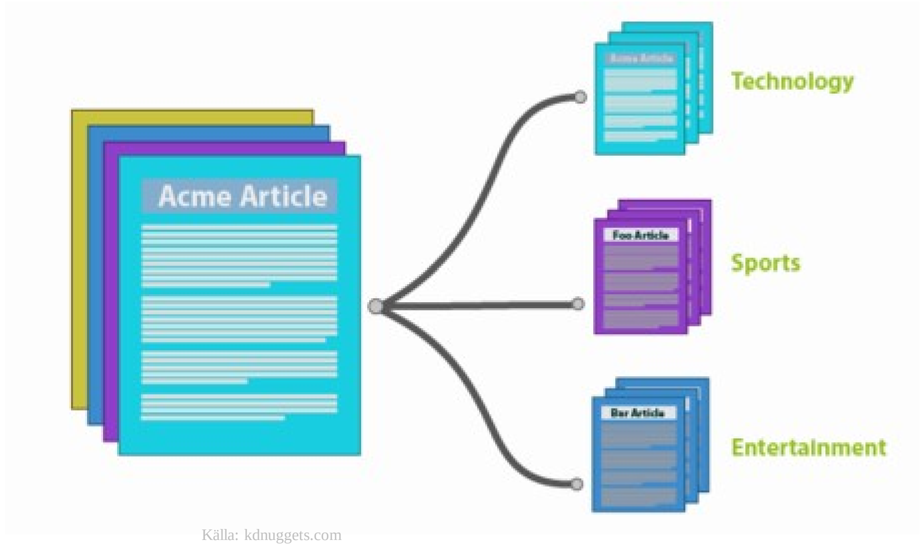
Naïve Bayes classifiers
Decision trees

Lecture 2b

Naive Bayes classifiers: motivation

- Consider n labeled text documents
  - $Y = \{0,1\}$, $0 = \text{"}Science\ fiction\text{"}, 1 = \text{"}Comedy\text{"}$
  - $X = \{X_1, \ldots X_{100}\}$ does the document contain the keyword (0=No,1=Yes)
    - X_1 corr. ”space”, X_2 corr. ”fun”,…



Källa: kdnuggets.com

- Want to classify a new document

Naive Bayes classifiers: motivation

Chance of observing a given combination of words in science fiction

Idea: use Bayes classifier

$$p(Y = y|X) = \frac{P(X|Y = y)P(Y = y)}{\sum_j P(X|Y = y_j)P(Y = y_j)}$$

Proportion of science fiction documents

Naive Bayes classifiers: motivation

- Attempt 1:
  - Model $P\left(X = (x_1, \ldots x_p) \middle| Y = y_i\right)$ and $P(Y = y_i)$ as unknown parameters
  - Use data to derive those with Maximum Likelihood
  - Classify by use of the posterior distribution

- How many parameters?
  - How many different combinations of X? 2^p
  - Amount of $P\left(X = (x_1, \ldots x_p) \middle| Y = y_i\right)$ is $2 * 2^p - 2$
    - Probabilities for each Y sum up to one
- If $p = 100$, 10^{30} parameters need to be estimated→ ouch!

Naive Bayes classifiers

- Naive Bayes assumption: conditional independence

$$P\big(X=(x_1,\dots x_p)\big|Y=y\big)=\prod_{i=1}^{p} P(X_i=x_i|Y=y)$$

- How many parameters now?
  - $P(X_i=x_i|Y=y), i=1,\dots p, x_i=\{0,1\}, y=\{0,1\}$ $2*p$

- Is Naive Bayes assumption always valid?
  - P(Space,ship|SciFi)= P(Space|SciFi)*P(Ship|SciFi) ?

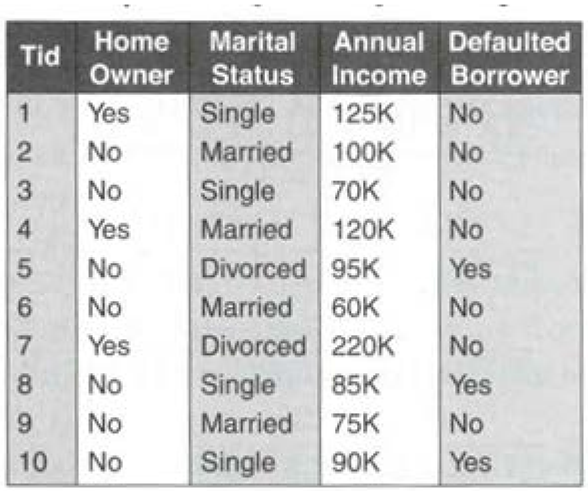
Naive Bayes classifiers - discrete inputs

- Given $D = \{(X_{m1}, \ldots X_{mp}, Y_m),\ m = 1, \ldots n\}$
- Assume $X_i \in \{x_1, \ldots x_J\}, i = 1, \ldots p, Y \in \{y_1 \ldots y_K\}$
- Denote $\theta_{ijk} = p(X_i = x_j | Y = y_k)$
  - How many parameters? $(J-1)Kp$
- Denote $\pi_k = p(Y = y_k)$

- Maximum likelihood: assume θ_{ijk} and π_k are constants
  - $\hat{\theta}_{ijk} = \frac{\#\{X_i = x_j \& Y = y_k\}}{\#\{Y = y_k\}}$
  - $\hat{\pi}_k = \frac{\#\{Y = y_k\}}{n}$
  - Classification using 0-1 loss: $\hat{Y} = \arg\max_y p(Y = y|X)$

Naive Bayes classifiers - discrete inputs

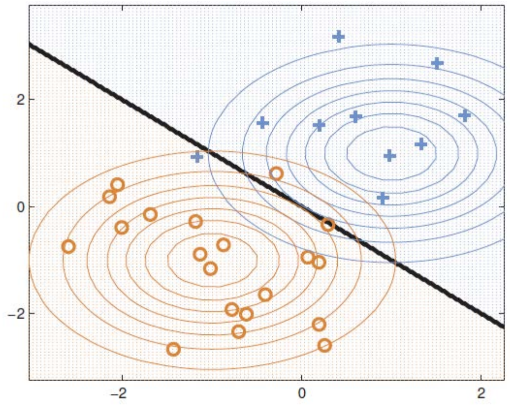
- **Example** Loan decision
  - Classify a person: Home Owner=No, Single=Yes



Tid	Home Owner	Marital Status	Annual Income	Defaulted Borrower
1	Yes	Single	125K	No
2	No	Married	100K	No
3	No	Single	70K	No
4	Yes	Married	120K	No
5	No	Divorced	95K	Yes
6	No	Married	60K	No
7	Yes	Divorced	220K	No
8	No	Single	85K	Yes
9	No	Married	75K	No
10	No	Single	90K	Yes

Naive Bayes – continuous inputs

- X_i are continuous
- Assumption A: $x_j|y = C$ are univariate Gaussian
  - $p(x_j|y = C_i, \theta) = N(x_j|\mu_{ij}, \sigma_{ij}^2)$
- Therefore $p(\boldsymbol{x}|y = C_i, \theta) = N(\boldsymbol{x}|\boldsymbol{\mu_i}, \boldsymbol{\Sigma_i})$
  - $\boldsymbol{\Sigma_i}$=diag$(\sigma_{i1}^2, \dots, \sigma_{ip}^2)$

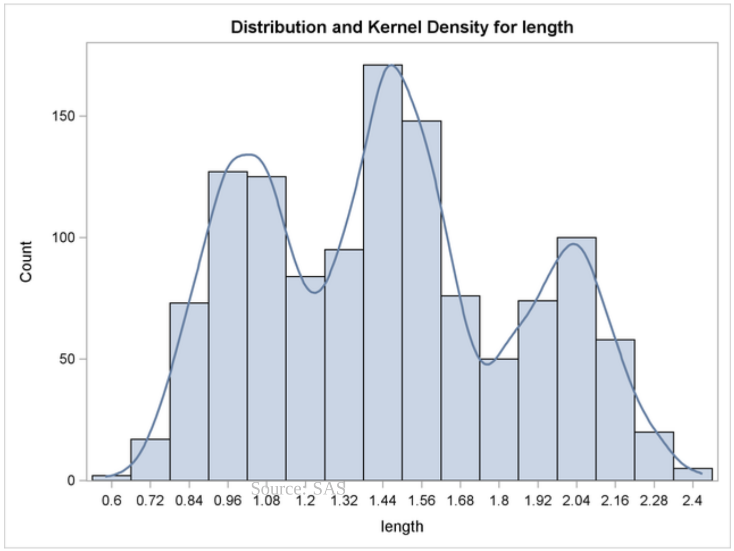


- Naive bayes is a special case of LDA (given A)
  - →MLE are means and variances (per class)

Naive Bayes – continuous inputs

- Assumption B: $p(x_j|y = C)$ are unknown functions of x_j that can be estimated from data
  - Nonparametric density estimation (kernel for ex.)

1. Estimate $p\left(X_i = x_j \middle| Y = y_k\right)$ using nonparametric methods
2. Estimate $p(Y = y_k)$ as class proportions
3. Use Bayes rule and 0-1 loss to classify



Naive Bayes in R

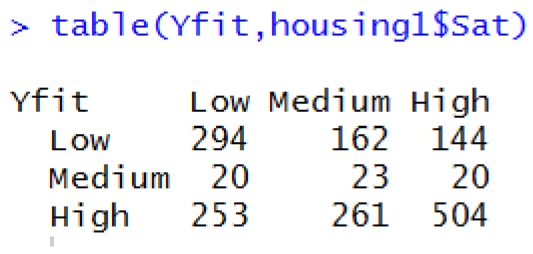
- naiveBayes in package **e1071**

Example: Satisfaction of householders with their present housing circumstances

```
library(MASS)
library(e1071)
n=dim(housing)[1]
ind=rep(1:n, housing[,5])
housing1=housing[ind,-5]

fit=naiveBayes(Sat~., data=housing1)
fit

Yfit=predict(fit, newdata=housing1)
table(Yfit,housing1$Sat)
```



```
> table(Yfit,housing1$Sat)

Yfit     Low Medium High
  Low    294    162  144
  Medium  20     23   20
  High   253    261  504
```

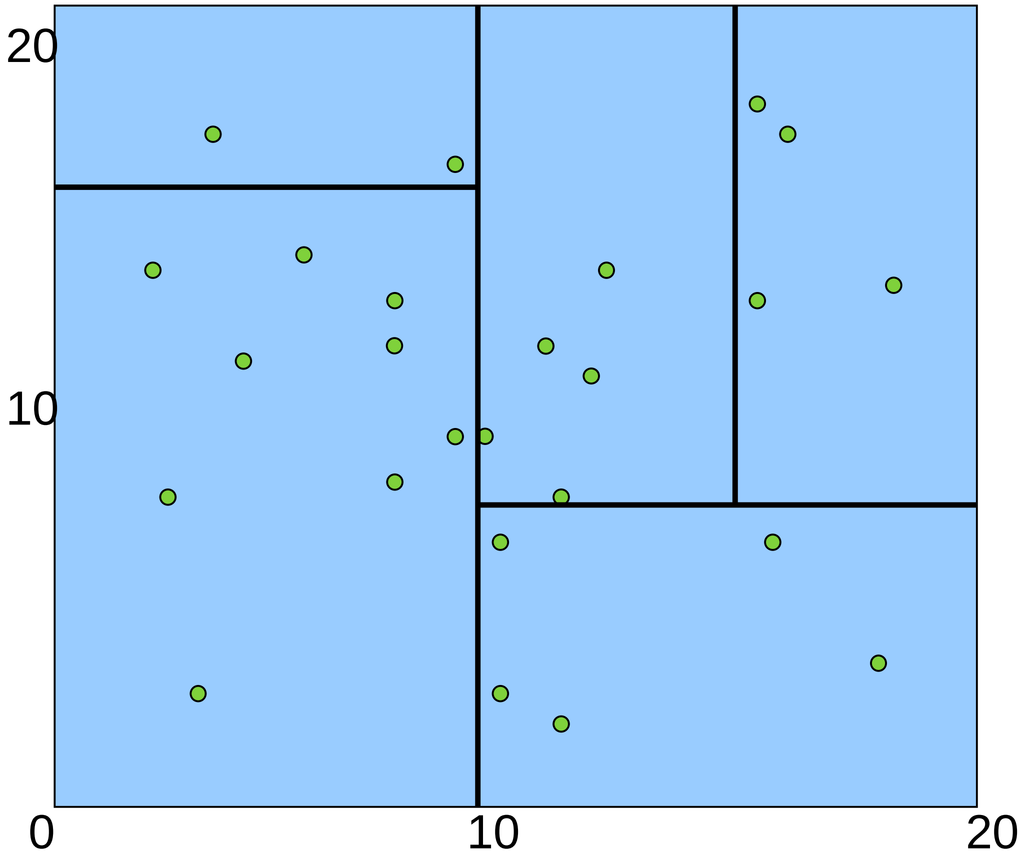
Decision trees

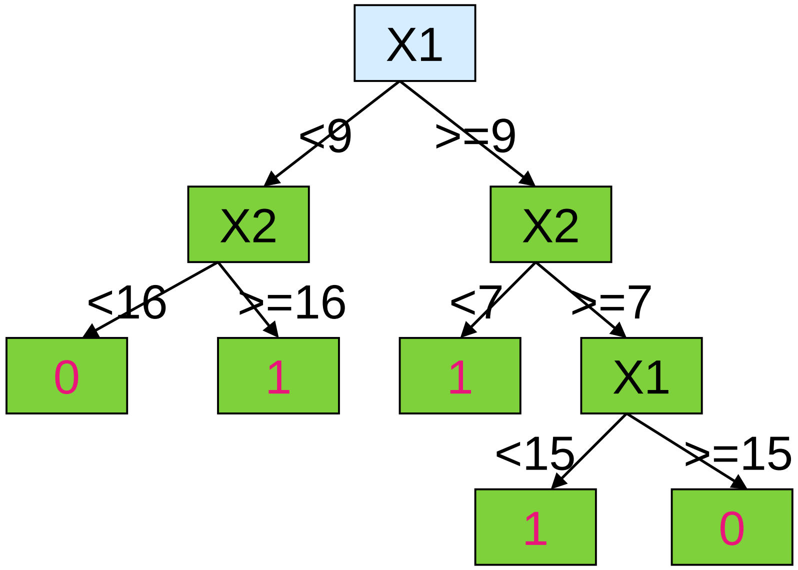
Idea

Split the domain of predictor set into the set of hypercubes (rectangles, cubes) and define the target value to be constant within each hypercube

- Regression trees:
  - Target is a continuous variable
- Classification trees
  - Target is a class (qualitative) variable

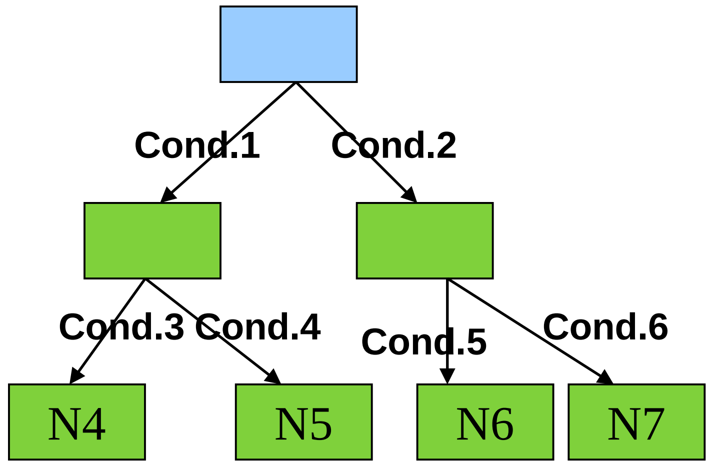
Classification tree toy example



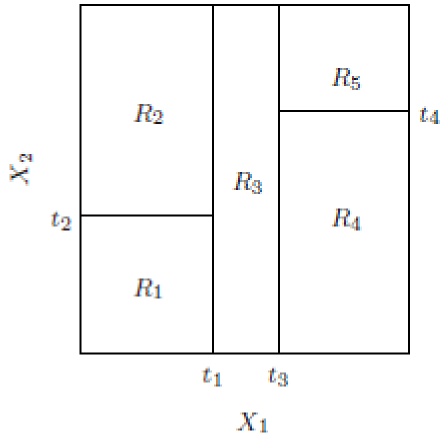


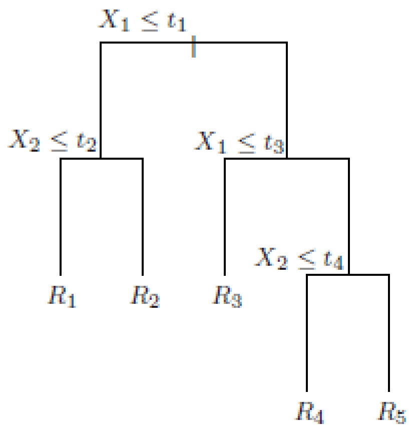
Definitions

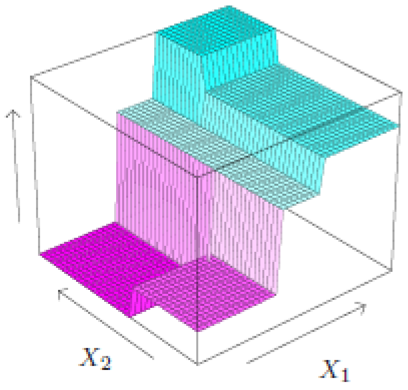
- Root node
- Nodes
- Leaves (terminal nodes)
- Parent node, child node
- Decision rules
- A value is assigned to the leaves



Regression tree toy example







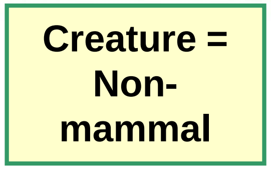
A classification problem

Create a classification tree that would describe the following patterns

ID	x1	x2	x3	x4	x5	x6	x7	y
Name	Body temperature	Skin cover	Gives birth	Aquatic creature	Aerial creature	Has legs	Hibernates	Class label
human	warm-blooded	hair	yes	no	no	yes	no	mammal
python	cold-blooded	scales	no	no	no	no	yes	non-mammal
salmon	cold-blooded	scales	no	yes	no	no	no	non-mammal
whale	warm-blooded	hair	yes	yes	no	no	no	mammal
frog	cold-blooded	none	no	semi	no	yes	yes	non-mammal
komodo	cold-blooded	scales	no	no	no	yes	no	non-mammal
bat	warm-blooded	hair	yes	no	yes	yes	yes	mammal
pigeon	warm-blooded	feathers	no	no	yes	yes	no	non-mammal
cat	warm-blooded	fur	yes	no	no	yes	no	mammal
shark	cold-blooded	scales	yes	yes	no	no	no	non-mammal
turtle	cold-blooded	scales	no	semi	no	yes	no	non-mammal
penguin	warm-blooded	feathers	no	semi	no	yes	no	non-mammal
porcupine	warm-blooded	quills	yes	no	no	yes	yes	mammal
eel	cold-blooded	scales	no	yes	no	no	no	non-mammal
salamander	cold-blooded	none	no	semi	no	yes	yes	non-mammal

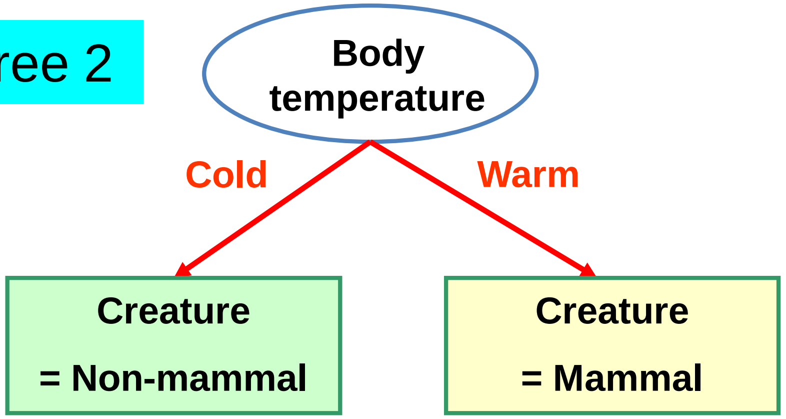
Several solutions

Tree 1



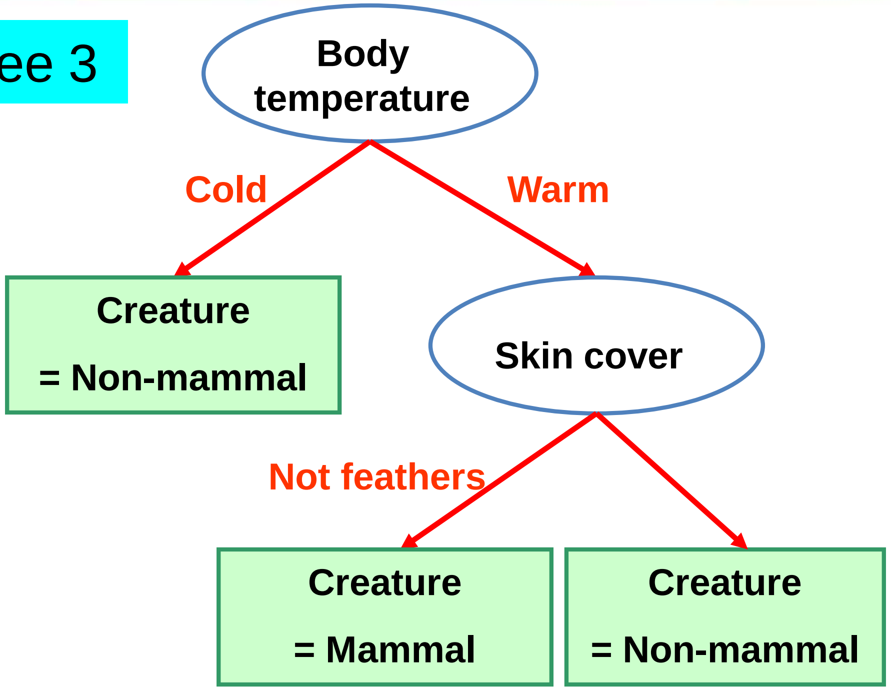
Large misclassification rate!

Tree 2



A lower misclassification rate

Tree 3



Zero misclassification

Green boxes represent pure nodes =nodes where observed values are the same

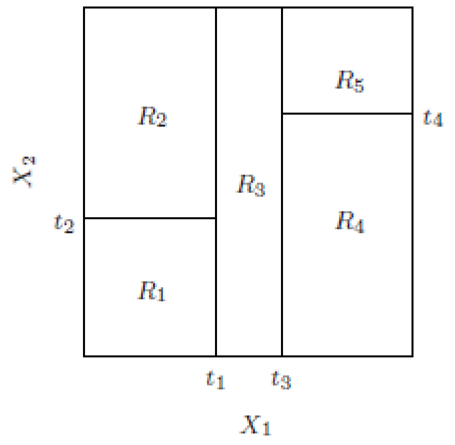
Decision trees

- A tree $T = < r_i, s_{r_i}, R_j, i = 1 \dots S, j = 1 \dots L >$
  - $x_{r_i} \leq s_{r_i}$ splitting rules (conditions), S- their amount
  - R_j-terminal nodes, L- their amount
  - labels μ_j in each terminal node

Model:

- $Y|T$ for R_j comes from exponential family with mean μ_j

- Fitting by MLE:
  - Step 1: Finding optimal tree
  - Step 2: Finding optimal labels in terminal nodes



Decision trees

Example:

- **Normal model** leads to regression trees
  - Objective: MSE
- **Multinoulli model** leads to classification trees
  - Objective: cross-entropy (deviance)

Classification trees

- Target is categorical

- Classification probability $\mathrm{p}_{\mathrm{mk}} = p(Y = k|X \in R_m)$ is estimated for every class in a node
- How to estimate p_{mk} for class k and node R_m?

Class proportions

$$\hat{p}_{mk} = \frac{1}{N_m} \sum_{x_i \in R_m} I(y_i = k)$$

- For any node (leave), a label can be assigned

$$k(m) = \arg\max_k \hat{p}_{mk}$$

Classification trees

- Impurity measure $\mathrm{Q}(R_m)$
  - R_m is a tree node (region)
  - Node can be split unless it is pure

Misclassification error:	$\frac{1}{N_m}\sum_{i\in R_m} I(y_i \neq k(m)) = 1 - \hat{p}_{mk(m)}$
Gini index:	$\sum_{k\neq k'} \hat{p}_{mk}\hat{p}_{mk'} = \sum_{k=1}^{K} \hat{p}_{mk}(1-\hat{p}_{mk})$
Cross-entropy or deviance:	$-\sum_{k=1}^{K} \hat{p}_{mk} \log \hat{p}_{mk}.$

- Note: In many sources, deviance is $\mathrm{Q}(R_m)\, N(R_m)$

Example: Cross –entropy is MLE of $Y_j|T \sim Multinomial(p_{j1}, \ldots p_{jc})$

Fitting regression trees: CART

Step 1: Finding optimal tree: grow the tree in order to minimize global objective

1. Let C_0 be a hypercube containing all observations
2. Let queue $C=\{C_0\}$
3. Pick up some C_i from C and find a variable X_j and value *s* that split C_j into two hypercubes

$$R_1(j,s) = \{X | X_j \leq s\} \text{ and } R_2(j,s) = \{X | X_j > s\}$$

and solve

$$\min_{j,s}[N_1 Q(R_1) + N_2 Q(R_2)]$$

4. Remove C_j from C and add R_1 and R_2
5. Repeat 3-4 as many times as needed (or until each cube has only 1 observation)

CART: comments

- Greedy algorithm (optimal tree is not found)
- The largest tree will interpolate the data $\rightarrow$ large trees = overfitting the data
- Too small trees=underfitting (important structure may not be captured)
- Optimal tree length?

Optimal trees

- **Postpruning**

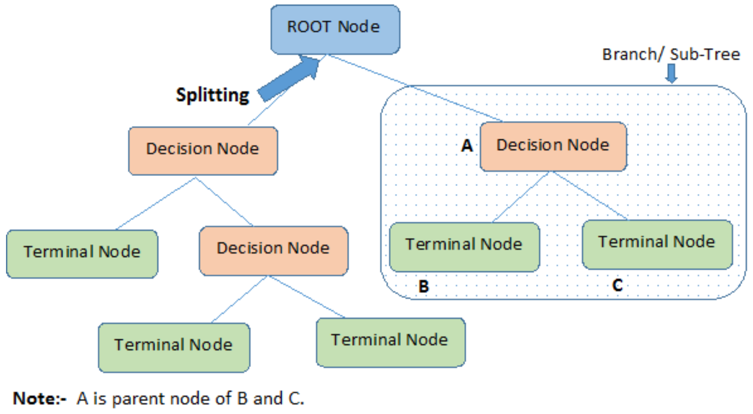
Weakest link pruning:

1. Merge two leaves that have smallest *N(parent)*Q(parent)-N(leave1)Q(leave1)-N(leave2)Q(leave2)*
2. For the current tree T, compute

$$I(T) = \sum_{R_i \in leaves} N(R_i)Q(R_i) + \alpha|T|$$

$|T|$ =#leaves

3. Repeat 1-2 until the tree with one leave is obtained
4. Select the tree with smallest I(T)



Source: http://www.analyticsvidhya.com

How to find the optimal α? Cross validation!

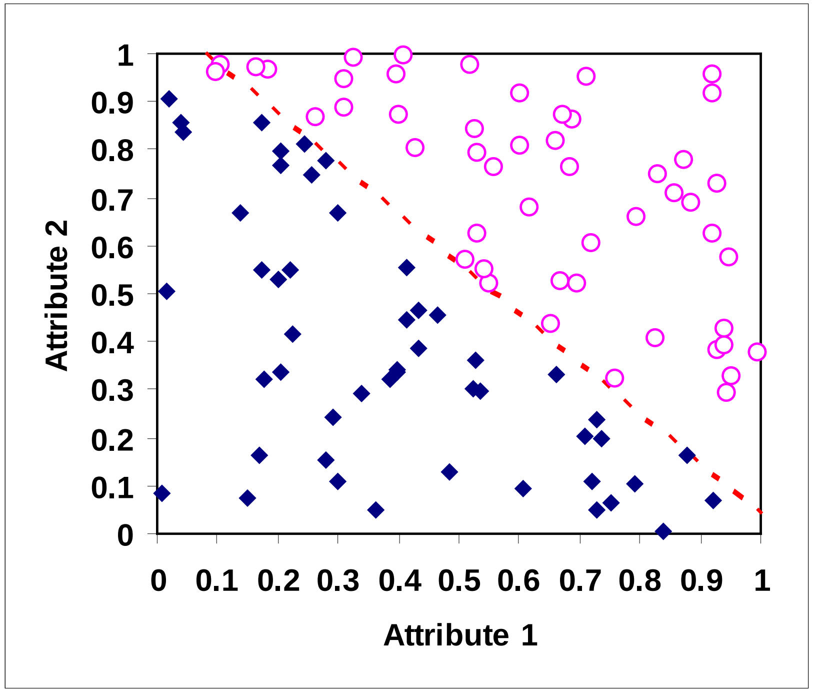
Decision trees: comments

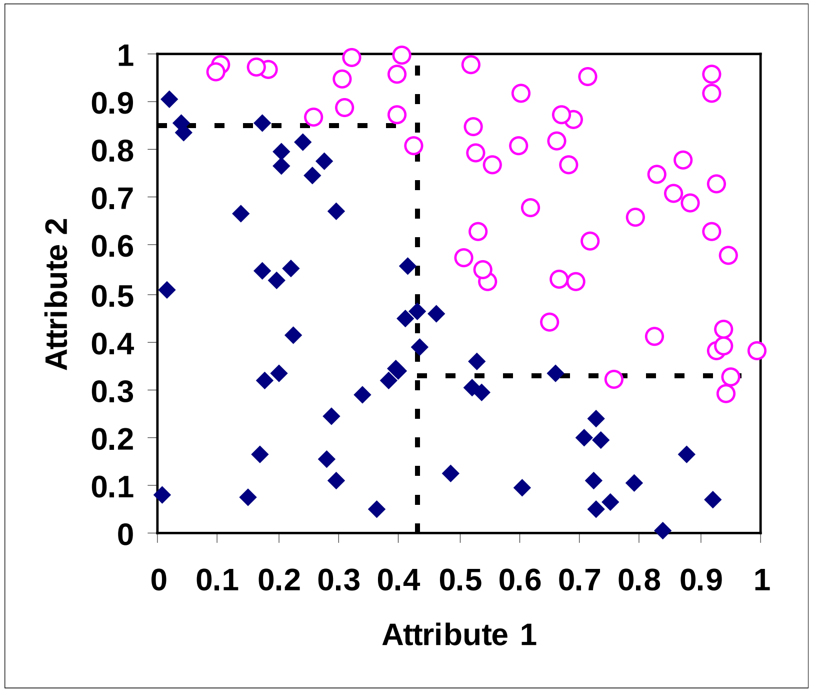
- Similar algorithms work for regression trees – replace $N \cdot Q(R)$ by $SSE(R)$
- Easy to interpret
- Easy to handle all types of predictors in one model
- **Automatic variable selection**
- Relatively robust to outliers
- Handle large datasets

- Trees have high variance: a small change in response → totally different tree
- Greedy algorithms → fit may be not so good
- Lack of smoothness

Decision trees: issues

- Large trees may be needed to model an easy system:





Decision trees in R

- **tree** package
  - Alternative: **rpart**

tree(formula, data, weights, control, split = c("deviance", "gini"), ...)

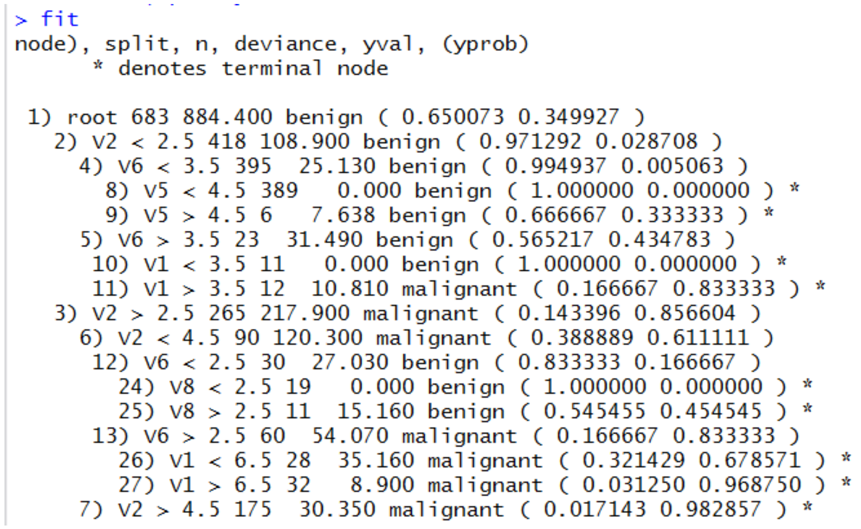
print(), summary(), plot(), text()

Example: breast cancer as a function av biological measurements

```
library(tree)
n=dim(biopsy)[1]
fit=tree(class~., data=biopsy)
plot(fit)
text(fit, pretty=0)
fit
summary(fit)
```

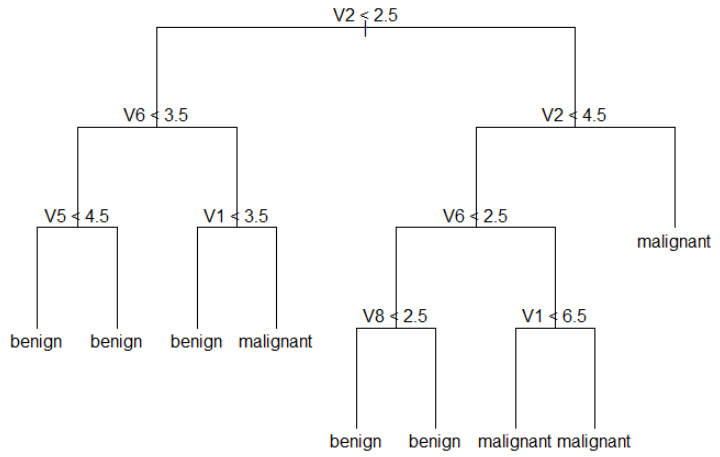
Decision trees in R

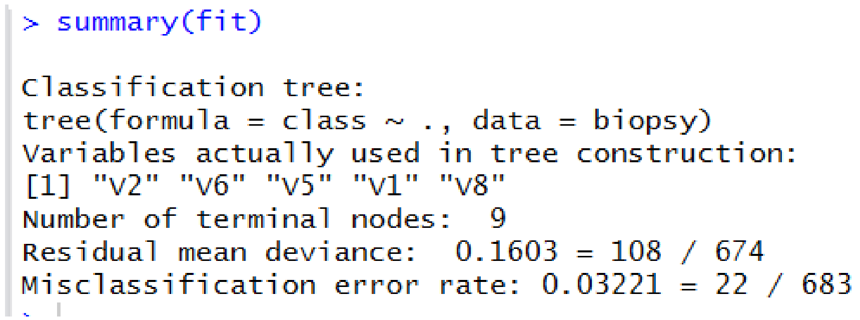
- Adjust the splitting in the tree with *control* parameter (leaf size for ex)



```
> fit
node), split, n, deviance, yval, (yprob)
      * denotes terminal node

 1) root 683 884.400 benign ( 0.650073 0.349927 )
   2) V2 < 2.5 418 108.900 benign ( 0.971292 0.028708 )
     4) V6 < 3.5 395  25.130 benign ( 0.994937 0.005063 )
       8) V5 < 4.5 389   0.000 benign ( 1.000000 0.000000 ) *
       9) V5 > 4.5 6   7.638 benign ( 0.666667 0.333333 ) *
     5) V6 > 3.5 23  31.490 benign ( 0.565217 0.434783 )
      10) V1 < 3.5 11   0.000 benign ( 1.000000 0.000000 ) *
      11) V1 > 3.5 12  10.810 malignant ( 0.166667 0.833333 ) *
   3) V2 > 2.5 265 217.900 malignant ( 0.143396 0.856604 )
     6) V2 < 4.5 90 120.300 malignant ( 0.388889 0.611111 )
      12) V6 < 2.5 30  27.030 benign ( 0.833333 0.166667 )
        24) V8 < 2.5 19   0.000 benign ( 1.000000 0.000000 ) *
        25) V8 > 2.5 11  15.160 benign ( 0.545455 0.454545 ) *
      13) V6 > 2.5 60  54.070 malignant ( 0.166667 0.833333 )
        26) V1 < 6.5 28  35.160 malignant ( 0.321429 0.678571 ) *
        27) V1 > 6.5 32   8.900 malignant ( 0.031250 0.968750 ) *
     7) V2 > 4.5 175  30.350 malignant ( 0.017143 0.982857 ) *
```





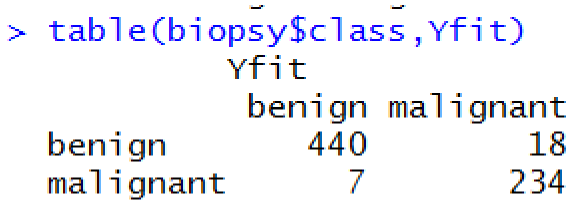
```
> summary(fit)

Classification tree:
tree(formula = class ~ ., data = biopsy)
Variables actually used in tree construction:
[1] "V2" "V6" "V5" "V1" "V8"
Number of terminal nodes:  9
Residual mean deviance:  0.1603 = 108 / 674
Misclassification error rate: 0.03221 = 22 / 683
```

Decision trees in R

- Misclassification results

```
Yfit=predict(fit, newdata=biopsy, type="class")
table(biopsy$class,Yfit)
```



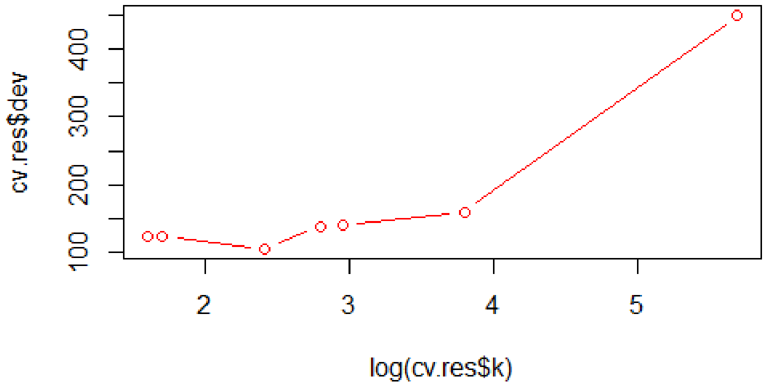
```
> table(biopsy$class,Yfit)
           Yfit
            benign malignant
  benign       440        18
  malignant      7       234
```

Decision trees in R

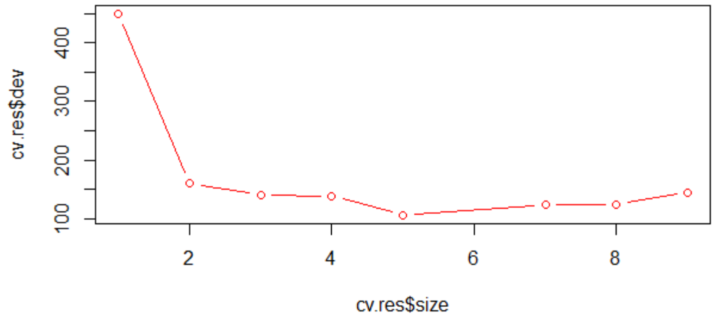
- Selecting optimal tree by penalizing
  - Cv.tree()

```
set.seed(12345)
ind=sample(1:n, floor(0.5*n))
train=biopsy[ind,]
valid=biopsy[-ind,]

fit=tree(class~., data=train)
set.seed(12345)
cv.res=cv.tree(fit)
plot(cv.res$size, cv.res$dev, type="b",
col="red")
plot(log(cv.res$k), cv.res$dev,
type="b", col="red")
```



What is optimal number of leaves?



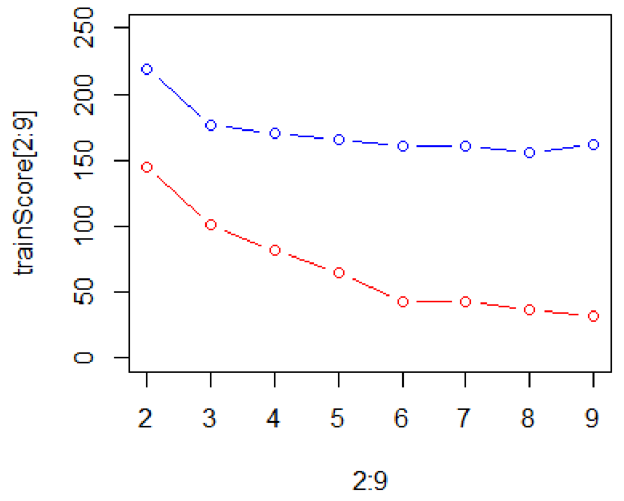
Decision trees in R

- Selecting optimal tree by train/validation

```
fit=tree(class~., data=train)

trainScore=rep(0,9)
testScore=rep(0,9)

for(i in 2:9) {
  prunedTree=prune.tree(fit,best=i)
  pred=predict(prunedTree, newdata=valid,
type="tree")
  trainScore[i]=deviance(prunedTree)
  testScore[i]=deviance(pred)
}
plot(2:9, trainScore[2:9], type="b", col="red",
ylim=c(0,250))
points(2:9, testScore[2:9], type="b", col="blue")
```

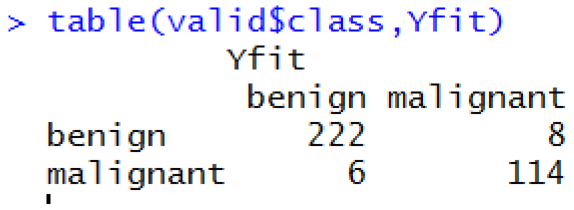


What is optimal number of leaves?

Decision trees in R

- Final tree: 5 leaves

```
finalTree=prune.tree(fit, best=5)
Yfit=predict(finalTree, newdata=valid,
type="class")
table(valid$class,Yfit)
```



```
> table(valid$class,Yfit)
           Yfit
            benign malignant
  benign       222         8
  malignant      6       114
```