Hierarchical Clustering

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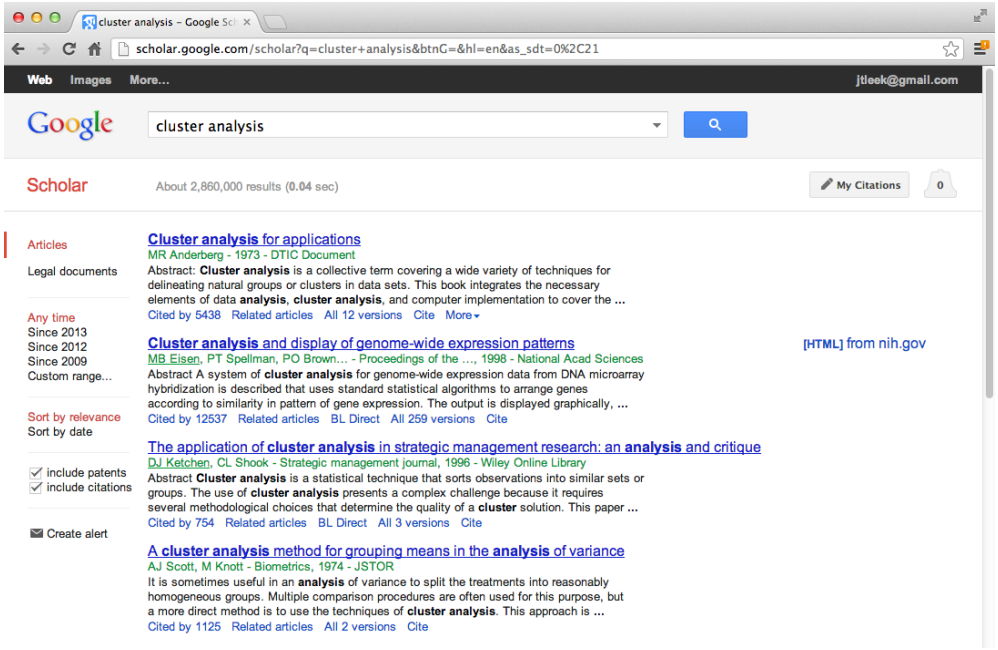
Can we find things that are close together?

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



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

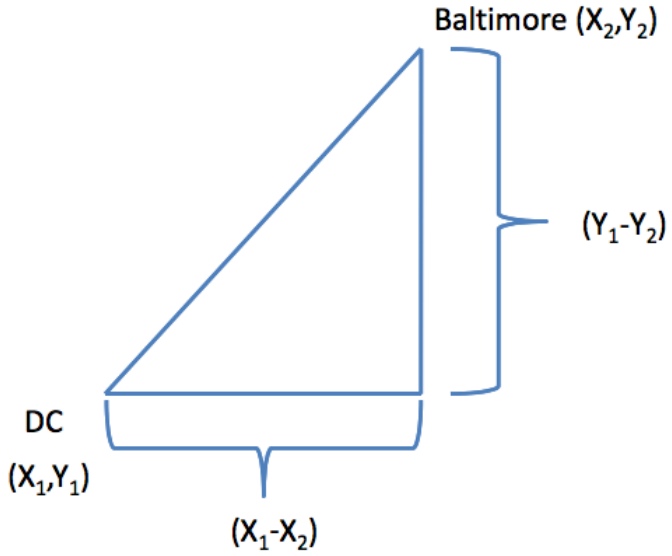
Hierarchical clustering

- 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

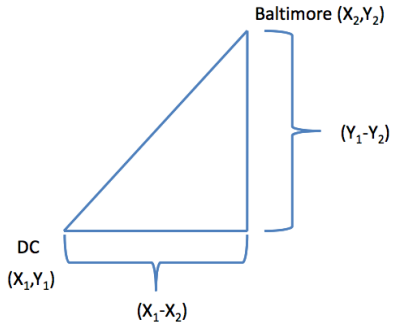
Example distances - Euclidean



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

Example distances - Euclidean

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

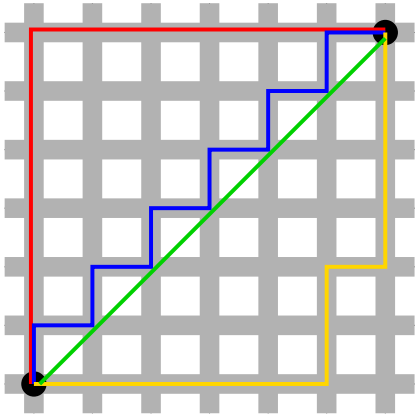


In general:

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

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

Example distances - Manhattan



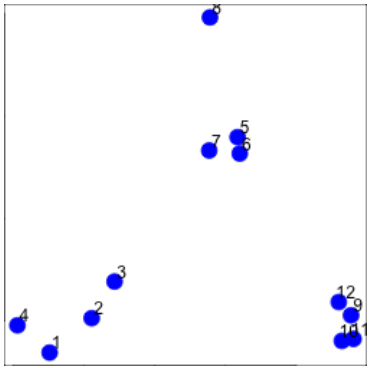
In general:

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

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))
```



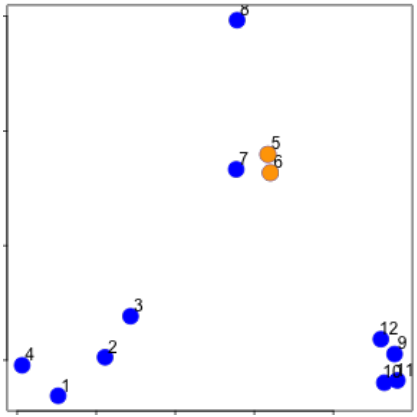
Hierarchical clustering - `dist`

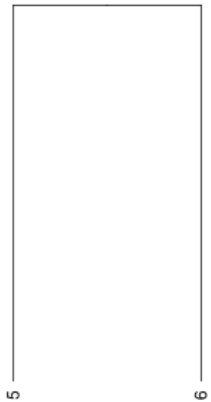
- Important parameters: *x*,*method*

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

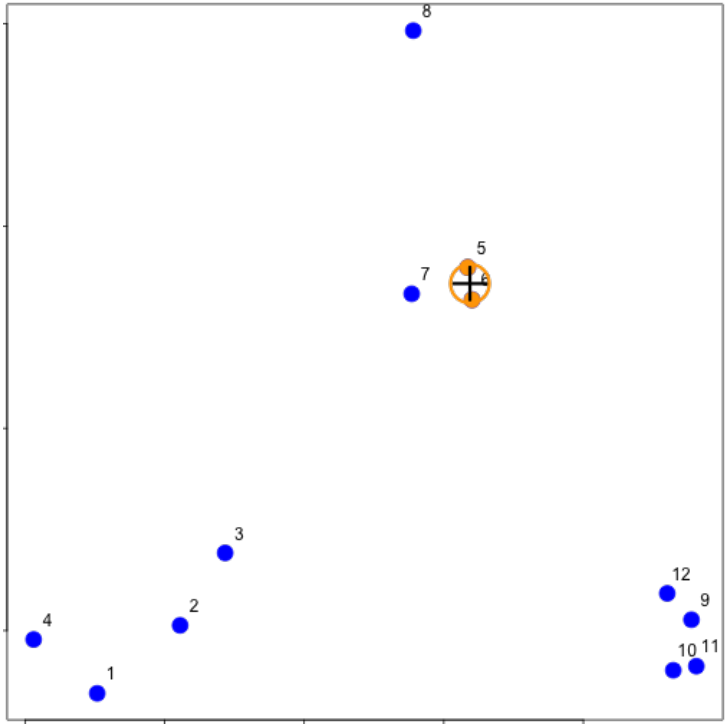
```
##          1       2       3       4       5       6       7       8       9
## 2  0.34121
## 3  0.57494 0.24103
## 4  0.26382 0.52579 0.71862
## 5  1.69425 1.35818 1.11953 1.80667
## 6  1.65813 1.31960 1.08339 1.78081 0.08150
## 7  1.49823 1.16621 0.92569 1.60132 0.21110 0.21667
## 8  1.99149 1.69093 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
```

Hierarchical clustering - #1

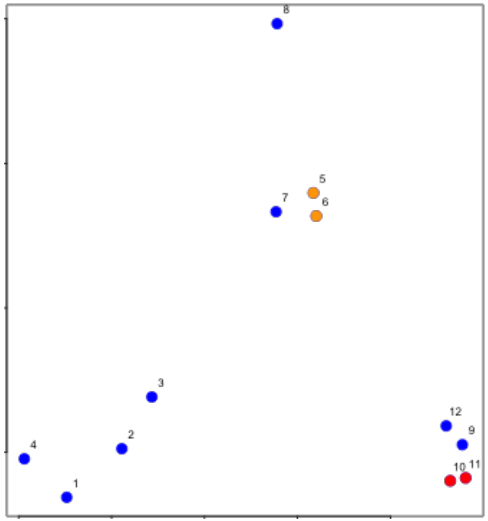


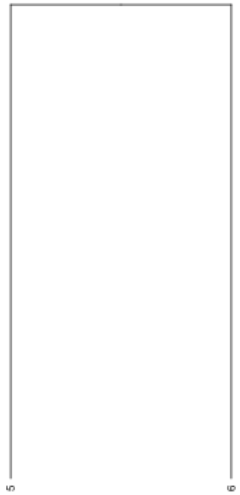


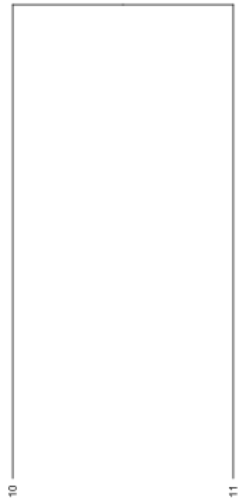
Hierarchical clustering - #2



Hierarchical clustering - #3

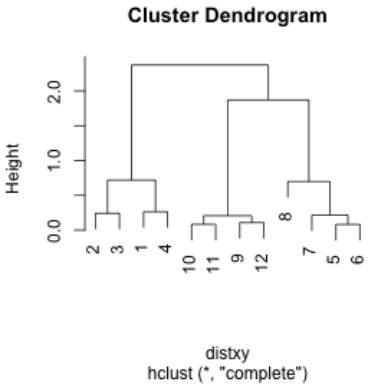






Hierarchical clustering - hclust

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

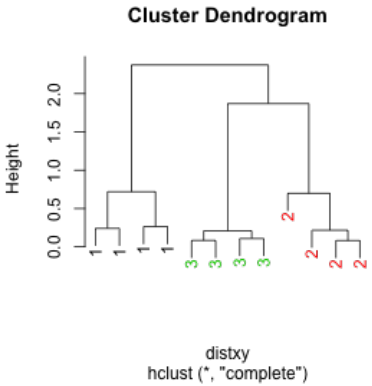


Prettier dendrograms

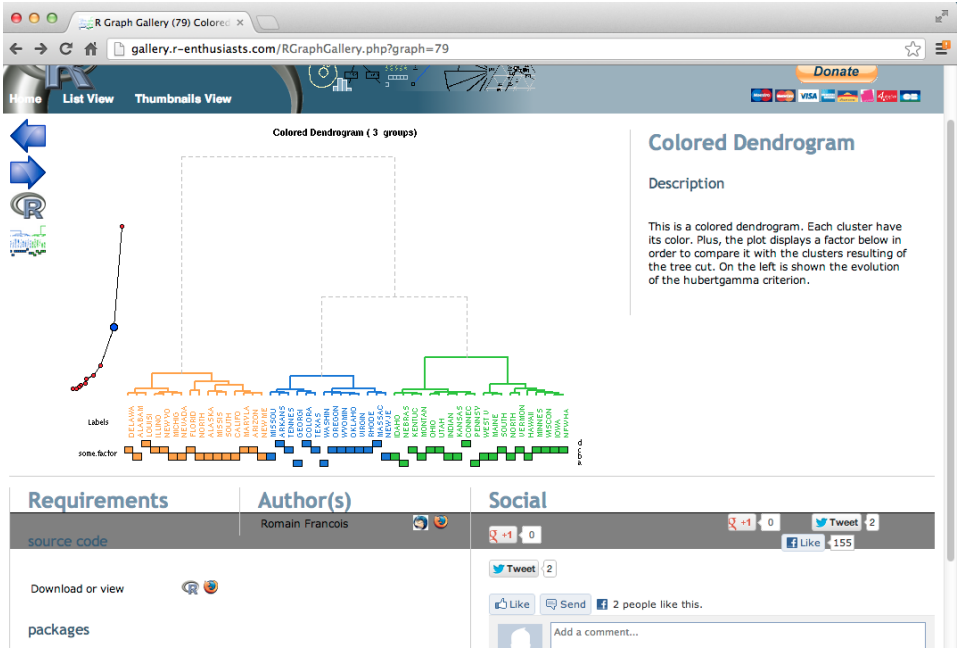
```
myplclust <- function(hclust, lab = hclust$labels, lab.col = rep(1, length(hclust$labels)),
    hang = 0.1, ...) {
    ## modifiction of plclust for plotting hclust objects *in colour*!  Copyright
    ## Eva KF Chan 2009 Arguments: hclust: hclust object lab: a character vector
    ## of labels of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

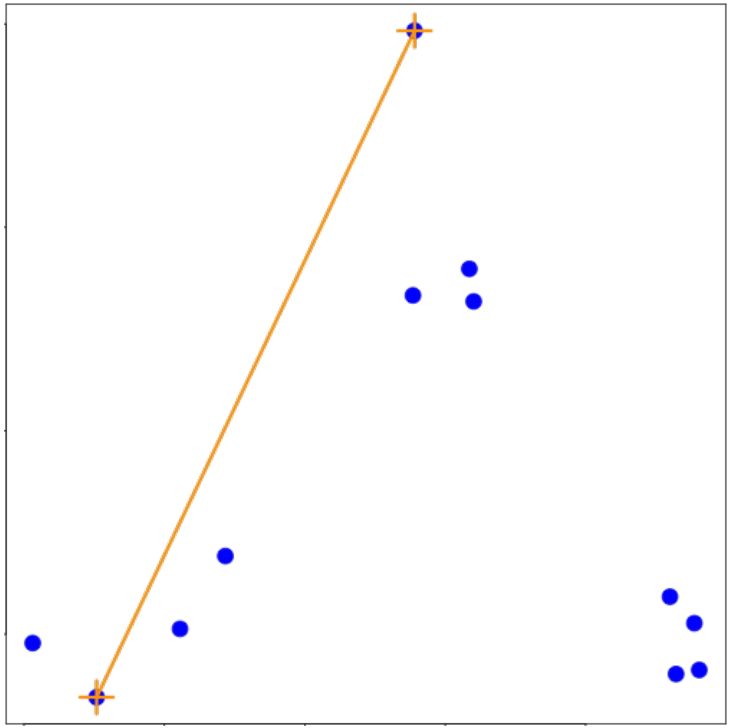


Even Prettier dendrograms

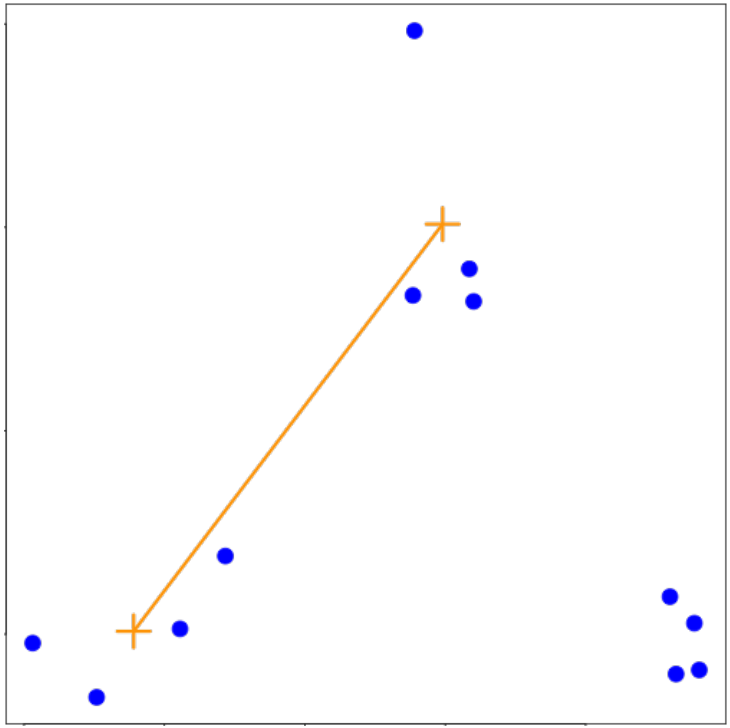


http://gallery.r-enthusiasts.com/RGraphGallery.php?graph=79

Merging points - complete

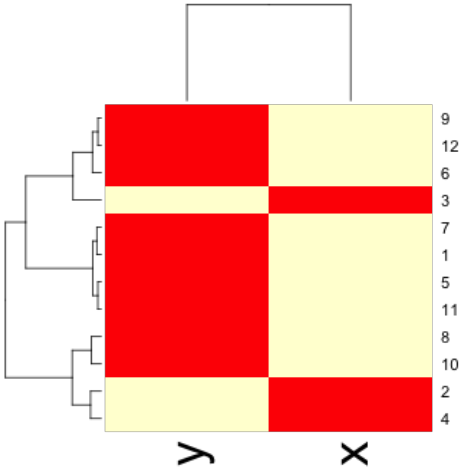


Merging points - average



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