Single Linkage Clustering

Parismita Das

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Single Linkage Criterion

In Single Linlage Criterion of Agglomerative Hierarchical clustering, The distance between the elements of each cluster is minimised. As the Naive single linkage clustering has a worst case time complexity of O(N^3). It becomes useless for large data which are frequency used in the field of bioinformatics.

Here by restricting the data to h-band similarity matrix and using min-heap we reduce the time complexity to O(plogp + ph)

The Input

The input is taken as Cosine Similarity matrix which is then converted into Distance Matrix in file adjClust-Band_heap.R

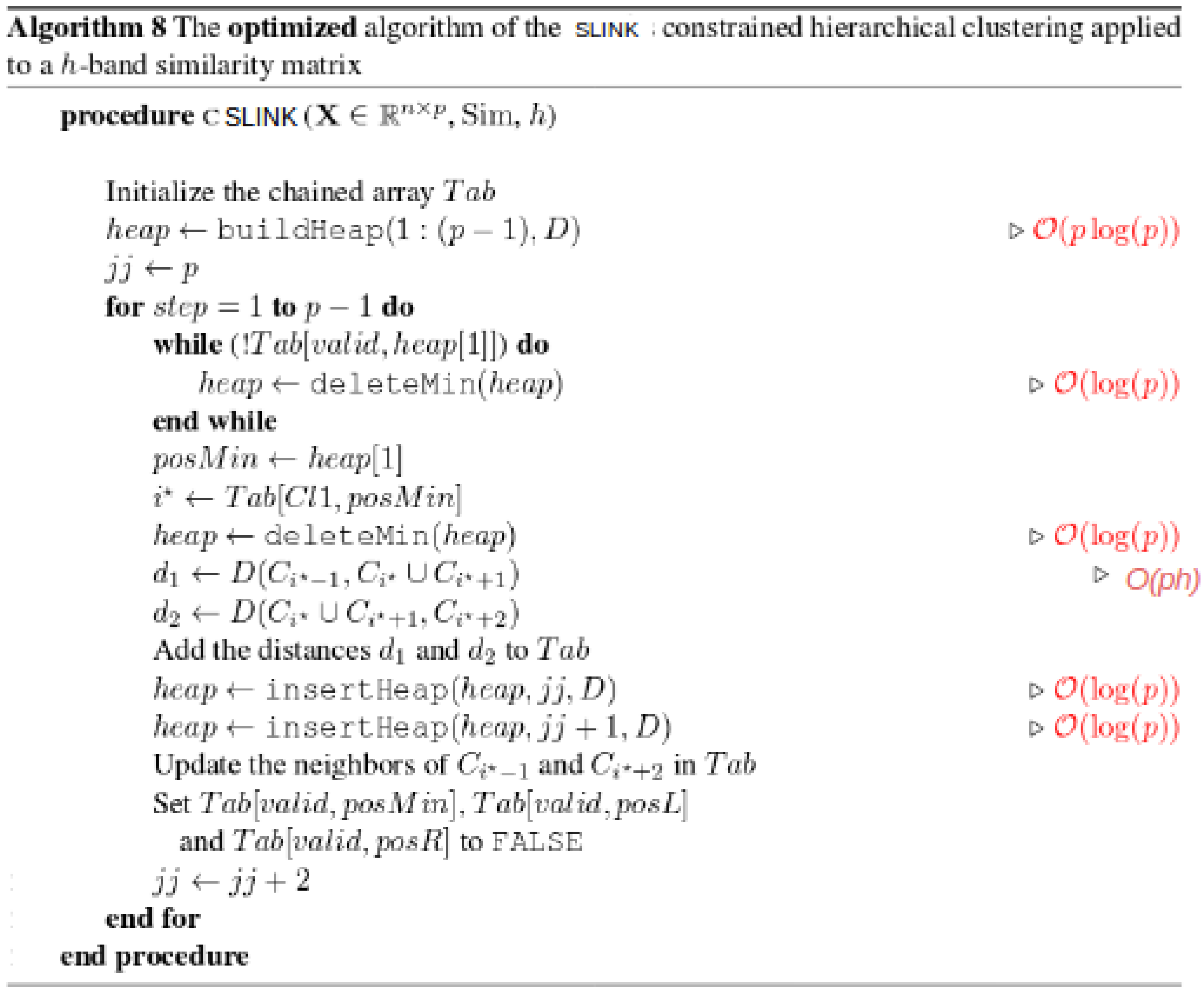
```
matL <- .toMatLeft(xt, p, h)     ## a matrix p x h (with zeros at the bottom) of the LD values
dissim <- as.numeric(1 - matL)    ## cosine distance metric
```

The Output

The output is a hclust object with details of gain, height, label, merge data, order etc.

```
tree <- list(traceW=traceW,
                 gains=gains,
                 merge = res,
                 height = height,
                 seqdist = height,
                 order = 1:p,
                 labels = paste("",1:p),
                 method = "adjclust-heaps",
                 call = match.call(),
                 dist.method = attr(D, "method"))
    class(tree) <- "hclust"
```

The Algorithm



Algorithm 8 The **optimized** algorithm of the SLINK constrained hierarchical clustering applied to a h-band similarity matrix

```
procedure cSLINK($\mathbf{X} \in \mathbb{R}^{n \times p}$, Sim, $h$)

    Initialize the chained array $Tab$
    $heap \leftarrow$ buildHeap($1:(p-1), D$)                    ▷ $\mathcal{O}(p\log(p))$
    $jj \leftarrow p$
    for $step = 1$ to $p-1$ do
        while (!$Tab[valid, heap[1]]$) do
            $heap \leftarrow$ deleteMin($heap$)                  ▷ $\mathcal{O}(\log(p))$
        end while
        $posMin \leftarrow heap[1]$
        $i^\star \leftarrow Tab[Cl1, posMin]$
        $heap \leftarrow$ deleteMin($heap$)                      ▷ $\mathcal{O}(\log(p))$
        $d_1 \leftarrow D(C_{i^\star-1}, C_{i^\star} \cup C_{i^\star+1})$        ▷ O(ph)
        $d_2 \leftarrow D(C_{i^\star} \cup C_{i^\star+1}, C_{i^\star+2})$
        Add the distances $d_1$ and $d_2$ to $Tab$
        $heap \leftarrow$ insertHeap($heap, jj, D$)              ▷ $\mathcal{O}(\log(p))$
        $heap \leftarrow$ insertHeap($heap, jj+1, D$)            ▷ $\mathcal{O}(\log(p))$
        Update the neighbors of $C_{i^\star-1}$ and $C_{i^\star+2}$ in $Tab$
        Set $Tab[valid, posMin]$, $Tab[valid, posL]$
          and $Tab[valid, posR]$ to FALSE
        $jj \leftarrow jj + 2$
    end for
end procedure
```

Computation of Minimum Distance via SLINK

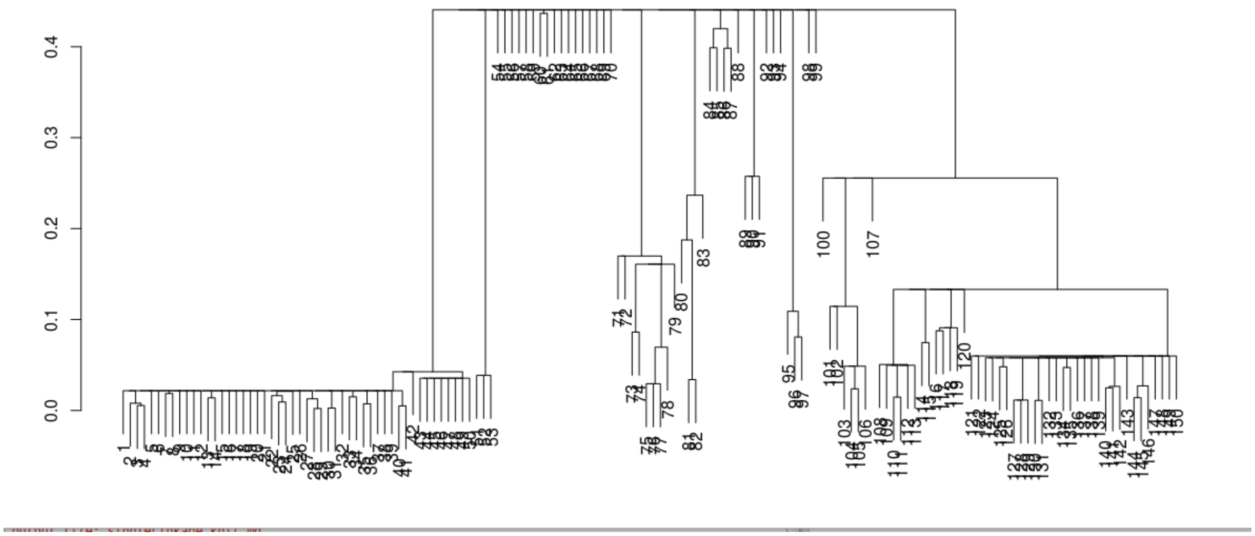
```
  for(int i=mini;i<=maxi;i++)
  {
    for(int j=minj-i;(j<=maxj-i)&&(j<=h);j++)
    {
    res = MIN(DIS(i,j,p),res);
    }
}
```

Where the number of items in cluster I is mini - maxi and cluster J is minj - maxj. In loop-2 the constrain that the difference between index of item must not exceed h is applied.

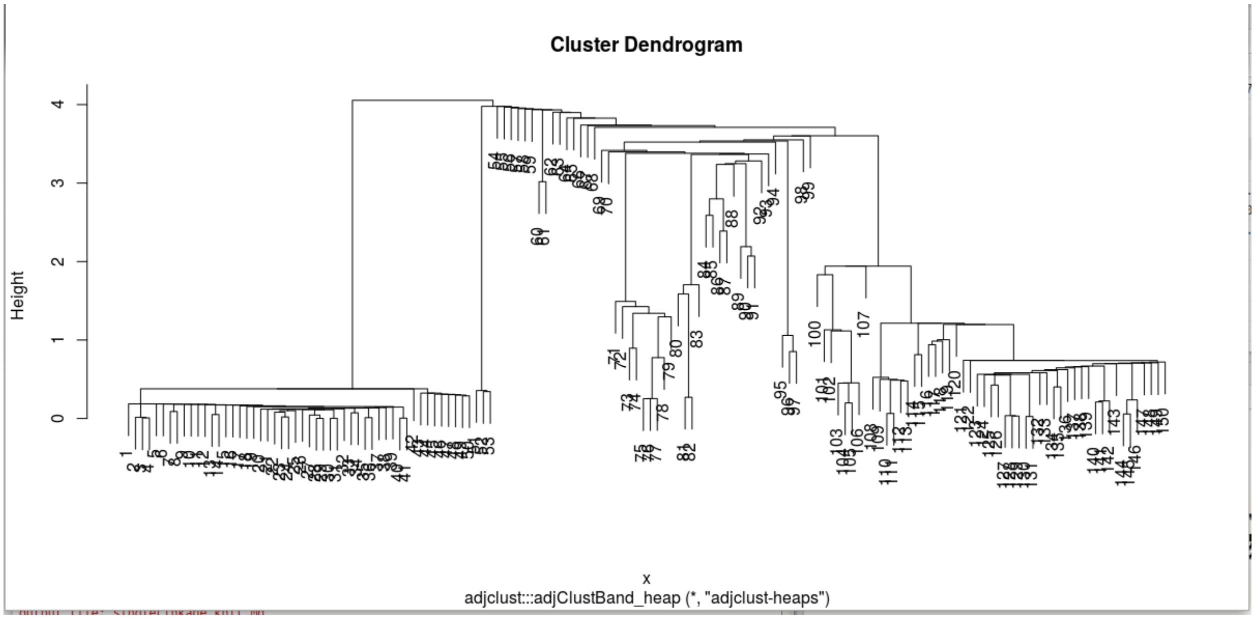
Comparision with Rioja

Taking parameter h as the width of the matrix we get similar results as chclust function of rioja with conslink method.

- The output by rioja chclust (conslink)



- The output by adjClustBand_heap

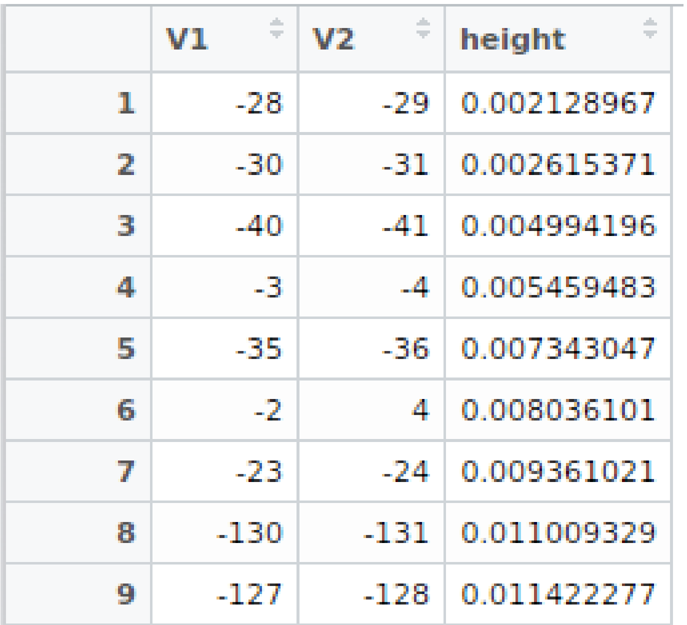


Comparing the Merge Data of both the functions we get same values initially and it deviates a little at higher heights.

- The Merge Data by chclust (conslink)

```
#Recalculating the similarity matrix as s_re = 2-2*s' and rechecking the rioja cluster value
s_re <- 2 - 2*s_scaled
```

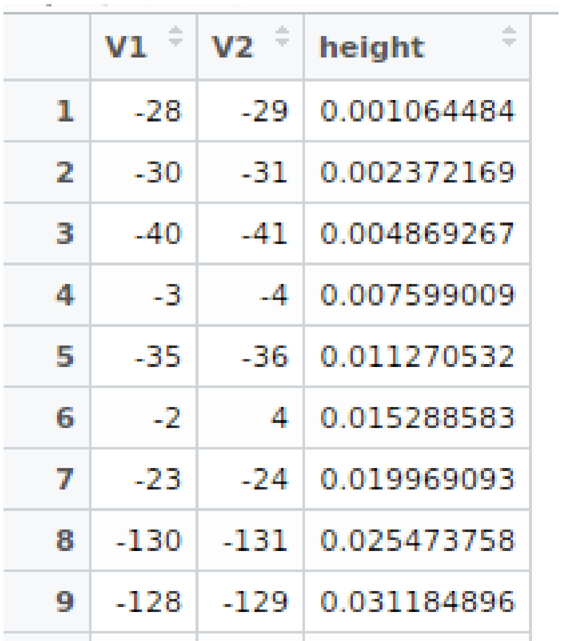
```
#rioja hclust object
diss <- as.dist(s_re)
clust <- chclust(diss, method = "conslink")
View(cbind(clust$merge ,height = clust$height))
```



	V1	V2	height
1	-28	-29	0.002128967
2	-30	-31	0.002615371
3	-40	-41	0.004994196
4	-3	-4	0.005459483
5	-35	-36	0.007343047
6	-2	4	0.008036101
7	-23	-24	0.009361021
8	-130	-131	0.011009329
9	-127	-128	0.011422277

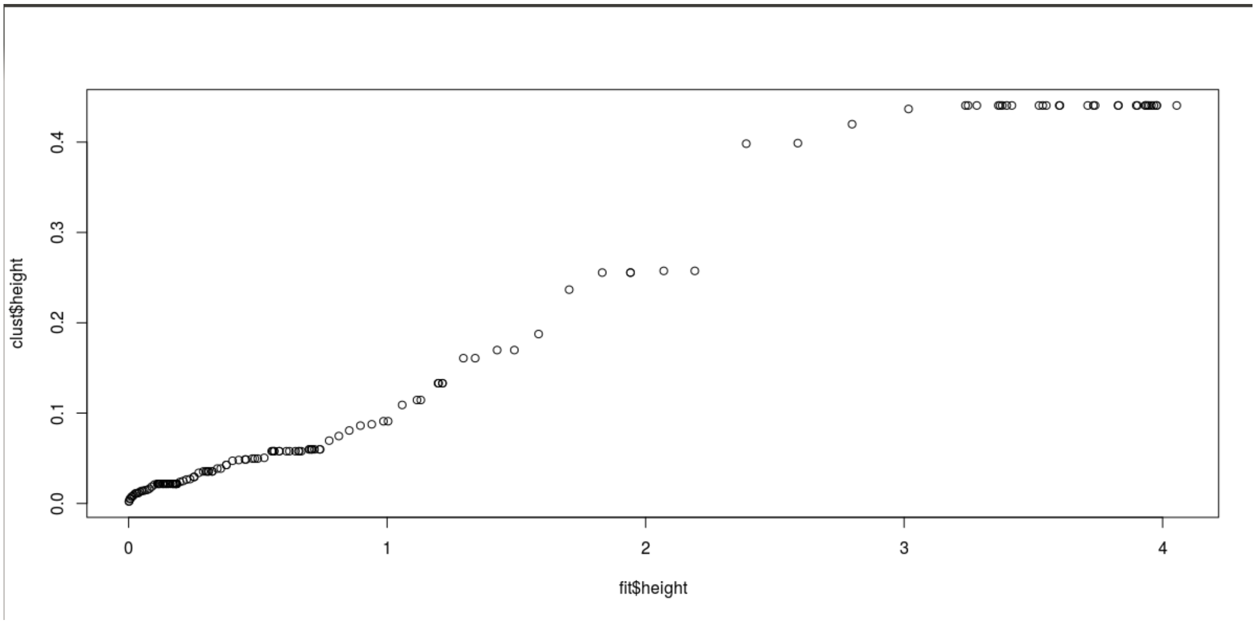
- The Merge Data by adjClustBand_heap

```
# hclust object using adjClustBand_heap function
# where s_scaled is the similatrity matrix
h<- ncol(s_scaled)
fit <- chaclust(s_scaled,h,f = 1)
plot(fit)
View(cbind(fit$merge ,height = fit$height))
```



	V1	V2	height
1	-28	-29	0.001064484
2	-30	-31	0.002372169
3	-40	-41	0.004869267
4	-3	-4	0.007599009
5	-35	-36	0.011270532
6	-2	4	0.015288583
7	-23	-24	0.019969093
8	-130	-131	0.025473758
9	-128	-129	0.031184896

However there is slight difference between the heights of clusters that are merged via chclust and adjBancClust_heap. To show the relation between the heights we see the scatter plot between there heights:



From the plot , as we can see its almost a straight line till a certain height, thus the adjBancClust_heap single linkage method is working fine and the height obtained is proportional to that obtained by rioja.

But after a certain height ie, 3 for adjBancClust_heap and 0.4 for chclust. The chclust function of rioja approximates all height above 0.4 to be at 0.4, thus we get a constant slope plot as seen.

In adjClustBand_heap that approsimation is not done hence we get a bit different result than rioja as seen in dendrograms formed.

Hence we can conclude that the applied single linkage method gives same result as that of rioja thus proving its correctness.

References:

- https://tel.archives-ouvertes.fr/tel-01288568/en
- http://www.geeksforgeeks.org/greedy-algorithms-set-5-prims-minimum-spanning-tree-mst-2/