Decision Trees
Announcements

HW6 and P6 will be released soon
Recap on the K-NN algorithm

K-NN can have complicated nonlinear decision boundaries

[1-NN decision boundary in prelim]
Recap on the K-NN algorithm

K-NN can have complicated nonlinear decision boundaries

k-NN is expensive in computation and memory

[1-NN decision boundary in prelim]
Objective today

Decision tree — more efficient algorithm that
(1) splits space into regions with the same label, (2) is very fast in test time
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Decision tree — more efficient algorithm that (1) splits space into regions with the same label, (2) is very fast in test time
Outline of Today

1. Decision tree in classification

2. Decision tree in regression

3. Demos of decision tree
Overview of the Decision Tree algorithm
How to split a tree node

Consider k-class classification, i.e., \( y \in \{1, 2, \ldots, k\} \)

\[ S = \{x, y\} \]
How to split a tree node

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\( x[1] \leq \tau \)

\( x[1] > \tau \)

\( S_L \)

\( S_R \)
How to split a tree node

Consider k-class classification, i.e., \( y \in \{1,2,\ldots,k\} \)

\[
S = \{x, y\}
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\[
x[1] \leq \tau \quad \text{or} \quad x[1] > \tau
\]

\[
S_L + S_R = S, \quad S_L \cap S_R = \emptyset
\]
How to split a tree node

Consider k-class classification, i.e., $y \in \{1,2,\ldots,k\}$

$$S = \{x, y\}$$

$x[1] \leq \tau$ \hspace{1cm} $x[1] > \tau$

Goal: do an axis aligned split such that diversity of labels in leafs are reduced.

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How to split a tree node

Consider k-class classification, i.e., $y \in \{1,2,\ldots,k\}$

Goal: do an axis aligned split such that diversity of labels in leafs are reduced

How to mathematically quantify “diversity”? 

$S = \{x, y\}$

$x[1] \leq \tau$  
$x[1] > \tau$

$S_L + S_R = S$, $S_L \cap S_R = \emptyset$
Detour: Entropy

Given a set $S = \{x_i, y_i\}_{i=1}^n, y_i \in \{1,2,\ldots,k\}$, measure the diversity of labels via entropy
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Given a set $S = \{x_i, y_i\}_{i=1}^n$, $y_i \in \{1, 2, \ldots, k\}$, measure the diversity of labels via entropy

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   (Probability of $y$ being label $i$)

2. Entropy: $H(S) = \sum_{i=1}^k -p_i \ln(p_i)$
Detour: Entropy

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   (Probability of $y$ being label $i$)

2. Entropy: $H(S) = \sum_{i=1}^k -p_i \ln(p_i)$

   High entropy means “diverse, chaos, uncertain”
Entropy

Consider a Bernoulli distribution

\[ P(y = 1) = p, \quad P(y = 0) = 1 - p \]

Entropy \( H(y) \):
Entropy

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Entropy \( H(y) \): 

\[ -P(y = 1) \cdot \ln P(y = 1) - P(y = 0) \cdot \ln P(y = 0) \]
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\[ = -p \ln p - (1 - p)\ln(1 - p) \]
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Entropy \( H(y) \):

\[
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\]

\[
= - p \ln p - (1 - p) \ln(1 - p)
\]
Entropy

Consider a categorical distribution

\[ y \in \{1, 2, \ldots, k\}, \quad P(y = i) = p_i \geq 0, \quad \sum_{i=1}^{k} p_i = 1 \]

Q: when is entropy maximized?

\[ H = -\sum_{i=1}^{k} p_i \ln p_i \]

\[ p_1 = \frac{1}{k} \ldots = p_k = \frac{1}{k} \]
Consider a split, i.e, dim $i$ and threshold $\tau$, 

$$S = \{x, y\}$$

$$x[i] \leq \tau$$

$$x[i] > \tau$$

$S_L$

$S_R$

Optimization:
Consider a split, i.e., dim $i$ and threshold $\tau$,

$$
S = \{x, y\} \\
H(S) = \sum_{i=1}^{k} -p_i \ln p_i \\
S = \{x, y\} = \{x_i \leq \tau, x_i > \tau\} \\
S_L \\
S_R
$$

Optimization:

$$
p_i = \frac{\# \text{ of } \text{ins} \in S}{|S|}
$$
Consider a split, i.e., dim $i$ and threshold $\tau$,

$$S = \{x, y\}$$

$$H(S) = \sum_{i=1}^{k} -p_i \ln p_i$$

**Optimization:**

$$\frac{|S_L|}{|S|} H(S_L) + \frac{|S_R|}{|S|} H(S_R)$$
Consider a split, i.e., dim $i$ and threshold $\tau$,

$$H(S) = \sum_{i=1}^{k} -p_i \ln p_i$$

where $S = \{x, y\}$.

Optimization:

Find a split $(i, \tau)$ such that

$$\left(\frac{S_L}{S}H(S_L) + \frac{S_R}{S}H(S_R)\right)$$

is the smallest.
Consider a split, i.e., dim $i$ and threshold $\tau$,

$$\begin{align*}
S &= \{x, y\} \\
S_L &= \text{if } x[i] \leq \tau \\
S_R &= \text{if } x[i] > \tau \\
H(S) &= \sum_{i=1}^{k} -p_i \ln p_i \\
\frac{|S_L|}{|S|} H(S_L) + \frac{|S_R|}{|S|} H(S_R)
\end{align*}$$

Optimization:

Find a split $(i, \tau)$ such that

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Consider a split, i.e., dim $i$ and threshold $\tau$, $S = \{x, y\}$

\[ H(S) = \sum_{i=1}^{k} -p_i \ln p_i \]

\[ S_L = \{x \mid x[i] \leq \tau\} \]
\[ S_R = \{x \mid x[i] > \tau\} \]

\[
\frac{S_L}{S}H(S_L) + \frac{S_R}{S}H(S_R)
\]

**Optimization:**

Find a split $(i, \tau)$ such that $\frac{S_L}{S}H(S_L) + \frac{S_R}{S}H(S_R)$ is the smallest

**Q:** how many splits we need to check? $n$ points
Put everything together — ID3 algorithm

Input: training set $S = \{x, y\}$

Decision_tree($S$):
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- If all $y$ in $S$ are the same
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  Done, and return this label
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**Decision_tree($S$):**

- If all $y$ in $S$ are the same
  
  Done, and return this label

- Else:
  
  Find a split $(i, \tau)$ that minimizes weighted entropy

\[
\frac{|S_L|}{|S|} H(S_L) + \frac{|S_R|}{|S|} H(S_R)
\]
Input: training set $S = \{x, y\}$

**Decision_tree($S$):**

- If all $y$ in $S$ are the same
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  Find a split $(i, \tau)$ that minimizes weighted entropy

  Call $\text{Decision_tree}(S_L)$ & $\text{Decision_tree}(S_R)$
Put everything together — ID3 algorithm

Input: training set $S = \{x, y\}$

**Decision_tree($S$):**

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  Find a split $(i, \tau)$ that minimizes weighted entropy

Call $\text{Decision_tree}(S_L) \& \text{Decision_tree}(S_R)$
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1. Decision tree in classification

2. Decision tree in regression

3. Demos of decision tree
Regression

How to split the note, i.e., what is the diversity measure?
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Consider a set of training points $S = \{x_i, y_i\}_{i=1}^m, y_i \in \mathbb{R}$.
Regression

How to split the note, i.e., what is the diversity measure?

Consider a set of training points $S = \{x_i, y_i\}_{i=1}^m, y_i \in \mathbb{R}$

Define the sample mean $\hat{y}_S = \sum_{i=1}^m y_i / m$
Regression

How to split the note, i.e., what is the diversity measure?

Consider a set of training points $S = \{x_i, y_i\}_{i=1}^m, y_i \in \mathbb{R}$

Define the sample mean $\hat{y}_S = \frac{1}{m} \sum_{i=1}^{m} y_i$

Impurity: sample variance $\text{Var} (S) = \frac{1}{m} \sum_{i=1}^{m} (y_i - \hat{y}_S)^2$

$\Rightarrow \text{Var} (y) \quad \text{when} \quad m \to \infty$
Regression Tree

Regression_Tree(S):
Regression Tree

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- IF $|S| \leq k$:
  - Set leaf value to be $\bar{y}_S$
Regression Tree

Regression_Tree( S ):

- IF \( S \leq k \):
  - Set leaf value to be \( \bar{y}_S \)
- ELSE:
Regression Tree

Regression_Tree( S ):

- IF \( |S| \leq k \):
  Set leaf value to be \( \bar{y}_S \)

- ELSE:
  For all \((i, \tau)\), find the split such that minimizes
  \[
  \frac{S_L}{S} \text{Var} (S_L) + \frac{S_R}{S} \text{Var} (S_R)
  \]
Regression_Tree:

- IF \( |S| \leq k \):
  - Set leaf value to be \( \bar{y}_S \)
- ELSE:
  - For all \((i, \tau)\), find the split such that minimizes \( \frac{|S_L|}{|S|} \text{Var}(S_L) + \frac{|S_R|}{|S|} \text{Var}(S_R) \)
  - Call Regression_Tree(\( S_L \)) & Regression_Tree(\( S_R \))
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Issue of Decision Trees

Decision Tree can have high variance, i.e., overfilling!
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Decision Tree can have high variance, i.e., overfitting!
Take-home messages

1. Decision tree algorithms splits space into axis-aligned regions
   Each region ideally should only contain one unique label

2. Split a node such that the entropy of labels in the leafs are minimized

3. Can easily overfit as the depth of the tree increases
   (limiting the depth of the tree is a good regularization)