Decision Tree Construction

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Overview

- Introduction
- Construction of decision trees
  - Top-down decision tree construction schema, split selection, pruning, data access, missing values
- Evaluation
  - Comparison with other methods
  - Predictive accuracy, complexity, training time, selection bias

Classification Example

- Example training database
  - Two predictor attributes: Age and Car-type (**S**port, **M**inivan and **T**ruck)
  - Age is ordered, Car-type is categorical attribute
  - Class label indicates whether person bought product
  - Dependent attribute is *categorical*

Age	Car	Class
20	M	Yes
30	M	Yes
25	T	No
30	S	Yes
40	S	Yes
20	T	No
30	M	Yes
25	M	Yes
40	M	Yes
20	S	No

Regression Example

- Example training database
  - Two predictor attributes: Age and Car-type (**S**port, **M**inivan and **T**ruck)
  - Spent indicates how much person spent during a recent visit to the web site
  - Dependent attribute is *numerical*

Age	Car	Spent
20	M	\$200
30	M	\$150
25	T	\$300
30	S	\$220
40	S	\$400
20	T	\$80
30	M	\$100
25	M	\$125
40	M	\$500
20	S	\$420

Types of Variables

- *Numerical*: Domain is ordered and can be represented on the real line (e.g., age, income)
- *Nominal* or *categorical*: Domain is a finite set without any natural ordering (e.g., occupation, marital status, race)
- *Ordinal*: Domain is ordered, but absolute differences between values is unknown (e.g., preference scale, severity of an injury)

Definitions

- Random variables X_1, …, X_k (*predictor variables*) and Y (*dependent variable*)
- X_i has domain dom(X_i), Y has domain dom(Y)
- P is a probability distribution on dom(X_1) x … x dom(X_k) x dom(Y)
  Training database D is a random sample from P
- A *predictor* d is a function
  d: dom(X_1) … dom(X_k) → dom(Y)

Classification Problem

- If Y is categorical, the problem is a *classification problem*, and we use C instead of Y. $|dom(C)| = J$.
- C is called the *class label*, d is called a *classifier.*
- Take r be record randomly drawn from P. Define the *misclassification rate* of d: $RT(d,P) = P(d(r.X_1, \ldots, r.X_k) != r.C)$
- Problem definition: Given dataset D that is a random sample from probability distribution P, find classifier d such that RT(d,P) is minimized.

Regression Problem

- If Y is numerical, the problem is a *regression problem.*
- Y is called the dependent variable, d is called a *regression function.*
- Take r be record randomly drawn from P. Define mean squared error rate of d: $RT(d,P) = E(r.Y - d(r.X_1, \ldots, r.X_k))^2$
- Problem definition: Given dataset D that is a random sample from probability distribution P, find regression function d such that RT(d,P) is minimized.

Goals and Requirements

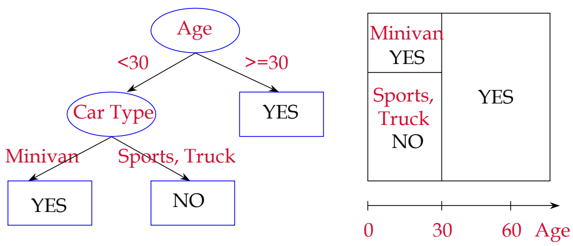
Goals:

- To produce an accurate classifier/regression function
- To understand the structure of the problem

Requirements on the model:

- High accuracy
- Understandable by humans, interpretable
- Fast construction for very large training databases

What are Decision Trees?



Decision Trees

- A *decision tree* T encodes d (a classifier or regression function) in form of a tree.
- A node t in T without children is called a *leaf node*. Otherwise t is called an *internal node*.

Internal Nodes

- Each internal node has an associated *splitting predicate*. Most common are binary predicates.
  Example predicates:
  - Age <= 20
  - Profession in {student, teacher}
  - 5000*Age + 3*Salary – 10000 > 0

Internal Nodes: Splitting Predicates

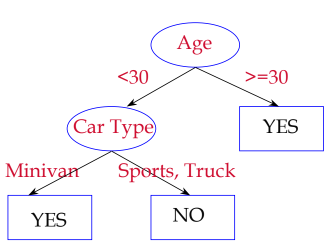
- Binary Univariate splits:
  - Numerical or ordered X: X <= c, c in dom(X)
  - Categorical X: X in A, A subset dom(X)
- Binary Multivariate splits:
  - Linear combination split on numerical variables:
    $\Sigma a_i X_i <= c$
- k-ary (k>2) splits analogous

Leaf Nodes

Consider leaf node t

- Classification problem: Node t is labeled with one class label c in dom(C)
- Regression problem: Two choices
  - Piecewise constant model:
    t is labeled with a constant y in dom(Y).
  - Piecewise linear model:
    t is labeled with a linear model
    $Y = y_t + \Sigma a_i X_i$

Example



Encoded classifier:

If (age<30 and
carType=Minivan)
Then YES

If (age <30 and
(carType=Sports or
carType=Truck))
Then NO

If (age >= 30)
Then NO

Evaluation of Misclassification Error

Problem:

- In order to quantify the quality of a classifier d, we need to know its misclassification rate RT(d,P).
- But unless we know P, RT(d,P) is unknown.
- Thus we need to estimate RT(d,P) as good as possible.

Resubstitution Estimate

The *Resubstitution estimate* R(d,D) estimates RT(d,P) of a classifier d using D:

- Let D be the training database with N records.
- $R(d,D) = 1/N \Sigma I(d(r.X) != r.C))$
- Intuition: R(d,D) is the proportion of training records that is misclassified by d
- Problem with resubstitution estimate: Overly optimistic; classifiers that overfit the training dataset will have very low resubstitution error.

Test Sample Estimate

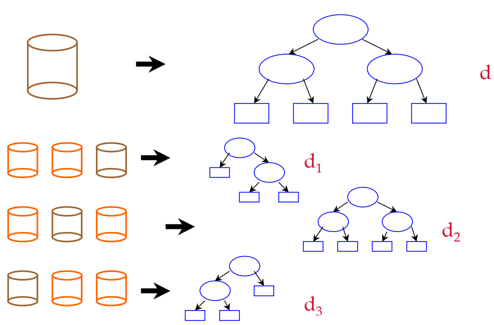
- Divide D into D_1 and D_2
- Use D_1 to construct the classifier d
- Then use resubstitution estimate $R(d,D_2)$ to calculate the estimated misclassification error of d
- Unbiased and efficient, but removes D_2 from training dataset D

V-fold Cross Validation

Procedure:
- Construct classifier d from D
- Partition D into V datasets $D_1, \ldots, D_V$
- Construct classifier d_i using $D \setminus D_i$
- Calculate the estimated misclassification error $R(d_i,D_i)$ of d_i using test sample D_i

Final misclassification estimate:
- Weighted combination of individual misclassification errors:
$R(d,D) = 1/V\ \Sigma\ R(d_i,D_i)$

Cross-Validation: Example



Cross-Validation

- Misclassification estimate obtained through cross-validation is usually nearly unbiased
- Costly computation (we need to compute d, and $d_1, \ldots, d_V$); computation of d_i is nearly as expensive as computation of d
- Preferred method to estimate quality of learning algorithms in the machine learning literature

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- Introduction
- Construction of decision trees
  - **Top-down decision tree construction schema**
  - Split selection
  - Pruning
  - Data access
  - Missing values
- Evaluation

Decision Tree Construction

- Top-down tree construction schema:
  - Examine training database and find best splitting predicate for the root node
  - Partition training database
  - Recurse on each child node

Top-Down Tree Construction

BuildTree(Node *t*, Training database *D*,
Split Selection Method *S*)

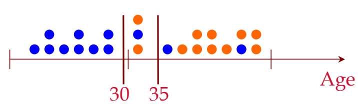
(1) Apply *S* to *D* to find splitting criterion
(2) **if** (*t* is not a leaf node)
(3) Create children nodes of *t*
(4) Partition *D* into children partitions
(5) Recurse on each partition
(6) **endif**

Decision Tree Construction

- Three algorithmic components:
  - Split selection (CART, C4.5, QUEST, CHAID, CRUISE, …)
  - Pruning (direct stopping rule, test dataset pruning, cost-complexity pruning, statistical tests, bootstrapping)
  - Data access (CLOUDS, SLIQ, SPRINT, RainForest, BOAT, UnPivot operator)

Split Selection Method

- Numerical or ordered attributes: Find a split point that separates the (two) classes



(Yes: No:)

Split Selection Method (Contd.)

- Categorical attributes: How to group?

Sport: Truck: Minivan:

(Sport, Truck) -- (Minivan)

(Sport) --- (Truck, Minivan)

(Sport, Minivan) --- (Truck)

Pruning Method

- For a tree T, the misclassification rate R(T,P) and the mean-squared error rate R(T,P) depend on P, but not on D.
- The goal is to do well on records randomly drawn from P, not to do well on the records in D
- If the tree is too large, it overfits D and does not model P. The pruning method selects the tree of the right size.

Data Access Method

- Recent development: Very large training databases, both in-memory and on secondary storage
- Goal: Fast, efficient, and scalable decision tree construction, using the complete training database.

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  - **Split selection**
  - Pruning
  - Data access
  - Missing values
- Evaluation

Split Selection Methods

- Multitude of split selection methods in the literature
- In this tutorial:
  - CART
  - QUEST
  - CHAID

Split Selection Methods: CART

- Classification And Regression Trees (Breiman, Friedman, Ohlson, Stone, 1984; considered "the" reference on decision tree construction)
- Commercial version sold by Salford Systems (www.salford-systems.com)
- Many other, slightly modified implementations exist (e.g., IBM Intelligent Miner implements the CART split selection method)

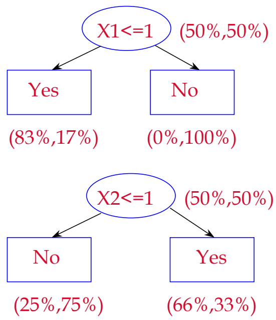
CART Split Selection Method

Motivation: We need a way to choose quantitatively between different splitting predicates

- Idea: Quantify the *impurity* of a node
- Method: Select splitting predicate that generates children nodes with minimum impurity from a space of possible splitting predicates

Intuition: Impurity Function

X1	X2	Class
1	1	Yes
1	2	Yes
1	2	Yes
1	2	Yes
1	2	Yes
1	1	No
2	1	No
2	1	No
2	2	No
2	2	No



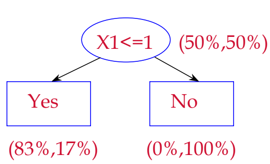
Impurity Function

- Let p(j|t) be the proportion of class j training records at node t
- Node impurity measure at node t:

  i(t) = phi(p(1|t), …, p(J|t))
- phi is symmetric
- Maximum value at arguments (J^{-1}, …, J^{-1}) (maximum impurity)
- phi(1,0,…,0) = … =phi(0,…,0,1) = 0 (node has records of only one class; “pure” node)

Example

- Root node t:
  p(1|t)=0.5; p(2|t)=0.5
  Left child node t:
  P(1|t)=0.83; p(2|t)=-.17
- Impurity of root node: phi(0.5,0.5)
- Impurity of left child node: phi(0.83,0.17)
- Impurity of right child node: phi(0.0,1.0)



Goodness of a Split

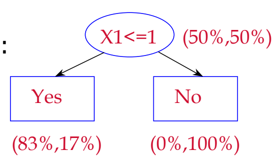
Consider node t with impurity phi(t)

The *reduction in impurity* through splitting predicate s (t splits into children nodes t_L with impurity phi(t_L) and t_R with impurity phi(t_R)) is:

$\Delta_{phi}(s,t) = \text{phi}(t) - p_L\ \text{phi}(t_L) - p_R\ \text{phi}(t_R)$

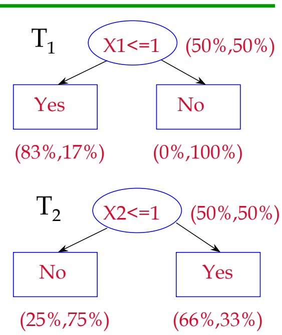
Example (Contd.)

- Impurity of root node: phi(0.5,0.5)
- Impurity of whole tree: 0.6* phi(0.83,0.17) + 0.4 * phi(0,1)
- Impurity reduction: phi(0.5,0.5) - 0.6* phi(0.83,0.17) - 0.4 * phi(0,1)



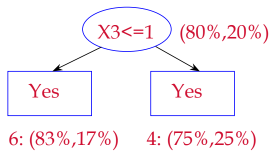
Error Reduction as Impurity Function

- Possible impurity function: Resubstitution error R(T,D).
- Example:
  R(no tree, D) = 0.5
  R(T_1,D) = 0.6*0.17
  R(T_2,D) = 0.4*0.25 + 0.6*0.33



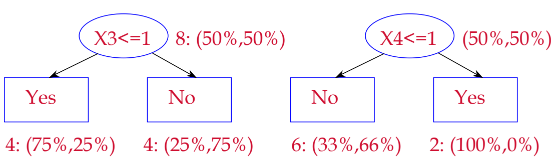
Problems with Resubstitution Error

- Obvious problem: There are situations where no split can decrease impurity
- Example: R(no tree, D) = 0.2 $R(T_1,D)$ $=0.6*0.17+0.4*0.25$ $=0.2$



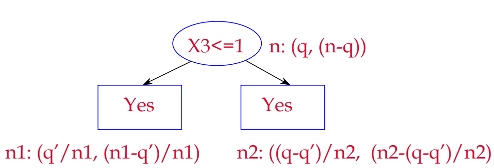
Problems with Resubstitution Error

- More subtle problem:



Problems with Resubstitution Error

Root node: n records, q of class 1
Left child node: n1 records, q' of class 1
Right child node: n2 records, (q-q') of class 1, n1+n2 = n



Problems with Resubstitution Error

Tree structure:
- Root node: n records (q/n, (n-q))
- Left child: n1 records (q'/n1, (n1-q')/n1)
- Right child: n2 records ((q-q')/n2, (n2-q')/n2)

Impurity before split:
- Error: q/n

Impurity after split:
- Left child: n1/n * q'/n1 = q'/n
- Right child: n2/n * (q-q')/n2 = (q-q')/n
- Total error: q'/n + (q-q')/n = q/n

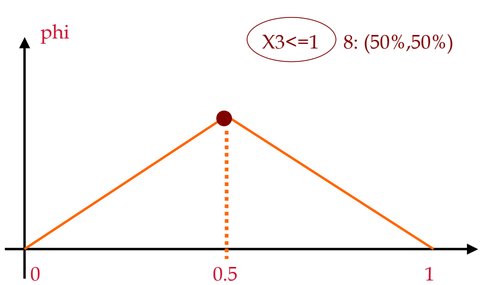
Problems with Resubstitution Error

Heart of the problem:

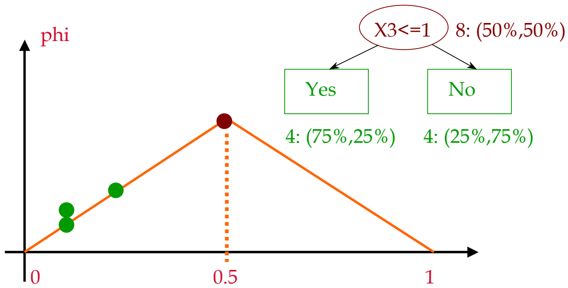
Assume two classes:
- phi(p(1|t), p(2|t)) = phi(p(1|t), 1-p(1|t)) = phi (p(1|t))

Resubstitution errror has the following property:
- phi(p1 + p2) = phi(p1)+phi(p2)

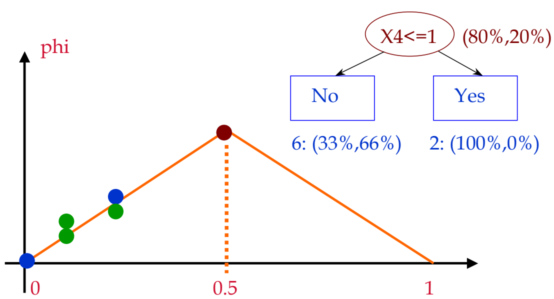
Example: Only Root Node



Example: Split (75,25), (25,75)



Example: Split (33,66), (100,0)



Remedy: Concavity

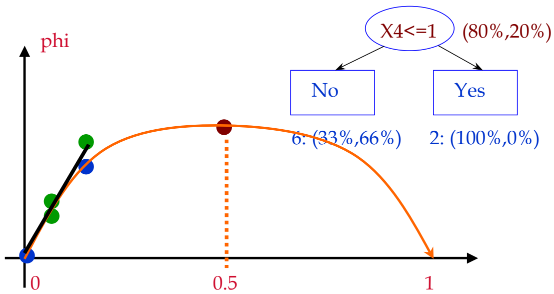
Use impurity functions that are concave:

phi″ < 0

Example impurity functions

- Entropy:
  phi(t) = - Σ p(j|t) log(p(j|t))
- Gini index:
  phi(t) = Σ p(j|t)²

Example Split With Concave Phi



Nonnegative Decrease in Impurity

Theorem: Let phi(p_1, …, p_J) be a strictly concave function on j=1, …, J, $\Sigma_j p_j = 1$.

Then for any split s:

$$\Delta_{phi}(s,t) >= 0$$

With equality if and only if:

$$p(j|t_L) = p(j|t_R) = p(j|t), j = 1, \ldots, J$$

Note: Entropy and gini-index are concave.

CART Univariate Split Selection

- Use gini-index as impurity function
- For each numerical or ordered attribute X, consider all binary splits s of the form
  X <= x
  where x in dom(X)
- For each categorical attribute X, consider all binary splits s of the form
  X in A, where A subset dom(X)
- At a node t, select split s* such that Δ_{phi}(s*,t) is maximal over all s considered

CART: Shortcut for Categorical Splits

Computational shortcut if |Y|=2.

- Theorem: Let X be a categorical attribute with dom(X) = {b_1, …, b_k}, |Y|=2, phi be a concave function, and let
  $p(X=b_1) <= \ldots <= p(X=b_k)$.
  Then the best split is of the form:
  X in {b_1, b_2, …, b_l} for some l < k
- Benefit: We need only to check k-1 subsets of dom(X) instead of $2^{(k-1)}$-1 subsets

CART Multivariate Split Selection

- For numerical predictor variables, examine splitting predicates s of the form:
  $\Sigma_i a_i X_i <= c$
  with the constraint:
  $\Sigma_i a_i^2 = 1$
- Select splitting predicate s* with maximum decrease in impurity.

Problems with CART Split Selection

- Biased towards variables with more splits (M-category variable has 2^{M-1}-1) possible splits, an M-valued ordered variable has (M-1) possible splits
- Computationally expensive for categorical variables with large domains

Split Selection Methods: QUEST

- Quick, Unbiased, Efficient, Statistical Tree (Loh and Shih, Statistica Sinica, 1997) Freeware, available at www.stat.wisc.edu/~loh Also implemented in SPSS.
- Main new ideas:
  - Separate splitting predicate selection into variable selection and split point selection
  - Use statistical significance tests instead of impurity function

QUEST Variable Selection

Let β be a selected significance level. Let $X_1, \ldots, X_l$ be numerical predictor variables, and let $X_{l+1}, \ldots, X_k$ be categorical predictor variables.

1. Find p-value from ANOVA F-test for each numerical variable.
2. Find p-value for each X^2-test for each categorical variable.
3. Choose variable $X_{k'}$ with overall smallest p-value $p_{k'}$

QUEST Variable Selection

4. Choose $X_{k'}$ as splitting variable if $p_{k'} < \beta/k$ (first Bonferroni correction).
5. Otherwise, find p-values for Levene's F-test for each numerical predictor variable. Let $X_{k''}$ have the smallest such p-value $p_{k''}$.
6. If $p_{k''} < \beta/(k+l)$, split on $X_{k''}$ (second Bonferroni correction)
7. Else split on $X_{k'}$

QUEST Split Point Selection

CRIMCOORD transformation of categorical variables into numerical variables:

1. Take categorical variable X with domain $dom(X)=\{x_1, \ldots, x_l\}$
2. For each record in the training database, create vector $(v_1, \ldots, v_l)$ where $v_i = I(X=x_i)$
3. Find principal components of set of vectors V
4. Project the dimensionality-reduced data onto the largest discriminant coordinate dx_i
5. Replace X with numeral dx_i in the rest of the algorithm

CRIMCOORDs: Examples

- Values(X|Y=1) = $\{4c_1,c_2,5c_3\}$, values(X|Y=2) = $\{2c_1, 2c_2, 6c_3\}$
  $dx_1 = 1$, $dx_2 = -1$, $dx_3 = -0.3$
- Values(X|Y=1) = $\{5c_1,5c_3\}$, values(X|Y=2) = $\{5c_1, 5c_3\}$
  $dx_1 = 1$, $dx_2 = 0$, $dx_3 = 1$
- Values(X|Y=1) = $\{5c_1,5c_3\}$, values(X|Y=2) = $\{5c_1, c_2, 5c_3\}$
  $dx_1 = 1$, $dx_2 = -1$, $dx_3 = 1$

Why CRIMCOORD Transformation?

Advantages

- Avoid exponential subset search from CART
- Each dx_i has the form $\Sigma\, b_i\, I(X=x_i)$ for some $b_1, \ldots, b_l$, thus there is a 1-1 correspondence between subsets of X and a dx_i

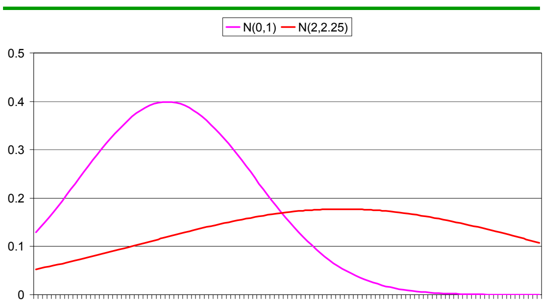
QUEST Split Point Selection

- Assume X is the selected variable (either numerical, or categorical transformed to CRIMCOORDS)
- Group J>2 classes into two superclasses
- Now problem is reduced to one-dimensional two-class problem
  - Use exhaustive search for the best split point (like in CART)
  - Use quadratic discriminant analysis (QDA, see next slide)

QUEST Split Point Selection: QDA

- Let x_1, x_2 and s_1^2, s_2^2 the means and variances for the two superclasses
- Make normal distribution assumption, and find intersections of the two normal distributions $N(x_1,s_1^2)$ and $N(x_2,s_2^2)$
- QDA splits the X-axis into three intervals
- Select as split point the root that is closer to the sample means

Illustration: QDA Splits



QUEST Linear Combination Splits

- Transform all categorical variables to CRIMCOORDS
- Apply PCA to the correlation matrix of the data
- Drop the smallest principal components, and project the remaining components onto the largest CRIMCOORD
- Group J>2 classes into two superclasses
- Find split on largest CRIMCOORD using ES or QDA

Key Differences CART/QUEST

Feature	QUEST	CART
Variable selection	F and X^2 tests	ES
Split point selection	QDA or ES	ES
Categorical variables	CRIMCOORDS	ES
Monotone transformations for numerical variables	Not invariant	Invariant
Ordinal Variables	No	Yes

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  - Split Selection
  - **Pruning**
  - Data Access
  - Missing Values
- Evaluation

Pruning Methods

- Test dataset pruning
- Direct stopping rule
- Cost-complexity pruning
- MDL pruning
- Pruning by randomization testing

Top-Down and Bottom-Up Pruning

Two classes of methods:

- Top-down pruning: Stop growth of the tree at the right size. Need a statistic that indicates when to stop growing a subtree.
- Bottom-up pruning: Grow an overly large tree and then chop off subtrees that "overfit" the training data.

Stopping Policies

A stopping policy indicates when further growth of the tree at a node t is counterproductive.

- All records are of the same class
- The attribute values of all records are identical
- All records have missing values
- At most one class has a number of records larger than a user-specified number
- All records go to the same child node if t is split (only possible with some split selection methods)

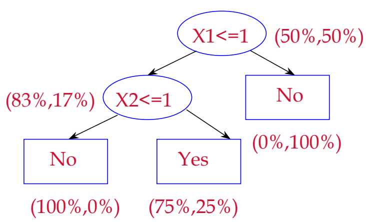
Test Dataset Pruning

- Use an independent test sample D′ to estimate the misclassification cost using the resubstitution estimate R(T,D′) at each node
- Select the subtree T′ of T with the smallest expected cost

Test Dataset Pruning Example

Test set:

X1	X2	Class
1	1	Yes
1	2	Yes
1	2	Yes
1	2	Yes
1	1	Yes
1	2	No
2	1	No
2	1	No
2	2	No
2	2	No



Only root: 10% misclassification
Full tree: 30% misclassification

Reduced Error Pruning

(Quinlan, C4.5, 1993)

- Assume observed misclassification rate at a node is p
- Replace p (pessimistically) with the upper 75% confidence bound p′, assuming a binomial distribution
- Then use p′ to estimate error rate of the node

Cost Complexity Pruning

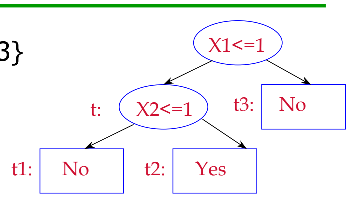
(Breiman, Friedman, Olshen, Stone, 1984)

Some more tree notation

- t: node in tree T
- leaf(T): set of leaf nodes of T
- |leaf(T)|: number of leaf nodes of T
- T_t: subtree of T rooted at t
- {t}: subtree of T_t containing only node t

Notation: Example

leaf(T) = {t1,t2,t3}
|leaf(T)|=3
Tree rooted at node t: T_t
Tree consisting of only node t: {t}
leaf(T_t)={t1,t2}
leaf({t})={t}



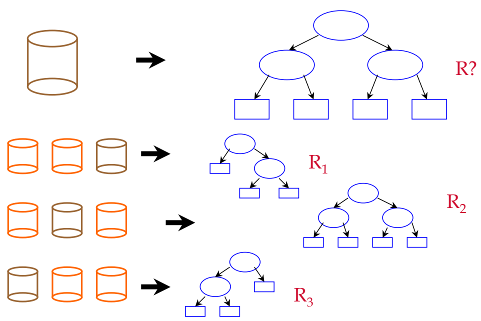
Cost-Complexity Pruning

- Test dataset pruning is the ideal case, if we have a large test dataset. But:
  - We might not have a large test dataset
  - We want to use all available records for tree construction
- If we do not have a test dataset, we do not obtain "honest" classification error estimates
- Remember cross-validation: Re-use training dataset in a clever way to estimate the classification error.

Cost-Complexity Pruning

1. /* cross-validation step */
   Construct tree T using D
2. Partition D into V subsets $D_1, \ldots, D_V$
3. for (i=1; i<=V; i++)
   Construct tree T_i from (D \ D_i)
   Use D_i to calculate the estimate $R(T_i, D \setminus D_i)$
   endfor
4. /* estimation step */
   Calculate R(T,D) from $R(T_i, D \setminus D_i)$

Cross-Validation Step

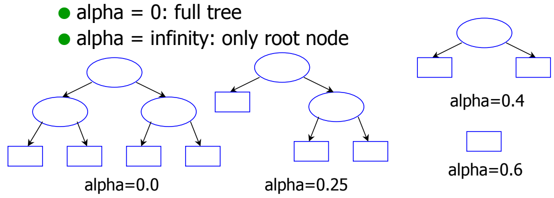


Cost-Complexity Pruning

- Problem: How can we relate the misclassification error of the CV-trees to the misclassification error of the large tree?
- Idea: Use a parameter that has the same meaning over different trees, and relate trees with similar parameter settings.
- Such a parameter is the cost-complexity of the tree.

Cost-Complexity Pruning

- Cost complexity of a tree T:
  $R_{alpha}(T) = R(T) + alpha\ |leaf(T)|$
- For each A, there is a tree that minimizes the cost complexity:
  - alpha = 0: full tree
  - alpha = infinity: only root node

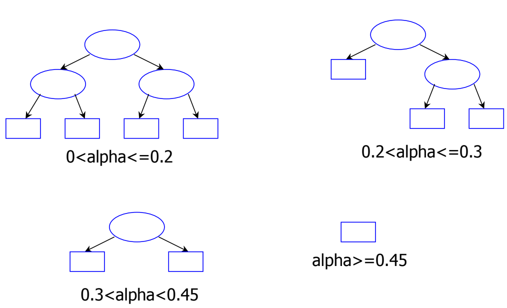


Cost-Complexity Pruning

- When should we prune the subtree rooted at t?
  - $R_{alpha}(\{t\}) = R(t) + alpha$
  - $R_{alpha}(T_t) = R(T_t) + alpha\ |leaf(T_t)|$
  - Define

    $g(t) = (R(t)-R(T_t)) / (|leaf(T_t)|-1)$
- Each node has a critical value g(t):
  - Alpha < g(t): leave subtree T_t rooted at t
  - Alpha >= g(t): prune subtree rooted at t to {t}
- For each alpha we obtain a unique minimum cost-complexity tree.

Example Revisited



Cost Complexity Pruning

1. Let $T^1 > T^2 > \ldots > \{t\}$ be the nested cost-complexity sequence of subtrees of T rooted at t.
   Let $alpha_1 < \ldots < alpha_k$ be the sequence of associated critical values of alpha. Define $alpha_{k'}$=squareroot($alpha_k$ * $alpha_{k+1}$)
2. Let T_i be the tree grown from D \ D_i
3. Let $T^i(alpha_{k'})$ be the minimal cost-complexity tree for $alpha_{k'}$

Cost Complexity Pruning

4. Let $R'(T_i)(alpha_{k'}))$ be the misclassification cost of $T_i(alpha_{k'})$ based on D_i
5. Define the V-fold cross-validation misclassification estimate as follows: $R^*(T^k) = 1/V\ \Sigma_i\ R'(T_i(alpha_{k'}))$
6. Select the subtree with the smallest estimated CV error

k-SE Rule

- Let T* be the subtree of T that minimizes the misclassification error $R(T_k)$ over all k
- But $R(T_k)$ is only an estimate:
  - Estimate the estimated standard error SE(R(T*)) of R(T*)
  - Let T** be the smallest tree such that R(T**) <= R(T*) + k*SE(R(T*)); use T** instead of T*
  - Intuition: A smaller tree is easier to understand.

Cost Complexity Pruning

Advantages:

- No independent test dataset necessary
- Gives estimate of misclassification error, and chooses tree that minimizes this error

Disadvantages:

- Originally devised for small datasets; is it still necessary for large datasets?
- Computationally very expensive for large datasets (need to grow V trees from nearly all the data)

Pruning Using the MDL Principle

(Mehta, Rissanen, Agrawal, KDD 1996)
Also used before by Fayyad, Quinlan, and others.

- MDL: Minimum Description Length Principle
- Idea: Think of the decision tree as encoding the class labels of the records in the training database
- MDL Principle: The best tree is the tree that encodes the records using the fewest bits

How To Encode a Node

Given a node t, we need to encode the following:

- Nodetype: One bit to encode the type of each node (leaf or internal node)

For an internal node:

- Cost(P(t)): The cost of encoding the splitting predicate P(t) at node t

For a leaf node:

- n*E(t): The cost of encoding the records in leaf node t with n records from the training database (E(t) is the entropy of t)

How To Encode a Tree

Recursive definition of the minimal cost of a node:

- Node t is a leaf node:

  $cost(t)= n*E(t)$

- Node t is an internal node with children nodes t_1 and t_2. Choice: Either make t a leaf node, or take the best subtrees, whatever is cheaper:

  $cost(t) =$
  $\min(n*E(t), 1+cost(P(t))+cost(t_1)+cost(t_2))$

How to Prune

1. Construct decision tree to its maximum size
2. Compute the MDL cost for each node of the tree bottom-up
3. Prune the tree bottom-up:
   If cost(t)=n*E(t), make t a leaf node.
   Resulting tree is the final tree output by the pruning algorithm.

Performance Improvements: PUBLIC

(Shim and Rastogi, VLDB 1998)

- MDL bottom-up pruning requires construction of a complete tree before the bottom-up pruning can start
- Idea: Prune the tree during (not after) the tree construction phase
- Why is this possible?
  - Calculate a lower bound on cost(t) and compare it with n*E(t)

PUBLIC Lower Bound Theorem

- Theorem: Consider a classification problem with k predictor attributes and J classes. Let T_t be a subtree with s internal nodes, rooted at node t, let n_i be the number of records with class label i. Then

  $cost(T_t) >= 2*s+1+s*log\ k + \Sigma\ n_i$
- Lower bound on $cost(T_t)$ is thus the minimum of:
  - n*E+1 (t becomes a leaf node)
  - $2*s+1+s*log\ k + \Sigma\ n_i$ (subtree at t remains)

Large Datasets Lead to Large Trees

- Oates and Jensen (KDD 1998)
- Problem: Constant probability distribution P, datasets $D_1, D_2, \ldots, D_k$ with
  $|D_1| < |D_2| < \ldots < |D_k|$
  $|D_k| = c\ |D_{k-1}| = \ldots = c^k\ |D_1|$
- Observation: Trees grow
  $|T_1| < |T_2| < \ldots < |T_k|$
  $|T_k| = c'\ |T_{k-1}| = \ldots = c'^k\ |T_1|$
- But: No gain in accuracy due to larger trees
  $R(T_1,D_1) \sim R(T_2,D_2) \sim \ldots \sim R(T_k, D_k)$

Pruning By Randomization Testing

- Reduce pruning decision at each node to a hypothesis test
- Generate empirical distribution of the hypothesis under the null hypothesis for a node n:

Randomization Pruning

Node n with subtree T(n) and pruning statistic S(n)

For (i=0; i<K; i++)

1. Randomize class labels of the data at n
2. Build and prune a tree rooted at n
3. Calculate pruning statistic $S_i(n)$

Compare S(n) to empirical distribution of $S_i(n)$ to estimate significance of S(n)

If S(n) is not significant enough compared to a significance level alpha, then prune T(n) to n

Overview

- Introduction
- Construction of Decision Trees
  - Top-down decision tree construction schema
  - Split Selection
  - Pruning
  - **Data Access**
  - Missing Values
- Evaluation

SLIQ

Shafer, Agrawal, Mehta (EDBT 1996)

- Motivation:
  - Scalable data access method for CART
  - To find the best split we need to evaluate the impurity function at all possible split points for each numerical attribute, at each node of the tree
  - Idea: Avoids re-sorting at each node of the three through pre-sorting and maintenance of sort orders

SLIQ: Pre-Sorting

Age	Car	Class
20	M	Yes
30	M	Yes
25	T	No
30	S	Yes
40	S	Yes
20	T	No
30	M	Yes
25	M	Yes
40	M	Yes
20	S	No

Age	Ind
20	1
20	6
20	10
25	3
25	8
30	2
30	4
30	7
40	5
40	9

Ind	Class	Leaf
1	Yes	1
2	Yes	1
3	No	1
4	Yes	1
5	Yes	1
6	No	1
7	Yes	1
8	Yes	1
9	Yes	1
10	No	1

SLIQ: Evaluation of Splits

Age	Ind
20	1
20	6
20	10
25	3
25	8
30	2
30	4
30	7
40	5
40	9

Ind	Class	Leaf
1	Yes	2
2	Yes	2
3	No	2
4	Yes	3
5	Yes	3
6	No	2
7	Yes	2
8	Yes	2
9	Yes	2
10	No	3

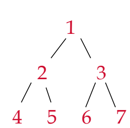
Node2	Yes	No
Left	2	0
Right	3	2

Node3	Yes	No
Left	0	1
Right	2	0

SLIQ: Splitting of a Node

Age	Ind
20	1
20	6
20	10
25	3
25	8
30	2
30	4
30	7
40	5
40	9

Ind	Class	Leaf
1	Yes	4
2	Yes	5
3	No	5
4	Yes	7
5	Yes	7
6	No	4
7	Yes	7
8	Yes	7
9	Yes	7
10	No	6



SLIQ: Summary

- Uses vertical partitioning to avoid re-sorting
- Main-memory resident data structure with schema (class label, leaf node index)
  Very likely to fit in-memory for nearly all training databases

SPRINT

Shafer, Agrawal, Mehta (VLDB 1996)

- Motivation:
  - Scalable data access method for CART
  - Improvement over SLIQ to avoid main-memory data structure

SPRINT: Algorithm Overview

- Create vertical partitions called attribute lists for each attribute
- Pre-sort the attribute lists

Recursive tree construction:

1. Scan all attribute lists at node t to find the best split
2. Partition current attribute lists over children nodes while maintaining sort orders
3. Recurse

SPRINT Attribute Lists

Age	Car	Class
20	M	Yes
30	M	Yes
25	T	No
30	S	Yes
40	S	Yes
20	T	No
30	M	Yes
25	M	Yes
40	M	Yes
20	S	No

Age	Class	Ind
20	Yes	1
20	No	6
20	No	10
25	No	3
25	Yes	8
30	Yes	2
30	Yes	4
30	Yes	7
40	Yes	5
40	Yes	9

Car	Class	Ind
M	Yes	1
M	Yes	2
T	No	3
S	Yes	4
S	Yes	5
T	No	6
M	Yes	7
M	Yes	8
M	Yes	9
S	No	10

SPRINT: Evaluation of Splits

Age	Class	Ind
20	Yes	1
20	No	6
20	No	10
25	No	3
25	Yes	8
30	Yes	2
30	Yes	4
30	Yes	7
40	Yes	5
40	Yes	9

Node1	Yes	No
Left	1	2
Right	6	1

SPRINT: Splitting of a Node

1. Scan all attribute lists to find the best split
2. Partition the attribute list of the splitting attribute X
3. For each attribute X_i != X

Perform the partitioning step of a hash-join between the attribute list of X and the attribute list of X_i

SPRINT: Hash-Join Partitioning

Age	Class	Ind	
20	Yes	1	
20	No	6	Right Child
20	No	10	Right Child
25	No	3	R
25	Yes	8	
30	Yes	2	
30	Yes	4	R
30	Yes	7	
40	Yes	5	R
40	Yes	9	

Car	Class	Ind
M	Yes	1
M	Yes	2
M	Yes	7
M	Yes	8
M	Yes	9

SPRINT: Summary

- Scalable data access method for CART split selection method
- Completely scalable, can be (and has been) implemented "inside" a database system
- Hash-join partitioning step expensive (each attribute, at each node of the tree)

RainForest: Motivation

(Gehrke, Ramakrishnan, Ganti, VLDB 1998)

- Example training database
  - Two predictor attributes: Age and Car-type (**S**port, **M**inivan and **T**ruck)
  - Age is ordered, Car-type is categorical attribute
  - Class label indicates whether person bought product

Age	Car	Class
20	M	Yes
30	M	Yes
25	T	No
30	S	Yes
40	S	Yes
20	T	No
30	M	Yes
25	M	Yes
40	M	Yes
20	S	No

RainForest: AVC-Set

Training Database

Age	Car	Class
20	M	Yes
30	M	Yes
25	T	No
30	S	Yes
40	S	Yes
20	T	No
30	M	Yes
25	M	Yes
40	M	Yes
20	S	No

AVC-Sets

Age	Yes	No
20	1	2
25	1	1
30	3	0
40	2	0

Car	Yes	No
Sport	2	1
Truck	0	2
Minivan	5	0

Refined RainForest Top-Down Schema

BuildTree(Node *n*, Training database *D*,
Split Selection Method ***S***)

[(1) Apply ***S*** to *D* to find splitting criterion]
(1a) **for** each predictor attribute *X*
(1b) Call *S*.findSplit(AVC-set of *X*)
(1c) **endfor**
(1d) *S*.chooseBest();
(2) **if** (*n* is not a leaf node) ...

S: C4.5, CART, CHAID, FACT, ID3, GID3, QUEST, etc.

RainForest Data Access Method

Assume datapartition at a node is D. Then the following steps are carried out:

1. Construct AVC-group of the node
2. Choose splitting attribute and splitting predicate
3. Partition D across the children

RainForest Summary

- Works best if the AVC-group of the root node fits in-memory
- Feasible (but slow) if each individual AVC-set of the root node fits in-memory
- If training database is very large, use hybrid between RainForest and SPRINT
- Scales broad class of split selection methods

Overview

- Introduction
- Construction of Decision Trees
  - Top-down decision tree construction schema
  - Split Selection
  - Pruning
  - Data Access
  - **Missing Values**
- Evaluation

Missing Values

- What is the problem?
  - During computation of the splitting predicate, we can selectively ignore records with missing values (note that this has some problems)
  - But if a record r misses the value of the variable in the splitting attribute, r can not participate further in tree construction

Algorithms for missing values address this problem.

Mean and Mode Imputation

Assume record r has missing value r.X, and splitting variable is X.

- Simplest algorithm:
  - If X is numerical (categorical), impute the overall mean (mode)
- Improved algorithm:
  - If X is numerical (categorical), impute the mean(X|t.C) (the mode(X|t.C))

Surrogate Splits (CART)

Assume record r has missing value r.X, and splitting predicate is P_X.

- Idea: Find splitting predicate $Q_{X'}$ involving another variable X' != X that is most similar to P_X.
  - Similarity sim(Q,P|D) between splits Q and P:
    Sim(Q,P|D) = |{r in D: P(r) and Q(r)}|/|D|
  - 0 <= sim(Q,P|D) <= 1
  - Sim(P,P) = 1

Surrogate Splits: Example

Consider splitting predicate X1 <= 1.

Sim((X1 <= 1), (X2 <= 1)|D) = (3+4)/10

Sim((X1 <= 1), (X2 <= 2)|D) = (6+3)/10

(X2 <= 2) is the preferred surrogate split.

X1	X2	Class
1	1	Yes
1	1	Yes
1	1	Yes
1	2	Yes
1	2	Yes
1	2	No
2	2	No
2	3	No
2	3	No
2	3	No

Overview

- Introduction
- Construction of decision trees
- Evaluation
  - **Predictive accuracy, complexity, training time, selection bias**

Choice of Classification Algorithm?

- Example study: (Lim, Loh, and Shih, Machine Learning 2000)
  - 33 classification algorithms
  - 16 (small) data sets (UC Irvine ML Repository)
  - Each algorithm applied to each data set
- Experimental measurements:
  - Classification accuracy
  - Computational speed
  - Classifier complexity

Classification Algorithms

- Tree-structure classifiers:
  - IND, S-Plus Trees, C4.5, FACT, QUEST, CART, OC1, LMDT, CAL5, T1
- Statistical methods:
  - LDA, QDA, NN, LOG, FDA, PDA, MDA, POL
- Neural networks:
  - LVQ, RBF

Experimental Details

- 16 primary data sets, created 16 more data sets by adding noise
- Converted categorical predictor variables to 0-1 dummy variables if necessary
- Error rates for 6 data sets estimated from supplied test sets, 10-fold cross-validation used for the other data sets

Ranking by Mean Error Rate

Rank	Algorithm	Mean Error	Time
1	Polyclass	0.195	3 hours
2	Quest Multivariate	0.202	4 min
3	Logistic Regression	0.204	4 min
6	LDA	0.208	10 s
8	IND CART	0.215	47 s
12	C4.5 Rules	0.220	20 s
16	Quest Univariate	0.221	40 s
…			

Other Results

- Number of leaves for tree-based classifiers varied widely (median number of leaves between 5 and 32 (removing some outliers))
- Mean misclassification rates for top 26 algorithms are not statistically significantly different, bottom 7 algorithms have significantly lower error rates

Problem: Variable Selection Bias

- Exhaustive search is biased towards variables with more splits (M-category variable has $2^{M-1}-1$) possible splits, an M-valued ordered variable has (M-1) possible splits
- ES is biased towards variables with more missing values
- This is a serious problem, since users want to interpret the tree!

Variable Selection Bias: Null Case

X_i	Dist.	k			
		5	10	15	20
X_1	N(0,1)	.41	.25	.12	.05
X_2	E(0,1)	.42	.26	.12	.05
X_3	U{4}	.04	.02	.01	.00
X_4	C{2}	.02	.01	.01	.00
X_5	C{k}	.11	.46	.74	.90

Example: Teaching Assistant Data

- 151 teaching assistant evaluations over five semesters
- Response is TA evaluation score (above or below average)
- Predictor Variables:
  - English (TA is native English speaker)
  - Course (26 categories)
  - Instructor (25 categories)
  - Session (regular or summer session)
  - NumberResp (number of respondents)

Statistical Significance of Predictors

Predictor	P-value
English	0.005
Session	0.010
Course	0.019
Instructor	0.171
NumberResp	0.992

TA-Data: Decision Tree Results

- Exhaustive search split selection method:
  - First split is on Course
  - One of the splits on the second level is on Instructor
- Less biased split selection method (QUEST): Splits on English

Bias in Split Selection for ES

Assume: No correlation with the class label.

- Question: Should we choose Age or Car?
- Answer: We should choose both of them equally likely!

Age	Yes	No
20	15	15
25	15	15
30	15	15
40	15	15

Car	Yes	No
Sport	20	20
Truck	20	20
Minivan	20	20

Formal Definition of the Bias

- Bias: "Odds of choosing X_1 and X_2 as split variable when neither X_1 nor X_2 is correlated with the class label"
- Formally:
  $Bias(X_1,X_2) = Log_{10}(P(X_1,X_2)/(1-P(X_1,X_2))$,
  $P(X_1,X_2)$: probability of choosing variable X_1 over X_2

We would like: $Bias(X_1,X_2) = 0$ in the Null Case

Formal Definition of the Bias (Contd.)

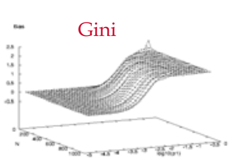
- Example: Synthetic data with two categorical predictor variables
  - X_1: 10 categories
  - X_2: 2 categories
- For each category: Same probability of choosing "Yes" (no correlation)

Car	Yes	No
Car1		
Car2		
Car3		
…		
Car10		

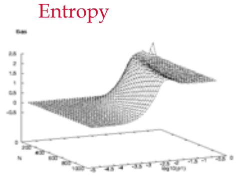
State	Yes	No
CA		
NY		

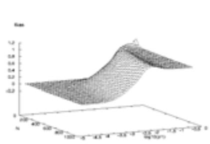
Evidence of the Bias

Gini



Entropy





Gain Ratio

One Explanation

Theorem: (Expected Value of the Gini Gain)
Assume:

- Two classlabels
- n: number of categories
- N: number of records
- p1: probability of having classlabel "Yes"

Then: E(ginigain) = 2p(1-p)*(n-1)/N

Expected ginigain increases linearly with number of categories!

Bias Correction: Intuition

- Value of the splitting criteria is biased under the Null Hypothesis.
- Idea: Use p-value of the criterion: Probability that the value of the criterion under the Null Case is as extreme as the observed value

Method:

1. Compute criterion (gini, entropy, etc.)
2. Compute p-value
3. Choose splitting variable

Correction Through P-Value

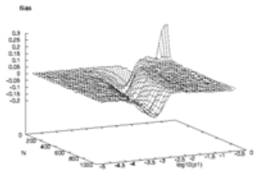
- New p-value criterion:
  - Maintains "good" properties of your favorite splitting criterion
  - Theorem: The correction through the p-value is nearly unbiased.

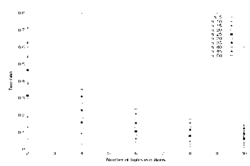
Computation:

1. Exact (randomization statistic; very expensive to compute)
2. Bootstrapping (Monte Carlo simulations; computationally expensive; works only for small p-values)
3. Asymptotic approximations (G^2 for entropy, Chi^2 distribution for Chi^2 test; don't work well in boundary conditions)
4. Tight approximations (cheap, often work well in practice)

Tight Approximation

- Experimental evidence shows that Gamma distribution approximates gini-gain very well.
- We can calculate:
  - Expected gain: $E(gain) = 2p(1-p)*(n-1)/N$
  - Variance of gain: $Var(gain) = 4p(1-p)/N^2[(1-6p-6p^2) * (sum\ 1/N_i - (2n-1)/N) + 2(n-1)p(1-p)]$





Problem: ES and Missing Value

Consider a training database with the following schema: $(X_1, \ldots, X_k, C)$

- Assume the projection onto (X_1, C) is the following:

  {(1, Class1), (2, Class2), (NULL, $Class_{13}$), …, (NULL, $Class_{1N}$)}
  (X_1 has missing values except for the first two records)

- Exhaustive search will very likely split on X_1!

Problem: ES and Missing Value

Consider a training database with the following schema: $(X_1, \ldots, X_k, C)$

- Assume the projection onto (X_1, C) is the following:

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  (X_1 has missing values except for the first two records)

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Concluding Remarks

- Many application of decision trees
- There are many algorithms available for:
  - Split selection
  - Pruning
  - Handling Missing Values
  - Data Access
- Decision tree construction still active research area (after 20+ years!)
- Challenges: Performance, scalability, evolving datasets, new applications

Questions?

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