

Hierarchical clustering

Jeffrey Leek, Assistant Professor of Biostatistics
Johns Hopkins Bloomberg School of Public Health

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

The screenshot shows a Google Scholar search results page for the query "cluster analysis". The browser address bar shows the URL: scholar.google.com/scholar?q=cluster+analysis&btnG=&hl=en&as_sdt=0%2C21. The search results show approximately 2,860,000 results. The left sidebar contains filters for "Articles", "Legal documents", "Any time" (with sub-options: Since 2013, Since 2012, Since 2009, Custom range...), "Sort by relevance" (with sub-option: Sort by date), and checkboxes for "include patents" and "include citations". There is also a "Create alert" button. The main content area lists several articles:

- 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 ...
Cited by 5438 Related articles All 12 versions Cite More
- Cluster analysis and display of genome-wide expression patterns**
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_sdt=1%2C21

3/21

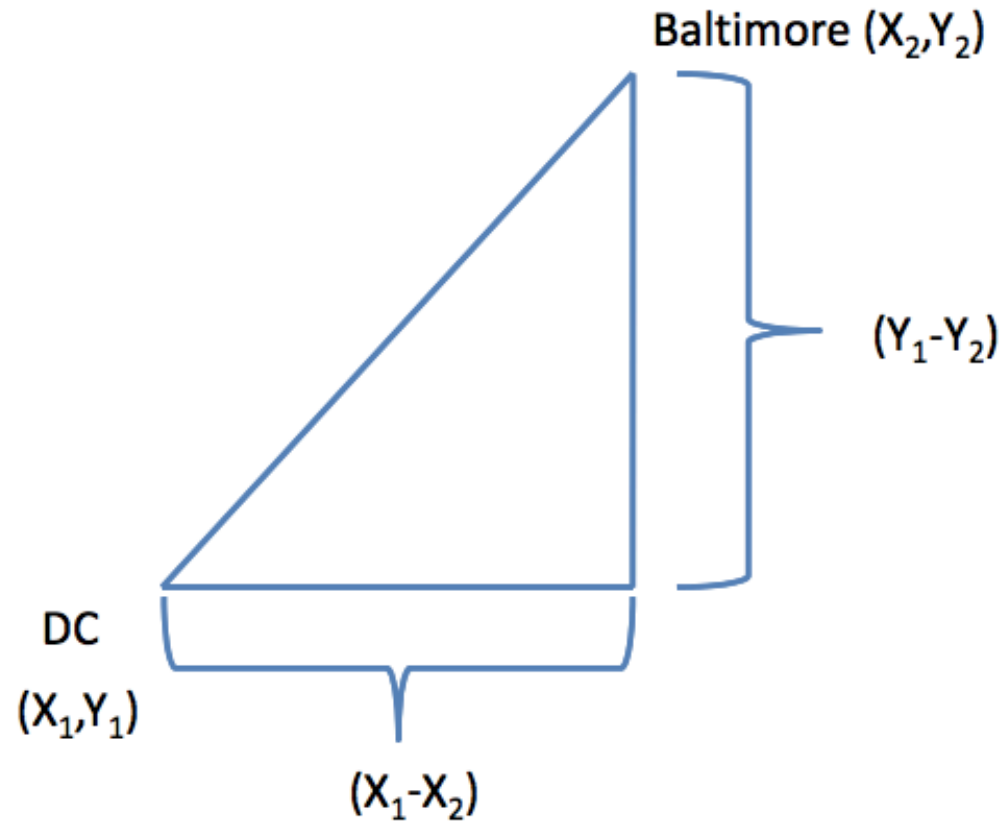
Hierarchical clustering

- 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

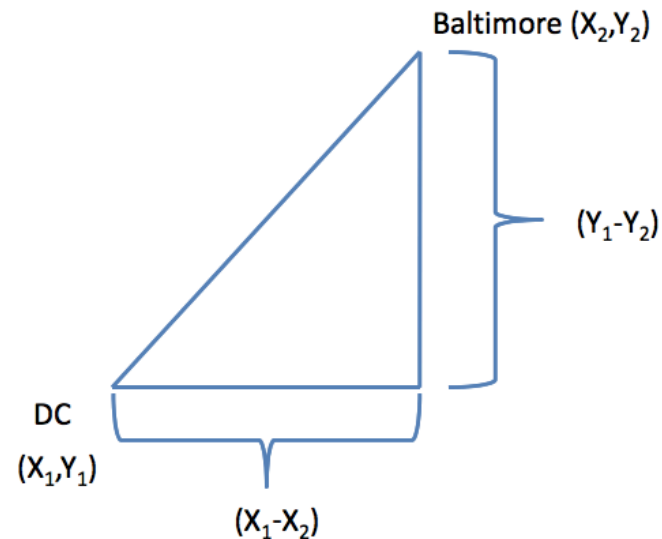
Example distances - Euclidean



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

Example distances - Euclidean

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

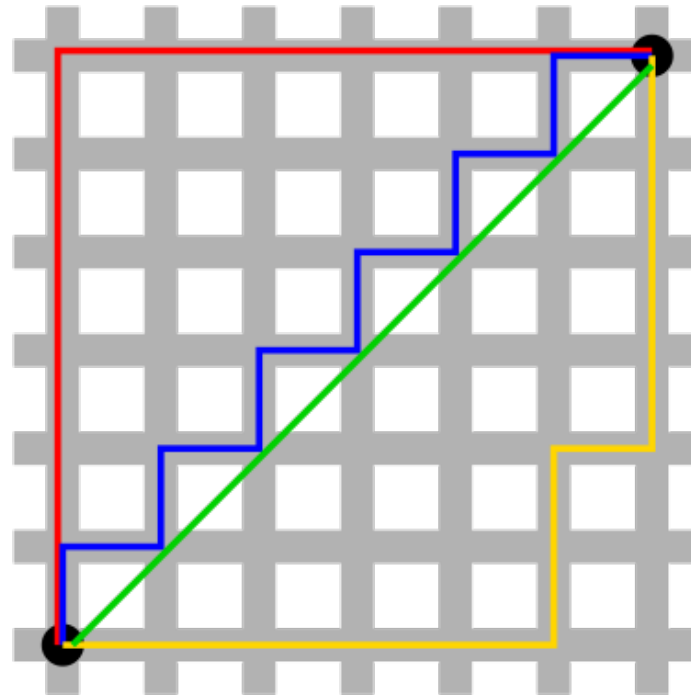


In general:

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

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

Example distances - Manhattan



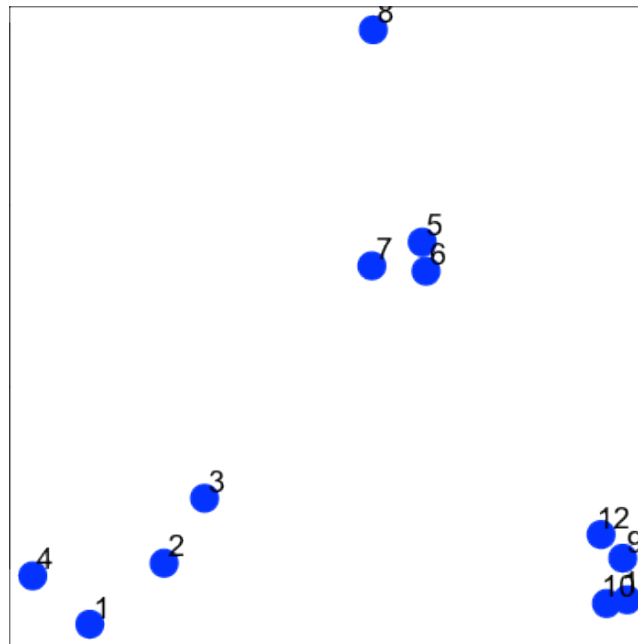
In general:

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

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

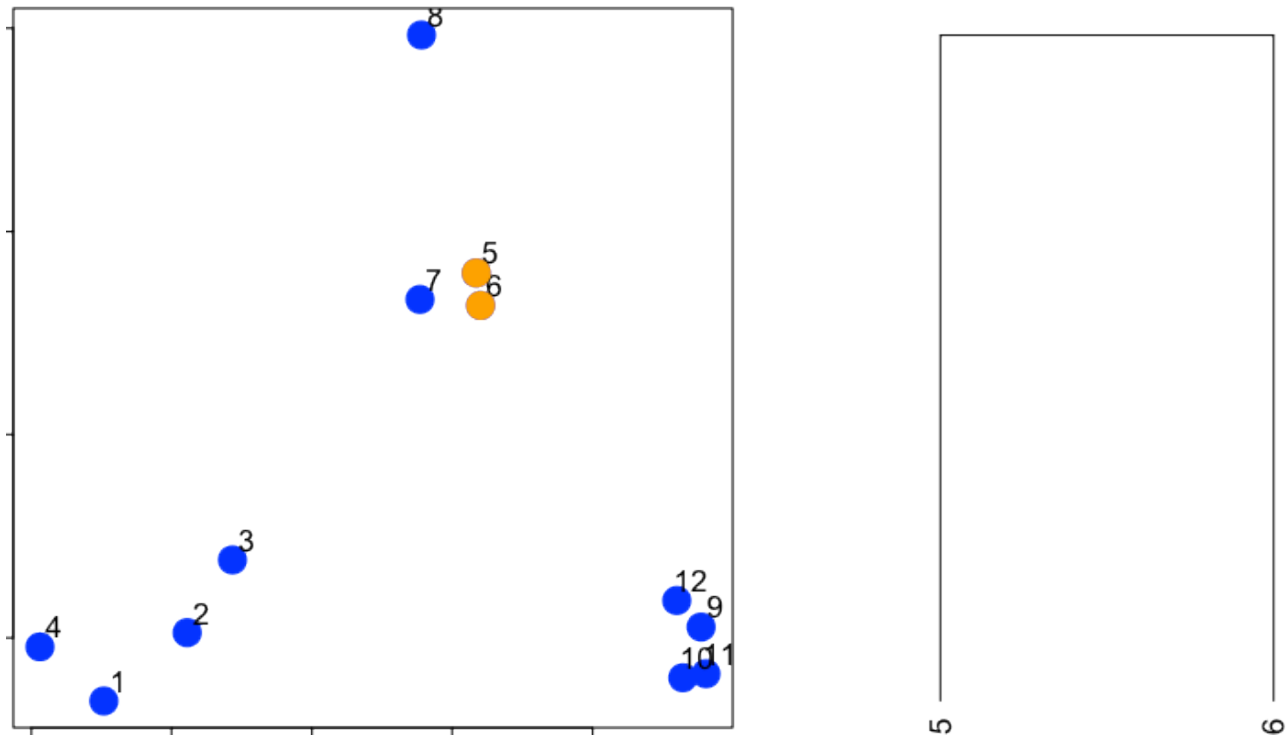
- Important parameters: *x, method*

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

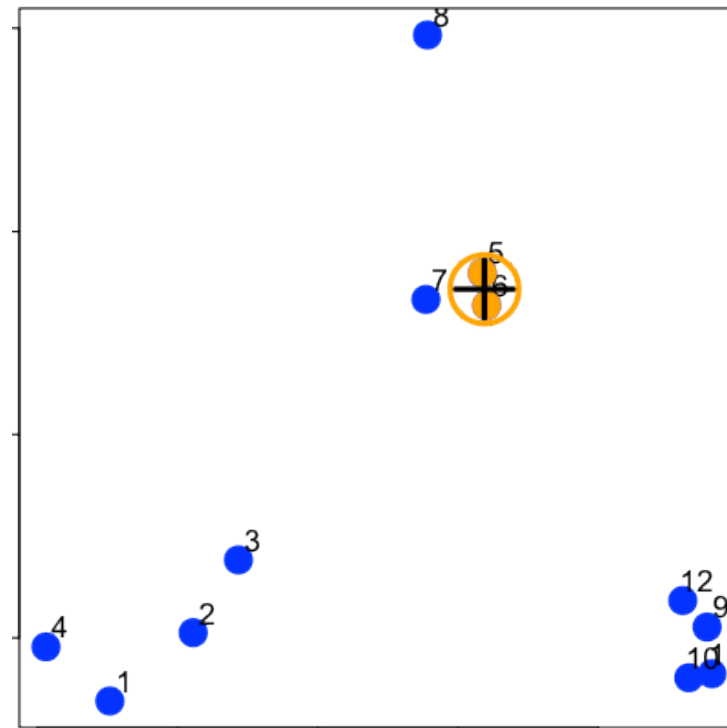
```

      1      2      3      4      5      6      7      8      9      10      11
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 0.08318
12 2.05664 1.74663 1.58659 2.27232 1.07701 1.00777 1.17740 1.66224 0.10849 0.19129 0.20803
```

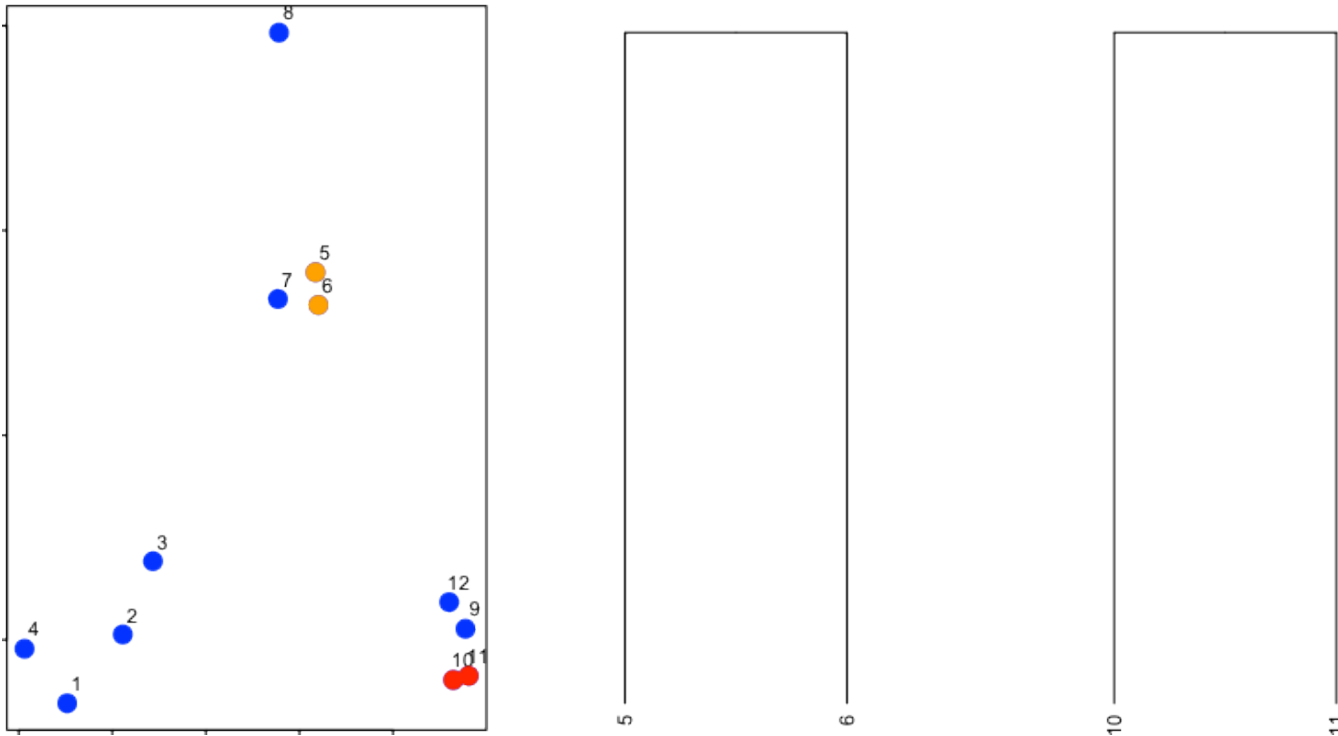
Hierarchical clustering - #1



Hierarchical clustering - #2

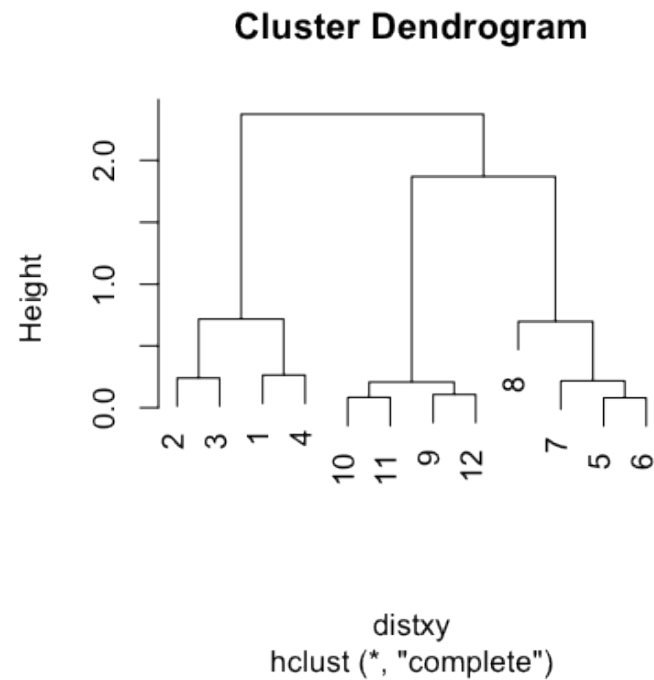


Hierarchical clustering - #3



Hierarchical clustering - hclust

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

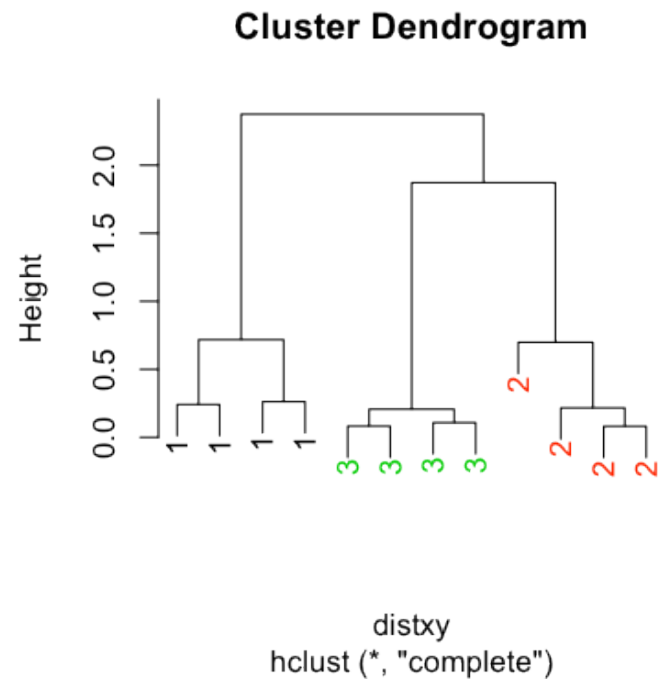


Prettier dendrograms

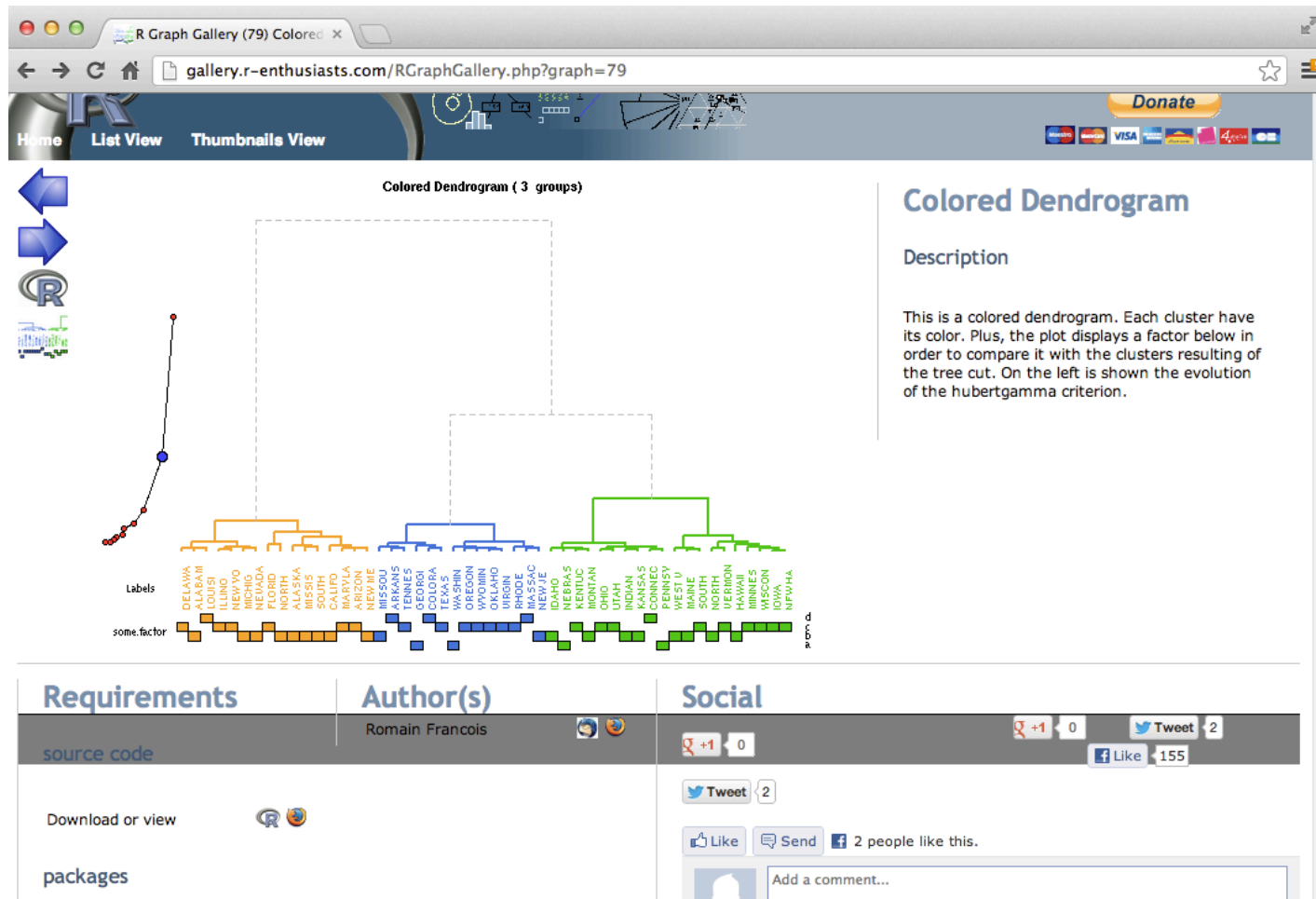
```
myplclust <- function( hclust, lab=hclust$labels, lab.col=rep(1,length(hclust$labels)), hang=0.1,...
  ## modifiction of plclust for plotting hclust objects *in colour*!
  ## Copyright Eva KF Chan 2009
  ## Arguments:
  ##   hclust:      hclust object
  ##   lab:         a character vector of labels 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, ... )
}
```

Hierarchical clustering - hclust

```
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))
```

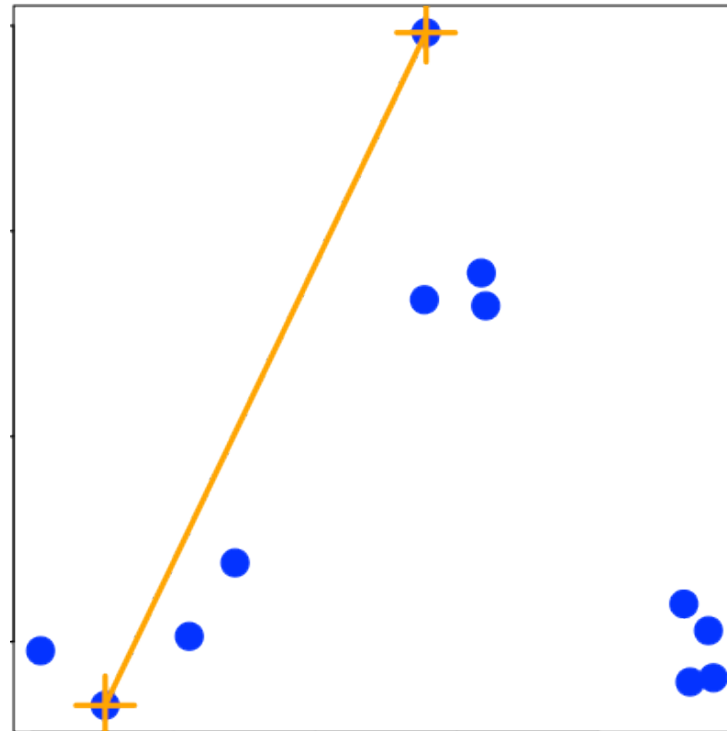


Even Prettier dendrograms

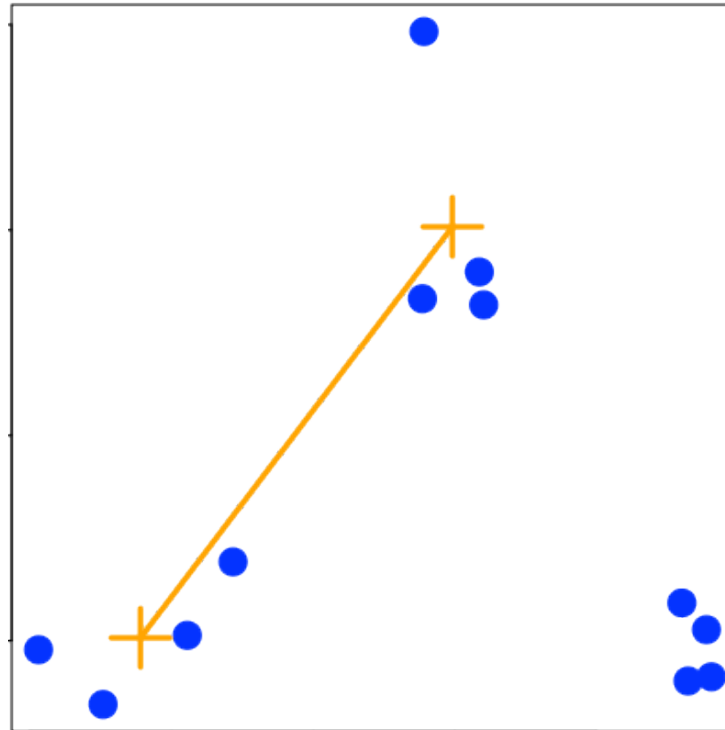


<http://gallery.r-enthusiasts.com/RGraphGallery.php?graph=79>

Merging points - complete

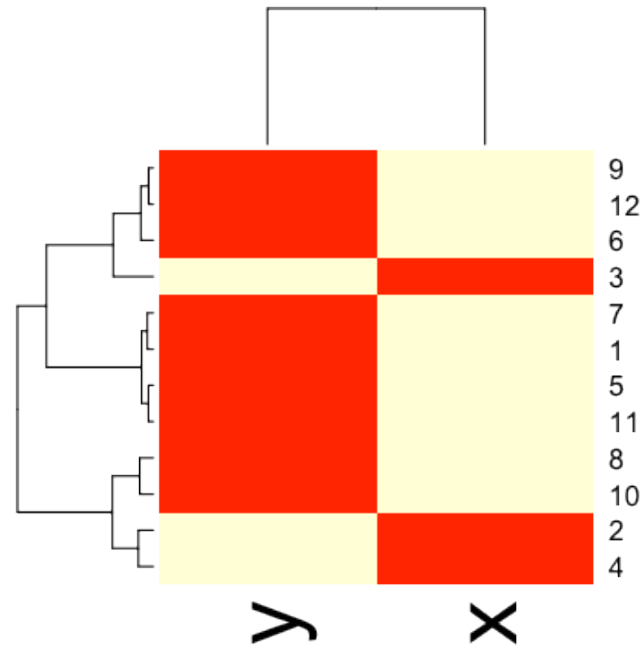


Merging points - average



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](#)