



# Clustering Gerarchico

Alberto Borghese

Università degli Studi di Milano  
Laboratorio di Sistemi Intelligenti Applicati (AIS-Lab)  
Dipartimento di Scienze dell'Informazione  
[alberto.borghese@unimi.it](mailto:alberto.borghese@unimi.it)




A.A. 2012-2013 1/51 <http:\\homes.dsi.unimi.it\\~borghese\\>




# Riassunto

**Hierarchical clustering**

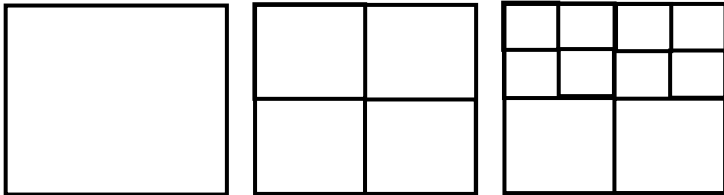
A.A. 2012-2013 2/51 <http:\\homes.dsi.unimi.it\\~borghese\\>




## Algoritmi gerarchici: QTD




- Quad Tree Decomposition;
- Suddivisione gerarchica dello spazio delle feature, mediante splitting dei cluster;
- Criterio di splitting ( $\sim$ distanza tra cluster).



A.A. 2012-2013 3/51





## Algoritmi gerarchici: QTD



- Clusterizzazione immagini RGB, 512x512;
- Pattern: pixel (x,y);
- Feature: canali R, G, B.
- Distanza tra due pattern (non euclidea):  
 $\text{dist}(p1, p2) =$   
 $\text{dist}([R1 \ G1 \ B1], [R2 \ G2 \ B2]) =$   
 $\max(|R1-R2|, |G1-G2|, |B1-B2|).$

A.A. 2012-2013 4/51

## Algoritmi gerarchici: QTD



$p1 = [0 \ 100 \ 250]$   
 $p2 = [50 \ 100 \ 200]$   
 $p3 = [255 \ 150 \ 50]$

$\text{dist}(p1, p2) = \text{dist}([R1 \ G1 \ B1], [R2 \ G2 \ B2]) =$   
 $\max(|R1-R2|, |G1-G2|, |B1-B2|) = \max([50 \ 0 \ 50]) = 50.$

$\text{dist}(p2, p3) = 205.$

$\text{dist}(p3, p1) = 255.$

A.A. 2012-2013 5/51

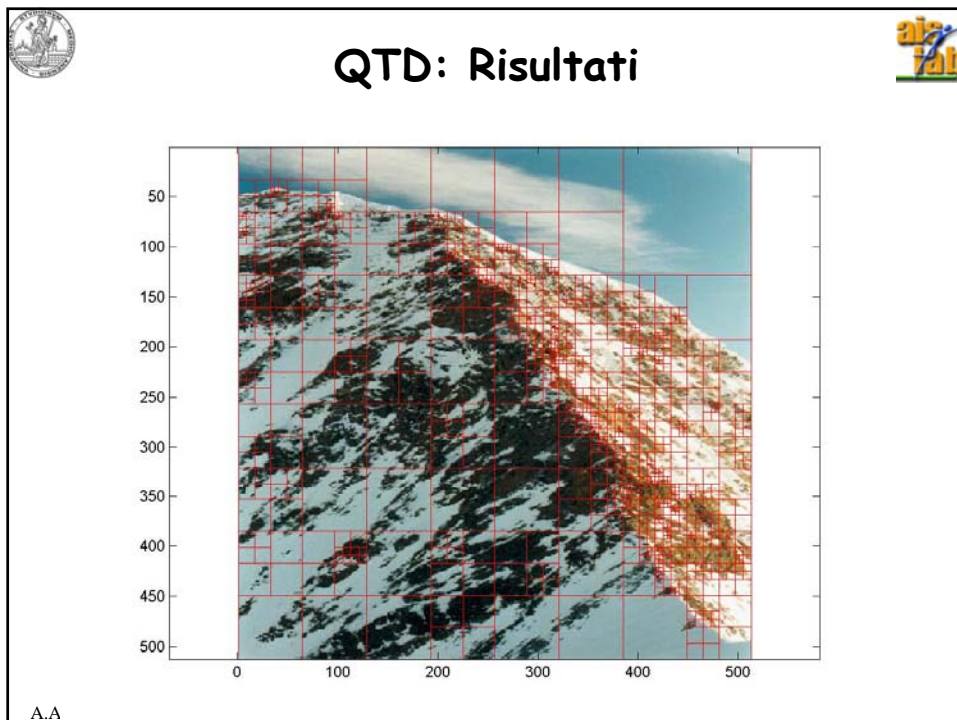
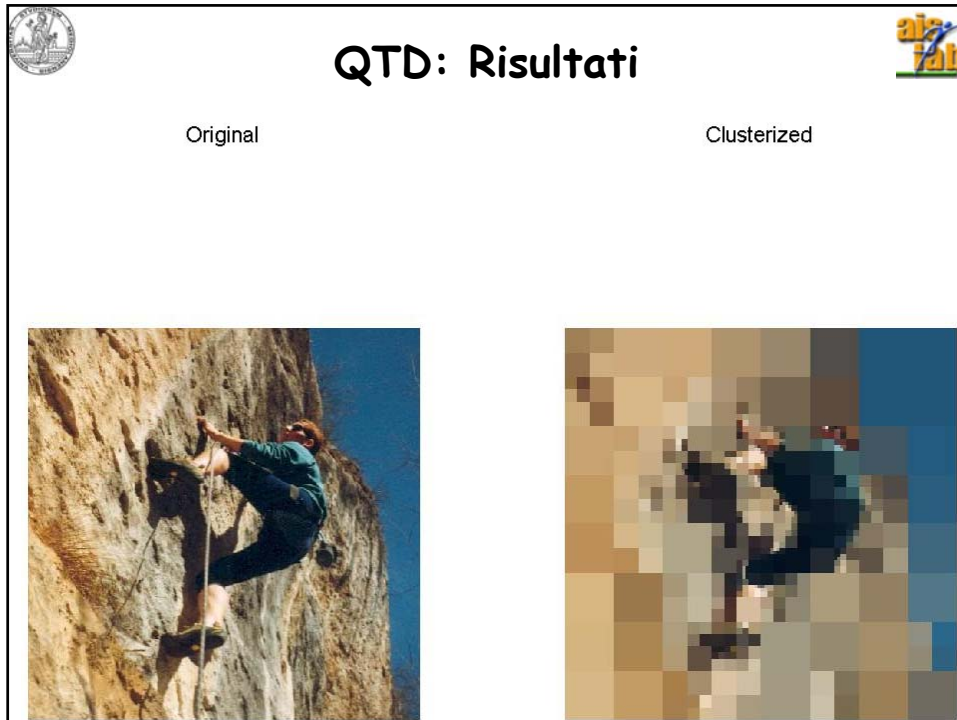



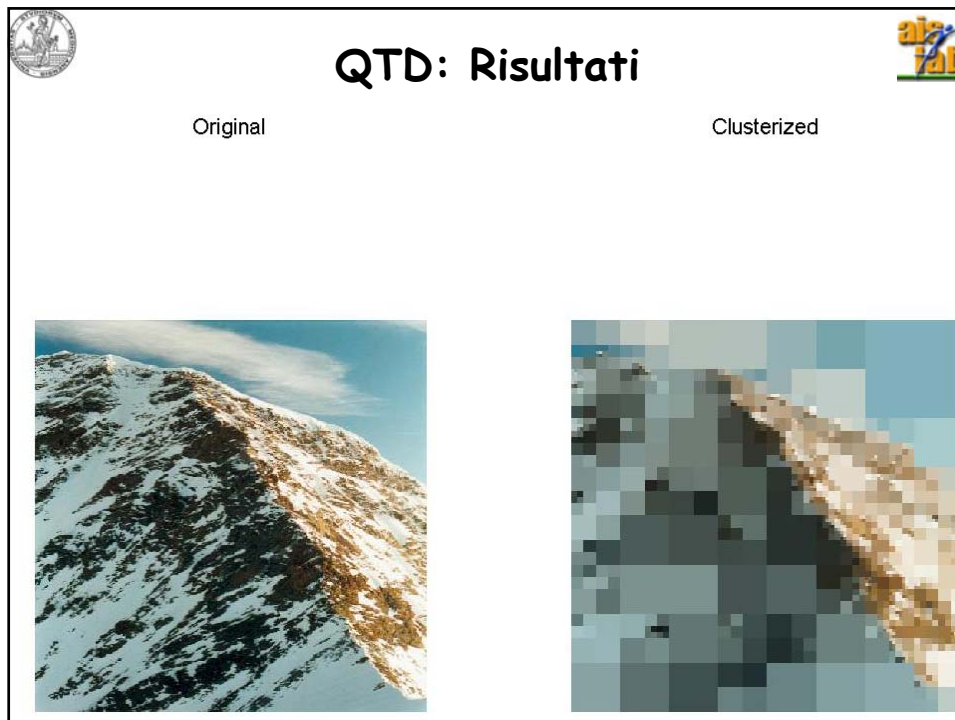
## Algoritmi gerarchici: QTD

Criterio di splitting: se due pixel all'interno dello stesso cluster distano più di una determinata soglia, il cluster viene diviso in 4 cluster.

Esempio applicazione: segmentazione immagini, compressione immagini, analisi locale frequenze immagini...

A.A. 2012-2013 6/51







**Hierarchical Clustering**

- In brief, HC algorithms build a whole hierarchy of clustering solutions
  - ◆ Solution at level  $k$  is a *refinement* of solution at level  $k-1$
- Two main classes of HC approaches:
  - ◆ Agglomerative: solution at level  $k$  is obtained from solution at level  $k-1$  by merging two clusters
  - ◆ Divisive: solution at level  $k$  is obtained from solution at level  $k-1$  by splitting a cluster into two parts
    - ⇒ Less used because of computational load

A.A. 2012-2013 10/51 <http://homes.dsi.unimi.it/~borgnese/>

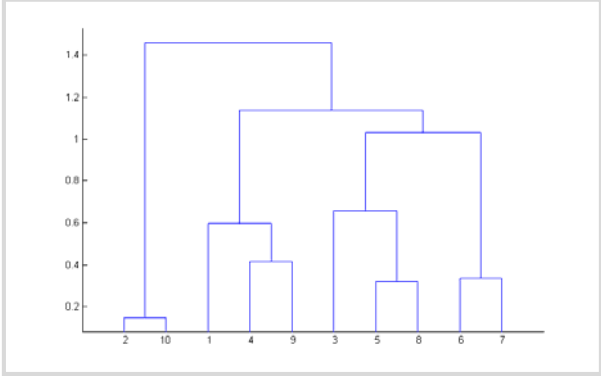


## The 3 steps of agglomerative clustering




1. At start, each input pattern is assigned to a singleton cluster
2. At each step, the two *closest* clusters are merged into one
  - ◆ So the number of clusters is decreased by one at each step
3. At the last step, only one cluster is obtained


The clustering process is represented by a *dendrogram*



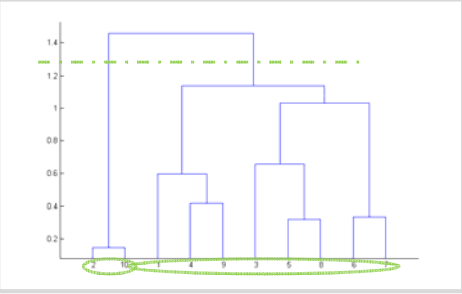
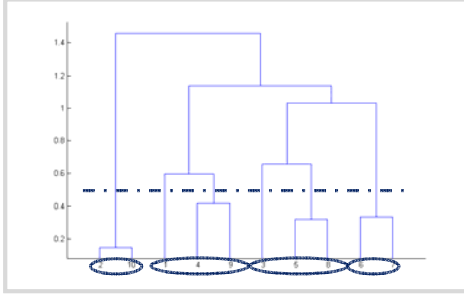
A.A. 2012-2013
11/51
<http://homes.dsi.unimi.it/~borghese/>





## How to obtain the final solution



- The resulting dendrogram has to be cut at some level to get the final clustering:
  - ◆ Cut criterion: number of desired clusters, or threshold on some features of resulting clusters

A.A. 2012-2013
12/51
<http://homes.dsi.unimi.it/~borghese/>






## Dissimilarity criteria

- Different distances/indices of dissimilarity (*point wise*) ...
  - ◆ E.g. euclidean, city-block, correlation...
- ... and agglomeration criteria: Merge clusters  $C_i$  and  $C_j$  such that  $diss(i, j)$  is minimum (*cluster wise*)
  - ◆ Single linkage:
    - ⊖  $diss(i, j) = \min d(x, y)$ , where  $x$  is in  $C_i$ ,  $y$  in cluster  $C_j$
  - ◆ Complete linkage:
    - ⊖  $diss(i, j) = \max d(x, y)$ , where  $x$  is in cluster  $i$ ,  $y$  in cluster  $j$
  - ◆ Group Average (GA) and Weighted Average (WA) Linkage:
    - ⊖  $diss(i, j) = \frac{\sum_{x \in C_i} \sum_{y \in C_j} w_i w_j d(x, y)}{\sum_{x \in C_i} \sum_{y \in C_j} w_i w_j}$ 

GA:  $w_i = w_j = 1$   
 WA:  $w_i = n_i, w_j = n_j$


A.A. 2012-2013 13/51 http://homes.dsi.unimi.it/~borghese/


## Cluster wise dissimilarity

- Other agglomeration criteria: Merge clusters  $C_i$  and  $C_j$  such that  $diss(i, j)$  is minimum
  - ◆ Centroid Linkage:
    - ⊖  $diss(i, j) = d(\mu_i, \mu_j)$
  - ◆ Median Linkage:
    - ⊖  $diss(i, j) = d(\text{center}_i, \text{center}_j)$ , where each  $\text{center}_i$  is the average of the centers of the clusters composing  $C_i$
  - ◆ Ward's Method:
    - ⊖  $diss(i, j) = \text{increase in the total error sum of squares (ESS) due to the merging of } C_i \text{ and } C_j$
- Single, complete, and average linkage: *graph methods*
  - ◆ *All points in clusters are considered*
- Centroid, median, and Ward's linkage: *geometric methods*
  - ◆ *Clusters are summed up by their centers*

A.A. 2012-2013 14/51 http://homes.dsi.unimi.it/~borghese/



## Ward's method



It is also known as minimum variance method.

Each merging step minimizes the increase in the total ESS:

$$ESS_i = \sum_{x \in C_i} (x - \mu_i)^2 \quad ESS = \sum_i ESS_i$$


When merging clusters  $C_i$  and  $C_j$ , the increase in the total ESS is:

$$\Delta ESS = ESS_{i,j} - ESS_i - ESS_j$$


Spherical, compact clusters are obtained.

The solution at each level  $k$  is an approximation to the optimal solution for that level (the one minimizing ESS)

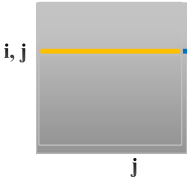
A.A. 2012-2013
15/51
<http://homes.dsi.unimi.it/~borghese/>



## How HC operates





- HC algorithms operate on a dissimilarity matrix:
  - ◆ For each pair of existant clusters, their dissimilarity value is stored
- When clusters  $C_i$  and  $C_j$  are merged, only dissimilarities for the new resulting cluster have to be computed
  - ◆ The rest of the matrix is left untouched



A.A. 2012-2013
16/51
<http://homes.dsi.unimi.it/~borghese/>



## The Lance-William recursive formulation



Used for iterative implementation. The dissimilarity value between newly formed cluster  $\{C_i, C_j\}$  and every other cluster  $C_k$  is computed as:

$$diss(k, (i, j)) = \alpha_i diss(k, i) + \alpha_j diss(k, j) + \beta diss(i, j) + \gamma |diss(k, i) - diss(k, j)|$$

Only values already stored in the dissimilarity matrix are used. Different sets of coefficients correspond to different criteria.

Criterion	$\alpha_i$	$\alpha_j$	$\beta$	$\gamma$
Single Link.	$\frac{1}{2}$	$\frac{1}{2}$	0	$-\frac{1}{2}$
Complete Link.	$\frac{1}{2}$	$\frac{1}{2}$	0	$\frac{1}{2}$
Group Avg.	$n_i/(n_i+n_j)$	$n_j/(n_i+n_j)$	0	0
Weighted Avg.	$\frac{1}{2}$	$\frac{1}{2}$	0	0
Centroid	$n_i/(n_i+n_j)$	$n_j/(n_i+n_j)$	$-n_i n_j / (n_i+n_j)^2$	0
Median	$\frac{1}{2}$	$\frac{1}{2}$	$-\frac{1}{4}$	0
Ward	$(n_i+n_k)/(n_i+n_j+n_k)$	$(n_j+n_k)/(n_i+n_j+n_k)$	$-n_k/(n_i+n_j+n_k)$	0

A.A. 2012-2013 17/51 <http://homes.dsi.unimi.it/~borghese/>

## Characteristics of HC

- Pros:
  - ◆ Independence from initialization
  - ◆ No need to specify a desired number of clusters from the beginning
- Cons:
  - ◆ Computational complexity at least  $O(N^2)$
  - ◆ Sensitivity to outliers
  - ◆ No reconsideration of possibly misclassified points
  - ◆ Possibility of inversion phenomena and multiple solutions

A.A. 2012-2013 18/51 <http://homes.dsi.unimi.it/~borghese/>



# Riassunto



Hierarchical clustering