CS256 – Midterm Exam Study Guide

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Chapter #04 – Classification: Basic Concepts, Decision Trees, and Model Evaluation

Classification	Training Set	Model	Test Set	Example Classification Techniques
Task of assigning objects to one of several predefined categories.	A collection of records. Each **record** contains a set of attributes one of which is the **class**.	A function from the value of record attributes to the class attribute.	A collection of records used to determine the accuracy of the classification model.	1. **Neural Networks** 2. **Decision Tree** 3. **Rule Based Classifier** 4. **Memory Based Reasoning** 5. **Support Vector Machines** 6. **Naïve Bayes and Bayesian Belief Networks**

Induction

Using a training set to generate a model.

Deduction

Process of applying a model to a training set.

Decision Tree Induction

- **Greedy Strategy**
- **Key Decision #1:** Attribute to expand next
- **Key Decision #2:** When to stop expanding

Hunt's Decision Tree Induction Algorithm:

- Let D_t be the set of training records that reach a node t.

1. If D_t contains records that **all belong to the same class y_t**, then t is a leaf node with class value y_t.
2. If D_t is an **empty set**, then t is a leaf node with default value y_d.
3. If D_t contains **records that belong to more than one class and there are no attributes left**, then t is a leaf node with default value is a leaf node with default value y_d.
4. If D_t contains **records that belong to more than one class**, then use an attribute test to split the data into smaller subsets. Recursively apply the same procedure above.

Attribute Types

- **Binary** – Attribute with exactly two possible values.
- **Nominal** – Two or more class values with no intrinsic Order
- **Ordinal** – Two or more class values that can be ordered or ranked
- **Continuous** – Quantitative attribute that can be measured along a continuum.

Splitting Nominal and Ordinal Attributes

- **Binary** – Divides attribute values into two subsets. **This requires the additional step of finding optimal partitioning.**
- **Multi-way** – Use as many partitions as distinct values.

Splitting Based on Continuous Attributes

- **Discretization** – Form an ordinal categorical attribute.
  - **Static** – Discretize once at the beginning
  - **Dynamic** – Ranges can be found by equal interval bucketing, equal frequency bucketing, or clustering.
- **Binary Decision** (A < v or A >v) – Consider all possible splits and find the best cut.
  - **Binary Decision Procedure:** Go between each training set record value and calculate the GINI index if the splitting point was at that value. **Select the splitting point with the lowest $\text{GINI}_{\text{SPLIT}}$ value.**
    - **Computationally inefficient** $O(n)$ – where n is the number of records.

Homogeneity/Low Impurity – Extent to which nodes in the decision tree have the same class value/distribution.

Nodes with high levels of homogeneity (i.e. low levels of impurity) are preferred.

Impurity Measures

For all of these metrics, a lower score is generally preferable.

GINI Index

$$GINI(t) = 1 - \sum_{j=1}^{n_c} \left(p(j|t)\right)^2$$

- t – Node in the decision tree
- j – Class value
- n_c – Number of class values
- $p(j|t)$ – Probability (i.e. relative frequency) of class value j in node t

Minimum Value: 0 when:

$$\exists j\left(p(j|t) = 1\right)$$

Maximum Value: $1 - \frac{1}{n_c}$ when:

$$\forall j\left(p(j|t) = \frac{1}{n_c}\right)$$

$\text{GINI}_{\text{SPLIT}}$

$$GINI_{SPLIT} = \sum_{i=1}^{k} \frac{n_i}{n} \cdot GINI(i)$$

- i – Child node
- n – Number of records in parent node. Note:

$$n = \sum_{i=1}^{k} n_i$$

- n_i – Number of child nodes (i.e. attribute partitions)
- $GINI(i)$ – GINI index value of node i.

Minimum Value: 0 when:

$$\forall i\left(GINI(i) = 0\right)$$

Maximum Value: $1 - \frac{1}{n_c}$ when:

$$\forall i\left(GINI(i) = 1 - \frac{1}{n_c}\right)$$

Entropy

$$Entropy(t) = -\sum_{j=1}^{n_c} p(j|t) \cdot log_2\left(p(j|t)\right)$$

- t – Node in the decision tree
- j – Class value
- n_c – Number of class values
- $p(j|t)$ – Probability (i.e. relative frequency) of class value j in node t

Minimum Value: 0 when:

$$\exists j\left(p(j|t) = 1\right)$$

Maximum Value: $\log_2(n_c)$ when:

$$\forall j\left(p(j|t) = \frac{1}{n_c}\right)$$

Information Gain

$$GAIN_{SPLIT}(t) = Entropy(p) - \left(\sum_{i=1}^{k} \frac{n_i}{n} \cdot Entropy(i)\right)$$

- p – Parent node in the decision tree
- i – Child node in the decision tree
- k – Number of child nodes
- n_i – Number of records in child node i
- n – Number of records in parent node p

$$n = \sum_{i=1}^{k} n_i$$

Key Note: A higher $GAIN_{SPLIT}$ is preferable unlike with the other metrics where a lower value was better.

Disadvantage of Information Gain: Tends to prefer splits that result in a large number of partitions, each being small but pure (i.e. overfitting)

Normalizing for Split Size

$$GainRATIO_{Split} = \frac{Gain_{SPLIT}(t)}{SplitINFO}$$

$$SplitINFO = -\sum_{i=1}^{k} \frac{n_i}{n} \cdot log_2\left(\frac{n_i}{n}\right)$$

$Split_{INFO}$ penalizes a large split by reducing the gain.

Classification Error

$$Error(t) = 1 - max_j(p(j|t))$$

- t – Node in the decision tree
- j – Class value
- $p(j|t)$ – Probability (i.e. relative frequency) of class value j in node t

Minimum Value: 0 when:
$\exists j(p(j|t) = 1)$

Maximum Value: $1 - \frac{1}{n_c}$ when:
$\forall j\left(p(j|t) = \frac{1}{n_c}\right)$

Stopping Criteria for Decision Tree Induction

Three Stopping Criteria for Decision Tree Induction

- **When all records in a node have the same class value**
- **When all records in a node have similar attribute values.**
- **Early Termination**

Underfitting – When a model is too simple, both training and test errors are large.

Overfitting – When a model becomes too complex (e.g. too large a tree), the test error begins to increase even though the training error decreases.

- **Result:** Training error is **NOT** representative for generalization error.

Causes of Overfitting

- **Noise**
- **Insufficient training records** (i.e. lack of representative samples)

Resubstitution Error

Error on the **training** set.

Single Leaf Node Error: $e(t)$
Total Resubstitution Error: $e(T)$

$$e(T) = \sum e(t)$$

Generalization Error

Error on the **testing** data.

Single Leaf Node Error: $e'(t)$
Total Generalization Error: $e'(T)$

$$e'(T) = \sum e'(t)$$

Generalization Error Estimation

Optimistic Estimation

Training error is equal to the testing error.

$$\sum e(t) = \sum e'(t)$$

Pessimistic Estimation

Assign a penalty term to ea.

$$e'(t) = e(t) + 0.5$$

Total Pessimistic Error

$$e'^{(T)} = \sum(e(t)) + N \cdot 0.5$$

N – Number of leaf nodes.

Reduced Error Pruning

Use a validation set to estimate the generalization error.

Occam's Razor

Given two models with similar generalization errors, one should prefer the simpler model over the more complex model.

This is because more complex model has a greater chance of fitting accidentally by errors in the data.

Pre-pruning (Early Stopping Rule)

- **Stop the induction algorithm before it becomes a full tree.**
- **Typical Stopping Rules:**
  - All remaining records have the same class value
  - All attribute values are the same.
- **More restrictive conditions:**
  - Number of instances is below a user-specified threshold.
  - Expanding the current node does not improve impurity measures (e.g. GINI Index, Information Gain)
  - Class distribution of instances are independent of available features.

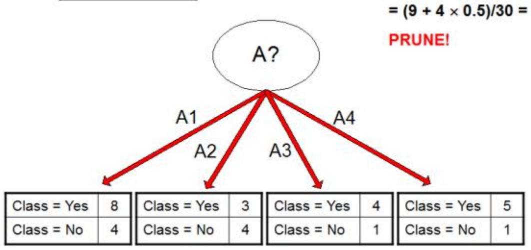
Post-pruning (Early Stopping Rule)

- **Grow the decision tree to its entirety.**
- Trim nodes in the tree in a **bottom-up fashion.**
- Only **trim nodes if by trimming the estimate of the generalization error improves.**
- New leaf node's **class label is determined from the majority class of instances in the merged node.**

Example of Post-Pruning

Class = Yes	20
Class = No	10
Error = 10/30	

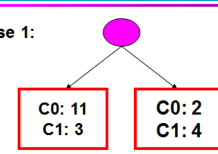
Training Error (Before splitting) = 10/30
Pessimistic error = (10 + 0.5)/30 = 10.5/30
Training Error (After splitting) = 9/30
Pessimistic error (After splitting)
= (9 + 4 × 0.5)/30 = 11/30
PRUNE!



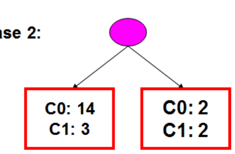
Examples of Post-pruning

- Optimistic error?
  Don't prune for both cases
- Pessimistic error?
  Don't prune case 1, prune case 2
- Reduced error pruning?
  Depends on validation set

Case 1:



Case 2:



Handling Missing Attribute Values

Issues Associated with Missing Attribute Values

- Affects how impurity measures are computed
- Affects how to distribute instances with missing value to child nodes.
- Affects how to test instance with missing value is classified.

Computing Impurity Measure

- Calculate entropies (i.e. information gain) with element with missing value EXCLUDED.
- Multiply by scalar of elements included over total number of elements (in below example 9 elements included over 10 total elements hence 0.9):

Computing Impurity Measure

Tid	Refund	Marital Status	Taxable Income	Class
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	?	Single	90K	Yes

Missing value

Before Splitting:
Entropy(Parent)
= -0.3 log(0.3)-(0.7)log(0.7) = 0.8813

	Class = Yes	Class = No
Refund=Yes	0	3
Refund=No	2	4
Refund=?	1	0

Split on Refund:

Entropy(Refund=Yes) = 0

Entropy(Refund=No)
= -(2/6)log(2/6) – (4/6)log(4/6) = 0.9183

Entropy(Children)
= 0.3 (0) + 0.6 (0.9183) = 0.551

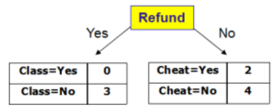
Gain = 0.9 × (0.8813 – 0.551) = 0.3303

Distribute Instances

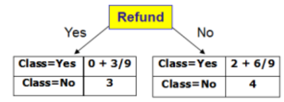
- Split the missing record between the two child nodes
- Percentage of child node that goes to each child is portion to the relative frequency of that attribute value.

Distribute Instances

Tid	Refund	Marital Status	Taxable Income	Class
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No



Tid	Refund	Marital Status	Taxable Income	Class
10	?	Single	90K	Yes



Probability that Refund=Yes is 3/9

Probability that Refund=No is 6/9

Assign record to the left child with weight = 3/9 and to the right child with weight = 6/9

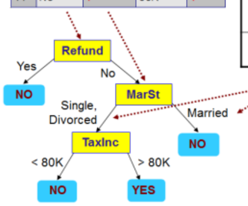
Classifying New/Unseen Records with Missing Data

- Pick the most likely of child nodes and use continue down that portion of the tree.

Classify Instances

New record:

Tid	Refund	Marital Status	Taxable Income	Class
11	No	?	85K	?



	Married	Single	Divorced	Total
Class=No	3	1	0	4
Class=Yes	6/9	1	1	2.67
Total	3.67	2	1	6.67

Probability that Marital Status = Married is 3.67/6.67

Probability that Marital Status ={Single,Divorced} is 3/6.67

Data Fragmentation – At each level of the tree, the number of instances gets smaller. At leaf nodes, the number of instances could be too small to be statistically significant.

Oblique Decision Tree – Test condition in a node may involve multiple attributes.
- **Advantage** – Most expressive decision tree
- **Disadvantage** – Finding optimal test condition is computationally expensive.

Tree Induction: NP Hard

Alternate Strategies
- Bottom Up Tree Generation
- Bidirectional Tree Generation
  - Inside-out Bidirectional
  - Outside-in Bidirectional

Expressiveness – Decision trees do not generalize well to certain types of functions including a parity function which would require a complete tree.

Decision Boundary – Borderline between two neighboring regions of different classes. In non-oblique decision trees, this is parallel to access since it involves a single attribute at a time.

Tree Replication – In a decision tree, a subtree may appear in multiple branches. This leads to unnecessary memory usage.

Performance Evaluation

- Focus on the predictive capability of a model.

Confusion Matrix

		Predicted Class	
		Class = Yes	Class=No
Actual Class	Class = Yes	a	b
	Class=No	c	d

a – True Positive (TP)
b – False Negative (FN)
c – False Positive (FP)
d – True Negative (TN)

Accuracy

$$Accuracy = \frac{A + D}{A + B + C + D}$$

$$Accuracy = \frac{TP + TN}{TP + FN + FP + TN}$$

- Accuracy only tells part of the story.
  - Example: Two Class Problem
    - Number of Class 0 Examples: 9990
    - Number of Class 1 Examples: 10
    - If the model predicts everything as class 0, its accuracy is 99.9% but it cannot detect any class 1.

Cost Matrix

		Predicted Class	
		Class = Yes	Class=No
Actual Class	Class = Yes	C(Y|Y)	C(N|Y)
	Class=No	C(Y|N)	C(N|N)

- $C(j \mid k)$– Cost of predicting class "j" given the actual class is "k".

$$TotalCost = a \cdot C(Y|Y) + b \cdot C(N|Y) + c \cdot C(Y|N) + d \cdot C(N|N)$$

- Cost matrix can be a better performance evaluation as it accounts for different costs of depending on the type of error.

$$Precision\ (p) = \frac{a}{a + c}$$

- **Precision** – Accuracy of positive predictions. Biased towards C(Y|Y) & C(Y|N).
  - **a** – True positive.
  - **c** – False positive.

$$Recall\ (r) = \frac{a}{a + b}$$

- **Precision** – Accuracy of records with positive class value. Biased towards C(Y|Y) & C(N|Y).
  - **a** – True positive.
  - **b** – False negative.

$$F\_Measure\ (F) = \frac{2 \cdot r \cdot p}{r + p} = \frac{a + c}{2 \cdot a + b + c}$$

- **F-Measure** – Biased two all except C(N|N) (i.e. true negative)
  - **r** – Recall
  - **p** – Precision
  - **c** – False Positive

$$WA = \frac{w_1 \cdot a + w_4 \cdot d}{w_1 \cdot a + w_2 \cdot b + w_3 \cdot c + w_4 \cdot d}$$ n – Number of instances covered by rule n_c – Number of positive instances covered by rule.	**Proportionality of Cost and Accuracy** • Cost and accuracy are proportional if: $C(Y\|Y) = C(N\|N)$ and $C(Y\|N) = C(N\|Y)$	**Sample Size and Model Performance** • **Learning Curve** – Shows how model accuracy changes (and varies) with sample size. • **Effects of Small Sample Size:** ○ **Bias in the estimate** ○ **Variance in the estimate.**

Methods for Model Comparison

Holdout – Reserve 2/3 of labelled examples for training and 1/3 for testing.

Disadvantages
- **Uses on a subset of the labelled examples** when training the model.
- Model **dependent on the composition of the training and test sets**.
- **Training and test sets are not independent** since come from same original set. If one class value is over- or under-represented in either set, it will skew the results.

Random Subsampling – Repeats the whole out method multiple times with replacement.

Disadvantages:
- Still **uses only a subset of the labelled examples** to build the model.
- **No control of how many times each record appears in the training and test sets**. If a particular record is always in the training set, it may skew the model.

Accuracy of k Random Subsamplings

$$acc_{sub} = \frac{1}{k} \cdot \sum_{i=1}^{k} acc_i$$

- k – Number of iterations
- acc_i – Accuracy of the i^{th} iteration.

Cross Validation – Partition the labelled dataset into *k* disjoint subsets.
- **k-Fold** – Train on k-1 partitions and test on the remaining one.
- **Leave-One-Out** – The number of partitions equals the number of training samples.

Accuracy of k-Fold Cross Validation

$$acc_{sub} = \frac{1}{k} \cdot \sum_{i=1}^{k} acc_i$$

- k – Number of iterations
- acc_i – Accuracy of the i^{th} iteration.

Disadvantages:
- **Computationally expensive** as process is repeated *k* times.
- Depending on size of partition (e.g. 1 for Leave-One-Out), **accuracy from iteration to iteration** can vary significantly.

Bootstrap –	

Minimum Description Length	$WeightedDistance = \frac{1}{d^2}$

Chapter #05 – Additional Classification Techniques

Rule-Based Classifiers

Classifies records using a collection of "if…then…" rules. Form of Rule: $(Condition) \rightarrow y$ • **Condition** (**Antecedent**, **LHS**) – Conjunction of attributes. • y (**Consequent**, **RHS**) – Class value.	**Cover** – A rule r covers an instance x if the attributes of x satisfy the condition (LHS) of the rule. **Coverage of a Rule** – Fraction of records that satisfy the antecedent of a rule. **Accuracy of a Rule** – For records covered by a rule, it is the fraction of records that have the matching class value.	**Mutually Exclusive Rule Set** – Rules in the set are independent of each other such that **each record is covered by at most one rule**. **Exhaustive Rule Set** – A set of rules that covers every possible combination of attribute values. Hence, **each record is covered by at least one rule**.	

$$Accuracy = \frac{n_c}{n}$$ n – Number of instances covered by rule n_c – Number of positive instances covered by rule.	$$Laplace = \frac{n_c + 1}{n + k}$$ n – Number of instances covered by rule n_c – Number of positive instances covered by rule. k – Number of classes	$$m\_estimate = \frac{n_c + p \cdot k}{n + k}$$ n – Number of instances covered by rule n_c – Number of positive instances covered by rule. k – Number of classes p – Prior probability of positive class.

	$WeightedDistance = \frac{1}{d^2}$

	ROC Curve	

Bootstrap –	• Used to illustrate the performance of a binary classifier.
	• Two Dimensional
	  ○ **X-Axis** – False Positive Rate
	  ○ **Y-Axis** – True Positive Rate	

Miscellaneous

Decision Tree Algorithm		
Advantages • **Inexpensive to construct** • **Extremely fast at classifying unknown records.** • **Easy to interpret for small sized trees.** • **Accuracy is comparable to other classification techniques for many simple datasets.** (Since everything comes right from the data) **Disadvantages** • **May not generalize well for certain types of functions** (e.g. Parity function requires a complete tree) • **May be insufficient for modelling continuous variables** that do not allow oblique nodes.		