Machine Learning Techniques (機器學習技法)



Lecture 9: Decision Tree Hsuan-Tien Lin (林軒田) htlin@csie.ntu.edu.tw

Department of Computer Science & Information Engineering

National Taiwan University (國立台灣大學資訊工程系)



Roadmap

- Embedding Numerous Features: Kernel Models
- 2 Combining Predictive Features: Aggregation Models

Lecture 8: Adaptive Boosting

optimal re-weighting for diverse hypotheses and adaptive linear aggregation to boost 'weak' algorithms

Lecture 9: Decision Tree

- Decision Tree Hypothesis
- Decision Tree Algorithm
- Decision Tree Heuristics in C&RT
- Decision Tree in Action

Oistilling Implicit Features: Extraction Models

What We Have Done

blending: aggregate after getting g_t ;

_	aggregation type	blending	
-	uniform	voting/averaging	
-	non-uniform	linear	
-	conditional	stacking	

What We Have Done

blending: aggregate after getting g_t ; learning: aggregate as well as getting g_t

aggregation type	blending	learning
uniform	voting/averaging	Bagging
non-uniform	linear	AdaBoost
conditional	stacking	

What We Have Done

blending: aggregate after getting g_t ; learning: aggregate as well as getting g_t

aggregation type	blending	learning
uniform	voting/averaging	Bagging
non-uniform	linear	AdaBoost
conditional	stacking	Decision Tree

What We Have Done

blending: aggregate after getting g_t ; learning: aggregate as well as getting g_t

aggregation type	blending	learning
uniform	voting/averaging	Bagging
non-uniform	linear	AdaBoost
conditional	stacking	Decision Tree

decision tree: a traditional learning model that realizes conditional aggregation

Decision Tree Hypothesis

Decision Tree for Watching MOOC Lectures



Decision Tree Hypothesis

Decision Tree for Watching MOOC Lectures



Decision Tree Hypothesis

Decision Tree for Watching MOOC Lectures

$$G(\mathbf{x}) = \sum_{t=1}^{T} \boldsymbol{q}_t(\mathbf{x}) \cdot \boldsymbol{g}_t(\mathbf{x})$$

 base hypothesis g_t(x): leaf at end of path t, a constant here



Decision Tree Hypothesis

Decision Tree for Watching MOOC Lectures

$$G(\mathbf{x}) = \sum_{t=1}^{T} \boldsymbol{q}_t(\mathbf{x}) \cdot \boldsymbol{g}_t(\mathbf{x})$$

- base hypothesis g_t(x): leaf at end of path t, a constant here
- condition q_t(x):
 [is x on path t?]]



Decision Tree Hypothesis

Decision Tree for Watching MOOC Lectures

$$G(\mathbf{x}) = \sum_{t=1}^{T} \boldsymbol{q}_t(\mathbf{x}) \cdot \boldsymbol{g}_t(\mathbf{x})$$

- base hypothesis g_t(x): leaf at end of path t, a constant here
- condition q_t(x):
 [is x on path t?]
- usually with simple internal nodes



Decision Tree Hypothesis

Decision Tree for Watching MOOC Lectures

$$G(\mathbf{x}) = \sum_{t=1}^{T} \boldsymbol{q}_t(\mathbf{x}) \cdot \boldsymbol{g}_t(\mathbf{x})$$

- base hypothesis g_t(x): leaf at end of path t, a constant here
- condition q_t(x):
 [is x on path t?]
- usually with simple internal nodes



decision tree: arguably one of the most human-mimicking models

Decision Tree Hypothesis

Recursive View of Decision Tree Path View: $G(\mathbf{x}) = \sum_{t=1}^{T} [\mathbf{x} \text{ on path } t] \cdot \text{leaf}_t(\mathbf{x})$



Decision Tree Hypothesis

Recursive View of Decision Tree Path View: $G(\mathbf{x}) = \sum_{t=1}^{T} [[\mathbf{x} \text{ on path } t]] \cdot \text{leaf}_t(\mathbf{x})$



Recursive View

$$G(\mathbf{x}) = \sum_{c=1}^{C} \llbracket b(\mathbf{x}) = c \rrbracket \cdot G_c(\mathbf{x})$$

Decision Tree Hypothesis

Recursive View of Decision Tree Path View: $G(\mathbf{x}) = \sum_{t=1}^{T} [[\mathbf{x} \text{ on path } t]] \cdot \text{leaf}_t(\mathbf{x})$



Recursive View

$$G(\mathbf{x}) = \sum_{c=1}^{C} \llbracket b(\mathbf{x}) = c \rrbracket \cdot \mathbf{G}_{c}(\mathbf{x})$$

• G(x): full-tree hypothesis

Decision Tree Hypothesis

Recursive View of Decision Tree Path View: $G(\mathbf{x}) = \sum_{t=1}^{T} [[\mathbf{x} \text{ on path } t]] \cdot \text{leaf}_t(\mathbf{x})$



Recursive View

$$G(\mathbf{x}) = \sum_{c=1}^{C} \llbracket b(\mathbf{x}) = c \rrbracket \cdot G_c(\mathbf{x})$$

• G(x): full-tree hypothesis

Decision Tree Hypothesis

Recursive View of Decision Tree Path View: $G(\mathbf{x}) = \sum_{t=1}^{T} [x \text{ on path } t] \cdot \text{leaf}_t(\mathbf{x})$



Recursive View

$$G(\mathbf{x}) = \sum_{c=1}^{C} \llbracket b(\mathbf{x}) = c \rrbracket \cdot \mathbf{G}_{c}(\mathbf{x})$$

- *G*(**x**): full-tree hypothesis
- *b*(**x**): branching criteria
- *G_c*(**x**): sub-tree hypothesis at the *c*-th branch

Decision Tree Hypothesis

Recursive View of Decision Tree Path View: $G(\mathbf{x}) = \sum_{t=1}^{T} [[\mathbf{x} \text{ on path } t]] \cdot \text{leaf}_t(\mathbf{x})$



Recursive View

$$G(\mathbf{x}) = \sum_{c=1}^{C} \llbracket b(\mathbf{x}) = c \rrbracket \cdot G_c(\mathbf{x})$$

- G(x): full-tree hypothesis
- *b*(**x**): branching criteria
- *G_c*(**x**): sub-tree hypothesis at the *c*-th branch

tree = (root, sub-trees),

Decision Tree Hypothesis

Recursive View of Decision Tree Path View: $G(\mathbf{x}) = \sum_{t=1}^{T} [[\mathbf{x} \text{ on path } t]] \cdot \text{leaf}_t(\mathbf{x})$



Recursive View

$$G(\mathbf{x}) = \sum_{c=1}^{C} \llbracket b(\mathbf{x}) = c \rrbracket \cdot \mathbf{G}_{c}(\mathbf{x})$$

- G(x): full-tree hypothesis
- *b*(**x**): branching criteria
- *G_c*(**x**): sub-tree hypothesis at the *c*-th branch

tree = (root, sub-trees), just like what your data structure instructor would say :-)

Disclaimers about Decision Tree

Usefulness

 human-explainable: widely used in business/medical data analysis

Disclaimers about Decision Tree

Usefulness

- human-explainable: widely used in business/medical data analysis
- simple: even freshmen can implement one :-)

Disclaimers about Decision Tree

Usefulness

- human-explainable: widely used in business/medical data analysis
- simple: even freshmen can implement one :-)
- efficient in prediction and training

Disclaimers about Decision Tree

Usefulness

- human-explainable: widely used in business/medical data analysis
- simple: even freshmen can implement one :-)
- efficient in prediction and training

However.....

Disclaimers about Decision Tree

Usefulness

- human-explainable: widely used in business/medical data analysis
- simple: even freshmen can implement one :-)
- efficient in prediction and training

However.....

 heuristic: mostly little theoretical explanations

Disclaimers about Decision Tree

Usefulness

- human-explainable: widely used in business/medical data analysis
- simple: even freshmen can implement one :-)
- efficient in prediction and training

However.....

- heuristic: mostly little theoretical explanations
- heuristics:
 'heuristics selection' confusing to beginners

Disclaimers about Decision Tree

Usefulness

- human-explainable: widely used in business/medical data analysis
- simple: even freshmen can implement one :-)
- efficient in prediction and training

However.....

- heuristic: mostly little theoretical explanations
- heuristics:
 'heuristics selection' confusing to beginners
- arguably no single representative algorithm

Disclaimers about Decision Tree

Usefulness

- human-explainable: widely used in business/medical data analysis
- simple: even freshmen can implement one :-)
- efficient in prediction and training

However.....

- heuristic: mostly little theoretical explanations
- heuristics:
 'heuristics selection' confusing to beginners
- arguably no single representative algorithm

decision tree: mostly heuristic but useful on its own

Fun Time

The following C-like code can be viewed as a decision tree of three leaves.

```
if (income > 100000) return true;
else {
   if (debt > 50000) return false;
   else return true;
}
```

What is the output of the tree for (income, debt) = (98765, 56789)?

1 true	3 98765
2 false	4 56789

Fun Time

The following C-like code can be viewed as a decision tree of three leaves.

```
if (income > 100000) return true;
else {
  if (debt > 50000) return false;
  else return true;
}
```

What is the output of the tree for (income, debt) = (98765, 56789)?

1 true	3 98765
2 false	4 56789

Reference Answer: (2)

You can simply trace the code. The tree expresses a complicated boolean condition [[income > 100000 or debt ≤ 50000].

Decision Tree Algorithm

A Basic Decision Tree Algorithm

$$G(\mathbf{x}) = \sum_{c=1}^{C} \llbracket b(\mathbf{x}) = c \rrbracket \mathbf{G}_{c}(\mathbf{x})$$

function DecisionTree(data $\mathcal{D} = \{(\mathbf{x}_n, y_n)\}_{n=1}^N$)

Decision Tree Algorithm

A Basic Decision Tree Algorithm

$$G(\mathbf{x}) = \sum_{c=1}^{C} \llbracket b(\mathbf{x}) = c \rrbracket \mathbf{G}_{c}(\mathbf{x})$$

function DecisionTree(data $\mathcal{D} = \{(\mathbf{x}_n, y_n)\}_{n=1}^N$)

1 learn branching criteria $b(\mathbf{x})$

Decision Tree Algorithm

A Basic Decision Tree Algorithm

$$G(\mathbf{x}) = \sum_{c=1}^{C} \llbracket b(\mathbf{x}) = c \rrbracket \mathbf{G}_{c}(\mathbf{x})$$

function DecisionTree(data $\mathcal{D} = \{(\mathbf{x}_n, y_n)\}_{n=1}^N$)

1 learn branching criteria $b(\mathbf{x})$

2 split \mathcal{D} to C parts $\mathcal{D}_c = \{(\mathbf{x}_n, y_n) : b(\mathbf{x}_n) = c\}$

Decision Tree Algorithm

A Basic Decision Tree Algorithm

$$G(\mathbf{x}) = \sum_{c=1}^{C} \llbracket b(\mathbf{x}) = c \rrbracket \mathbf{G}_{c}(\mathbf{x})$$

function DecisionTree(data $\mathcal{D} = \{(\mathbf{x}_n, y_n)\}_{n=1}^N$)

1 learn branching criteria $b(\mathbf{x})$

- 2 split \mathcal{D} to C parts $\mathcal{D}_c = \{(\mathbf{x}_n, y_n) : b(\mathbf{x}_n) = c\}$
- **③** build sub-tree G_c ← DecisionTree(\mathcal{D}_c)

Decision Tree Algorithm

A Basic Decision Tree Algorithm

$$G(\mathbf{x}) = \sum_{c=1}^{C} \llbracket b(\mathbf{x}) = c \rrbracket \mathbf{G}_{c}(\mathbf{x})$$

function DecisionTree(data $\mathcal{D} = \{(\mathbf{x}_n, y_n)\}_{n=1}^N$)

learn branching criteria b(x)
 split D to C parts D_c = {(x_n, y_n): b(x_n) = c}
 build sub-tree G_c ← DecisionTree(D_c)
 return G(x) = ∑_{c=1}^C [[b(x) = c]] G_c(x)

Decision Tree Algorithm

A Basic Decision Tree Algorithm

$$G(\mathbf{x}) = \sum_{c=1}^{C} \llbracket b(\mathbf{x}) = c \rrbracket \mathbf{G}_{c}(\mathbf{x})$$

function DecisionTree(data $\mathcal{D} = \{(\mathbf{x}_n, \mathbf{y}_n)\}_{n=1}^N$) if termination criteria met

return base hypothesis $g_t(\mathbf{x})$

else

- 1 learn branching criteria $b(\mathbf{x})$
- 2 split \mathcal{D} to C parts $\mathcal{D}_c = \{(\mathbf{x}_n, \mathbf{y}_n) : \mathbf{b}(\mathbf{x}_n) = c\}$
- ⁽³⁾ build sub-tree G_c ← DecisionTree(D_c)

 $e \text{term} G(\mathbf{x}) = \sum_{c=1}^{C} \left[b(\mathbf{x}) = c \right] G_c(\mathbf{x})$

Decision Tree Algorithm

A Basic Decision Tree Algorithm

$$G(\mathbf{x}) = \sum_{c=1}^{C} \llbracket b(\mathbf{x}) = c \rrbracket \mathbf{G}_c(\mathbf{x})$$

function DecisionTree(data $\mathcal{D} = \{(\mathbf{x}_n, y_n)\}_{n=1}^N$) if termination criteria met

return base hypothesis $g_t(\mathbf{x})$

else

- 1 learn branching criteria $b(\mathbf{x})$
- 2 split \mathcal{D} to C parts $\mathcal{D}_c = \{(\mathbf{x}_n, y_n) : b(\mathbf{x}_n) = c\}$
- **③** build sub-tree G_c ← DecisionTree(\mathcal{D}_c)

4 return $G(\mathbf{x}) = \sum_{c=1}^{C} \llbracket \mathbf{b}(\mathbf{x}) = c \rrbracket G_c(\mathbf{x})$

four choices: number of branches, branching criteria, termination criteria, & base hypothesis

Hsuan-Tien Lin (NTU CSIE)

Machine Learning Techniques
Decision Tree Algorithm

Classification and Regression Tree (C&RT)

function DecisionTree(data $\mathcal{D} = \{(\mathbf{x}_n, \mathbf{y}_n)\}_{n=1}^N$) if termination criteria met

return base hypothesis $g_t(\mathbf{x})$

else ...

2 split \mathcal{D} to C parts $\mathcal{D}_c = \{(\mathbf{x}_n, y_n) : \mathbf{b}(\mathbf{x}_n) = c\}$

Decision Tree Algorithm

Classification and Regression Tree (C&RT)

function DecisionTree(data $\mathcal{D} = \{(\mathbf{x}_n, \mathbf{y}_n)\}_{n=1}^N$) if termination criteria met

return base hypothesis $g_t(\mathbf{x})$

else ...

2 split
$$\mathcal{D}$$
 to C parts $\mathcal{D}_c = \{(\mathbf{x}_n, y_n) : b(\mathbf{x}_n) = c\}$

Decision Tree Algorithm

Classification and Regression Tree (C&RT)

function DecisionTree(data $\mathcal{D} = \{(\mathbf{x}_n, \mathbf{y}_n)\}_{n=1}^N$) if termination criteria met

return base hypothesis $g_t(\mathbf{x})$

else ...

2 split
$$\mathcal{D}$$
 to C parts $\mathcal{D}_c = \{(\mathbf{x}_n, y_n) : b(\mathbf{x}_n) = c\}$

two simple choices

• C = 2 (binary tree)

Decision Tree Algorithm

Classification and Regression Tree (C&RT)

function DecisionTree(data $\mathcal{D} = \{(\mathbf{x}_n, y_n)\}_{n=1}^N$) if termination criteria met

return base hypothesis $g_t(\mathbf{x})$

else ...

2 split \mathcal{D} to C parts $\mathcal{D}_c = \{(\mathbf{x}_n, y_n) : b(\mathbf{x}_n) = c\}$

- C = 2 (binary tree)
- $g_t(\mathbf{x}) = E_{in}$ -optimal constant

Decision Tree Algorithm

Classification and Regression Tree (C&RT)

function DecisionTree(data $\mathcal{D} = \{(\mathbf{x}_n, \mathbf{y}_n)\}_{n=1}^N$) if termination criteria met

return base hypothesis $g_t(\mathbf{x})$

else ...

2 split \mathcal{D} to C parts $\mathcal{D}_c = \{(\mathbf{x}_n, y_n) : b(\mathbf{x}_n) = c\}$

- C = 2 (binary tree)
- $g_t(\mathbf{x}) = E_{in}$ -optimal constant
 - binary/multiclass classification (0/1 error): majority of {*y_n*}

Decision Tree Algorithm

Classification and Regression Tree (C&RT)

function DecisionTree(data $\mathcal{D} = \{(\mathbf{x}_n, \mathbf{y}_n)\}_{n=1}^N$) if termination criteria met

return base hypothesis $g_t(\mathbf{x})$

else ...

2 split \mathcal{D} to C parts $\mathcal{D}_c = \{(\mathbf{x}_n, y_n) : b(\mathbf{x}_n) = c\}$

- C = 2 (binary tree)
- $g_t(\mathbf{x}) = E_{in}$ -optimal constant
 - binary/multiclass classification (0/1 error): majority of {*y_n*}
 - regression (squared error): average of {y_n}

Decision Tree Algorithm

Classification and Regression Tree (C&RT)

function DecisionTree(data $\mathcal{D} = \{(\mathbf{x}_n, \mathbf{y}_n)\}_{n=1}^N$) if termination criteria met

return base hypothesis $g_t(\mathbf{x})$

else ...

2 split \mathcal{D} to C parts $\mathcal{D}_c = \{(\mathbf{x}_n, y_n) : \mathbf{b}(\mathbf{x}_n) = c\}$

two simple choices

- C = 2 (binary tree)
- $g_t(\mathbf{x}) = E_{in}$ -optimal constant
 - binary/multiclass classification (0/1 error): majority of {*y_n*}
 - regression (squared error): average of {y_n}

disclaimer: **C&RT** here is based on **selected components** of **CART**TM of California Statistical Software

Hsuan-Tien Lin (NTU CSIE)

Machine Learning Techniques

function DecisionTree(data $\mathcal{D} = \{(\mathbf{x}_n, y_n)\}_{n=1}^N$) if termination criteria met

return base hypothesis $g_t(\mathbf{x}) = E_{in}$ -optimal constant

else ...

- **1** learn branching criteria $b(\mathbf{x})$
- 2 split \mathcal{D} to 2 parts $\mathcal{D}_c = \{(\mathbf{x}_n, y_n) : \mathbf{b}(\mathbf{x}_n) = c\}$

function DecisionTree(data $\mathcal{D} = \{(\mathbf{x}_n, y_n)\}_{n=1}^N$) if termination criteria met

return base hypothesis $g_t(\mathbf{x}) = E_{in}$ -optimal constant

else ...

- **1** learn branching criteria $b(\mathbf{x})$
- 2 split \mathcal{D} to 2 parts $\mathcal{D}_c = \{(\mathbf{x}_n, y_n) : b(\mathbf{x}_n) = c\}$

more simple choices

function DecisionTree(data $\mathcal{D} = \{(\mathbf{x}_n, \mathbf{y}_n)\}_{n=1}^N$) if termination criteria met

return base hypothesis $g_t(\mathbf{x}) = E_{in}$ -optimal constant

else ...

- learn branching criteria $b(\mathbf{x})$
- 2 split \mathcal{D} to 2 parts $\mathcal{D}_c = \{(\mathbf{x}_n, y_n) : b(\mathbf{x}_n) = c\}$

more simple choices

• simple internal node for *C* = 2: {1,2}-output decision stump

function DecisionTree(data $\mathcal{D} = \{(\mathbf{x}_n, \mathbf{y}_n)\}_{n=1}^N$) if termination criteria met

return base hypothesis $g_t(\mathbf{x}) = E_{in}$ -optimal constant else ...

- 1 learn branching criteria $b(\mathbf{x})$
- 2 split \mathcal{D} to 2 parts $\mathcal{D}_c = \{(\mathbf{x}_n, y_n) : b(\mathbf{x}_n) = c\}$

more simple choices

- simple internal node for *C* = 2: {1,2}-output decision stump
- 'easier' sub-tree: branch by purifying

function DecisionTree(data $\mathcal{D} = \{(\mathbf{x}_n, \mathbf{y}_n)\}_{n=1}^N$) if termination criteria met

return base hypothesis $g_t(\mathbf{x}) = E_{in}$ -optimal constant else ...

- 1 learn branching criteria $b(\mathbf{x})$
- 2 split \mathcal{D} to 2 parts $\mathcal{D}_c = \{(\mathbf{x}_n, y_n) : b(\mathbf{x}_n) = c\}$

more simple choices

- simple internal node for *C* = 2: {1,2}-output decision stump
- 'easier' sub-tree: branch by purifying

$$b(\mathbf{x}) = \operatorname*{argmin}_{\text{decision stumps } h(\mathbf{x})} \sum_{c=1}^{2} |\mathcal{D}_c \text{ with } h| \cdot \operatorname{impurity}(\mathcal{D}_c \text{ with } h)$$

function DecisionTree(data $\mathcal{D} = \{(\mathbf{x}_n, \mathbf{y}_n)\}_{n=1}^N$) if termination criteria met

return base hypothesis $g_t(\mathbf{x}) = E_{in}$ -optimal constant else ...

- 1 learn branching criteria $b(\mathbf{x})$
- 2 split \mathcal{D} to 2 parts $\mathcal{D}_c = \{(\mathbf{x}_n, y_n) : b(\mathbf{x}_n) = c\}$

more simple choices

- simple internal node for C = 2: {1,2}-output decision stump
- 'easier' sub-tree: branch by purifying

$$\boldsymbol{b}(\mathbf{x}) = \operatorname*{argmin}_{\text{decision stumps } h(\mathbf{x})} \sum_{c=1}^{2} |\mathcal{D}_c \text{ with } h| \cdot \operatorname{impurity}(\mathcal{D}_c \text{ with } h)$$

C&RT: bi-branching by purifying

Hsuan-Tien Lin (NTU CSIE)

Machine Learning Techniques

Decision Tree Algorithm Impurity Functions



Decision Tree Algorithm Impurity Functions

by *E*_{in} of optimal constant

• regression error:

impurity(
$$\mathcal{D}$$
) = $\frac{1}{N} \sum_{n=1}^{N} (y_n - \bar{y})^2$

with \overline{y} = average of $\{y_n\}$

Decision Tree Algorithm Impurity Functions

by E_{in} of optimal constant

• regression error:

impurity(
$$\mathcal{D}$$
) = $\frac{1}{N} \sum_{n=1}^{N} (y_n - \bar{y})^2$

with \bar{y} = average of $\{y_n\}$

classification error:

impurity(
$$\mathcal{D}$$
) = $\frac{1}{N} \sum_{n=1}^{N} [y_n \neq y^*]$
with y^* = majority of $\{y_n\}$

Decision Tree Algorithm Impurity Functions

by E_{in} of optimal constant

• regression error:

impurity(
$$\mathcal{D}$$
) = $\frac{1}{N} \sum_{n=1}^{N} (y_n - \bar{y})^2$

with \bar{y} = average of $\{y_n\}$

classification error:

impurity(
$$\mathcal{D}$$
) = $\frac{1}{N} \sum_{n=1}^{N} [y_n \neq y^*]$
with y^* = majority of $\{y_n\}$

for classification



Decision Tree Algorithm Impurity Functions

by E_{in} of optimal constant for classification regression error: impurity(\mathcal{D}) = $\frac{1}{N} \sum_{n=1}^{N} (y_n - \bar{y})^2$ with \overline{y} = average of $\{y_n\}$ classification error: classification error: impurity(\mathcal{D}) = $\frac{1}{N} \sum_{n=1}^{N} [[y_n \neq y^*]]$ $1 - \max_{1 \le k \le K} \frac{\sum_{n=1}^{N} \left[\left[y_n = k \right] \right]}{N}$ with $y^* =$ majority of $\{y_n\}$ -optimal $k = y^*$ only

Decision Tree Algorithm Impurity Functions

by E_{in} of optimal constant

• regression error:

impurity(
$$\mathcal{D}$$
) = $\frac{1}{N} \sum_{n=1}^{N} (y_n - \bar{y})^2$

with \overline{y} = average of $\{y_n\}$

classification error:

impurity(
$$\mathcal{D}$$
) = $\frac{1}{N} \sum_{n=1}^{N} \llbracket y_n \neq y^* \rrbracket$

with y^* = majority of $\{y_n\}$

for classification

• Gini index:

$$1 - \sum_{k=1}^{K} \left(\frac{\sum_{n=1}^{N} \left[y_n = k \right]}{N} \right)^2$$

- -all k considered together
- classification error:

$$1 - \max_{1 \le k \le K} \frac{\sum_{n=1}^{N} \llbracket y_n = k \rrbracket}{N}$$

—optimal $k = y^*$ only

Decision Tree Algorithm Impurity Functions

by E_{in} of optimal constant

• regression error:

impurity(
$$\mathcal{D}$$
) = $\frac{1}{N} \sum_{n=1}^{N} (y_n - \bar{y})^2$

with \overline{y} = average of $\{y_n\}$

classification error:

impurity(
$$\mathcal{D}$$
) = $\frac{1}{N} \sum_{n=1}^{N} \llbracket y_n \neq y^* \rrbracket$

with y^* = majority of $\{y_n\}$

for classification

• Gini index:

$$1 - \sum_{k=1}^{K} \left(\frac{\sum_{n=1}^{N} \left[y_n = k \right]}{N} \right)^2$$

- -all k considered together
- classification error:

$$1 - \max_{1 \le k \le K} \frac{\sum_{n=1}^{N} \llbracket y_n = k \rrbracket}{N}$$

—optimal $k = y^*$ only

popular choices: Gini for classification, regression error for regression

Hsuan-Tien Lin (NTU CSIE)

Machine Learning Techniques

function DecisionTree(data $\mathcal{D} = \{(\mathbf{x}_n, y_n)\}_{n=1}^N$) if termination criteria met

return base hypothesis $g_t(\mathbf{x}) = E_{in}$ -optimal constant else ...

Iearn branching criteria

$$\mathbf{b}(\mathbf{x}) = \underset{\text{decision stumps } h(\mathbf{x})}{\operatorname{argmin}} \sum_{c=1}^{2} |\mathcal{D}_{c} \text{ with } h| \cdot \underset{c=1}{\operatorname{impurity}} (\mathcal{D}_{c} \text{ with } h)$$

'forced' to terminate when

function DecisionTree(data $\mathcal{D} = \{(\mathbf{x}_n, y_n)\}_{n=1}^N$) if termination criteria met

return base hypothesis $g_t(\mathbf{x}) = E_{in}$ -optimal constant else ...

Iearn branching criteria

$$\mathbf{b}(\mathbf{x}) = \operatorname*{argmin}_{\text{decision stumps } h(\mathbf{x})} \sum_{c=1}^{2} |\mathcal{D}_{c} \text{ with } h| \cdot \operatorname{impurity}(\mathcal{D}_{c} \text{ with } h)$$

'forced' to terminate when

• all y_n the same: impurity = 0 $\implies g_t(\mathbf{x}) = y_n$

function DecisionTree(data $\mathcal{D} = \{(\mathbf{x}_n, y_n)\}_{n=1}^N$) if termination criteria met

return base hypothesis $g_t(\mathbf{x}) = E_{in}$ -optimal constant else ...

Iearn branching criteria

$$D(\mathbf{x}) = \operatorname*{argmin}_{\text{decision stumps } h(\mathbf{x})} \sum_{c=1}^{2} |\mathcal{D}_{c} \text{ with } h| \cdot \operatorname{impurity}(\mathcal{D}_{c} \text{ with } h)$$

'forced' to terminate when

- all y_n the same: impurity = 0 $\Longrightarrow g_t(\mathbf{x}) = y_n$
- all x_n the same: no decision stumps

function DecisionTree(data $\mathcal{D} = \{(\mathbf{x}_n, y_n)\}_{n=1}^N$) if termination criteria met

return base hypothesis $g_t(\mathbf{x}) = E_{in}$ -optimal constant else ...

Iearn branching criteria

$$\mathcal{D}(\mathbf{x}) = \underset{\text{decision stumps } h(\mathbf{x})}{\operatorname{argmin}} \sum_{c=1}^{2} |\mathcal{D}_c \text{ with } h| \cdot \operatorname{impurity}(\mathcal{D}_c \text{ with } h)$$

'forced' to terminate when

- all y_n the same: impurity = 0 $\Longrightarrow g_t(\mathbf{x}) = y_n$
- all x_n the same: no decision stumps

C&RT: **fully-grown tree** with constant leaves that come from **bi-branching** by **purifying**

Hsuan-Tien Lin (NTU CSIE)

Machine Learning Techniques

Fun Time

For the Gini index,
$$1 - \sum_{k=1}^{K} \left(\frac{\sum_{n=1}^{N} \left[y_n = k \right]}{N} \right)^2$$
. Consider $K = 2$, and let

 $\mu = \frac{N_1}{N}$, where N_1 is the number of examples with $y_n = 1$. Which of the following formula of μ equals the Gini index in this case?

1
$$2\mu(1-\mu)$$

2 $2\mu^2(1-\mu)$
3 $2\mu(1-\mu)^2$
4 $2\mu^2(1-\mu)^2$

Fun Time

For the Gini index,
$$1 - \sum_{k=1}^{K} \left(\frac{\sum_{n=1}^{N} \left[y_n = k \right]}{N} \right)^2$$
. Consider $K = 2$, and let

 $\mu = \frac{N_1}{N}$, where N_1 is the number of examples with $y_n = 1$. Which of the following formula of μ equals the Gini index in this case?

1
$$2\mu(1-\mu)$$

2 $2\mu^2(1-\mu)$
3 $2\mu(1-\mu)^2$
4 $2\mu^2(1-\mu)^2$

Reference Answer: (1)

Simplify $1 - (\mu^2 + (1 - \mu)^2)$ and the answer should pop up.

Decision Tree Heuristics in C&RT

Basic C&RT Algorithm

function DecisionTree(data $\mathcal{D} = \{(\mathbf{x}_n, y_n)\}_{n=1}^N$) if cannot branch anymore

return $g_t(\mathbf{x}) = E_{in}$ -optimal constant

else

learn branching criteria

$$b(\mathbf{x}) = \operatorname*{argmin}_{\text{decision stumps } h(\mathbf{x})} \sum_{c=1}^{2} |\mathcal{D}_c \text{ with } h| \cdot \operatorname{impurity}(\mathcal{D}_c \text{ with } h)$$

2 split \mathcal{D} to 2 parts $\mathcal{D}_c = \{(\mathbf{x}_n, y_n) : \mathbf{b}(\mathbf{x}_n) = c\}$

⁽³⁾ build sub-tree G_c ← DecisionTree(D_c)

4 return $G(\mathbf{x}) = \sum_{c=1}^{2} \llbracket b(\mathbf{x}) = c \rrbracket G_c(\mathbf{x})$

Hsuan-Tien Lin (NTU CSIE)

Decision Tree Heuristics in C&RT

Basic C&RT Algorithm

function DecisionTree(data $\mathcal{D} = \{(\mathbf{x}_n, y_n)\}_{n=1}^N$) if cannot branch anymore

return $g_t(\mathbf{x}) = E_{in}$ -optimal constant

else

Iearn branching criteria

$$b(\mathbf{x}) = \underset{\text{decision stumps } h(\mathbf{x})}{\operatorname{argmin}} \sum_{c=1}^{2} |\mathcal{D}_c \text{ with } h| \cdot \underset{c=1}{\operatorname{impurity}} (\mathcal{D}_c \text{ with } h)$$

2 split \mathcal{D} to 2 parts $\mathcal{D}_c = \{(\mathbf{x}_n, y_n) : b(\mathbf{x}_n) = c\}$

③ build sub-tree G_c ← DecisionTree(\mathcal{D}_c)

4 return $G(\mathbf{x}) = \sum_{c=1}^{2} \llbracket b(\mathbf{x}) = c \rrbracket G_c(\mathbf{x})$

easily handle binary classification, regression, & multi-class classification

Hsuan-Tien Lin (NTU CSIE)

Machine Learning Techniques

Decision Tree Heuristics in C&RT

Regularization by Pruning fully-grown tree: $E_{in}(G) = 0$ if all \mathbf{x}_n different

Regularization by Pruning

fully-grown tree: $E_{in}(G) = 0$ if all \mathbf{x}_n different

but overfit (large E_{out}) because low-level trees built with small D_c

Regularization by Pruning

fully-grown tree: $E_{in}(G) = 0$ if all \mathbf{x}_n different but overfit (large E_{out}) because low-level trees built with small \mathcal{D}_c

• need a **regularizer**, say, $\Omega(G) = \text{NumberOfLeaves}(G)$

Regularization by Pruning

fully-grown tree: $E_{in}(G) = 0$ if all \mathbf{x}_n different but overfit (large E_{out}) because low-level trees built with small \mathcal{D}_c

- need a **regularizer**, say, $\Omega(G) = \text{NumberOfLeaves}(G)$
- want regularized decision tree:

argmin
$$E_{in}(G) + \lambda \Omega(G)$$

all possible G

Regularization by Pruning

fully-grown tree: $E_{in}(G) = 0$ if all \mathbf{x}_n different but overfit (large E_{out}) because low-level trees built with small \mathcal{D}_c

- need a **regularizer**, say, $\Omega(G) = \text{NumberOfLeaves}(G)$
- want regularized decision tree:

argmin
$$E_{in}(G) + \lambda \Omega(G)$$

-called pruned decision tree

Regularization by Pruning

fully-grown tree: $E_{in}(G) = 0$ if all \mathbf{x}_n different but overfit (large E_{out}) because low-level trees built with small \mathcal{D}_c

- need a **regularizer**, say, $\Omega(G) = \text{NumberOfLeaves}(G)$
- want regularized decision tree:

argmin $E_{in}(G) + \lambda \Omega(G)$ all possible G

-called pruned decision tree

cannot enumerate all possible G computationally:
 —often consider only

Regularization by Pruning

fully-grown tree: $E_{in}(G) = 0$ if all \mathbf{x}_n different but overfit (large E_{out}) because low-level trees built with small \mathcal{D}_c

- need a **regularizer**, say, $\Omega(G) = \text{NumberOfLeaves}(G)$
- want regularized decision tree:

argmin $E_{in}(G) + \lambda \Omega(G)$ all possible G

-called pruned decision tree

- cannot enumerate all possible G computationally:
 —often consider only
 - G⁽⁰⁾ = fully-grown tree

Regularization by Pruning

fully-grown tree: $E_{in}(G) = 0$ if all \mathbf{x}_n different but overfit (large E_{out}) because low-level trees built with small \mathcal{D}_c

- need a **regularizer**, say, $\Omega(G) = \text{NumberOfLeaves}(G)$
- want regularized decision tree:

argmin $E_{in}(G) + \lambda \Omega(G)$ all possible G

-called pruned decision tree

- cannot enumerate all possible G computationally: —often consider only
 - $G^{(0)}$ = fully-grown tree
 - $G^{(i)} = \operatorname{argmin}_{G} E_{in}(G)$ such that G is **one-leaf removed** from $G^{(i-1)}$
Regularization by Pruning

fully-grown tree: $E_{in}(G) = 0$ if all \mathbf{x}_n different but overfit (large E_{out}) because low-level trees built with small \mathcal{D}_c

- need a **regularizer**, say, $\Omega(G) = \text{NumberOfLeaves}(G)$
- want regularized decision tree:

argmin $E_{in}(G) + \lambda \Omega(G)$ all possible *G*

-called pruned decision tree

- cannot enumerate all possible G computationally: —often consider only
 - $G^{(0)}$ = fully-grown tree
 - $G^{(i)} = \operatorname{argmin}_{G} E_{in}(G)$ such that G is **one-leaf removed** from $G^{(i-1)}$

systematic choice of λ ?

Hsuan-Tien Lin (NTU CSIE)

Machine Learning Techniques

Regularization by Pruning

fully-grown tree: $E_{in}(G) = 0$ if all \mathbf{x}_n different but overfit (large E_{out}) because low-level trees built with small \mathcal{D}_c

- need a **regularizer**, say, $\Omega(G) = \text{NumberOfLeaves}(G)$
- want regularized decision tree:

argmin $E_{in}(G) + \lambda \Omega(G)$ all possible *G*

-called pruned decision tree

- cannot enumerate all possible G computationally:
 —often consider only
 - $G^{(0)}$ = fully-grown tree
 - $G^{(i)} = \operatorname{argmin}_{G} E_{in}(G)$ such that G is **one-leaf removed** from $G^{(i-1)}$

systematic choice of λ ? validation

Hsuan-Tien Lin (NTU CSIE)

Machine Learning Techniques

Decision Tree Heuristics in C&RT

Branching on Categorical Features

numerical features

blood pressure: 130, 98, 115, 147, 120

Decision Tree Heuristics in C&RT

Branching on Categorical Features

numerical features

blood pressure: 130, 98, 115, 147, 120

branching for numerical

decision stump

$$b(\mathbf{x}) = \llbracket x_i \leq \theta \rrbracket + 1$$

with $\theta \in \mathbb{R}$

Branching on Categorical Features

numerical features

blood pressure: 130, 98, 115, 147, 120

branching for numerical

decision stump

$$b(\mathbf{x}) = \llbracket x_i \leq \theta \rrbracket + 1$$

with $\theta \in \mathbb{R}$

categorical features

major symptom: fever, pain, tired, sweaty

Branching on Categorical Features

numerical features

blood pressure: 130, 98, 115, 147, 120

categorical features

major symptom: fever, pain, tired, sweaty

branching for numerical

decision stump

$$b(\mathbf{x}) = \llbracket x_i \leq \theta \rrbracket + 1$$

with $\theta \in \mathbb{R}$

branching for categorical

decision subset

Branching on Categorical Features

numerical features

blood pressure: 130, 98, 115, 147, 120

categorical features

major symptom: fever, pain, tired, sweaty

branching for numerical

decision stump

$$\mathbf{b}(\mathbf{x}) = \llbracket x_i \leq \mathbf{\theta} \rrbracket + 1$$

with $\theta \in \mathbb{R}$

branching for categorical

decision subset

$$\boldsymbol{b}(\mathbf{x}) = \llbracket x_i \in \boldsymbol{S} \rrbracket + 1$$

with $S \subset \{1, 2, ..., K\}$

Branching on Categorical Features

numerical features

blood pressure: 130, 98, 115, 147, 120

categorical features

major symptom: fever, pain, tired, sweaty

branching for numerical

decision stump

$$\mathbf{b}(\mathbf{x}) = \llbracket x_i \leq \theta \rrbracket + 1$$

with $\theta \in \mathbb{R}$

branching for categorical

decision subset

$$\mathbf{b}(\mathbf{x}) = \llbracket x_i \in \mathbf{S} \rrbracket + 1$$

with $S \subset \{1, 2, \dots, K\}$

C&RT (& general decision trees): handles categorical features easily

Decision Tree Heuristics in C&RT

Missing Features by Surrogate Branch possible $b(\mathbf{x}) = [weight \le 50kg]$

Decision Tree Heuristics in C&RT

Missing Features by Surrogate Branch possible $b(\mathbf{x}) = [weight \le 50kg]$

Decision Tree Heuristics in C&RT

Missing Features by Surrogate Branch possible $b(\mathbf{x}) = [weight \le 50kg]$

if weight missing during prediction:

what would human do?

Decision Tree Heuristics in C&RT

Missing Features by Surrogate Branch possible $b(\mathbf{x}) = [weight \le 50kg]$

- what would human do?
 - go get weight

Missing Features by Surrogate Branch possible $b(\mathbf{x}) = [weight \le 50kg]$

- what would human do?
 - go get weight
 - or, use threshold on height instead, because threshold on height \approx threshold on weight

Missing Features by Surrogate Branch possible $b(\mathbf{x}) = [weight \le 50 \text{kg}]$

- what would human do?
 - go get weight
 - or, use threshold on height instead, because threshold on height ≈ threshold on weight
- surrogate branch:
 - maintain surrogate branch b₁(**x**), b₂(**x**), ... ≈ best branch b(**x**) during training

Missing Features by Surrogate Branch possible $b(\mathbf{x}) = [weight \le 50kg]$

- what would human do?
 - go get weight
 - or, use threshold on height instead, because threshold on height ≈ threshold on weight
- surrogate branch:
 - maintain surrogate branch b₁(**x**), b₂(**x**), ... ≈ best branch b(**x**) during training
 - allow missing feature for b(x) during prediction by using surrogate instead

Missing Features by Surrogate Branch possible $b(\mathbf{x}) = [weight \le 50kg]$

if weight missing during prediction:

- what would human do?
 - go get weight
 - or, use threshold on height instead, because threshold on height ≈ threshold on weight
- surrogate branch:
 - maintain surrogate branch b₁(**x**), b₂(**x**), ... ≈ best branch b(**x**) during training
 - allow missing feature for b(x) during prediction by using surrogate instead

C&RT: handles missing features easily

Fun Time

For a categorical branching criteria $\mathbf{b}(\mathbf{x}) = [[\mathbf{x}_i \in \mathbf{S}]] + 1$ with

 $S = \{1, 6\}$. Which of the following is the explanation of the criteria?

- if *i*-th feature is of type 1 or type 6, branch to first sub-tree; else branch to second sub-tree
- if *i*-th feature is of type 1 or type 6, branch to second sub-tree; else branch to first sub-tree
- if *i*-th feature is of type 1 and type 6, branch to second sub-tree; else branch to first sub-tree
- if *i*-th feature is of type 1 and type 6, branch to first sub-tree; else branch to second sub-tree

Fun Time

For a categorical branching criteria $\mathbf{b}(\mathbf{x}) = [[\mathbf{x}_i \in \mathbf{S}]] + 1$ with

 $S = \{1, 6\}$. Which of the following is the explanation of the criteria?

- if *i*-th feature is of type 1 or type 6, branch to first sub-tree; else branch to second sub-tree
- if *i*-th feature is of type 1 or type 6, branch to second sub-tree; else branch to first sub-tree
- if *i*-th feature is of type 1 and type 6, branch to second sub-tree; else branch to first sub-tree
- if *i*-th feature is of type 1 and type 6, branch to first sub-tree; else branch to second sub-tree

Reference Answer: (2)

Note that ' \in S' is an 'or'-style condition on the elements of S in human language.

Decision Tree in Action



Decision Tree in Action



Decision Tree in Action



Decision Tree in Action



Decision Tree in Action



Decision Tree in Action



Decision Tree in Action



Decision Tree in Action



Decision Tree in Action



Decision Tree in Action



Decision Tree in Action

A Simple Data Set



C&RT: 'divide-and-conquer'

Hsuan-Tien Lin (NTU CSIE)

Machine Learning Techniques

Decision Tree in Action

A Complicated Data Set



C&RT



initially

Decision Tree in Action

A Complicated Data Set



C&RT



Decision Tree in Action

A Complicated Data Set



C&RT



Decision Tree in Action

A Complicated Data Set



C&RT



Decision Tree in Action

A Complicated Data Set



C&RT

AdaBoost-Stump

C&RT: even more efficient than AdaBoost-Stump

Hsuan-Tien Lin (NTU CSIE)

Machine Learning Techniques

Practical Specialties of C&RT

• human-explainable

Practical Specialties of C&RT

- human-explainable
- multiclass easily
Decision Tree

Practical Specialties of C&RT

- human-explainable
- multiclass easily
- categorical features easily

Decision Tree

Practical Specialties of C&RT

- human-explainable
- multiclass easily
- categorical features easily
- missing features easily

Practical Specialties of C&RT

- human-explainable
- multiclass easily
- categorical features easily
- missing features easily
- efficient non-linear training (and testing)

Practical Specialties of C&RT

- human-explainable
- multiclass easily
- categorical features easily
- missing features easily
- efficient non-linear training (and testing)

—almost no other learning model share all such specialties, except for other decision trees

Practical Specialties of C&RT

- human-explainable
- multiclass easily
- categorical features easily
- missing features easily
- efficient non-linear training (and testing)

—almost no other learning model share all such specialties, except for other decision trees

another popular decision tree algorithm: C4.5, with different choices of heuristics

Fun Time

Which of the following is not a specialty of C&RT without pruning?

- 1 handles missing features easily
- 2 produces explainable hypotheses
- 3 achieves low E_{in}
- 4 achieves low E_{out}

Fun Time

Which of the following is not a specialty of C&RT without pruning?

- handles missing features easily
- 2 produces explainable hypotheses
- 3 achieves low E_{in}
- 4 achieves low E_{out}

Reference Answer: (4)

The first two choices are easy; the third comes from the fact that fully grown C&RT greedy minimizes E_{in} (almost always to 0). But as you may imagine, overfitting may happen and E_{out} may not always be low.

Summary

- Embedding Numerous Features: Kernel Models
- 2 Combining Predictive Features: Aggregation Models

Lecture 9: Decision Tree

- Decision Tree Hypothesis

 express path-conditional aggregation

 Decision Tree Algorithm

 recursive branching until termination to base
 - Decision Tree Heuristics in C&RT pruning, categorical branching, surrogate
 - Decision Tree in Action

explainable and efficient

- next: aggregation of aggregation?!
- Oistilling Implicit Features: Extraction Models