Topics in Artificial Intelligence:

# Machine Learning Techniques for Data Mining

B Semester 2000

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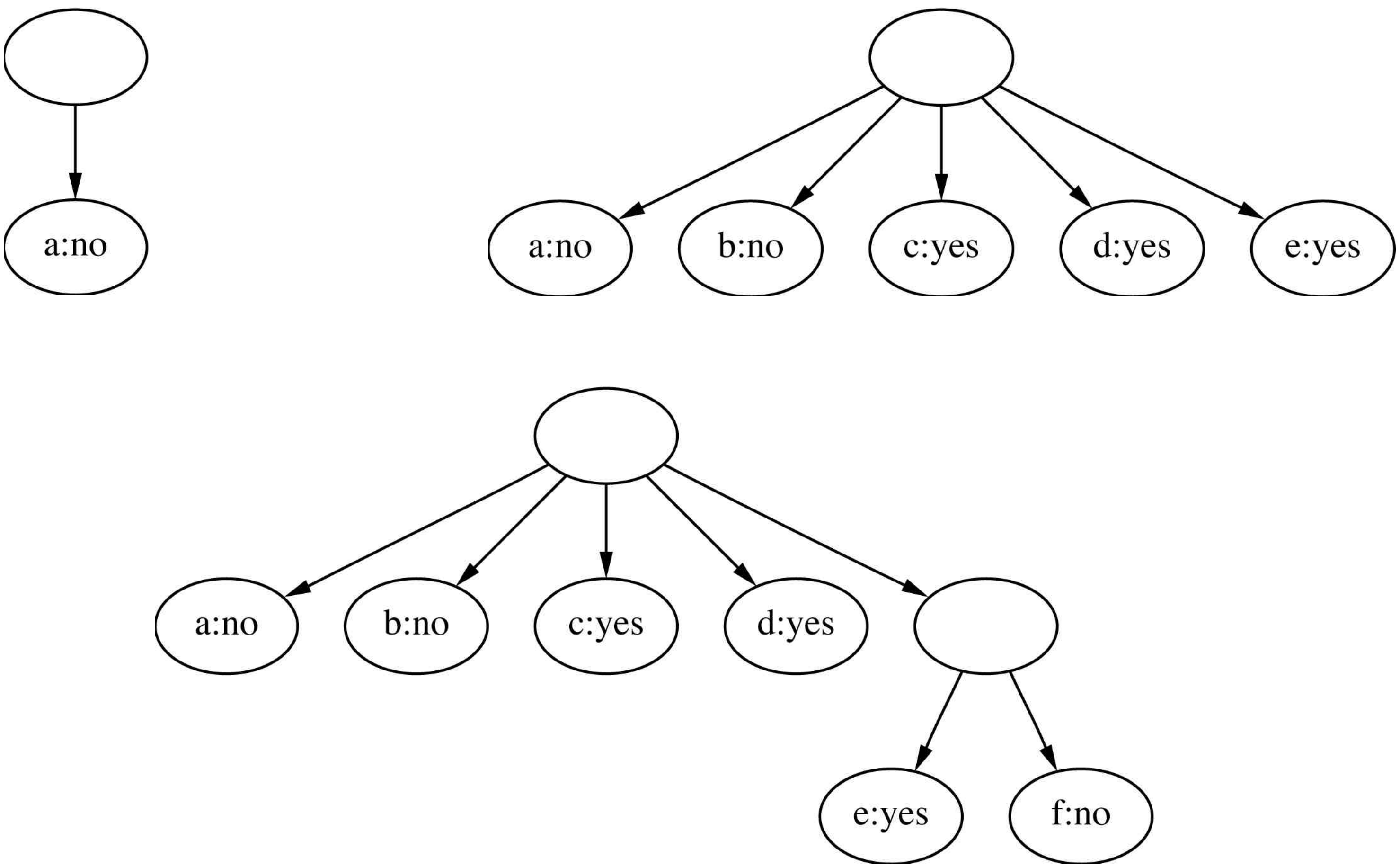
# Incremental clustering

- COBWEB/CLASSIT: incrementally forms a hierarchy of clusters
- In the beginning tree consists of empty root node
- Instances are added one by one, and the tree is updated appropriately at each stage
- Updating involves finding the right leaf for an instance (possibly restructuring the tree)
- Updating decisions are based on *category utility*

# Clustering the weather data

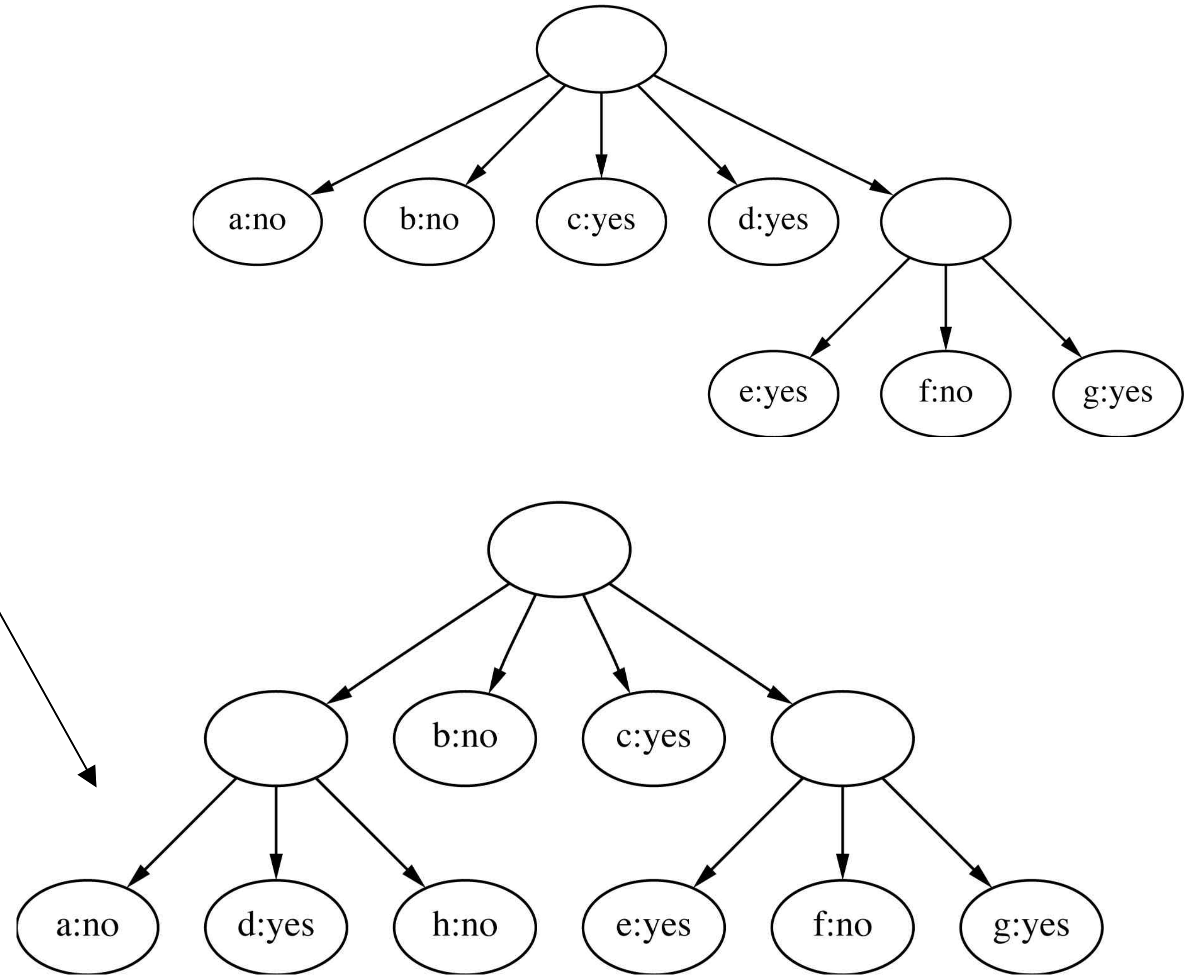
| ID code | Outlook | Temp. | Humidity | Windy |
|---|---|---|---|---|
| A | Sunny | Hot | High | False |
| B | Sunny | Hot | High | True |
| C | Overcast | Hot | High | False |
| D | Rainy | Mild | High | False |
| E | Rainy | Cool | Normal | False |
| F | Rainy | Cool | Normal | True |
| G | Overcast | Cool | Normal | True |
| H | Sunny | Mild | High | False |
| I | Sunny | Cool | Normal | False |
| J | Rainy | Mild | Normal | False |
| K | Sunny | Mild | Normal | True |
| L | Overcast | Mild | High | True |
| M | Overcast | Hot | Normal | False |
| N | Rainy | Mild | High | True |

# Steps 1-3



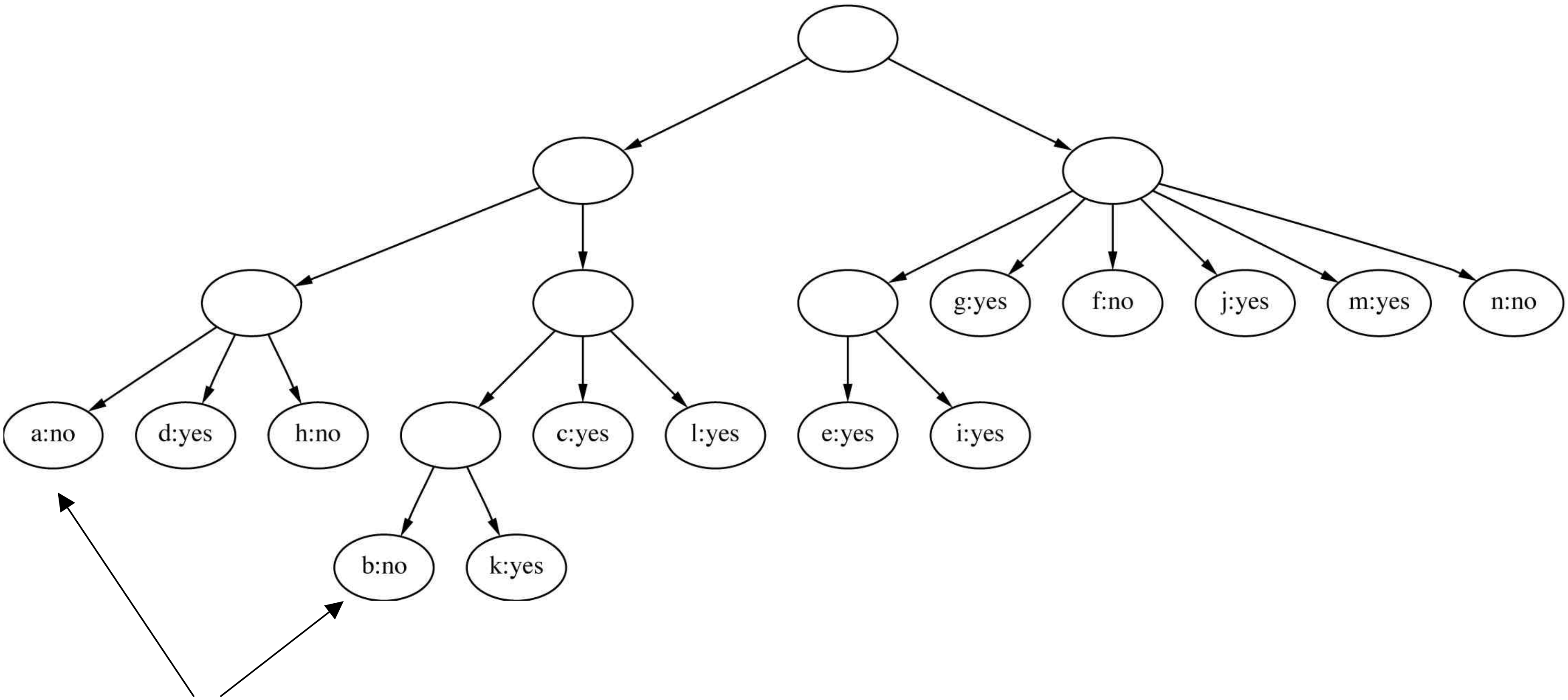
# Steps 3-4

Best host and
runner-up have
been *merged*



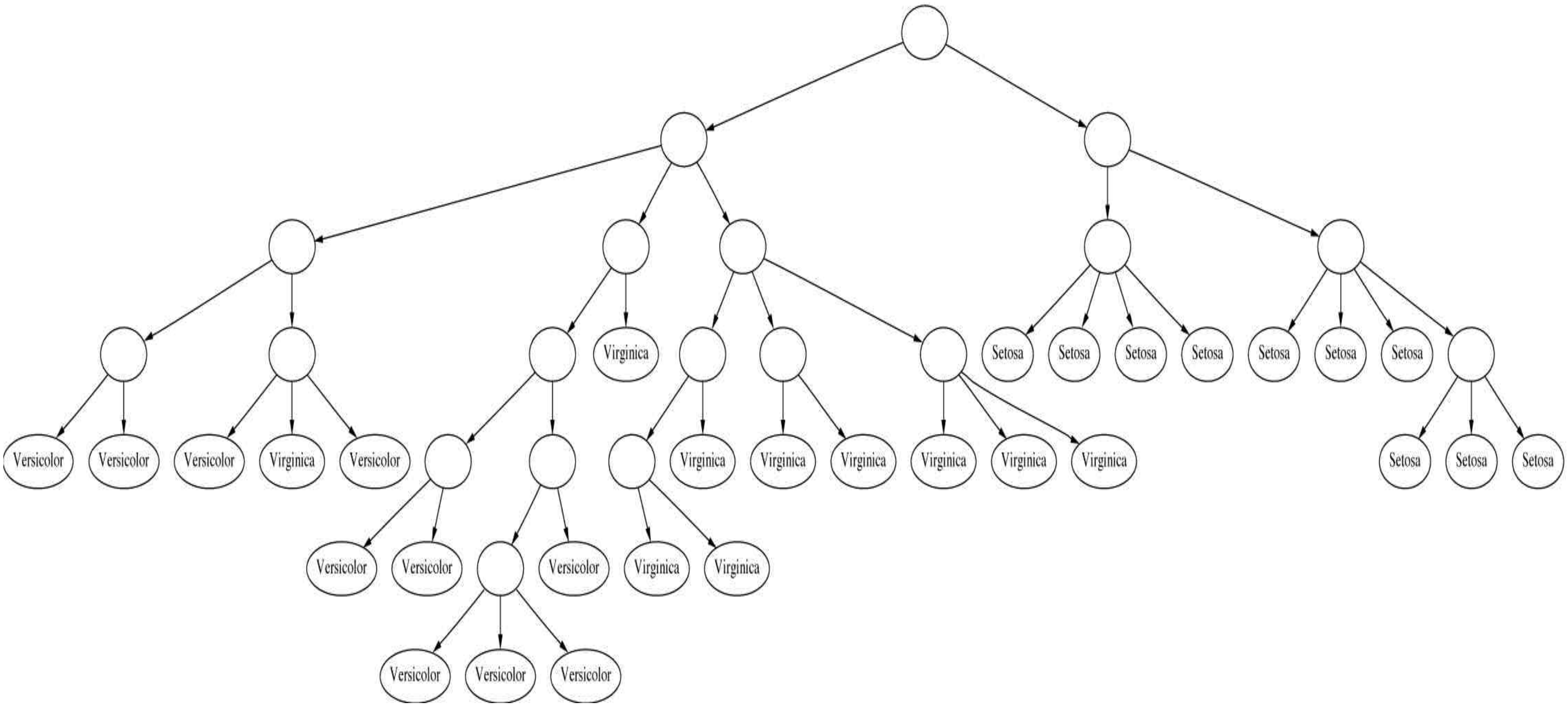

Note: *splitting* the best host is considered if merging doesn't help

# The final hierarchy

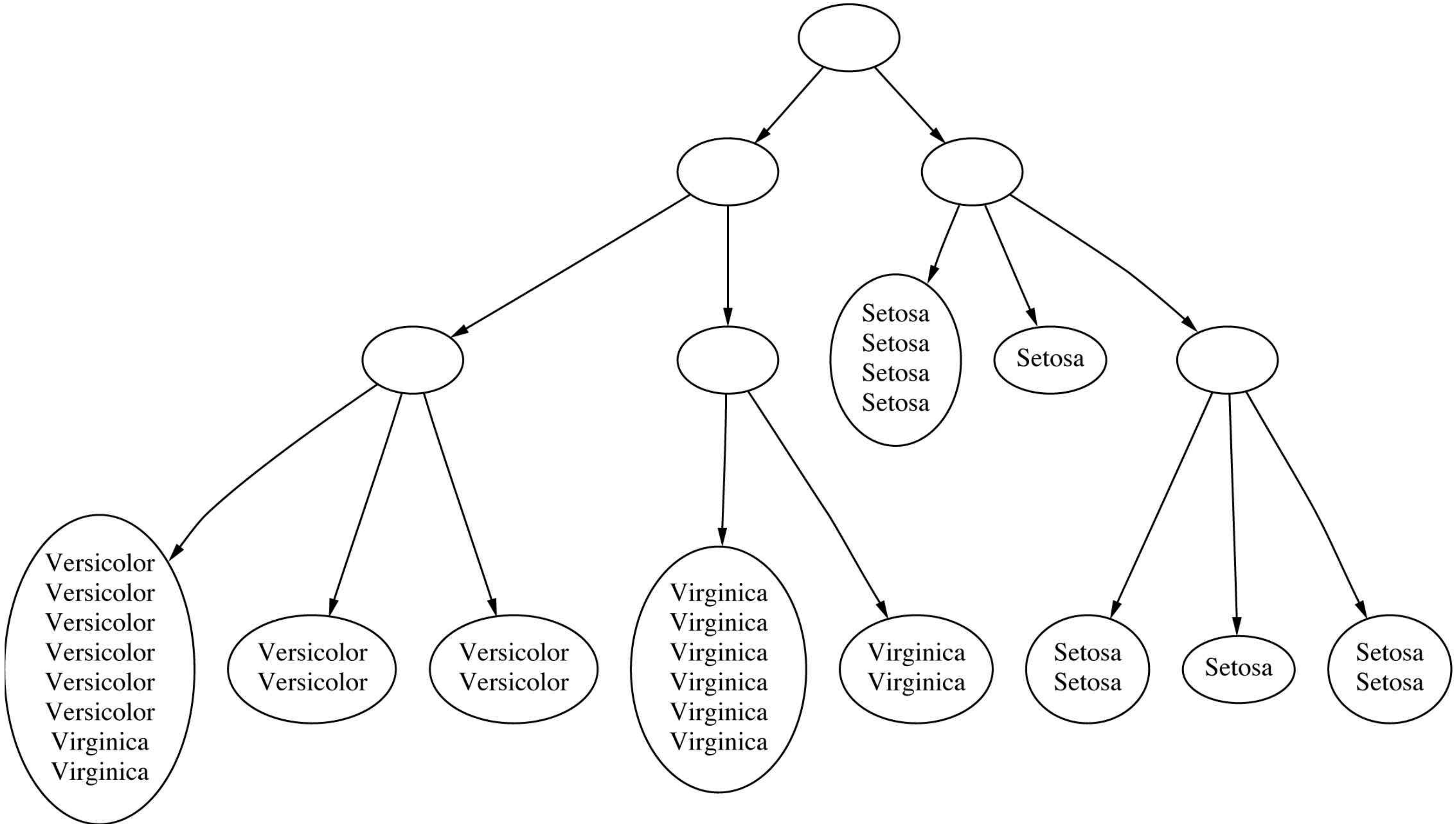



***a and b are actually very similar***

# Clustering (parts) of the iris data



# Clustering the iris data with cutoff



# Category utility

- Category utility is a kind of quadratic loss function defined on conditional probabilities:

$$CU(C_1, C_2, ..., C_k) = \frac{\sum_l \Pr[C_l] \sum_i \sum_j (\Pr[a_i = v_{ij} \mid C_l]^2 - \Pr[a_i = v_{ij}]^2)}{k}$$

- If every instance gets put into a different category the numerator becomes (m = #attributes):

$$m - \Pr[a_i = v_{ij}]^2 \longleftarrow \textbf{\textit{maximum}}$$

# Numeric attributes

- We assume normal distribution: $f(a) = \frac{1}{\sqrt{2\pi}\sigma} e^{\frac{(a-\mu)^2}{2\sigma^2}}$
- Then we get: $\sum_j \Pr[a_i = v_{ij}]^2 \Leftrightarrow \int f(a_i)^2 da_i = \frac{1}{2\sqrt{\pi}\sigma_i}$
- Thus

$$CU = \frac{\sum_l \Pr[C_l] \sum_i \sum_j (\Pr[a_i = v_{ij} \mid C_l]^2 - \Pr[a_i = v_{ij}]^2)}{k}$$

  is

$$CU = \frac{\sum_l \Pr[C_l] \frac{1}{2\sqrt{\pi}} \sum_i \left( \frac{1}{\sigma_{il}} - \frac{1}{\sigma_i} \right)}{k}$$

- *Acuity* parameter: prespecified minimum variance

# Probability-based clustering

- Problems with above heuristic approach:
  - Division by *k?*
  - Order of examples?
  - Are restructuring operations sufficient?
  - Is result at least *local* minimum of category utility?
- From a probabilistic perspective, we want to find the most likely clusters given the data
- Also: instance only has certain probability of belonging to a particular cluster

# Finite mixtures

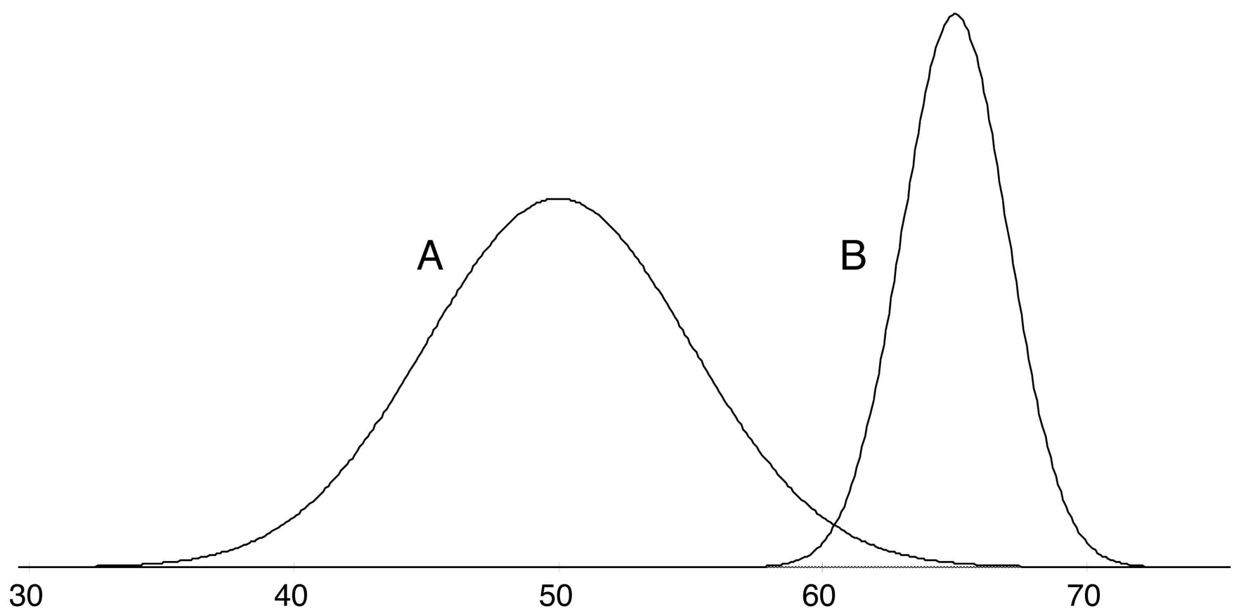
- Probabilistic clustering algorithms model the data using a *mixture* of distributions
- Each cluster is represented by one distribution
  - The distribution governs the probabilities of attributes values in the corresponding cluster
- They are called *finite mixtures* because there is only a finite number of clusters being represented
- Usually individual distributions are normal distribut.
- Distributions are combined using cluster weights

# A two-class mixture model

data

| | | | | | | | | | | | |
|---|---|---|---|---|---|---|---|---|---|---|---|
| A | 51 | B | 62 | B | 64 | A | 48 | A | 39 | A | 51 |
| A | 43 | A | 47 | A | 51 | B | 64 | B | 62 | A | 48 |
| B | 62 | A | 52 | A | 52 | A | 51 | B | 64 | B | 64 |
| B | 64 | B | 64 | B | 62 | B | 63 | A | 52 | A | 42 |
| A | 45 | A | 51 | A | 49 | A | 43 | B | 63 | A | 48 |
| A | 42 | B | 65 | A | 48 | B | 65 | B | 64 | A | 41 |
| A | 46 | A | 48 | B | 62 | B | 66 | A | 48 | | |
| A | 45 | A | 49 | A | 43 | B | 65 | B | 64 | | |
| A | 45 | A | 46 | A | 40 | A | 46 | A | 48 | | |

model




$m_A$=50, $s_A$ =5, $p_A$=0.6 $m_B$=65, $s_B$ =2, $p_B$=0.4

# Using the mixture model

- The probability of an instance *x* belonging to cluster *A* is:

$$\Pr[A \mid x] = \frac{\Pr[x \mid A]\Pr[A]}{\Pr[x]} = \frac{f(x;\mu_A,\sigma_A)\,p_A}{\Pr[x]}$$

with

$$f(x;\mu,\sigma) = \frac{1}{\sqrt{2\pi}\sigma} e^{\frac{(x-\mu)^2}{2\sigma^2}}$$

- The *likelihood* of an instance given the clusters is:

$$\Pr[x \mid \text{the distributions}] = \sum_i \Pr[x \mid \text{cluster}_\text{i}]\Pr[\text{cluster}_\text{i}]$$

# Learning the clusters

- Assume we know that there are *k* clusters
- To learn the clusters we need to determine their parameters
  - I.e. their means and standard deviations
- We actually have a performance criterion: the likelihood of the training data given the clusters
- Fortunately, there exists an algorithm that finds a local maximum of the likelihood

# The EM algorithm

- *EM algorithm*: expectation-maximization algorithm
  - Generalization of *k*-means to probabilistic setting
- Similar iterative procedure:
  1. Calculate cluster probability for each instance (expectation step)
  2. Estimate distribution parameters based on the cluster probabilities (maximization step)
- Cluster probabilities are stored as instance weights

# More on EM

- Estimating parameters from weighted instances:

$$\mu_A = \frac{w_1 x_1 + w_2 x_2 + \ldots + w_n x_n}{w_1 + w_2 + \ldots + w_n}$$

$$\sigma_A{}^2 = \frac{w_1 (x_1 - \mu)^2 + w_2 (x_2 - \mu)^2 + \ldots + w_n (x_n - \mu)^2}{w_1 + w_2 + \ldots + w_n}$$

- Procedure stops when log-likelihood saturates
- Log-likelihood:

$$\sum_i \log(p_A \Pr[x_i \mid A] + p_B \Pr[x_i \mid B])$$

# Extending the mixture model

- Using more then two distributions: easy
- Several attributes: easy if independence is assumed
- Correlated attributes: difficult
  - Modeled jointly using a bivariate normal distribution with a (symmetric) covariance matrix
  - With $n$ attributes this requires estimating $n+n(n+1)/2$ parameters
- Nominal attributes: easy if independent

# More on extensions

- Correlated nominal attributes: difficult
  - Two correlated attributes result in $v_1 v_2$ parameters
- Missing values: easy
- Distributions other than the normal distribution can be used:
  - “log-normal” if predetermined minimum is given
  - “log-odds” if bounded from above and below
  - Poisson for attributes that are integer counts
- Cross-validation can be used to estimate *k*!!

# Bayesian clustering

- Problem: overfitting possible if number of parameters gets large
- *Bayesian approach*: every parameter has a prior probability distribution
  - Gets incorporated into the overall likelihood figure and thereby penalizes introduction of parameters
- Example: Laplace estimator for nominal attributes
- Can also have prior on number of clusters!
- Actual implementation: NASA's AUTOCLASS

# Discussion

- Clusters can be interpreted by using supervised learning in a post-processing step
- Can be used to fill in missing values
- May be advantageous to make attributes more independent in pre-processing step
  - I.e. using *principal component analysis*
- Big advantage of probabilistic clustering schemes:
  - Likelihood of data can be estimated and used to compare different clustering models