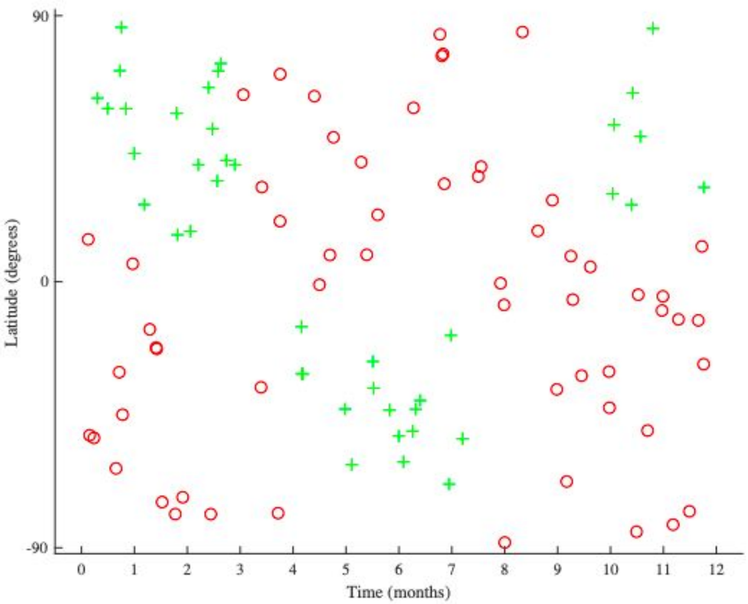
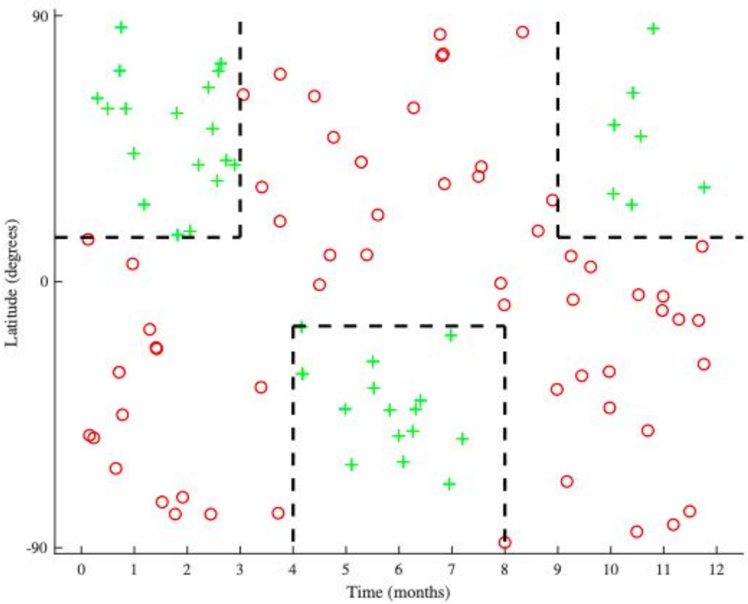
CS229
Decision Trees

May 14, 2021

Decision Trees: nonlinear classifier





Decision Trees: canonical situation

- No linear separation line
- Want to divide input space into “regions”
- Can do this by dividing input space into disjoint regions R_i

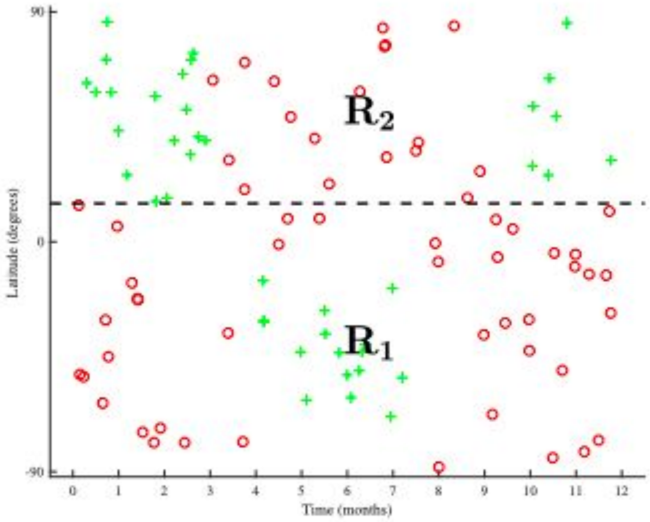
$$\mathcal{X} = \bigcup_{i=0}^{n} R_i$$

$$\text{s.t.} \qquad R_i \cap R_j = \emptyset \ \text{ for } \ i \neq j$$

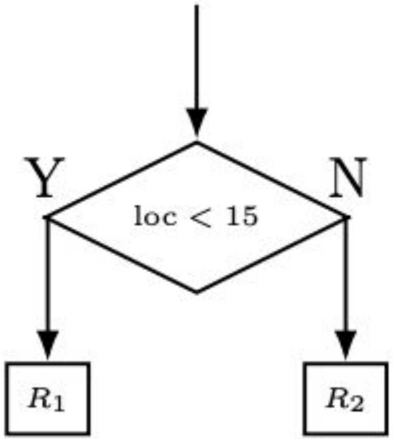
Recursively splitting regions

- Parent region R_p
- "Children" regions R_1 and R_2
- Split on feature X_j

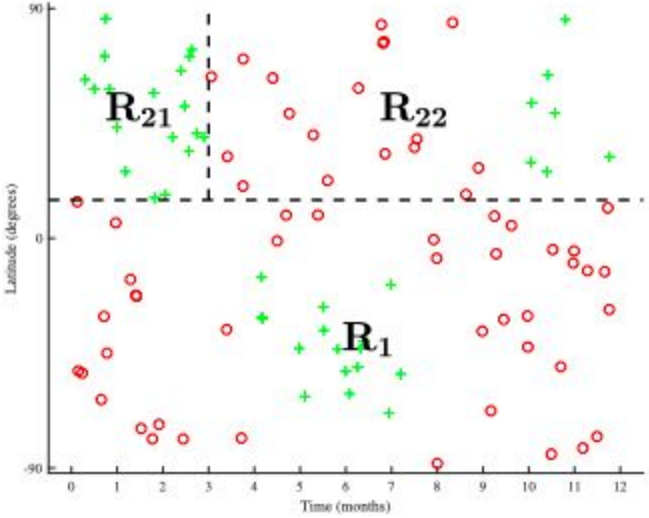
$$R_1 = \{X \mid X_j < t, X \in R_p\}$$
$$R_2 = \{X \mid X_j \geq t, X \in R_p\}$$



90
0
-90
0
1
2
3
4
5
6
7
8
9
10
11
12
Time (months)
Latitude (degrees)
$\mathbf{R_2}$
$\mathbf{R_1}$

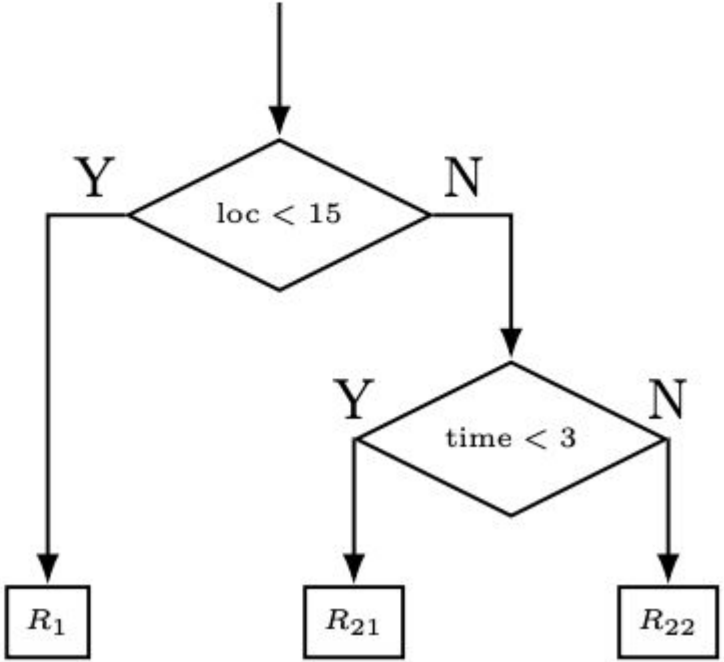


Y
N
loc < 15
R_1
R_2

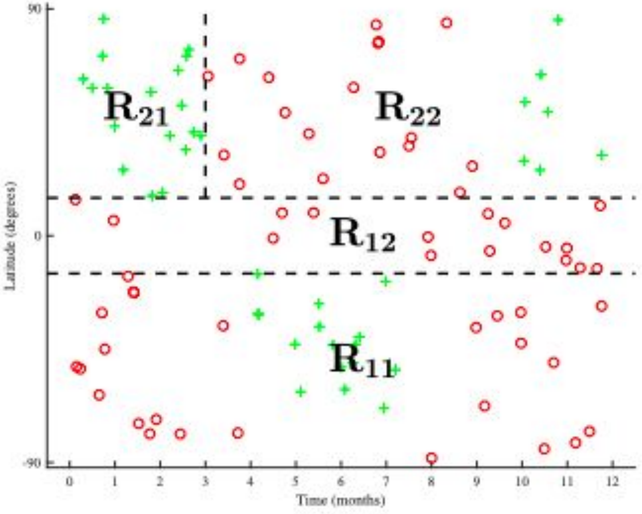


R_{21}
R_{22}
R_1
90
0
-90
Latitude (degrees)
0 1 2 3 4 5 6 7 8 9 10 11 12
Time (months)

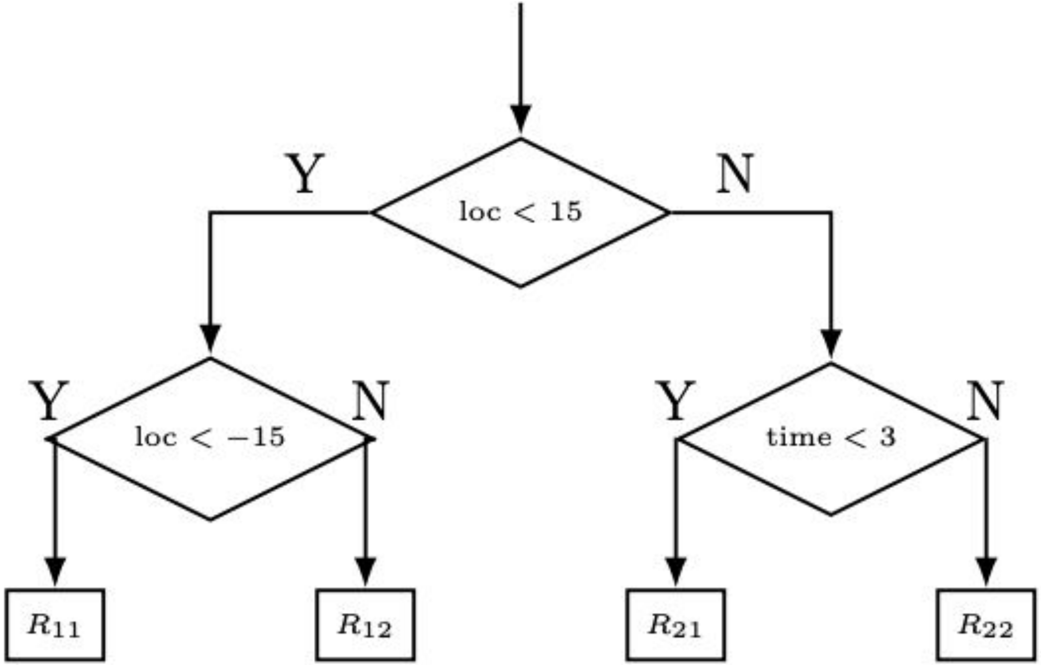
(b)



loc < 15
Y
N
time < 3
Y
N
R_1
R_{21}
R_{22}



90
0
-90
Latitude (degrees)
0 1 2 3 4 5 6 7 8 9 10 11 12
Time (months)
R21
R22
R12
R11



Y
N
loc < 15
Y
N
loc < −15
Y
N
time < 3
R11
R12
R21
R22

How ‘good’ is a split?

- Need to define a loss function L on a region
- Loss of the parent region $L(R_p)$ must be higher than that of child regions R_1 and R_2
- When deciding which attribute to split on, pick the one which maximizes the ‘gain’ in the loss
    - **Greedy splitting**

$$L(R_p) - \frac{|R_1|L(R_1) + |R_2|L(R_2)}{|R_1| + |R_2|}$$

Why greedy splitting?

- Checking every possible way of splitting every single feature in every possible order is computationally intractable!
- Greedy splitting is much easier: just compute the loss for each feature you want to consider splitting on

Entropy loss

- Looks like the cross-entropy loss that you have seen before
- $\hat{p}_c$ is the prevalence of class c in region R
- $L_{cross}(R) = 0$ if all the data in region R belongs to a single class

$$L_{cross}(R) = -\sum_{c} \hat{p}_c \log_2 \hat{p}_c$$

Entropy loss

- Note that the entropy loss is convex
- Can be shown that, under reasonable conditions, weighted average of children's loss is always less than parent's loss

$$L(R_p) - \frac{|R_1|L(R_1) + |R_2|L(R_2)}{|R_1| + |R_2|}$$

Common alternative: Gini impurity

- Closely related to entropy loss
- Default splitting loss for many ML libraries like scikit-learn

$$I_G(\hat{p}) = \sum_{i=1}^{c} \hat{p}_i \left(\sum_{k \neq c} \hat{p}_k \right) = \sum_{i=1}^{c} \hat{p}_i (1 - \hat{p}_i)$$

What about regression?

- Same growth process, but final prediction is now the mean of all datapoints in region: $\hat{y} = \frac{\sum_{i \in R} y_i}{|R|}$
- Use least-squares loss to split:

$$L_{squared}(R) = \frac{\sum_{i \in R} (y_i - \hat{y})^2}{|R|}$$

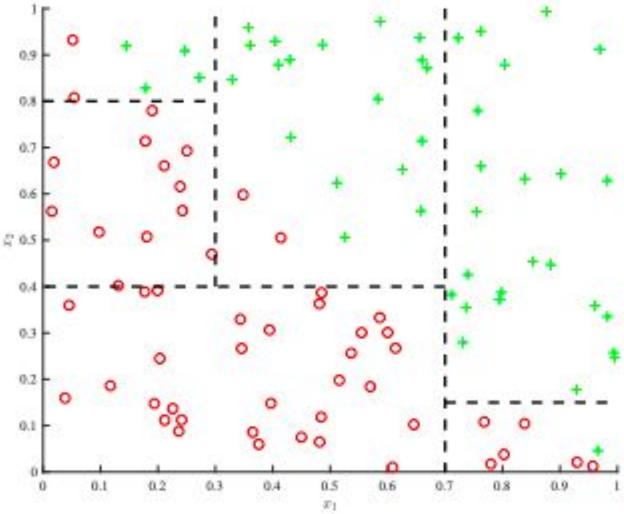
Regularization

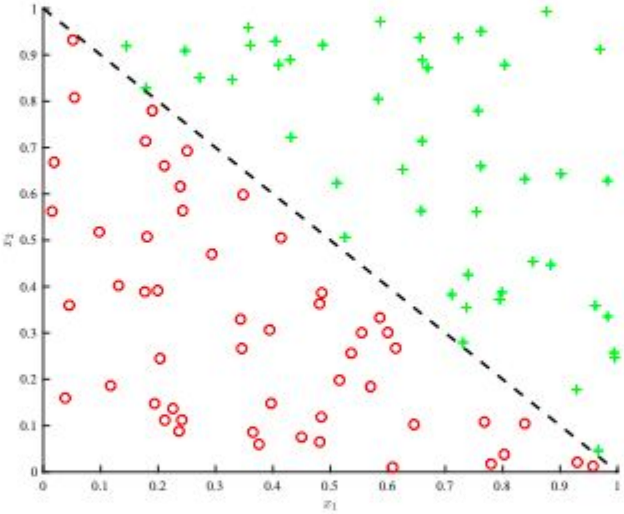
- Decision trees are highly prone to overfitting! High variance, low bias
- **Minimum leaf size**
  - Do not split R if its cardinality falls below a fixed threshold
- **Maximum depth**
  - Do not split R if more than a fixed threshold of splits were already taken to reach R
- **Maximum number of nodes**
  - Stop if a tree has more than a fixed threshold of leaf nodes

Runtime Complexity

- n examples, f features and a tree of depth d
- Test time complexity: O(d)
  - If balanced tree, O(d)=O(log n)
- Train time complexity: O(nfd)
  - Relatively fast since data matrix size is O(nf)

Decision trees lack “additive” structure





Random Forests

- Decision trees are prone to overfitting, so use a randomized ensemble of decision trees
  - Typically works a lot better than a single tree
- Each tree can use feature and sample bagging
  - Randomly select a subset of the data to grow tree
  - Randomly select a set of features
  - Decreases the correlation between different trees in the forest

Live Demo!

A few words about boosting...

- Iteratively add simple “weak” classifiers to improve classification performance
- After adding weak classifier, evaluate performance and reweight training samples
- Weak classifier can be decision tree of depth 1 (decision stump)
- Theoretically, can achieve zero training loss!
- Python libraries: LightGBM, XGBoost
- More in the boosting pdf notes!

Thank you