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
77,F,140,0,125,100,40,30,1,1,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,1,1	1

…

Supervised Learning

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

57,M,195,0,125,95,39,25,0,1,0,0,0,1,0,0,0,0,0,1,1,0,0,0,0,0,0,0,0	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	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
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

- 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	?

- 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

$\neq$

Supervised Learning

Clustering

=

Unsupervised Learning

Supervised Learning

Train Set:

57,M,195,0,125,95,39,25,0,1,0,0,0,1,0,0,0,0,0,0,1,1,0,0,0,0,0,0,0,0	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
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,160,1,130,105,38,20,1,0,0,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0	?

Un-Supervised Learning

Train Set:

57,M,195,0,125,95,39,25,0,1,0,0,0,1,0,0,0,0,0,0,1,1,0,0,0,0,0,0,0,0	~~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,135,0,120,95,36,28,0,0,0,0,0,0,0,0,0,0,0,1,1,0,0,0,0,0,0,1,0,0	~~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~~

…

Test Set:

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

Un-Supervised Learning

Train Set:

57,M,195,0,125,95,39,25,0,1,0,0,0,1,0,0,0,0,0,0,1,1,0,0,0,0,0,0,0,0 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,135,0,120,95,36,28,0,0,0,0,0,0,0,0,0,0,0,1,1,0,0,0,0,0,0,1,0,0 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,140,0,125,100,40,30,1,1,0,0,0,0,0,0,0,0,0,1,0,0,0,0,0,0,0,0,0,1,1 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

Data Set:

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

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

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,165,0,110,80,41,30,0,0,0,0,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0

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,250,1,130,100,38,26,1,1,0,0,0,1,1,0,0,0,0,0,0,0,0,0,0,0,0,0,0,0

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,195,0,125,95,39,25,0,1,0,0,0,1,0,0,0,0,0,1,1,0,0,0,0,0,0,0,0

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

...

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

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

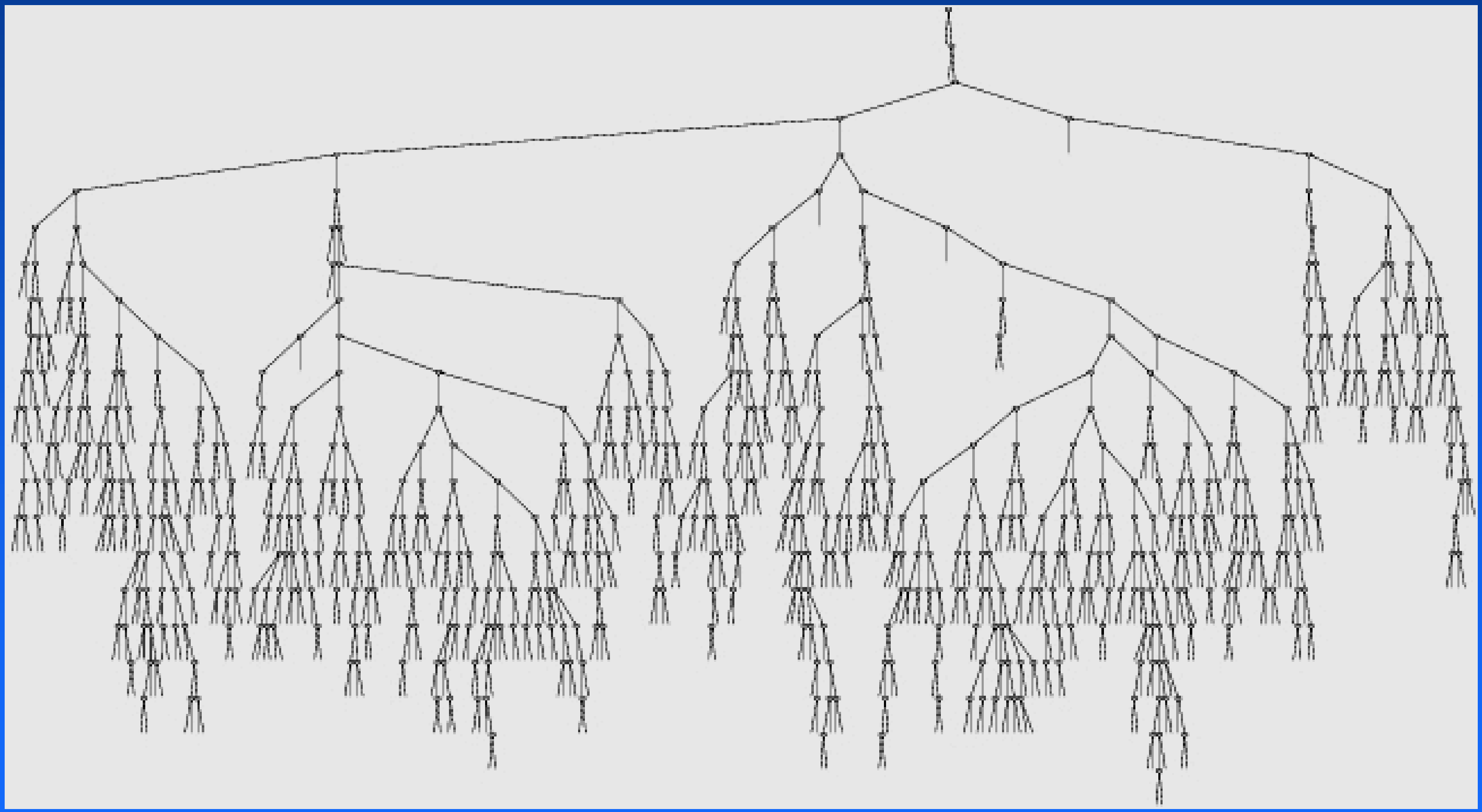
Agglomerative Clustering

- 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

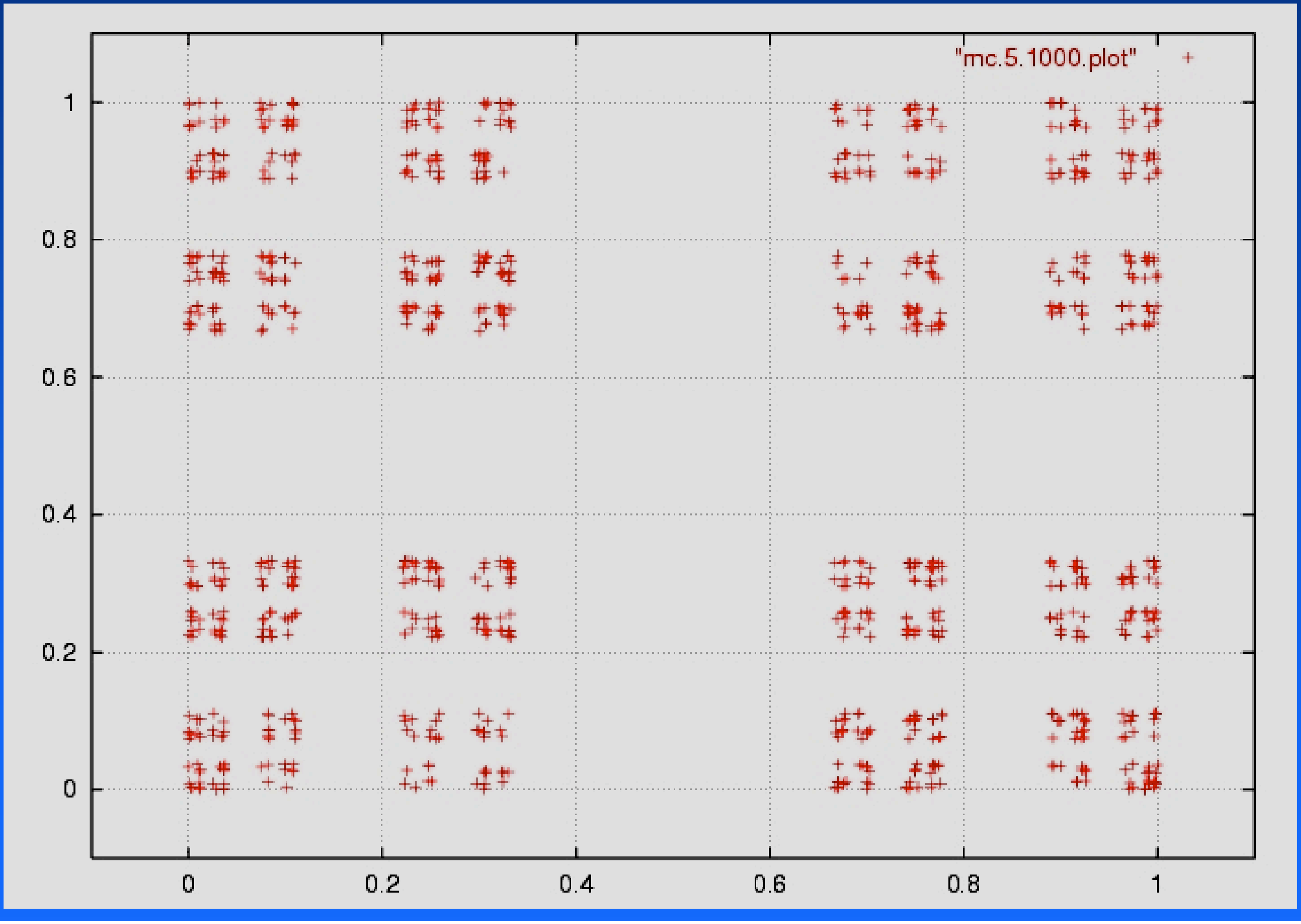
$$Mean\_Internal\_Dist(c) = \frac{\sum_{i \in c} \sum_{j \in c, i \neq j} Dist(i,j)}{\sum_{i \in c} \sum_{j \in c, i \neq j} 1}$$

Mean Point Happiness

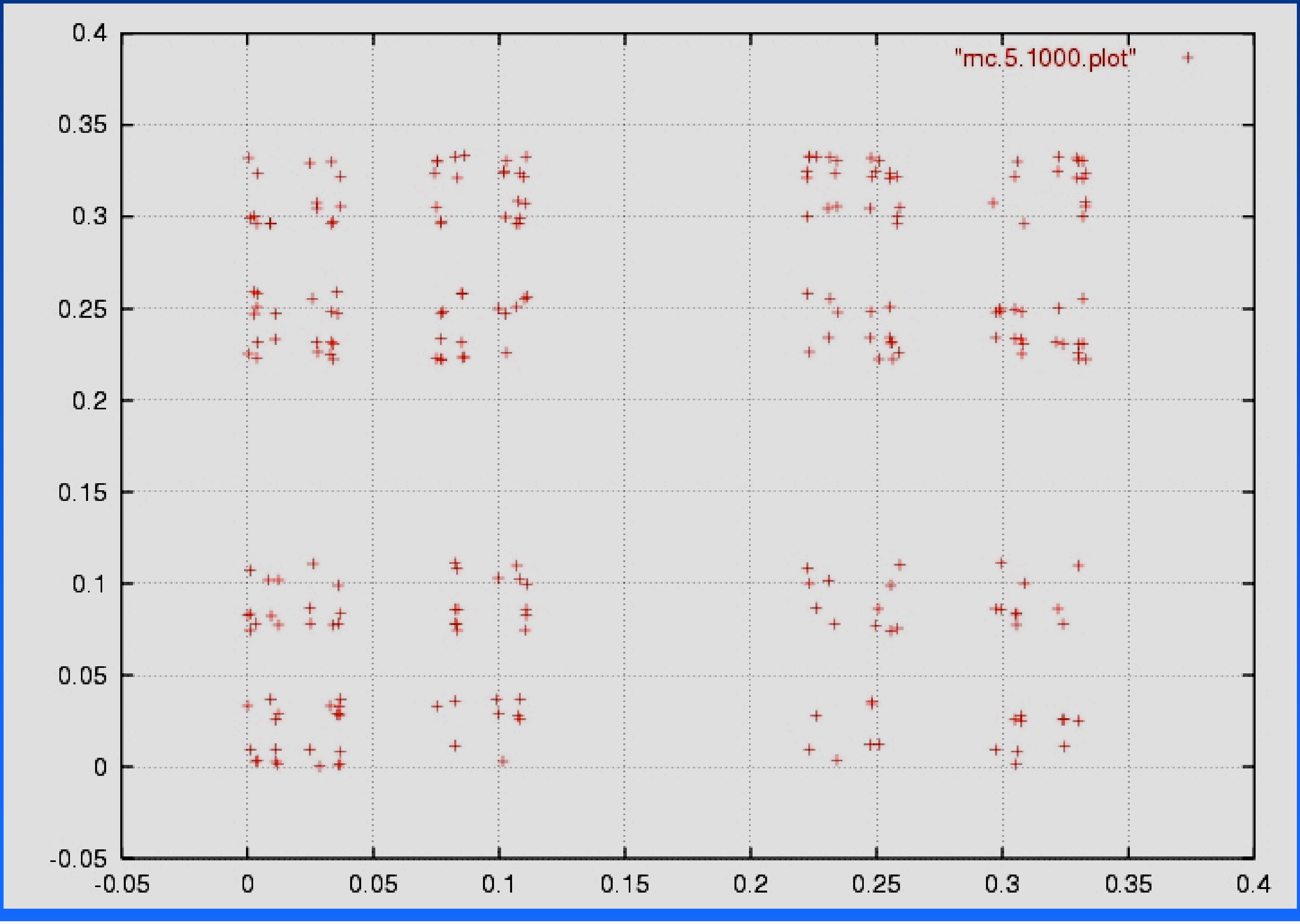
$$\square_{ij} = \left\{ \begin{array}{ll} 1 & when\ cluster(i) = cluster(j) \\ 0 & when\ cluster(i) \neq cluster(j) \end{array} \right\}$$

$$Mean\_Happiness = \frac{\sum_i \sum_j \square_{ij} \bullet Dist(i,j)}{\sum_i \sum_j \square_{ij}}$$

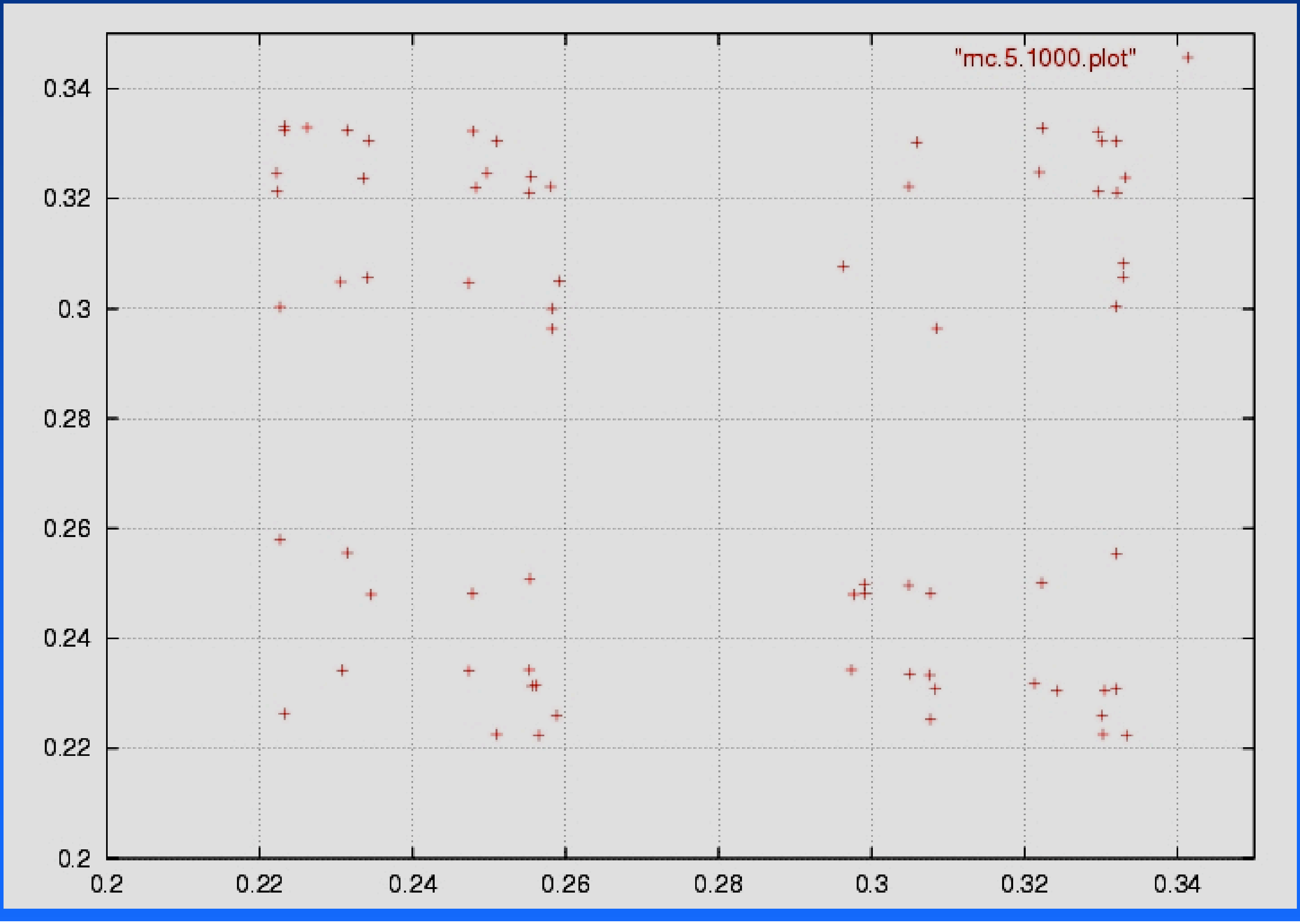
Recursive Clusters



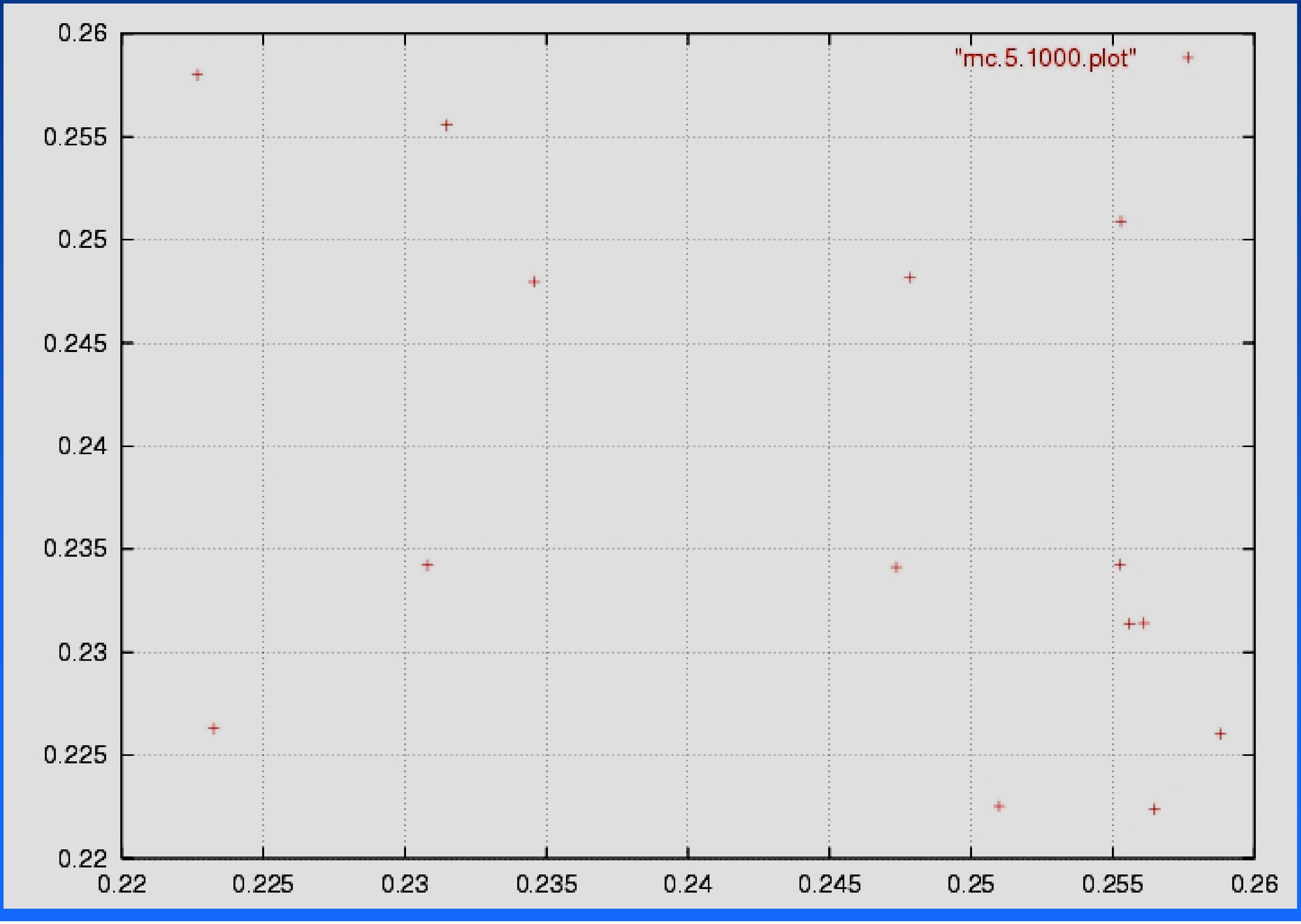
Recursive Clusters



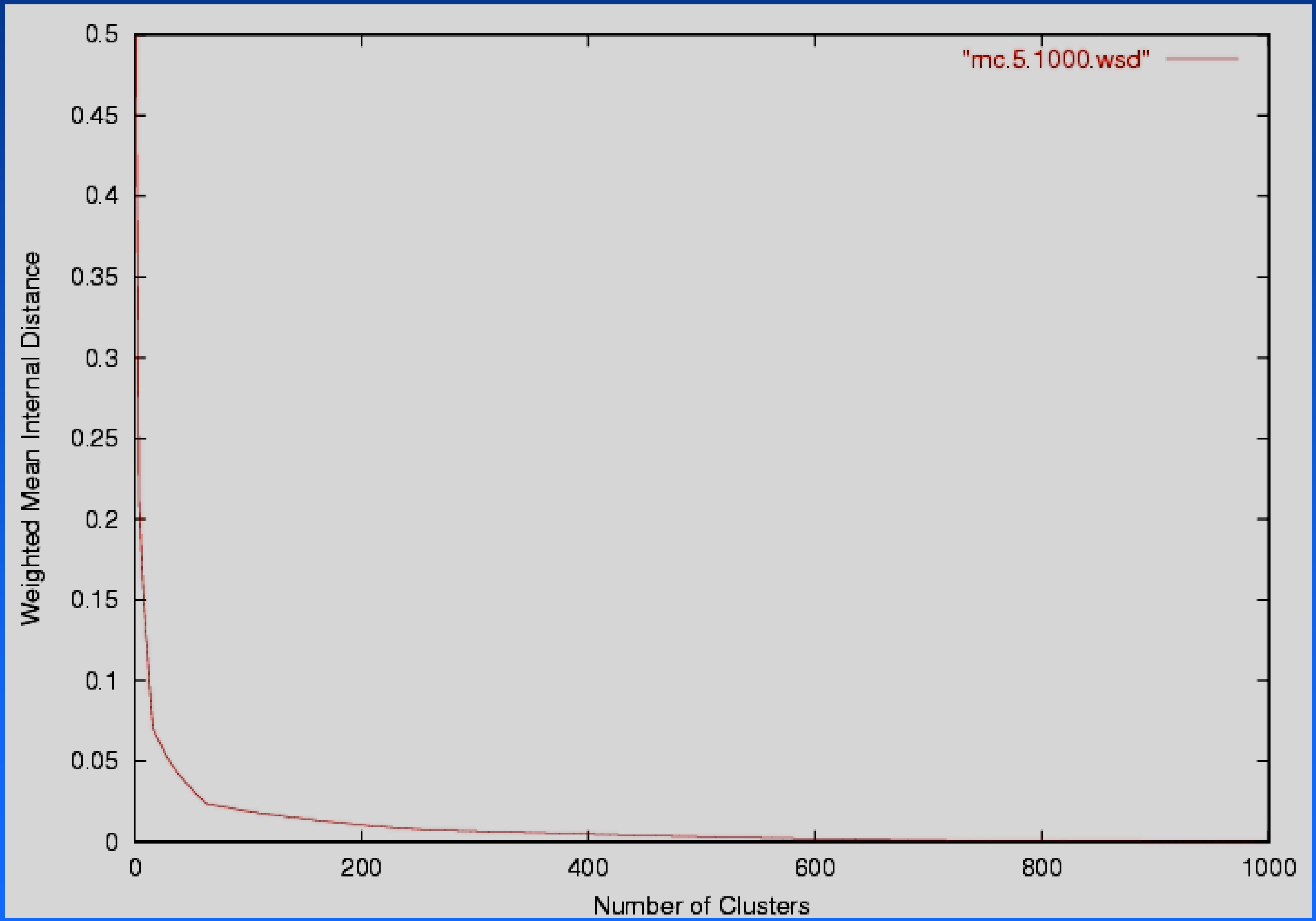
Recursive Clusters



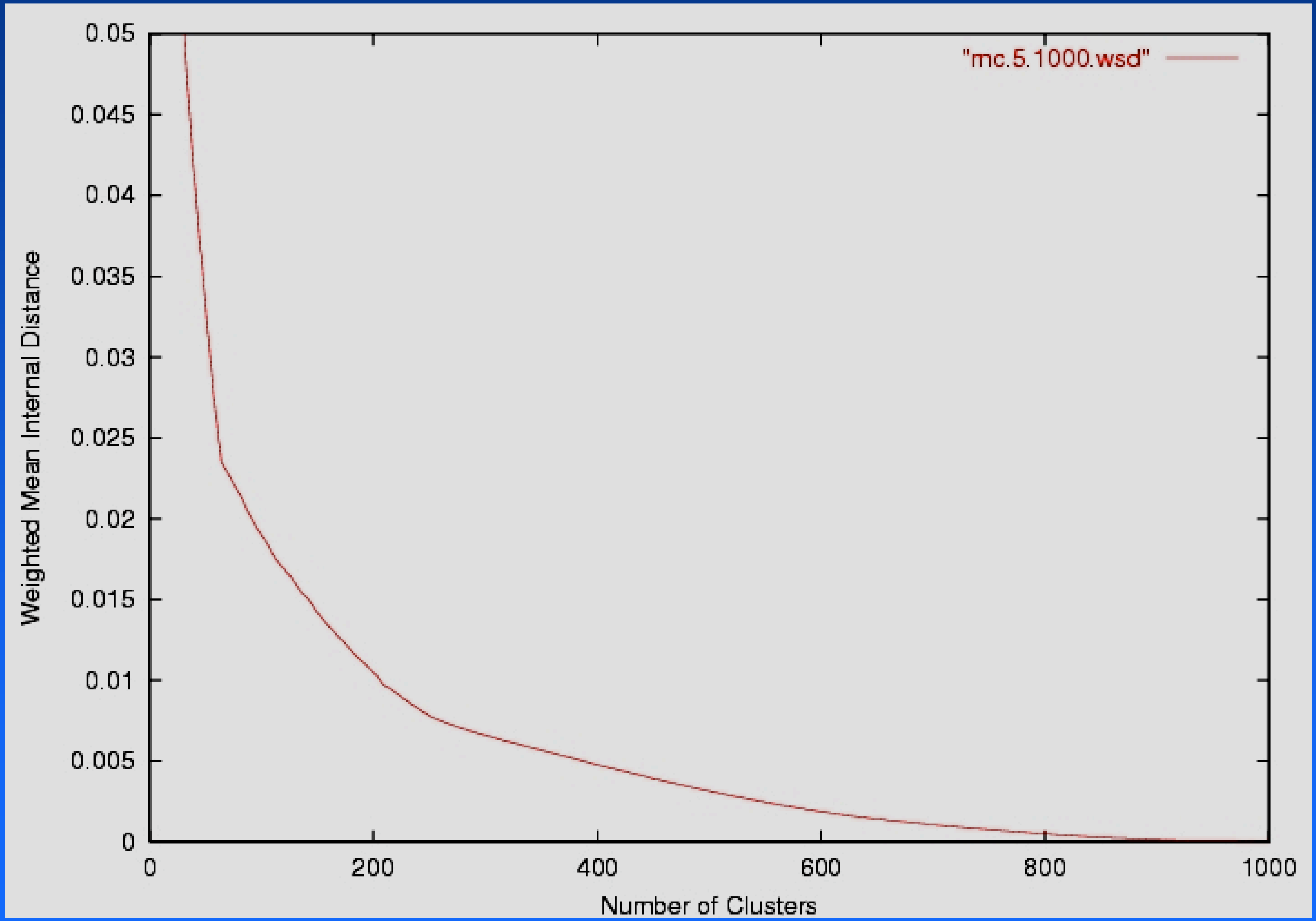
Recursive Clusters



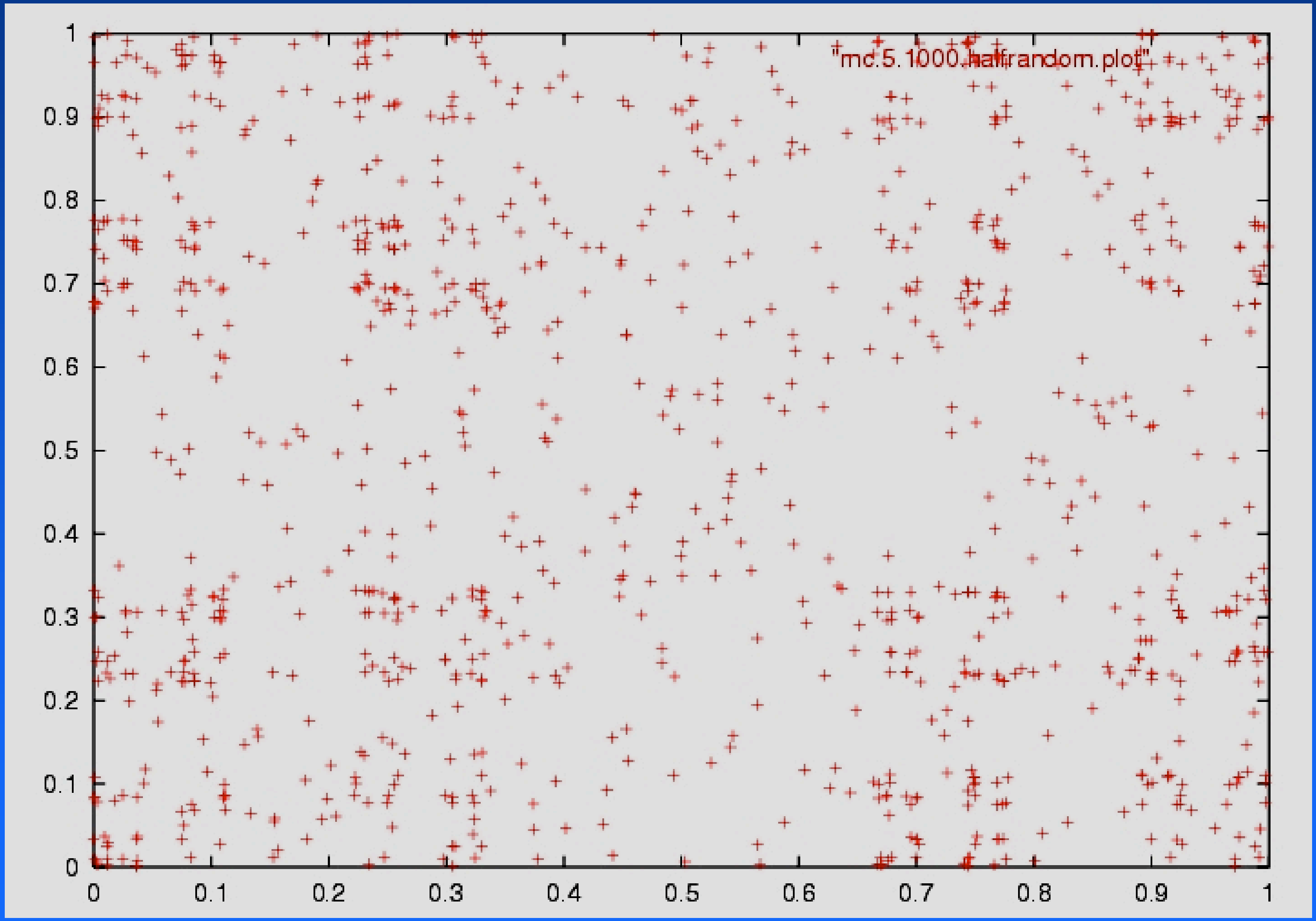
Mean Point Happiness



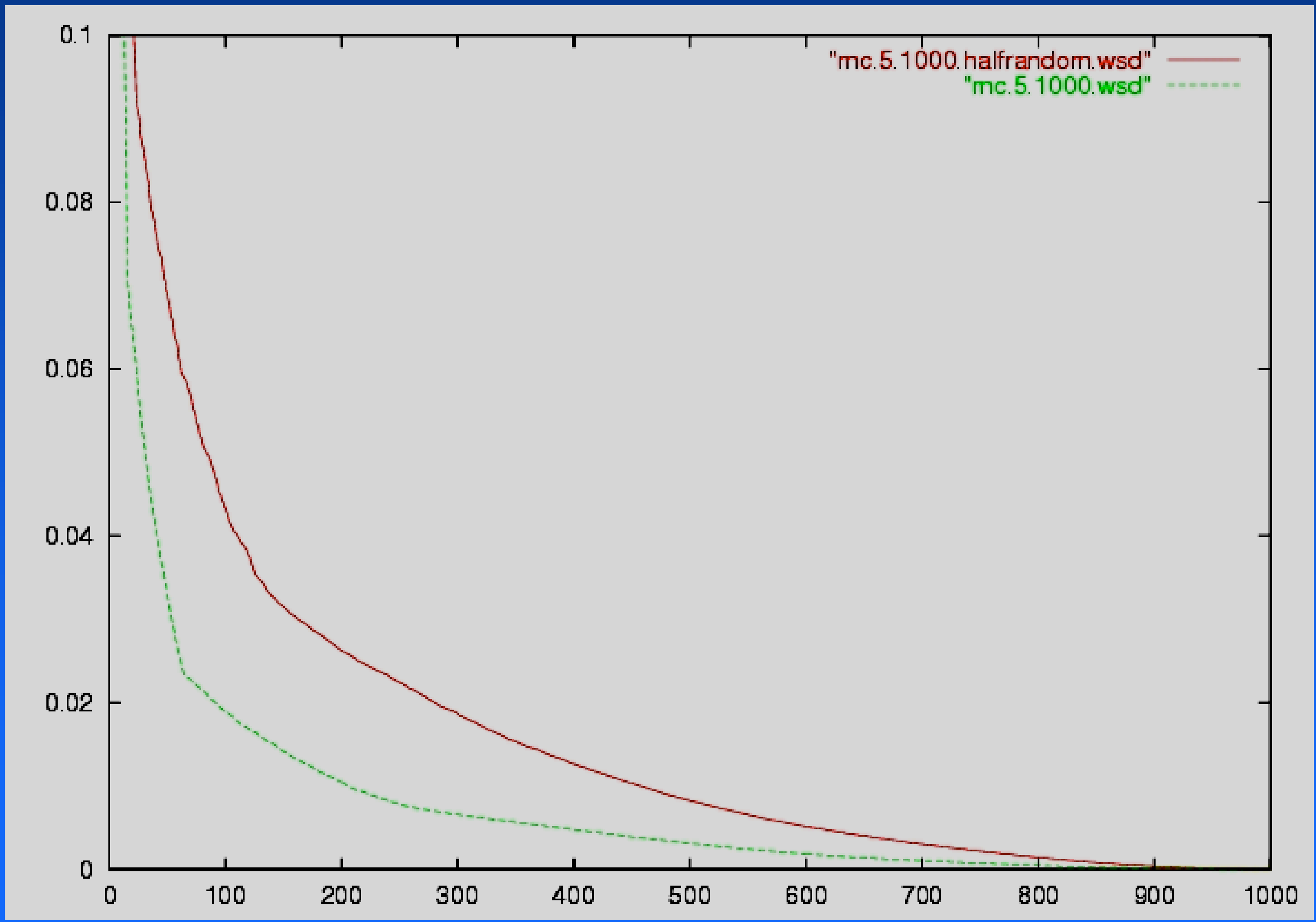
Mean Point Happiness



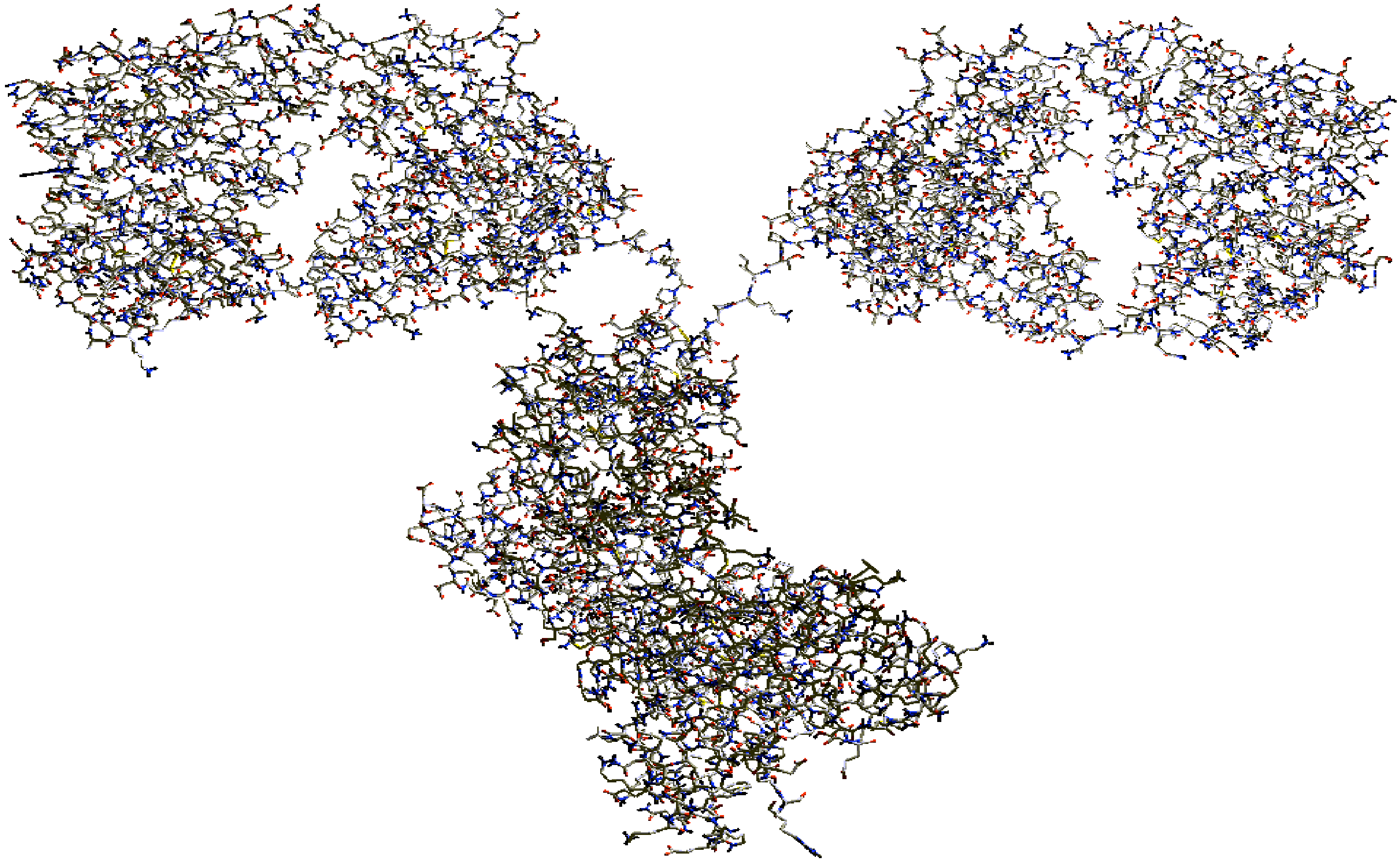
Recursive Clusters + Random Noise

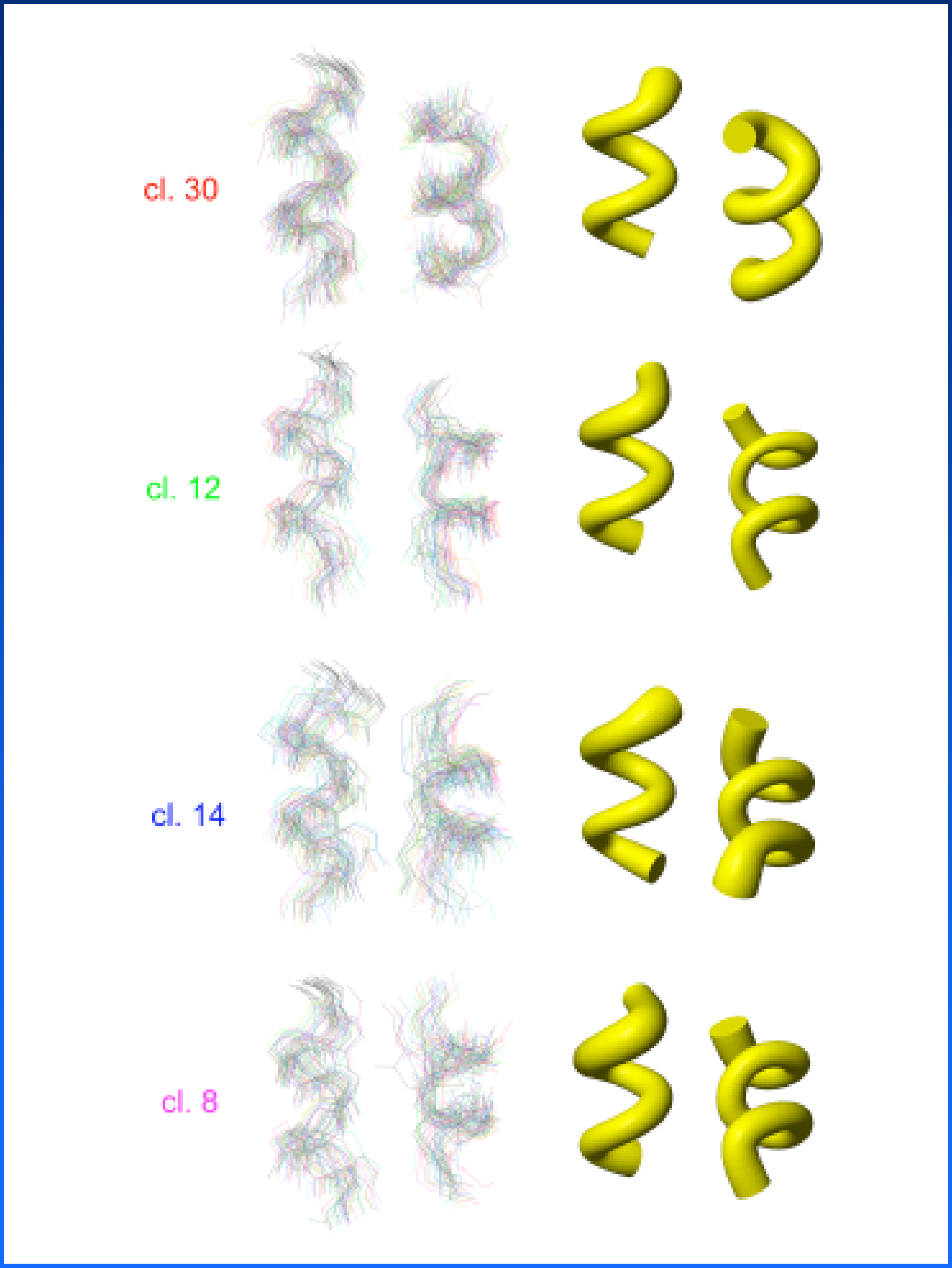


Recursive Clusters + Random Noise



Clustering Proteins

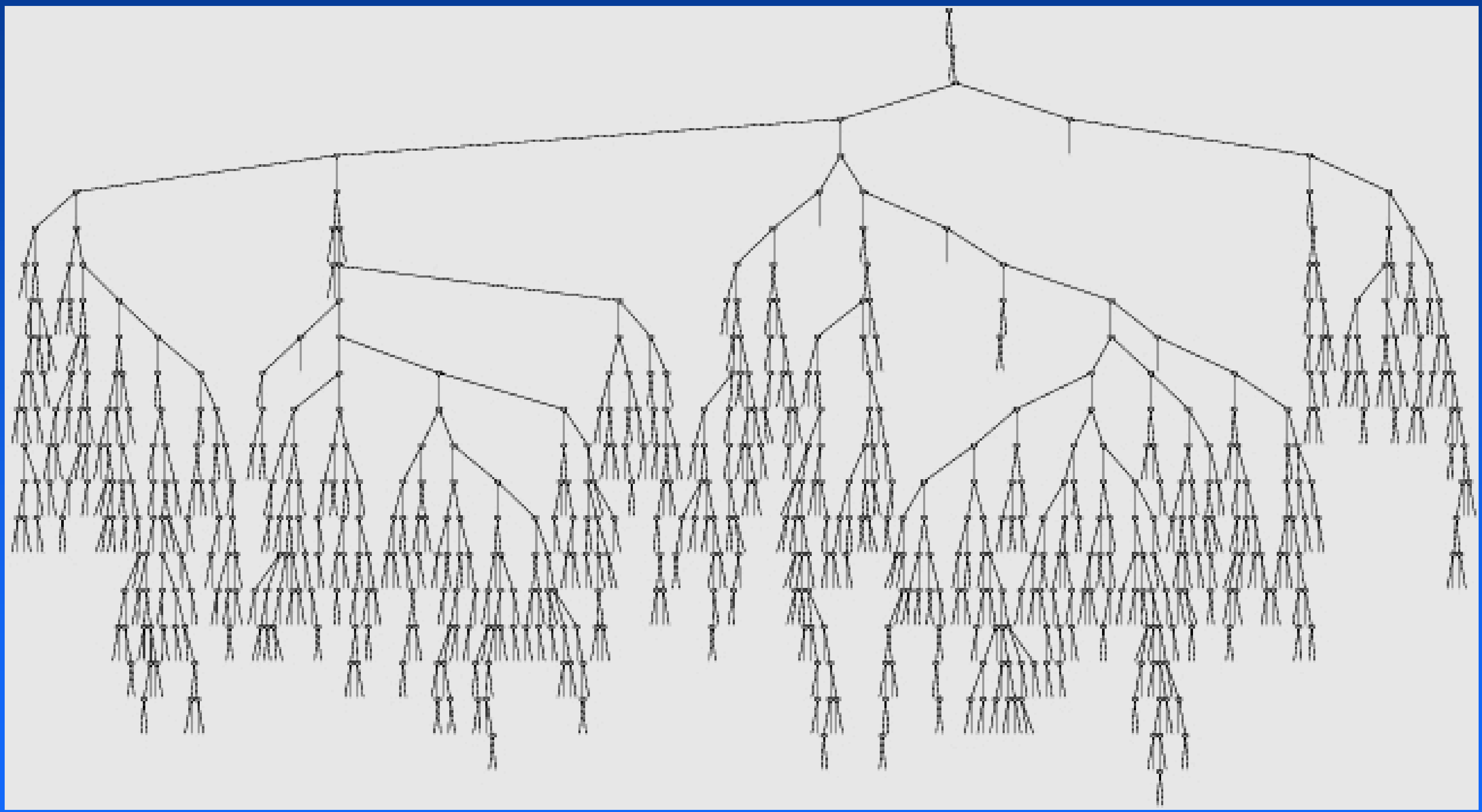



cl. 30
cl. 12
cl. 14
cl. 8

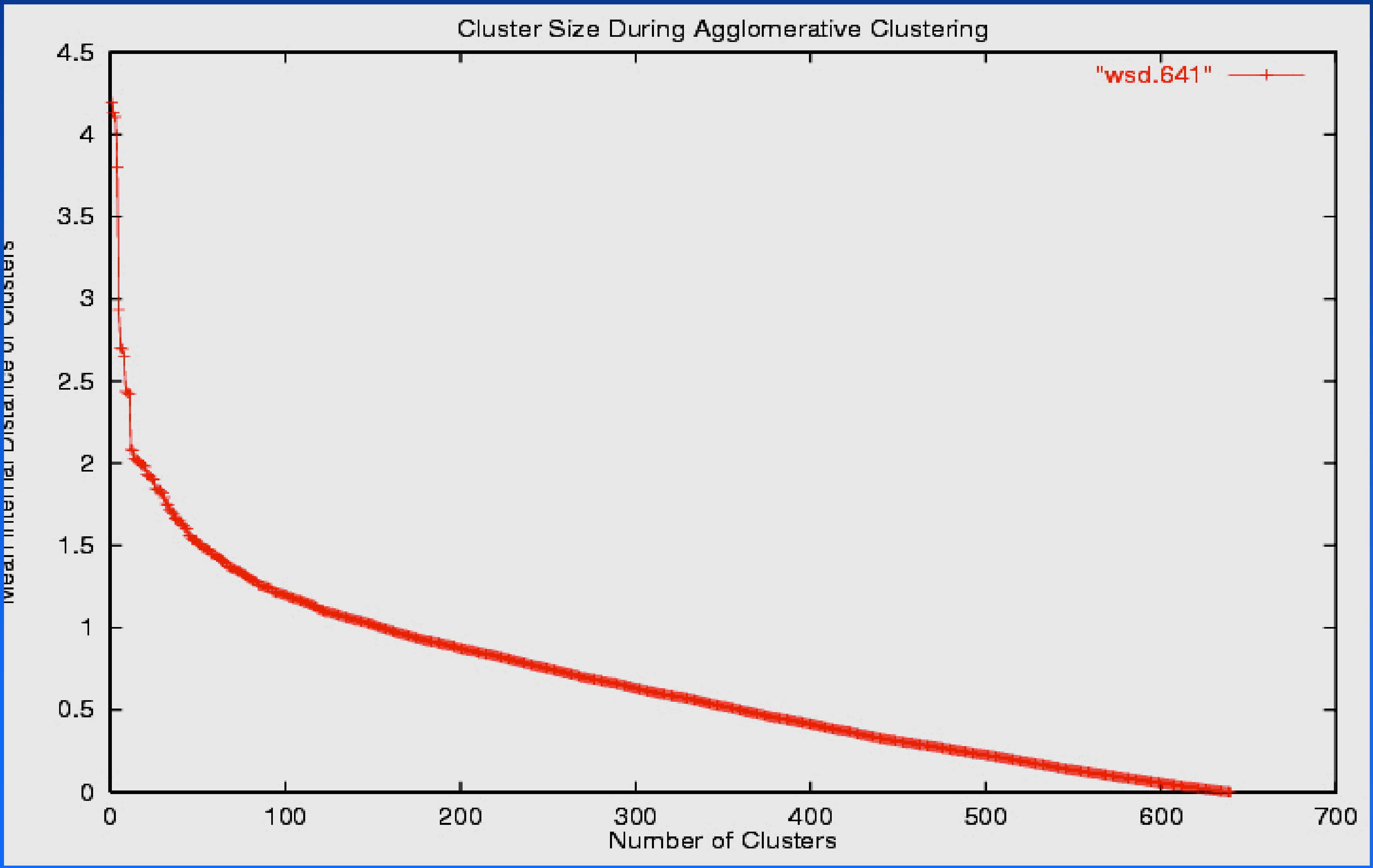
Distance Between Helices

- 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

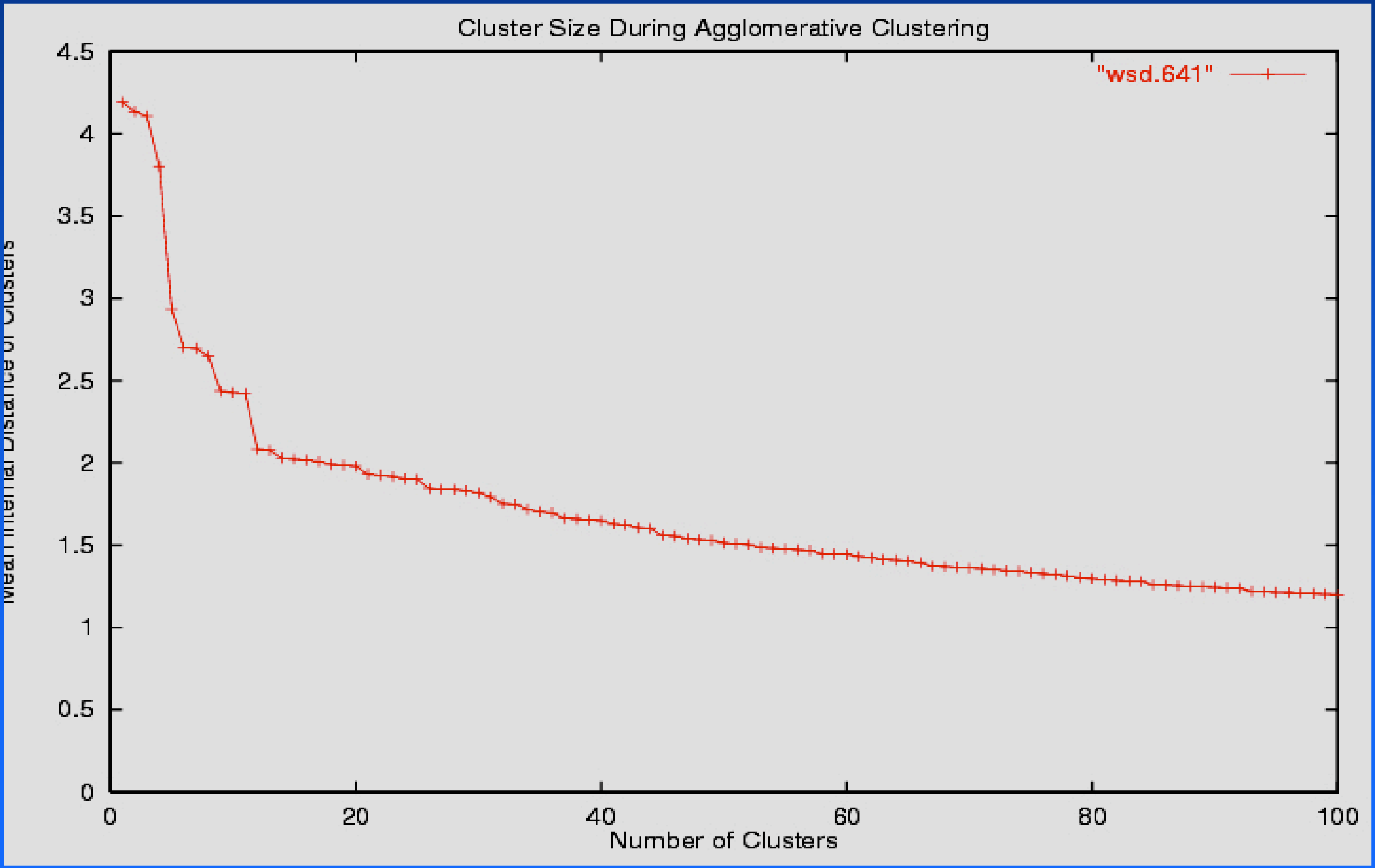
Agglomerative Clustering of Proteins



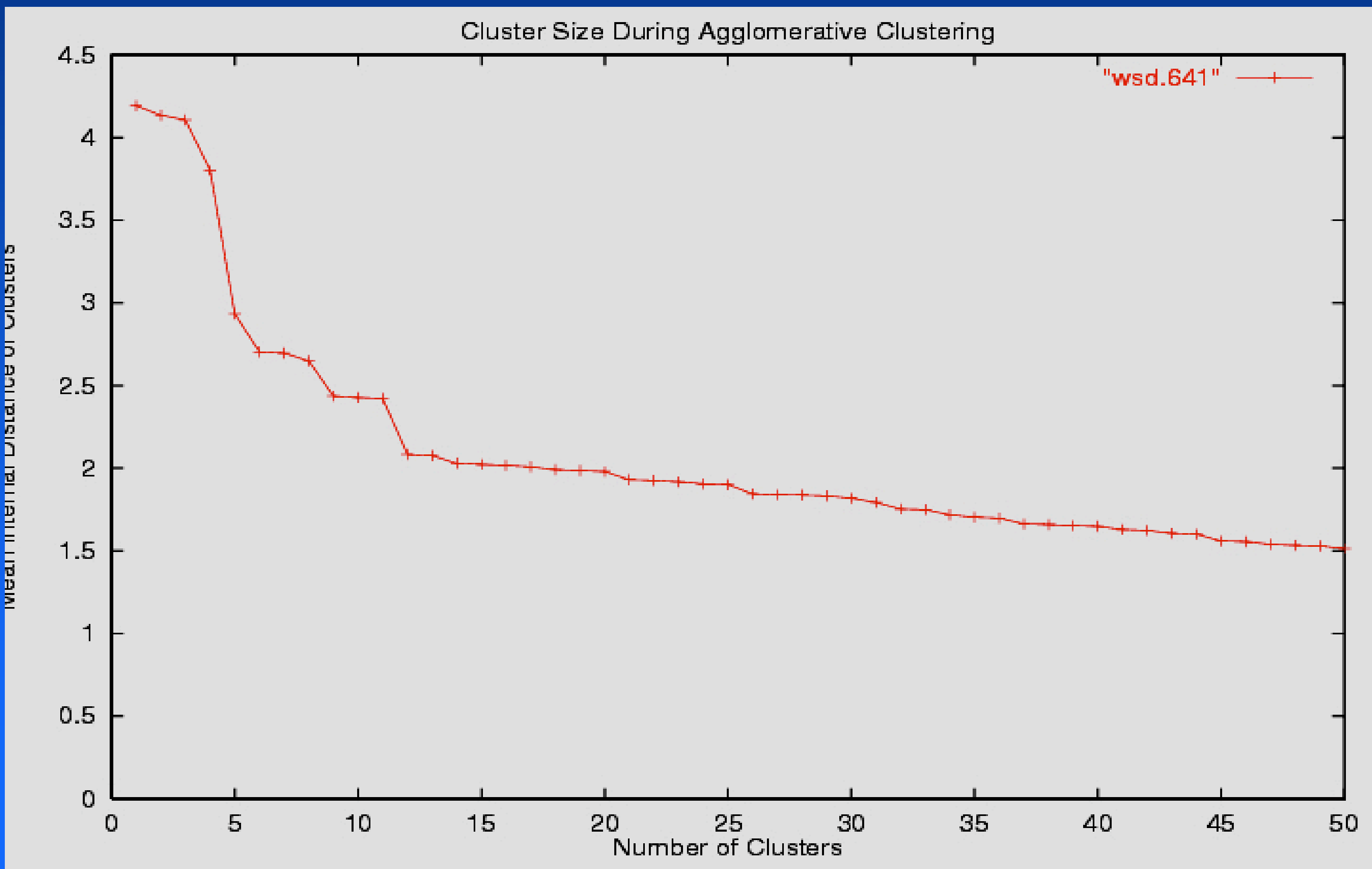
Agglomerative Clustering of Proteins



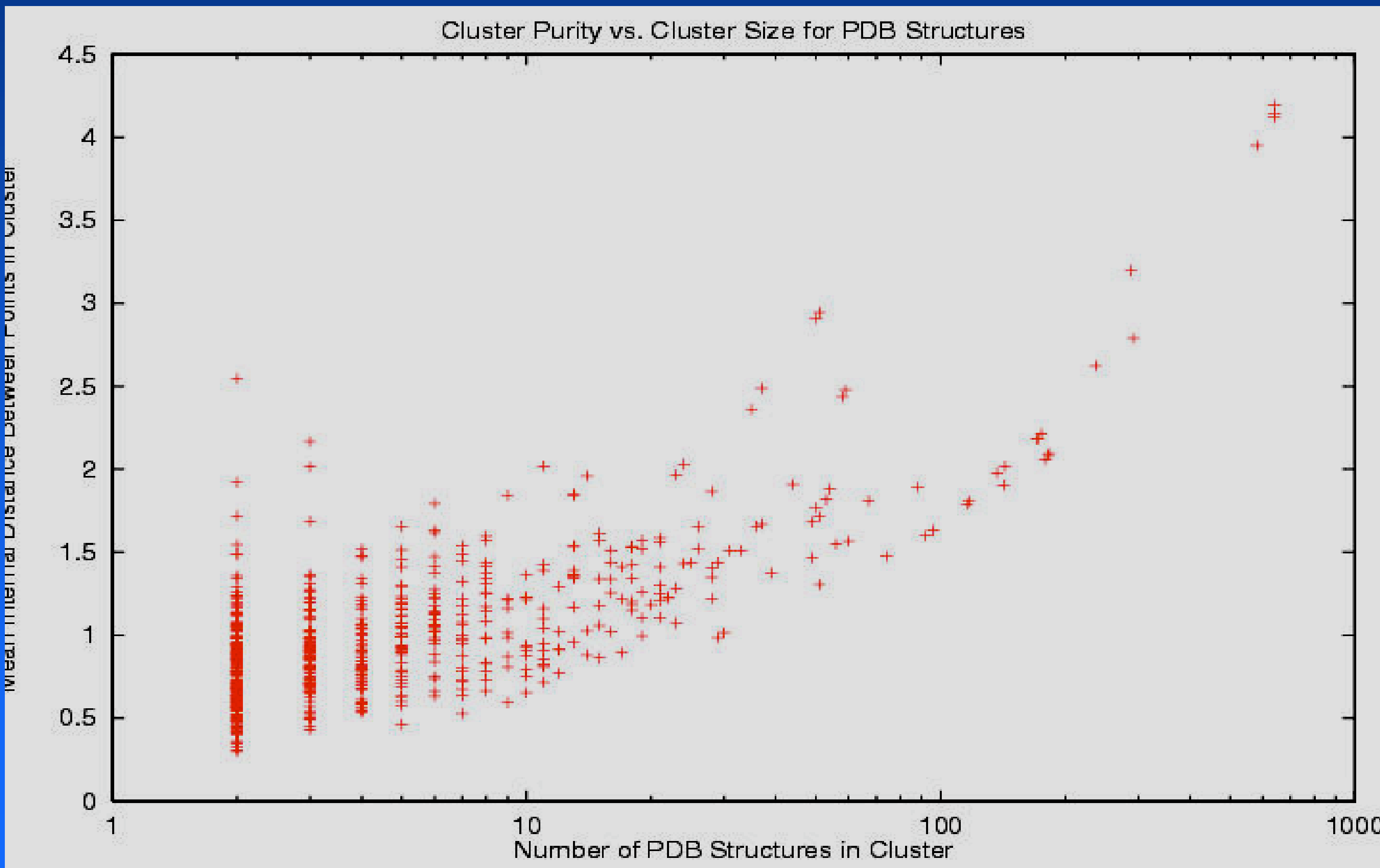
Agglomerative Clustering of Proteins



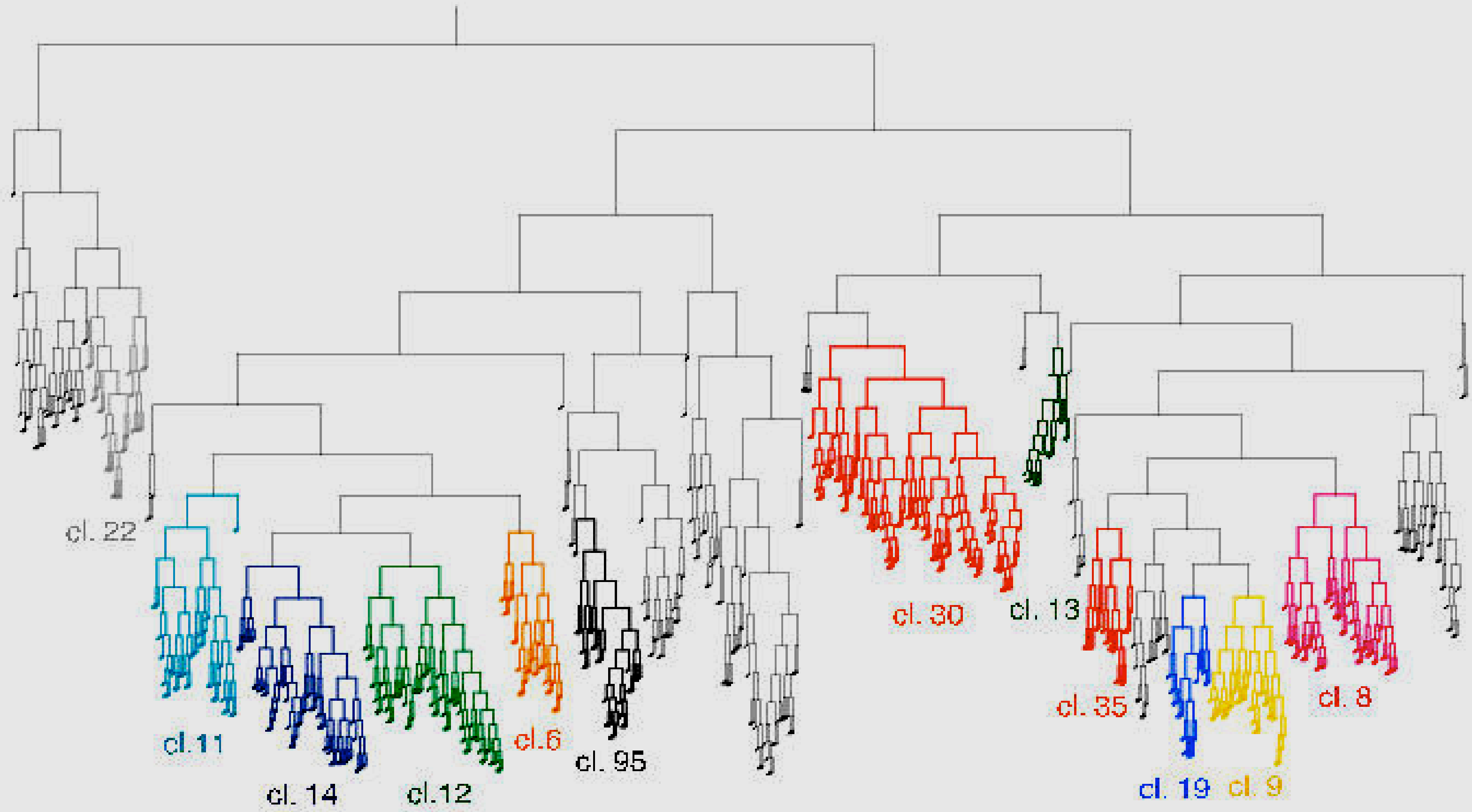
Agglomerative Clustering of Proteins



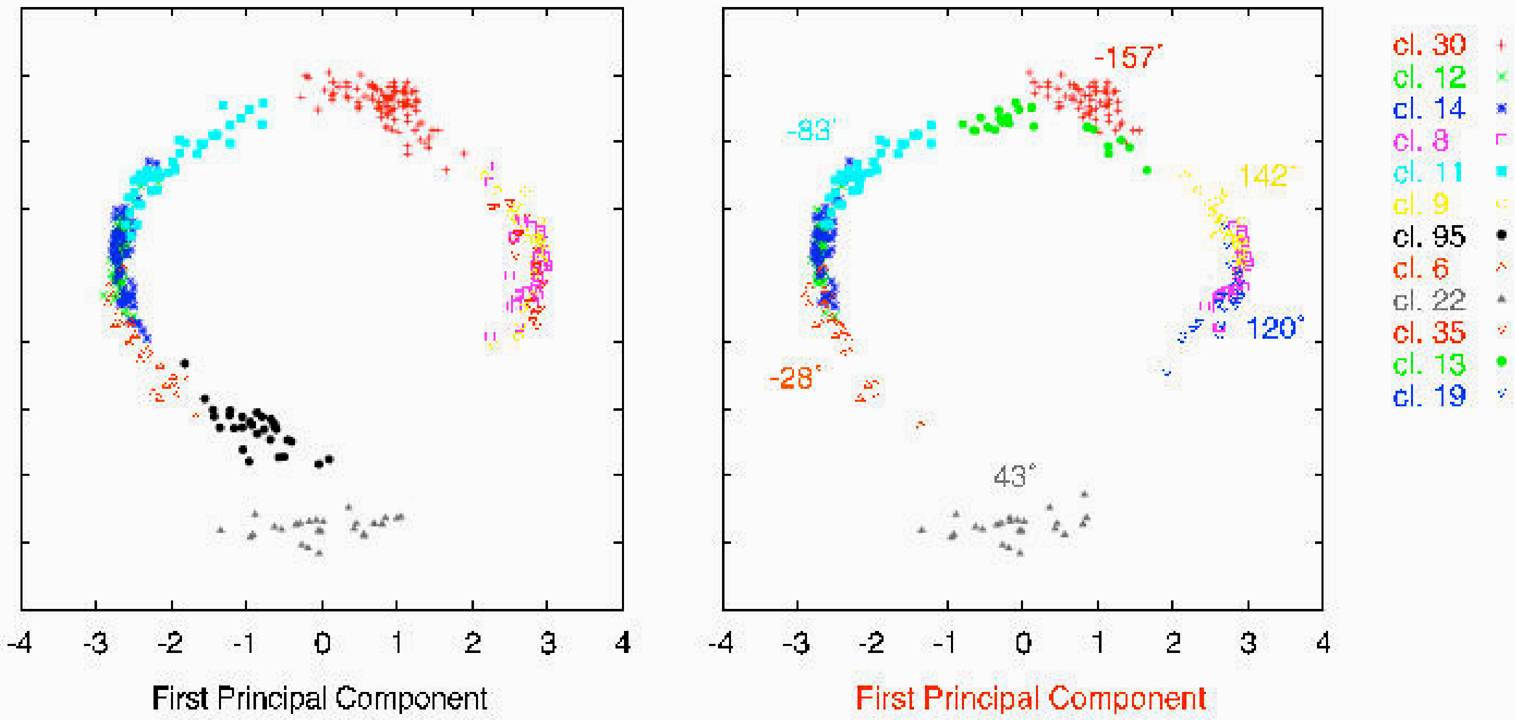
Agglomerative Clustering of Proteins



Agglomerative Clustering of Helix Pairs



Multidimensional Scaling of helix pairs by RMSD



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)

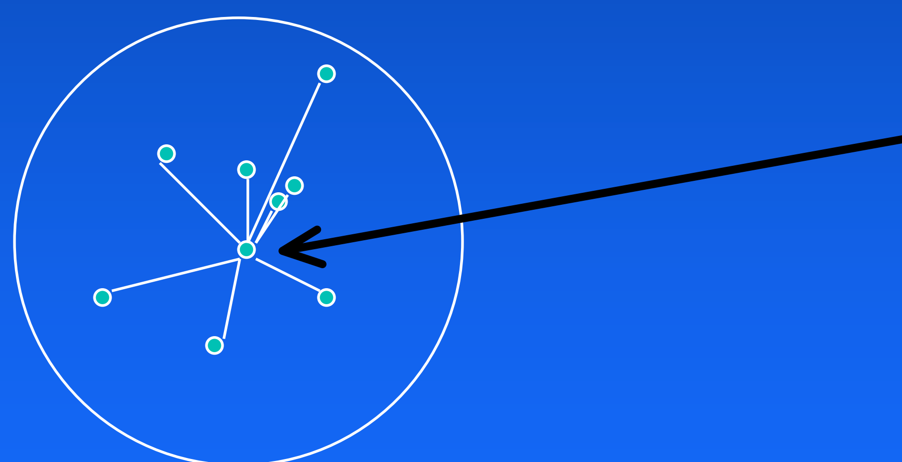
- Initialize model parameters:
  - means
  - std_devs
  - ...
- Assign points probabilistically to each cluster
- Update cluster parameters from weighted points
- Repeat until convergence to local minimum

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

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



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)