



Dominant Sets and Pairwise Clustering

Marcello Pelillo

Computer Vision and Pattern Recognition Group

Dipartimento di Informatica

Università Ca' Foscari, Venezia

joint work with Massimiliano Pavan



Talk's Outline

- Dominant sets and their characterization
- Evolutionary game dynamics for clustering
- Experiments on intensity/color/texture image segmentation
- Extension of the framework to hierarchical clustering
- Experiments on the (hierarchical) organization of an image database

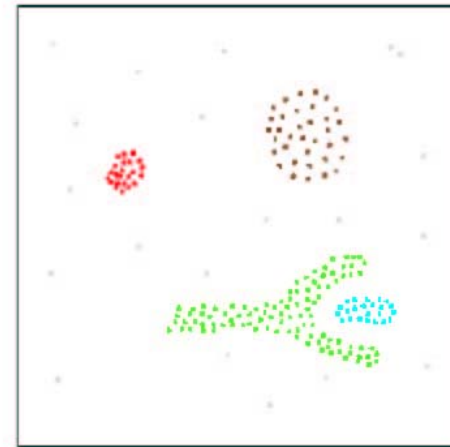
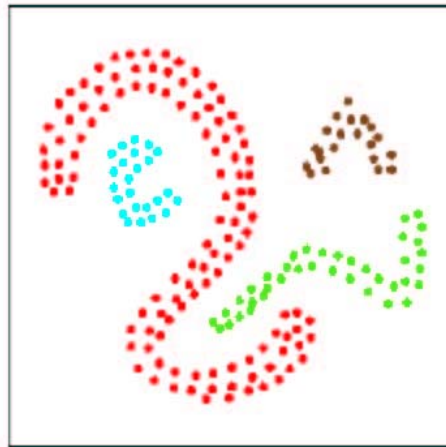
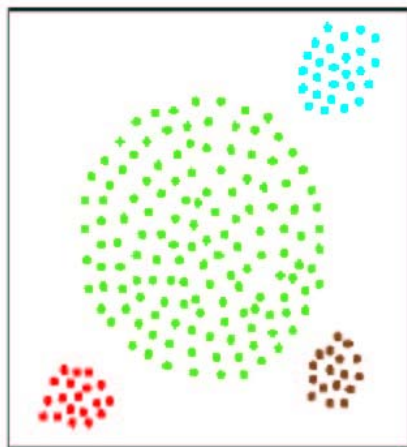


The (Pairwise) Clustering Problem

Given:

- a set of n “objects”
- an $n \times n$ matrix of pairwise similarities

Goal: Partition the input objects into maximally homogeneous groups (i.e., **clusters**).





Applications

Clustering problems abound in many areas of computer science and engineering.

A short list of applications domains:

- Image processing and computer vision
- Computational biology and bioinformatics
- Information retrieval
- Data mining
- Signal processing
- Machine learning
- ...



What is a Cluster?

No universally accepted definition of a “cluster”.

Informally, a cluster should satisfy two criteria:

Internal criterion: all objects *inside* a cluster should be highly similar to each other.

External criterion: all objects *outside* a cluster should be highly dissimilar to the ones inside.



Clustering as a Graph-Theoretic Problem

We represent the data to be clustered as an undirected edge-weighted graph with no self-loops $G = (V, E, w)$, where $V = \{1, \dots, n\}$ is the vertex set, $E \subseteq V \times V$ is the edge set, and $w : E \rightarrow \mathbb{R}_+^*$ is the (positive) weight function.

We represent the graph G with the corresponding weighted adjacency (or similarity) matrix, which is the $n \times n$ symmetric matrix $A = (a_{ij})$ defined as:

$$a_{ij} = \begin{cases} w(i, j), & \text{if } (i, j) \in E \\ 0, & \text{otherwise.} \end{cases}$$



An Illustrative Example: The Binary Case

Suppose the similarity matrix is a binary matrix.

In this case, the notion of a cluster coincide with that of a *maximal clique*.

Given an unweighted undirected graph $G=(V,E)$:

A *clique* is a subset of mutually adjacent vertices

A *maximal clique* is a clique that is not contained in a larger one

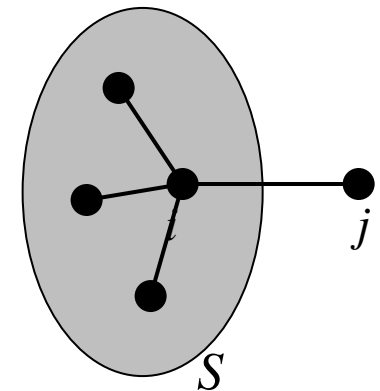
How to generalize the notion of a maximal clique to weighted graphs?



Basic Definitions

Let $S \subseteq V$ be a non-empty subset of vertices and $i \in S$. The (average) weighted degree of i w.r.t. S is defined as:

$$\text{awdeg}_S(i) = \frac{1}{|S|} \sum_{j \in S} a_{ij} .$$



Moreover, if $j \notin S$ we define:

$$\phi_S(i, j) = a_{ij} - \text{awdeg}_S(i) .$$

Intuitively, $\phi_S(i, j)$ measures the similarity between nodes j and i , with respect to the average similarity between node i and its neighbors in S .



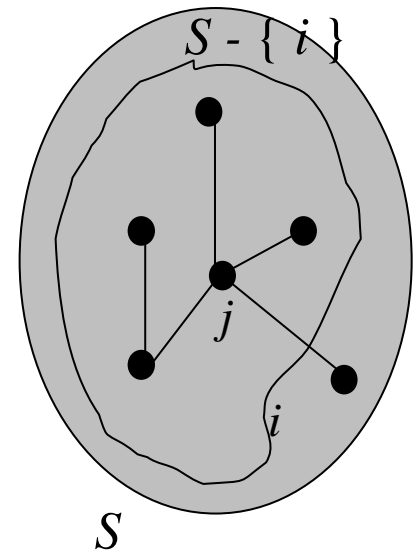
Assigning Node Weights / 1

Let $S \subseteq V$ be a non-empty subset of vertices and $i \in S$. The **weight** of i w.r.t. S is

$$w_S(i) = \begin{cases} 1, & \text{if } |S| = 1 \\ \sum_{j \in S \setminus \{i\}} \phi_{S \setminus \{i\}}(j, i) w_{S \setminus \{i\}}(j), & \text{otherwise.} \end{cases}$$

Moreover, the **total weight** of S is defined to be:

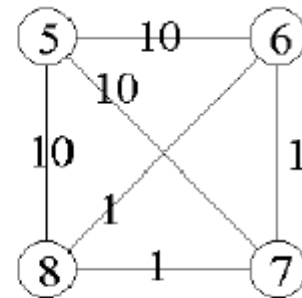
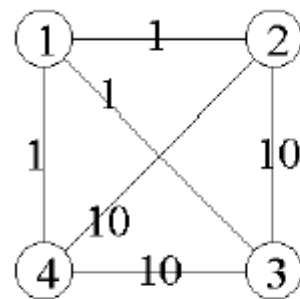
$$W(S) = \sum_{i \in S} w_S(i).$$





Assigning Node Weights / 2

Intuitively, $w_S(i)$ gives us a measure of the overall similarity between vertex i and the vertices of $S \setminus \{i\}$ with respect to the overall similarity among the vertices in $S \setminus \{i\}$.



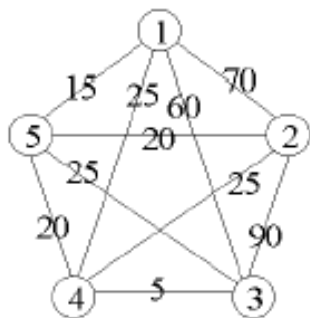
$$w_{\{1,2,3,4\}}(1) < 0 \text{ and } w_{\{5,6,7,8\}}(5) > 0.$$



Dominant Sets

A non-empty subset of vertices $S \subseteq V$ such that $W(T) > 0$ for any non-empty $T \subseteq S$, is said to be **dominant** if:

1. $w_S(i) > 0$, for all $i \in S$ (internal homogeneity)
2. $w_{S \cup \{i\}}(i) < 0$, for all $i \notin S$ (external inhomogeneity)



Dominant sets \equiv clusters

The set $\{1, 2, 3\}$ is dominant.

For 0/1 matrices: dominant sets \equiv (strictly) maximal cliques



From Dominant Sets to Local Optima (and Back) / 1

Given an edge-weighted graph $G = (V, E, w)$ and its weighted adjacency matrix A , consider the following **Standard Quadratic Program (StQP)**:

$$\begin{array}{ll} \text{maximize} & f(\mathbf{x}) = \mathbf{x}'A\mathbf{x} \\ \text{subject to} & \mathbf{x} \in \Delta \end{array}$$

where

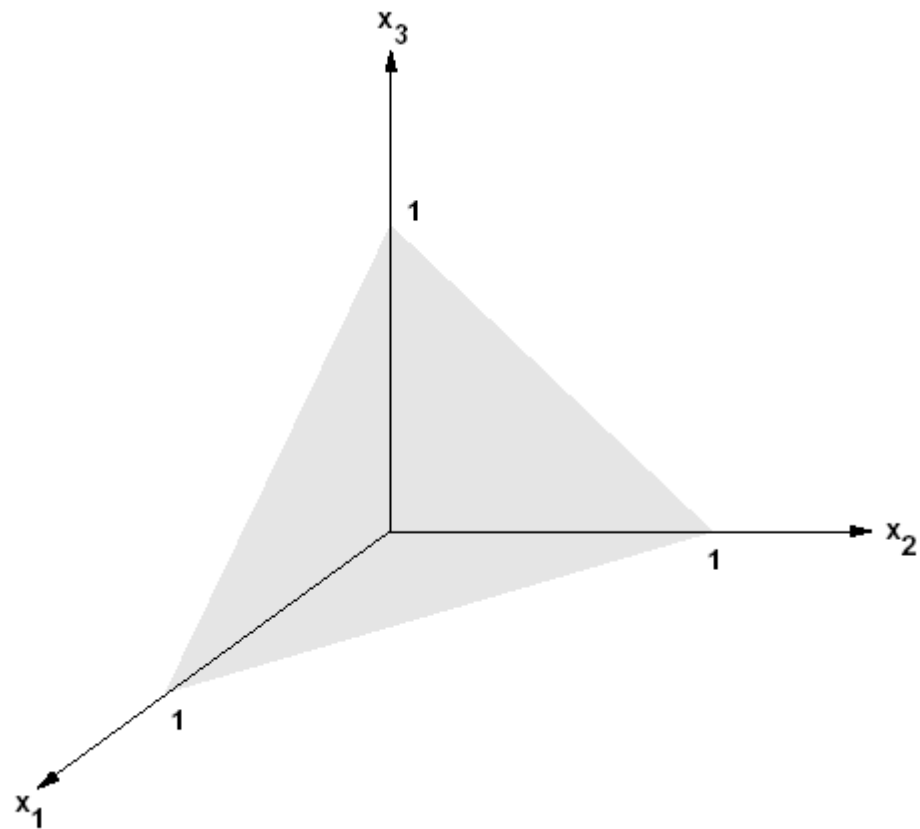
$$\Delta = \left\{ \mathbf{x} \in \mathbf{R}^n : \mathbf{e}'\mathbf{x} = 1 \text{ and } x_i \geq 0 \forall i \in V \right\}$$

is the standard simplex of \mathbf{R}^n and $\mathbf{e} = (1, 1, \dots, 1)'$.

Note. Other approaches to clustering lead to similar quadratic optimization problems (e.g., Sarkar and Boyer, 1998).



The Standard Simplex (when $n = 3$)





From Dominant Sets to Local Optima (and Back) / 2

Theorem *If S is a dominant subset of vertices, then its weighted characteristics vector \mathbf{x}^S , defined as*

$$x_i^S = \begin{cases} \frac{w_S(i)}{W(S)}, & \text{if } i \in S \\ 0, & \text{otherwise} \end{cases}$$

is a strict local maximizer of f in Δ .

Conversely, if \mathbf{x}^ is a strict local maximizer of f in Δ then its support*

$$\sigma = \sigma(\mathbf{x}^*) \doteq \{i \in V : x_i^* \neq 0\}$$

is a dominant set, provided that $w_{\sigma \cup \{i\}}(i) \neq 0$ for all $i \notin \sigma$.

Generalization of Motzkin-Straus theorem from graph theory



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Replicator Equations

Developed in evolutionary game theory to model the evolution of behavior in animal conflicts (Hofbauer & Sigmund, 1998).

Let $W = (w_{ij})$ be a non-negative real-valued $n \times n$ matrix.

Continuous-time version:

$$\frac{d}{dt}x_i(t) = x_i(t) \left[(W\mathbf{x}(t))_i - \mathbf{x}(t)'W\mathbf{x}(t) \right]$$

Discrete-time version:

$$x_i(t+1) = x_i(t) \frac{(W\mathbf{x}(t))_i}{\mathbf{x}(t)'W\mathbf{x}(t)}$$

Δ is invariant under both dynamics, and they have the same stationary points.



The Fundamental Theorem of Natural Selection

If $W = W'$, then the function

$$F(\mathbf{x}) = \mathbf{x}'W\mathbf{x}$$

is strictly increasing along any non-constant trajectory of both continuous-time and discrete-time replicator dynamics.

In other words, $\forall t \geq 0$:

$$\frac{d}{dt}F(\mathbf{x}(t)) > 0$$

for the continuous-time dynamics, and

$$F(\mathbf{x}(t + 1)) > F(\mathbf{x}(t))$$

for the discrete-time dynamics, unless $\mathbf{x}(t)$ is a stationary point.



Grouping by Replicator Equations

Let A denote the weighted adjacency matrix of the similarity graph.

Let

$$W = A \quad (= W' \geq 0) .$$

The replicator systems, starting from an arbitrary initial state, will eventually converge to a maximizer of the function $f(\mathbf{x}) = \mathbf{x}' A \mathbf{x}$, over the simplex.

This will correspond to a dominant set in the graph, and hence to a cluster of vertices.



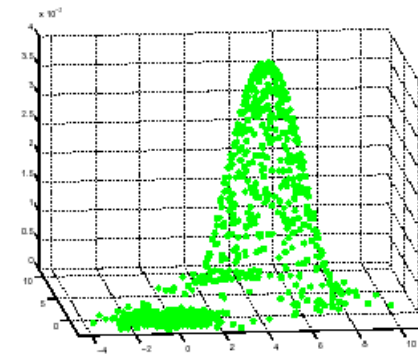
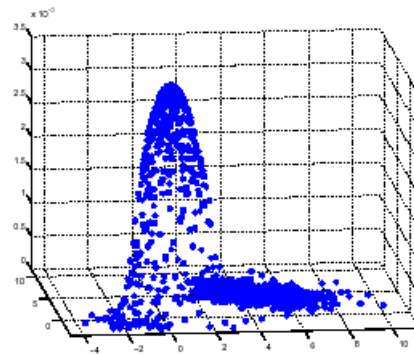
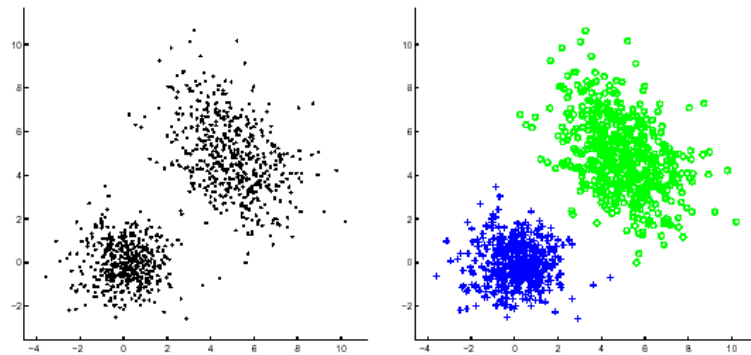
A MATLAB Implementation

```
distance=inf;
while distance>epsilon
    old_x=x;
    x = x.*(A*x);
    x = x./sum(x);
    distance=pdist([x,old_x]');
end
```



Characteristic Vectors

Note. The components of the weighted characteristic vectors give us a measure of the participation of the corresponding vertices in the cluster, while the value of the objective function provides a measure of the cohesiveness of the cluster (*cfr.* Sarkar and Boyer, 1998).





Separating Structure for Clutter

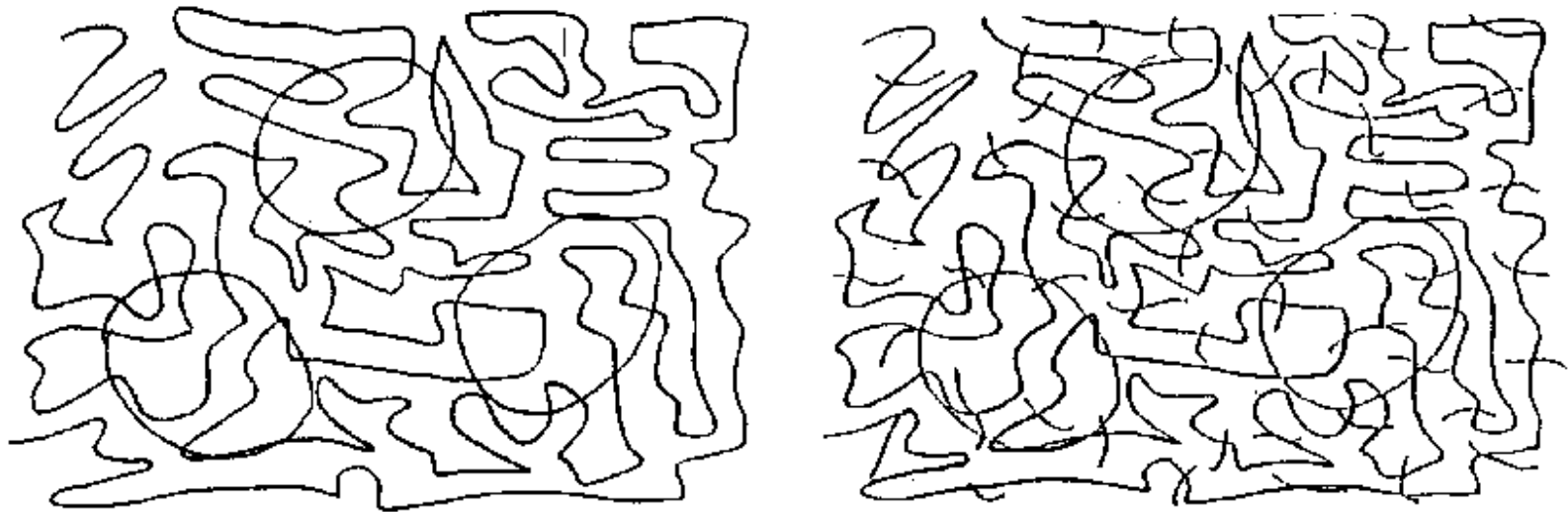


Figure 1a. Three prominent blobs are perceived immediately and with little effort. Locally, the blobs are similar to the background contours. (adopted from Mahoney (1986))

Figure 1b. Intersections were added to illustrate that the blobs are not distinguished by virtue of their intersections with the background curves.



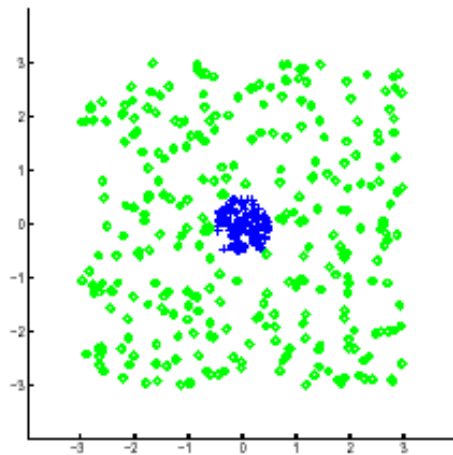
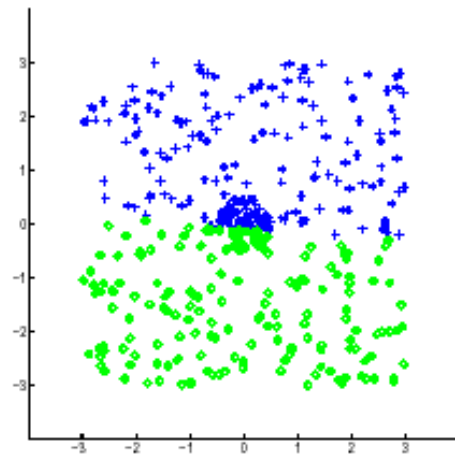
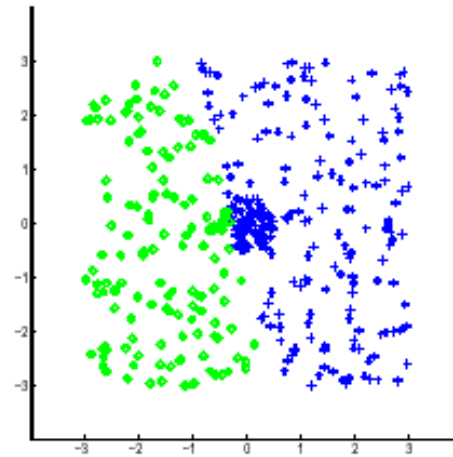
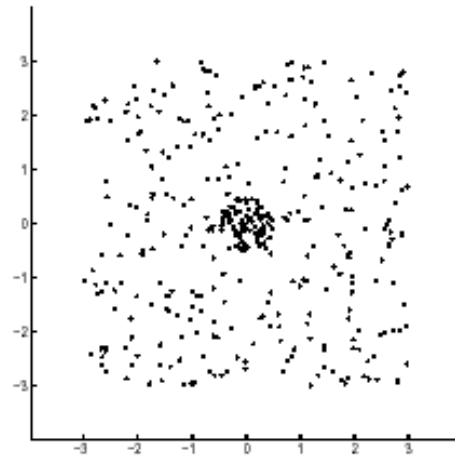
Figure 2. A circle in a background of 200 randomly placed and oriented segments. The circle is still perceived immediately although its contour is fragmented.

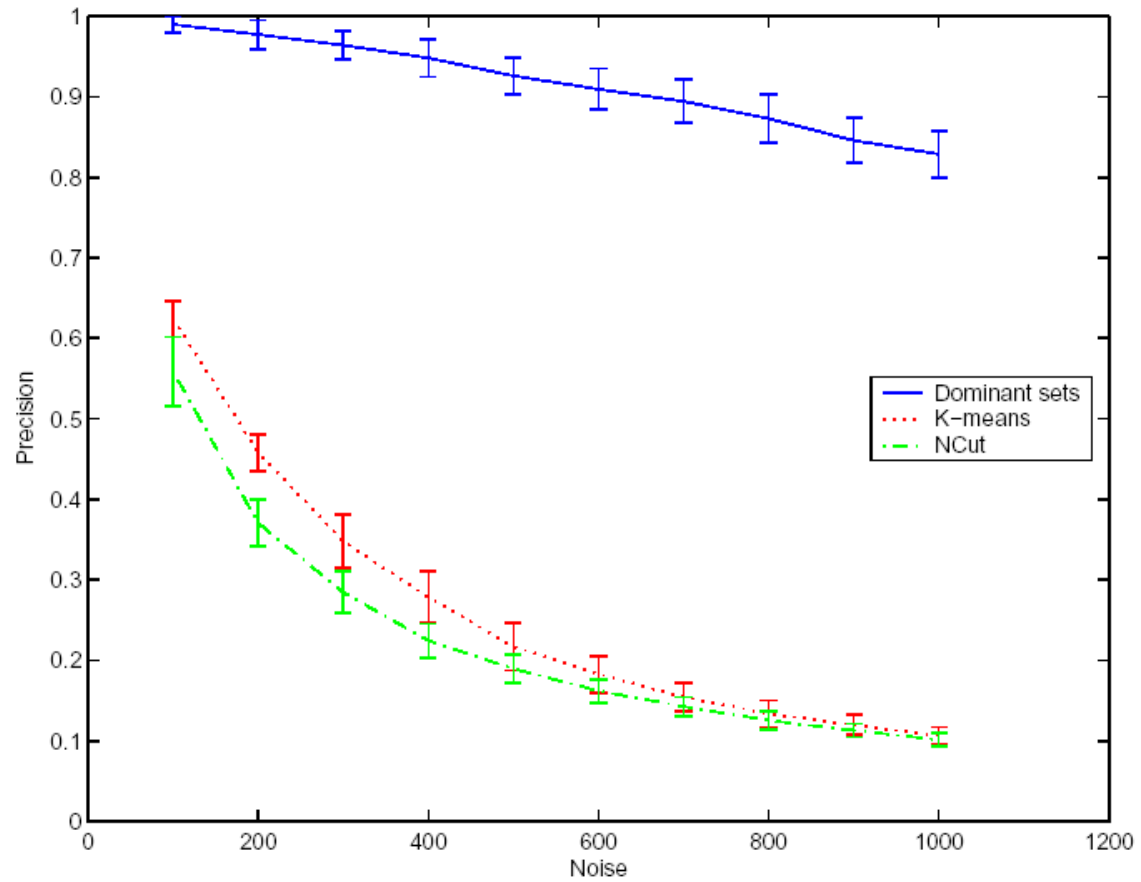


Figure 3. An edge image of a car in a cluttered background. Our attention is drawn immediately to the region of interest. It seems that the car need not be recognized to attract our attention. The car also remains salient when parallel lines and small blobs are removed, and when the less textured region surrounding parts of the car is filled in with more texture.



Separating Structure from Clutter







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Image Segmentation

Image segmentation problem:

Decompose a given image into *segments*, i.e. regions containing “similar” pixels.

First step in many
computer vision problems



Example: Segments might be regions of the image depicting the same object.

Semantics Problem: *How should we infer objects from segments?*



Image Segmentation

An image is represented as an edge-weighted undirected graph, where vertices correspond to individual pixels and the edge-weights reflect the “similarity” between pairs of vertices.

Our clustering algorithm basically consists of iteratively finding a dominant set in the graph using replicator dynamics and then removing it from the graph, until all vertices have been clustered.

On average, the algorithm took only a few seconds to converge, on a machine equipped with a 750 MHz Intel Pentium III.



Experimental Setup

The similarity between pixels i and j was measured by:

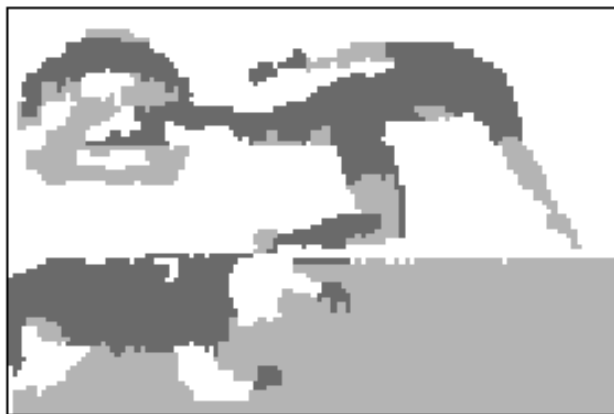
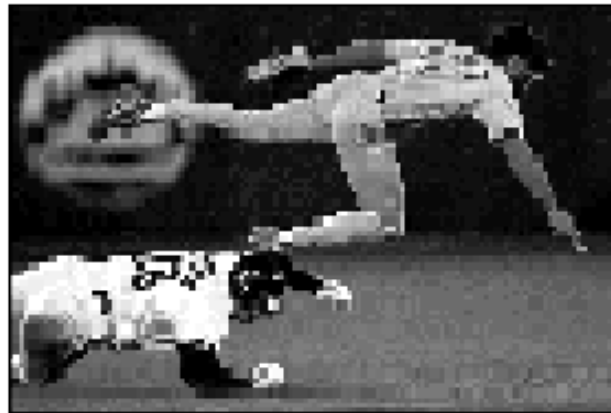
$$w(i, j) = \exp\left(\frac{-\|\mathbf{F}(i) - \mathbf{F}(j)\|_2^2}{\sigma^2}\right)$$

where σ is a positive real number which affects the decreasing rate of w , and:

- $\mathbf{F}(i) \equiv$ (normalized) intensity of pixel i , for **intensity segmentation**
- $\mathbf{F}(i) = [v, vs \sin(h), vs \cos(h)](i)$, where h, s, v are the HSV values of pixel i , for **color segmentation**
- $\mathbf{F}(i) = [|I * f_1|, \dots, |I * f_k|](i)$ is a vector based on texture information at pixel i , the f_i being DOOG filters at various scales and orientations, for **texture segmentation**



Intensity Segmentation Results



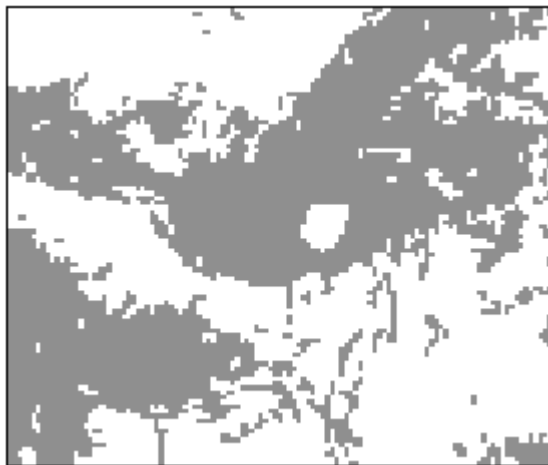
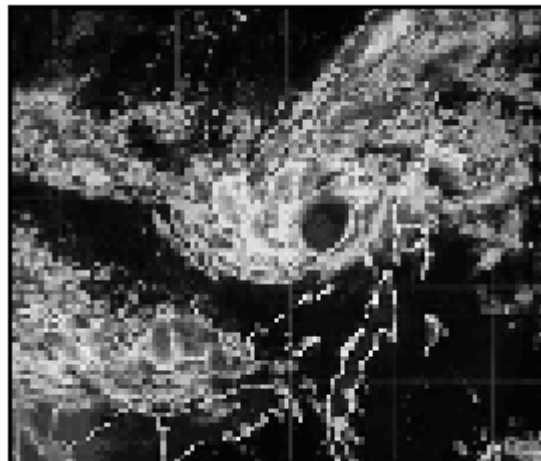
Dominant sets



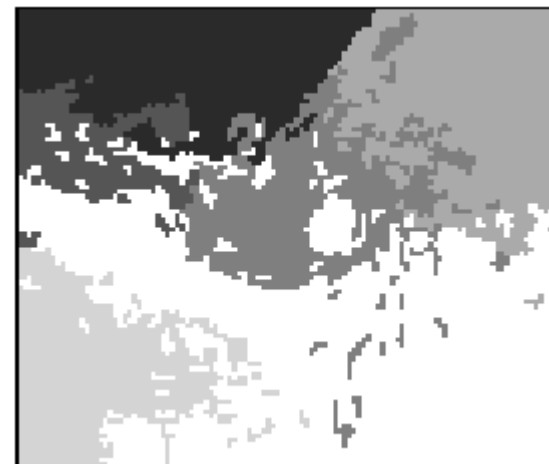
Ncut



Intensity Segmentation Results (97 x 115)



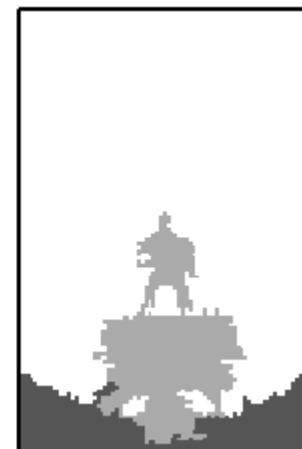
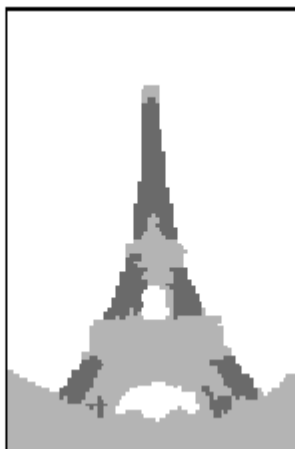
Dominant sets



Ncut



Color Segmentation Results (125 x 83)



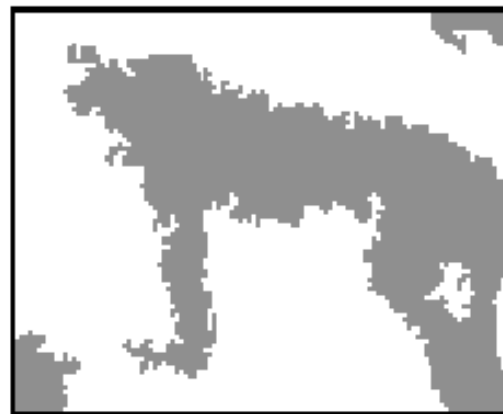
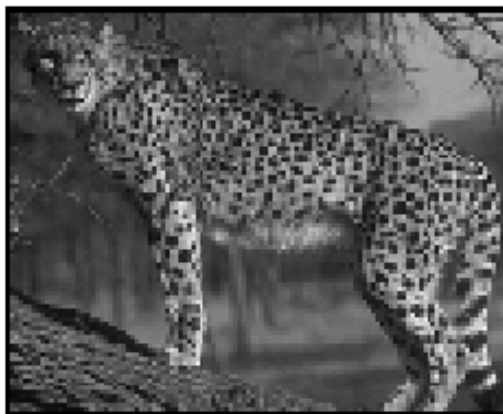
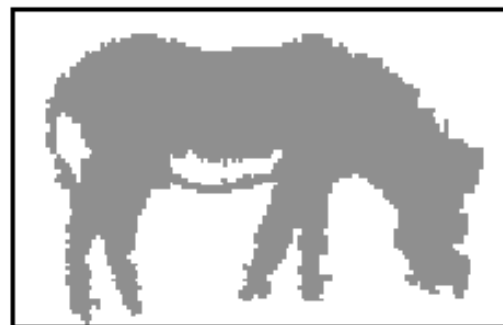
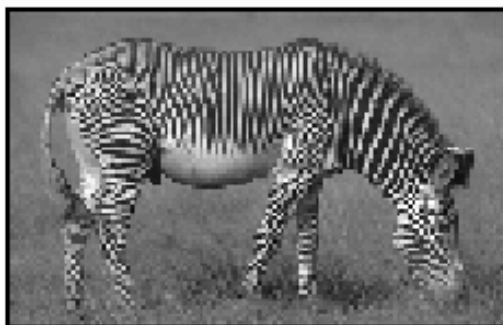
Original image

Dominant sets

Ncut



Texture Segmentation Results (approx. 90 x 120)





Ncut Results



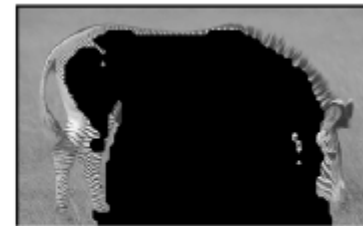
(a)



(b)



(c)



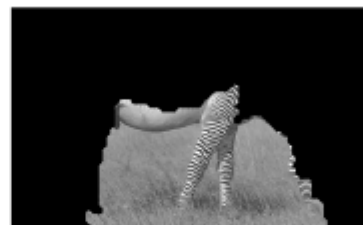
(d)



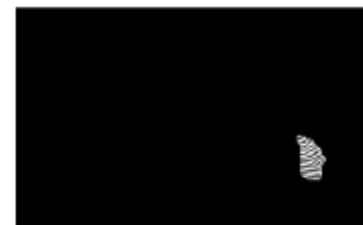
(e)



(f)



(g)



(h)



Dealing with Large Data Sets

We address the problem of grouping *out-of-sample* (i.e., unseen) examples after the clustering process has taken place.

This may serve to:

1. substantially reduce the computational burden associated to the processing of very large data sets, by extrapolating the complete grouping solution from a small number of samples,
2. deal with dynamic situations whereby data sets need to be updated continually.



Grouping Out-of-Sample Data

Recall that the sign of $w_{S \cup \{i\}}(i)$ provides an indication as to whether i is tightly or loosely coupled with the vertices in S .

Accordingly, we use the following rule for predicting cluster membership of unseen data i :

if $w_{S \cup \{i\}}(i) > 0$, then assign vertex i to cluster S .

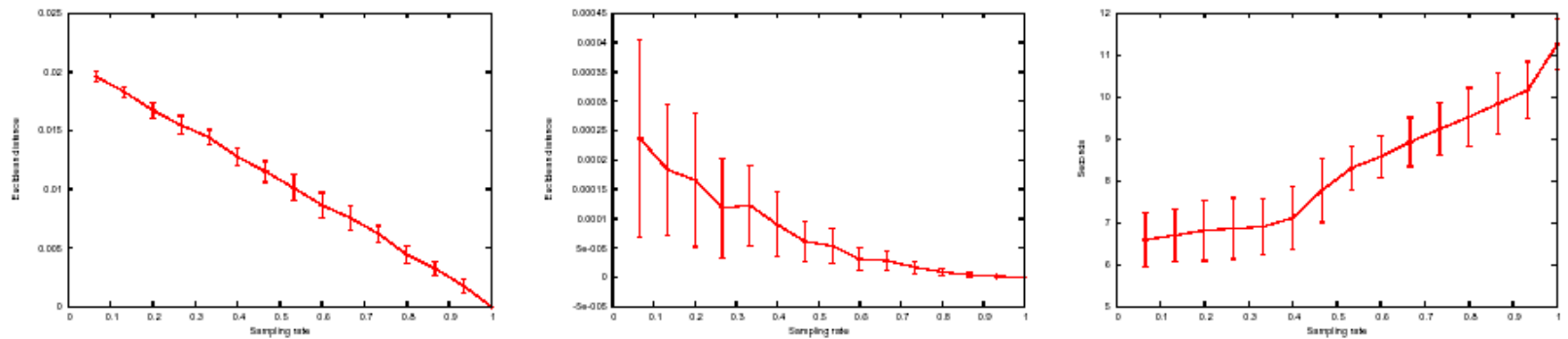


Figure 2: Evaluating the quality of our approximations on a 150-point cluster. Average distance between approximated and actual cluster membership (left) and cohesiveness (middle) as a function of sampling rate. Right: average CPU time as a function of sampling rate.

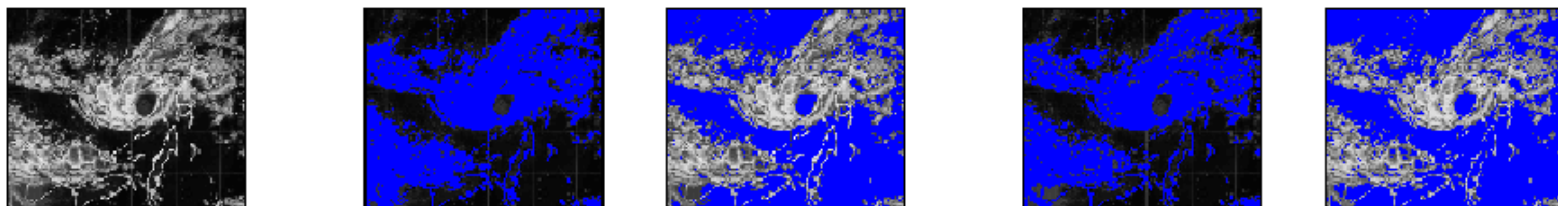


Figure 4: Segmentation results on a 115×97 weather radar image. From left to right: original image, the two regions found on the sampled image (sampling rate = 0.5%), and the two regions obtained on the whole image (sampling rate = 100%).



Results on Berkeley Database Images (321 x 481)



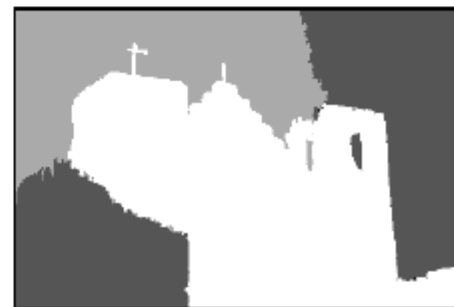
GCE = 0.05, LCE = 0.04



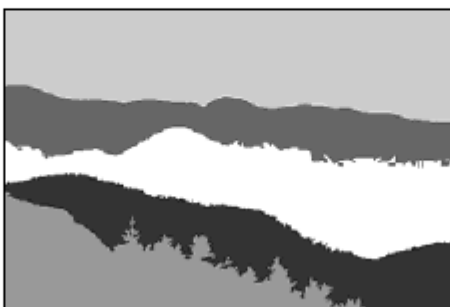
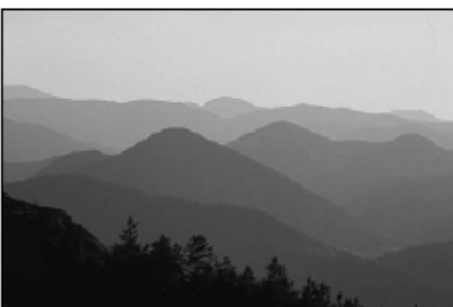
GCE = 0.08, LCE = 0.05



GCE = 0.11, LCE = 0.09



GCE = 0.36, LCE = 0.27



GCE = 0.09, LCE = 0.08



GCE = 0.31, LCE = 0.22



Results on Berkeley Database Images (321 x 481)



GCE = 0.12, LCE = 0.12



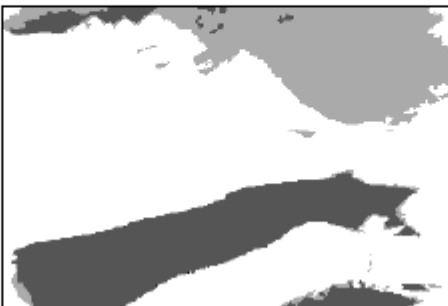
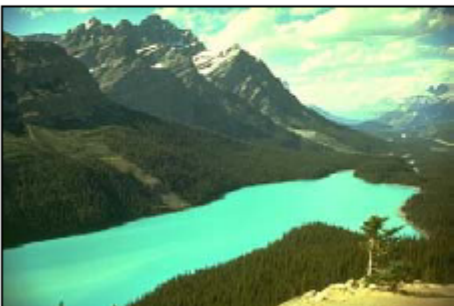
GCE = 0.19, LCE = 0.13



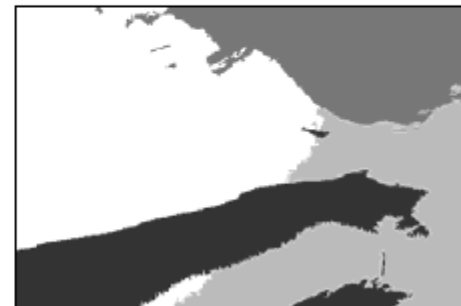
GCE = 0.31, LCE = 0.26



GCE = 0.35, LCE = 0.29



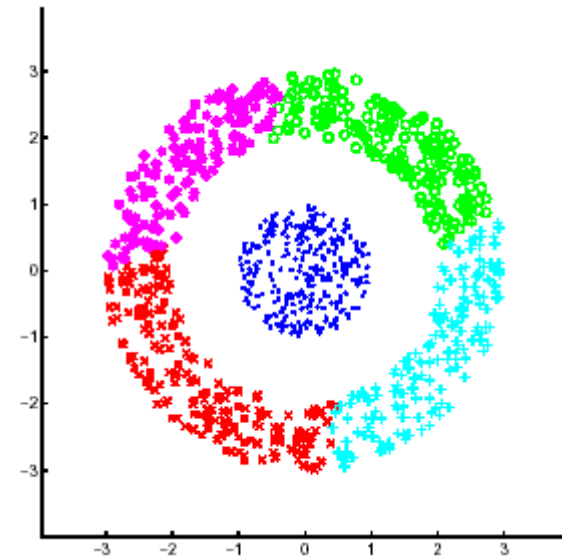
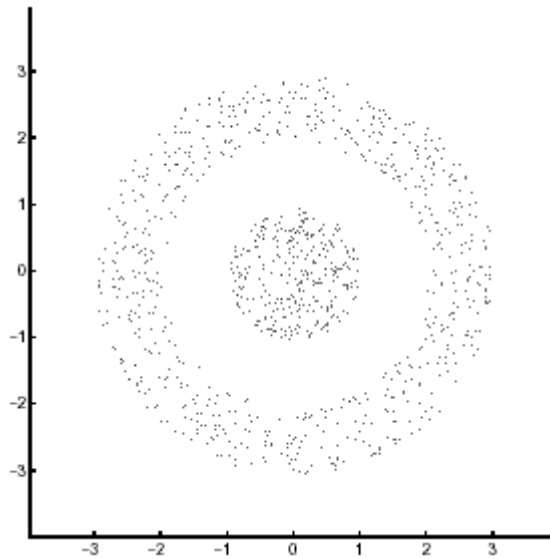
GCE = 0.09, LCE = 0.09



GCE = 0.16, LCE = 0.16

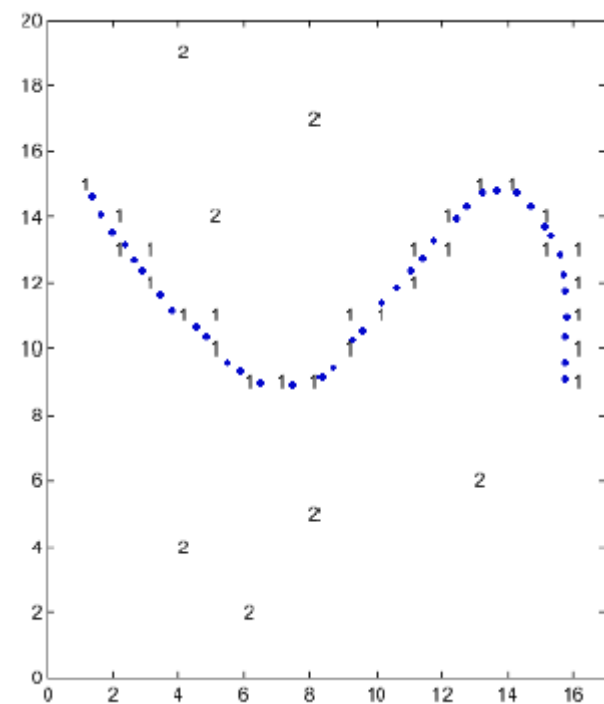
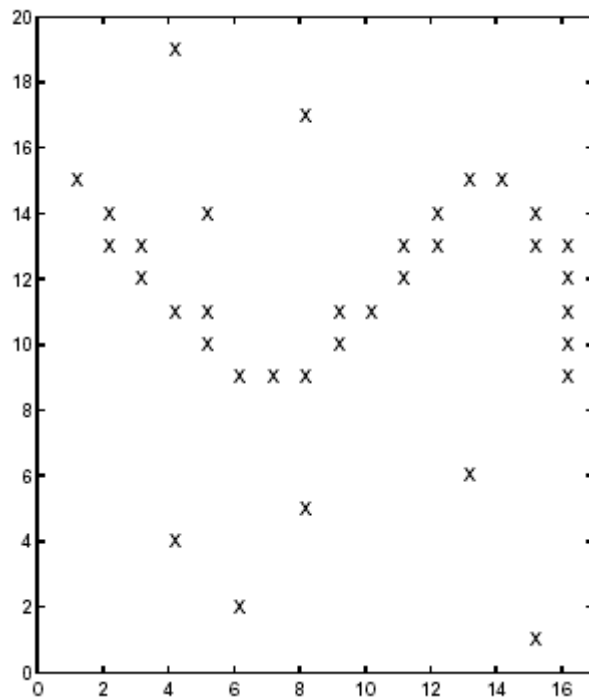


Capturing Elongated Structures / 1





Capturing Elongated Structures / 2





“Closing” the Similarity Graph

Basic idea: Transform the original similarity graph G into a “closed” version thereof (G_{closed}), whereby edge-weights take into account chained (path-based) structures.

Unweighted (0/1) case:

$$G_{\text{closed}} = \text{Transitive Closure of } G$$

Note: G_{closed} can be obtained from:

$$A + A^2 + \dots + A^n$$



Weighted Closure of G

Observation: When G is weighted, the ij -entry of A^k represents the sum of the total weights on the paths of length k between vertices i and j .

Hence, our choice is:

$$A_{\text{closed}} = A + A^2 + \dots + A^n$$



Example: Without Closure ($\sigma = 2$)

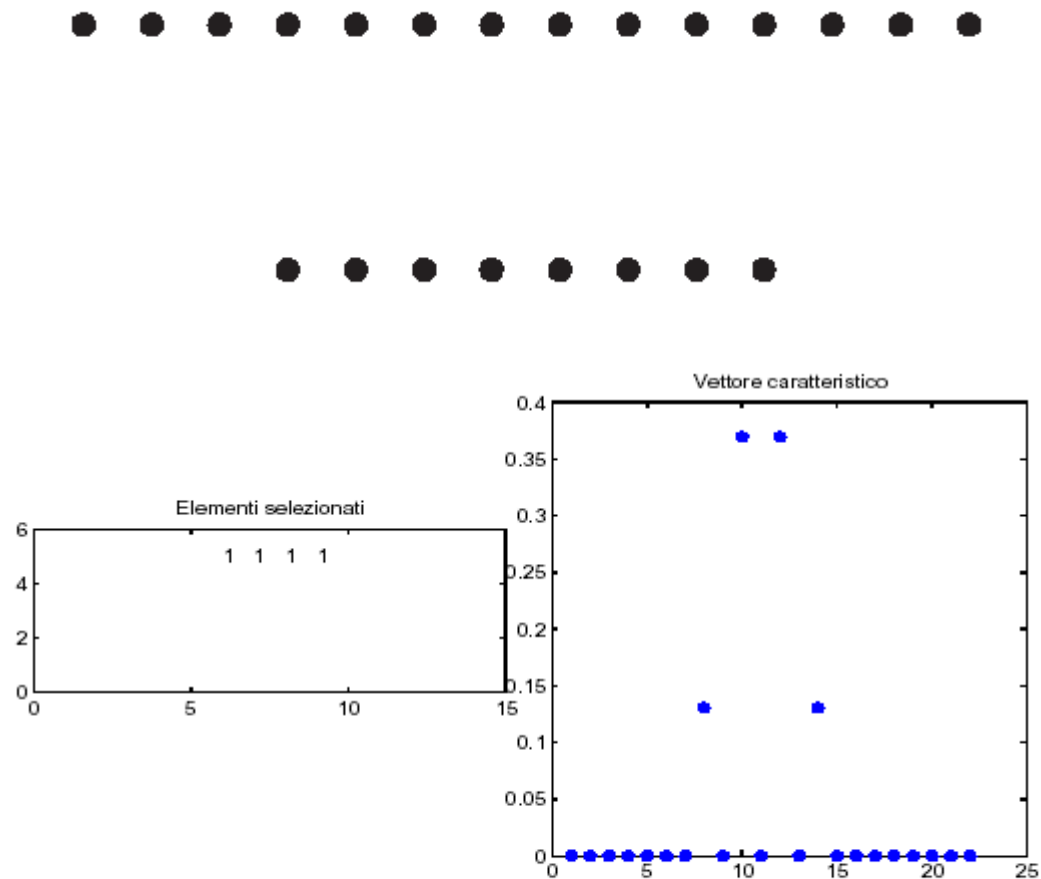


Figura 4.11: Cluster senza chiusura: $\sigma = 2$



Example: Without Closure ($\sigma = 4$)

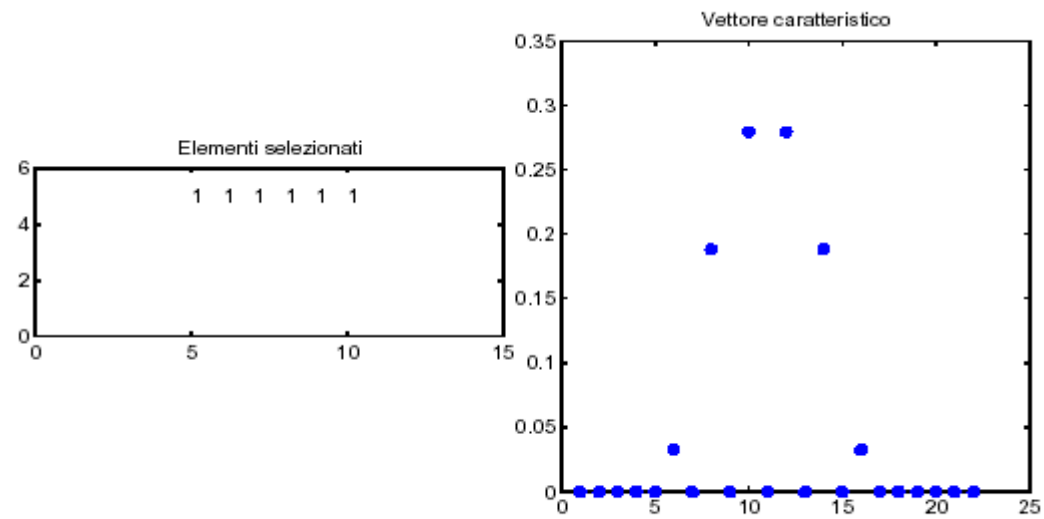
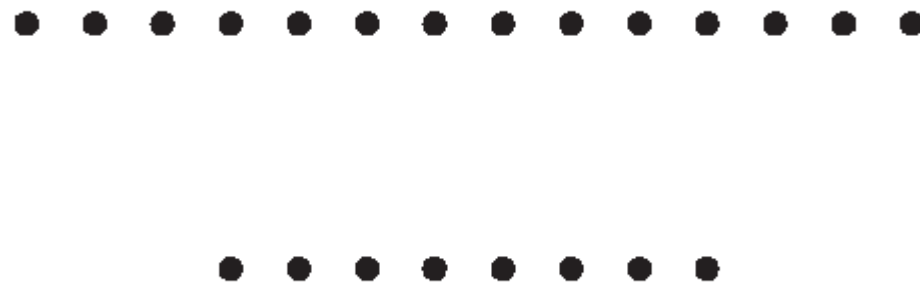


Figura 4.12: Cluster senza chiusura: $\sigma = 4$



Example: Without Closure ($\sigma = 8$)

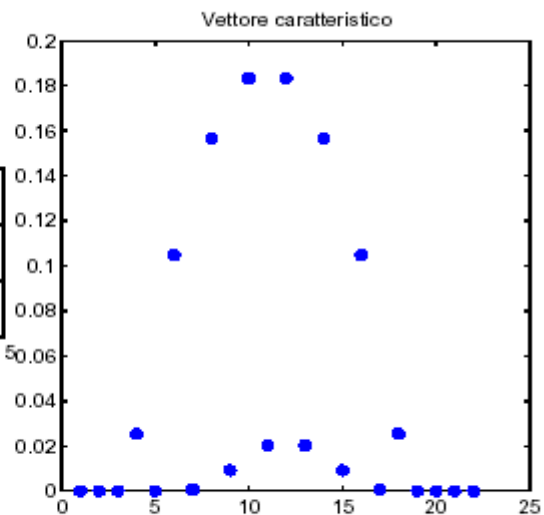
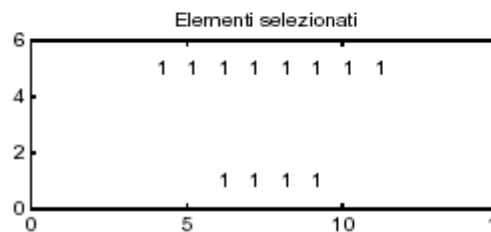


Figura 4.13: Cluster senza chiusura: $\sigma = 8$



Example: With Closure ($\sigma = 0.5$)

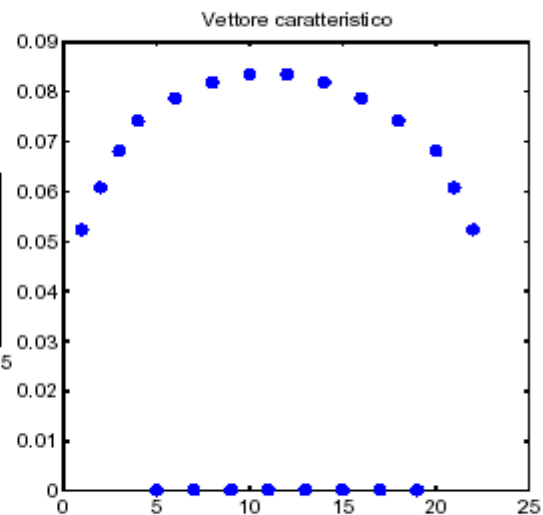
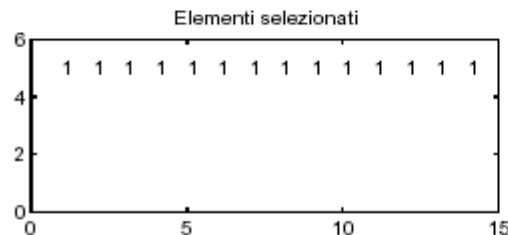
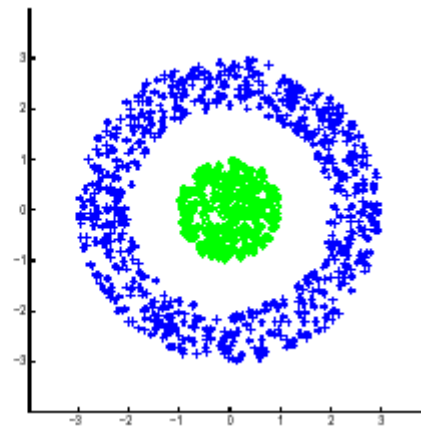
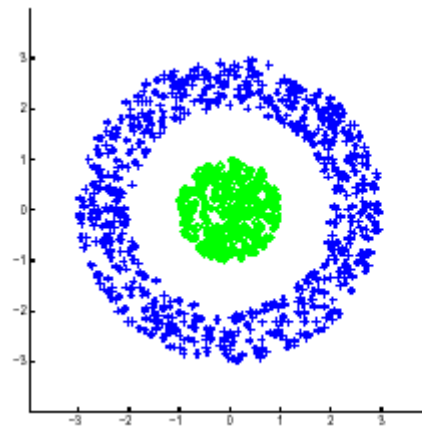
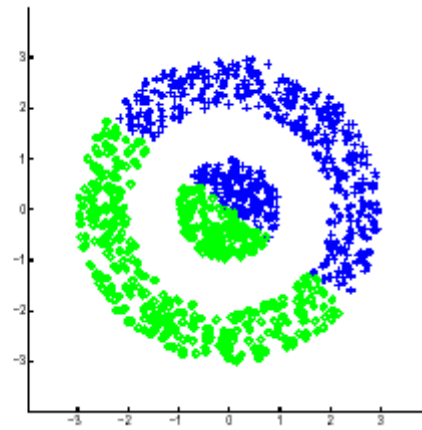
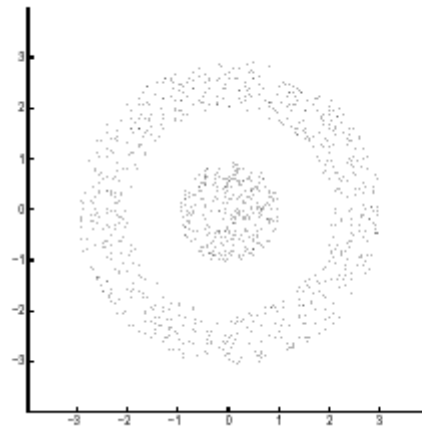


Figura 4.14: Cluster mediante chiusura: $\sigma = 0,5$





Grouping Edge Elements

Here, the elements to be grouped are **edgels** (edge elements).

We used Herault/Horaud (1993) similarities, which combine the following four terms:

1. Co-circularity
2. Smoothness
3. Proximity
4. Contrast

Comparison with Mean-Field Annealing (MFA).

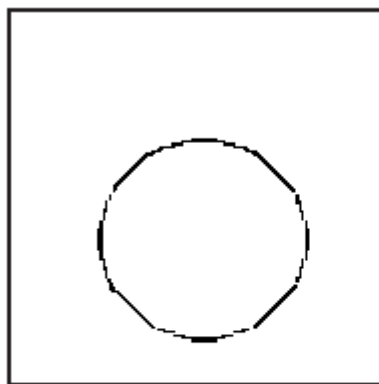


Immagine originale
204 edge

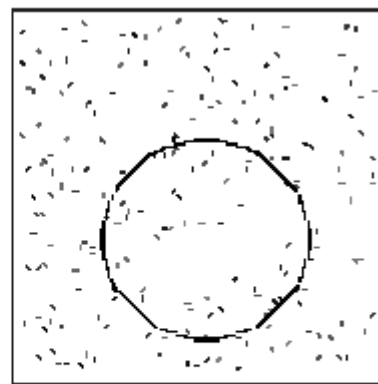
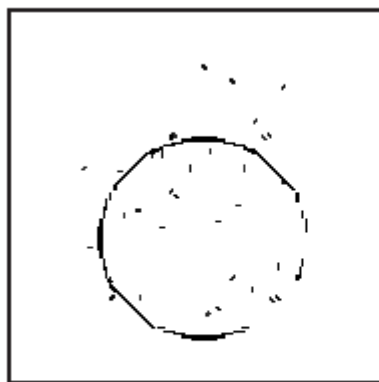
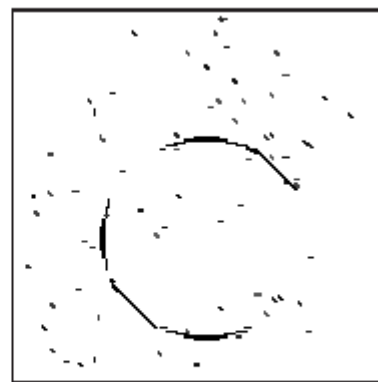


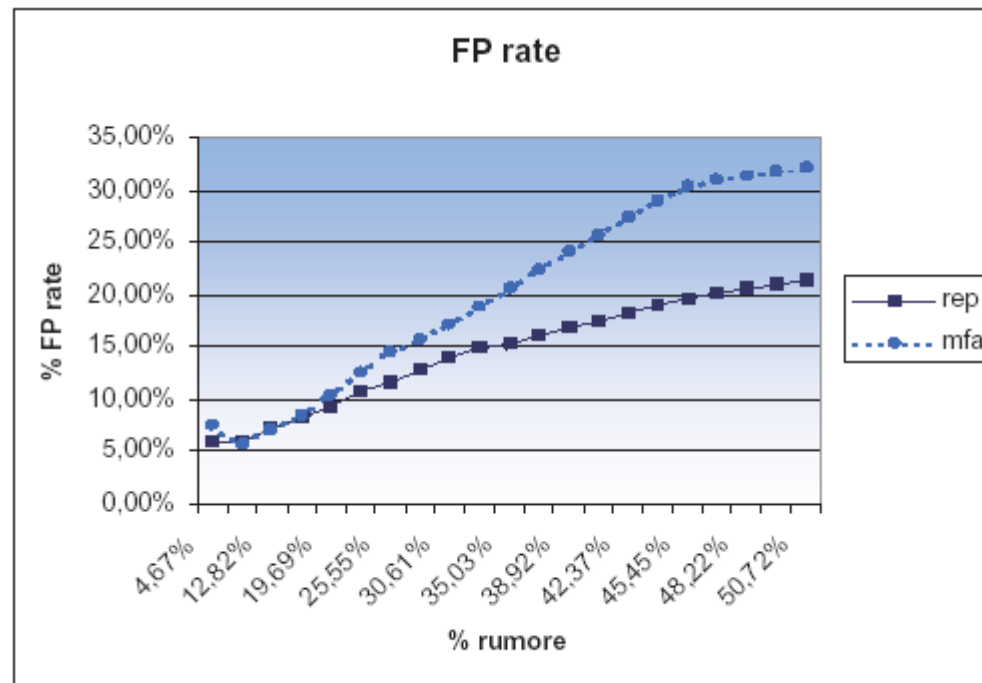
Immagine con rumore al 50%



Insiemi dominanti
FP rate: 16,67%



Mean Field Annealing
FP rate: 34, 31%



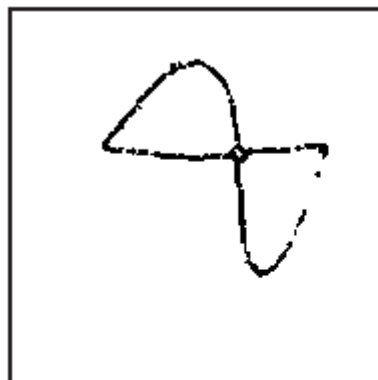


Immagine originale
278 edge

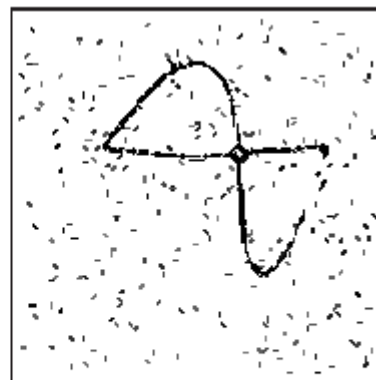
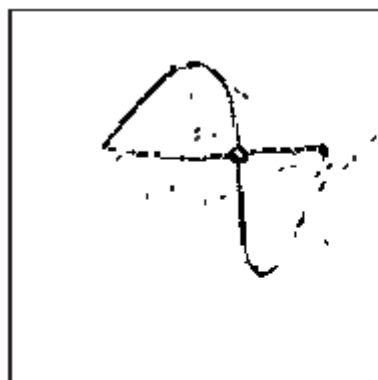
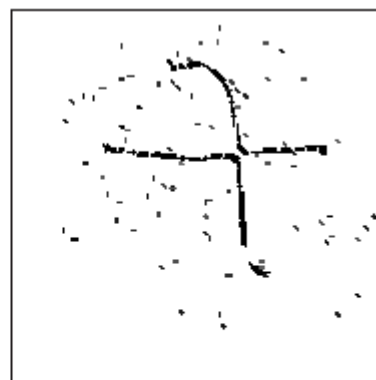


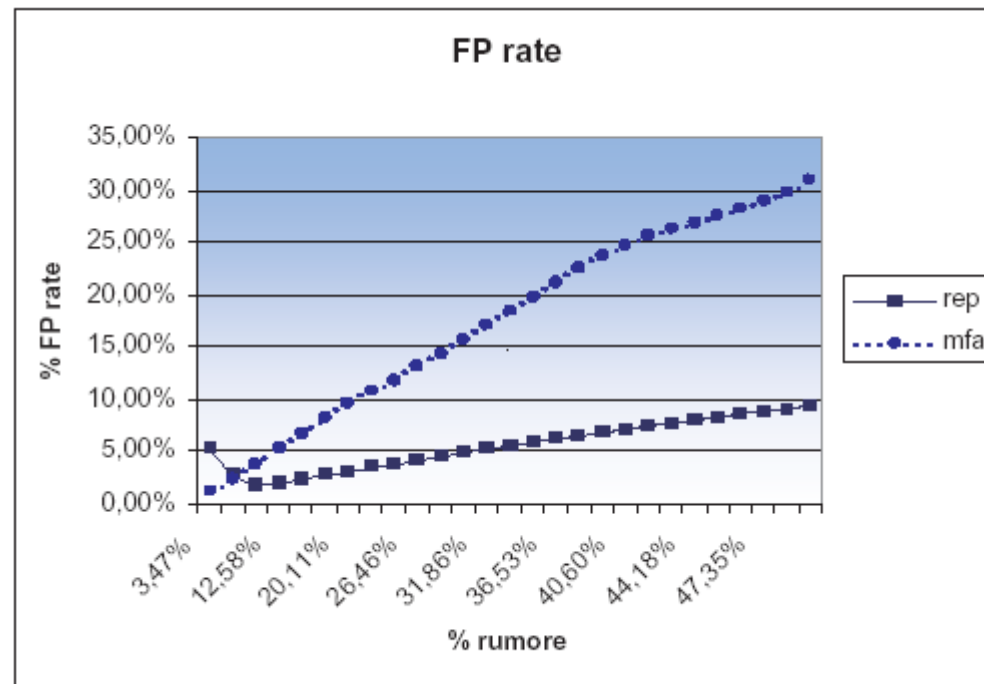
Immagine con rumore al 50%



Insiemi dominanti
FP rate: 8,99%



Mean Field Annealing
FP rate: 29,5%





Talk's Outline

- Dominant sets and their characterization
- Evolutionary game dynamics for clustering
- Experiments on intensity/color/texture image segmentation
- **Extension of the framework to hierarchical clustering**
- Experiments on the (hierarchical) organization of an image database



Building a Hierarchy: A Family of Quadratic Programs

Consider the following family of StQP's:

$$\begin{array}{ll} \text{maximize} & f_\alpha(\mathbf{x}) = \mathbf{x}'(A - \alpha I)\mathbf{x} \\ \text{subject to} & \mathbf{x} \in \Delta \end{array}$$

where $\alpha \geq 0$ is a parameter and I is the identity matrix.

The objective function f_α consists of:

- a **data term** ($\mathbf{x}'A\mathbf{x}$) which favors solutions with high internal coherency
- a **regularization term** ($-\alpha\mathbf{x}'\mathbf{x}$) which acts as an entropic factor: it is concave and, on the simplex Δ , it is maximized at the barycenter and it attains its minimum value at the vertices of Δ



An Observation

The solutions of the StQP remain the same if the matrix $A - \alpha I$ is replaced with $A - \alpha I + \kappa ee'$, where κ is an arbitrary constant, since

$$\mathbf{x}'(A - \alpha I + \kappa ee')\mathbf{x} = \mathbf{x}'(A - \alpha I)\mathbf{x} + \kappa$$

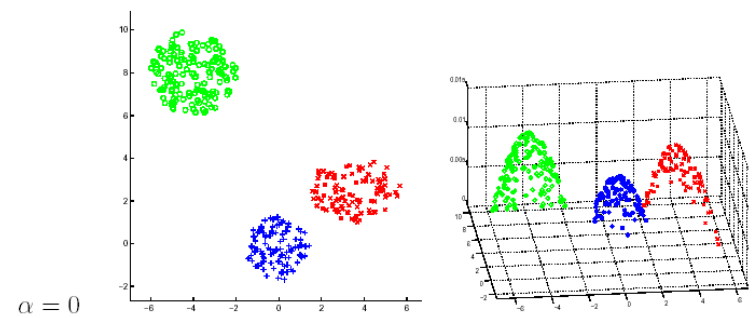
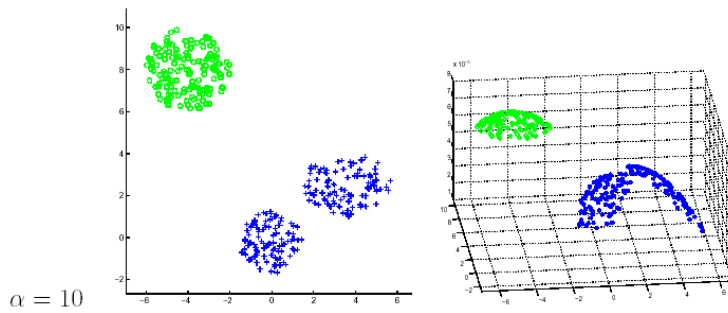
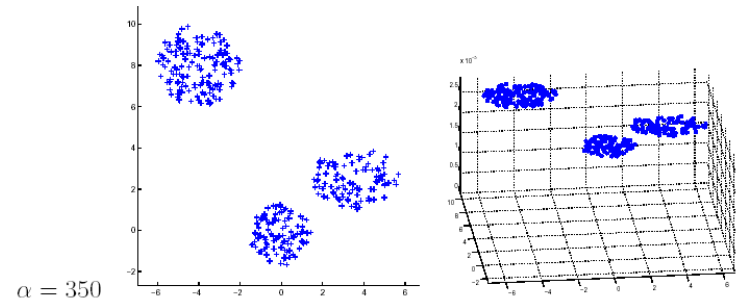
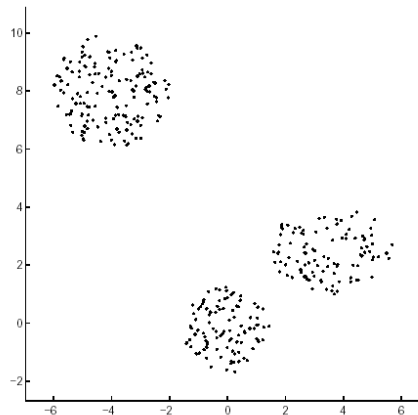
for all $\mathbf{x} \in \Delta$.

In particular, if $\kappa = \alpha$ the resulting matrix is nonnegative and has a null diagonal.

Hence all (strict) solutions of the StQP correspond to dominant sets for the scaled similarity matrix $A + \alpha(ee' - I)$ having the off-diagonal entries equal to $a_{ij} + \alpha$.



The effects of α





Bounds for the Regularization Parameter / 1

When α is large enough the regularization term $(-\alpha \mathbf{x}'\mathbf{x})$ dominates, and the only solution of the StQP is in the interior of Δ : this corresponds to a unique large cluster which comprises all the data points.

Proposition *If*

$$\alpha > \lambda_{\max}(A)$$

then f_α is a strictly concave function in \mathbb{R}^n , and the only solution \mathbf{x} of the StQP belongs to the interior of Δ , i.e., $\sigma(\mathbf{x}) = V$.



Bounds for the Regularization Parameter / 2

Given a subset of vertices $S \subseteq V$, the face of Δ corresponding to S is defined as:

$$\Delta_S = \{\mathbf{x} \in \Delta : \sigma(\mathbf{x}) \subseteq S\}$$

and its relative interior is:

$$\text{int}(\Delta_S) = \{\mathbf{x} \in \Delta : \sigma(\mathbf{x}) = S\} .$$

Theorem *Let $S \subset V$ be a proper subset of vertices ($S \neq V$), and let A_S denote the submatrix of A formed by the rows and columns indexed by the elements of S . If*

$$\alpha > \lambda_{\max}(A_S)$$

then there is no point $\mathbf{x} \in \text{int}(\Delta_S)$ that is a local maximizer of f_α in Δ .



Bounds for the Regularization Parameter / 3

Suppose for simplicity that $a_{ij} \leq 1$ for all $i, j \in V$, i.e.

$$0 \leq A \leq \mathbf{e}\mathbf{e}^T - I.$$

For any $S \subseteq V$ we get:

$$\lambda_{\max}(A_S) \leq \lambda_{\max}(\mathbf{e}\mathbf{e}^T - I) = |S| - 1$$

Hence, if we want to avoid clusters of size $|S| \leq m < |V|$ we could let

$$\alpha > m - 1$$

In so doing, no face Δ_S with $|S| \leq m$ will contain solutions of the StQP, in other words:

at this scale *all* clusters will have more than m data points



The Landscape of f_α

Key observation: For any fixed α , the energy landscape of f_α is populated by two kinds of solutions:

- solutions which correspond to dominant sets for the original matrix A
- solutions which do not correspond to any dominant set for the original matrix A , although they are dominant for the scaled matrix $A + \alpha(ee' - I)$

The latter represent large subsets of points that are not sufficiently coherent to be dominant with respect to A , and hence they should be split.



Sketch of the Hierarchical Clustering Algorithm

Basic idea: start with a sufficiently large α and adaptively decrease it during the clustering process:

- 1) let α be a large positive value (e.g., $\alpha > |V| - 1$)
- 2) find a partition of the data into α -clusters
- 3) for all the α -clusters that are not 0-clusters recursively repeat step 2) with decreased α



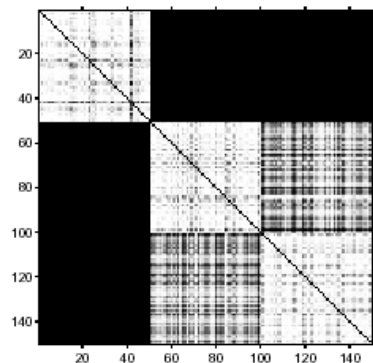
Pseudo-code of the Algorithm

```
Algorithm HIER_CLUSTERING(  $V, A$  )  
begin  
  if  $V$  is dominant then return  $V$   
  let  $\alpha > |V| - 1$   
  repeat  
    decrease  $\alpha$   
    if  $\alpha < 0$  then  $\alpha \leftarrow 0$   
     $V_1, \dots, V_k \leftarrow \text{SPLIT}( V, A, \alpha )$   
  until  $k > 1$   
  return  $\bigcup_{i=1}^k \{ \text{HIER\_CLUSTERING}( V_i, A_{V_i} ) \}$   
end
```

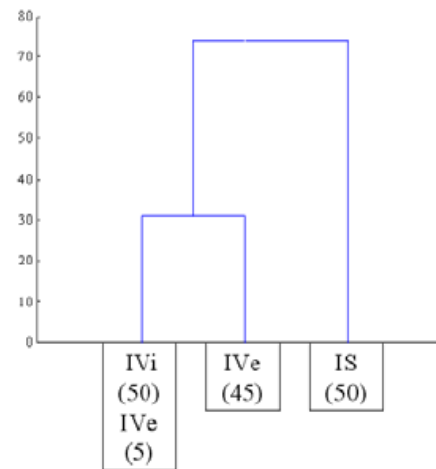


Results on the IRIS dataset / 1

This data set, attributed to Fisher (1936), is a classic benchmark in the machine learning literature. The data set contains 3 classes of 50 instances each, where each class refers to a type of iris plant. The three classes are Iris Setosa (IS), Iris Versicolour (IVe), and Iris Virginica (IVi). Each data item is a 4-dimensional real vector representing as many measurements of an Iris flower. Class IS is linearly separable from the other two (IVe and IVi), but IVe and IVi are not linearly separable.



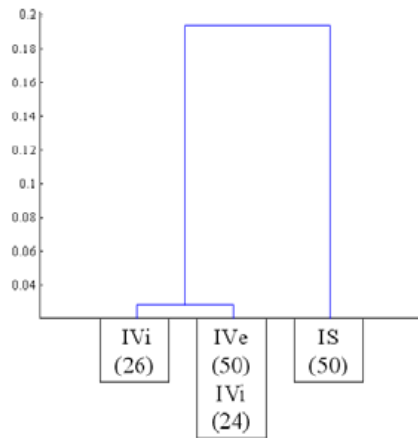
Similarity matrix



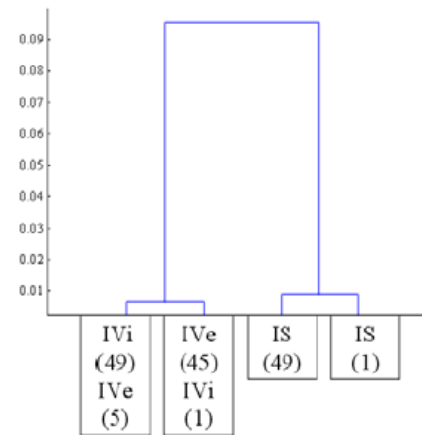
Dominant sets



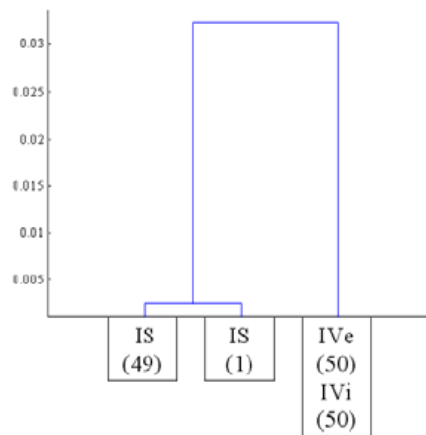
Results on the IRIS dataset / 2



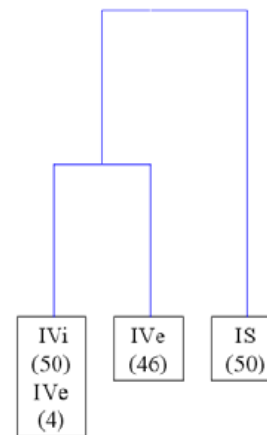
Complete-link



Average-link



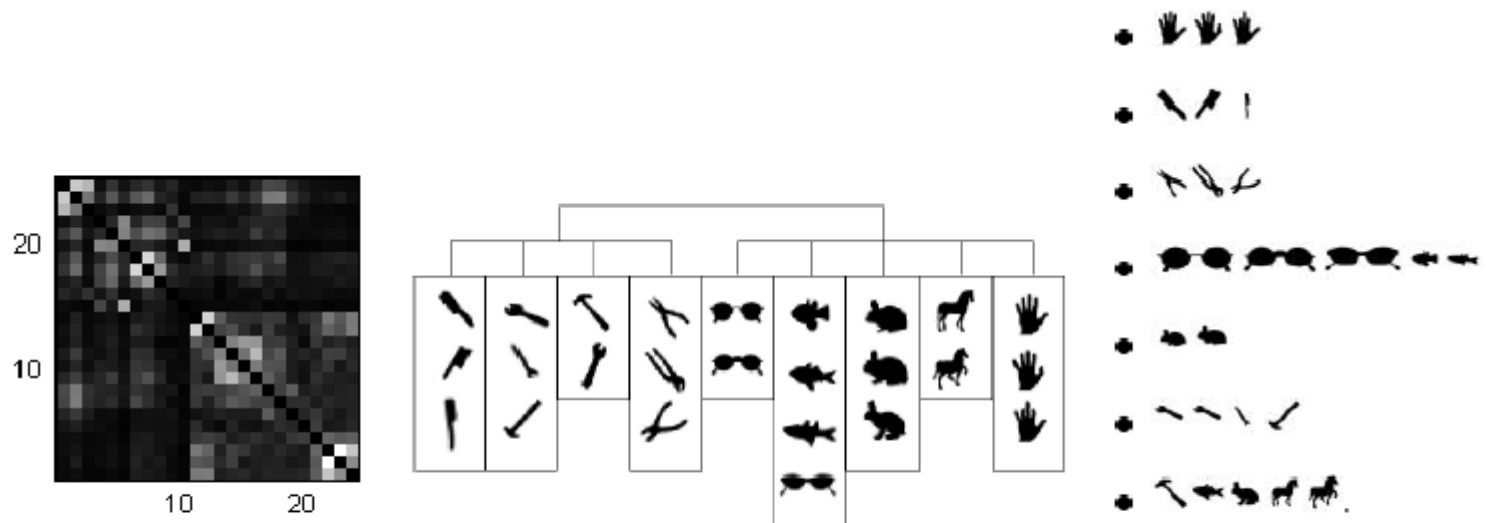
Single-link



NCut



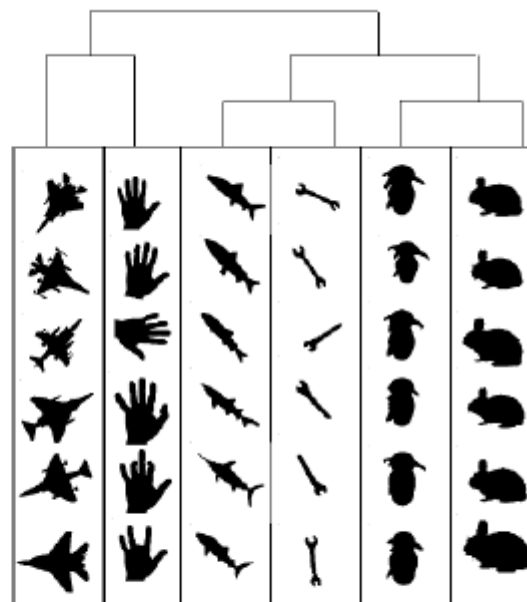
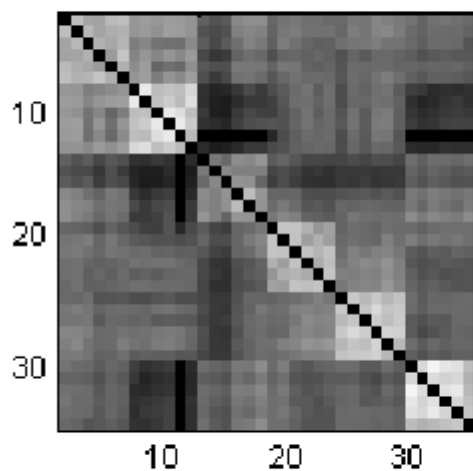
Luo and Hancock's Similarities (CVPR'01)



Left: Similarity matrix used in the experiment. Middle: Hierarchy produced by our algorithm. Right: (Flat) partition produced by Luo and Hancock.



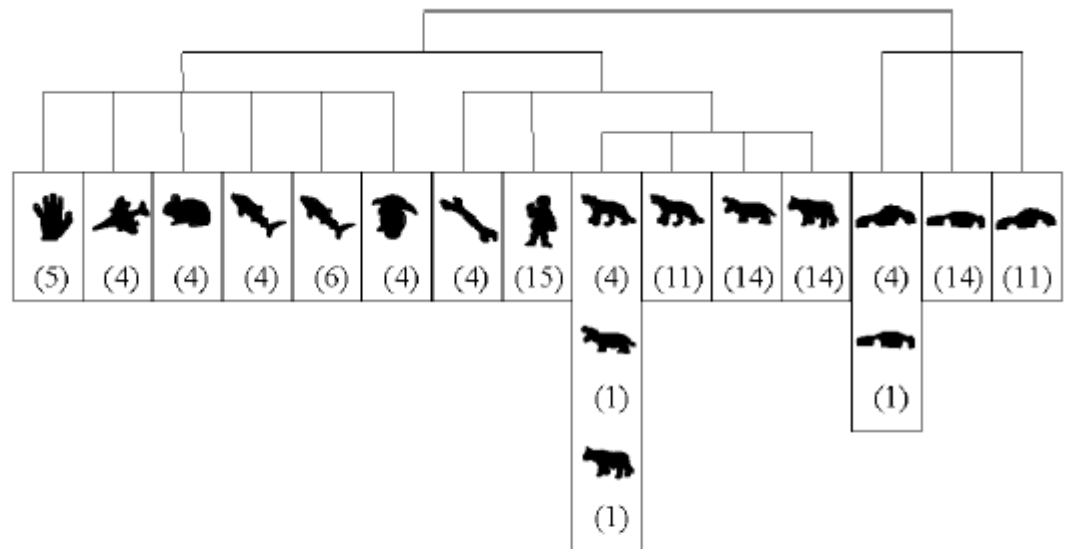
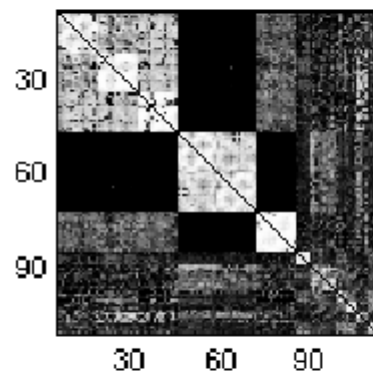
Klein and Kimia's Similarities (SODA'01)



Left: Similarity matrix used in the experiment. Right: Hierarchy produced by our algorithm.



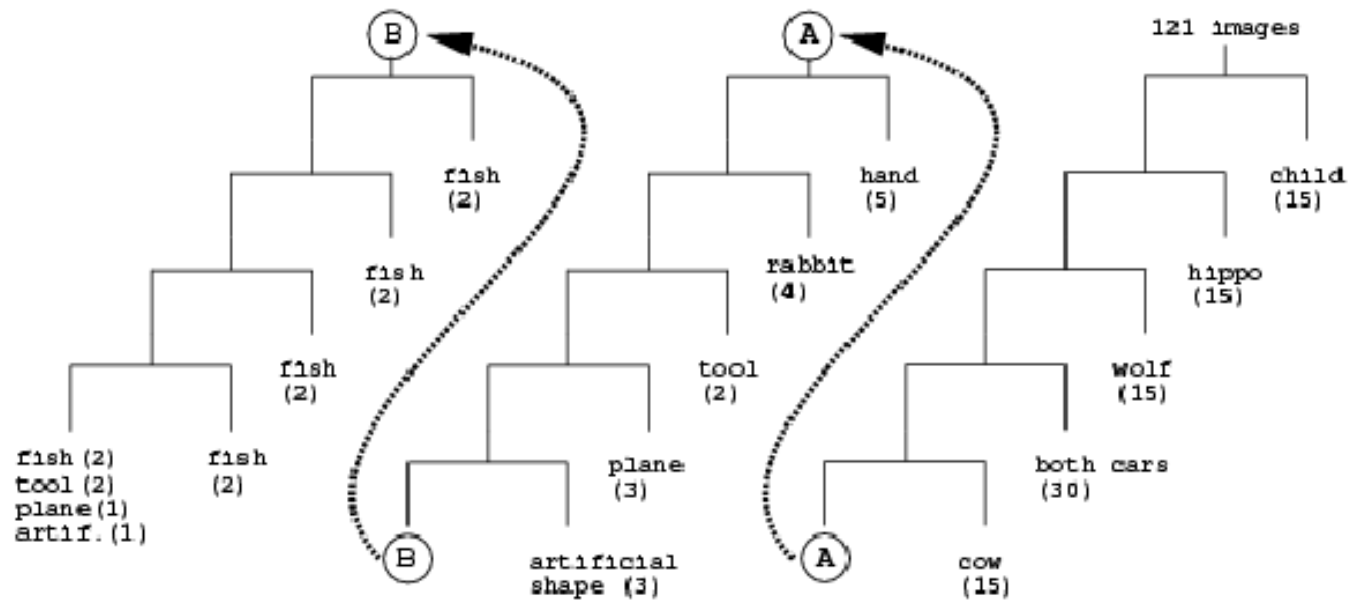
Gdalyahu and Weinshall's Similarities (PAMI 01)



Left: Similarity matrix used in the experiment (courtesy of Y. Gdalyahu). Right: Hierarchy produced by our algorithm.

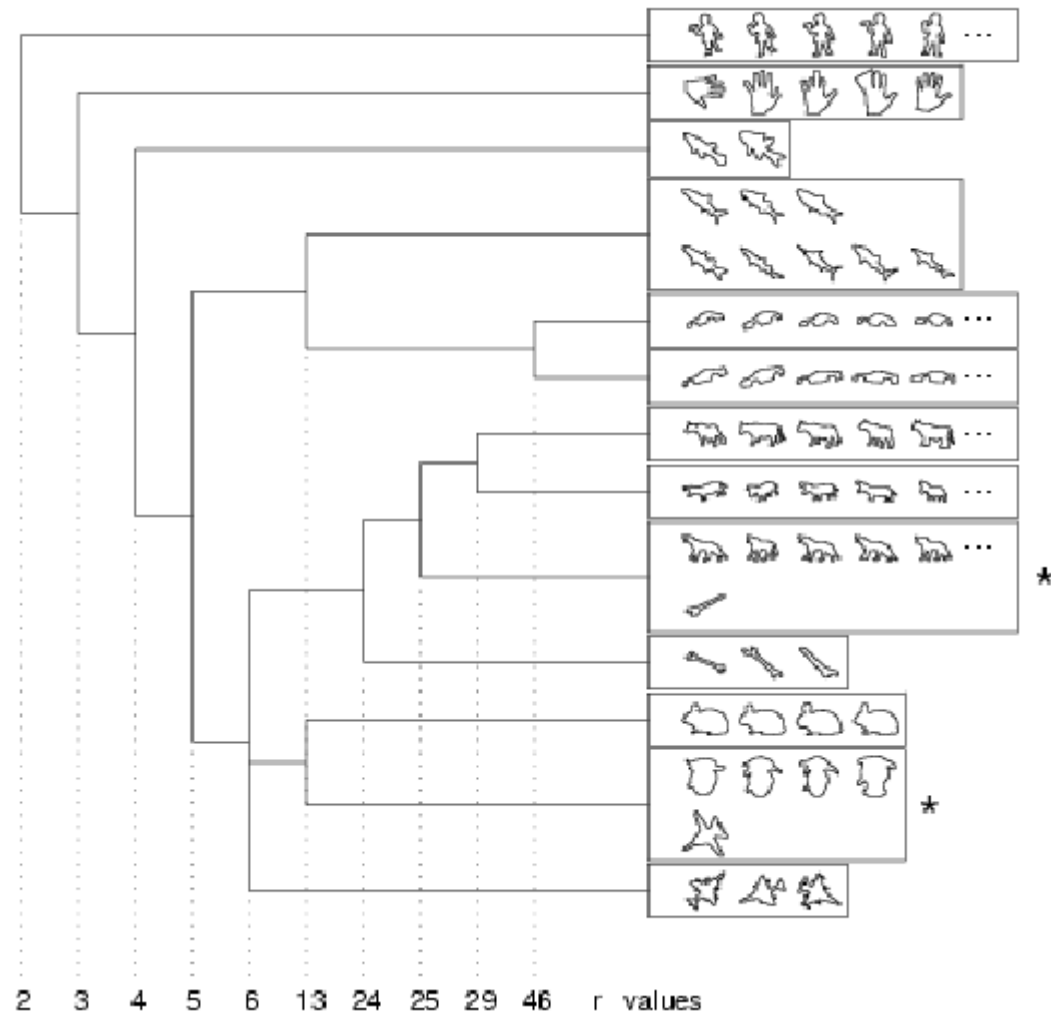


Factorization Results (Perona and Freeman, 98)





Typical-cut Results (From Gdalyahu, 1999)





Conclusions

- Introduced the notion of a **dominant set** of vertices in an edge-weighted graph, and defined a new notion of a cluster.
- Established a connection between the (combinatorial) problem of finding dominant sets and (continuous) quadratic programming.
- Used straightforward parallel dynamics from evolutionary game theory that can be coded in a few lines of MATLAB.
- Demonstrated potential of the approach on image segmentation.
- Extended the framework to hierarchical clustering
- Demonstrated its potential on the problem of organizing a shape database.



On-going and Future Projects

- Grouping with asymmetric affinities: Game theory
- Clustering on hypergraphs (high-order relations)
- Graph matching, object recognition and tracking
- Video segmentation



Other Applications of Dominant-Set Clustering

Bioinformatics

Identification of protein binding sites

R. Zauhar, M. Bruist, Univ. of Sciences Philadelphia, USA (2005)

Clustering gene expression profiles

T. Li et al, Fudan University, Hong Kong (2005)

Security and video surveillance

Detection of anomalous activities in video streams

R. Hamid et al., Georgia Institute of Tehcnology, USA (2005)

Detection of malicious activities in the internet

F. Pouget, Insitut Eurécom (2006)

Content-based image retrieval

G. Giacinto, F. Roli, University of Cagliari, Italy (2007)



References

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- M. Pavan, M. Pelillo. Dominant sets and hierarchical clustering. *Proc. IEEE International Conference on Computer Vision*, Nice, France, 2003.
- M. Pavan, M. Pelillo. Efficient out-of-sample extension of dominant-set clusters. In: *Advances in Neural Information Processing Systems 17* (MIT Press, 2005).
- A. Torsello, S. Rota Bulò, M. Pelillo. Grouping with asymmetric affinities: A game-theoretic perspective. *Proc. IEEE Computer Society Conference on Computer Vision and Pattern Recognition*, New York, NY, 2006.
- M. Pavan, M. Pelillo. Dominant sets and pairwise clustering. *IEEE Transactions on Pattern Analysis and Machine Intelligence* 29(1):167-172, 2007.