${\rm INFO~6105}$ Data Science Engineering Methods and Tools

Lecture 8 Classification Trees

Ebrahim Nasrabadi nasrabadi@northeastern.edu

> College of Engineering Northeastern University

> > Fall 2019

$$y_i \in \{\mathcal{C}_1, \ldots, \mathcal{C}_K\}.$$

• Tree-base methods can be applied to multi-class classification problems where

$$y_i \in \{\mathcal{C}_1, \ldots, \mathcal{C}_K\}.$$

• Classification tees work much like regression trees. We need to modify

$$y_i \in \{\mathcal{C}_1, \ldots, \mathcal{C}_K\}.$$

- Classification tees work much like regression trees. We need to modify
 - ▶ criterion for splitting nodes. Instead of minimizing the RSS, we minimize a classification loss function.

$$y_i \in \{\mathcal{C}_1, \ldots, \mathcal{C}_K\}.$$

- Classification tees work much like regression trees. We need to modify
 - ▶ criterion for splitting nodes. Instead of minimizing the RSS, we minimize a classification loss function.
 - method for pruning tree.

$$y_i \in \{\mathcal{C}_1, \ldots, \mathcal{C}_K\}.$$

- Classification tees work much like regression trees. We need to modify
 - ▶ criterion for splitting nodes. Instead of minimizing the RSS, we minimize a classification loss function.
 - ▶ method for pruning tree.
- We predict the response by majority vote, i.e., pick the most common class in every region.

 \bullet Let node j represent the region R_j with N_j observations.

- Let node j represent the region R_j with N_j observations.
- Let \hat{p}_{jk} be the proportion of observations within R_j in class k, i.e.,

$$\hat{p}_{jk} = \frac{1}{N_j} \sum_{i: x_i \in R_j} \mathbf{1}(y_i = k)$$

- Let node j represent the region R_j with N_j observations.
- Let \hat{p}_{jk} be the proportion of observations within R_j in class k, i.e.,

$$\hat{p}_{jk} = \frac{1}{N_j} \sum_{i: x_i \in R_j} \mathbf{1}(y_i = k)$$

• The class prediction in region R_j is:

$$\hat{y}_{R_j} = \arg\max_{k} \hat{p}_{jk}$$



- Let node j represent the region R_j with N_j observations.
- Let \hat{p}_{jk} be the proportion of observations within R_j in class k, i.e.,

$$\hat{p}_{jk} = \frac{1}{N_j} \sum_{i: x_i \in R_j} \mathbf{1}(y_i = k)$$

• The class prediction in region R_j is:

$$\hat{y}_{R_j} = \arg\max_k \hat{p}_{jk}$$

• The class probability distribution in region R_j is:

$$(\hat{p}_{j1}, \hat{p}_{j2}, \dots, \hat{p}_{jK})$$



• Misclassification rate:

$$\sum_{j=1}^{|T|} q_j \sum_{i: x_j \in R_j} \mathbf{1}(y_i \neq \hat{y}_{R_j})$$

where q_j is the proportion of observations in R_j .

• Misclassification rate:

$$\sum_{j=1}^{|T|} q_j \sum_{i: x_j \in R_j} \mathbf{1}(y_i \neq \hat{y}_{R_j})$$

where q_j is the proportion of observations in R_j .

• The cross-entropy

$$-\sum_{j=1}^{|T|} q_{j} \sum_{k=1}^{K} \hat{p}_{jk} \log{(\hat{p}_{jk})}$$

• Misclassification rate:

$$\sum_{j=1}^{|T|} q_j \sum_{i: x_j \in R_j} \mathbf{1}(y_i \neq \hat{y}_{R_j})$$

where q_j is the proportion of observations in R_j .

• The cross-entropy

$$-\sum_{j=1}^{|T|} q_{j} \sum_{k=1}^{K} \hat{p}_{jk} \log{(\hat{p}_{jk})}$$

• The Gini index

$$\sum_{j=1}^{|T|} q_j \sum_{k=1}^{K} \hat{p}_{jk} (1 - \hat{p}_{jk})$$

◆ロト ◆団ト ◆豆ト ◆豆ト を めんぐ

• The Gini index and cross-entropy are better measures of the purity of a region, i.e. they are low when the region is mostly one category.

- The Gini index and cross-entropy are better measures of the purity of a region, i.e. they are low when the region is mostly one category.
- They take on a small value if all of \hat{p}_{jk} 's are close to zero except one that is close to one.

- The Gini index and cross-entropy are better measures of the purity of a region, i.e. they are low when the region is mostly one category.
- They take on a small value if all of \hat{p}_{jk} 's are close to zero except one that is close to one.
- Motivation for Gini index: If instead of predicting the most likely class, we predict a random sample from the distribution

$$(\hat{p}_{j1},\hat{p}_{j2},\ldots,\hat{p}_{jK}),$$

the Gini index is the expected misclassification rate.

- The Gini index and cross-entropy are better measures of the purity of a region, i.e. they are low when the region is mostly one category.
- They take on a small value if all of \hat{p}_{jk} 's are close to zero except one that is close to one.
- Motivation for Gini index: If instead of predicting the most likely class, we predict a random sample from the distribution

$$(\hat{p}_{j1},\hat{p}_{j2},\ldots,\hat{p}_{jK}),$$

the Gini index is the expected misclassification rate.

• It is typical to use the Gini index or cross-entropy for growing the tree, while using the misclassification rate when pruning the tree.

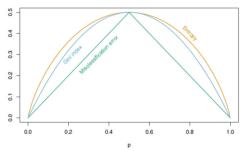
←ロト ←団ト ← 重ト 重 り へ ○

Misclassification Rate =
$$1 - \max(p, 1 - p)$$

Gini index = $2p(1 - p)$
Cross-entropy = $-p \log p - (1 - p) \log(1 - p)$

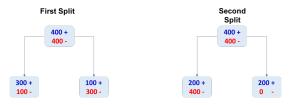
Misclassification Rate =
$$1 - \max(p, 1 - p)$$

Gini index = $2p(1 - p)$
Cross-entropy = $-p \log p - (1 - p) \log(1 - p)$



Example

• Consider a two-class problem with 400 observations in each class and two splits as:



Example

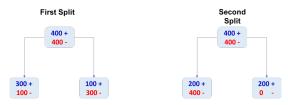
• Consider a two-class problem with 400 observations in each class and two splits as:



• Both splits produce a misclassification rate of 0.25, but the second split produces a pure node and is probably preferable.

Example

• Consider a two-class problem with 400 observations in each class and two splits as:



- Both splits produce a misclassification rate of 0.25, but the second split produces a pure node and is probably preferable.
- Both the Gini index and cross-entropy are lower for the second split. For this reason, either the Gini index or cross-entropy are typically used when growing the tree.

• Consider a node t with size N_t and impurity Q_t .

- Consider a node t with size N_t and impurity Q_t .
- For some variable j and split point s, we split node t into two nodes, say t_L and t_R with sizes N_{t_L} and N_{t_R} and impurities Q_{t_L} and Q_{t_R}

- Consider a node t with size N_t and impurity Q_t .
- For some variable j and split point s, we split node t into two nodes, say t_L and t_R with sizes N_{t_L} and N_{t_R} and impurities Q_{t_L} and Q_{t_R}
- The average decrease of impurity is

$$\Delta(j,s) = Q_t - \frac{1}{N_t} \left(\frac{N_{t_L}}{N_t} Q_{t_R} + \frac{N_{t_L}}{N_t} Q_{t_R} \right)$$

- Consider a node t with size N_t and impurity Q_t .
- For some variable j and split point s, we split node t into two nodes, say t_L and t_R with sizes N_{t_L} and N_{t_R} and impurities Q_{t_L} and Q_{t_R}
- The average decrease of impurity is

$$\Delta(j,s) = Q_t - \frac{1}{N_t} \left(\frac{N_{t_L}}{N_t} Q_{t_R} + \frac{N_{t_L}}{N_t} Q_{t_R} \right)$$

• We select at each step the splitting variable j and the split point s that maximizes $\Delta(j,s)$ or, equivalently, that minimizes the average impurity

$$\frac{N_{t_L}}{N_t}Q_{t_R} + \frac{N_{t_L}}{N_t}Q_{t_R}$$

4 ロ ト 4 回 ト 4 重 ト 4 重 ・ 夕 Q や

• When splitting a categorical variable having q unordered values, there are $2^{q-1}-1$ possible partitions of the q values into two groups.

- When splitting a categorical variable having q unordered values, there are $2^{q-1} 1$ possible partitions of the q values into two groups.
- It becomes computationally expensive for large q.

- When splitting a categorical variable having q unordered values, there are $2^{q-1}-1$ possible partitions of the q values into two groups.
- It becomes computationally expensive for large q.
- In the 2-class case, this computation can be simplified.

- When splitting a categorical variable having q unordered values, there are $2^{q-1}-1$ possible partitions of the q values into two groups.
- It becomes computationally expensive for large q.
- In the 2-class case, this computation can be simplified.
 - ▶ We order the predictor values according to the proportion falling in positive class.

- When splitting a categorical variable having q unordered values, there are $2^{q-1} 1$ possible partitions of the q values into two groups.
- It becomes computationally expensive for large q.
- In the 2-class case, this computation can be simplified.
 - ▶ We order the predictor values according to the proportion falling in positive class.
 - ▶ Then we split this predictor as if it were an ordered predictor.

- When splitting a categorical variable having q unordered values, there are $2^{q-1}-1$ possible partitions of the q values into two groups.
- It becomes computationally expensive for large q.
- In the 2-class case, this computation can be simplified.
 - ▶ We order the predictor values according to the proportion falling in positive class.
 - ▶ Then we split this predictor as if it were an ordered predictor.
 - ▶ One can show this gives the optimal split, in terms of cross-entropy or Gini index, among all possible $2^{q-1} 1$ splits.

• The partitioning algorithm tends to favor categorical predictors with many levels q;

- The partitioning algorithm tends to favor categorical predictors with many levels q;
- \bullet the number of partitions grows exponentially in q,

- The partitioning algorithm tends to favor categorical predictors with many levels q;
- the number of partitions grows exponentially in q,
- the more choices we have, the more likely we can find a good one for the data at hand

- The partitioning algorithm tends to favor categorical predictors with many levels q;
- the number of partitions grows exponentially in q,
- the more choices we have, the more likely we can find a good one for the data at hand
- ullet This can lead to severe overfitting if q is large, and such variables should be avoided

• Very easy to interpret

- Very easy to interpret
- Easy to visualize (especially if they are small).

- Very easy to interpret
- Easy to visualize (especially if they are small).
- Handle qualitative predictors without the need to create dummy variables

- Very easy to interpret
- Easy to visualize (especially if they are small).
- Handle qualitative predictors without the need to create dummy variables
- Invariant to monotone transformation of predictor variables

- Very easy to interpret
- Easy to visualize (especially if they are small).
- Handle qualitative predictors without the need to create dummy variables
- Invariant to monotone transformation of predictor variables
- Unfortunately, trees generally do not have the same level of predictive accuracy as some of the other modern regression and classification approaches.