# Robust Single Linkage Algorithm and Extract Flat Clustering

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#### Introduction

- There are many sources of almost unlimited data:
  - Images from the web.
  - Speech recorded by a microphone.
  - Records of credit card or other transactions.
- Noise points occasionally draw 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  $\infty$ :

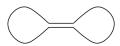
- Construct a graph  $G_r$  with nodes  $\{x_i : r(x_i) \le r\}$ . Include edge  $(x_i, x_i)$  if  $||x_i x_i|| \le \alpha r$ .
- **2** Let  $\mathbb{C}_n(r)$  be the connected components of  $G_r$ .

#### 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  $||x_i - x_j|| \le \alpha r$ .

#### New distance function

#### Effect 1: thin bridges



For any set Z, let  $Z_{\sigma}$  be all points within distance  $\sigma$  of it.

Figure 1: "Thin bridge" effect.

#### **Definition**

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

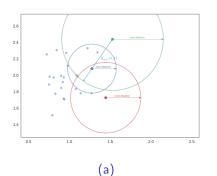
$$d_{\text{mrd}_k}(x_i, x_j) = \max\{core_k(x_i), core_k(x_j), ||x_i - x_j||\}$$

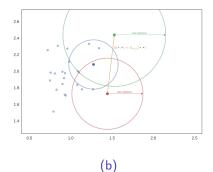
## Mutual reachability distance

#### **Definition**

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

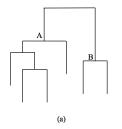
$$d_{\mathrm{mrd}_k}(x_i, x_j) = \max\{core_k(x_i), core_k(x_j), ||x_i - x_j||\}$$

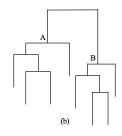


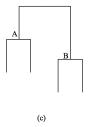


#### Condense tree

- 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.







## 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 ← H[left].childrenSize;
                     right \leftarrow nodeList[r].child2;
                     rightCount ← H[right].childrenSize;
                     if leftCount > minClusterSize and rightCount > minClusterSize then
                                          T[p++] \leftarrow (nextLabel, ++nextLabel, 1/distance, leftCount); T[p++] \leftarrow (nextLabel, ++nextLabel, ++
                                                1/distance, rightCount):
                    end
                     if leftCount < minClusterSize then
                                          for tmpNode in BFS(left) do
                                                              if tmpNode is leaf then
                                                                                     T[p++] \leftarrow (nextLabel, tmpNode, 1/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/distance, 1):
                                                               end
                                                               Ignore tmpNode;
                                          end
                     end
```

end

## Cluster stability

#### Definition

Let  $\lambda=\frac{1}{d_{\mathrm{mrd}_k}}$ . For each cluster we give  $\lambda_{\mathrm{birth}}$  and  $\lambda_p$  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, \lambda, children Size)
Output: S[n] \leftarrow stability of every node in condense tree
for r \leftarrow 0 to n do
     currChild \leftarrow T[r].child;
     \operatorname{curr} \lambda \leftarrow \mathsf{T}[r].\lambda;
     if currChild = prevChild then
           \min \lambda \leftarrow \min(\min \lambda, \operatorname{curr} \lambda);
     else
           birth\lambda[currChild] \leftarrow min\lambda;
           prevChild \leftarrow currChild;
           \min \lambda \leftarrow \operatorname{curr} \lambda;
     end
end
for r \leftarrow 0 to n do
     S[r] \leftarrow S[r] + T[r] \cdot \lambda - birth \lambda [T[r] \cdot parent] \times T[r] \cdot children Size;
end
```

## Flat clustering

#### **Definition**

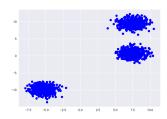
Set SC(C) is the sum of the stabilities of the child cluster of cluster C.

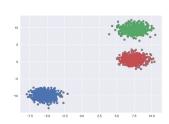
$$SC(C) = \sum_{q \in C} S(q)$$

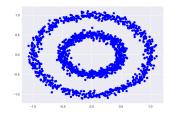
## Flat clustering algorithm

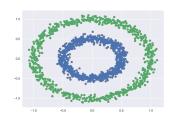
```
Input: S[n] \leftarrow stability condense tree sorted in reverse topological order
Output: L[n] \leftarrow True cluster is selected; False otherwise
L \leftarrow \{True\};
for r \leftarrow 0 to n do
    childList \leftarrow {list of node whose parent is r};
    subtreeStabilities \leftarrow \sum_{c \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
```

## Experiment

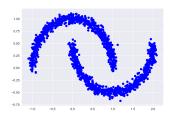


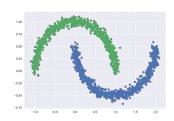


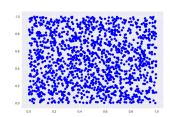


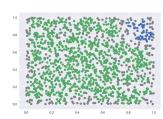


## Experiment (cont.)

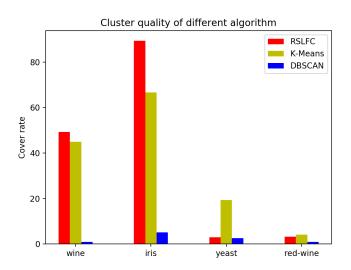








## Experiment (cont.)



#### 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).