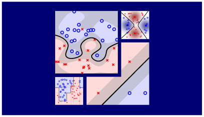
Machine Learning Techniques
(機器學習技法)



Lecture 9: Decision Tree

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Roadmap

1. 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

3. Distilling Implicit Features: Extraction Models

What We Have Done

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

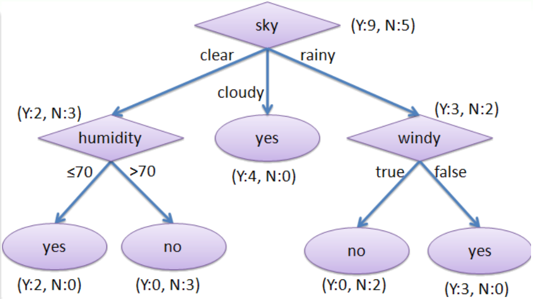
aggregation type	blending	learning
uniform	voting/averaging	Bagging
non-uniform	linear	AdaBoost
conditional	stacking	**Decision Tree**

decision tree: a traditional learning model that realizes **conditional aggregation**

Decision Tree for Playing Golf

$$G(\mathbf{x}) = \sum_{t=1}^{T} q_t(\mathbf{x}) \cdot g_t(\mathbf{x})$$

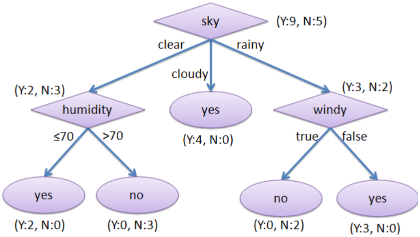
- **base hypothesis** $g_t(\mathbf{x})$: leaf at end of path t, a **constant** here
- **condition** $q_t(\mathbf{x})$: $[\![$is $\mathbf{x}$ on path t?$]\!]$
- usually with **simple internal nodes**



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

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

$$G(\mathbf{x}) = \sum_{c=1}^{C} [\![b(\mathbf{x}) = c]\!] \cdot G_c(\mathbf{x})$$

- $G(\mathbf{x})$: full-tree hypothesis
- $b(\mathbf{x})$: branching criteria
- $G_c(\mathbf{x})$: 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
- simple: **even freshmen can implement one :-)**
- efficient in prediction and **training**

However......

- heuristic: mostly **little theoretical** explanations
- heuristic**s**: 'heuristic**s** 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
2. false
3. 98765
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 ($\mathtt{income}, \mathtt{debt}$) = $(98765, 56789)$?

1. true
2. false
3. 98765
4. 56789

Reference Answer: 2

You can simply trace the code. The tree expresses a complicated boolean condition $[\![\mathtt{income} > 100000 \text{ or } \mathtt{debt} \leq 50000]\!]$.

A Basic Decision Tree Algorithm

$$G(\mathbf{x}) = \sum_{c=1}^{C} [\![b(\mathbf{x}) = c]\!] \, G_c(\mathbf{x})$$

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 $G_c \leftarrow$ DecisionTree($\mathcal{D}_c$)
4. return $G(\mathbf{x}) = \sum_{c=1}^{C} [\![b(\mathbf{x}) = c]\!] \, G_c(\mathbf{x})$

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

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

two simple choices

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

Branching in C&RT: Purifying

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

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

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

C&RT: **bi-branching** by **purifying**

Impurity Functions

by E_{in} of optimal constant

- regression error:

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

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

- classification error:

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

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

for classification

- Gini index:

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

—all k considered together

- classification error:

$$1 - \max_{1\leq k\leq K}\frac{\sum_{n=1}^{N}[\![y_n = k]\!]}{N}$$

—optimal $k = y^*$ only

popular choices: **Gini** for classification, **regression error** for regression

Termination in C&RT

function DecisionTree(data $\mathcal{D} = \{(\mathbf{x}_n, y_n)\}_{n=1}^{N}$)
if termination criteria met
return base hypothesis $g_t(\mathbf{x}) = E_{\text{in}}$-optimal constant
else ...
1. learn branching criteria

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

'forced' to terminate when

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

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

Fun Time

For the Gini index, $1 - \frac{1}{K}\sum_{k=1}^{K}\left(\frac{\sum_{n=1}^{N}[\![y_n = k]\!]}{N}\right)^2$. 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. $\mu \cdot (1-\mu) + \frac{1}{2}$
2. $\mu \cdot (1-\mu) - \frac{1}{2}$
3. $\mu \cdot (1-\mu) \cdot \frac{1}{2}$
4. $\mu \cdot (1-\mu) / \frac{1}{2}$

Fun Time

For the Gini index, $1 - \frac{1}{K}\sum_{k=1}^{K}\left(\frac{\sum_{n=1}^{N}[\![y_n = k]\!]}{N}\right)^2$. 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. $\mu \cdot (1 - \mu) + \frac{1}{2}$
2. $\mu \cdot (1 - \mu) - \frac{1}{2}$
3. $\mu \cdot (1 - \mu) \cdot \frac{1}{2}$
4. $\mu \cdot (1 - \mu) / \frac{1}{2}$

Reference Answer: 1

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

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

1. learn branching criteria

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

2. split $\mathcal{D}$ to 2 parts $\mathcal{D}_c = \{(\mathbf{x}_n, y_n) : b(\mathbf{x}_n) = c\}$
3. build sub-tree $G_c \leftarrow$ DecisionTree($\mathcal{D}_c$)
4. return $G(\mathbf{x}) = \sum_{c=1}^{2} [\![b(\mathbf{x}) = c]\!] \, G_c(\mathbf{x})$

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

Regularization by Pruning

fully-grown tree: $E_{\text{in}}(G) = 0$ 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:

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

—called **pruned** decision tree

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

systematic choice of λ? **validation**

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

$$b(\mathbf{x}) = [\![x_i \le \theta]\!] + 1$$

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

branching for categorical

decision subset

$$b(\mathbf{x}) = [\![x_i \in S]\!] + 1$$

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

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

Missing Features by Surrogate Branch

possible $b(\mathbf{x}) = [\![\text{weight} \leq 50\text{kg}]\!]$

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 $b_1(\mathbf{x}), b_2(\mathbf{x}), \ldots \approx$ best branch $b(\mathbf{x})$ during training
  - allow missing feature for $b(\mathbf{x})$ during prediction by using surrogate instead

C&RT: handles **missing features easily**

Fun Time

For a categorical branching criteria $b(\mathbf{x}) = [\![x_i \in S]\!] + 1$ with $S = \{1, 6\}$. Which of the following is the explanation of the criteria?

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

Fun Time

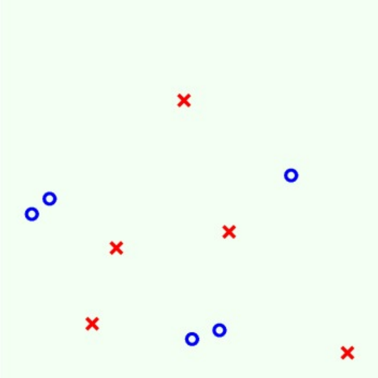
For a categorical branching criteria $b(\mathbf{x}) = [\![x_i \in S]\!] + 1$ with $S = \{1, 6\}$. Which of the following is the explanation of the criteria?

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

Reference Answer: 3

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

A Simple Data Set



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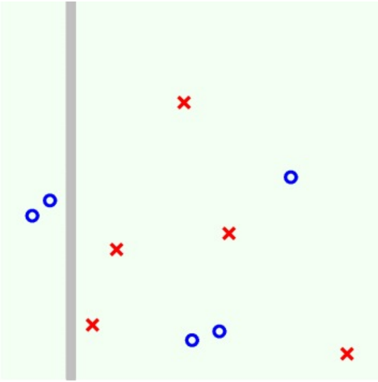

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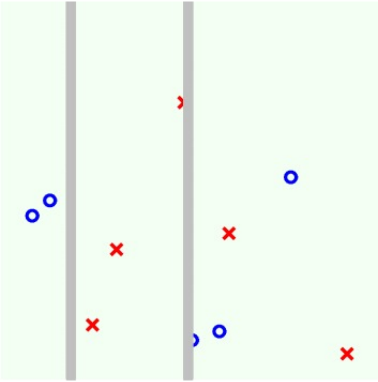

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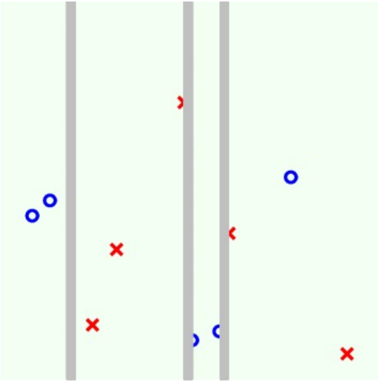

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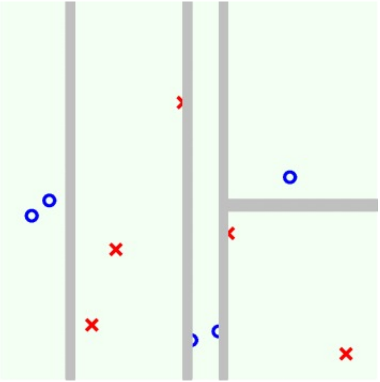

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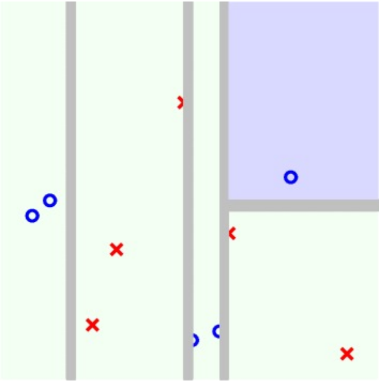

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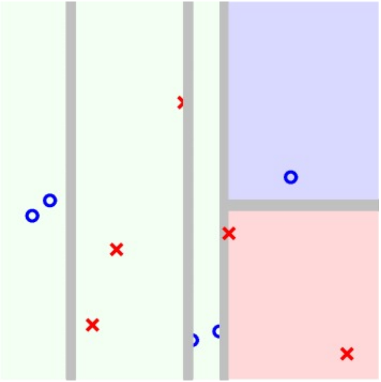

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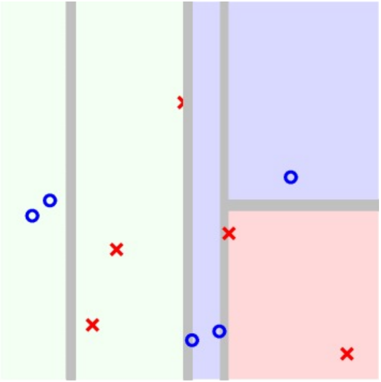

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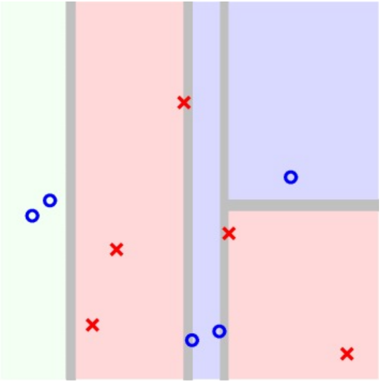

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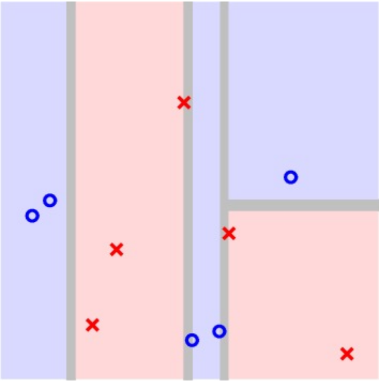

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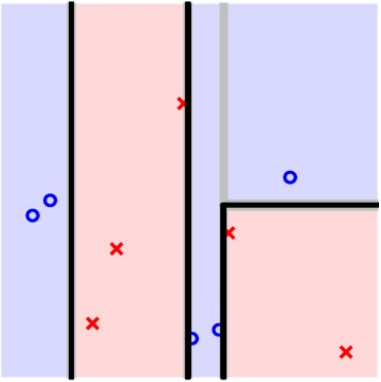
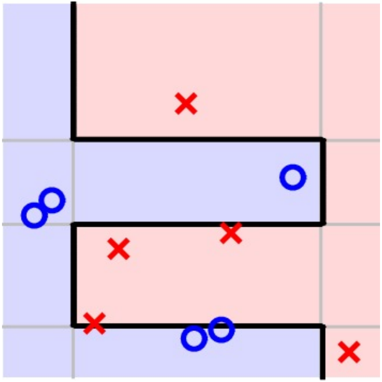


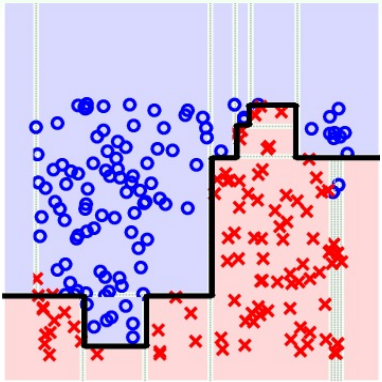
C&RT



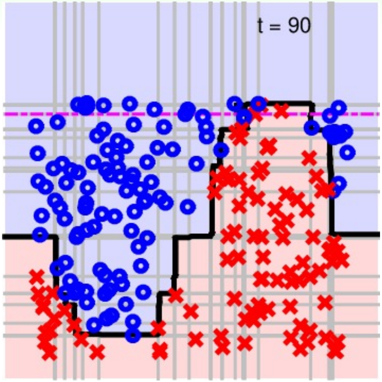
AdaBoost-Stump

C&RT: 'divide-and-conquer'

A Complicated Data Set



C&RT



AdaBoost-Stump

C&RT: even more efficient than AdaBoost-Stump

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?

1. 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

1. 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?!**

3. Distilling Implicit Features: Extraction Models