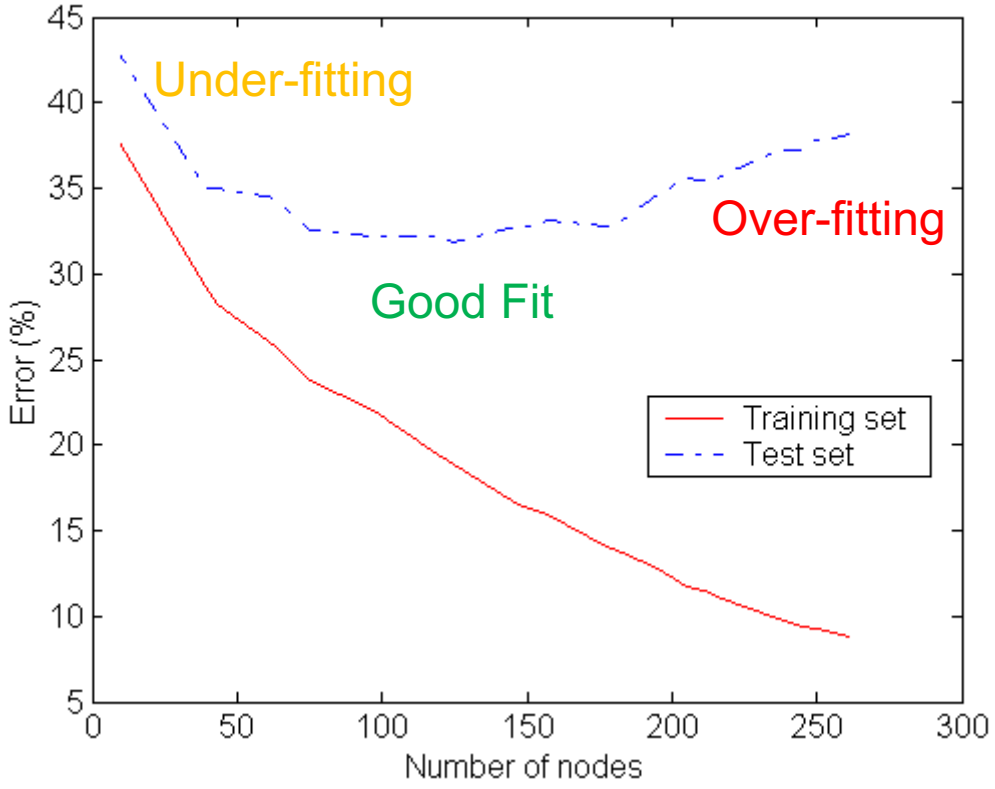
Under-fitting

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

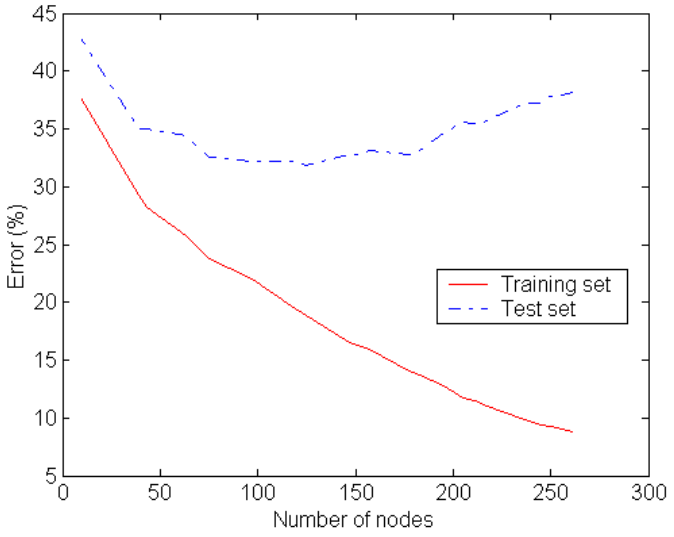
# Over-fitting



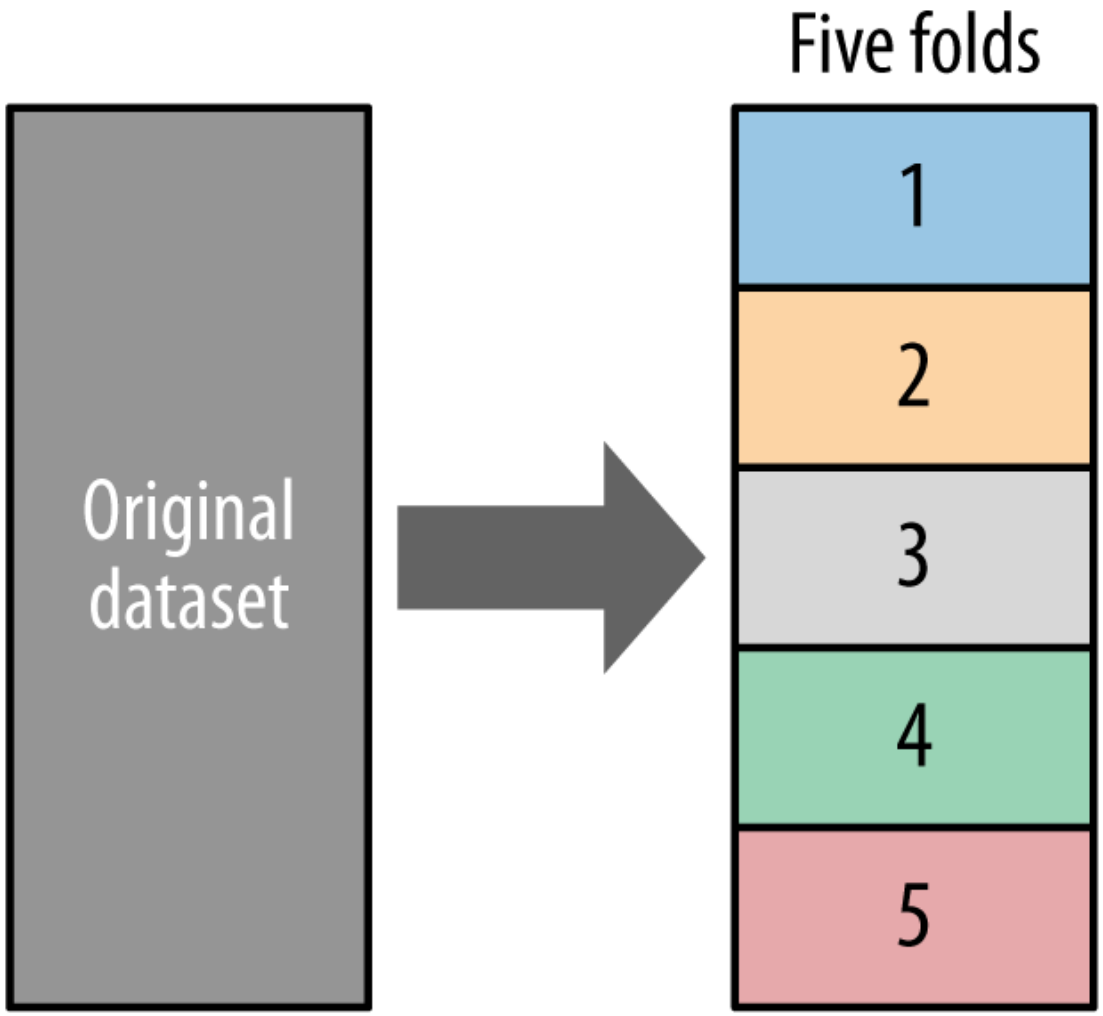

- Over-fitting: Model "memorizes" the properties of the particular training set rather than learning the underlying concept or phenomenon

# Holdout validation

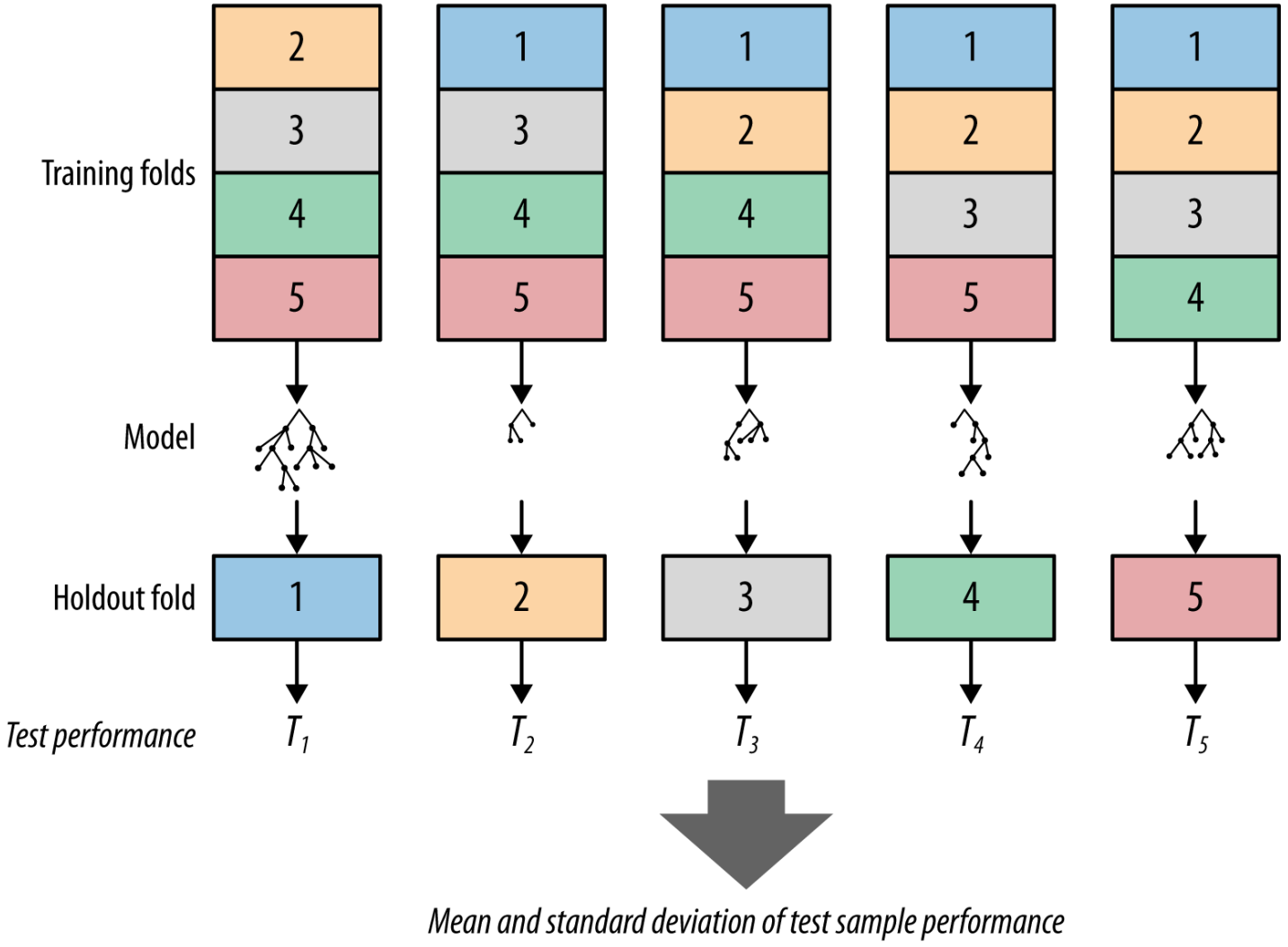
- We are interested in generalization
  - The performance on data not used for training
- Given only one data set, we hold out some data for evaluation
  - Holdout set for final evaluation is called the test set
- Accuracy on training data is sometimes called **"in-sample" accuracy**, vs. **"out-of-sample"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



# Cross-Validation



# Cross-Validation



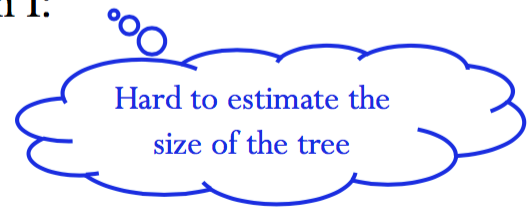
# From Holdout Evaluation to Cross-Validation

- 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:



# 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

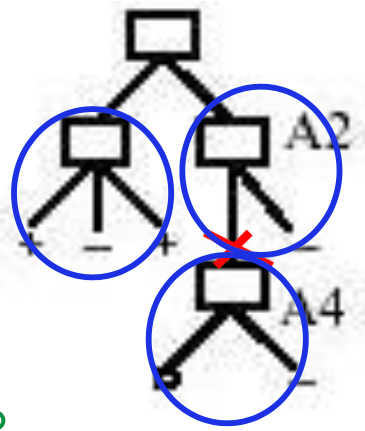
For option II:

- 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)) )

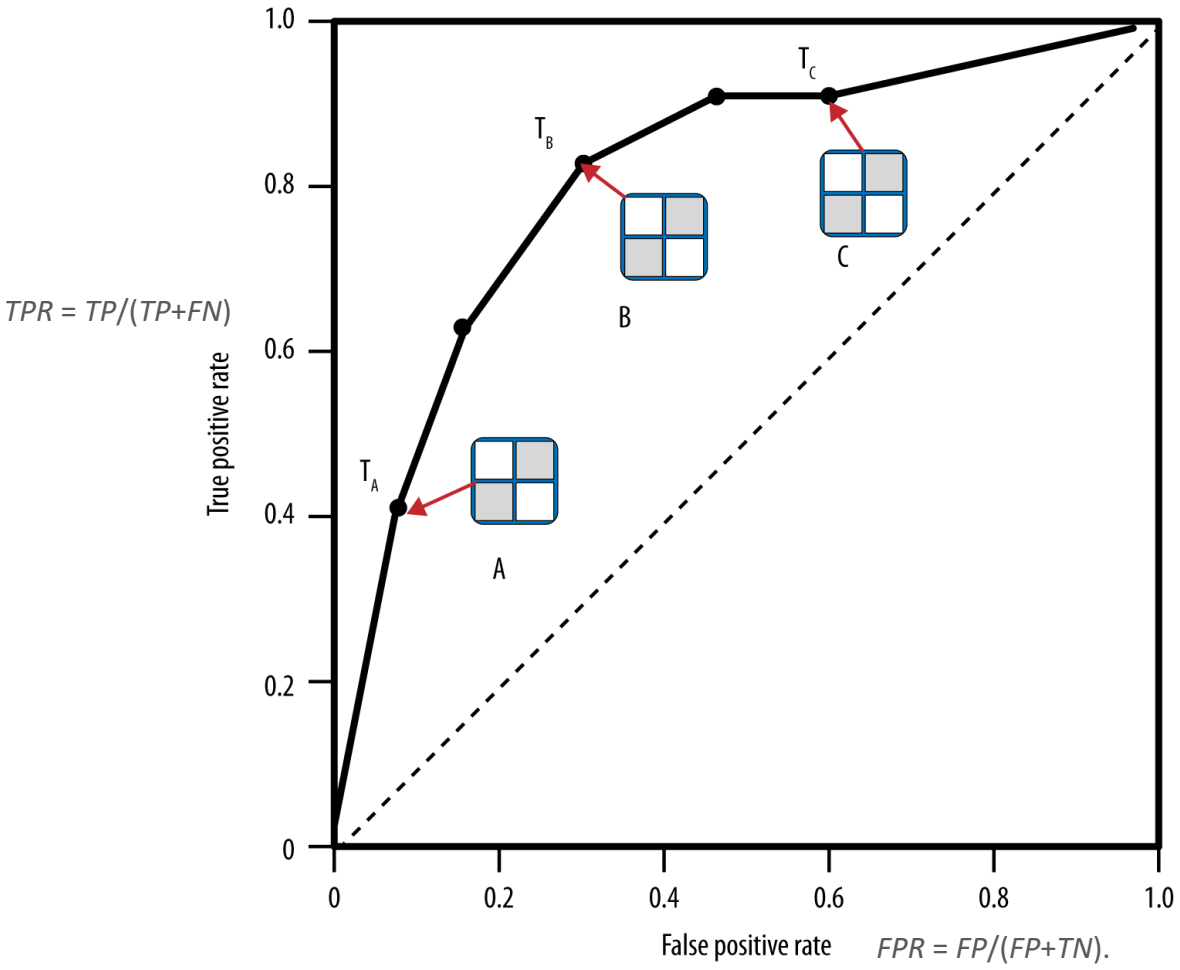
# Post-pruning (1). Reduced-Error pruning

- 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



# Generating ROC curve: Algorithm

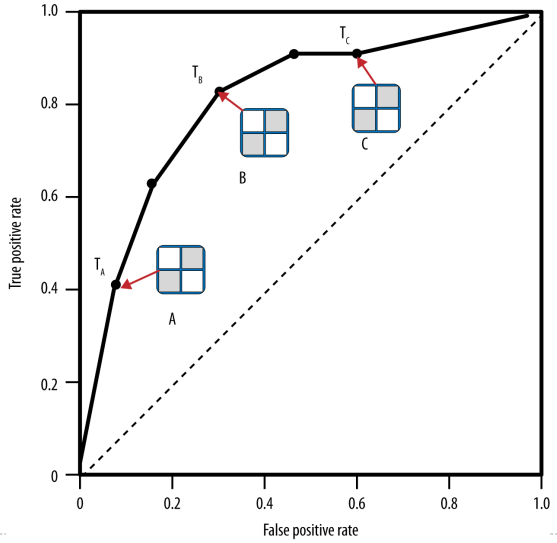
- For each test, count the number of true positives TP (positives with prediction above the cutoff) and false positives FP (negatives above the cutoff)
- Calculate TP rate (TP/P) and FP (FP/N) rate
- Plot current number of TP/P as a function of current FP/N

# ROC Graphs and Curves

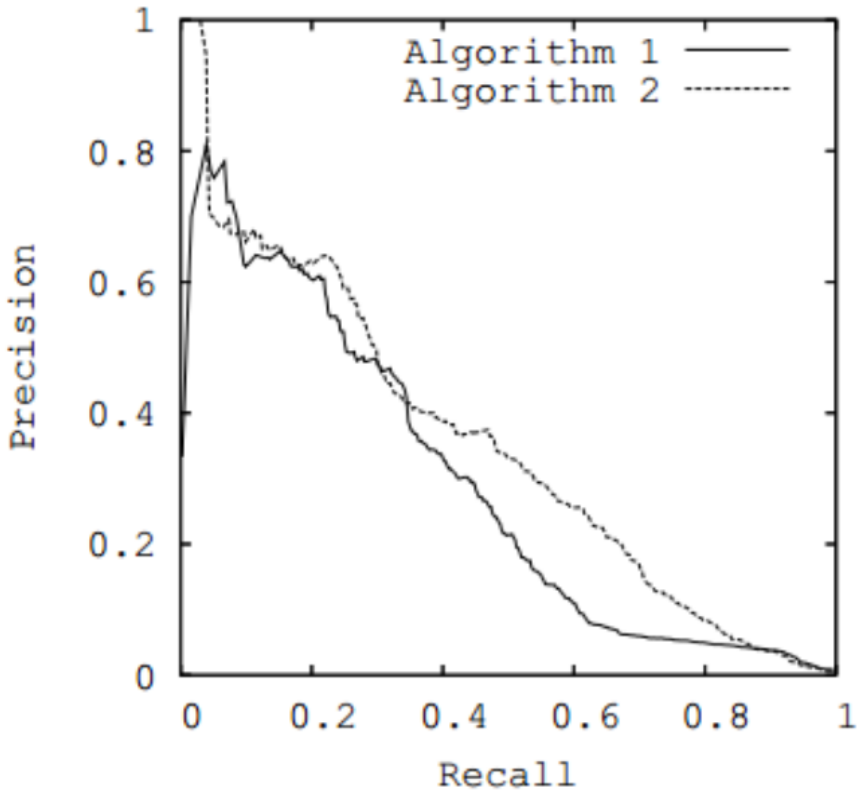
- ROC graphs decouple classifier performance from the conditions under which the classifiers will be used
- Not the most intuitive visualization for many business stakeholders

# 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?