Advanced Predictive Modeling Workshop

Tree-based Methods

March 27, 2017
San Diego, CA

Kudakwashe Chibanda, FCAS, MAAA
kudakwashe.chibanda@pwc.com

Jean-François Greeff, FASSA
jean.francois.greeff@pwc.com
Agenda

1. Decision trees
2. Ensembles
3. Classification examples
4. Regression examples
Decision trees

“If you dream of a forest, you better learn how to plant a tree”
Introduction

Is a region more than 20% black?

• Non-parametric classification/regression tools
• Create splits according to measures of homogeneity

Features

Is HS grad rate <78%?

• Simple to understand and interpret
• Flexible for non-linear or complex relationships

Advantages

Is HS grad rate >87%?

• Overfitting
• Unstable/Biased if certain classes of data dominate

Disadvantages

Is the county in the NE or South?

Decision Tree: The Obama-Clinton Divide (from NYT April, 2008)
Splitting Criteria

- Entropy measures the **disorderliness** for each variable level
- The **purer** the level for a given response, the more **predictable** the outcome
- The weighted average entropy across all levels of a variable gives us information
- Gini impurity is a purity measure that relies on **misclassification**
- It measures the probability that a randomly selected observation will be placed in the wrong bucket (i.e. misclassified)

- A large number of observations in a level can **bias** the information towards the entropy of the concentrated level
- To compensate, **Intrinsic Information** is calculated
- II takes size and number of levels into account i.e. penalizes large values/splits
- \( \text{Gain Ratio} = \frac{\text{Information Gain}}{\text{Intrinsic Information}} \)
- **p-values of Chi-Square** statistics can be used to split nodes
- Measure statistical significance of a variable’s levels and the response (i.e. test **null hypothesis of independence**)
- Insignificant splits are merged while significant ones are tested for further splits
Purity Measures Calculations

<table>
<thead>
<tr>
<th>Outlook</th>
<th>Yes</th>
<th>No</th>
<th>Total</th>
</tr>
</thead>
<tbody>
<tr>
<td>(x variable)</td>
<td>(y variable)</td>
<td>(by level)</td>
<td></td>
</tr>
<tr>
<td>Sunny (node i)</td>
<td>3</td>
<td>2</td>
<td>5</td>
</tr>
<tr>
<td>Overcast</td>
<td>4</td>
<td>0</td>
<td>4</td>
</tr>
<tr>
<td>Rainy</td>
<td>20</td>
<td>30</td>
<td>50</td>
</tr>
<tr>
<td>Total (t branch)</td>
<td>27</td>
<td>32</td>
<td>59</td>
</tr>
</tbody>
</table>

Entropy/Information measure purity of outcomes at each node, taking number and size of nodes into account

Information Gain and Gini also take purity at the branch (regardless of splits) into account

- **Entropy** \( H_y(i) \) = \( - \sum_y p(y|i) \log(y|i) \)
  - Entropy(sunny) = \( - \left( \frac{3}{5} \log \left( \frac{3}{5} \right) + \frac{2}{5} \log \left( \frac{2}{5} \right) \right) = 0.971 \)

- **Information** \( H(t) \) = \( - \sum_{i=0}^{c} p(i) H_y(i) \)
  - \( H(\text{Outlook}) = \frac{5}{59} * 0.971 + \frac{4}{59} * 0 + \frac{50}{59} * 0.971 = 0.905 \)

- **Information Gain** \( (IG(t)) = I(t) - H(t) \)
  - \( IG(t) = - \left( \frac{27}{59} \log \left( \frac{27}{59} \right) + \frac{32}{59} \log \left( \frac{32}{59} \right) \right) - 0.905 = 0.09 \)

- **Intrinsic Information** \( [II(t)] = \)
  - \( II(t) = - \left( \frac{5}{59} \log \left( \frac{5}{59} \right) + \frac{4}{59} \log \left( \frac{4}{59} \right) + \frac{50}{59} \log \left( \frac{50}{59} \right) \right) = 0.767 \)

- **Gain Ratio** \( ([GR(t)] = \frac{IG(t)}{II(t)} \)
  - \( GR(t) = \frac{0.09}{0.767} = 0.117 \)

- **Gini** \( (G(t) = 1 - \sum_y p(i|t)^2 \)
  - (prior to split)
  - \( G(t) = 1 - \left[ \left( \frac{27}{32} \right)^2 + \left( \frac{32}{59} \right)^2 \right] = 0.496 \)
Receiver Operating Characteristic (ROC)

• To measure predictive performance in binary classifier models, we rely on **confusion matrices**

• Using a selected **threshold**, we can bucket observations into each one of the four buckets as shown in the table

• Receiver Operator Curves (ROC) are commonly used to select a threshold

  • By plotting relationship between TPR and FPR, we can determine the point that **maximizes TPR while minimizing FPR**

  • We can also summarize the information by calculating **Area Under Curve (AUC)**

<table>
<thead>
<tr>
<th>Actual</th>
<th>Predicted</th>
<th>True Positive (TP)</th>
<th>False Negative (FN)</th>
<th>True Positive Rate (Sensitivity): $TPR = \frac{TP}{TP + FN}$</th>
</tr>
</thead>
<tbody>
<tr>
<td>False Positive (FP)</td>
<td>True Negative (TN)</td>
<td>False Positive Rate (Fall-out): $FPR = \frac{FP}{FP + TN}$</td>
<td></td>
<td></td>
</tr>
</tbody>
</table>
Types of Trees – ID3 and C4.5

**ID3**

- **Purity measure**: *Entropy*
- **Methodology**: at each node, calculate entropy for all variables. Select variable with minimum entropy
- **Splits**: can have multiple splits
- **Continuous/missing data**: no
- **Risks**: does not **prune**
  - **Fix**: use **stopping criteria** to avoid overfitting

**C4.5**

- **Purity measure**: *Information Gain*
- **Methodology & splits**: similar to ID3
- **Continuous/missing data**: yes
- **Risks**: susceptible to **outliers**
  - **Fix**: remove outliers
Classification And Regression Trees (CART)

**Classification Trees**

- **Purity measure**: *Gini impurity*
- **Methodology**: at each node, calculate gini for all variables. Select split with minimum gini
- **Splits**: *binary*
- **Continuous data**: requires splitting
- **Risks**: does not work for *multiple category* data
  - **Fix**: use CHAID/ID3

**Regression Trees**

- **Purity measure**: *Variance reduction*
- **Methodology**: For each variable, the split is determined by the point that *minimizes SSE*
- **Continuous/missing data**: yes
- **Risks**: *overfitting*
  - **Fix**: *prune* using Sum of Square Errors (SSE)
**Chi-square Automatic Interaction Detector (CHAID)**

**Step 1:** Discretize continuous variables. For categorical variables, pair levels

S O R W

**Step 2:** Perform Chi-Square test for each pair’s significance with response

S;O S;R R;O R;W S;W O;W

Significant?

Y/N Y/N Y/N Y/N Y/N Y/N

**Step 3:** Merge pair with least significance & repeat test until **stopping criteria**

(S+O); R (S+O); W

Y/N Y/N

**Step 4:** Test whether merged categories should be further split

(S+R); O

Y/N

**Step 5:** Repeat step 1-4 for every variable to determine optimal split

Step 6: Select root node based on variable with smallest $\chi^2$ with response

**Signature characteristic of CHAID is its ability to handle multiple categories**

Apply **Bonferroni Adjustment** to penalize for multiple testing
Classification Example
Ensembles
Weak Learners and Strong Classifiers

**Weak learners**
- Performs well only on a subset of the domain
- May be unstable with small perturbations in data
- May be biased in its predictions

**Strong classifiers**
- Performs well over the whole domain
- Stable across small changes in the data
- Unbiased in its predictions

Typically what we **have**

What we **want**
Illustration of Ensembling (1)

**Situation**
- Transmit binary signal from A to B
- Ensure that signal uncorrupted

**Ensemble approach**
- Use 3 independent signal carriers
- Majority vote (Choose bits where 2+ of three carriers agree)

**Consequence**
- Reconstruct signal with reduced error

<table>
<thead>
<tr>
<th>Signal</th>
<th>Accuracy</th>
</tr>
</thead>
<tbody>
<tr>
<td>Original signal</td>
<td>0100101001000110</td>
</tr>
<tr>
<td>Signal 1</td>
<td>0100001001000110</td>
</tr>
<tr>
<td>Signal 2</td>
<td>0100101001000111</td>
</tr>
<tr>
<td>Signal 3</td>
<td>0100100101000110</td>
</tr>
<tr>
<td>Combined Signal</td>
<td>0100101010100110</td>
</tr>
</tbody>
</table>

<table>
<thead>
<tr>
<th>Signal</th>
<th>Accuracy</th>
</tr>
</thead>
<tbody>
<tr>
<td>Original signal</td>
<td>0100101001000110</td>
</tr>
<tr>
<td>Signal 1</td>
<td>0100001010101010</td>
</tr>
<tr>
<td>Signal 2</td>
<td>0001110001111110</td>
</tr>
<tr>
<td>Signal 3</td>
<td>0100000000100100</td>
</tr>
<tr>
<td>Combined Signal</td>
<td>0100000000010110</td>
</tr>
</tbody>
</table>
Illustration of Ensembling (2)

- 3 signals with probability of corruption 30% per bit
  - \( P(\text{All correct}) = 0.7^3 = 34.29\% \)
  - \( P(2 \text{ correct}) = 3 \times (0.7^2 \times 0.3) = 44.09\% \)
  - \( P(1 \text{ correct}) = 3 \times (0.7^1 \times 0.3^2) = 18.90\% \)
  - \( P(\text{None correct}) = 0.3^3 = 2.70\% \)

- Correction made for 44.09% of the bits
- Expected accuracy of 78.38% per bit

Only if signals *uncorrelated*
Bagging
Bootstrap Aggregation

Algorithm
1. Create bootstrap resample of data
2. Fit model on each resample
3. Scoring:
   - Classification: Majority vote
   - Regression: Mean/Median score

Advantages
- Produces more stable predictions – i.e. reduces variance
- Less likely to over-fit data

Disadvantages
- Generates a “black box”
Random Forests
Bagging Decision Trees

- Introduced by Leo Breiman (2001)
- Uses bagging to improve decision trees
- De-correlates trees by sampling
  - Data with replacement
  - Columns/features at each node
- Produces out-of-bag error rates
- Produces variable importance measure
- Parameters to tune*:
  1. Number of trees
  2. Number of features to select at each node

* There are other parameters such as the sampling rate and maximum depth of the tree.
**Boosting**

**Algorithm**
- Rather than fitting models to bootstrap samples of the data – boosting fits sequential models focusing on areas of poor performance
- Subsequent models correct errors of previous models

**Advantages**
- Decrease bias in predictions

**Disadvantages**
- Generates a “black box”
- May be sensitive to outliers and noise

<table>
<thead>
<tr>
<th>AdaBoost</th>
<th>GBM</th>
</tr>
</thead>
<tbody>
<tr>
<td>Adaptive Boosting</td>
<td>Gradient Boosted</td>
</tr>
<tr>
<td></td>
<td>Machines / Models</td>
</tr>
<tr>
<td>Fits model to weighted</td>
<td>Fits model to the</td>
</tr>
<tr>
<td>distribution of the</td>
<td>residual of the prior</td>
</tr>
<tr>
<td>data. More weight is</td>
<td>models.</td>
</tr>
<tr>
<td>given to observations</td>
<td></td>
</tr>
<tr>
<td>that have the highest</td>
<td></td>
</tr>
<tr>
<td>error rate.</td>
<td></td>
</tr>
</tbody>
</table>
Gradient Boosted Trees
Boosting Decision Trees

- Introduced by Jerome Friedman (1999)
- Uses boosting to improve decision trees
- XGBoost algorithm most common
  - Stochastic gradient descent
  - Feature sub-sampling
- Parameters to tune*:  
  1. Number of trees
  2. Depth of trees
  3. Learning rate
**Stacking**
*Stacked generalization & Blending*

**Algorithm**
- Two stages of model fitting
  1. First Stage: Fit base learners to data
  2. Second Stage: Fit meta-learner to predictions of base learners

**Considerations**
- Different approaches to how the stacking is performed
- Careful consideration needs to be given to what data is used at what stages
- Need diverse models
Classification Example
Predictive Modeling Applications
Advanced Predictive Modeling Workshop

Tree-based Methods

Q&A

Kudakwashe Chibanda, FCAS, MAAA
kudakwashe.chibanda@pwc.com

Jean-François Greeff, FASSA
jean.francois.greeff@pwc.com