CS480/680: Introduction to Machine Learning

Lec 11: Decision Trees

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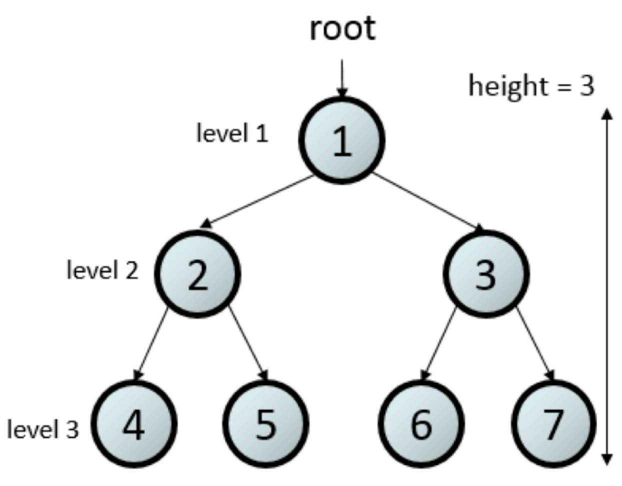
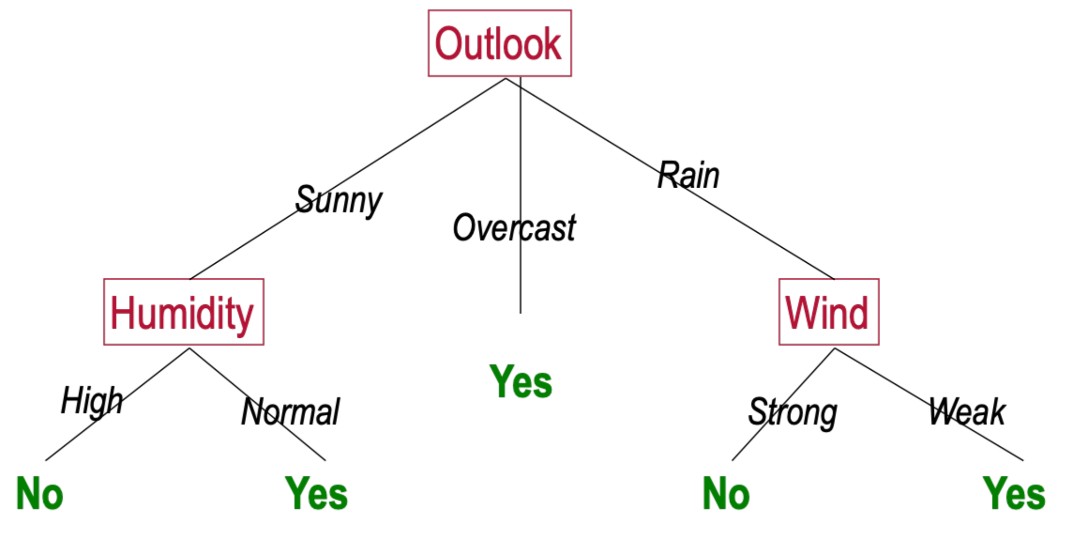
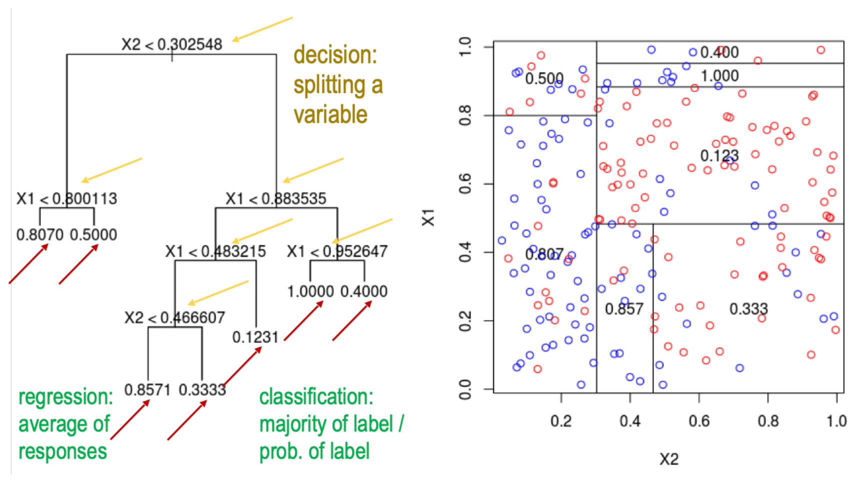
Trees Recalled





- Decision trees can represent any boolean function

Classification And Regression Tree

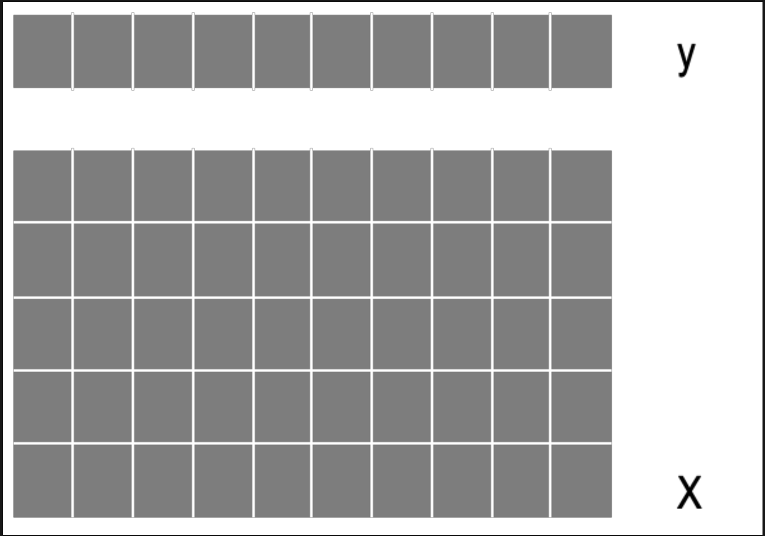


L. Breiman, J. H. Friedman, R. A. Olshen, and C. J. Stone. "Classification and Regression Trees". CRC, 1984.

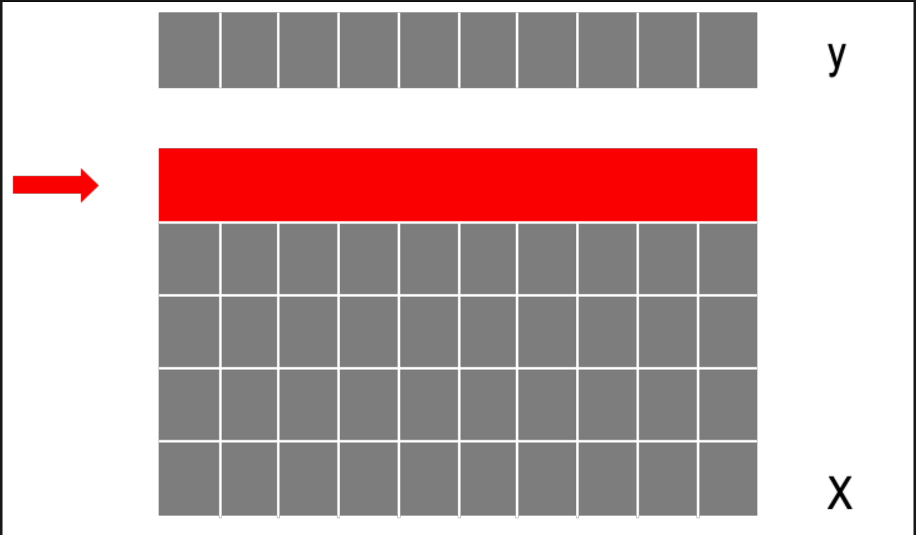
Learning Decision Trees

- Which variables to split at each stage?
- What threshold to use?
- When to stop?
  - regularization, e.g. early stopping
  - pruning
- What to put at the leaves?
  - classification: majority / probability
  - regression: average
  - can also simply store the training set

L. Hyafil and R. L. Rivest. "Constructing optimal binary decision trees is NP-complete". *Information Processing Letters*, vol. 5, no. 1 (1976), pp. 15–17.



- Splitting can only be based on $\mathbf{x}$
- Evaluation can be based on y as well



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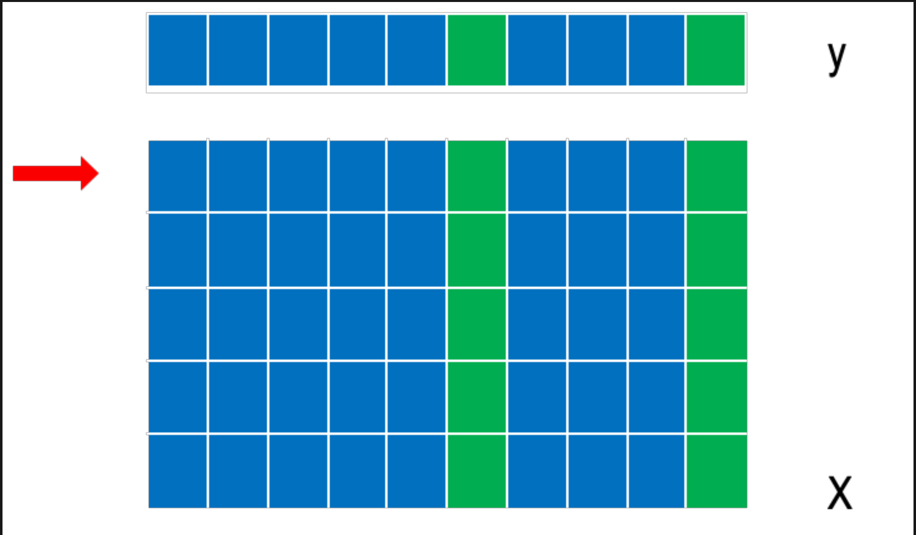

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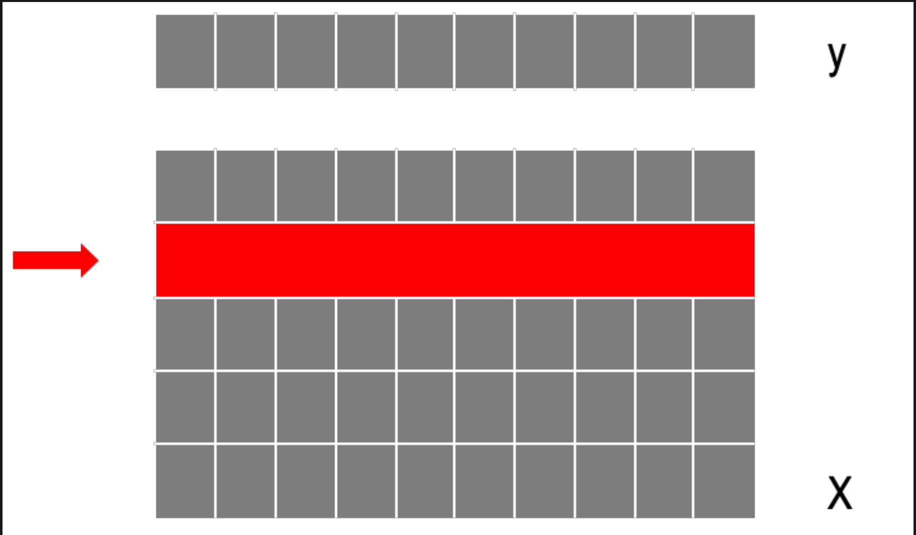

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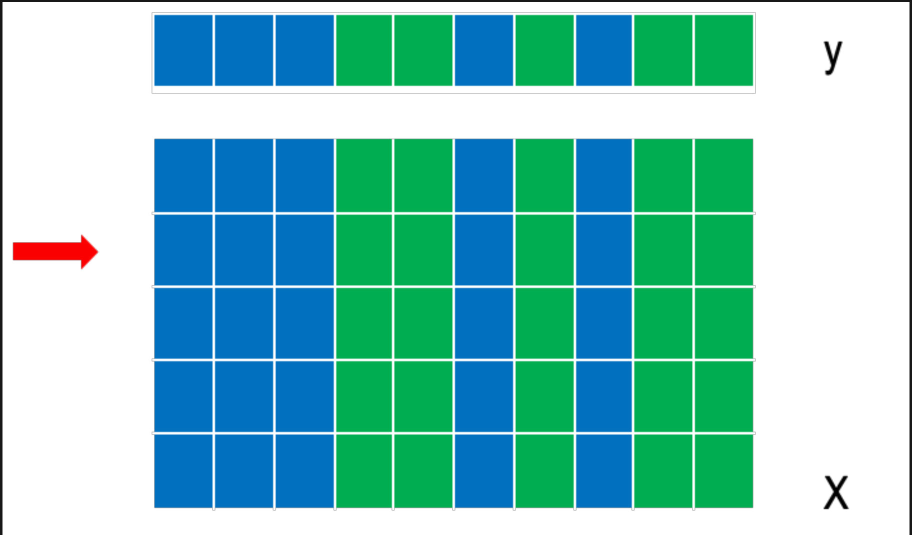

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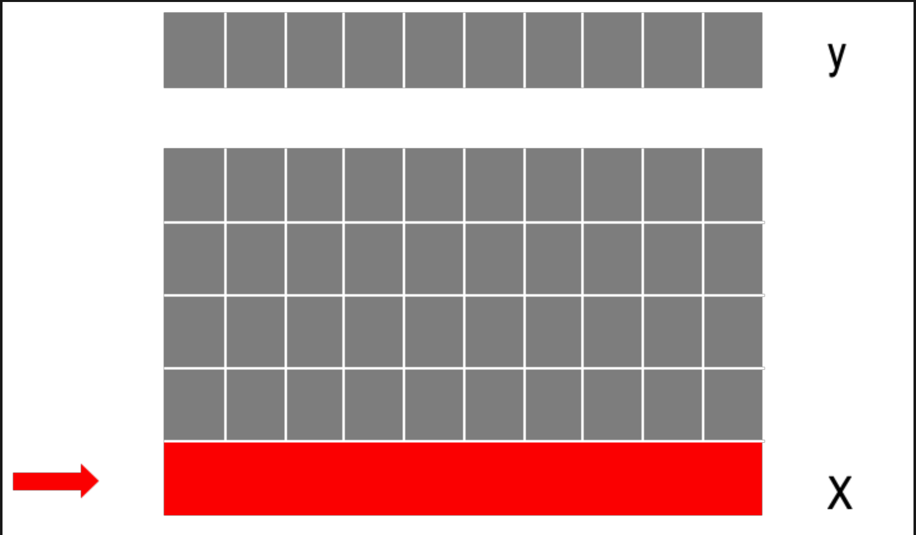

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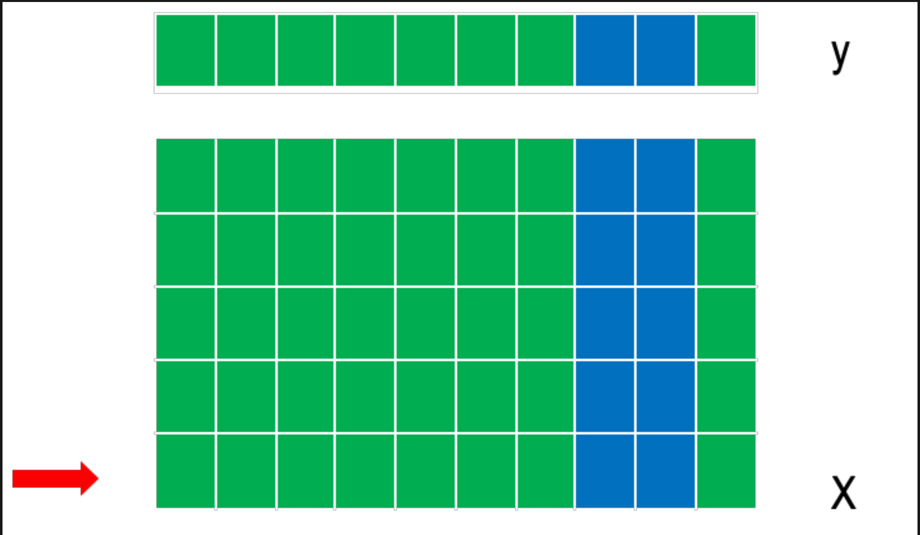

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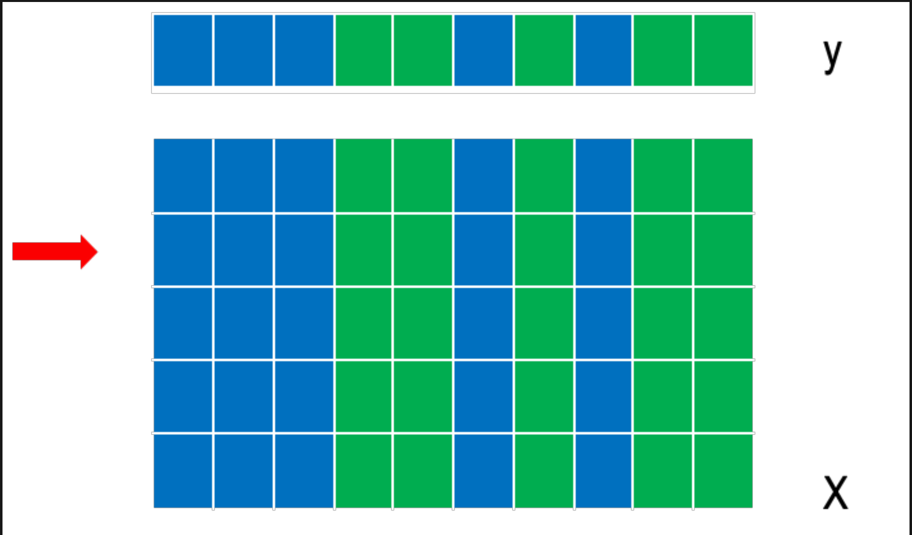

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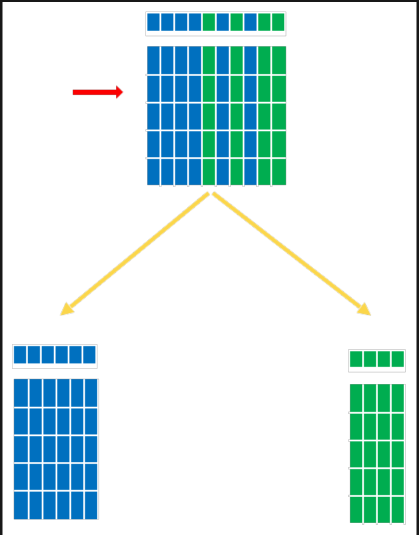

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Splitting by Minimizing

$$(j^*, t^*) = \operatorname*{argmin}_{j=1,\ldots,d} \min_{t \in T_j} \ \ell(\{\mathbf{x}_i, y_i\} : x_{ij} \le t) + \ell(\{\mathbf{x}_i, y_i\} : x_{ij} > t)$$

- Greedily choose the j-th feature to split
- Greedily choose a threshold $t \in T_j$ to split
  - what should T_j be? For categorical features?
- Partition training data into two disjoint parts: $x_{ij} \le t$ vs. $x_{ij} > t$
- Evaluate the resulting cost (objective)

Stopping Criterion

- Maximum depth exceeded
- Maximum runtime exceeded
- All childen nodes are (sufficiently) homogeneous
- All children nodes have too few training examples
- Reduction in cost stagnates:

$$\Delta := \ell(D) - \left(\frac{|\mathcal{D}_L|}{|\mathcal{D}|} \cdot \ell(\mathcal{D}_L) + \frac{|\mathcal{D}_R|}{|\mathcal{D}|} \cdot \ell(\mathcal{D}_R) \right)$$

- Cross-validation

Regression Cost

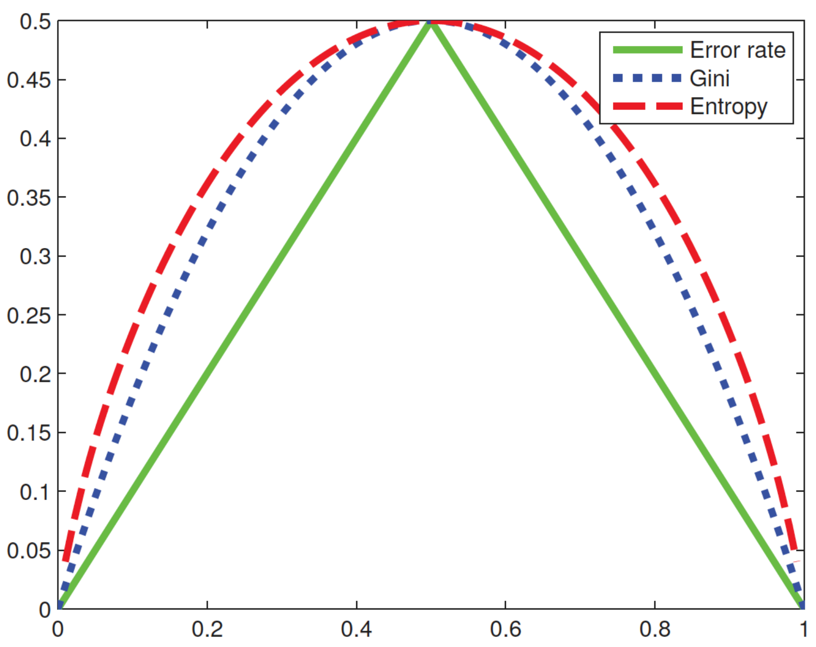
$$\ell(\mathcal{D}) := \left[\min_{y} \sum_{y_i \in \mathcal{D}} (y_i - y)^2\right] = \sum_{y_i \in \mathcal{D}} (y_i - \bar{y})^2, \quad \text{where} \quad \bar{y} = \frac{1}{|\mathcal{D}|} \sum_{y_i \in \mathcal{D}} y_i$$

- Can use any reasonable loss (other than the square loss)
- Can even fit a regression model on $\mathcal{D}$

Classification Cost

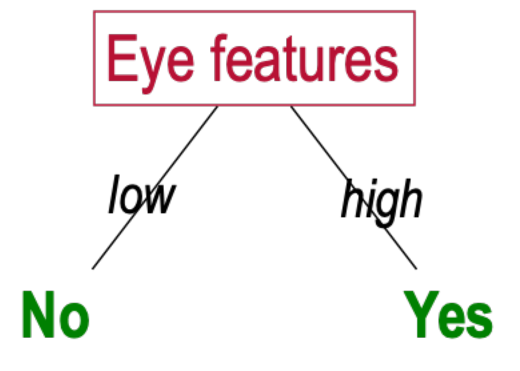
$$\hat{p}_k = \frac{1}{|\mathcal{D}|} \sum_{y_i \in \mathcal{D}} [\![y_i \in k]\!] , \qquad \hat{y} := \operatorname*{argmax}_{k=1,\ldots,c} \; \hat{p}_k$$

- Misclassification error: $\ell(\mathcal{D}) := 1 - \hat{p}_{\hat{y}}$, reduces to $\hat{p} \wedge (1 - \hat{p})$ if $c = 2$
- Gini index: $\ell(\mathcal{D}) := \sum_{k=1}^{c} \hat{p}_k (1 - \hat{p}_k) = 1 - \sum_{k=1}^{c} \hat{p}_k^2$, reduces to $2\hat{p}(1 - \hat{p})$ if $c = 2$
- Entropy: $\ell(\mathcal{D}) := -\sum_{k=1}^{c} \hat{p}_k \log \hat{p}_k$, reduces to $-\hat{p} \log \hat{p} - (1 - \hat{p}) \log(1 - \hat{p})$ if $c = 2$



0.5
0.45
0.4
0.35
0.3
0.25
0.2
0.15
0.1
0.05
0
0
0.2
0.4
0.6
0.8
1
Error rate
Gini
Entropy

Decision Stump



- A binary tree with depth 1
- Performs classification based on 1 feature
- Easy to train, interprettable, but underfits (addressed in next lecture)