Lecture 8: 29 April, 2021

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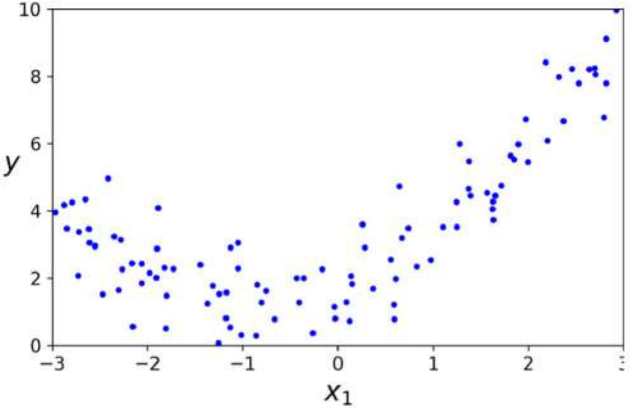
Data Mining and Machine Learning
April–July 2021

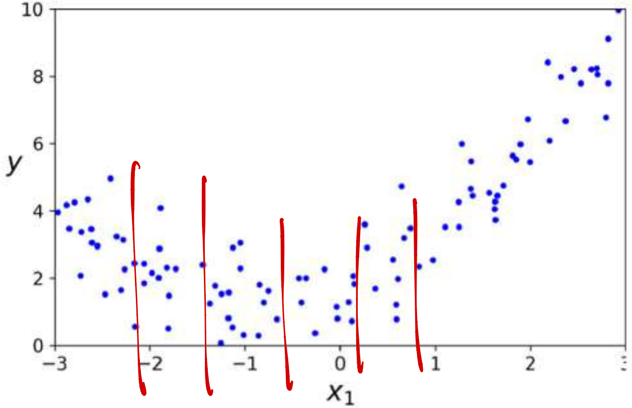
Decision trees for regression

- How do we use decision trees for regression?



Decision trees for regression

- How do we use decision trees for regression?
- Partition the input into intervals



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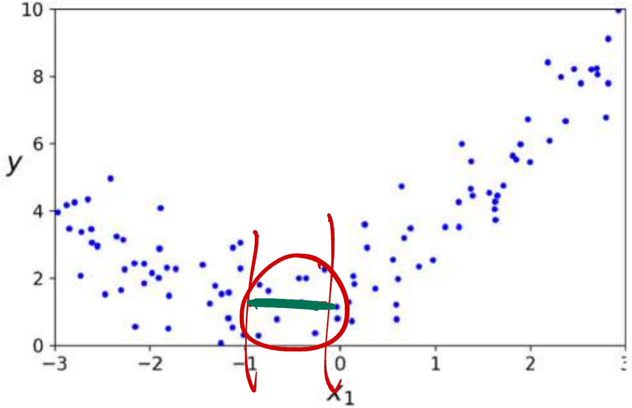
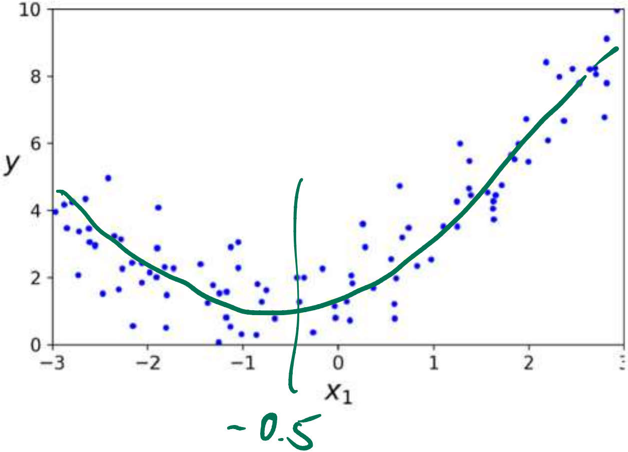
- For each interval, predict mean value of output, instead of majority class

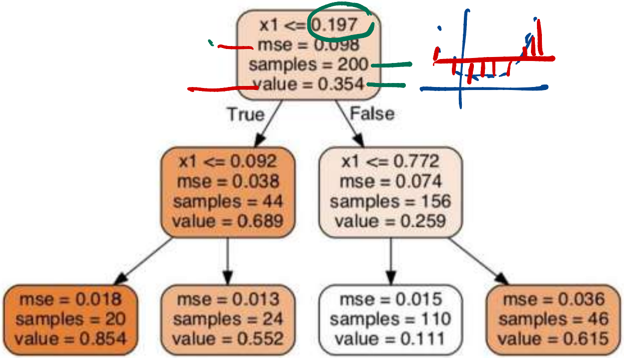


Decision trees for regression

- How do we use decision trees for regression?
- Partition the input into intervals
- For each interval, predict mean value of output, instead of majority class
- Regression tree



- Regression tree for noisy quadratic centered around $x_1 = 0.5$



Decision trees for regression

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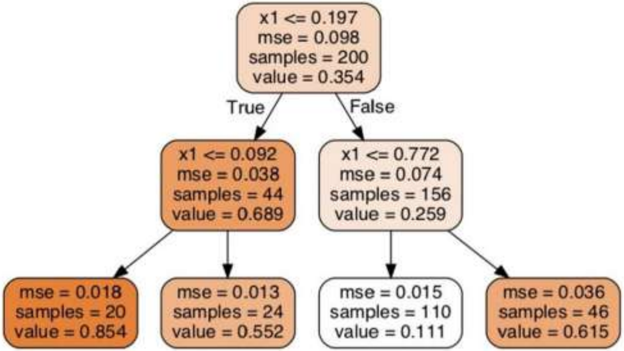
- For each node, the output is the mean y value for the current set of points



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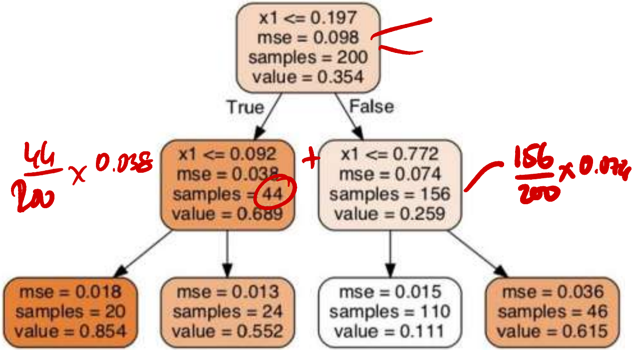
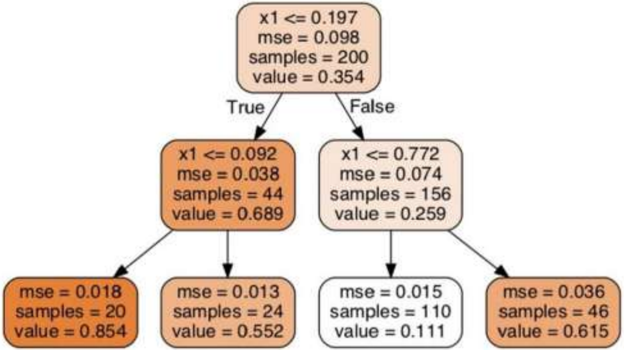


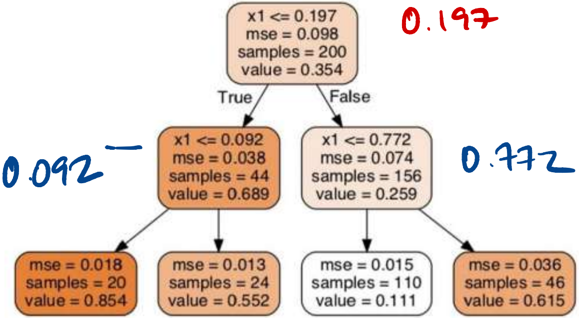
$\frac{44}{200} \times 0.038 + \frac{156}{200} \times 0.074$

Decision trees for regression

- Regression tree for noisy quadratic centered around $x_1 = 0.5$
- For each node, the output is the mean y value for the current set of points
- Instead of impurity, use mean squared error (MSE) as cost function
- Choose a split that minimizes MSE



- Approximation using regression tree

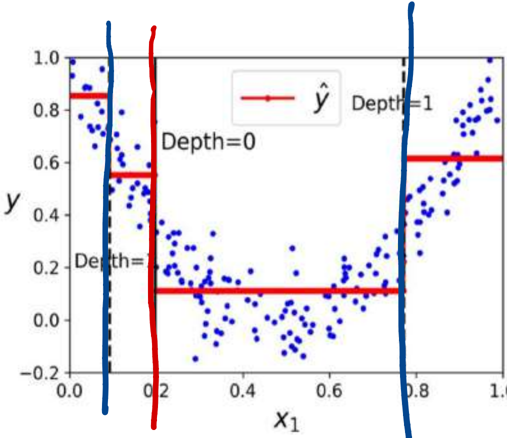


0.197

0.092

0.772

1 2 3 4



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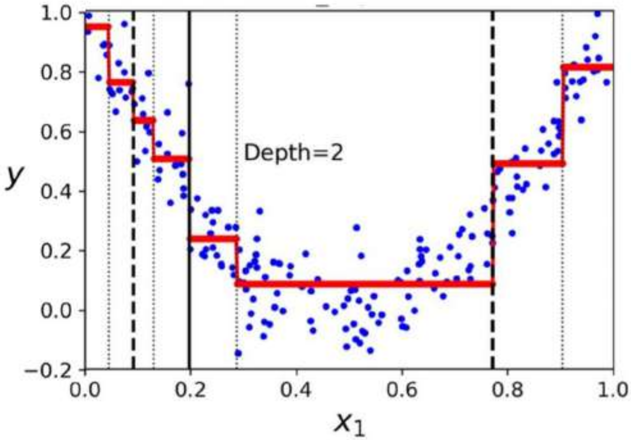
Regression trees

- Extend the regression tree one more level to get a finer approximation



Regression trees

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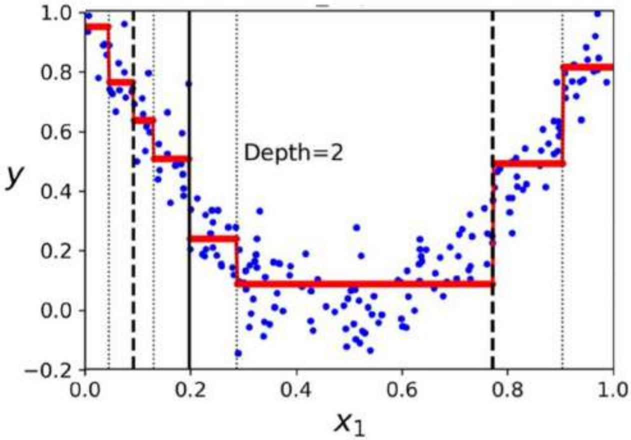


Regression trees

Entropy - Quinlan - C4.5

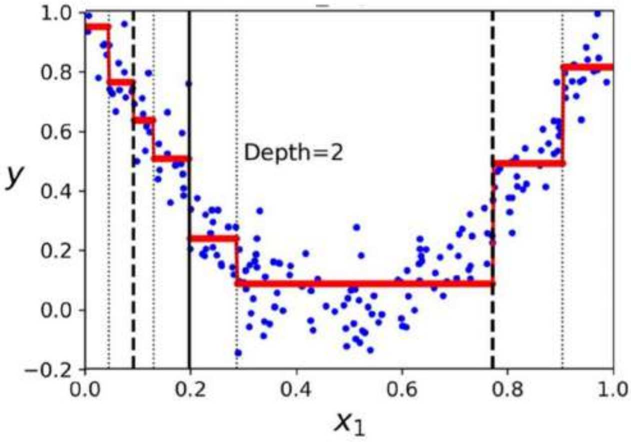
- Extend the regression tree one more level to get a finer approximation
- Set a threshold on MSE to decide when to stop
- Classification and Regression Trees (CART)

Python
R

Gini Index + Majority

MSE + Mean

Leo Breiman



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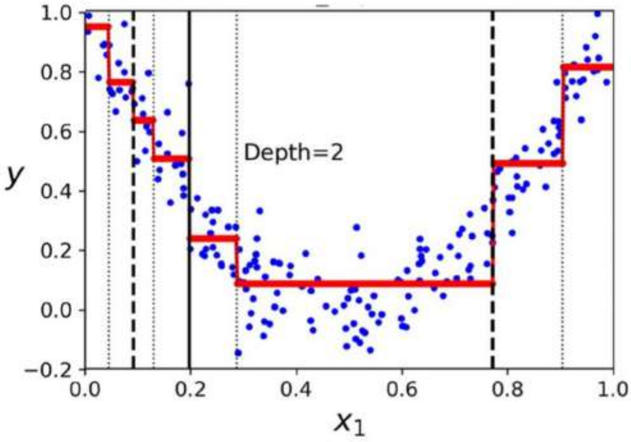
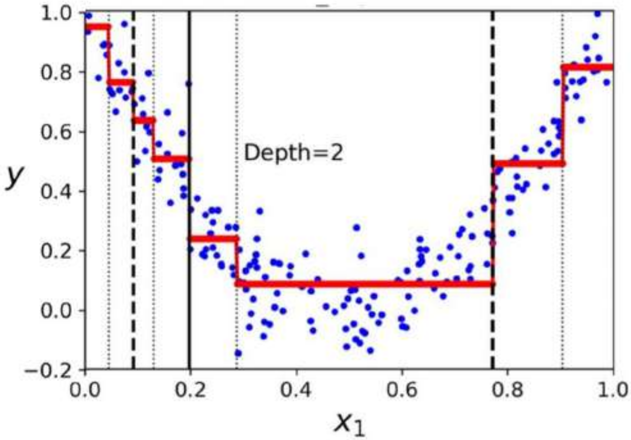
  - Combined algorithm for both use cases

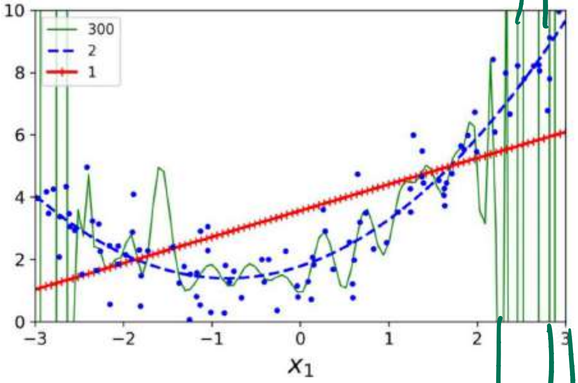


Regression trees

- Extend the regression tree one more level to get a finer approximation
- Set a threshold on MSE to decide when to stop
- Classification and Regression Trees (CART)
  - Combined algorithm for both use cases
- Programming libraries typically provide CART implementation



- Overfitting: model too specific to training data, does not generalize well



Overfitting

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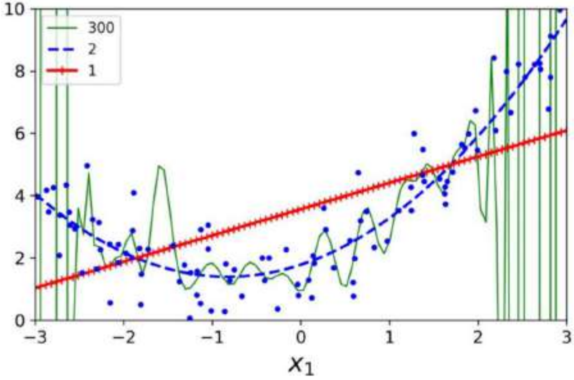
- Regression — use regularization to penalize model complexity



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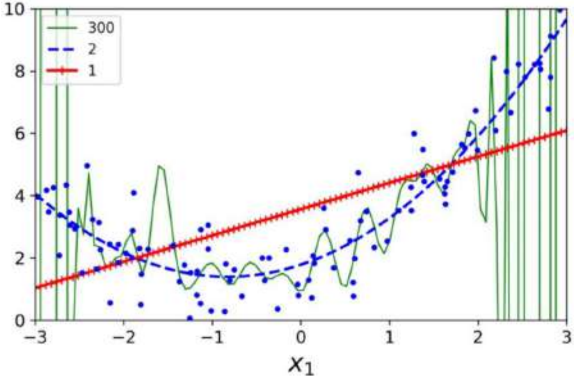

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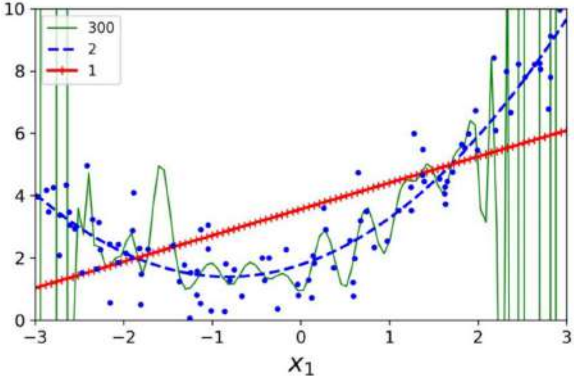
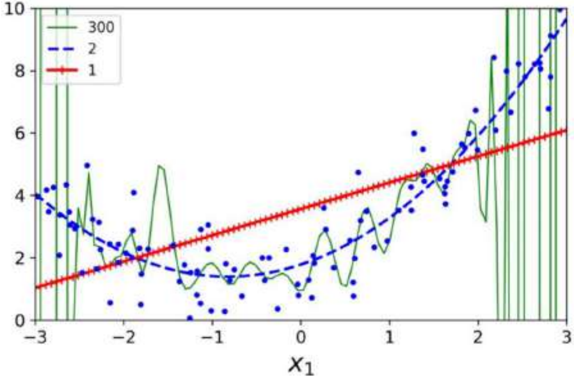


Overfitting

- Overfitting: model too specific to training data, does not generalize well
- Regression — use regularization to penalize model complexity
- What about decision trees?
- Deep, complex trees ask too many questions
- Prefer shallow, simple trees



Tree pruning

- Remove leaves to improve generalization

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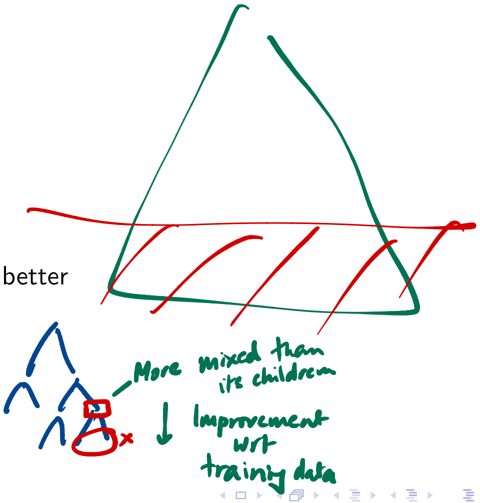
- Top-down pruning
  - Fix a maximum depth when building the tree
  - How to decide the depth in advance?

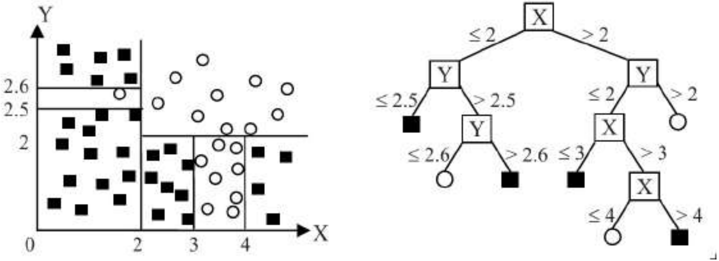
Tree pruning

- Remove leaves to improve generalization
- Top-down pruning – Fix # levels < K
    - Fix a maximum depth when building the tree
    - How to decide the depth in advance?
- Bottom-up pruning
    - Build the full tree
    - Remove a leaf if the reduced tree generalizes better
    - How do we measure this?



Tree pruning

Overfitted tree



Tree pruning

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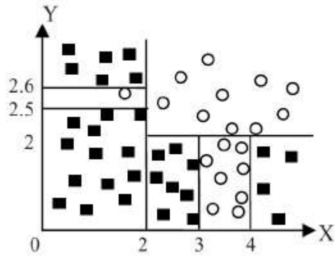
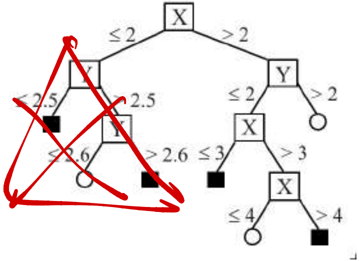
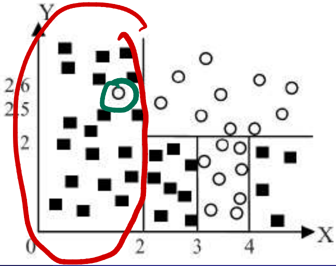
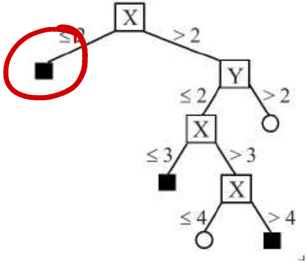




Pruned tree





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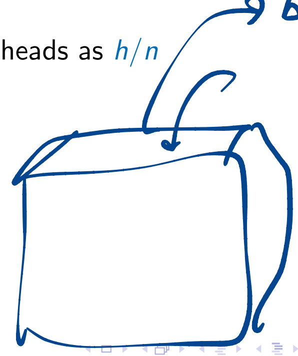
  - Estimate comes with a confidence interval: $h/n \pm \delta$

1000 balls

750 250

999 black 1 white or v.v.



black ball

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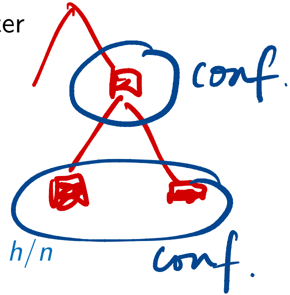

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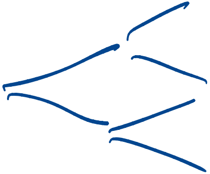
- Pruning leaves creates a larger impure sample one level above
- Does the confidence interval decrease (improve)?

Example: Predict party from voting pattern [Quinlan]

- Predict party affiliation of US legislators based on voting pattern
  - Read the tree from left to right



- physician fee freeze = n:
  - adoption of the budget resolution = y: democrat (151)
  - adoption of the budget resolution = u: democrat (1)
  - adoption of the budget resolution = n:
    - education spending = n: democrat (6)
    - education spending = y: democrat (9)
    - education spending = u: republican (1)
- physician fee freeze = y:
  - synfuels corporation cutback = n: republican (97/3) 100
  - synfuels corporation cutback = u: republican (4)
  - synfuels corporation cutback = y:
    - duty free exports = y: democrat (2)
    - duty free exports = u: republican (1)
    - duty free exports = n:
      - education spending = n: democrat (5/2)
      - education spending = y: republican (13/2)
      - education spending = u: democrat (1)
- physician fee freeze = u:
  - water project cost sharing = n: democrat (0)
  - water project cost sharing = y: democrat (4)
  - water project cost sharing = u:
    - mx missile = n: republican (0)
    - mx missile = y: democrat (3/1)
    - mx missile = u: republican (2)

Example: Predict party from voting pattern [Quinlan]

- Predict party affiliation of US legislators based on voting pattern
  - Read the tree from left to right
- After pruning, drastically simplified tree

In terms of confidence

```
physician fee freeze = n: democrat (168/2.6)
physician fee freeze = y: republican (123/13.9)
physician fee freeze = u:
|   mx missile = n: democrat (3/1.1)
|   mx missile = y: democrat (4/2.2)
|   mx missile = u: republican (2/1)
```

Example: Predict party from voting pattern [Quinlan]

- Predict party affiliation of US legislators based on voting pattern
  - Read the tree from left to right
- After pruning, drastically simplified tree
- Quinlan's comment on his use of sampling theory for post-pruning

Now, this description does violence to statistical notions of sampling and confidence limits, so the reasoning should be taken with a large grain of salt. Like many heuristics with questionable underpinnings, however, the estimates it produces seem frequently to yield acceptable results.

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Bayesian classifiers

- As before
  - Attributes $\{A_1, A_2, \ldots, A_k\}$ and
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Bayesian classifiers

- As before
  - Attributes $\{A_1, A_2, \ldots, A_k\}$ and
  - Classes $C = \{c_1, c_2, \ldots c_\ell\}$ $\ell = 2$
- Each class c_i defines a probabilistic model for attributes
  - $Pr(A_1 = a_1, \ldots, A_k = a_k \mid C = c_i)$
- Given a data item $d = (a_1, a_2, \ldots, a_k)$, identify the best class c for d
- Maximize $Pr(C = \underline{\underline{c_i}} \mid \underbrace{A_1 = a_1, \ldots, A_k = a_k}_{\text{Item}})$

Age	Home	Credit	Job	Loan
A_1	A_2	- -	A_k	Y/N C
Young	No	Poor	Yes	$\underline{\underline{C}}$

Yes No

$P(\text{Class} \mid \text{Item})$

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9 Y
6 N } 15

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- Generative model has associated parameters $\theta = (\theta_1, \ldots, \theta_m)$
  - Each class probability $Pr(c_j)$ is a parameter
  - Each conditional probability $Pr(a_1, \ldots, a_k \mid c_j)$ is a parameter

Choose $a_1, \ldots, a_k$ then c

Choose c then $a_1 \ldots a_k$

Data generated → gen c ⟶ gen $a_1 \ldots a_k$

Classify

Generative models

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- We need to estimate these parameters

Maximum Likelihood Estimators

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  - N coin tosses, H heads and T tails
  - Why is $\hat{\theta} = H/N$ the best estimate?

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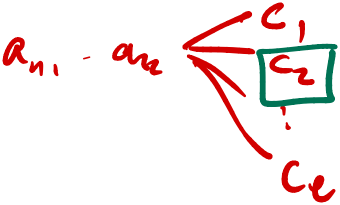
  - Given an estimate of θ, compute $Pr(\tau \mid \theta)$ — likelihood $L(\theta)$
- $\hat{\theta} = H/N$ maximizes this likelihood — $\arg\max\limits_{\theta} L(\theta) = \hat{\theta} = H/N$
  - Maximum Likelihood Estimator (MLE)

Bayesian classification

- Maximize $Pr(C = c_i \mid A_1 = a_1, \ldots, A_k = a_k)$



Bayesian classification

- Maximize $Pr(C = c_i \mid A_1 = a_1, \ldots, A_k = a_k)$
- By Bayes' rule,

$$\underline{Pr(C = c_i \mid A_1 = a_1, \ldots, A_k = a_k)}$$

$$= \frac{\overbrace{Pr(A_1 = a_1, \ldots, A_k = a_k \mid C = c_i)}^{\theta_j} \cdot \overbrace{Pr(C = c_i)}^{\theta_i}}{\underbrace{Pr(A_1 = a_1, \ldots, A_k = a_k)}_{?}}$$

$$P(A|B) = \frac{P(B|A) \cdot P(A)}{P(B)}$$

Bayesian classification

- Maximize $Pr(C = c_i \mid A_1 = a_1, \ldots, A_k = a_k)$
- By Bayes' rule,

$c_i \sim c_i$

$$Pr(C = c_i \mid A_1 = a_1, \ldots, A_k = a_k)$$

$$= \frac{Pr(A_1 = a_1, \ldots, A_k = a_k \mid C = c_i) \cdot Pr(C = c_i)}{Pr(A_1 = a_1, \ldots, A_k = a_k)}$$

$$= \frac{Pr(A_1 = a_1, \ldots, A_k = a_k \mid C = c_i) \cdot Pr(C = c_i)}{\sum_{j=1}^{\ell} Pr(A_1 = a_1, \ldots, A_k = a_k \mid C = c_j) \cdot Pr(C = c_j)}$$

$P(A|C)$ $\quad C < \begin{matrix} c_1 \\ c_2 \end{matrix}$

$P(A|c_1) \cdot P(c_1)$

$+ P(A|c_2)\, P(c_2)$

Bayesian classification

- Maximize $Pr(C = c_i \mid A_1 = a_1, \ldots, A_k = a_k)$
- By Bayes' rule,

$$Pr(C = c_i \mid A_1 = a_1, \ldots, A_k = a_k)$$

$$= \frac{Pr(A_1 = a_1, \ldots, A_k = a_k \mid C = c_i) \cdot Pr(C = c_i)}{Pr(A_1 = a_1, \ldots, A_k = a_k)}$$

Maximize

$$= \frac{Pr(A_1 = a_1, \ldots, A_k = a_k \mid C = c_i) \cdot Pr(C = c_i)}{\sum_{j=1}^{\ell} Pr(A_1 = a_1, \ldots, A_k = a_k \mid C = c_j) \cdot Pr(C = c_j)}$$

- Denominator is the same for all c_i, so sufficient to maximize

$$\underline{Pr(A_1 = a_1, \ldots, A_k = a_k \mid C = c_i)} \cdot \underline{Pr(C = c_i)}$$

Example

- To classify $A = g, B = q$

A	B	C
m	b	t
m	s	t
g	q	t
h	s	t
g	q	t
g	q	f
g	s	f
h	b	f
h	q	f
m	b	f

Example

- To classify $A = g, B = q$

- $Pr(C = t) = 5/10 = 1/2$
- $Pr(A = g, B = q \mid C = t) = 2/5$

P(θ_i) – count table

A	B	C
m	b	t
m	s	t
g	q	t
h	s	t
g	q	t
g	q	f
g	s	f
h	b	f
h	q	f
m	b	f

Example

- To classify $A = g, B = q$
- $Pr(C = t) = 5/10 = 1/2$
- $Pr(A = g, B = q \mid C = t) = 2/5$
- $Pr(A = g, B = q \mid C = t) \cdot Pr(C = t) = 1/5$

A	B	C
m	b	t
m	s	t
g	q	t
h	s	t
g	q	t
g	q	f
g	s	f
h	b	f
h	q	f
m	b	f

Example

- To classify $A = g, B = q$

- $Pr(C = t) = 5/10 = 1/2$
- $Pr(A = g, B = q \mid C = t) = 2/5$
- $Pr(A = g, B = q \mid C = t) \cdot Pr(C = t) = 1/5$

- $Pr(C = f) = 5/10 = 1/2$
- $Pr(A = g, B = q \mid C = f) = 1/5$

A	B	C
m	b	t
m	s	t
g	q	t
h	s	t
g	q	t
g	q	f
g	s	f
h	b	f
h	q	f
m	b	f

Example

- To classify $A = g, B = q$

- $Pr(C = t) = 5/10 = 1/2$
- $Pr(A = g, B = q \mid C = t) = 2/5$
- $Pr(A = g, B = q \mid C = t) \cdot Pr(C = t) = 1/5$ ✓

- $Pr(C = f) = 5/10 = 1/2$
- $Pr(A = g, B = q \mid C = f) = 1/5$
- $Pr(A = g, B = q \mid C = f) \cdot Pr(C = f) = 1/10$ ✓

A	B	C
m	b	t
m	s	t
g	q	t
h	s	t
g	q	t
g	q	f
g	s	f
h	b	f
h	q	f
m	b	f

Example

- To classify $A = g, B = q$

- $Pr(C = t) = 5/10 = 1/2$
- $Pr(A = g, B = q \mid C = t) = 2/5$
- $Pr(A = g, B = q \mid C = t) \cdot Pr(C = t) = 1/5$

- $Pr(C = f) = 5/10 = 1/2$
- $Pr(A = g, B = q \mid C = f) = 1/5$
- $Pr(A = g, B = q \mid C = f) \cdot Pr(C = f) = 1/10$

- Hence, predict $C = t$

A	B	C
m	b	t
m	s	t
g	q	t
h	s	t
g	q	t
g	q	f
g	s	f
h	b	f
h	q	f
m	b	f

Example . . .

- What if we want to classify $A = m, B = q$?

A	B	C
m	b	t
m	s	t
g	q	t
h	s	t
g	q	t
g	q	f
g	s	f
h	b	f
h	q	f
m	b	f

Example ...

- What if we want to classify $A = m, B = q$?
- $Pr(A = m, B = q \mid C = t) = 0$

A	B	C
m	b	t
m	s	t
g	q	t
h	s	t
g	q	t
g	q	f
g	s	f
h	b	f
h	q	f
m	b	f

Example ...

- What if we want to classify $A = m, B = q$?
- $Pr(A = m, B = q \mid C = t) = 0$
- Also $Pr(A = m, B = q \mid C = f) = 0$!

What to do?

A	B	C
m	b	t
m	s	t
g	q	t
h	s	t
g	q	t
g	q	f
g	s	f
h	b	f
h	q	f
m	b	f