# Unsupervised Learning
# and
# Data Mining

# Unsupervised Learning
# and
# Data Mining

***Clustering***

## Supervised Learning

- Decision trees
- Artificial neural nets
- K-nearest neighbor
- Support vectors
- Linear regression
- Logistic regression
- ...

## Supervised Learning

- F(x): true function (usually not known)
- D: training sample drawn from F(x)

| | |
|---|---|
| 57,M,195,0,125,95,39,25,0,1,0,0,0,1,0,0,0,0,0,0,1,1,0,0,0,0,0,0,0,0 | 0 |
| 78,M,160,1,130,100,37,40,1,0,0,0,1,0,1,1,1,0,0,0,0,0,0,0,0,0,0,0,0,0 | 1 |
| 69,F,180,0,115,85,40,22,0,0,0,0,0,1,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0 | 0 |
| 18,M,165,0,110,80,41,30,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0 | 0 |
| 54,F,135,0,115,95,39,35,1,1,0,0,0,1,0,0,0,1,0,0,0,0,1,0,0,0,1,0,0,0,0 | 1 |
| 84,F,210,1,135,105,39,24,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0,0,0 | 0 |
| 89,F,135,0,120,95,36,28,0,0,0,0,0,0,0,0,0,0,0,0,1,1,0,0,0,0,0,0,1,0,0 | 1 |
| 49,M,195,0,115,85,39,32,0,0,0,1,1,0,0,0,0,0,0,1,0,0,0,0,0,1,0,0,0,0 | 0 |
| 40,M,205,0,115,90,37,18,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0 | 0 |
| 74,M,250,1,130,100,38,26,1,1,0,0,0,1,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0 | 0 |
| 77,F,140,0,125,100,40,30,1,1,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,1,1 | 1 |
| … | |

## Supervised Learning

- F(x): true function (usually not known)
- D: training sample drawn from F(x)

| | |
|---|---|
| 57,M,195,0,125,95,39,25,0,1,0,0,0,1,0,0,0,0,0,0,1,1,0,0,0,0,0,0,0,0 | 0 |
| 78,M,160,1,130,100,37,40,1,0,0,0,1,0,1,1,1,0,0,0,0,0,0,0,0,0,0,0,0,0 | 1 |
| 69,F,180,0,115,85,40,22,0,0,0,0,0,1,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0 | 0 |
| 18,M,165,0,110,80,41,30,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0 | 0 |
| 54,F,135,0,115,95,39,35,1,1,0,0,0,1,0,0,0,1,0,0,0,0,1,0,0,0,1,0,0,0,0 | 1 |

- G(x): model learned from training sample D

| | |
|---|---|
| 71,M,160,1,130,105,38,20,1,0,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0 | ? |

- Goal: $E<(F(x)-G(x))^2>$ is small (near zero) for future samples drawn from F(x)

## Supervised Learning

Well Defined Goal:

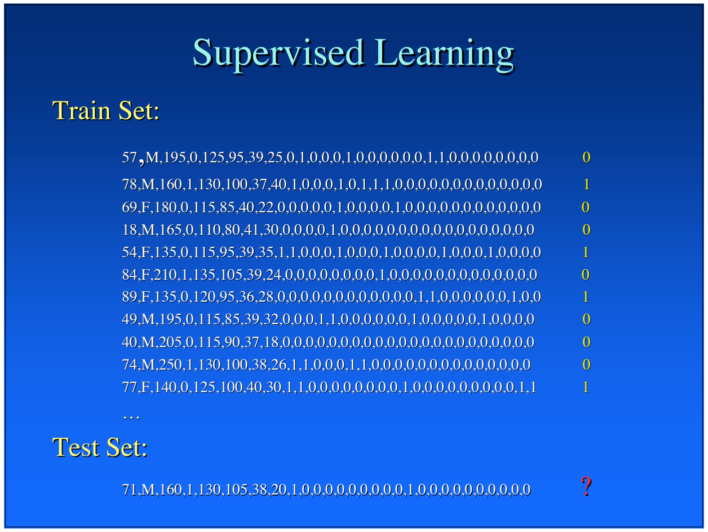
Learn G(x) that is a good approximation to F(x) from training sample D

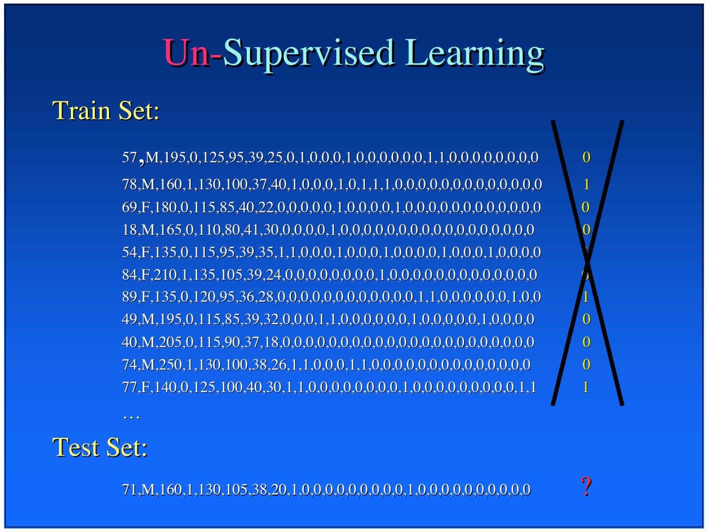
Know How to Measure Error:

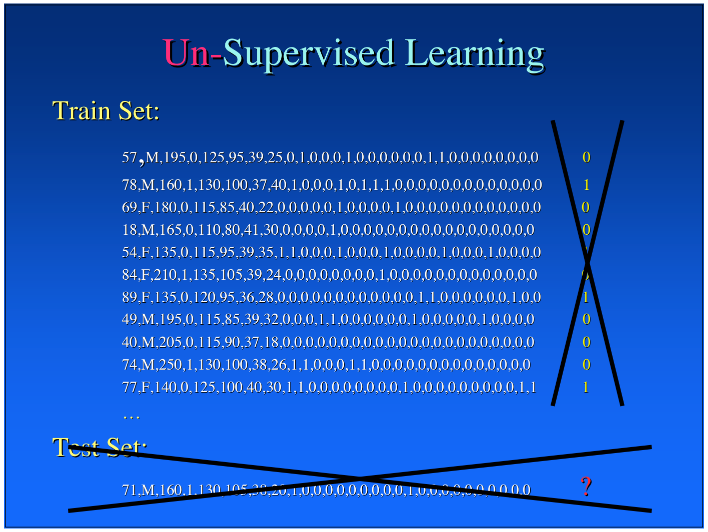
Accuracy, RMSE, ROC, Cross Entropy, ...

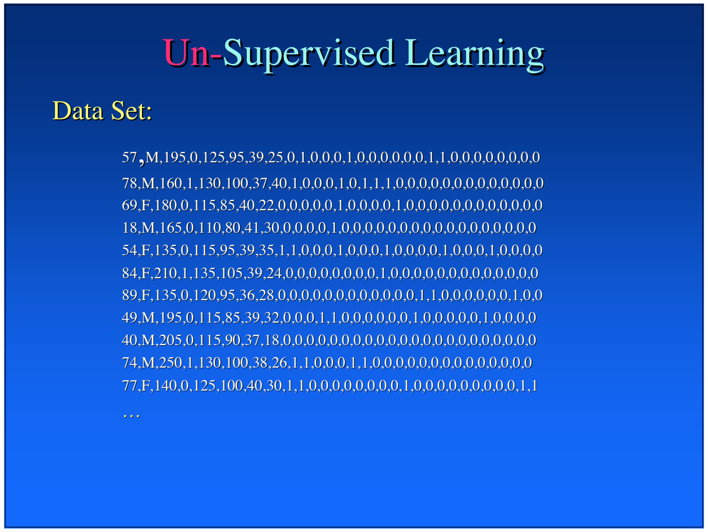
## Clustering ≠ Supervised Learning

## Clustering = Unsupervised Learning


Supervised Learning
Train Set:
57,M,195,0,125,95,39,25,0,1,0,0,0,1,0,0,0,0,0,1,1,0,0,0,0,0,0,0 0
78,M,160,1,130,100,37,40,1,0,0,0,1,0,1,1,1,0,0,0,0,0,0,0,0,0,0,0,0 1
69,F,180,0,115,85,40,22,0,0,0,0,0,1,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0 0
18,M,165,0,110,80,41,30,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0 0
54,F,135,0,115,95,39,35,1,1,0,0,0,1,0,0,0,1,0,0,0,0,1,0,0,0,1,0,0,0,0 1
84,F,210,1,135,105,39,24,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0,0,0 0
89,F,135,0,120,95,36,28,0,0,0,0,0,0,0,0,0,0,0,1,1,0,0,0,0,0,0,1,0,0 1
49,M,195,0,115,85,39,32,0,0,0,1,1,0,0,0,0,0,0,1,0,0,0,0,0,1,0,0,0,0 0
40,M,205,0,115,90,37,18,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0 0
74,M,250,1,130,100,38,26,1,1,0,0,0,1,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0 0
77,F,140,0,125,100,40,30,1,1,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,1,1 1
…
Test Set:
71,M,160,1,130,105,38,20,1,0,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0 ?


Un-Supervised Learning
Train Set:
57,M,195,0,125,95,39,25,0,1,0,0,0,1,0,0,0,0,0,1,1,0,0,0,0,0,0,0 0
78,M,160,1,130,100,37,40,1,0,0,0,1,0,1,1,1,0,0,0,0,0,0,0,0,0,0,0,0 1
69,F,180,0,115,85,40,22,0,0,0,0,0,1,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0 0
18,M,165,0,110,80,41,30,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0 0
54,F,135,0,115,95,39,35,1,1,0,0,0,1,0,0,0,1,0,0,0,0,1,0,0,0,1,0,0,0,0
84,F,210,1,135,105,39,24,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0,0,0
89,F,135,0,120,95,36,28,0,0,0,0,0,0,0,0,0,0,0,1,1,0,0,0,0,0,0,1,0,0 1
49,M,195,0,115,85,39,32,0,0,0,1,1,0,0,0,0,0,0,1,0,0,0,0,0,1,0,0,0,0 0
40,M,205,0,115,90,37,18,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0 0
74,M,250,1,130,100,38,26,1,1,0,0,0,1,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0 0
77,F,140,0,125,100,40,30,1,1,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,1,1 1
…
Test Set:
71,M,160,1,130,105,38,20,1,0,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0 ?


Un-Supervised Learning
Train Set:
57,M,195,0,125,95,39,25,0,1,0,0,0,1,0,0,0,0,0,1,1,0,0,0,0,0,0,0 0
78,M,160,1,130,100,37,40,1,0,0,0,1,0,1,1,1,0,0,0,0,0,0,0,0,0,0,0,0 1
69,F,180,0,115,85,40,22,0,0,0,0,0,1,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0 0
18,M,165,0,110,80,41,30,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0 0
54,F,135,0,115,95,39,35,1,1,0,0,0,1,0,0,0,1,0,0,0,0,1,0,0,0,1,0,0,0,0
84,F,210,1,135,105,39,24,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0,0,0
89,F,135,0,120,95,36,28,0,0,0,0,0,0,0,0,0,0,0,1,1,0,0,0,0,0,0,1,0,0 1
49,M,195,0,115,85,39,32,0,0,0,1,1,0,0,0,0,0,0,1,0,0,0,0,0,1,0,0,0,0 0
40,M,205,0,115,90,37,18,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0 0
74,M,250,1,130,100,38,26,1,1,0,0,0,1,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0 0
77,F,140,0,125,100,40,30,1,1,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,1,1 1
…
Test Set:
?


Un-Supervised Learning
Data Set:
57,M,195,0,125,95,39,25,0,1,0,0,0,1,0,0,0,0,0,1,1,0,0,0,0,0,0,0
78,M,160,1,130,100,37,40,1,0,0,0,1,0,1,1,1,0,0,0,0,0,0,0,0,0,0,0,0
69,F,180,0,115,85,40,22,0,0,0,0,0,1,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0
18,M,165,0,110,80,41,30,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0
54,F,135,0,115,95,39,35,1,1,0,0,0,1,0,0,0,1,0,0,0,0,1,0,0,0,1,0,0,0,0
84,F,210,1,135,105,39,24,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0,0,0
89,F,135,0,120,95,36,28,0,0,0,0,0,0,0,0,0,0,0,1,1,0,0,0,0,0,0,1,0,0
49,M,195,0,115,85,39,32,0,0,0,1,1,0,0,0,0,0,0,1,0,0,0,0,0,1,0,0,0,0
40,M,205,0,115,90,37,18,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0
74,M,250,1,130,100,38,26,1,1,0,0,0,1,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0
77,F,140,0,125,100,40,30,1,1,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,1,1
…

## Supervised vs. Unsupervised Learning

### Supervised

- y=F(x): true function
- D: labeled training set
- D: $\{x_i, y_i\}$
- y=G(x): model trained to predict labels D
- Goal:

  $E<(F(x)-G(x))^2> \approx 0$
- Well defined criteria: Accuracy, RMSE, ...

### Unsupervised

- Generator: true model
- D: unlabeled data sample
- D: $\{x_i\}$
- Learn

  ??????????
- Goal:

  ??????????
- Well defined criteria:

  ??????????

## What to Learn/Discover?

- Statistical Summaries
- Generators
- Density Estimation
- Patterns/Rules
- Associations
- Clusters/Groups
- Exceptions/Outliers
- Changes in Patterns Over Time or Location

## Goals and Performance Criteria?

- Statistical Summaries
- Generators
- Density Estimation
- Patterns/Rules
- Associations
- Clusters/Groups
- Exceptions/Outliers
- Changes in Patterns Over Time or Location

## Clustering

## Clustering

- Given:
  - Data Set D (training set)
  - Similarity/distance metric/information
- Find:
  - Partitioning of data
  - Groups of similar/close items

## Similarity?

- Groups of similar customers
  - Similar demographics
  - Similar buying behavior
  - Similar health
- Similar products
  - Similar cost
  - Similar function
  - Similar store
  - …
- Similarity usually is domain/problem specific

## Types of Clustering

- Partitioning
  - K-means clustering
  - K-medoids clustering
  - EM (expectation maximization) clustering
- Hierarchical
  - Divisive clustering (top down)
  - Agglomerative clustering (bottom up)
- Density-Based Methods
  - Regions of dense points separated by sparser regions of relatively low density

## Types of Clustering

- Hard Clustering:
  - Each object is in one and only one cluster
- Soft Clustering:
  - Each object has a probability of being in each cluster

## Two Types of Data/Distance Info

- N-dim vector space representation and distance metric

D1: 57,M,195,0,125,95,39,25,0,1,0,0,0,1,0,0,0,0,0,0,1,1,0,0,0,0,0,0,0,0
D2: 78,M,160,1,130,100,37,40,1,0,0,0,1,0,1,1,1,0,0,0,0,0,0,0,0,0,0,0,0,0
...
Dn: 18,M,165,0,110,80,41,30,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0

Distance (D1,D2) = ???

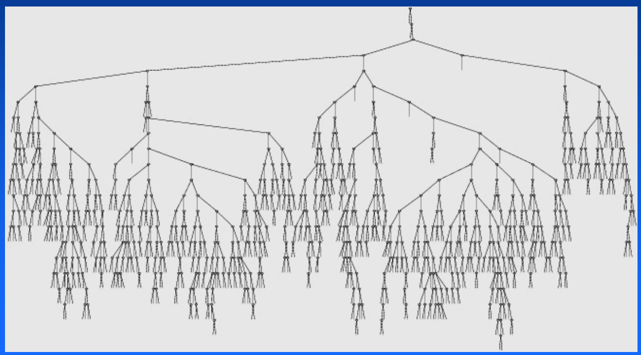
- Pairwise distances between points (no N-dim space)
  - Similarity/dissimilarity matrix (upper or lower diagonal)
  - Distance: 0 = near, ∞ = far
  - Similarity: 0 = far, ∞ = near

| -- | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | - | d | d | d | d | d | d | d | d | d |
| 2 | | - | d | d | d | d | d | d | d | d |
| 3 | | | - | d | d | d | d | d | d | d |
| 4 | | | | - | d | d | d | d | d | d |
| 5 | | | | | - | d | d | d | d | d |
| 6 | | | | | | - | d | d | d | d |
| 7 | | | | | | | - | d | d | d |
| 8 | | | | | | | | - | d | d |
| 9 | | | | | | | | | - | d |

## Agglomerative Clustering

- Put each item in its own cluster (641 singletons)
- Find all pairwise distances between clusters
- Merge the two *closest* clusters
- Repeat until everything is in one cluster
- Hierarchical clustering
- Yields a clustering with each possible # of clusters
- Greedy clustering: not optimal for any cluster size

## Agglomerative Clustering of Proteins



## Merging: Closest Clusters

- Nearest centroids
- Nearest medoids
- Nearest neighbors (shortest link)
- Nearest average distance (average link)
- Smallest greatest distance (maximum link)
- Domain specific similarity measure
  - word frequency, TFIDF, KL-divergence, ...
- Merge clusters that optimize criterion after merge
  - minimum mean_point_happiness

## Mean Distance Between Clusters

$$Mean\_Dist(c_1, c_2) = \frac{\sum_{i \in c_1} \sum_{j \in c_2} Dist(i, j)}{\sum_{i \in c_1} \sum_{j \in c_2} 1}$$

## Minimum Distance Between Clusters

$$Min\_Dist(c_1, c_2) = \underset{i \in c_1, j \in c_2}{MIN} (Dist(i, j))$$

## Mean Internal Distance in Cluster

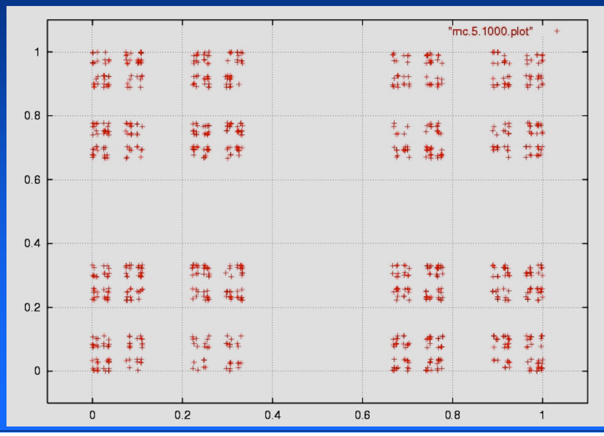
$$Mean\_Internal\_Dist(c) = \frac{\sum_{i \in c} \sum_{j \in c, i \neq j} Dist(i, j)}{\sum_{i \in c} \sum_{j \in c, i \neq j} 1}$$

## Mean Point Happiness

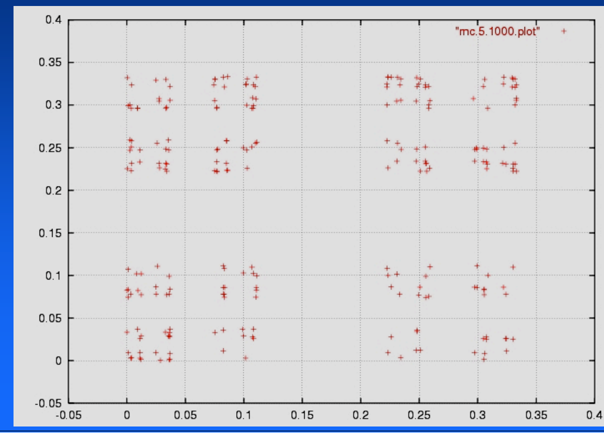
$$\delta_{ij} = \begin{cases} 1 & when\ cluster(i) = cluster(j) \\ 0 & when\ cluster(i) \neq cluster(j) \end{cases}$$

$$Mean\_Happiness = \frac{\sum_{i} \sum_{j \neq i} \delta_{ij} \bullet Dist(i, j)}{\sum_{i} \sum_{j \neq i} \delta_{ij}}$$

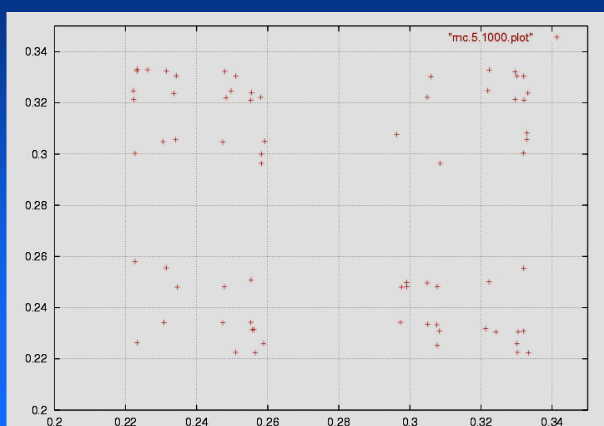
# Recursive Clusters



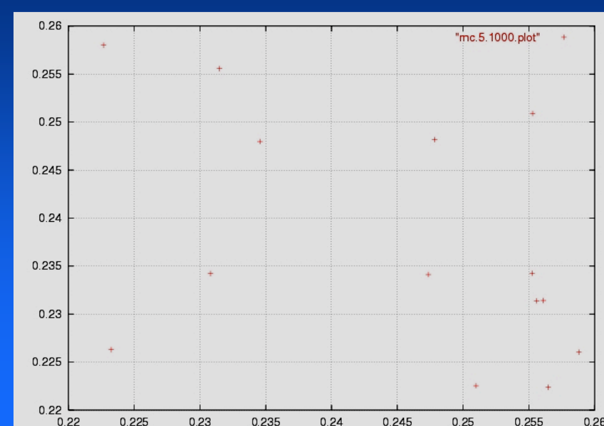

# Recursive Clusters



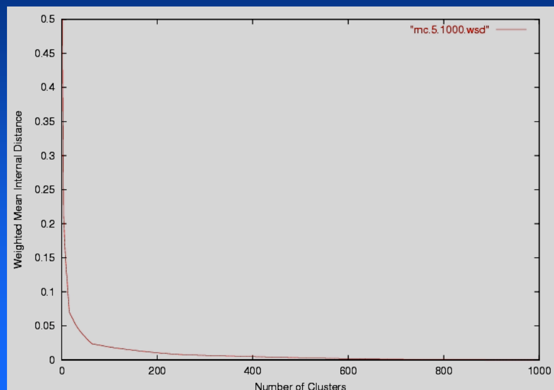

# Recursive Clusters



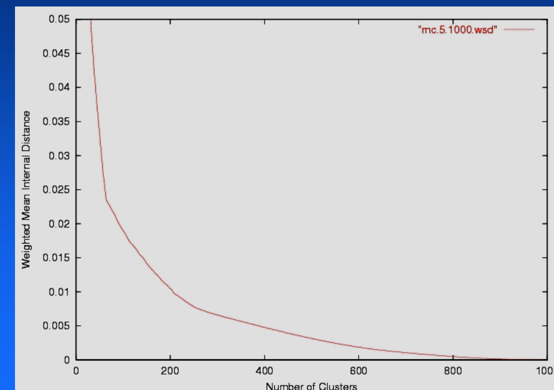

# Recursive Clusters



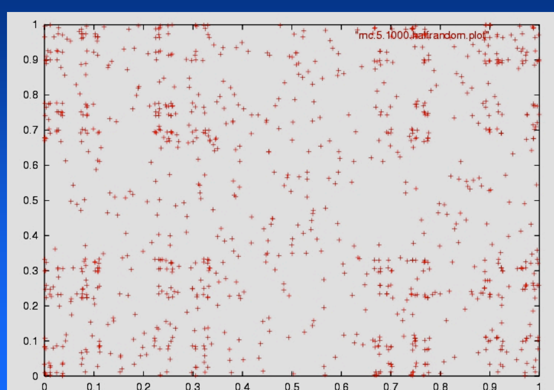
## Mean Point Happiness



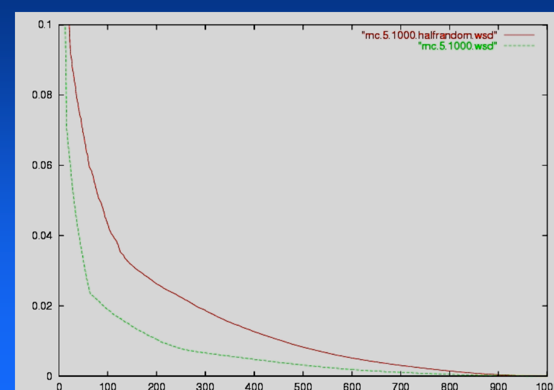

## Mean Point Happiness



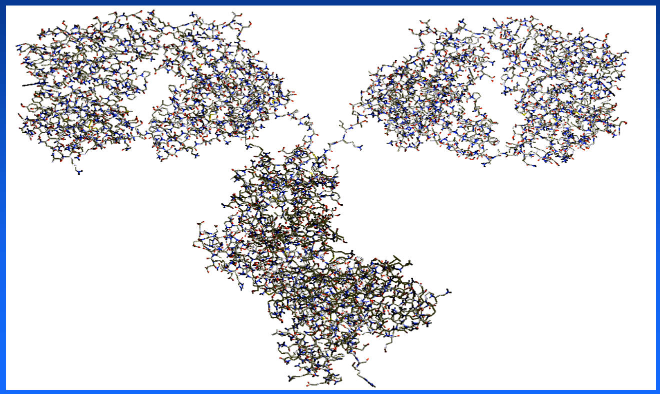

## Recursive Clusters + Random Noise

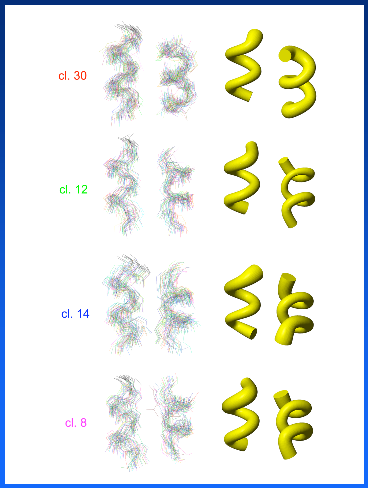



## Recursive Clusters + Random Noise



## Clustering Proteins



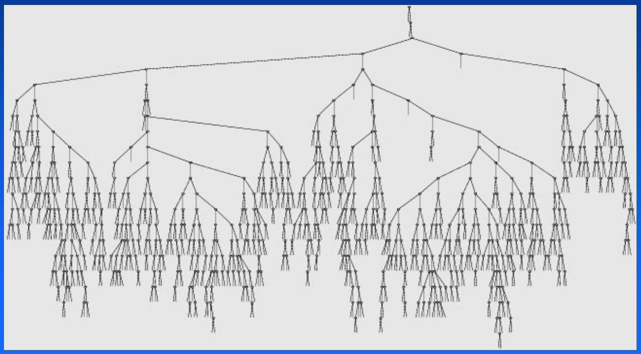



## Distance Between Helices

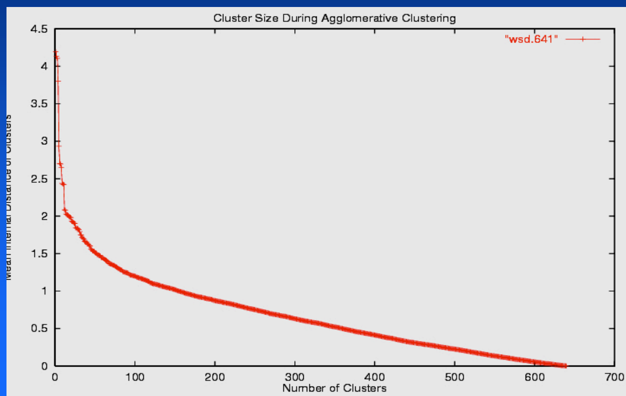
- Vector representation of protein data in 3-D space that gives x,y,z coordinates of each atom in helix
- Use a program developed by chemists (fortran) to convert 3-D atom coordinates into average atomic distances in angstroms between aligned helices
- 641 helices = 641 * 640 / 2

  = 205,120 pairwise distances

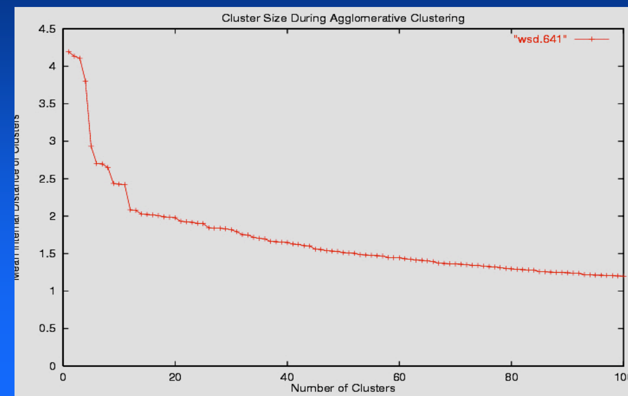
## Agglomerative Clustering of Proteins



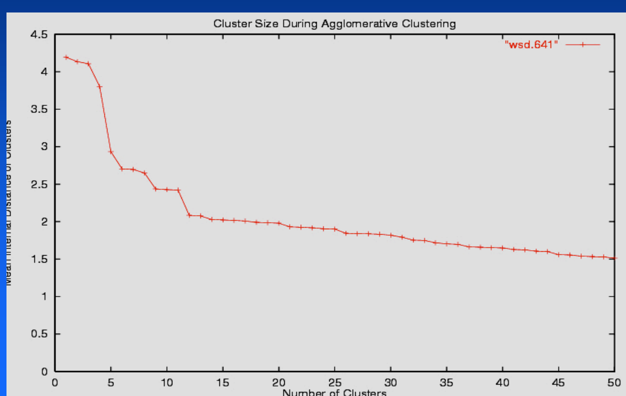
## Agglomerative Clustering of Proteins



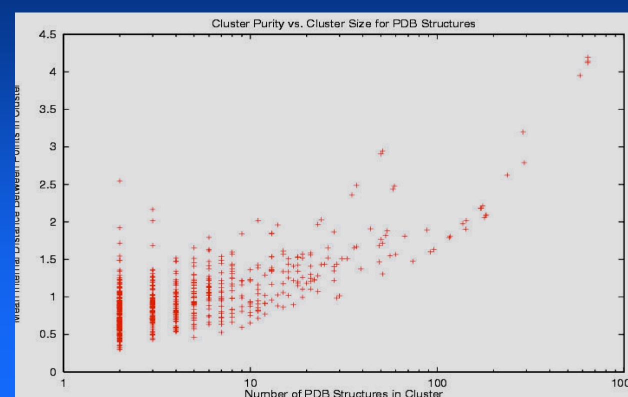

## Agglomerative Clustering of Proteins

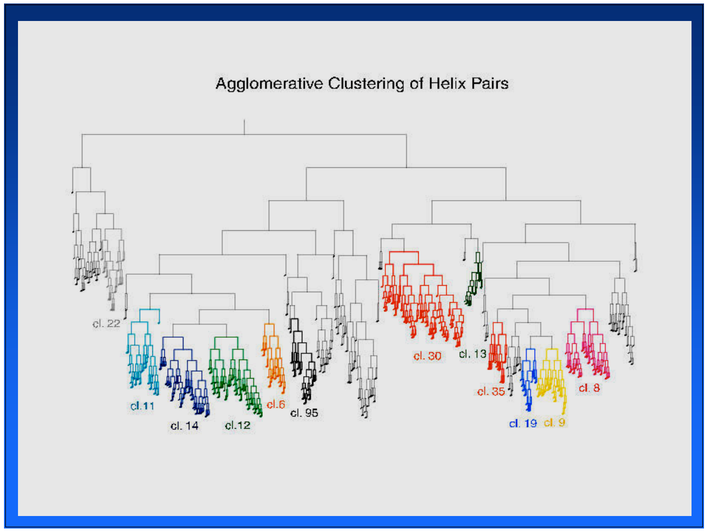


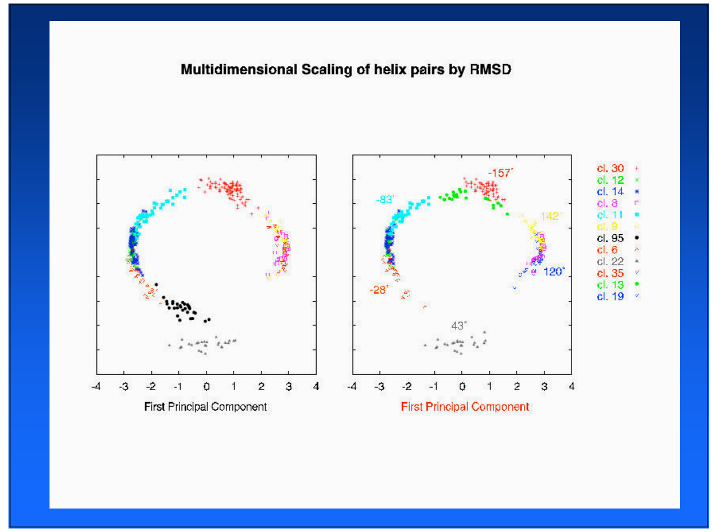

## Agglomerative Clustering of Proteins




## Agglomerative Clustering of Proteins






## Agglomerative Clustering

- Greedy clustering
  - once points are merged, never separated
  - suboptimal w.r.t. clustering criterion
- Combine greedy with iterative refinement
  - post processing
  - interleaved refinement

## Agglomerative Clustering

- Computational Cost
  - $O(N^2)$ just to read/calculate pairwise distances
  - N-1 merges to build complete hierarchy
    - + scan pairwise distances to find closest
    - + calculate pairwise distances between clusters
    - + fewer clusters to scan as clusters get larger
  - Overall $O(N^3)$ for simple implementations
- Improvements
  - sampling
  - dynamic sampling: add new points while merging
  - tricks for updating pairwise distances

## K-Means Clustering

- Inputs: data set and k (number of clusters)
- Output: each point assigned to one of k clusters

- K-Means Algorithm:
  - Initialize the k-means
    - assign from randomly selected points
    - randomly or equally distributed in space
  - Assign each point to nearest mean
  - Update means from assigned points
  - Repeat until convergence

## K-Means Clustering: Convergence

- Squared-Error Criterion

$$Squared\_Error = \sum_{c} \sum_{i \in c} (Dist(i, mean(c)))^2$$

- Converged when SE criterion stops changing
- Increasing K reduces SE - can't determine K by finding minimum SE
- Instead, plot SE as function of K

## K-Means Clustering

- Efficient
  - K << N, so assigning points is $O(K*N) < O(N^2)$
  - updating means can be done during assignment
  - usually # of iterations << N
  - Overall O(N*K*iterations) closer to O(N) than $O(N^2)$
- Gets stuck in local minima
  - Sensitive to initialization
- Number of clusters must be pre-specified
- Requires vector space date to calculate means

## Soft K-Means Clustering

- Instance of EM (Expectation Maximization)
- Like K-Means, except each point is assigned to each cluster with a probability
- Cluster means updated using weighted average
- Generalizes to Standard_Deviation/Covariance
- Works well if cluster models are known

## Soft K-Means Clustering (EM)

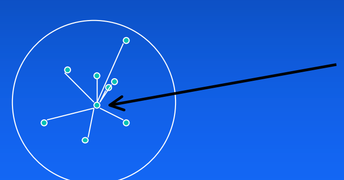
- Initialize model parameters:
  - means
  - std_devs
  - ...
- Assign points probabilistically to each cluster
- Update cluster parameters from weighted points
- Repeat until convergence to local minimum

## What do we do if we can't calculate cluster means?

| -- | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 |
|---|---|---|---|---|---|---|---|---|---|---|
| 1 | - | d | d | d | d | d | d | d | d | d |
| 2 | | - | d | d | d | d | d | d | d | d |
| 3 | | | - | d | d | d | d | d | d | d |
| 4 | | | | - | d | d | d | d | d | d |
| 5 | | | | | - | d | d | d | d | d |
| 6 | | | | | | - | d | d | d | d |
| 7 | | | | | | | - | d | d | d |
| 8 | | | | | | | | - | d | d |
| 9 | | | | | | | | | - | d |

## K-Medoids Clustering

$$Medoid(c) = pt \in c \text{ s.t. } MIN\left(\sum_{i \in c} Dist(i, pt)\right)$$



cluster
medoid

## K-Medoids Clustering

- Inputs: data set and k (number of clusters)
- Output: each point assigned to one of k clusters
- 
- Initialize k medoids
  - pick points randomly
- Pick medoid and non-medoid point at random
- Evaluate quality of swap
  - Mean point happiness
- Accept random swap if it improves cluster quality

## Cost of K-Means Clustering

- n cases; d dimensions; k centers; i iterations
- compute distance each point to each center: O(n*d*k)
- assign each of n cases to closest center: O(n*k)
- update centers (means) from assigned points: O(n*d*k)
- repeat i times until convergence
- overall: O(n*d*k*i)
- much better than $O(n^2)$-$O(n^3)$ for HAC
- sensitive to initialization - run many times
- usually don't know k - run many times with different k
- requires many passes through data set

## Graph-Based Clustering

## Scaling Clustering to Big Databases

- K-means is still expensive: O(n*d*k*I)
- Requires multiple passes through database
- Multiple scans may not be practical when:
  - database doesn't fit in memory
  - database is very large:
    - $10^4$-$10^9$ (or more) records
    - $>10^2$ attributes
  - expensive join over distributed databases

## Goals

- 1 scan of database
- early termination, on-line, anytime algorithm yields current best answer

# Scale-Up Clustering?

- Large number of cases (big n)
- Large number of attributes (big d)
- Large number of clusters (big c)