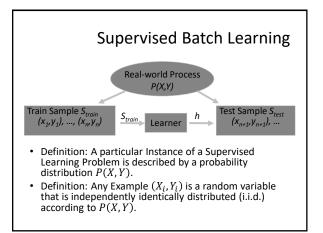
Empirical Risk Minimization, Model Selection, and Model Assessment

CS6780 – Advanced Machine Learning Spring 2019

> Thorsten Joachims Cornell University

Reading: Murphy 5.7-5.7.2.4, 6.5-6.5.3.1 Dietterich, T. G., (1998). Approximate Statistical Tests for Comparing Supervised Classification Learning Algorithms. Neural Computation, 10 (7) 1895-1924. (http://sci2s.ugr.es/keel/pdf/algorithm/articulo/dietterich1998.pdf



Training / Validation / Test Sample

• Definition: A Training / Test / Validation Sample $S = ((x_1, y_1), ..., (x_n, y_n))$ is drawn i.i.d. from P(X, Y).

$$P\left(S = \left((x_1, y_1), \dots, (x_n, y_n)\right)\right) = \prod_{i=1}^n P(X_i = x_i, Y_i = y_i)$$

Risk
• Definition: The Risk / Prediction Error / True
Error / Generalization Error of a hypothesis *h*
for a learning task
$$P(X, Y)$$
 is
 $Err_P(h) = \sum_{x,y} \Delta(y, h(x)) P(X = x, Y = y)$
• Definition: The Loss Eulertion $\Delta(y, \hat{y}) \in \Re$

• Definition: The Loss Function $\Delta(y, \hat{y}) \in \Re$ measures the quality of prediction \hat{y} if the true label is y.

Bayes Risk

• Given knowledge of P(X,Y), the true error of the best possible h is

$$Err_P(h_{bayes}) = E_{x \sim P(X)}[\min_{y \in Y} (1 - P(Y = y | X = x))]$$

for the 0/1 loss.

Three Roadmaps for Designing ML Methods

- Generative Model:
 - → Learn P(X, Y) from training sample, then h via Bayes Decision Rule.
- Discriminative Conditional Model:
 - → Learn P(Y|X) from training sample, then h via Bayes Decision Rule.
- Discriminative ERM Model:
 - ightarrow Learn h directly from training sample.

Empirical Risk

• Definition: The Empirical Risk / Error of hypothesis *h* on sample

$$S = ((x_1, y_1), \dots, (x_n, y_n))$$

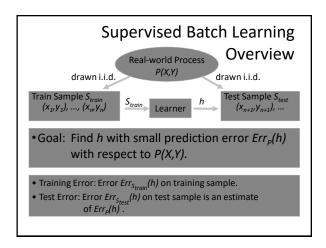
is

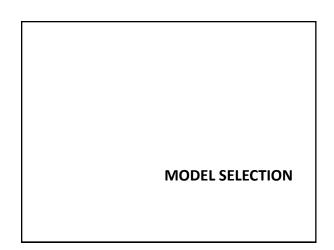
$$Err_{S}(h) = \frac{1}{n} \sum_{i=1}^{n} \Delta(y_{i}, h(x_{i}))$$

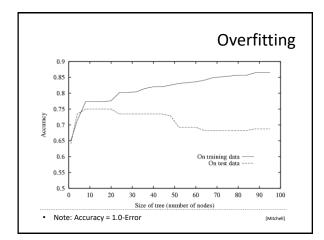
Empirical Risk Minimization

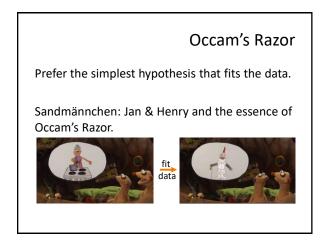
• Definition [ERM Principle]: Given a training sample $S = ((x_1, y_1), ..., (x_n, y_n)$ and a hypothesis space H, select the rule $h^{ERM} \in H$ that minimizes the empirical risk (i.e. training error) on S

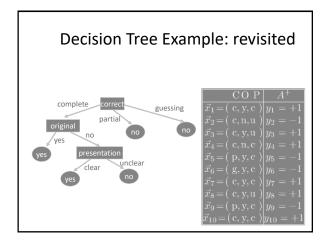
$$h^{ERM} = \min_{h \in H} \left[\frac{1}{n} \sum_{i=1}^{n} \Delta(y_i, h(y_i)) \right]$$

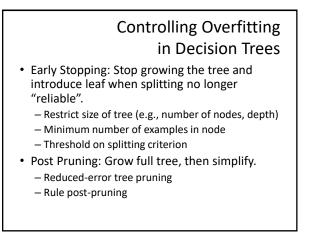


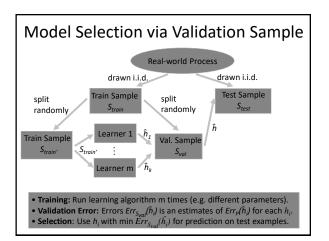


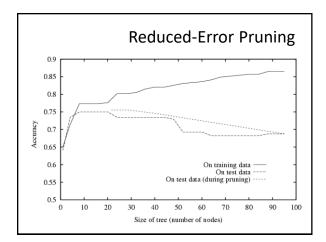










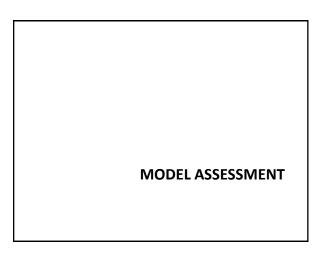


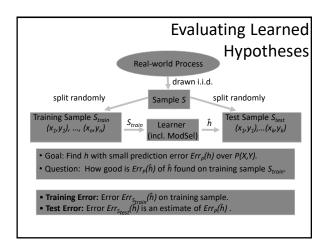
Text Classification Example "Corporate Acquisitions" Results

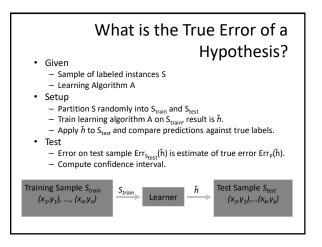
- Unpruned Tree (ID3 Algorithm):
 Size: 437 nodes Training Error: 0.0% Test Error: 11.0%
 - Early Stopping Tree (ID3 Algorithm):
- Size: 299 nodes Training Error: 2.6% Test Error: 9.8%
 Reduced-Error Pruning (C4.5 Algorithm):
- Size: 167 nodes Training Error: 4.0% Test Error: 10.8%
 Rule Post-Pruning (C4.5 Algorithm):
 - Size: 164 tests Training Error: 3.1% Test Error: 10.3%
 - Examples of rules

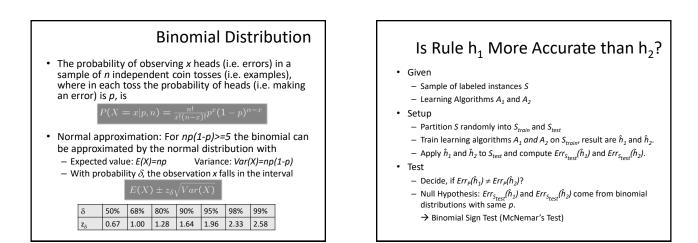
•

- IF vs = 1 THEN [99.4%]
- IF vs = 0 & export = 0 & takeover = 1 THEN + [93.6%]









Is Learning Algorithm A_1 better than A_2 ?

- Given
 - k samples $S_1 \dots S_k$ of labeled instances, all i.i.d. from P(X,Y). - Learning Algorithms A_1 and A_2
- Setup
 - For *i* from 1 to k
 - Partition S_i randomly into S_{train} and S_{test}
 - Train learning algorithms A_1 and A_2 on S_{train} , result are \hat{h}_1 and \hat{h}_2 .
 - Apply \hat{h}_1 and \hat{h}_2 to S_{test} and compute $Err_{s_{test}}(\hat{h}_1)$ and $Err_{s_{test}}(\hat{h}_2)$.
- Test
 - Decide, if $E_S(Err_P(A_1(S_{train}))) \neq E_S(Err_P(A_2(S_{train})))$?
 - Null Hypothesis: $Err_{S_{test}}(A_1(S_{train}))$ and $Err_{S_{test}}(A_2(S_{train}))$ come from same distribution over samples *S*. \rightarrow t-Test or Wilcoxon Signed-Rank Test

Approximation via K-fold Cross Validation

- Given
 - Sample of labeled instances S
 - Learning Algorithms A₁ and A₂
- Compute
 - Randomly partition S into k equally sized subsets $S_1 \dots S_k$
 - For *i* from 1 to k
 - Train A_1 and A_2 on $S_1 \dots S_{i+1} \dots S_k$ and get \hat{h}_1 and \hat{h}_2 .
 - Apply h
 ₁ and h
 ₂ to S_i and compute Err_{si}(h
 ₁) and Err_{si}(h
 ₂).
- Estimate
 - Average $Err_{S_i}(\hat{h}_1)$ is estimate of $E_S(Err_P(A_1(S_{train})))$
 - Average $Err_{s_i}(\hat{h}_2)$ is estimate of $E_s(Err_P(A_2(S_{train})))$
 - Count how often $Err_{s_i}(\hat{h}_1) > Err_{s_i}(\hat{h}_2)$ and $Err_{s_i}(\hat{h}_1) < Err_{s_i}(\hat{h}_2)$