Hierarchical Clustering

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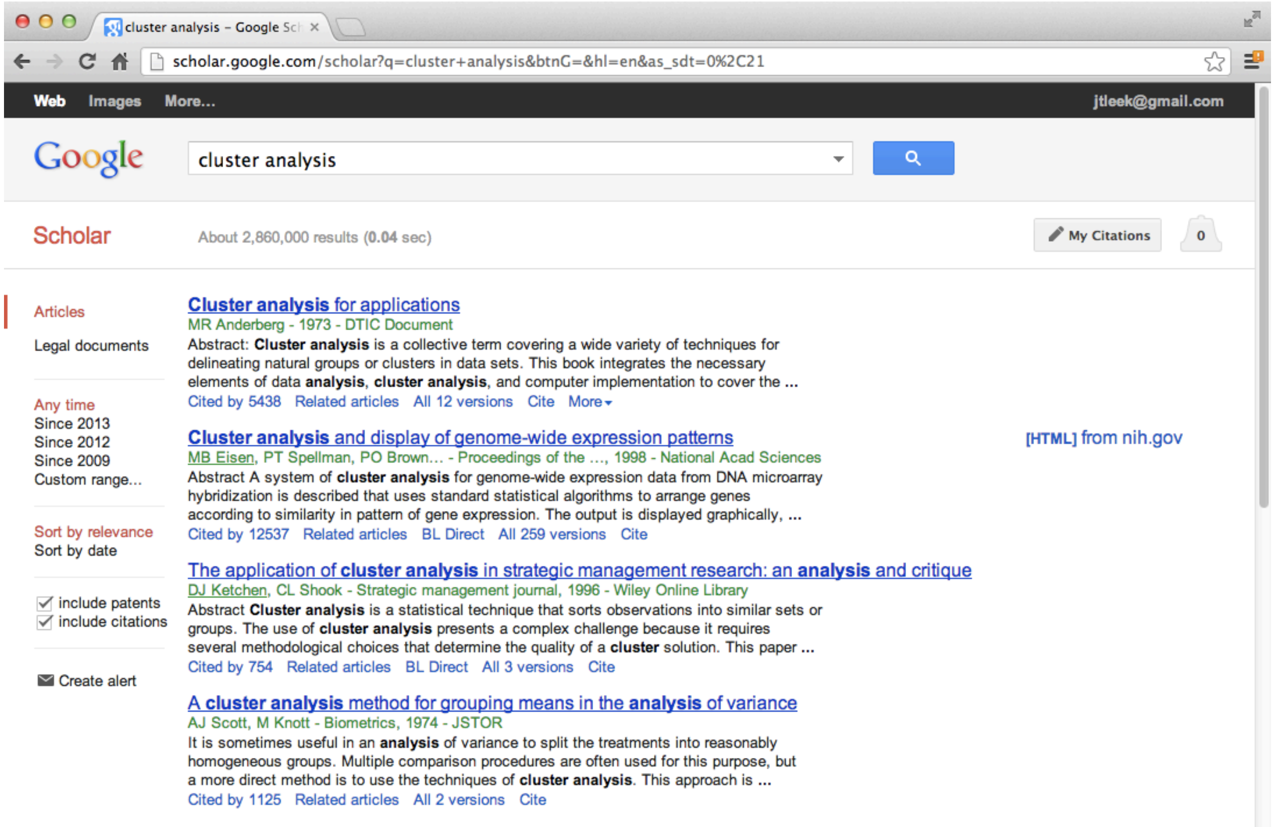
Can we find things that are close together?

Clustering organizes things that are **close** into groups

- How do we define close?
- How do we group things?
- How do we visualize the grouping?
- How do we interpret the grouping?

Hugely important/impactful



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Cluster analysis for applications
MR Anderberg - 1973 - DTIC Document
Abstract: **Cluster analysis** is a collective term covering a wide variety of techniques for delineating natural groups or clusters in data sets. This book integrates the necessary elements of data **analysis**, **cluster analysis**, and computer implementation to cover the ...
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Cluster analysis and display of genome-wide expression patterns
[HTML] from nih.gov
MB Eisen, PT Spellman, PO Brown... - Proceedings of the ..., 1998 - National Acad Sciences
Abstract A system of **cluster analysis** for genome-wide expression data from DNA microarray hybridization is described that uses standard statistical algorithms to arrange genes according to similarity in pattern of gene expression. The output is displayed graphically, ...
Cited by 12537 Related articles BL Direct All 259 versions Cite

The application of **cluster analysis** in strategic management research: an **analysis** and critique
DJ Ketchen, CL Shook - Strategic management journal, 1996 - Wiley Online Library
Abstract **Cluster analysis** is a statistical technique that sorts observations into similar sets or groups. The use of **cluster analysis** presents a complex challenge because it requires several methodological choices that determine the quality of a **cluster** solution. This paper ...
Cited by 754 Related articles BL Direct All 3 versions Cite

A **cluster analysis** method for grouping means in the **analysis** of variance
AJ Scott, M Knott - Biometrics, 1974 - JSTOR
It is sometimes useful in an **analysis** of variance to split the treatments into reasonably homogeneous groups. Multiple comparison procedures are often used for this purpose, but a more direct method is to use the techniques of **cluster analysis**. This approach is ...
Cited by 1125 Related articles All 2 versions Cite

http://scholar.google.com/scholar?hl=en&q=cluster+analysis&btnG=&as_sdt=1%2C21&as_sdtp=

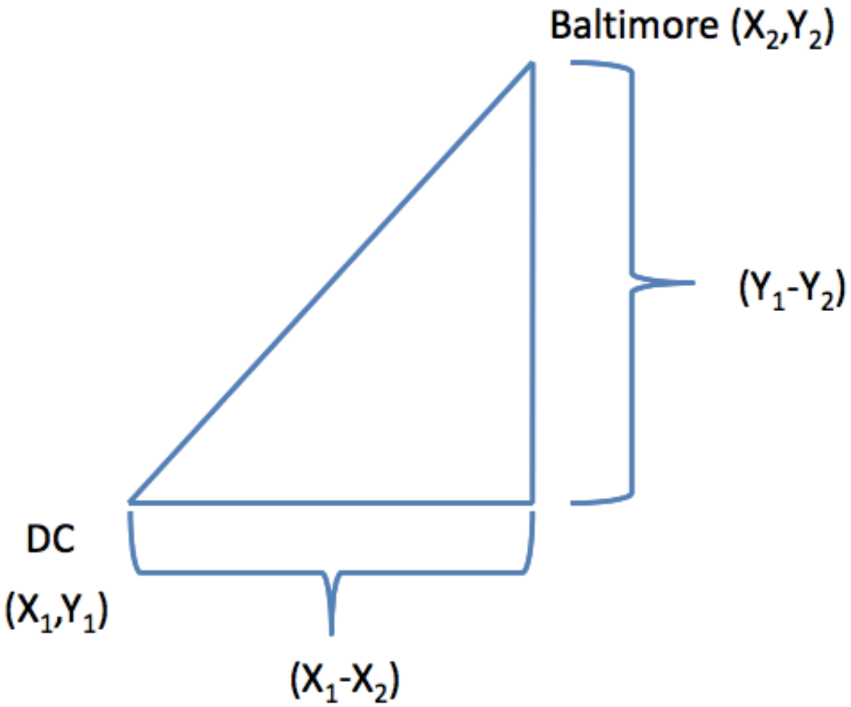
Hierarchical clustering

- An agglomerative approach
  - Find closest two things
  - Put them together
  - Find next closest
- Requires
  - A defined distance
  - A merging approach
- Produces
  - A tree showing how close things are to each other

How do we define close?

- Most important step
  - Garbage in -> garbage out
- Distance or similarity
  - Continuous - euclidean distance
  - Continuous - correlation similarity
  - Binary - manhattan distance
- Pick a distance/similarity that makes sense for your problem

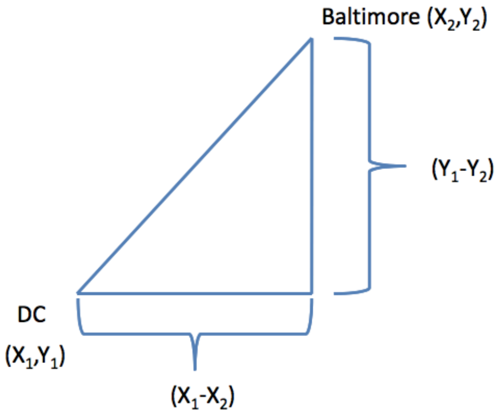
Example distances - Euclidean



http://rafalab.jhsph.edu/688/lec/lecture5-clustering.pdf

Example distances - Euclidean

$$\sqrt{(X_1 - X_2)^2 + (Y_1 - Y_2)^2}$$

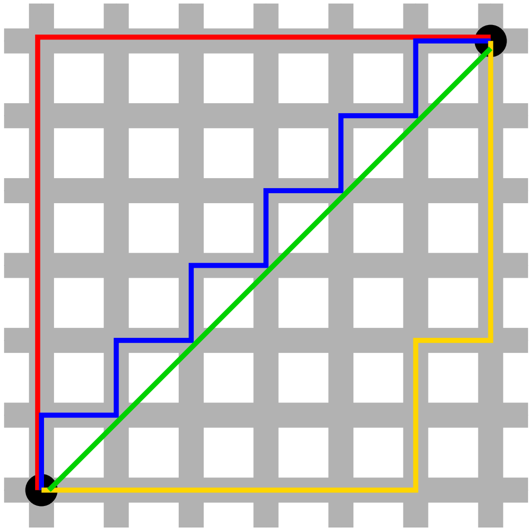


In general:

$$\sqrt{(A_1 - A_2)^2 + (B_1 - B_2)^2 + \ldots + (Z_1 - Z_2)^2}$$

http://rafalab.jhsph.edu/688/lec/lecture5-clustering.pdf

Example distances - Manhattan



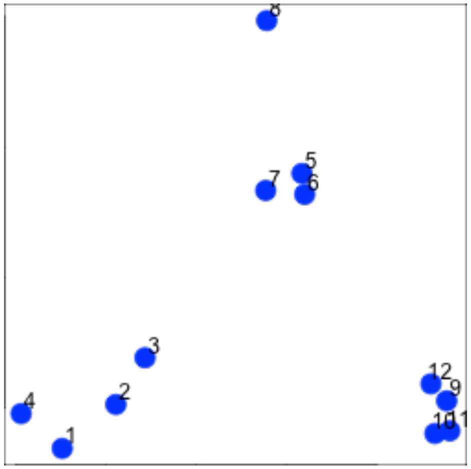
In general:

$$|A_1 - A_2| + |B_1 - B_2| + \ldots + |Z_1 - Z_2|$$

http://en.wikipedia.org/wiki/Taxicab_geometry

Hierarchical clustering - example

```
set.seed(1234)
par(mar = c(0, 0, 0, 0))
x <- rnorm(12, mean = rep(1:3, each = 4), sd = 0.2)
y <- rnorm(12, mean = rep(c(1, 2, 1), each = 4), sd = 0.2)
plot(x, y, col = "blue", pch = 19, cex = 2)
text(x + 0.05, y + 0.05, labels = as.character(1:12))
```



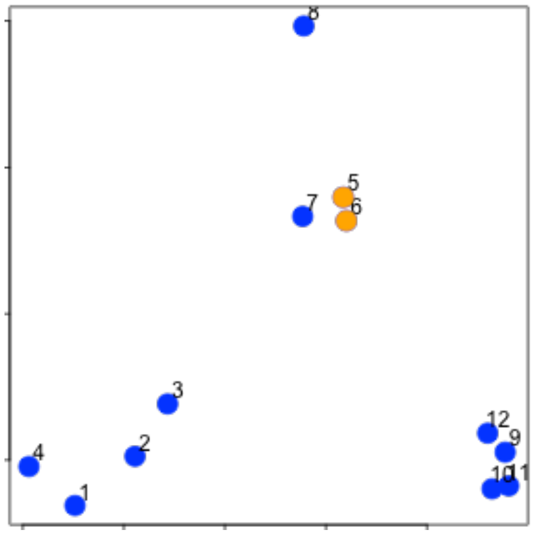
Hierarchical clustering - `dist`

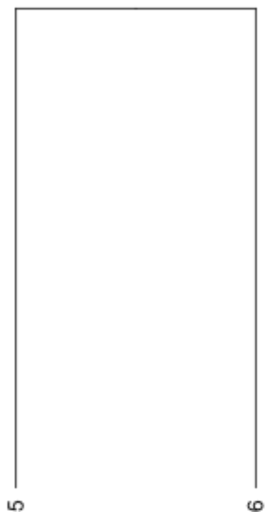
- Important parameters: *x*,*method*

```
dataFrame <- data.frame(x = x, y = y)
dist(dataFrame)
```

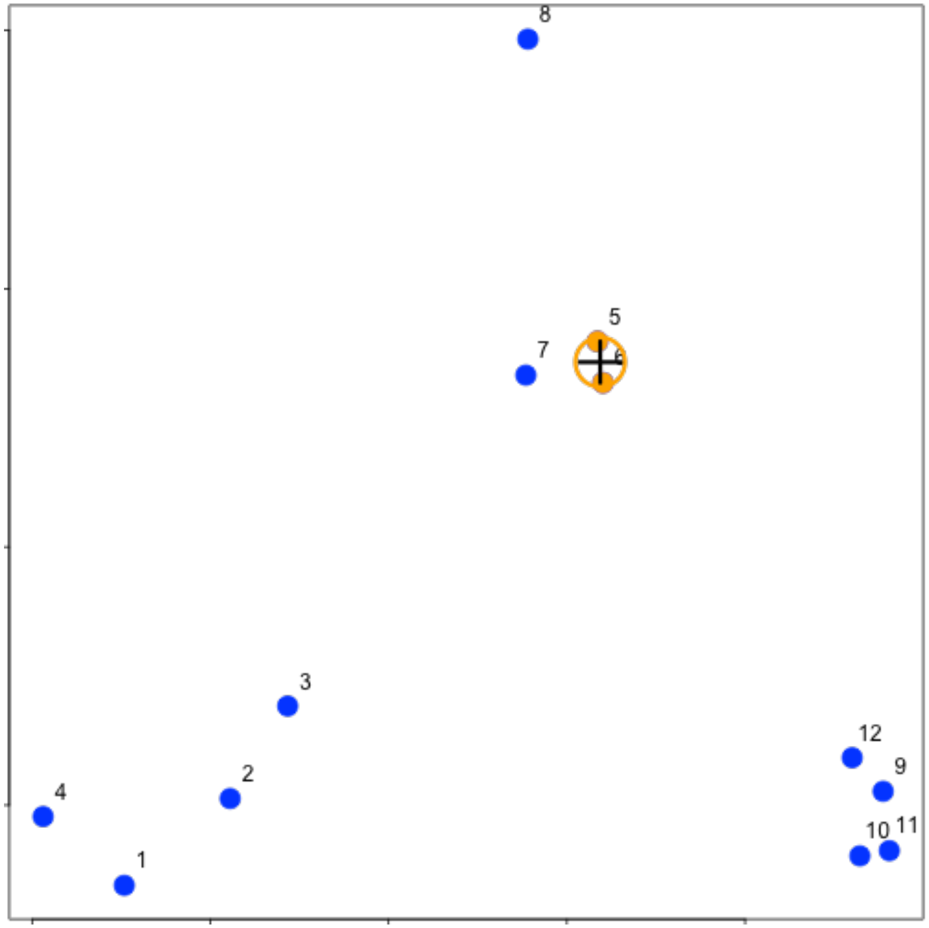
```
##          1       2       3       4       5       6       7       8       9
## 2  0.34121
## 3  0.57494 0.24103
## 4  0.26382 0.52579 0.71862
## 5  1.69425 1.35818 1.11953 1.80667
## 6  1.65813 1.31960 1.08339 1.78081 0.08150
## 7  1.49823 1.16621 0.92569 1.60132 0.21110 0.21667
## 8  1.99149 1.69093 1.45649 2.02849 0.61704 0.69792 0.65063
## 9  2.13630 1.83168 1.67836 2.35676 1.18350 1.11500 1.28583 1.76461
## 10 2.06420 1.76999 1.63110 2.29239 1.23848 1.16550 1.32063 1.83518 0.14090
## 11 2.14702 1.85183 1.71074 2.37462 1.28154 1.21077 1.37370 1.86999 0.11624
## 12 2.05664 1.74663 1.58659 2.27232 1.07701 1.00777 1.17740 1.66224 0.10849
##         10      11
## 2
## 3
## 4
## 5
```

Hierarchical clustering - #1

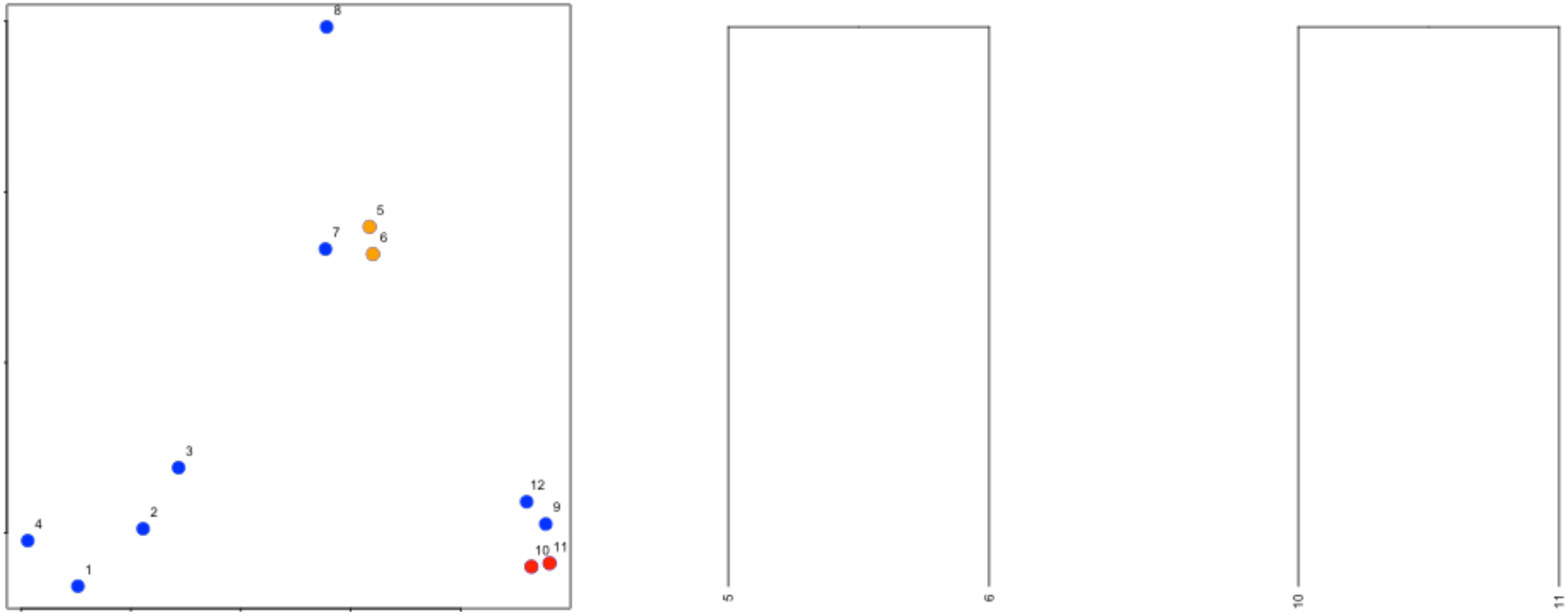




Hierarchical clustering - #2

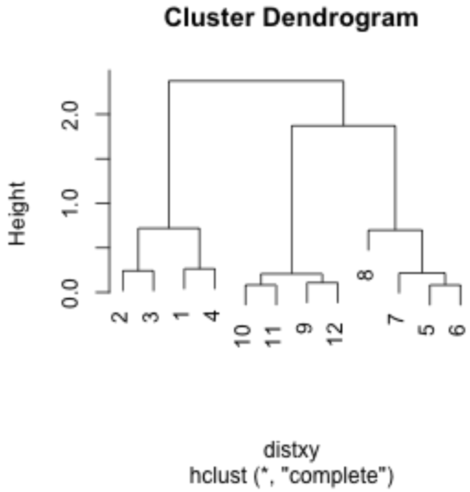


Hierarchical clustering - #3



Hierarchical clustering - hclust

```
dataFrame <- data.frame(x = x, y = y)
distxy <- dist(dataFrame)
hClustering <- hclust(distxy)
plot(hClustering)
```

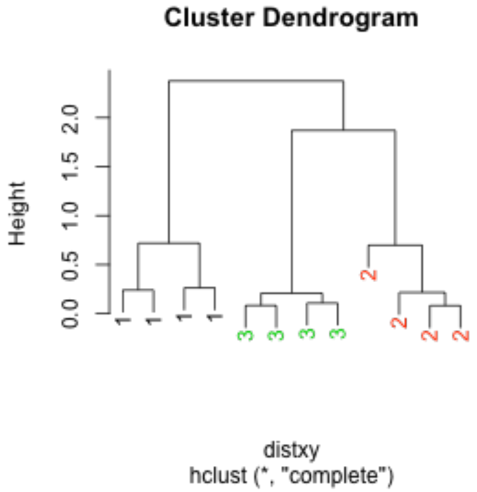


Prettier dendrograms

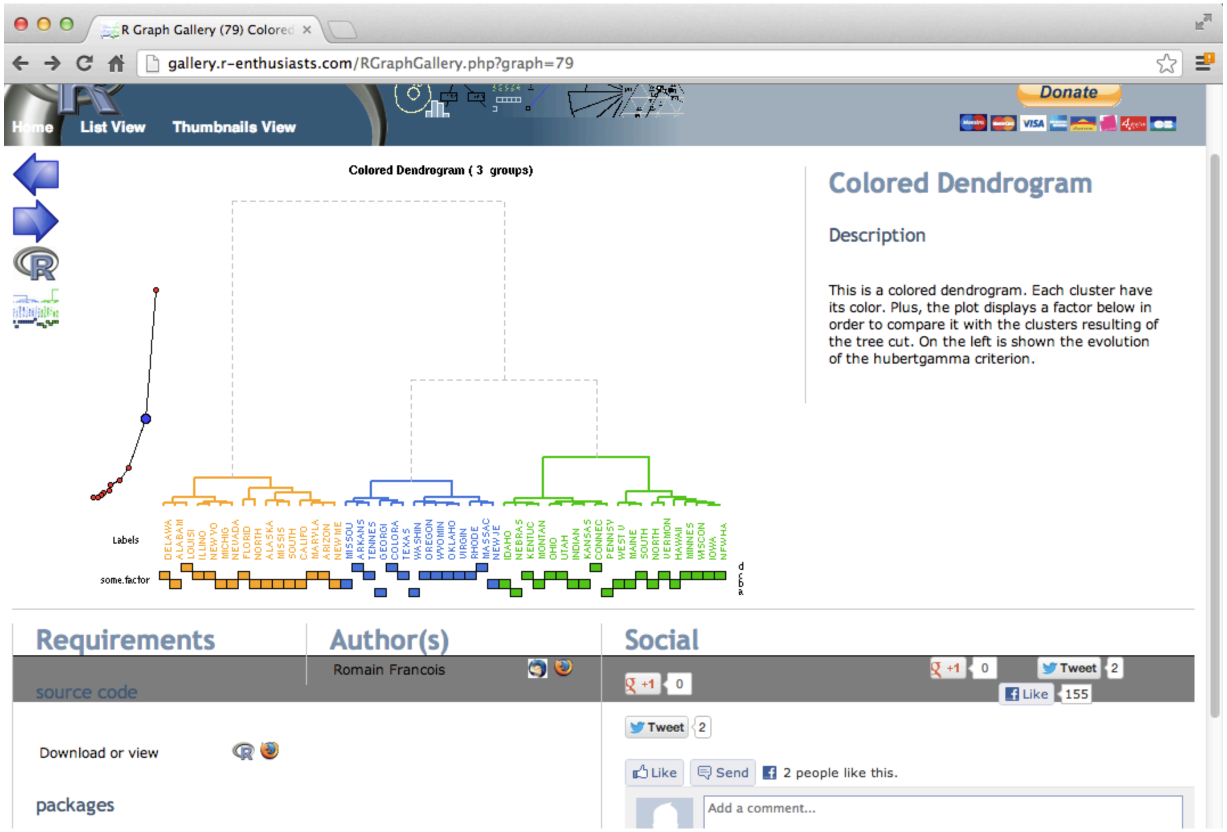
```
myplclust <- function(hclust, lab = hclust$labels, lab.col = rep(1, length(hclust$labels)),
    hang = 0.1, ...) {
    ## modifiction of plclust for plotting hclust objects *in colour*!  Copyright
    ## Eva KF Chan 2009 Arguments: hclust: hclust object lab: a character vector
    ## of labels of the leaves of the tree lab.col: colour for the labels;
    ## NA=default device foreground colour hang: as in hclust & plclust Side
    ## effect: A display of hierarchical cluster with coloured leaf labels.
    y <- rep(hclust$height, 2)
    x <- as.numeric(hclust$merge)
    y <- y[which(x < 0)]
    x <- x[which(x < 0)]
    x <- abs(x)
    y <- y[order(x)]
    x <- x[order(x)]
    plot(hclust, labels = FALSE, hang = hang, ...)
    text(x = x, y = y[hclust$order] - (max(hclust$height) * hang), labels = lab[hclust$order],
        col = lab.col[hclust$order], srt = 90, adj = c(1, 0.5), xpd = NA, ...)
}
```

Pretty dendrograms

```
dataFrame <- data.frame(x = x, y = y)
distxy <- dist(dataFrame)
hClustering <- hclust(distxy)
myplclust(hClustering, lab = rep(1:3, each = 4), lab.col = rep(1:3, each = 4))
```



Even Prettier dendrograms



Colored Dendrogram

Description

This is a colored dendrogram. Each cluster have its color. Plus, the plot displays a factor below in order to compare it with the clusters resulting of the tree cut. On the left is shown the evolution of the hubertgamma criterion.

Requirements

source code

Download or view

packages

Author(s)

Romain Francois

Social

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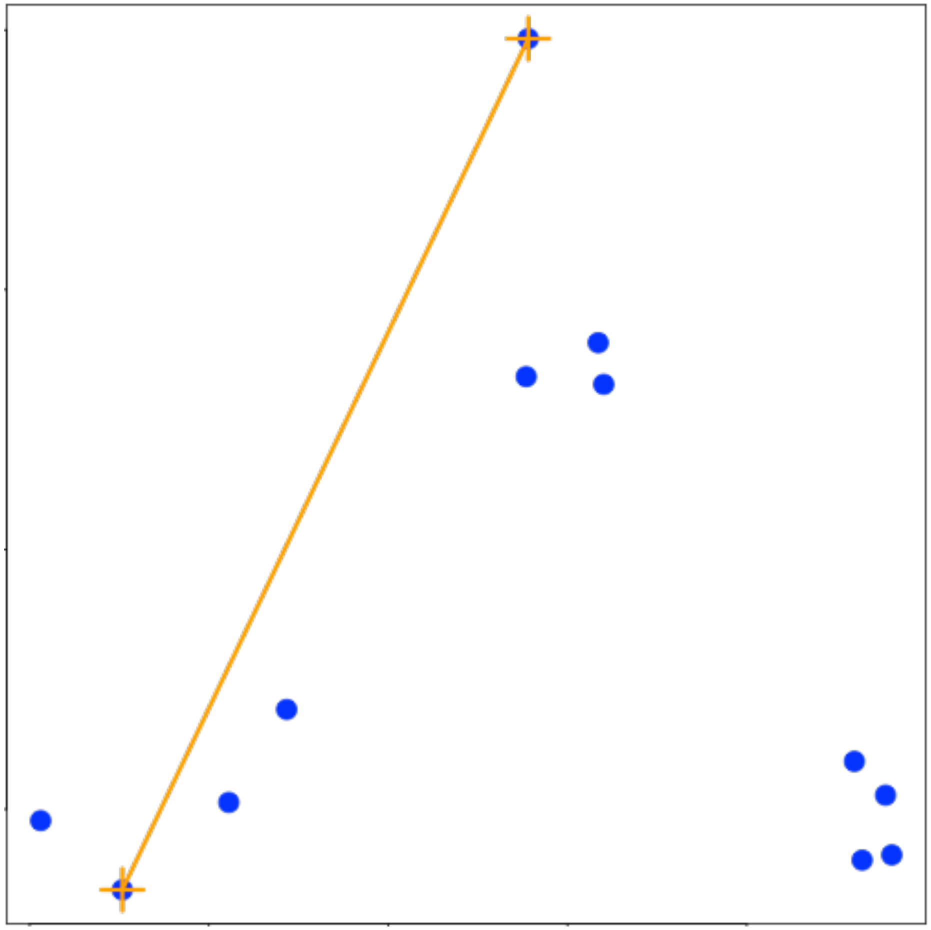
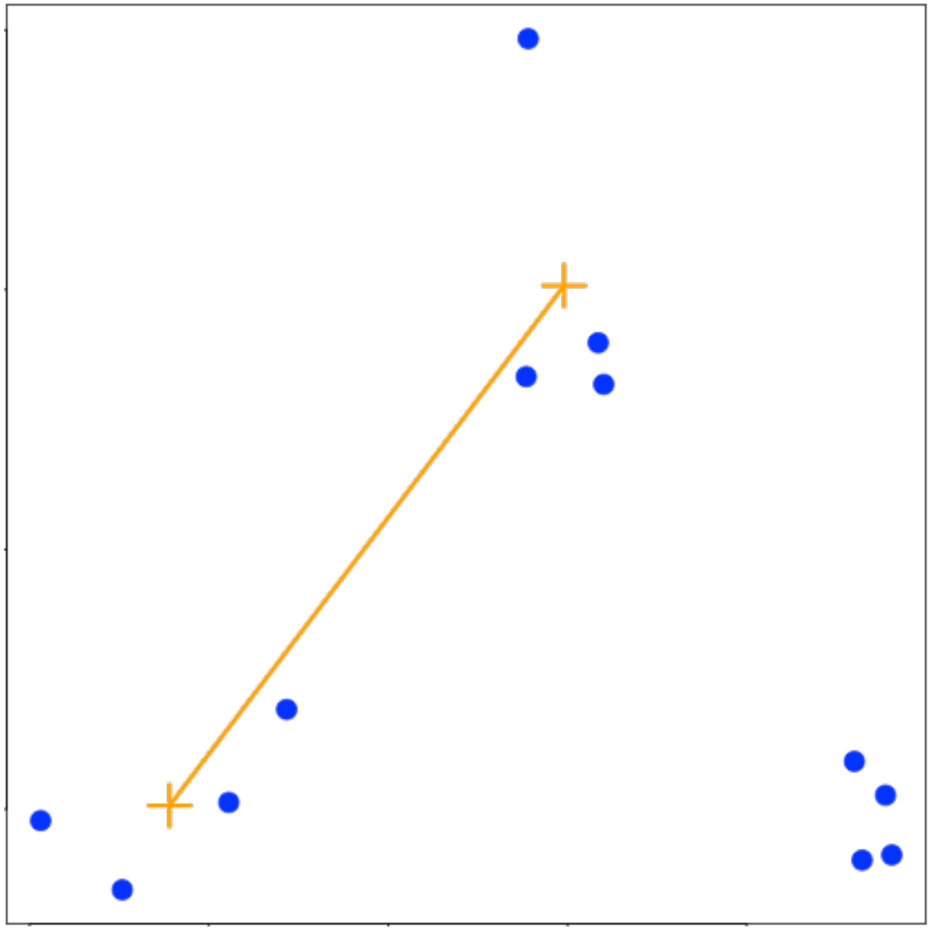
http://gallery.r-enthusiasts.com/RGraphGallery.php?graph=79

Merging points - complete

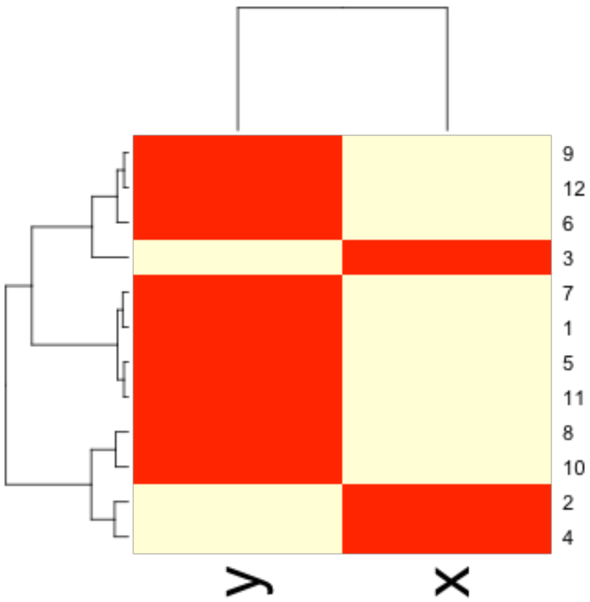


Merging points - average



heatmap()

```
dataFrame <- data.frame(x = x, y = y)
set.seed(143)
dataMatrix <- as.matrix(dataFrame)[sample(1:12), ]
heatmap(dataMatrix)
```



Notes and further resources

- Gives an idea of the relationships between variables/observations
- The picture may be unstable
  - Change a few points
  - Have different missing values
  - Pick a different distance
  - Change the merging strategy
  - Change the scale of points for one variable
- But it is deterministic
- Choosing where to cut isn't always obvious
- Should be primarily used for exploration
- Rafa's Distances and Clustering Video
- Elements of statistical learning