SML 201 – Week 12

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Contents

High-Dimensional Data

Definition

High-dimensional data (HD data) typically refers to data sets where *many variables* are simultaneously measured on any number of observations.

The number of variables is often represented by p and the number of observations by n.

HD data are collected into a $p \times n$ or $n \times p$ matrix.

Many methods exist for "large p, small n" data sets.

Examples

- Clinical studies
- Genomics (e.g., gene expression)
- Neuroimaging (e.g., fMRI)
- Finance (e.g., time series)
- Environmental studies
- Internet data (e.g., Netflix movie ratings)

Big Data vs HD Data

"Big data" are data sets that cannot fit into a standard computer's memory.

HD data were defined above.

They are not necessarily equivalent.

Cluster Analysis

Definition

Cluster analysis is the process of grouping objects (variables or observations) into groups based on measures of similarity.

Similar objects are placed in the same cluster, and dissimilar objects are placed in different clusters.

Cluster analysis methods are typically described by algorithms (rather than models or formulas).

Types of Clustering

Clustering can be categorized in various ways:

- Hard vs. soft
- Top-down vs bottom-up
- Partitioning vs. hierarchical agglomerative

Top-Down vs Bottom-Up

We will discuss two of the major clustering methods – *hierarchical clustering* and *K-means clustering*.

Hierarchical clustering is an example of *bottom-up* clustering in that the process begings with each object being its own cluster and then objects are joined in a hierarchical manner into larger and larger clusters.

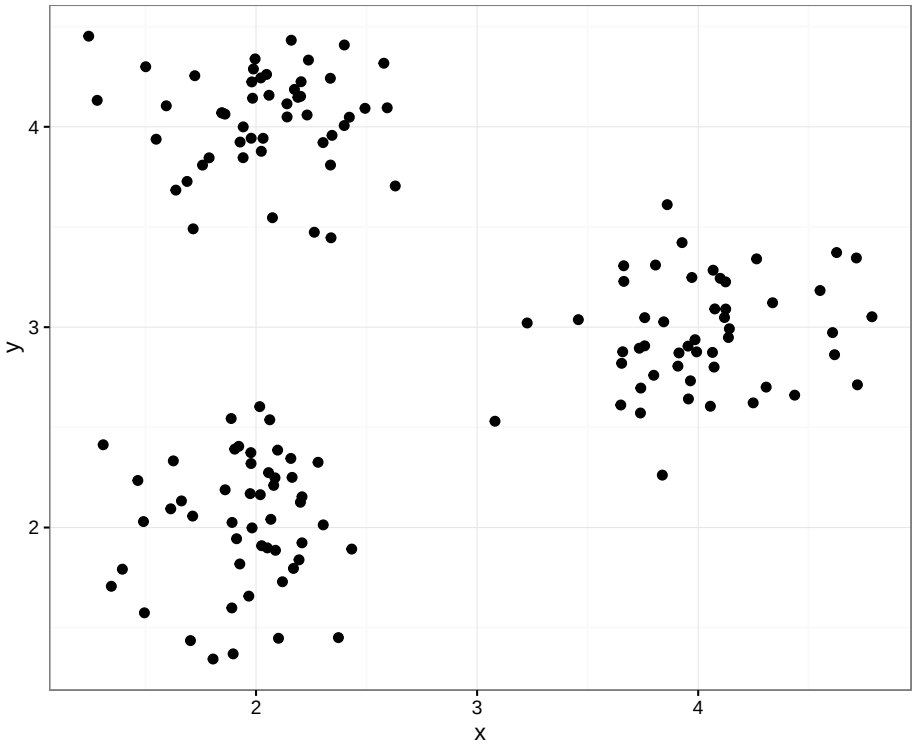
K-means clustering is an example of *top-down* clustering in that the number of clusters is chosen beforehand and then object are assigned to one of the K clusters.

Challenges

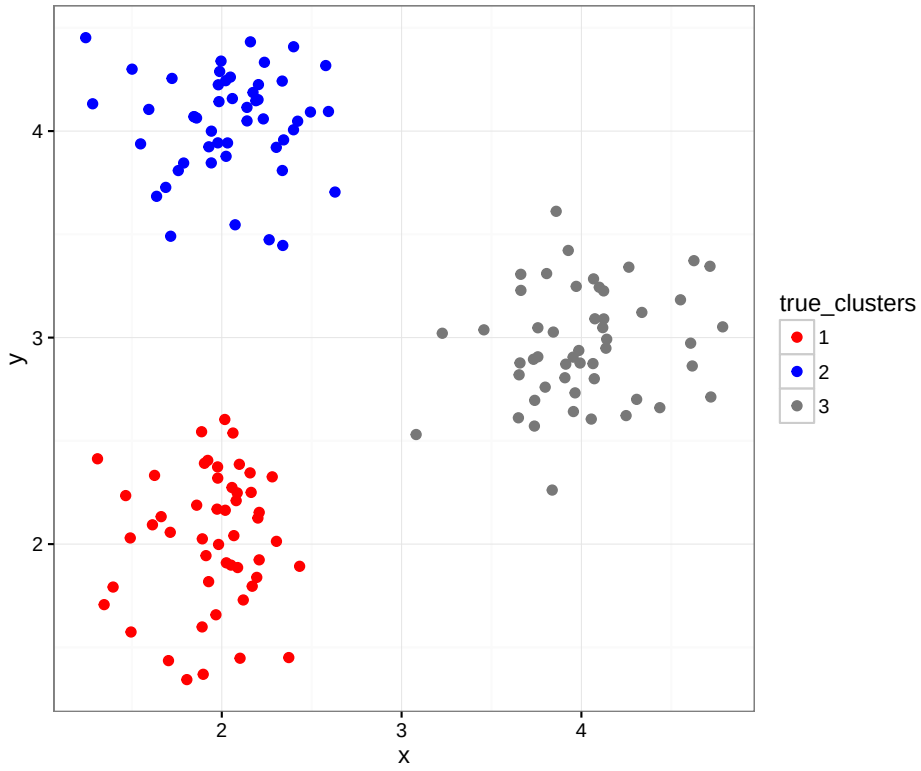
- Cluster analysis method
- Distance measure
- Number of clusters
- Convergence issues

Illustrative Data Sets

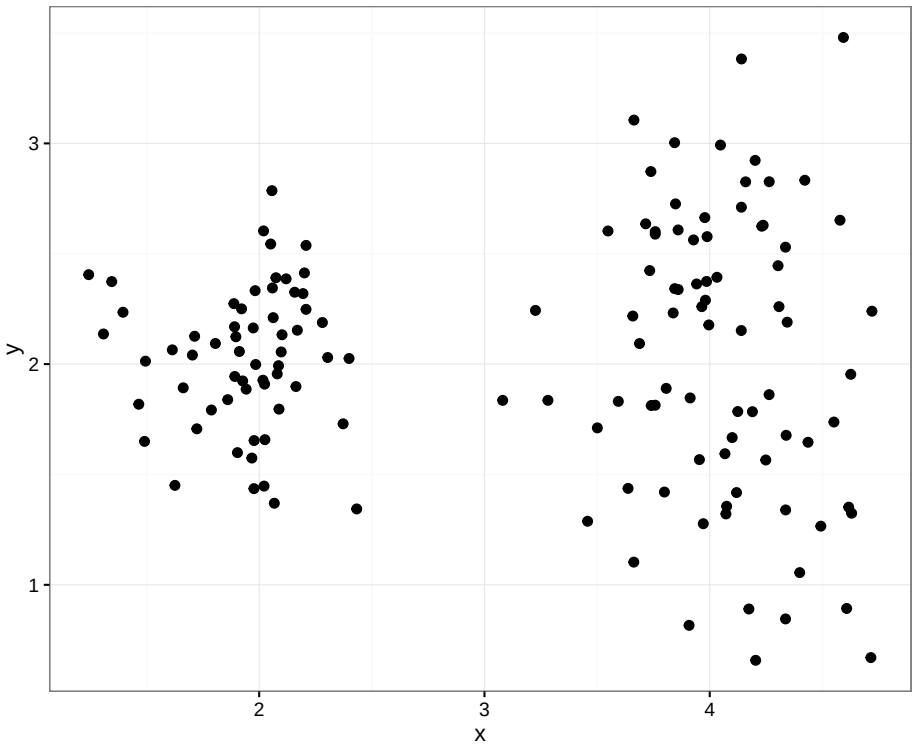
Simulated `data1`



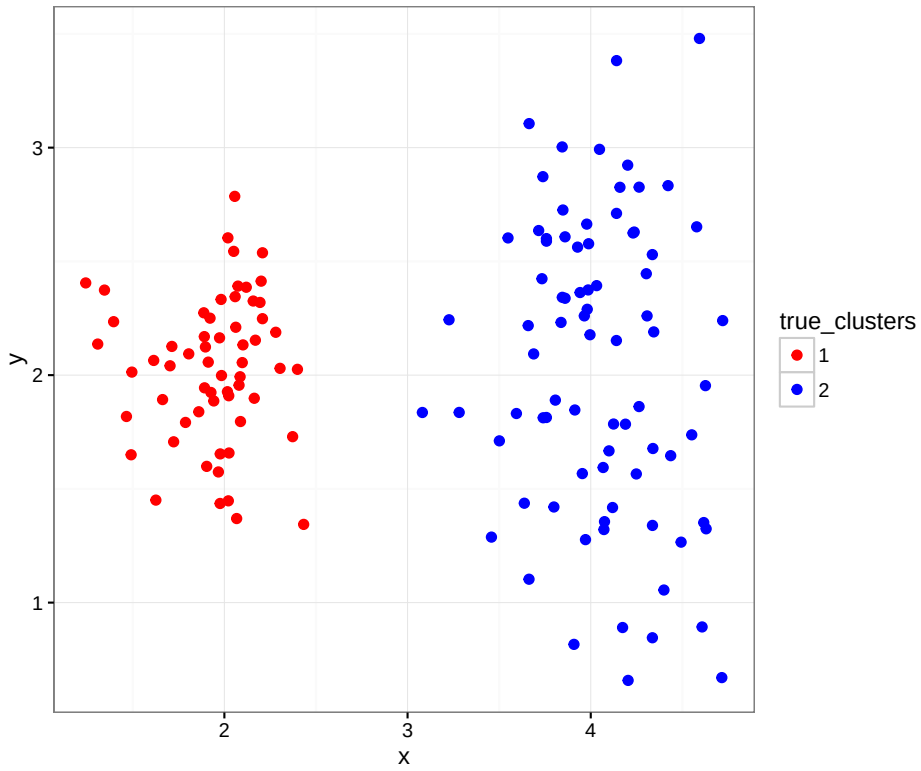
"True" Clusters `data1`



Simulated `data2`



"True" Clusters `data2`



Distance Measures

Objects

Most clustering methods require calculating a "distance" between two objects.

Let $\boldsymbol{a} = (a_1, a_2, \ldots, a_n)$ be one object and $\boldsymbol{b} = (b_1, b_2, \ldots, b_n)$ be another object.

We will assume both objects are composed of real numbers.

Euclidean

Euclidean distance is the shortest spatial distance between two objects in Euclidean space.

Euclidean distance is calculated as:

$$d(\boldsymbol{a}, \boldsymbol{b}) = \sqrt{\sum_{i=1}^{n} (a_i - b_i)^2}$$

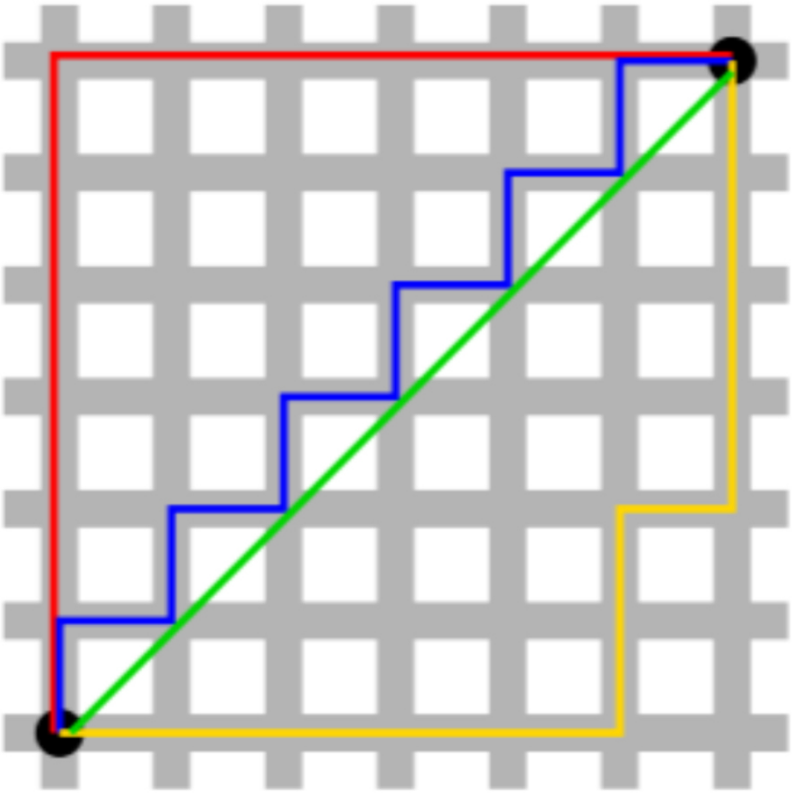
Manhattan

Manhattan distance is sometimes called taxicab distance. If you picture two locations in a city, it is the distance a taxicab must travel to get from one location to the other.

Manhattan distance is calculated as:

$$d(\boldsymbol{a}, \boldsymbol{b}) = \sum_{i=1}^{n} |a_i - b_i|$$

Euclidean vs Manhattan



Green is Euclidean. All others are Manhattan (and equal). Figure from *Exploratory Data Analysis with R.*

`dist()`

A distance matrix – which is the set of values resulting from a distance measure applied to all pairs of objects – can be obtained through the function `dist()`.

Default arguments for `dist()`:

```
> str(dist)
function (x, method = "euclidean", diag = FALSE, upper = FALSE,
    p = 2)
```

The key argument for us is `method=` which can take values `method="euclidean"` and `method="manhattan"` among others. See `?dist`.

Distance Matrix `data1`

```
> sub_data1 <- data1[1:4, c(1,2)]
> sub_data1
         x        y
1 2.085818 2.248086
2 1.896636 1.369547
3 2.097729 2.386383
4 1.491026 2.029814
> mydist <- dist(sub_data1)
> print(mydist)
          1         2         3
2 0.8986772
3 0.1388086 1.0365293
4 0.6335776 0.7749019 0.7037257
```

```
> (sub_data1[1,] - sub_data1[2,])^2 %>% sum() %>% sqrt()
[1] 0.8986772
```

Hierarchical Clustering

Strategy

Hierarchical clustering is a hierarchical agglomerative, bottom-up clustering method that strategically joins objects into larger and larger clusters, until all objects are contained in a single cluster.

Hierarchical clustering results are typically displayed as a dendrogram.

The number of clusters does not necessarily need to be known or chosen by the analyst.

Example: Cancer Subtypes

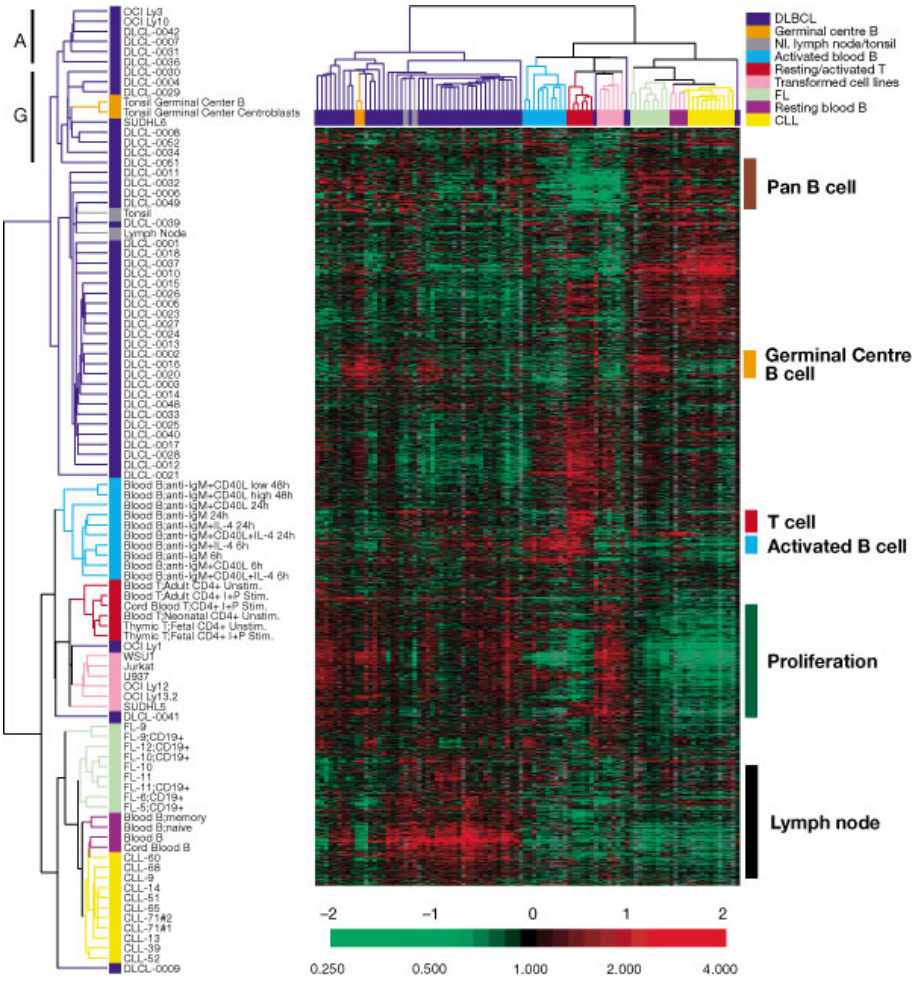


Figure from Alizadeh et al. (2000) *Nature*.

Algorithm

The algorithm for hierarchical clustering works as follows.

1. Start with each object assigned as its own cluster.
2. Calculate a distance between all pairs of clusters.
3. Join the two clusters with the smallest distance.
4. Repeat steps 2–3 until there is only one cluster.

At the very first iteration of the algorithm, all we need is some distance function (e.g., Euclidean or Manhattan) to determine the two objects that are closest.

But once clusters with more than one object are present, how do we calculate the distance between two clusters? This is where a key choice called the *linkage method or criterion* is needed.

Linkage Criteria

Suppose there are two clusters A and B and we have a distance function $d(\boldsymbol{a}, \boldsymbol{b})$ for all objects $\boldsymbol{a} \in A$ and $\boldsymbol{b} \in B$. Here are three ways (among many) to calculate a distance between clusters A and B:

$$\text{Complete:} \quad \max\{d(\boldsymbol{a}, \boldsymbol{b}) : \boldsymbol{a} \in A, \boldsymbol{b} \in B\} \tag{1}$$

$$\text{Single:} \quad \min\{d(\boldsymbol{a}, \boldsymbol{b}) : \boldsymbol{a} \in A, \boldsymbol{b} \in B\} \tag{2}$$

$$\text{Average:} \quad \frac{1}{|A||B|} \sum_{\boldsymbol{a} \in A} \sum_{\boldsymbol{b} \in B} d(\boldsymbol{a}, \boldsymbol{b}) \tag{3}$$

`hclust()`

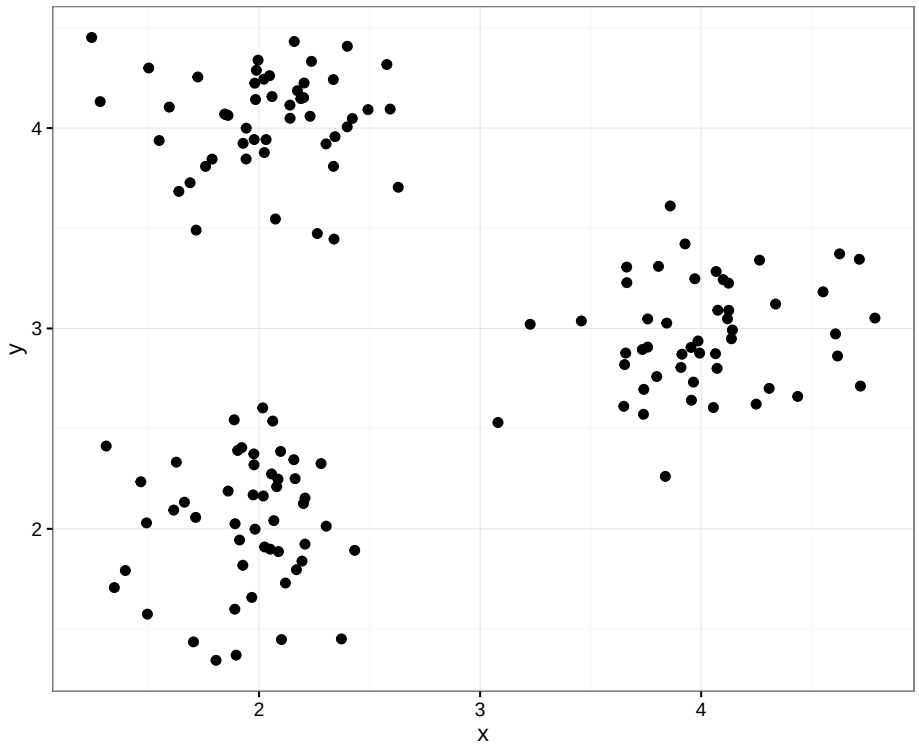
The `hclust()` function produces an R object that contains all of the information needed to create a complete hierarchical clustering.

Default arguments for `hclust()`:

```
> str(hclust)
function (d, method = "complete", members = NULL)
```

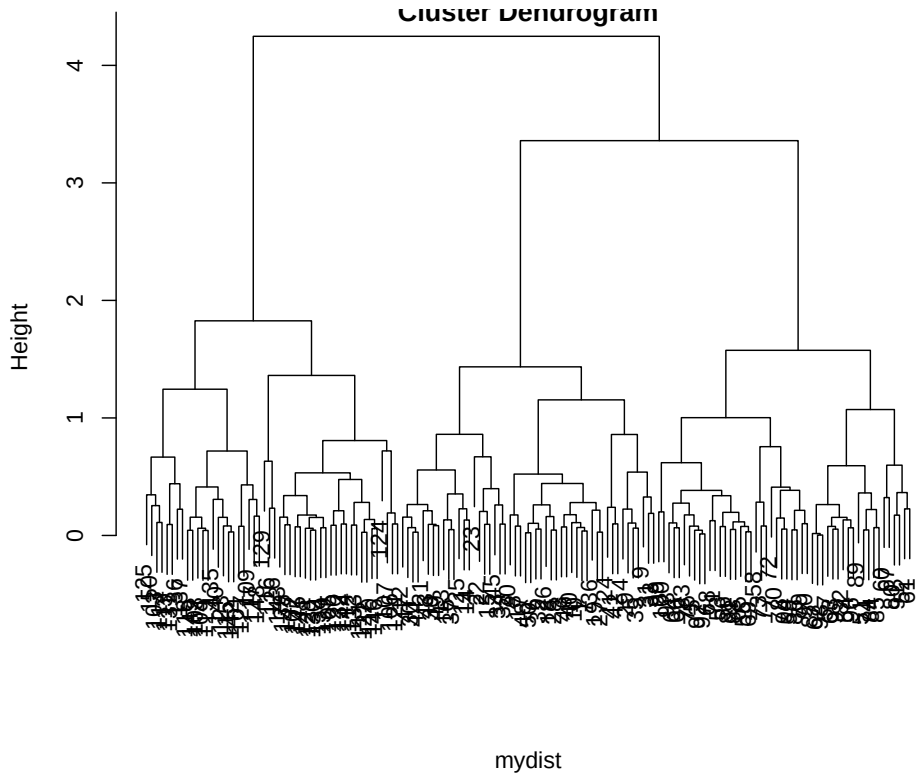
The primary input for `hclust()` is the `d` argument, which is a distance matrix (usually obtained from `dist()`). The `method` argument takes the linkage method, which includes `method="complete"`, `method="single"`, `method="average"`, etc. See `?hclust`.

Hierarchical Clustering of `data1`



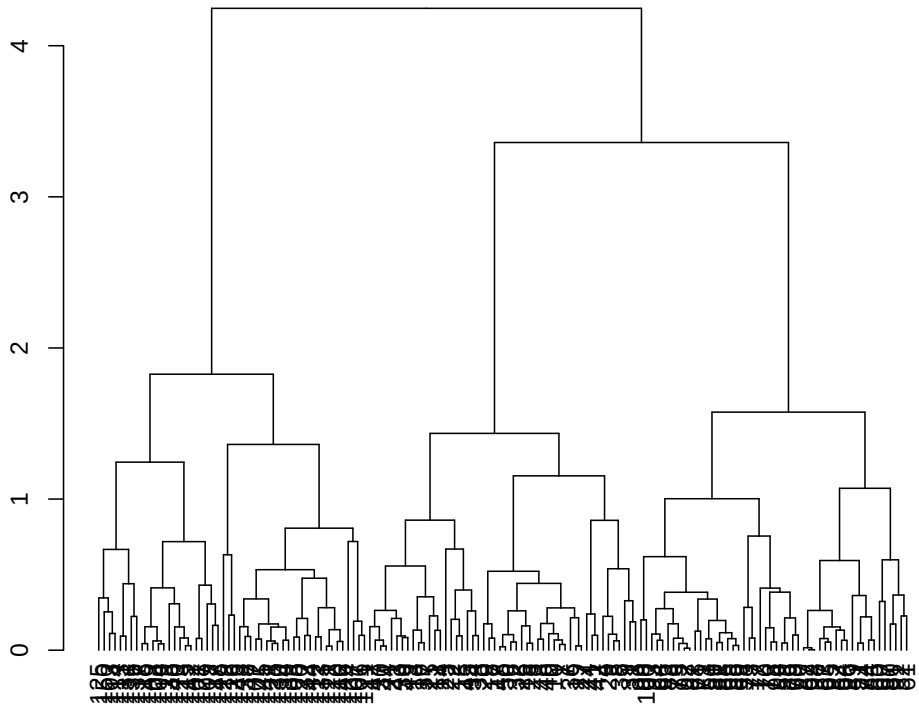
Standard `hclust()` Usage

```
> mydist <- dist(data1, method = "euclidean")
> myhclust <- hclust(mydist, method="complete")
> plot(myhclust)
```



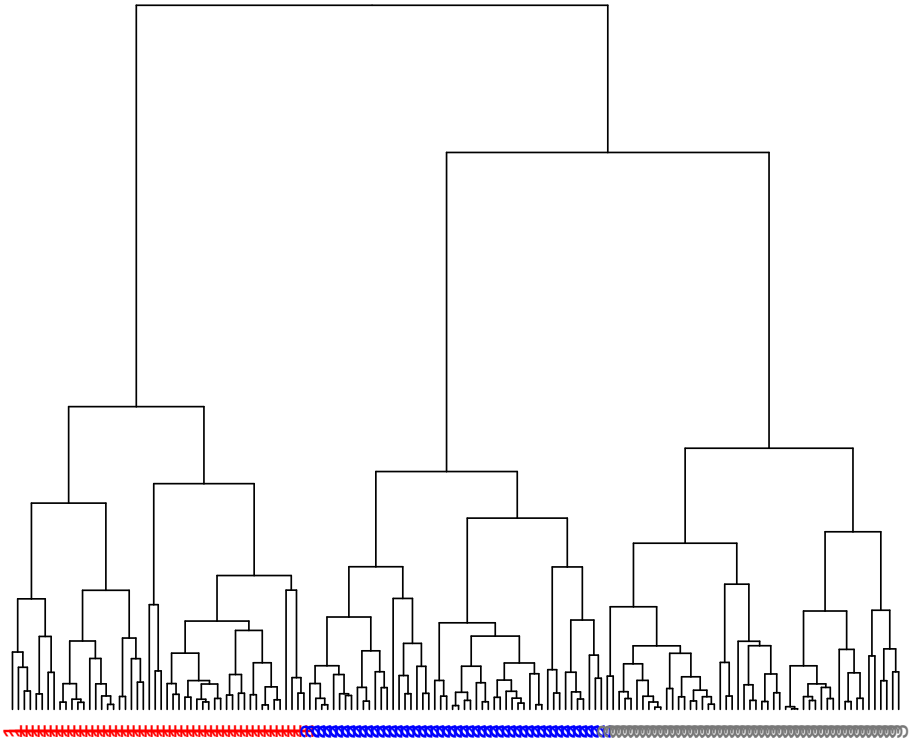
`as.dendrogram()`

```
> plot(as.dendrogram(myhclust))
```



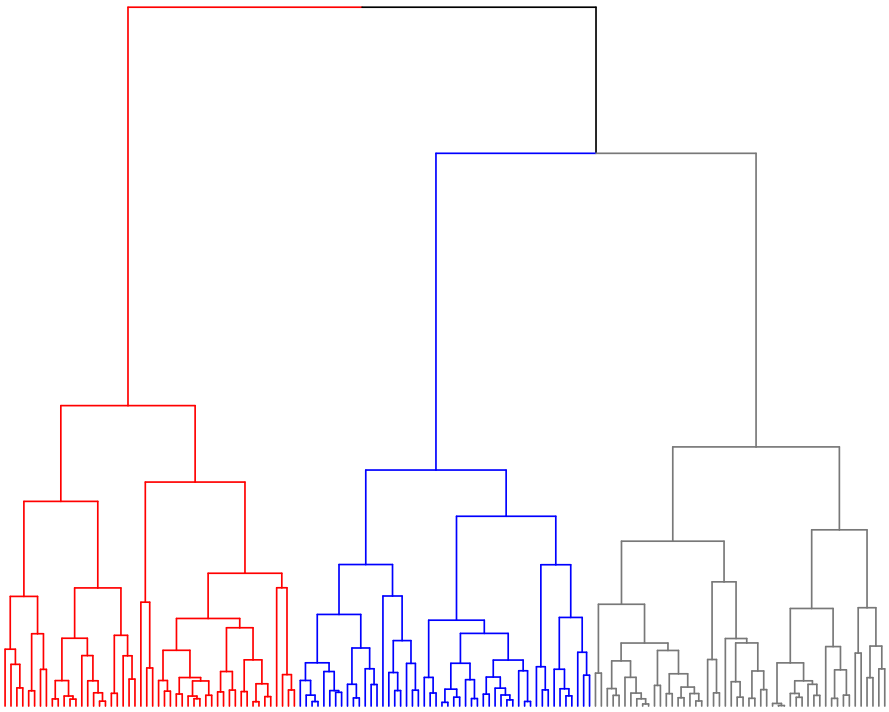
Modify the Labels

```
> library(dendextend)
> dend1 <- as.dendrogram(myhclust)
> labels(dend1) <- data1$true_clusters
> labels_colors(dend1) <-
+   c("red", "blue", "gray47")[as.numeric(data1$true_clusters)]
> plot(dend1, axes=FALSE, main=" ", xlab=" ")
```



Color the Branches

```
> dend2 <- as.dendrogram(myhclust)
> labels(dend2) <- rep(" ", nrow(data1))
> dend2 <- color_branches(dend2, k = 3, col=c("red", "blue", "gray47"))
> plot(dend2, axes=FALSE, main=" ", xlab=" ")
```

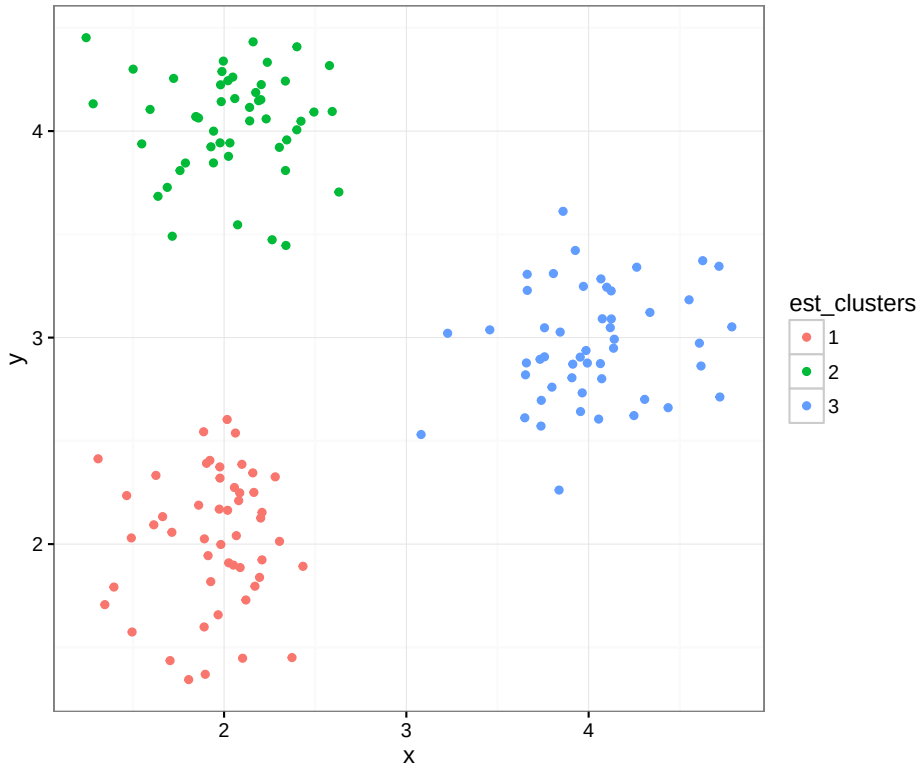


Cluster Assignments ($K = 3$)

```
> est_clusters <- cutree(myhclust, k=3)
> est_clusters
  [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 [30] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 2 2 2 2 2 2 2 2 2 2
 [59] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
 [88] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3
[117] 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3
[146] 3 3 3 3 3
```

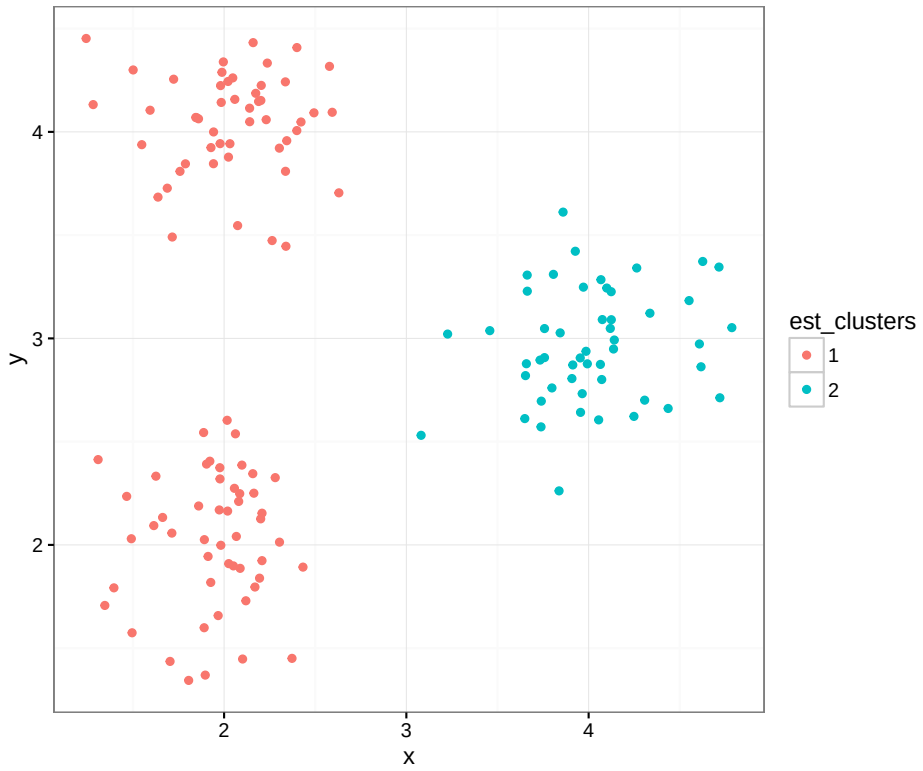
```
> est_clusters <- factor(est_clusters)
> p <- data1 %>%
+   mutate(est_clusters=est_clusters) %>%
+   ggplot()
> p + geom_point(aes(x=x, y=y, color=est_clusters))
```

Cluster Assignments ($K = 3$)



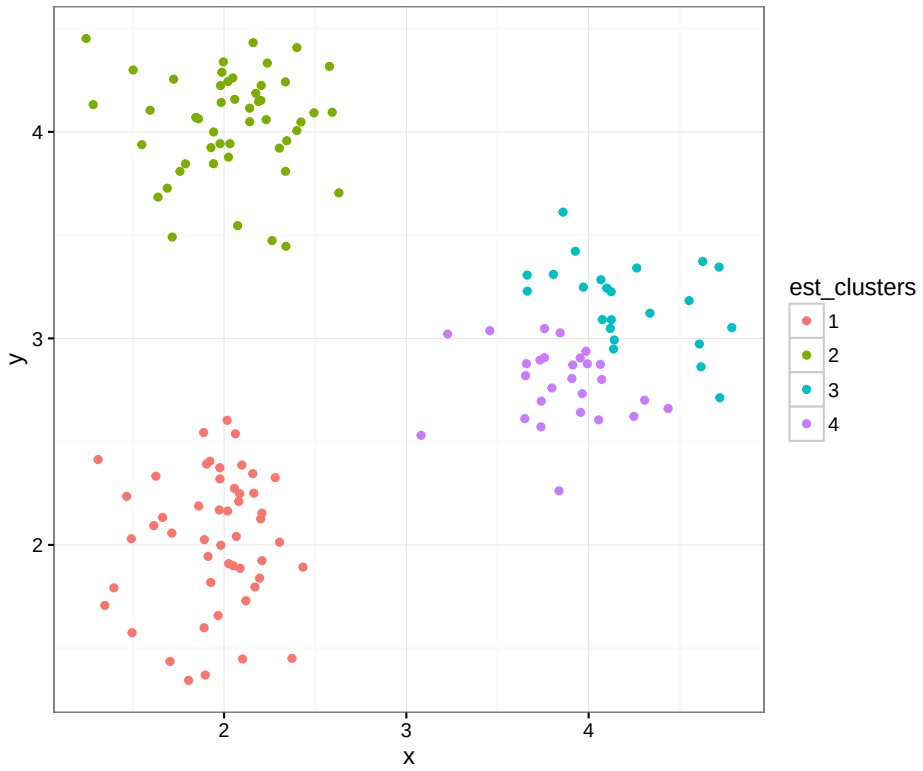
Cluster Assignments ($K = 2$)

```
> (data1 %>%
+    mutate(est_clusters=factor(cutree(myhclust, k=2))) %>%
+    ggplot()) + geom_point(aes(x=x, y=y, color=est_clusters))
```



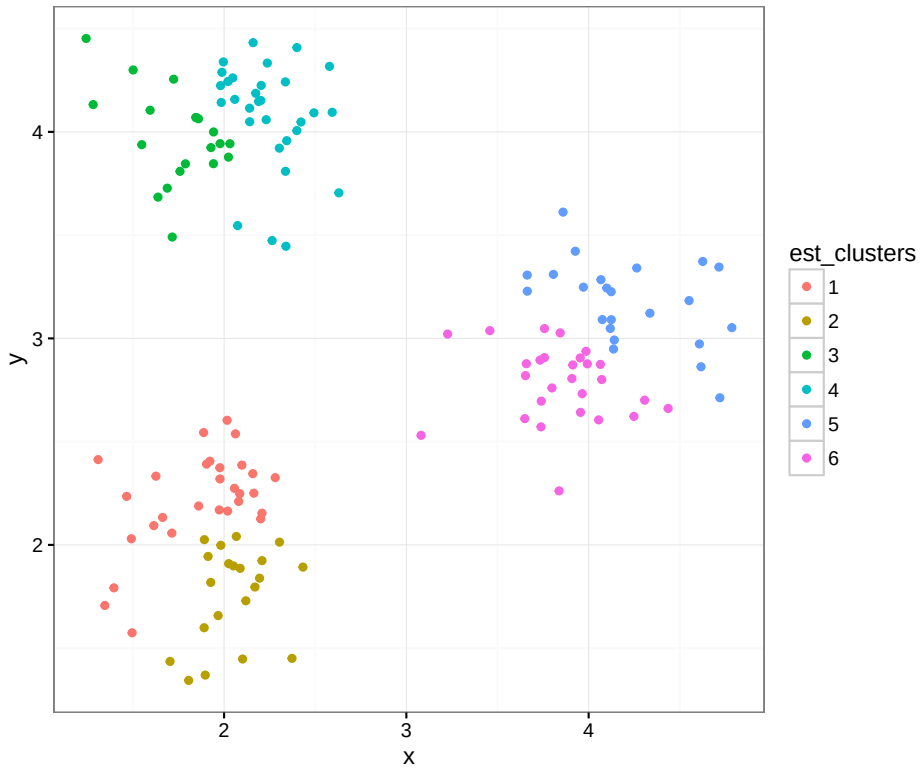
Cluster Assignments ($K = 4$)

```
> (data1 %>%
+    mutate(est_clusters=factor(cutree(myhclust, k=4))) %>%
+    ggplot()) + geom_point(aes(x=x, y=y, color=est_clusters))
```



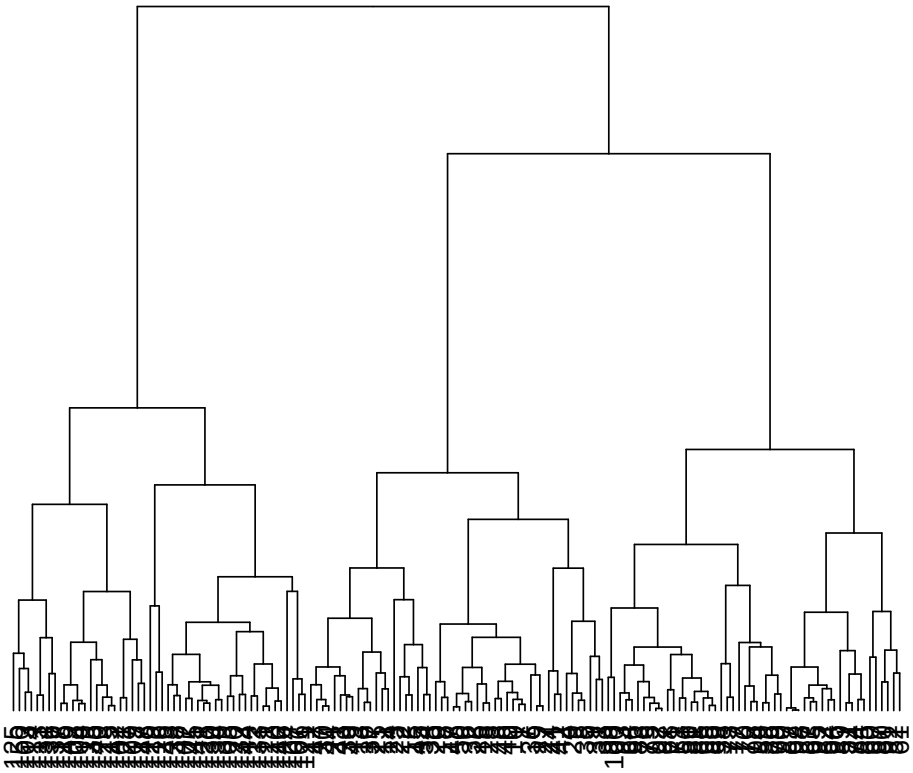
Cluster Assignments ($K = 6$)

```
> (data1 %>%
+    mutate(est_clusters=factor(cutree(myhclust, k=6))) %>%
+    ggplot()) + geom_point(aes(x=x, y=y, color=est_clusters))
```



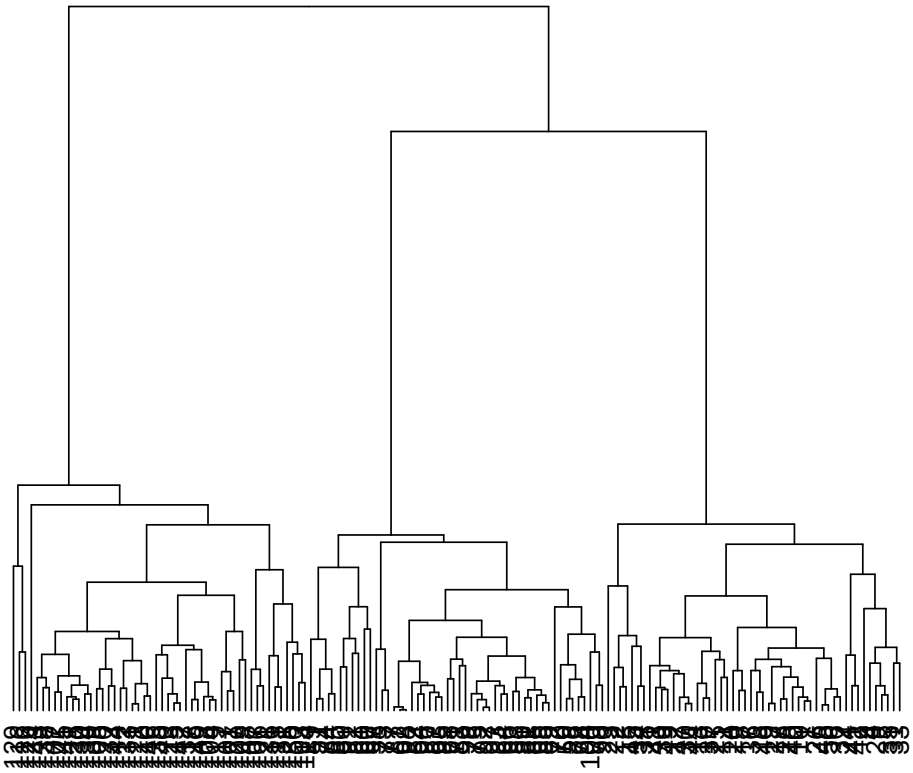
Linkage: Complete (Default)

```
> data1 %>% dist() %>% hclust(method="complete") %>%
+   as.dendrogram() %>% plot(axes=FALSE)
```



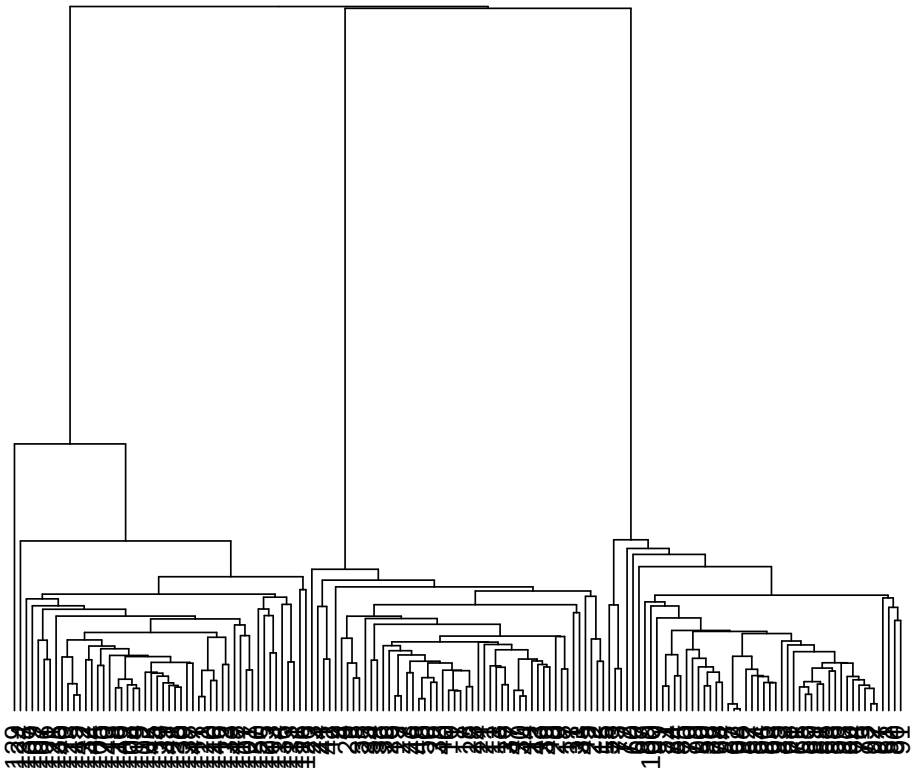
Linkage: Average

```
> data1 %>% dist() %>% hclust(method="average") %>%
+   as.dendrogram() %>% plot(axes=FALSE)
```



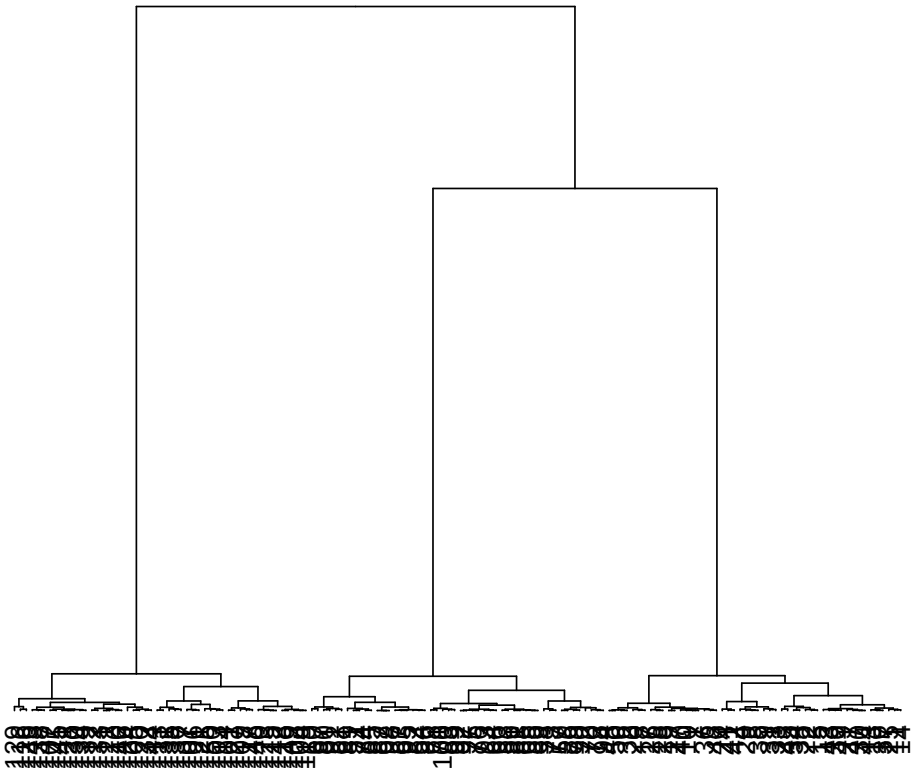
Linkage: Single

```
> data1 %>% dist() %>% hclust(method="single") %>%
+   as.dendrogram() %>% plot(axes=FALSE)
```

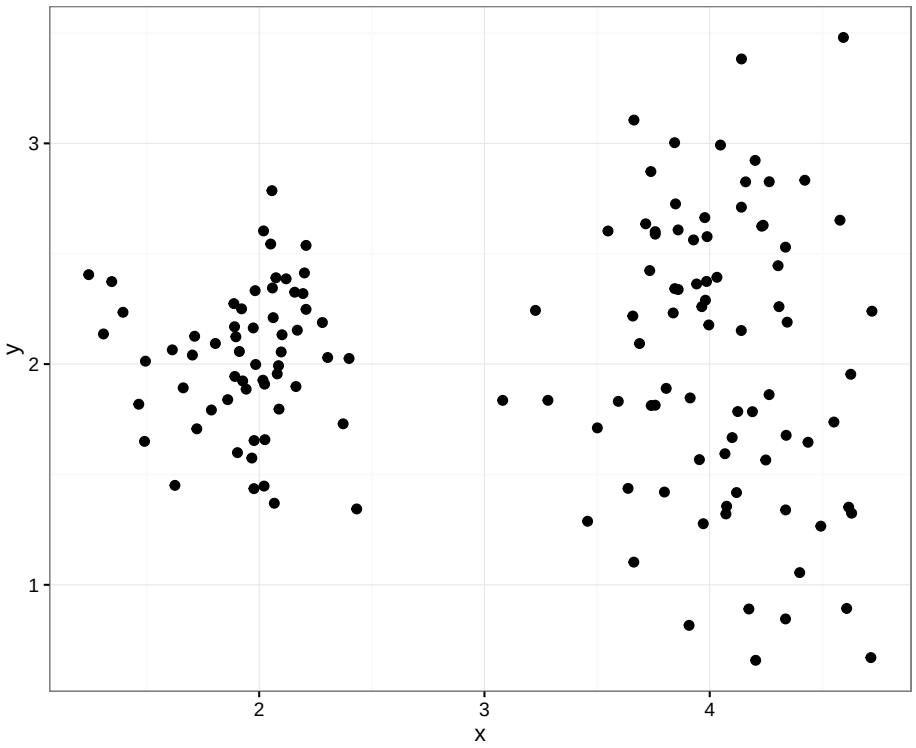


Linkage: Ward

```
> data1 %>% dist() %>% hclust(method="ward.D") %>%
+   as.dendrogram() %>% plot(axes=FALSE)
```

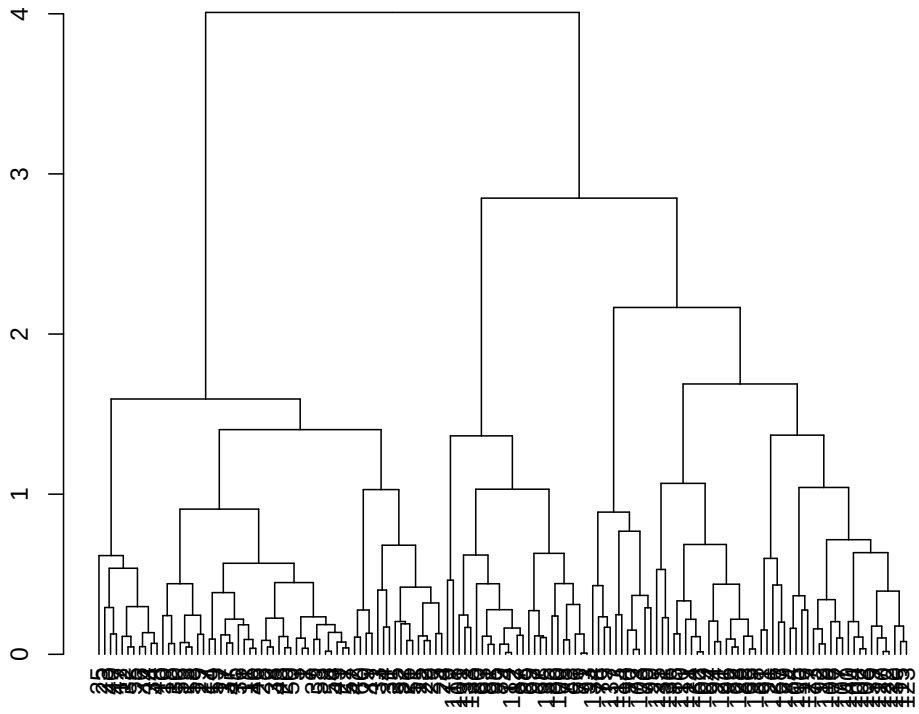


Hierarchical Clustering of `data2`



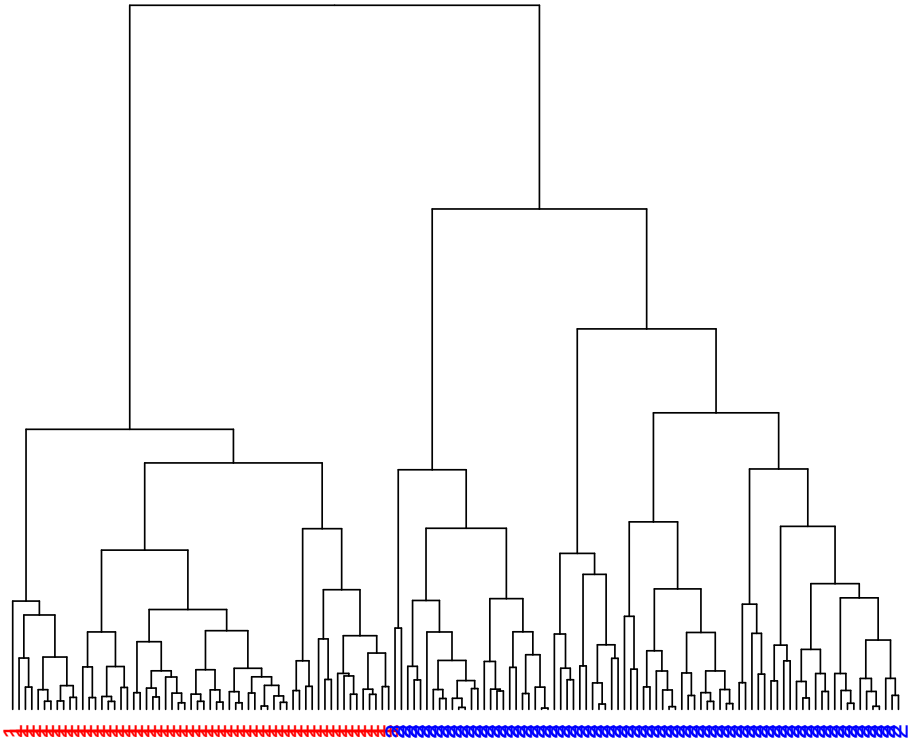
`as.dendrogram()`

```
> mydist <- dist(data2, method = "euclidean")
> myhclust <- hclust(mydist, method="complete")
> plot(as.dendrogram(myhclust))
```



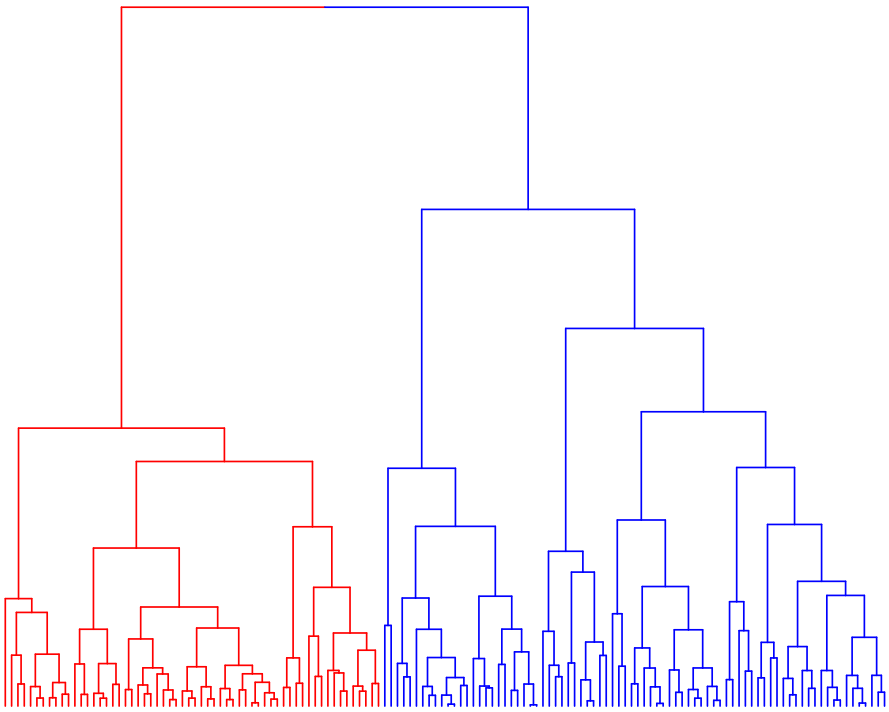
Modify the Labels

```
> library(dendextend)
> dend1 <- as.dendrogram(myhclust)
> labels(dend1) <- data2$true_clusters
> labels_colors(dend1) <-
+   c("red", "blue")[as.numeric(data2$true_clusters)]
> plot(dend1, axes=FALSE, main=" ", xlab=" ")
```



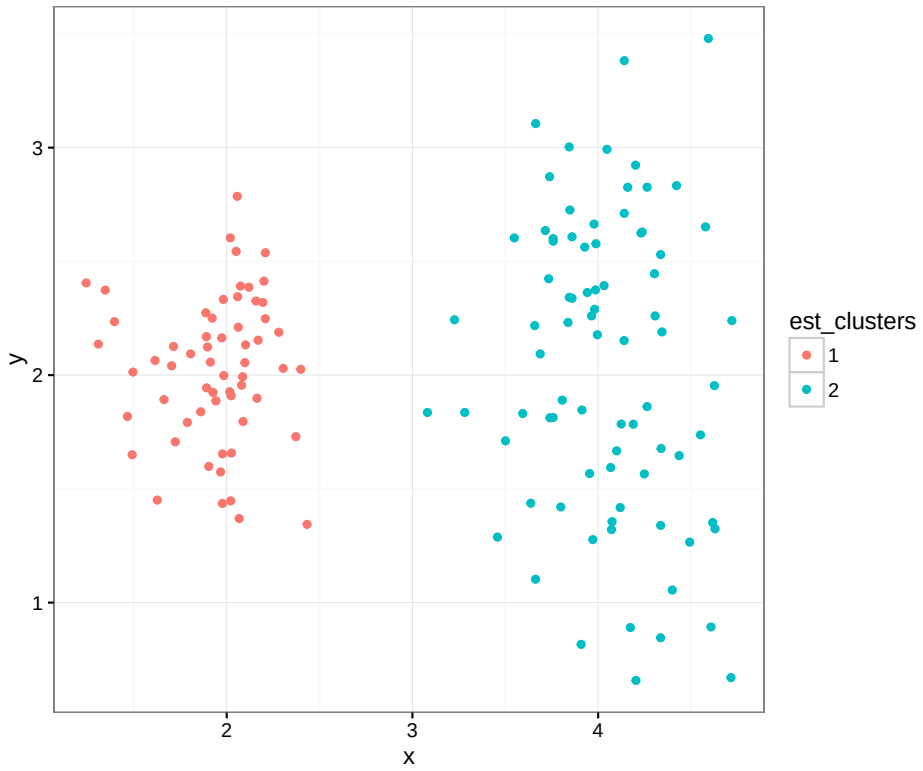
Color the Branches

```
> dend2 <- as.dendrogram(myhclust)
> labels(dend2) <- rep(" ", nrow(data2))
> dend2 <- color_branches(dend2, k = 2, col=c("red", "blue"))
> plot(dend2, axes=FALSE, main=" ", xlab=" ")
```



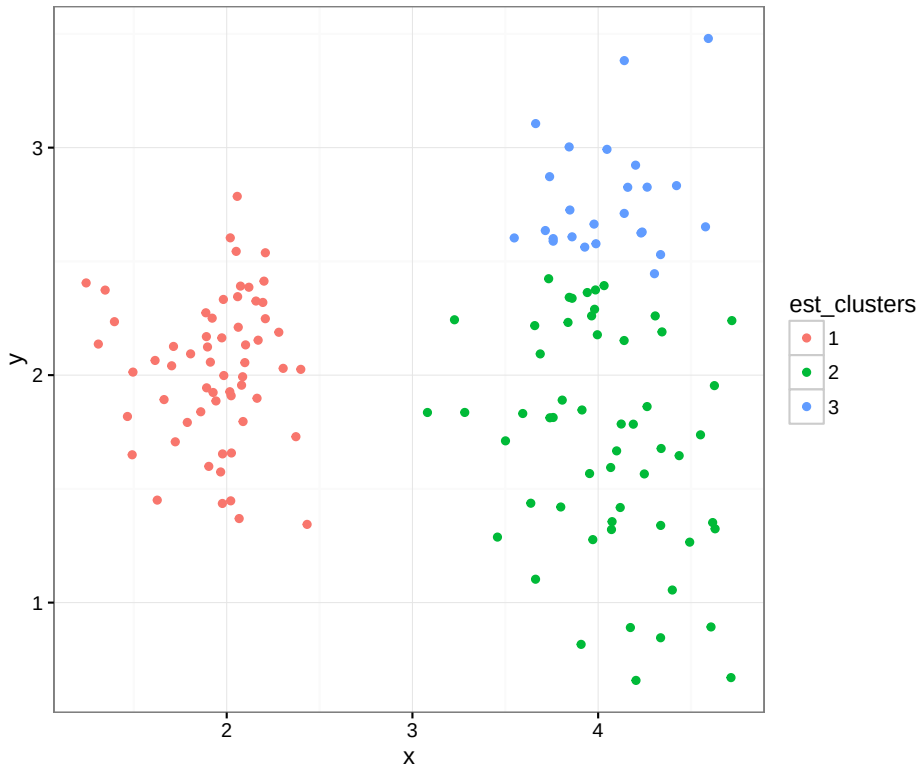
Cluster Assignments ($K = 2$)

```
> (data2 %>%
+    mutate(est_clusters=factor(cutree(myhclust, k=2))) %>%
+    ggplot()) + geom_point(aes(x=x, y=y, color=est_clusters))
```



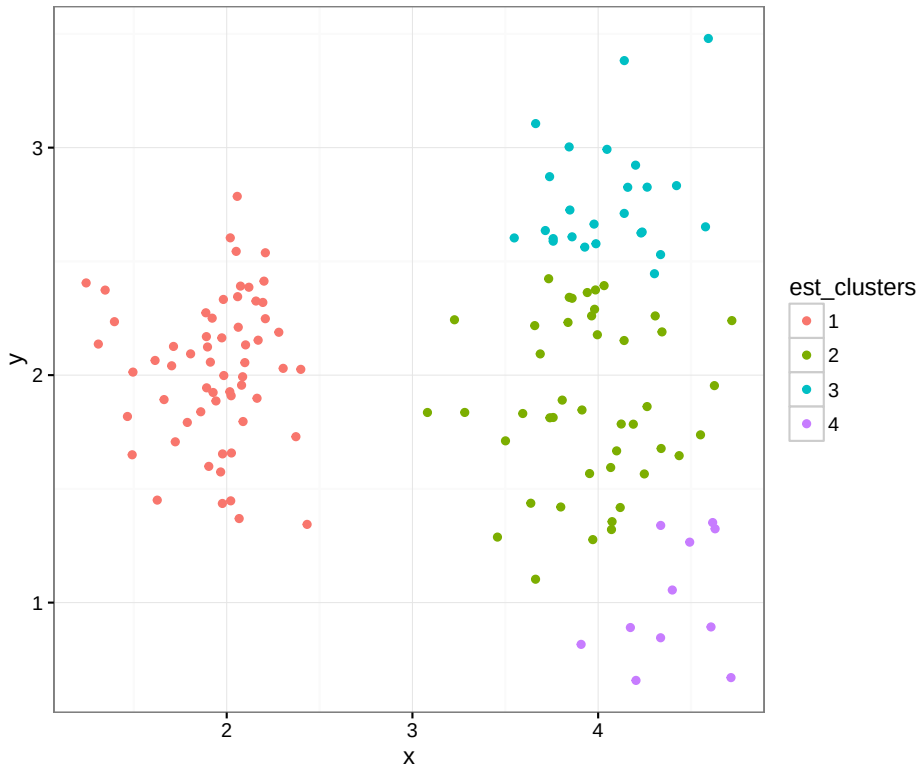
Cluster Assignments ($K = 3$)

```
> (data2 %>%
+    mutate(est_clusters=factor(cutree(myhclust, k=3))) %>%
+    ggplot()) + geom_point(aes(x=x, y=y, color=est_clusters))
```



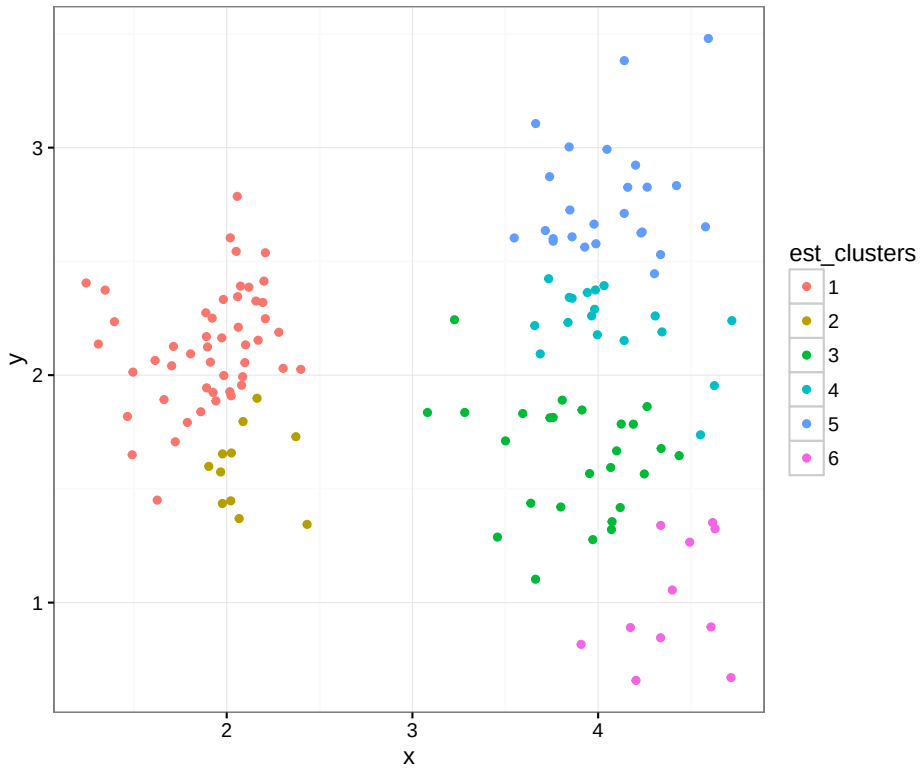
Cluster Assignments ($K = 4$)

```
> (data2 %>%
+    mutate(est_clusters=factor(cutree(myhclust, k=4))) %>%
+    ggplot()) + geom_point(aes(x=x, y=y, color=est_clusters))
```



Cluster Assignments ($K = 5$)

```
> (data2 %>%
+    mutate(est_clusters=factor(cutree(myhclust, k=6))) %>%
+    ggplot()) + geom_point(aes(x=x, y=y, color=est_clusters))
```



K-Means Clustering

Strategy

K-means clustering is a top-down, partitioning cluster analysis method that assigns each object to one of K clusters based on the distance between each object and the cluster centers, called *centroids*.

This is an iterative algorithm with potential random initial values.

The value of K is typically unknown and must be determined by the analyst.

Centroid

A centroid is the coordinate-wise average of all objects in a cluster.

Let A be a given cluster with objects $\boldsymbol{a} \in A$. Its centroid is:

$$\overline{\boldsymbol{a}} = \frac{1}{|A|} \sum_{\boldsymbol{a} \in A} \boldsymbol{a}$$

Algorithm

The number of clusters K must be chosen beforehand.

1. Initialize K cluster centroids.
2. Assign each object to a cluster by choosing the cluster with the smalllest distance (e.g., Euclidean) between the object and the cluster centroid.
3. Calculate new centroids based on the cluster assignments from Step 2.
4. Repeat Steps 2–3 until convergence.

Notes

The initialization of the centroids is typically random, so often the algorithm is run several times with new, random initial centroids.

Convergence is usually defined in terms of neglible changes in the centroids or no changes in the cluster assignments.

`kmeans()`

K-means clustering can be accomplished through the following function:

```
> str(kmeans)
function (x, centers, iter.max = 10L, nstart = 1L, algorithm = c("Hartigan-Wong",
    "Lloyd", "Forgy", "MacQueen"), trace = FALSE)
```

- `x`: the data to clusters, objects along rows
- `centers`: either the number of clusters K or a matrix giving initial centroids
- `iter.max`: the maximum number of iterations allowed
- `nstart`: how many random intial K centroids, where the best one is returned

`fitted()`

The cluster centroids or assigments can be extracted through the function `fitted()`, which is applied to the output of `kmeans()`.

The input of `fitted()` is the object returned by `kmeans()`. The key additional argument is called `method`.

When `method="centers"` it returns the centroids. When `method="classes"` it returns the cluster assignments.

K-Means Clustering of `data1`

```
> km1 <- kmeans(x=data1[,-3], centers=3, iter.max=100, nstart=5)
> est_clusters <- fitted(km1, method="classes")
> est_clusters
  [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 [30] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 3 3 3 3 3 3 3 3
 [59] 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3 3
 [88] 3 3 3 3 3 3 3 3 3 3 3 3 3 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
[117] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
[146] 2 2 2 2 2
```

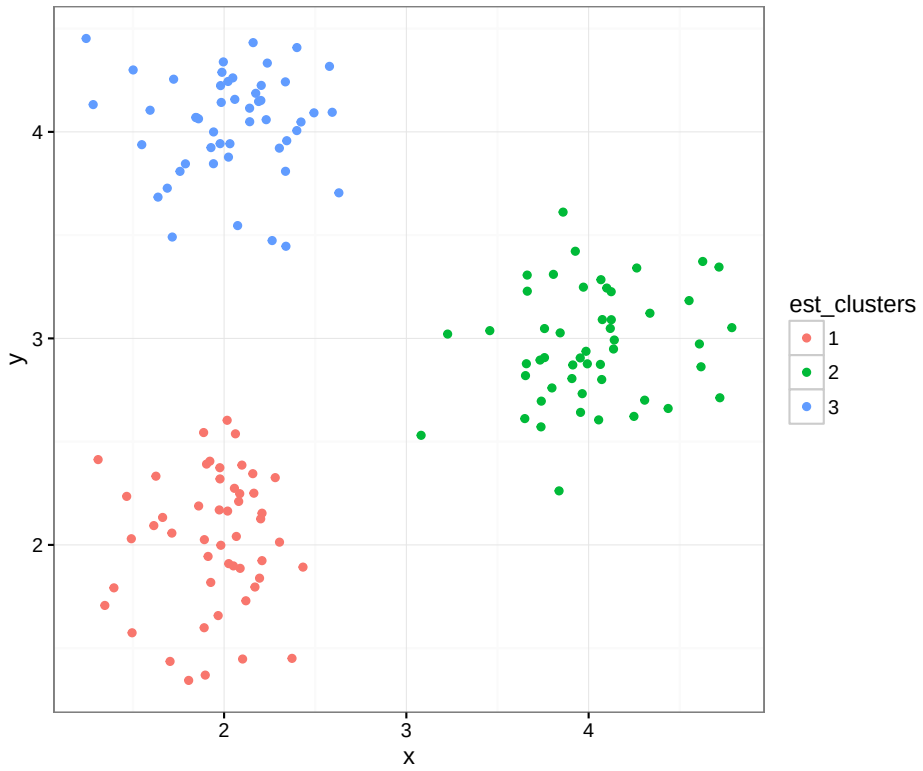
Centroids of `data1`

```
> centroids1 <- fitted(km1, method="centers") %>% unique()
> centroids1
         x        y
1 1.943184 2.028062
3 2.042872 4.037987
2 4.015934 2.962279
```

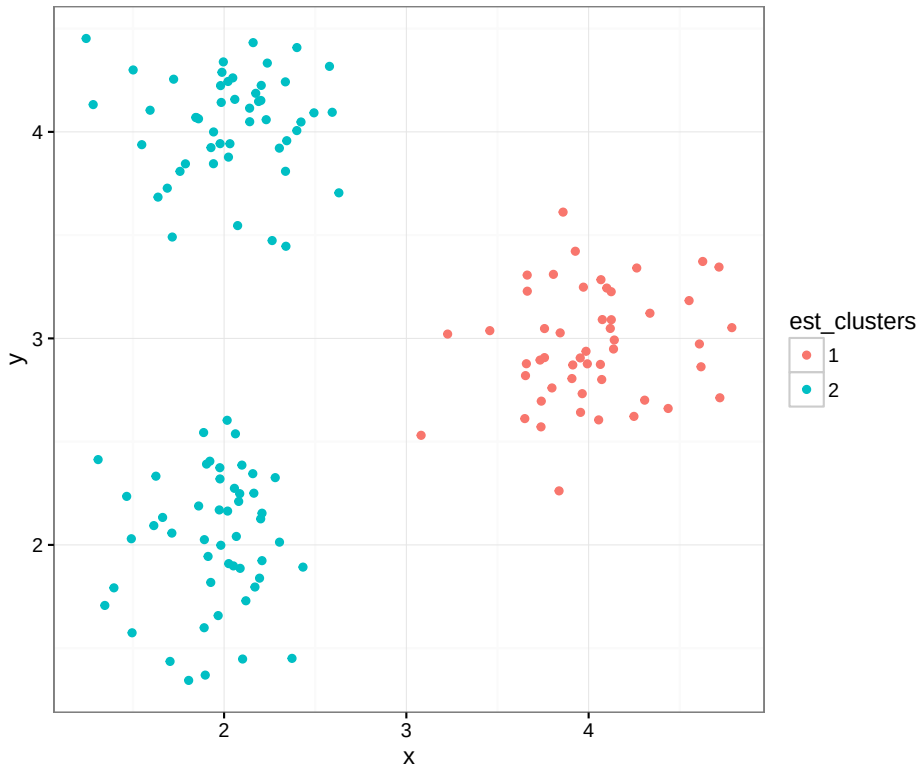
```
> est_clusters <- fitted(km1, method="classes")
> data1 %>% mutate(est_clusters = factor(est_clusters)) %>%
+   group_by(est_clusters) %>% summarize(mean(x), mean(y))
Source: local data frame [3 x 3]

  est_clusters  mean(x)  mean(y)
        (fctr)    (dbl)    (dbl)
1           1 1.943184 2.028062
2           2 4.015934 2.962279
3           3 2.042872 4.037987
```

Cluster Assignments ($K = 3$)

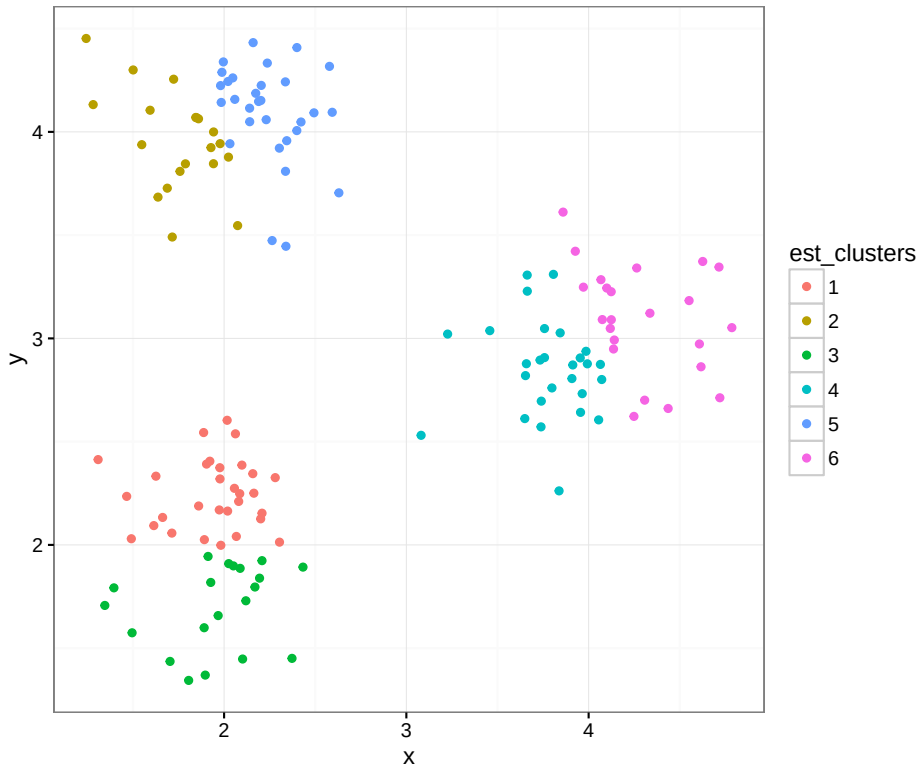
```
> est_clusters <- factor(est_clusters)
> ggplot(data1) + geom_point(aes(x=x, y=y, color=est_clusters))
```



Cluster Assignments ($K = 2$)



Cluster Assignments ($K = 6$)

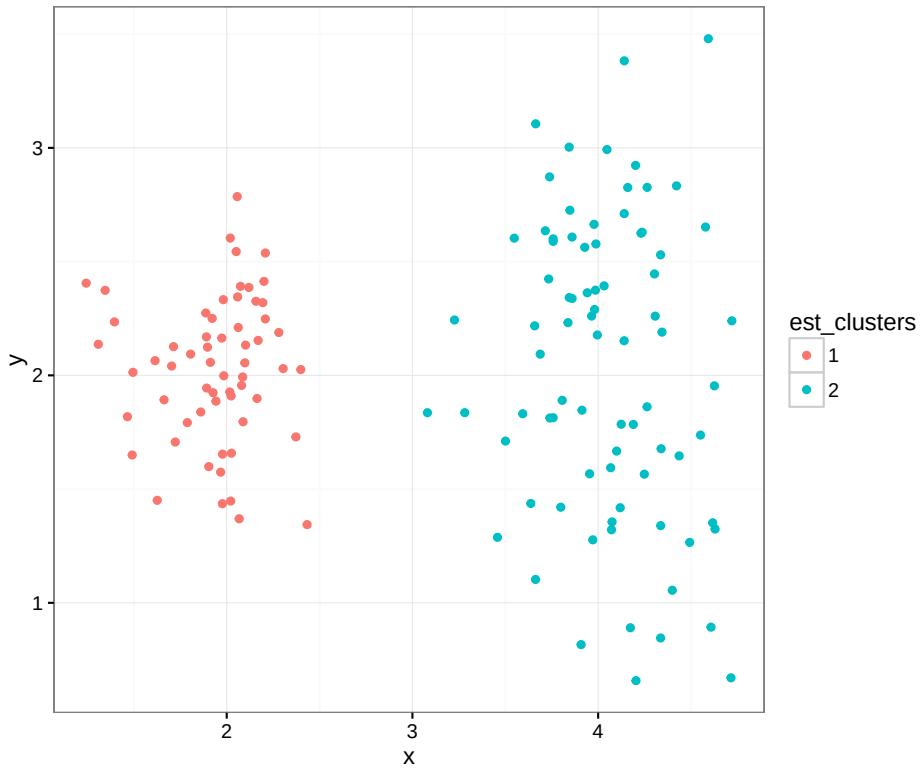


K-Means Clustering of `data2`

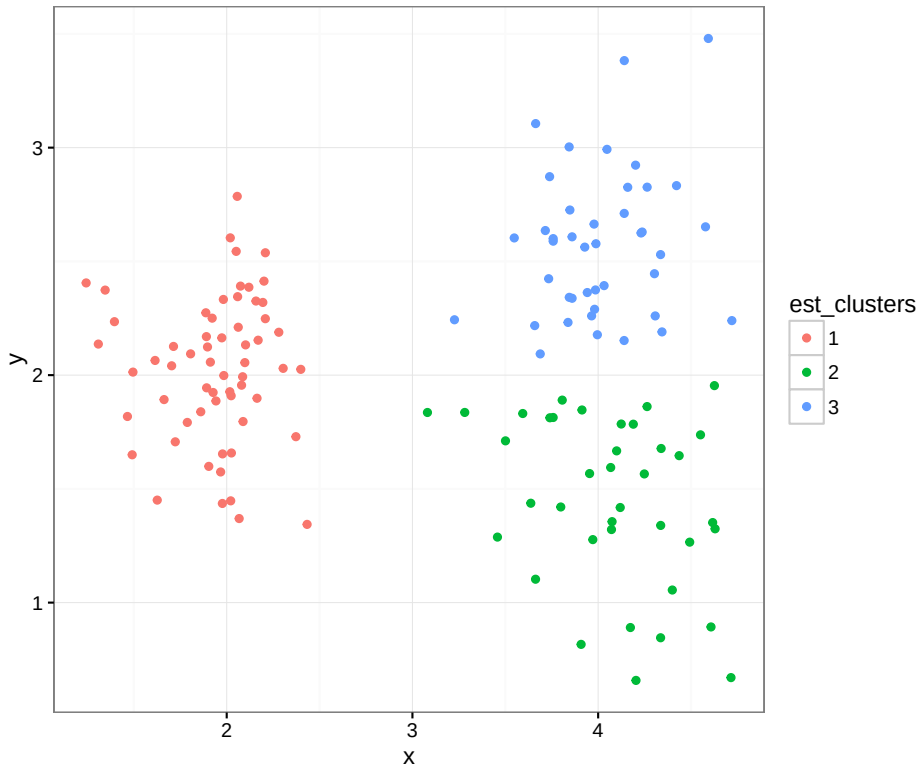
```
> km2 <- kmeans(x=data2[,-3], centers=2, iter.max=100, nstart=5)
> est_clusters <- fitted(km2, method="classes")
> est_clusters
  [1] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 [30] 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
 [59] 1 1 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
 [88] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
[117] 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2 2
```

Cluster Assignments ($K = 2$)

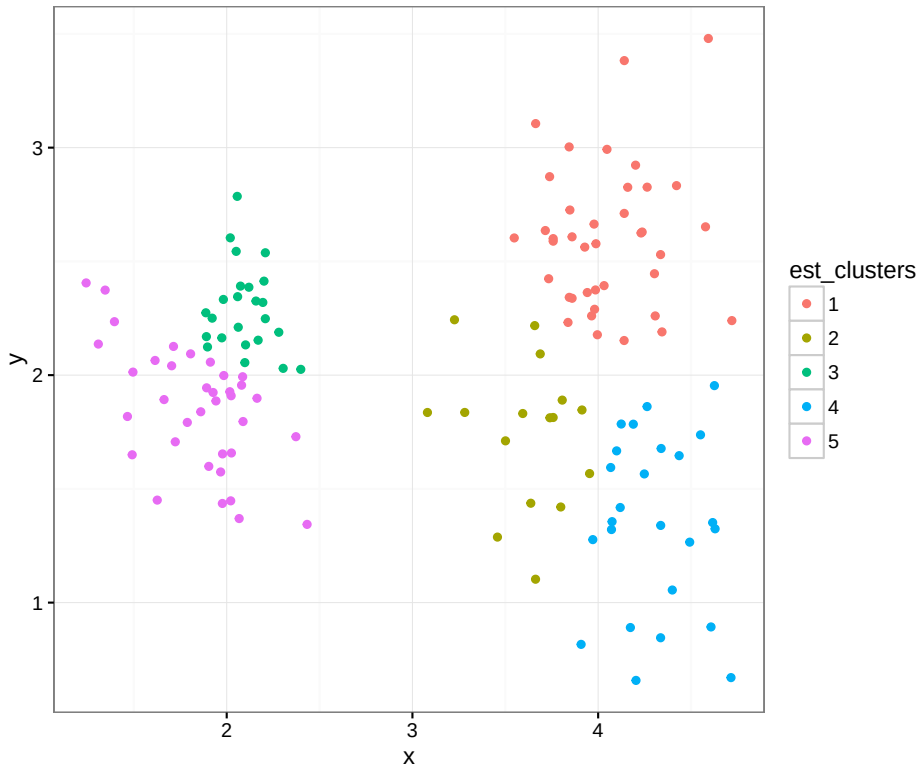
```
> est_clusters <- factor(est_clusters)
> ggplot(data2) + geom_point(aes(x=x, y=y, color=est_clusters))
```



Cluster Assignments ($K = 3$)



Cluster Assignments ($K = 5$)



Dimensionality Reduction

Weather Data

This is a subset of the weather data from Project 3:

```
> load("data/weather_data.RData")
> dim(weather_data)
[1] 2811   50
>
> weather_data[1:5, 1:7]
                  11       16  18       19  27  30       31
AG000060611 138.0000 175.0000 173 164.0000 218 160 163.0000
AGM00060369 158.0000 162.0000 154 159.0000 165 125 171.0000
AGM00060425 272.7619 272.7619 152 163.0000 163 108 158.0000
AGM00060444 128.0000 102.0000 100 111.0000 125  33 125.0000
AGM00060468 105.0000 122.0000  97 263.5714 155  52 263.5714
```

This matrix contains temperature data on 50 days and 2811 stations that were randomly selected.

Goal

The goal of dimensionality reduction is to extract low dimensional representations of high dimensional data that are useful for visualization, exploration, inference, or prediction.

The low dimensional representations should capture key sources of variation in the data.

Some Methods

- Cluster analysis
- Principal component analysis
- Singular value decomposition
- Vector quantization
- Self-organizing maps
- Multidimensional scaling
- Latent variable modeling

Principal Component Analysis

Goal

For a given set of variables, principal component analysis (PCA) finds (constrained) weighted sums of the variables that capture the maximum level of variation in the data.

Specifically, the first principal component is the weighted sum of the variables that results in a component with the highest variation.

This component is then regressed out of the data, and the second principal component is obtained on the resulting residuals.

This process is repeated until there is no variation left in the data.

Procedure

Suppose we have p variables, each with n observations:

$$\boldsymbol{x_1} = (x_{11}, x_{12}, \ldots, x_{1n}) \tag{4}$$
$$\boldsymbol{x_2} = (x_{21}, x_{22}, \ldots, x_{2n}) \tag{5}$$
$$\vdots \tag{6}$$
$$\boldsymbol{x_p} = (x_{p1}, x_{p2}, \ldots, x_{pn}) \tag{7}$$

Consider all possible weighted sums of these variables

$$\tilde{\boldsymbol{x}} = \sum_{i=1}^{p} w_i \boldsymbol{x_i}$$

where we constrain $\sum_{i=1}^{p} w_i^2 = 1$.

Procedure

The first principal component (PC1) is the set of weights that produces a vector $\tilde{\boldsymbol{x}}$ that maximizes

$$\tilde{x}_1^2 + \tilde{x}_2^2 + \cdots \tilde{x}_n^2.$$

Once this is found, then a least squares linear regression of each $\boldsymbol{x}_i$ on $\tilde{\boldsymbol{x}}$ (with no intercept) is performed and the residuals are obtained. The next principal component (PC2) is then calculated using the same procedure, and it is regressed out from the to obtain a new set of residuals for calculating PC3.

This iterative process is repeated to obtain up to $\min(p, n)$ PCs.

Singular Value Decomposition

Singular value decomposition (SVD) is a numerical matrix decomposition that can find all PCs at once.

This is an advanced topic.

See *Principal Component Analysis* by I.T. Jolliffe for a thorough account of PCA, including a clear explanation on the relationship between PCA and SVD (in Chapter 1).

Mean Centering and Covariance

PCA can be motivated and derived in terms of covariance matrices.

We will not cover that here, but it is definitely worth learning.

One thing we want to note is that it is usually the case that one centers each variable by its sample mean before performing PCA (i.e., subtract the variable's sample mean from each observation on that variable). This allows the optimization to be about maximizing sample variance of the component and provides the underlying connection to covariances.

My PCA Function

```
> pca <- function(x, space=c("rows", "columns"),
+                 center=TRUE, scale=FALSE) {
+   space <- match.arg(space)
+   if(space=="columns") {x <- t(x)}
+   x <- t(scale(t(x), center=center, scale=scale))
+   s <- svd(x)
+   loading <- s$u
+   colnames(loading) <- paste0("Loading", 1:ncol(loading))
+   rownames(loading) <- rownames(x)
+   pc <- diag(s$d) %*% t(s$v)
+   rownames(pc) <- paste0("PC", 1:nrow(pc))
+   colnames(pc) <- colnames(x)
+   pve <- s$d^2 / sum(s$d^2)
+   if(space=="columns") {pc <- t(pc); loading <- t(loading)}
+   return(list(pc=pc, loading=loading, pve=pve))
+ }
```

How It Works (Input)

Input:

- `x`: a matrix of numerical values
- `space`: either `"rows"` or `"columns"`, denoting which dimension contains the variables
- `center`: if `TRUE` then the variables are mean centered before calculating PCs
- `scale`: if `TRUE` then the variables are std dev scaled before calculating PCs

How It Works (Output)

Output is a list with the following items:

- `pc`: a matrix of all possible PCs
- `loading`: the weights or "loadings" that determined each PC
- `pve`: the proportion of variation explained by each PC

Note that the rows or columns of `pc` and `loading` have names to let you know on which dimension the values are organized.

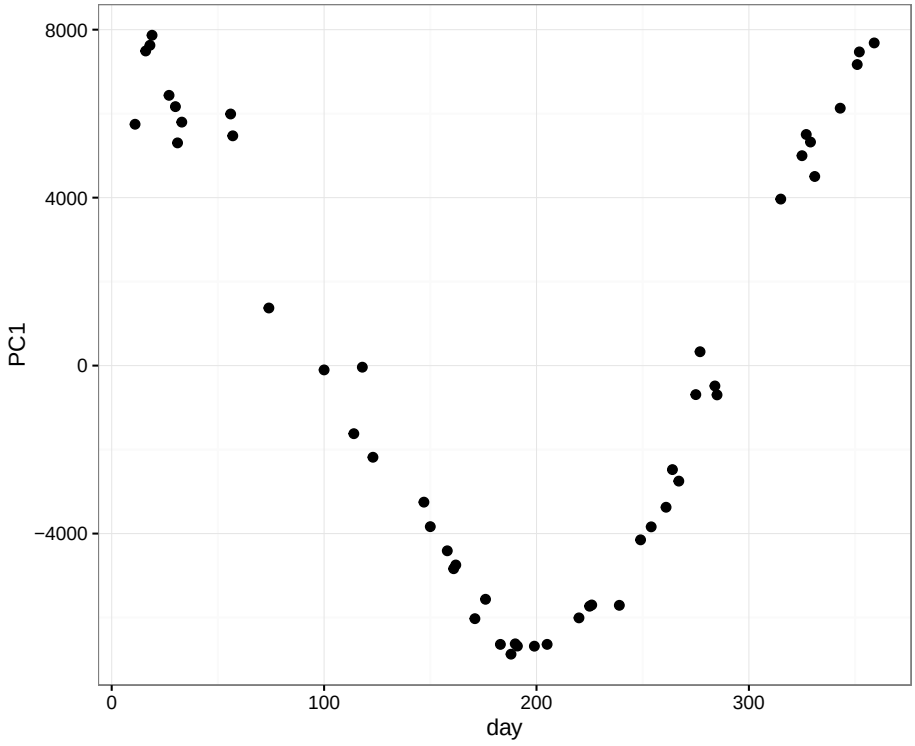
Application to Weather Data

```
> mypca <- pca(weather_data, space="rows")
>
> names(mypca)
[1] "pc"      "loading" "pve"
> dim(mypca$pc)
[1] 50 50
> dim(mypca$loading)
[1] 2811   50
```

```
> mypca$pc[1:3, 1:3]
           11         16         18
PC1 5747.5990  7492.4124  7628.1715
PC2 -766.4347 -1269.4797   285.8742
PC3 -196.7599  -365.3963 -1097.7858
> mypca$loading[1:3, 1:3]
                Loading1    Loading2     Loading3
AG000060611 -0.015172744 0.013033849 -0.011273121
AGM00060369 -0.009439176 0.016884418 -0.004611284
AGM00060425 -0.015779138 0.007026312 -0.009907972
```

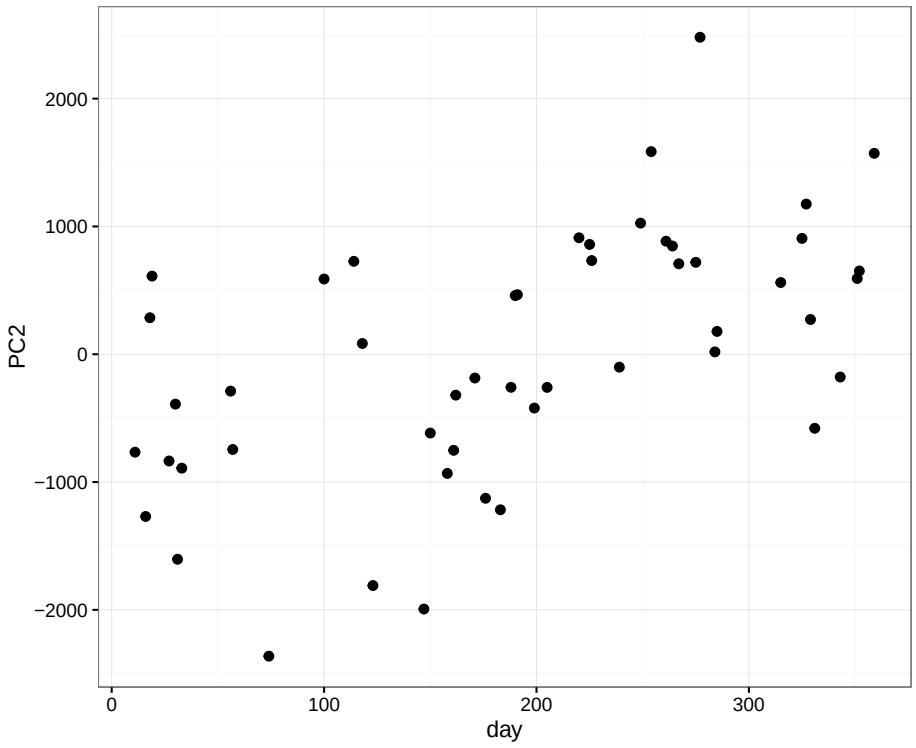
PC1 vs Time

```
> day_of_the_year <- as.numeric(colnames(weather_data))
> data.frame(day=day_of_the_year, PC1=mypca$pc[1,]) %>%
+   ggplot() + geom_point(aes(x=day, y=PC1), size=2)
```



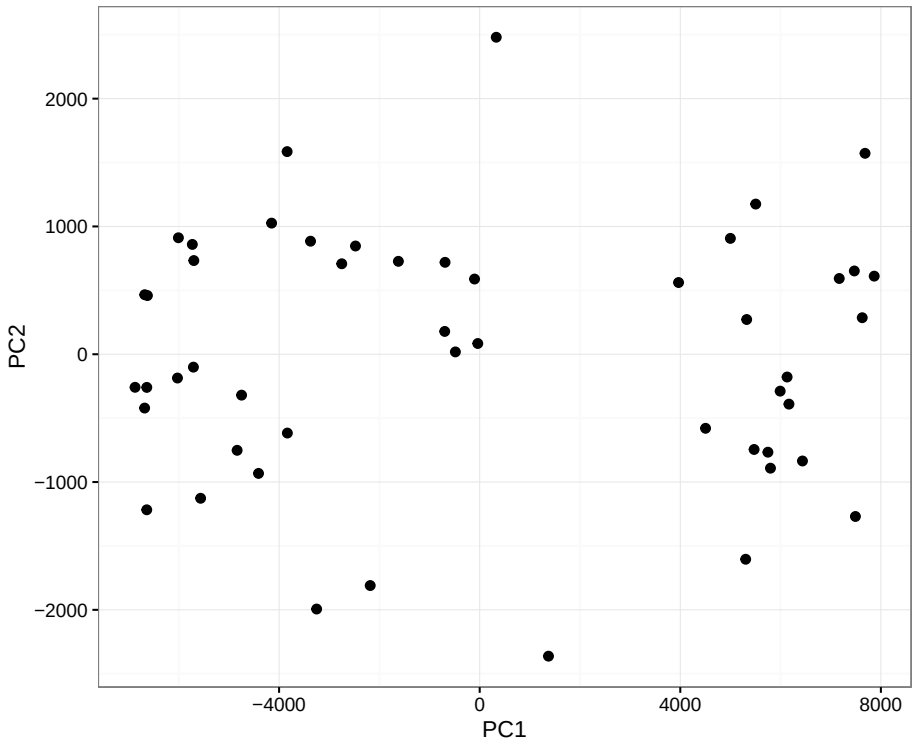
PC2 vs Time

```
> data.frame(day=day_of_the_year, PC2=mypca$pc[2,]) %>%
+   ggplot() + geom_point(aes(x=day, y=PC2), size=2)
```



PC1 vs PC2

```
> data.frame(PC1=mypca$pc[1,], PC2=mypca$pc[2,]) %>%
+   ggplot() + geom_point(aes(x=PC1, y=PC2), size=2)
```



PC Biplots

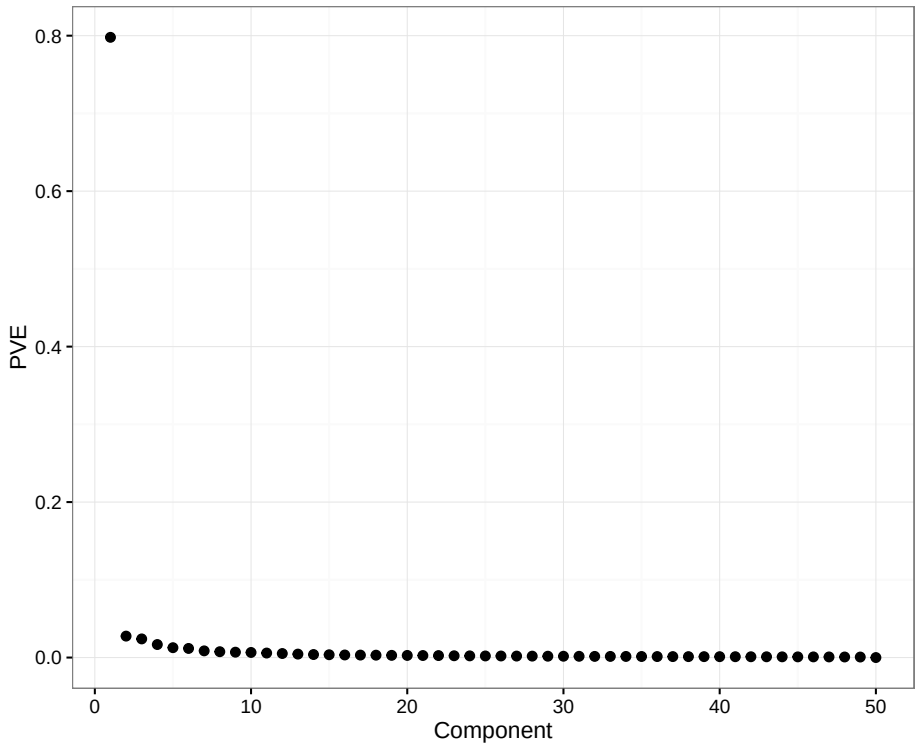
Sometimes it is really informative to plot a PC versus another PC (as in the previous slide). This is called a *PC biplot*.

It is possible that interesting subgroups or clusters of *observations* will emerge.

This does not appear to be the case in the weather data set, however, due to what we observe on the next slide.

Proportion of Variance Explained

```
> data.frame(Component=1:length(mypca$pve), PVE=mypca$pve) %>%
+   ggplot() + geom_point(aes(x=Component, y=PVE), size=2)
```



PCs Reproduce the Data

We can multiple the loadings matrix by the PCs matrix to reproduce the data:

```
> # mean centered weather data
> weather_data_mc <- weather_data - rowMeans(weather_data)
>
> # difference between the PC projections and the data
> # the small sum is just machine imprecision
> sum(abs(weather_data_mc - mypca$loading %*% mypca$pc))
[1] 3.572175e-08
```

Loadings

The sum of squared weights – i.e., loadings – equals one for each component:

```
> sum(mypca$loading[,1]^2)
[1] 1
>
> apply(mypca$loading, 2, function(x) {sum(x^2)})
```

```
 Loading1  Loading2  Loading3  Loading4  Loading5  Loading6
        1         1         1         1         1         1
 Loading7  Loading8  Loading9 Loading10 Loading11 Loading12
        1         1         1         1         1         1
Loading13 Loading14 Loading15 Loading16 Loading17 Loading18
        1         1         1         1         1         1
Loading19 Loading20 Loading21 Loading22 Loading23 Loading24
        1         1         1         1         1         1
Loading25 Loading26 Loading27 Loading28 Loading29 Loading30
        1         1         1         1         1         1
Loading31 Loading32 Loading33 Loading34 Loading35 Loading36
        1         1         1         1         1         1
Loading37 Loading38 Loading39 Loading40 Loading41 Loading42
        1         1         1         1         1         1
Loading43 Loading44 Loading45 Loading46 Loading47 Loading48
        1         1         1         1         1         1
Loading49 Loading50
        1         1
```

Pairs of PCs Have Correlaton Zero

PCs by contruction have sample correlation equal to zero:

```
> cor(mypca$pc[1,], mypca$pc[2,])
[1] 1.858194e-16
> cor(mypca$pc[1,], mypca$pc[3,])
[1] 9.762562e-17
> cor(mypca$pc[1,], mypca$pc[12,])
[1] -7.921241e-17
> cor(mypca$pc[5,], mypca$pc[27,])
[1] -2.43523e-16
> # etc...
```

Summary of SML 201

What Did We Learn?

- Basics of R
- Data wrangling
- Data visualization
- Exploratory data analysis
- Probability and random variables
- Statistical inference

- Formulating and fitting models
- Prediction / supervised learning
- Clustering / unsupervised learning
- Real data sets and questions are tough

R

Advanced R, Wickham

R Packages, Wickham

Introductory Statistics with R, Dalgaard

R Cookbook, Teetor

Visualization

R Graphics Cookbook, Chang

Visualizing Data, Cleveland

The Visual Display of Quantitative Information, Tufte

Modeling

Statistical Models: Theory and Practice, Freedman

Nonparametric Regression and Generalized Linear Models: A roughness penalty approach, Green and Silverman

Bayesian Data Analysis, Gelman et al.

Statistical Inference

All of Statistics, Wasserman

Statistical Inference, Casella and Berger

An Introduction to the Bootstrap, Efron and Tibshirani

A First Course in Bayesian Statistical Methods, Hoff

Machine Learning

An Introduction to Statistical Learning: with Applications in R, James et al.

Elements of Statistical Learning, Hastie, Tibshirani, and Friedman

Machine Learning: A Probabilistic Perspective, Murphy

Pattern Recognition and Machine Learning, Bishop

SML UG Certificate

http://csml.princeton.edu/education/undergraduate-certificate-program

- Requires five courses in total
- One fundamentals of statistics, one fundamentals of ML
- SML 201 currently counts as one of the three additional courses
- See the web site for further details

Extras

License

https://github.com/SML201/lectures/blob/master/LICENSE.md

Source Code

https://github.com/SML201/lectures/tree/master/week12

Session Information

```
> sessionInfo()
R version 3.2.3 (2015-12-10)
Platform: x86_64-apple-darwin13.4.0 (64-bit)
Running under: OS X 10.11.4 (El Capitan)

locale:
[1] en_US.UTF-8/en_US.UTF-8/en_US.UTF-8/C/en_US.UTF-8/en_US.UTF-8

attached base packages:
[1] stats     graphics  grDevices utils     datasets  methods
[7] base

other attached packages:
[1] dendextend_1.1.8 broom_0.4.0      dplyr_0.4.3
[4] ggplot2_2.1.0    knitr_1.12.3     magrittr_1.5
[7] devtools_1.11.1
```

```
loaded via a namespace (and not attached):
 [1] Rcpp_0.12.4       whisker_0.3-2     mnormt_1.5-4
 [4] munsell_0.4.3     lattice_0.20-33   colorspace_1.2-6
 [7] R6_2.1.2          highr_0.5.1       stringr_1.0.0
[10] plyr_1.8.3        tools_3.2.3       parallel_3.2.3
[13] grid_3.2.3        nlme_3.1-127      gtable_0.2.0
[16] psych_1.5.8       DBI_0.3.1         withr_1.0.1
[19] htmltools_0.3.5   lazyeval_0.1.10   yaml_2.1.13
[22] digest_0.6.9      assertthat_0.1    tidyr_0.4.1
[25] reshape2_1.4.1    formatR_1.3       memoise_1.0.0
[28] evaluate_0.8.3    rmarkdown_0.9.5.9 labeling_0.3
[31] stringi_1.0-1     scales_0.4.0
```