Università di Pisa

Data Mining and Machine Learning
Bioinspired computational methods
Biological data mining

Clustering with Constraints

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Some slides belong to the collection

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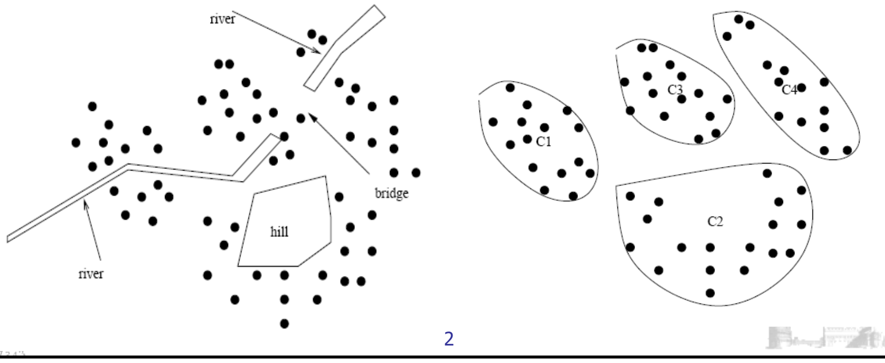
Why Constraint-Based Cluster Analysis?

- Need user feedback: Users know their applications the best
- Less parameters but more user-desired constraints:
  - A bank manager wishes to locate four ATMs in the area in the figure on the left: obstacle and desired clusters. Ignoring the obstacles will result in the clusters on the right



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Categorization of Constraints

- Constraints on instances: specifies how a pair or a set of instances should be grouped in the cluster analysis
  - Must-link vs. cannot link constraints
    - must-link(x, y): x and y should be grouped into one cluster
  - Constraints can be defined using variables, e.g.,
    - cannot-link(x, y) if distance(x, y) > d

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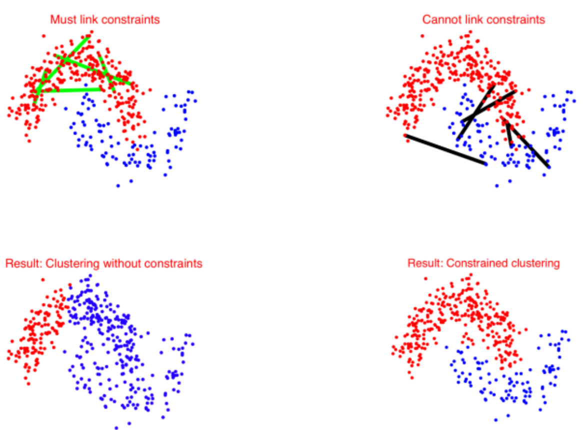
Categorization of Constraints

- Constraints on instances



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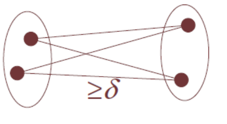
Categorization of Constraints

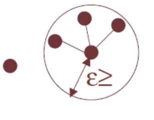
- Constraints on clusters: specify a requirement on the clusters
  - E.g., specify the min number of objects in a cluster, the max diameter of a cluster, the shape of a cluster (e.g., a convex), number of clusters (e.g., k)
  - δ-constraint (Minimum separation)
    - For any two clusters S_i, S_j, $\forall i, j$
    - For each two instances $s_p \in Si, s_q \in Sj, \forall p, q$
    - $D(s_p,s_q) >= \delta$
  - ε-constraint
    - For any cluster S_i, $|S_j| > 1$
    - $\forall p, s_p \in Si, \exists s_q \in Si$: $\varepsilon \geq D(sp,sq)$, $s_p <> s_q$

Categorization of Constraints

- Constraints on clusters can be converted to instance level constraints
  - δ-constraint (Minimum separation)
    - For every point x, must-link all points y such tha D(x,y) < δ, i.e., conjunction of must link (ML) constraints



  - ε-constraint
    - For every point x, must link to at least one point y such that D(x,y) <= ε, i.e. disjunction of ML constraints



  - Will generate many instance level constraints

Categorization of Constraints

- Constraints on similarity measurements: specifies a requirement that the similarity calculation must respect
  - E.g., to cluster people as moving objects in a plaza, while Euclidean distance is used to give the walking distance between two points, a constraint on similarity measurement is that the trajectory implementing the shortest distance cannot cross a wall.

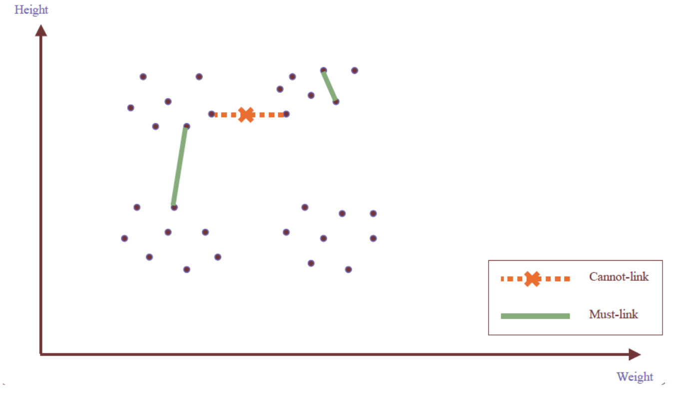
Categorization of Constraints

- Hard vs. soft constraints;
  - A constraint is hard if a clustering that violates the constraint is unacceptable.
  - A constraint is soft if a clustering that violates the constraint is not preferable but acceptable when no better solution can be found. Soft constraints are also called preferences.

Clustering with Constraints

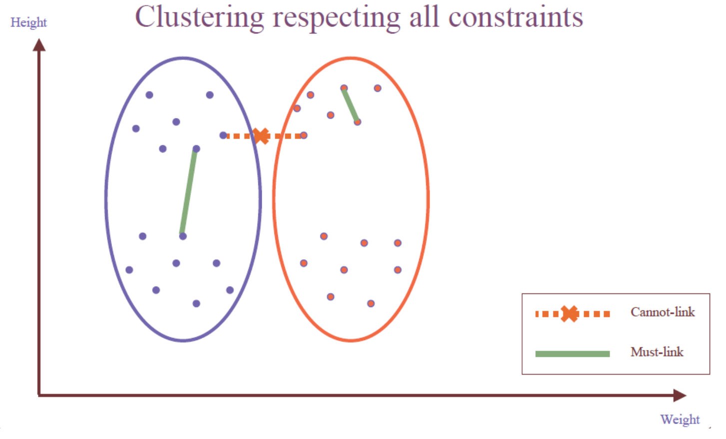
- Clustering with constraints:
  - Partition unlabeled data into clusters and use constraints to aid and bias clustering
- Goal
  - Examples in same cluster similar, separate clusters different and constraints are maximally respected
- Enforcing Constraints:
  - **Strict enforcement**: find best feasible clustering respecting all constraints
  - **Partial enforcement**: find best clustering maximally respecting constraints

Example: Enforcing Constraints



Example: Enforcing Constraints

Clustering respecting all constraints



Categorization of Constraints

- Conflicting or redundant constraints
  must-link(x, y) if dist(x, y) < 5
  cannot-link(x, y) if dist(x, y) > 3.
- If a data set has two objects, x, y, such that dist(x, y) = 4, then no clustering can satisfy both constraints simultaneously.
- How can we measure the quality and the usefulness of a set of constraints?
  - Informativeness: the amount of information carried by the constraints that is beyond the clustering model. Given a data set, D, a clustering method, A, and a set of constraints, C, the informativeness of C with respect to A on D can be measured by the fraction of constraints in C that are unsatisfied by the clustering computed by A on D.
  - Coherence of a set of constraints: the degree of agreement among the constraints themselves, which can be measured by the redundancy among the constraints

The Effects of Constraints on Clustering Solutions

- Constraints divide the set of all plausible solutions into two sets: feasible and infeasible: $S = S_F \cup S_I$
- Constraints effectively reduce the search space to S_F
- S_F all have a common property
- So it is not unexpected that we find solutions with a desired property and find them quickly.

Constraint-Based Clustering Methods (I): Handling Hard Constraints

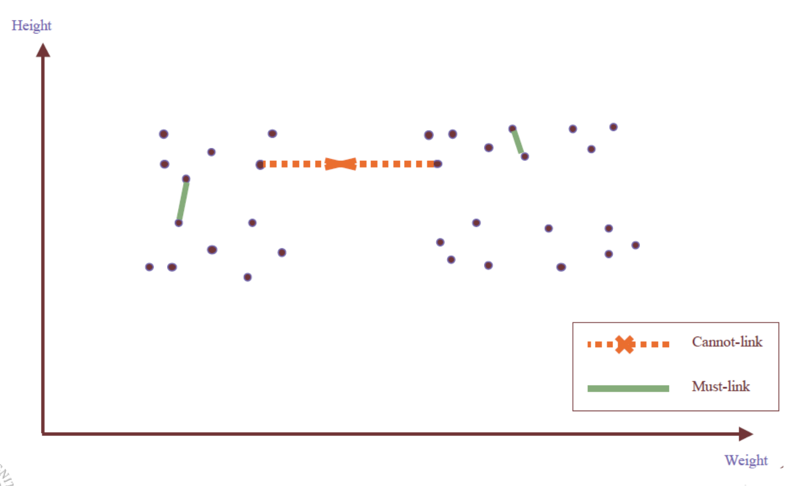
- Handling hard constraints: Strictly respect the constraints in cluster assignments
- The COP-k-means algorithm
  - Generate super-instances for must-link constraints
    - Compute the transitive closure of the must-link constraints
    - To represent such a subset, replace all those objects in the subset by the mean.
    - The super-instance also carries a weight, which is the number of objects it represents
  - Conduct modified k-means clustering to respect cannot-link constraints
    - Modify the center-assignment process in k-means to a nearest feasible center assignment
    - An object is assigned to the nearest center so that the assignment respects all cannot-link constraints

Constraint-Based Clustering Methods (I): Handling Hard Constraints

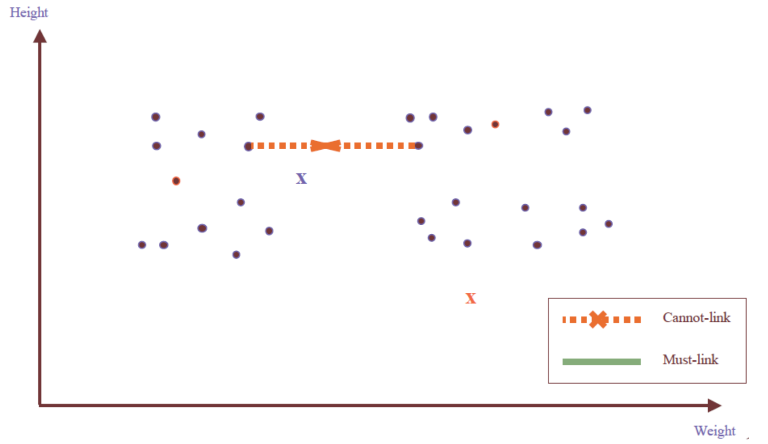
Input: S_u: unlabeled data, S_l: labeled data, k: the number of clusters to find, q: number of constraints to generate.
Output: A set partition of $S = S_u \cup S_l$ into k clusters so that all the constraints in $C = ML \cup CL$ are satisfied.

1. $ML = \emptyset, CL = \emptyset$
2. **loop** q times **do**
   (a) Randomly choose two distinct points x and y from S_l.
   (b) if(Label(x) = Label(y)) $ML = ML \cup \{x, y\}$ else $CL = CL \cup \{x, y\}$
3. Compute the transitive closure from ML to obtain the connected components $CC_1, ..., CC_r$.
4. For each i, $1 \leq i \leq r$, replace data points in CC_i with the average of the points in CC_i.
5. Randomly generate cluster centroids $C_1, \ldots, C_k$.
6. **loop** until convergence **do**
   (a) **for** i = 1 **to** $|S|$ **do**
      (a.1) Assign s_i to closest feasible cluster.
   (b) Recalculate $C_1, \ldots, C_k$.

Example: COP-K Means



Example: COP-K Means – ML Points Averaged



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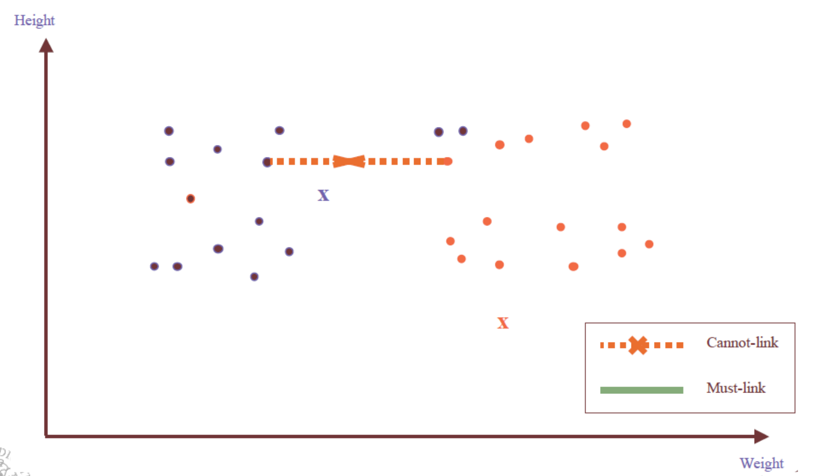
Example: COP-K Means – 3 Nearest Feasible Assignment



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Constraint-Based Clustering Methods (II): Handling Soft Constraints

- Treated as an optimization problem: When a clustering violates a soft constraint, a penalty is imposed on the clustering
- Overall objective: Optimizing the clustering quality, and minimizing the constraint violation penalty
- Ex. CVQE (Constrained Vector Quantization Error) algorithm: Conduct k-means clustering while enforcing constraint violation penalties

Constraint-Based Clustering Methods (III): Handling Soft Constraints

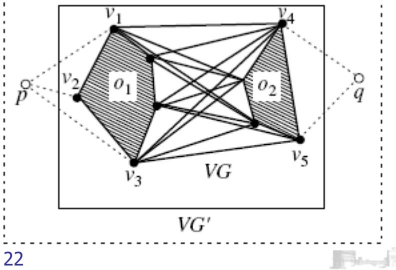
- Objective function: Sum of distance used in k-means, adjusted by the constraint violation penalties
  - Penalty of a must-link violation
    - If objects x and y must-be-linked but they are assigned to two different centers, c_1 and c_2, dist(c_1, c_2) is added to the objective function as the penalty
  - Penalty of a cannot-link violation
    - If objects x and y cannot-be-linked but they are assigned to a common center c, dist(c, c'), between c and c' is added to the objective function as the penalty, where c' is the closest cluster to c that can accommodate x or y

Speeding Up Constrained Clustering

- It is costly to compute some constrained clustering
- Ex. Clustering with obstacle objects: Tung, Hou, and Han. Spatial clustering in the presence of obstacles, ICDE'01
  - Cluster people as moving objects in a plaza.
  - Euclidean distance is used to measure the walking distance. However, constraint on similarity measurement is that the trajectory implementing the shortest distance cannot cross a wall.
  - Distance has to be derived by geometric computations: the computational cost is high if a large number of objects and obstacles are involved.
- A point p is visible from another point q if the straight line joining p and q does not intersect any obstacles.

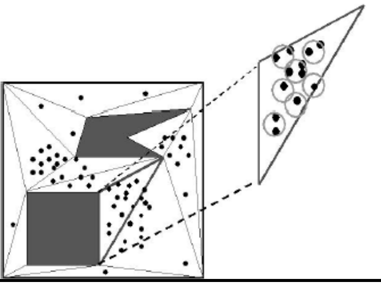
Speeding Up Constrained Clustering

- A visibility graph is the graph, VG = (V,E), such that each vertex of the obstacles has a corresponding node in V and two nodes, v_1 and v_2, in V are joined by an edge in E if and only if the corresponding vertices they represent are visible to each other.
- Let VG' = (V',E') be a visibility graph created from VG by adding two additional points, p and q, in V'. E' contains an edge joining two points in V' if the two points are mutually visible.
- The shortest path between two points, p and q, will be a subpath of VG'.



Speeding Up Constrained Clustering

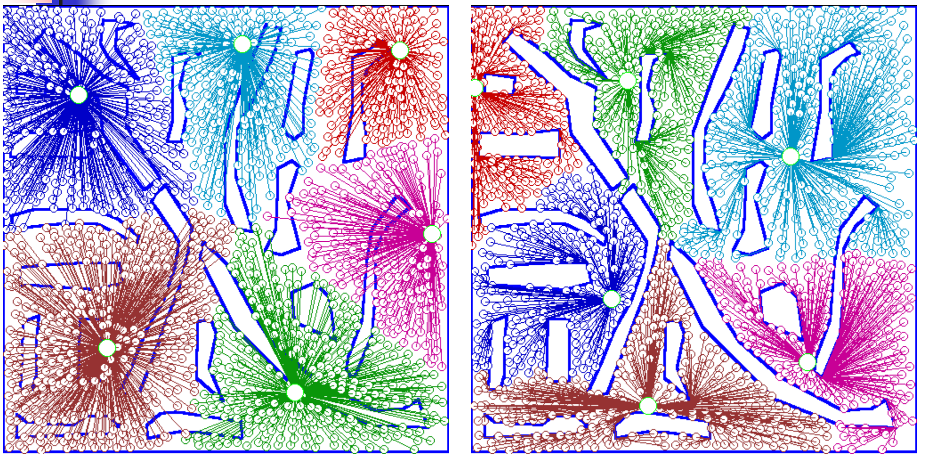
- To reduce the cost of distance computation between any two pairs of objects or points, several pre-processing and optimization techniques can be used.
- One method groups points that are close together into microclusters.
- This can be done by first triangulating the region R into triangles, and then grouping nearby points in the same triangle into microclusters, using a method similar to BIRCH or DBSCAN.



Speeding Up Constrained Clustering

- By processing microclusters rather than individual points, the overall computation is reduced.
- After that, precomputation can be performed to build two kinds of join indices based on the computation of the shortest paths:
  - (1) VV indices, for any pair of obstacle vertices, and
  - (2) MV indices, for any pair of microcluster and obstacle vertex.
- Use of the indices helps further optimize the overall performance.
- Using such precomputation and optimization strategies, the distance between any two points (at the granularity level of a microcluster) can be computed efficiently.
- Thus, the clustering process can be performed in a manner similar to a typical efficient k-medoids algorithm, such as CLARANS, and achieve good clustering quality for large data sets.

An Example: Clustering With Obstacle Objects



Not Taking obstacles into account   Taking obstacles into account