Robust Single Linkage Algorithm and Extract Flat Clustering

Taoran Xue

George Washington University

April 25, 2017

Introduction

- There are many sources of almost unlimited data:
  1. Images from the web.
  2. Speech recorded by a microphone.
  3. Records of credit card or other transactions.
- Noise points occasionally draws between two cluster

Minimum spanning tree

For each i, set $r(x_i)$ to the distance from x_i to its kth nearest neighbor.

As r grows from 0 to ∞:

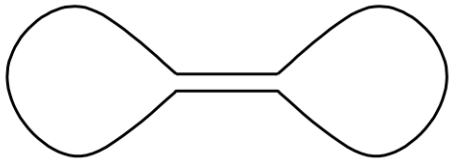
1. Construct a graph G_r with nodes $\{x_i : r(x_i) \leq r\}$. Include edge (x_i, x_j) if $\|x_i - x_j\| \leq \alpha r$.
2. Let $\mathbb{C}_n(r)$ be the connected components of G_r.

Definition

Set $r_k(x_i)$ to the distance to kth nearest neighbor. For any $r = \max\{r_k(x_i)\}$, connect points x_i and x_j, if $||x_i - x_j|| \leq \alpha r$.

New distance function

Effect 1: thin bridges



For any set Z, let Z_σ be all points within distance σ of it.

Figure 1: "Thin bridge" effect.

Definition

Set $core_k(x_i)$ to the distance to kth nearest neighbor.

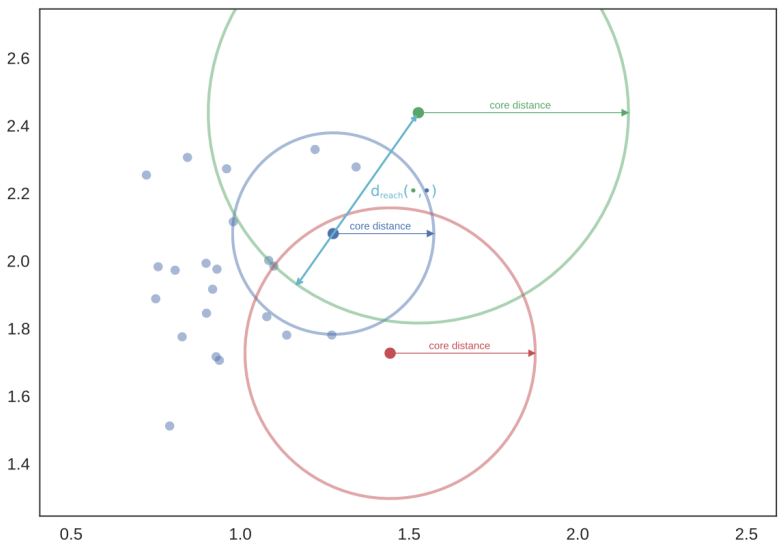
$$d_{\mathrm{mrd}_k}(x_i, x_j) = \max\{core_k(x_i), core_k(x_j), ||x_i - x_j||\}$$

Mutual reachability distance

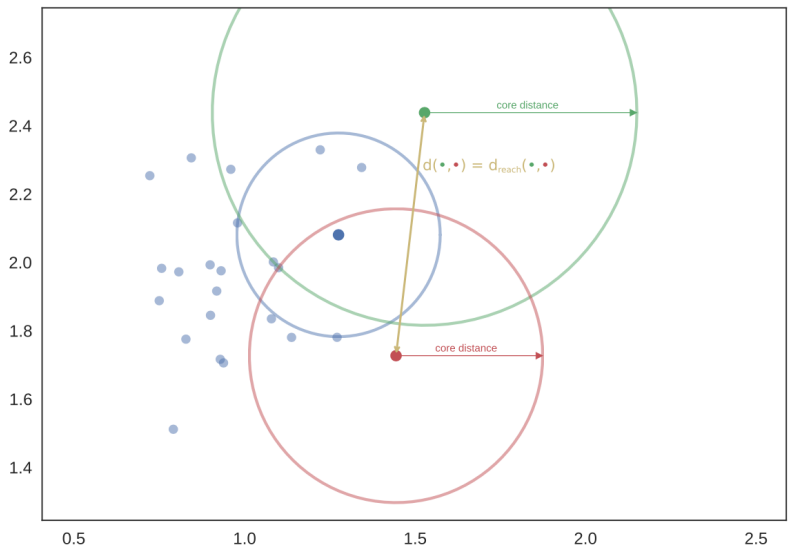
Definition

Set $core_k(x_i)$ to the distance to kth nearest neighbor.

$$d_{\mathrm{mrd}_k}(x_i, x_j) = \max\{core_k(x_i), core_k(x_j), ||x_i - x_j||\}$$



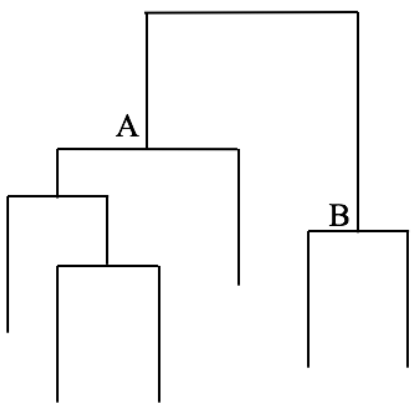
(a)



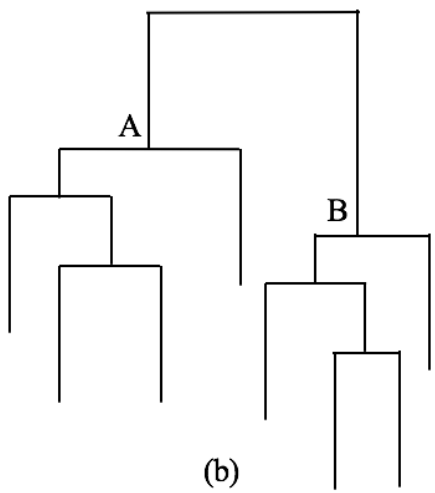
(b)

Condense tree

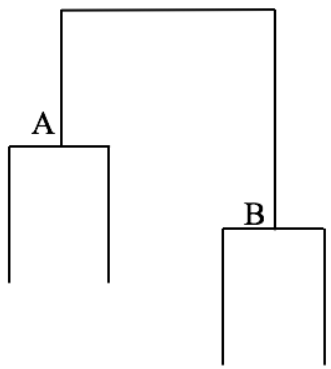
- If left child cluster point number is greater than minimum cluster size, but right side is not, Figure(a), keep the left branch and ignore right cluster;
- If left and right child clusters are both greater than minimum cluster size, Figure(b), we consider that a cluster split and let the split persist the whole tree;
- If left and right child clusters are both fewer than minimum cluster size, Figure(c), we ignore the two cluster.



(a)



(b)



(c)

Condense tree algorithm

Input: H[m] $\leftarrow$ hierarchy tree
Output: T[n] $\leftarrow$ condense tree
nodeList $\leftarrow$ `BFS(`H`)`;
for $r \leftarrow 0$ **to** m **do**
    if nodeList[r] *is ignored* **then**
        Pass;
    end
    left $\leftarrow$ nodeList[r].child1;
    leftCount $\leftarrow$ H[left].childrenSize;
    right $\leftarrow$ nodeList[r].child2;
    rightCount $\leftarrow$ H[right].childrenSize;
    if leftCount $\geq$ minClusterSize **and** rightCount $\geq$ minClusterSize **then**
        T[p++] $\leftarrow$ (nextLabel, ++nextLabel, $1/\mathrm{distance}$, leftCount); T[p++] $\leftarrow$ (nextLabel, ++nextLabel, $1/\mathrm{distance}$, rightCount);
    end
    if leftCount $<$ minClusterSize **then**
        for tmpNode **in** `BFS(left)` **do**
            if tmpNode *is leaf* **then**
                T[p++] $\leftarrow$ (nextLabel, tmpNode, $1/\mathrm{distance}$, 1);
            end
            Ignore tmpNode;
        end
    end
    if rightCount $<$ minClusterSize **then**
        for tmpNode **in** `BFS(right)` **do**
            if tmpNode *is leaf* **then**
                T[p++] $\leftarrow$ (nextLabel, tmpNode, $1/\mathrm{distance}$, 1);
            end
            Ignore tmpNode;
        end
    end
end

Cluster stability

Definition

Let $\lambda = \frac{1}{d_{\text{mrd}_k}}$. For each cluster we give λ_{birth} and λ_p to be the lambda value when the cluster split off then became it's own cluster, and the lambda value (if any) when the cluster split into smaller clusters respectively.

$$S(C) = \sum_{p \in C} (\lambda_p - \lambda_{\text{birth}})$$

Cluster stability algorithm

Input: T[n] $\leftarrow$ condense tree in reverse topological order contains a tuple of (parent,child,λ,childrenSize)
Output: S[n] $\leftarrow$ stability of every node in condense tree
for $r \leftarrow 0$ **to** n **do**
    currChild $\leftarrow$ T[r].child;
    currλ $\leftarrow$ T[r].λ;
    if currChild $=$ prevChild **then**
        minλ $\leftarrow$ `Min`(minλ, currλ);
    else
        birthλ[currChild] $\leftarrow$ minλ;
        prevChild $\leftarrow$ currChild;
        minλ $\leftarrow$ currλ;
    end
end
for $r \leftarrow 0$ **to** n **do**
    S[r] $\leftarrow$ S[r] + T[r].$\lambda$$-$birth$\lambda$[T[$r$].parent] $\times$T[r].childrenSize ;
end

Flat clustering

Definition

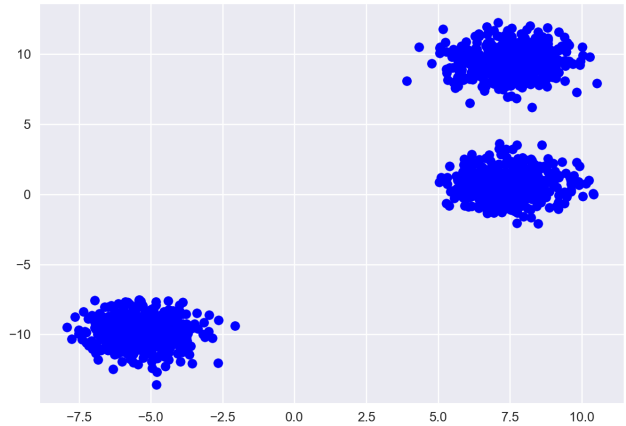
Set $SC(C)$ is the sum of the stabilities of the child cluster of cluster C.

$$SC(C) = \sum_{q \in C} S(c)$$

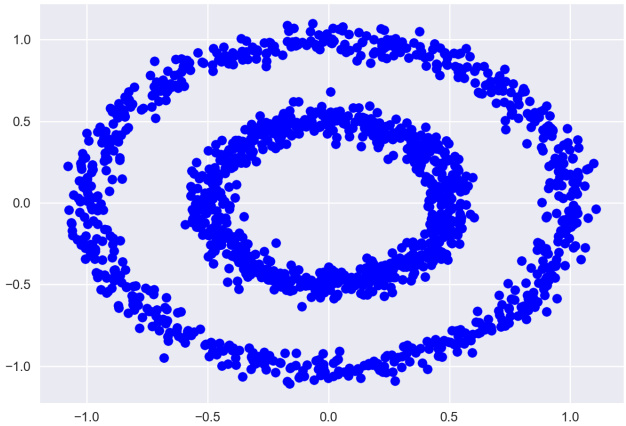
Flat clustering algorithm

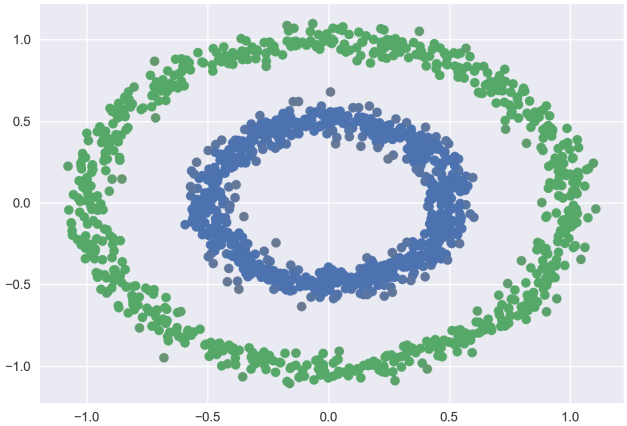
Input: S[n] $\leftarrow$ stability condense tree sorted in reverse topological order
Output: L[n] $\leftarrow$ **True** cluster is selected; **False** otherwise
L $\leftarrow$ {**True**};
for $r \leftarrow 0$ **to** n **do**
    childList $\leftarrow$ {list of node whose parent is r};
    subtreeStabilities $\leftarrow \sum_{c \in \text{childList}}$ S[c];
    if subtreeStabilities $>$ S[r] **then**
        L[r] $\leftarrow$ **False**;
        S[r] $\leftarrow$ subtreeStabilities;
    else
        for tmpNode **in** `BFS(`r`)` **do**
            if tmpNode $\neq r$ **then**
                L[tmpNode] $\leftarrow$ **False**
            end
        end
    end
end

Experiment

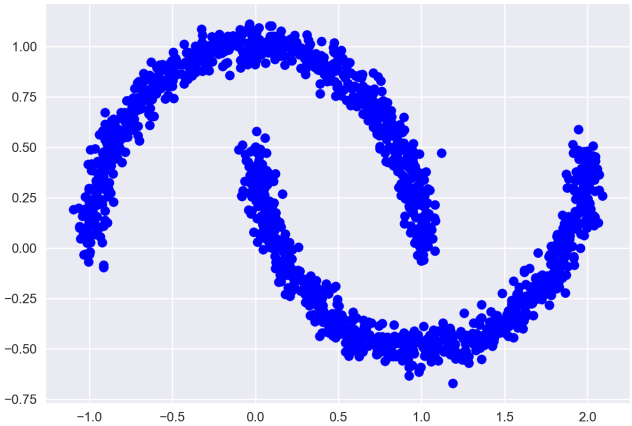

10
5
0
−5
−10
−7.5
−5.0
−2.5
0.0
2.5
5.0
7.5
10.0

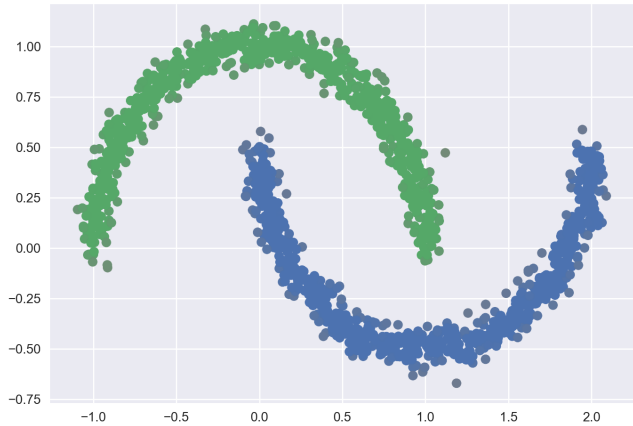

10
5
0
−5
−10
−7.5
−5.0
−2.5
0.0
2.5
5.0
7.5
10.0

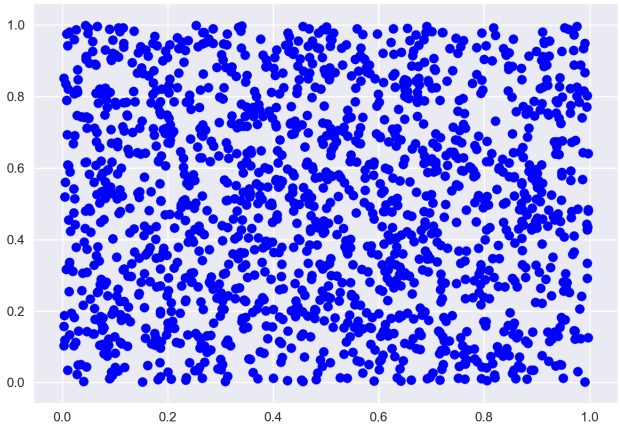

1.0
0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0

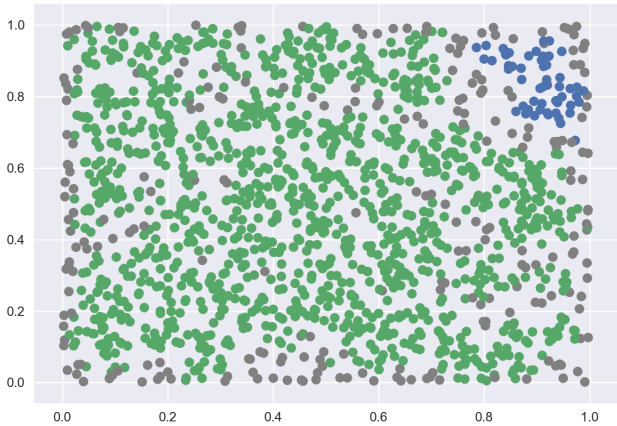

1.0
0.5
0.0
−0.5
−1.0
−1.0
−0.5
0.0
0.5
1.0

Experiment (cont.)

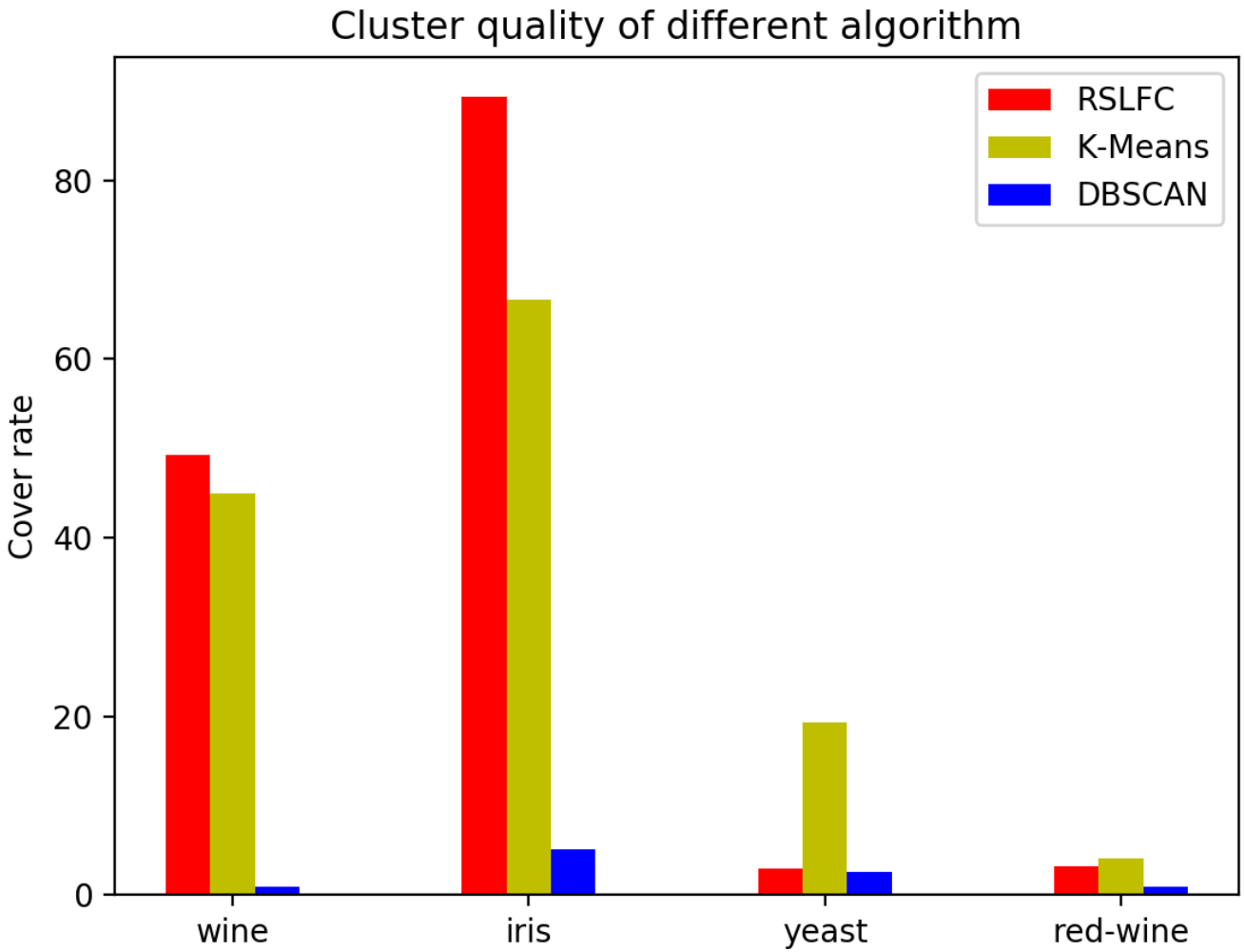








Experiment (cont.)



References

Campello, R. J., Moulavi, D., & Sander, J. (2013). Density-based clustering based on hierarchical density estimates. In *Pacific-asia conference on knowledge discovery and data mining* (pp. 160–172).

Chaudhuri, K., & Dasgupta, S. (2010). Rates of convergence for the cluster tree. In *Advances in neural information processing systems* (pp. 343–351).

McInnes, L., Healy, J., & Astels, S. (2017, mar). hdbscan: Hierarchical density based clustering. *The Journal of Open Source Software*, *2*(11).