Class 10

BUS 696

Prof. Jonathan Hersh

BUS 696: Class 10 Announcements

1. Exams

   - Still grading…

2. Final Projects

   - Nov 14th summary stats due

   - Must summarize training data -> having performed feature transformation and cleaning

BUS 696: Class 10 Outline

1. HBR AI Articles

2. Cleaning Factor Levels

3. Unsupervised Learning

   - K-means Clustering

   - Hierarchical Clustering

   - Principal Component Analysis

What is unsupervised learning?

- All of the machine learning we've encountered so far has been supervised learning such as regression

- This last lecture will describe **unsupervised learning**

- In unsupervised learning, we observe x_1, x_2, x_p, features but we don't observe any Ys
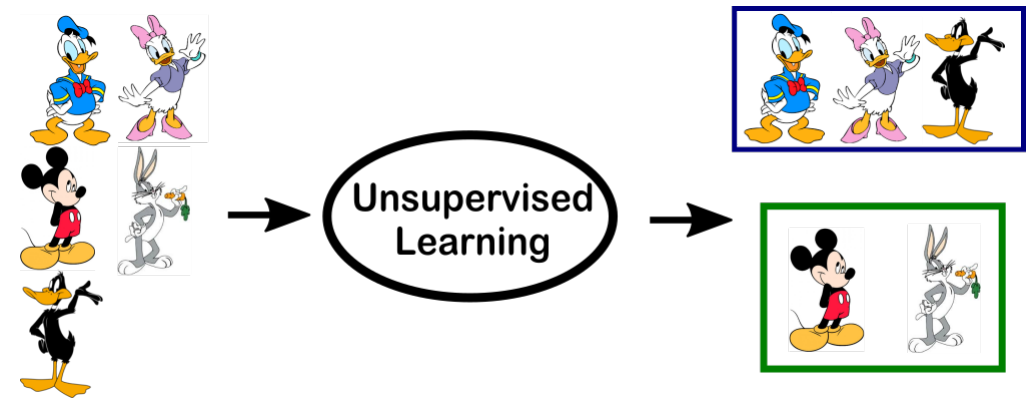
Goals of unsupervised learning

- **Since we don't observe $Y's$, we can't predict anything**

- The goal is more subtle here: can we discover interesting patterns in the data? Can we discover useful subgroups?

- We'll discuss two methods
  - **clustering**: a broad class of methods for discovering unknown subgroups
  - **principal component analysis**: a tool used for data visualization and dimension reduction

Supervised Learning

Unsupervised Learning

dataaspirant.wordpress.com

Challenge of unsupervised learning

- **Because we have no "truth", the end result is more subjective**

- **Some examples of unsupervised learning**
  - subgroup of breast cancer patients that by gene expression are drug resistant
  - groups of shoppers characterized by browsing and purchase histories
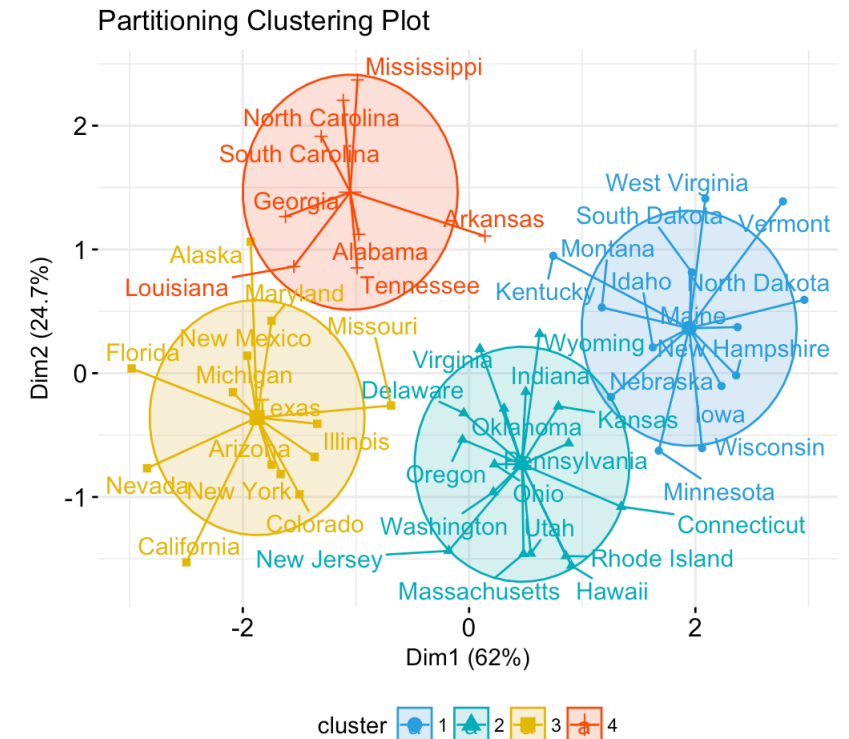 - movies grouped by ratings assigned by movie viewers

K-means clustering as a "game"

- Tell the computer how many groups (k) you think the data should be split into

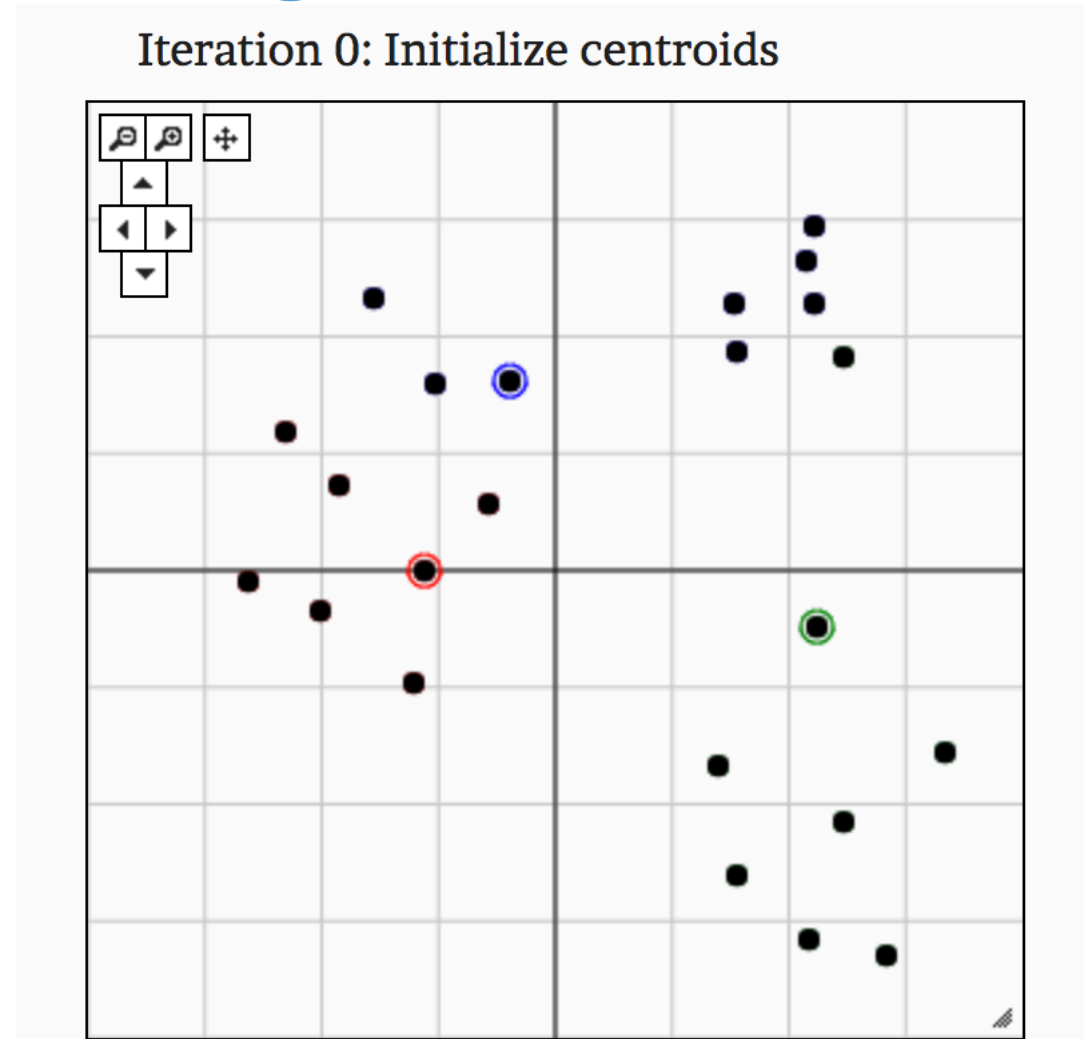- The computer splits the objects into k groups such that the groups are most similar

Partitioning Clustering Plot
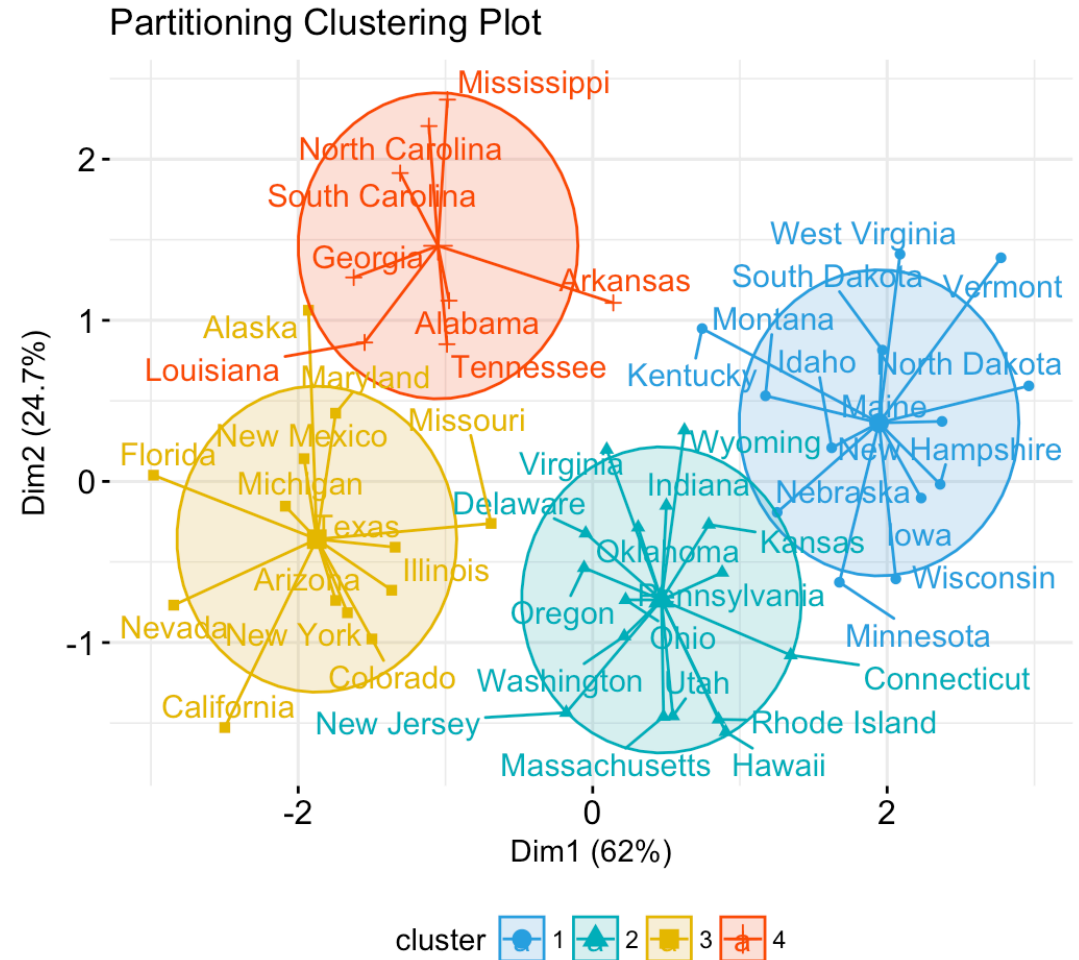
K-means clustering algorithm

1. Decide how many clusters we want. Call this K

2. Randomly assign a number, $1, . . . , K$, to each of the observations. (Initial cluster assignment)

3. Iterate until clusters stop changing:
   - **Expectation-step:** For each of the K clusters, compute the cluster centroid (center point, i.e. means for the k-th cluster)
   - **Maximization-step:** Assign each observation to the cluster whose centroid is closest (in Euclidean distance)
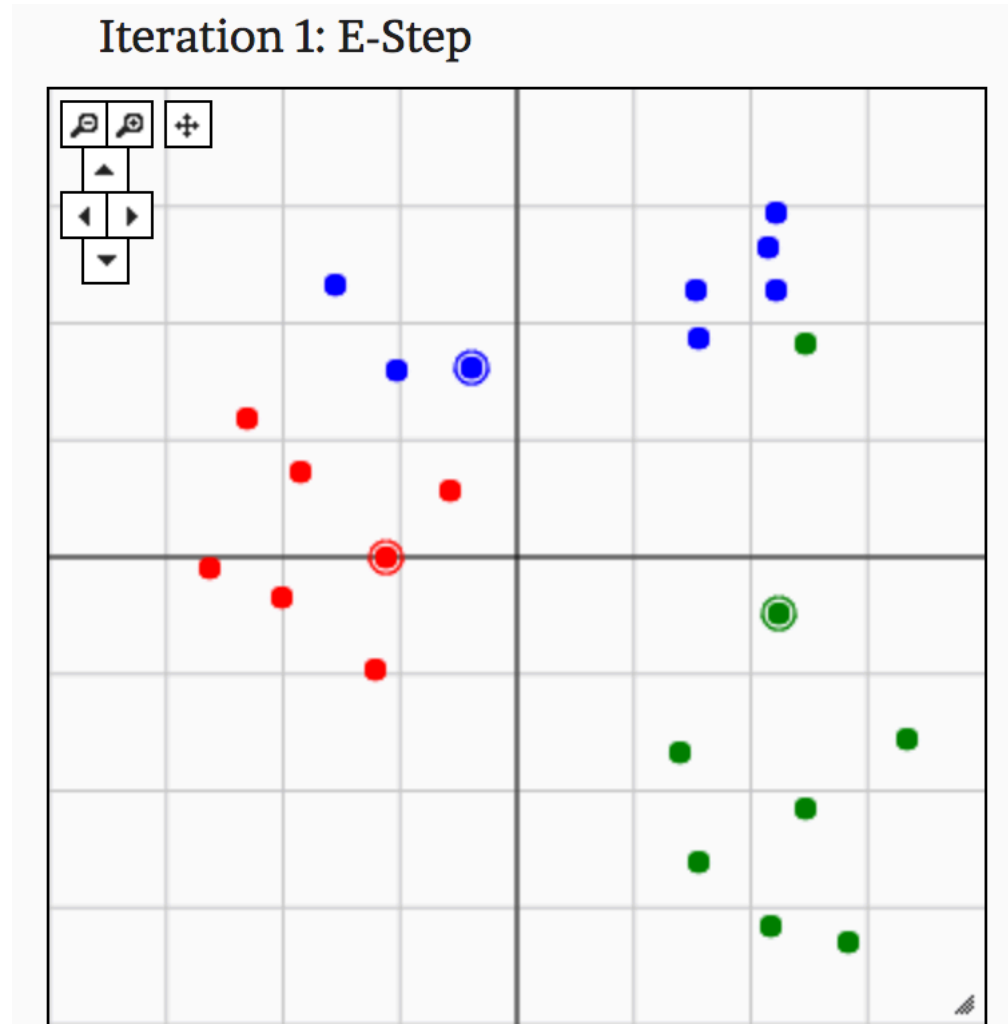

Partitioning Clustering Plot
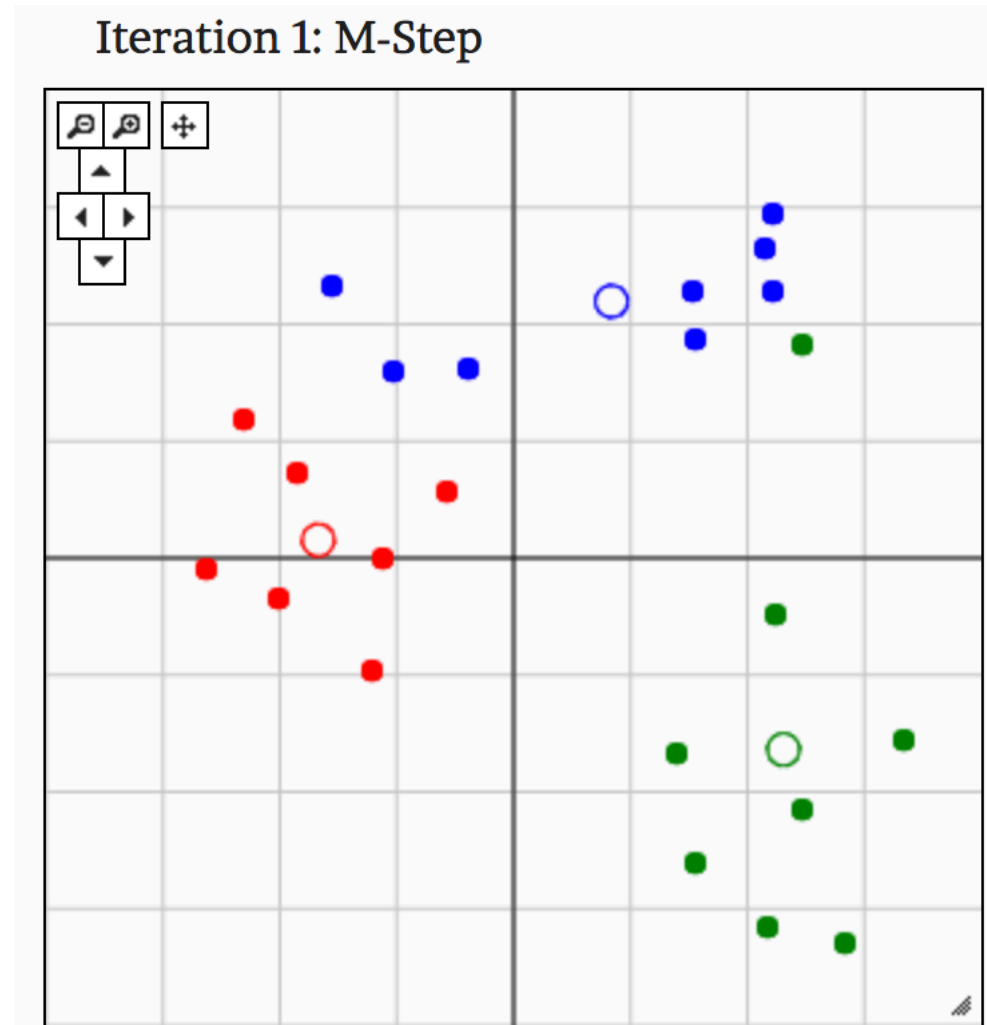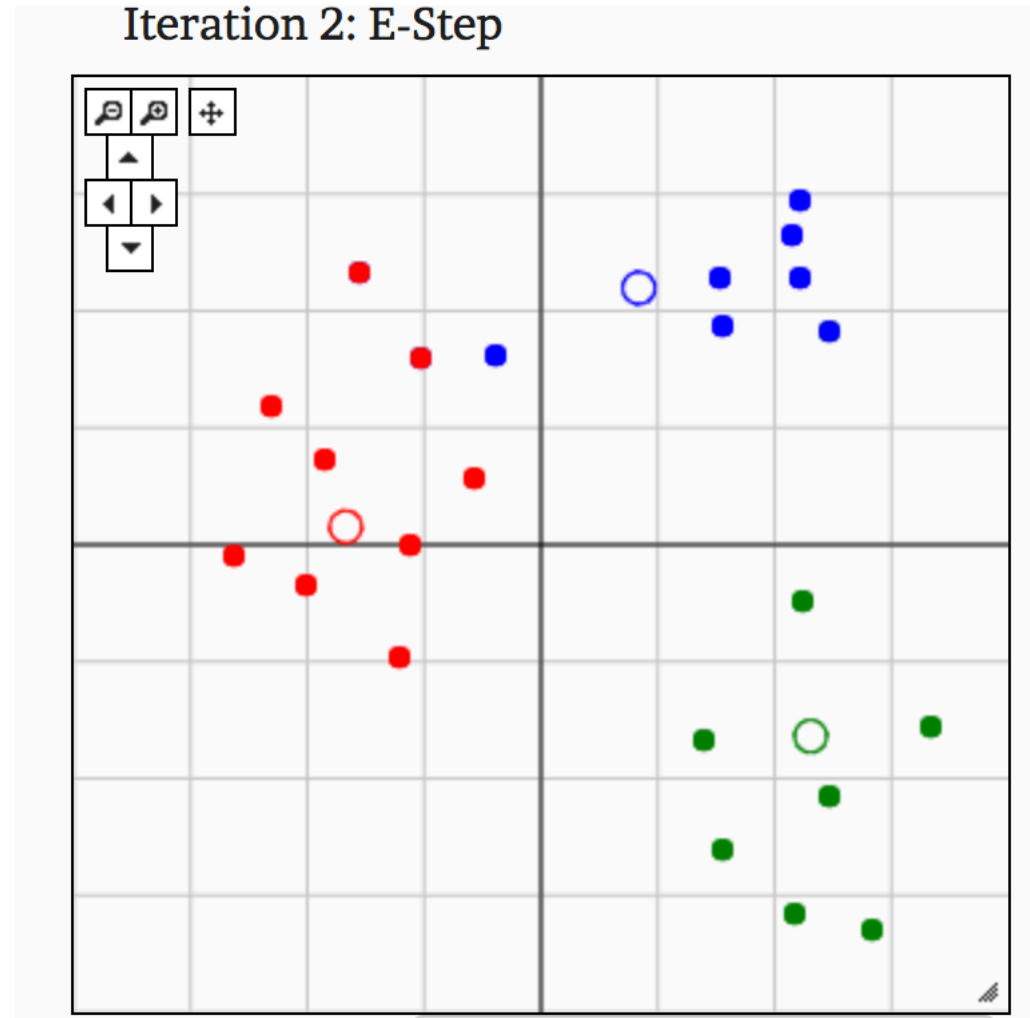
K-means clustering in action

Iteration 0: Initialize centroids

- From: http://util.io/k-means

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K-means clustering in action

Iteration 1: E-Step

- From: http://util.io/k-means

K-means clustering in action

Iteration 1: M-Step

- From: http://util.io/k-means

K-means clustering in action

- From: http://util.io/k-means

K-means clustering in action

- From: http://util.io/k-means

K-means clustering in action

- From: http://util.io/k-means

K-means clustering in action

Iteration 3: M-Step

- From: http://util.io/k-means

K-means clustering in action

Iteration 4: E-Step

- From: http://util.io/k-means
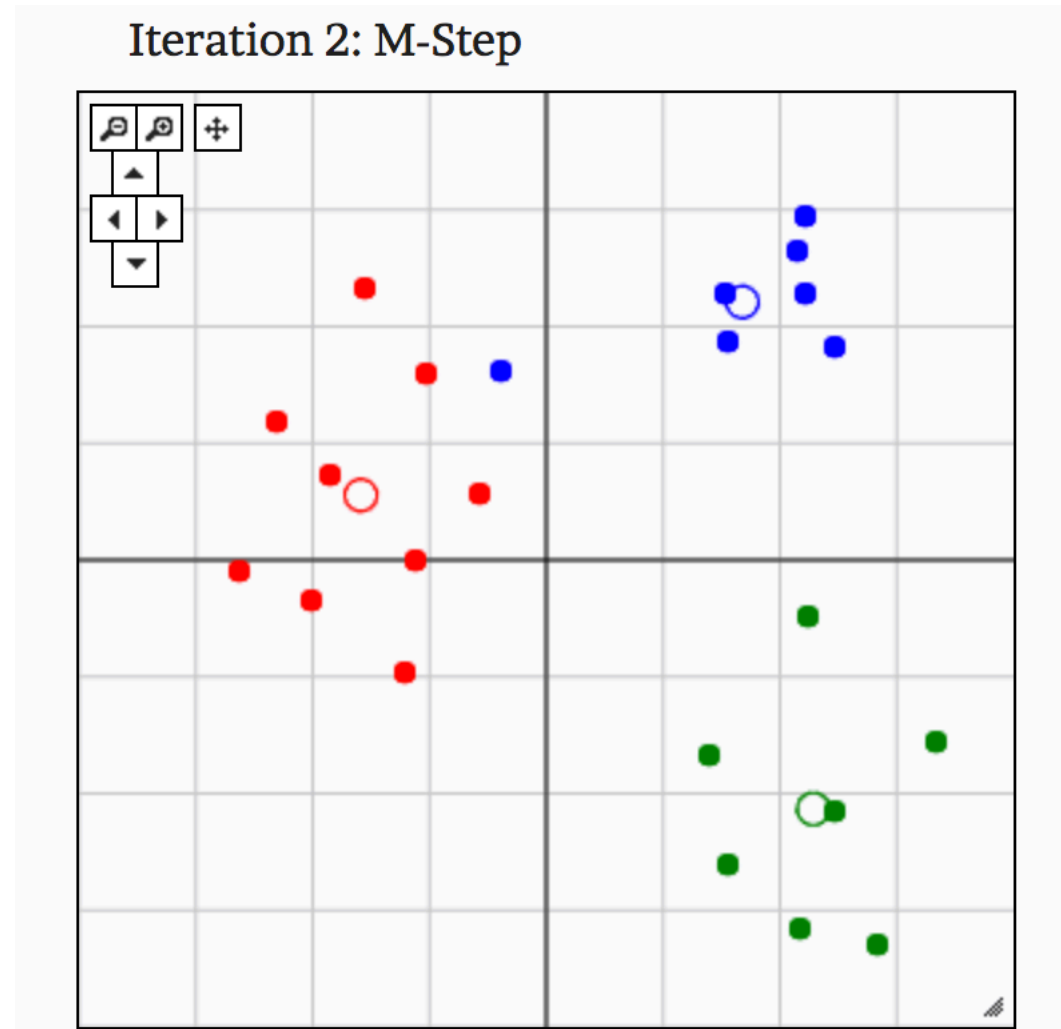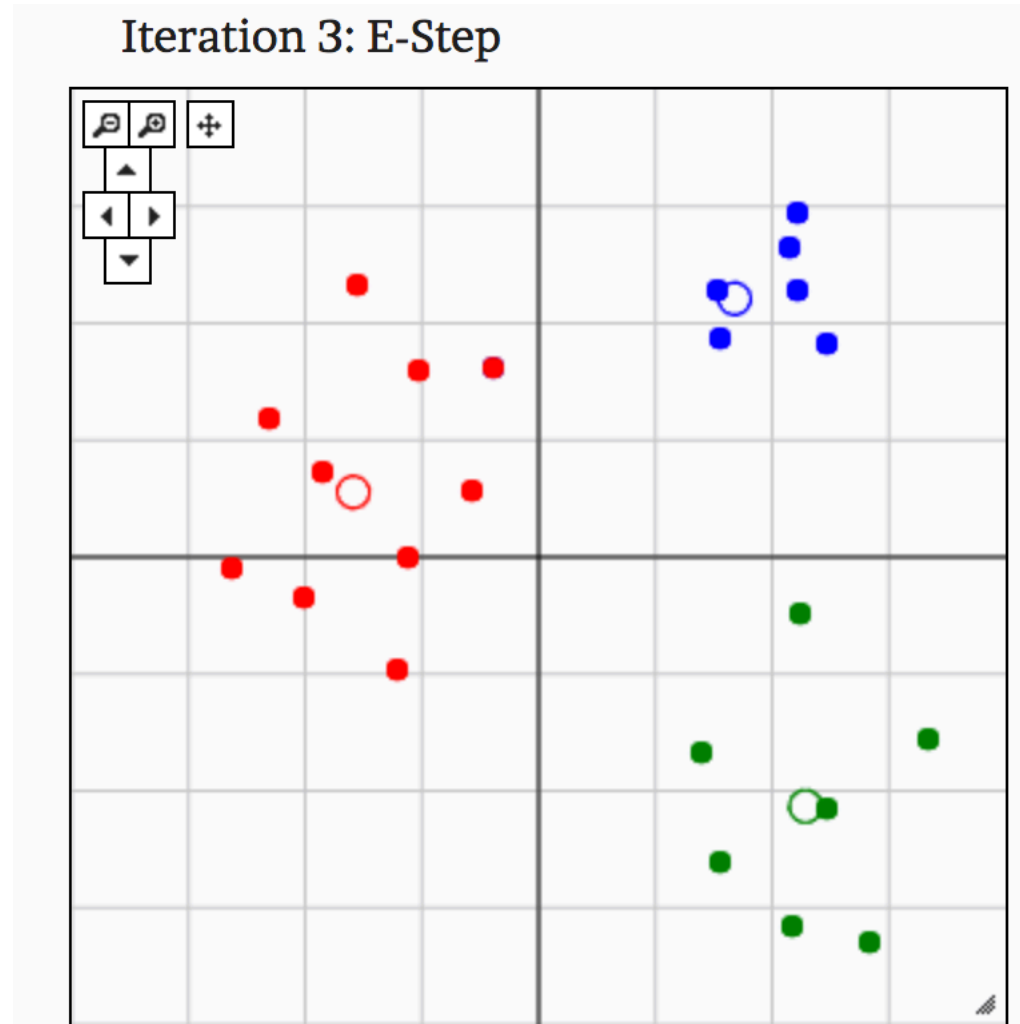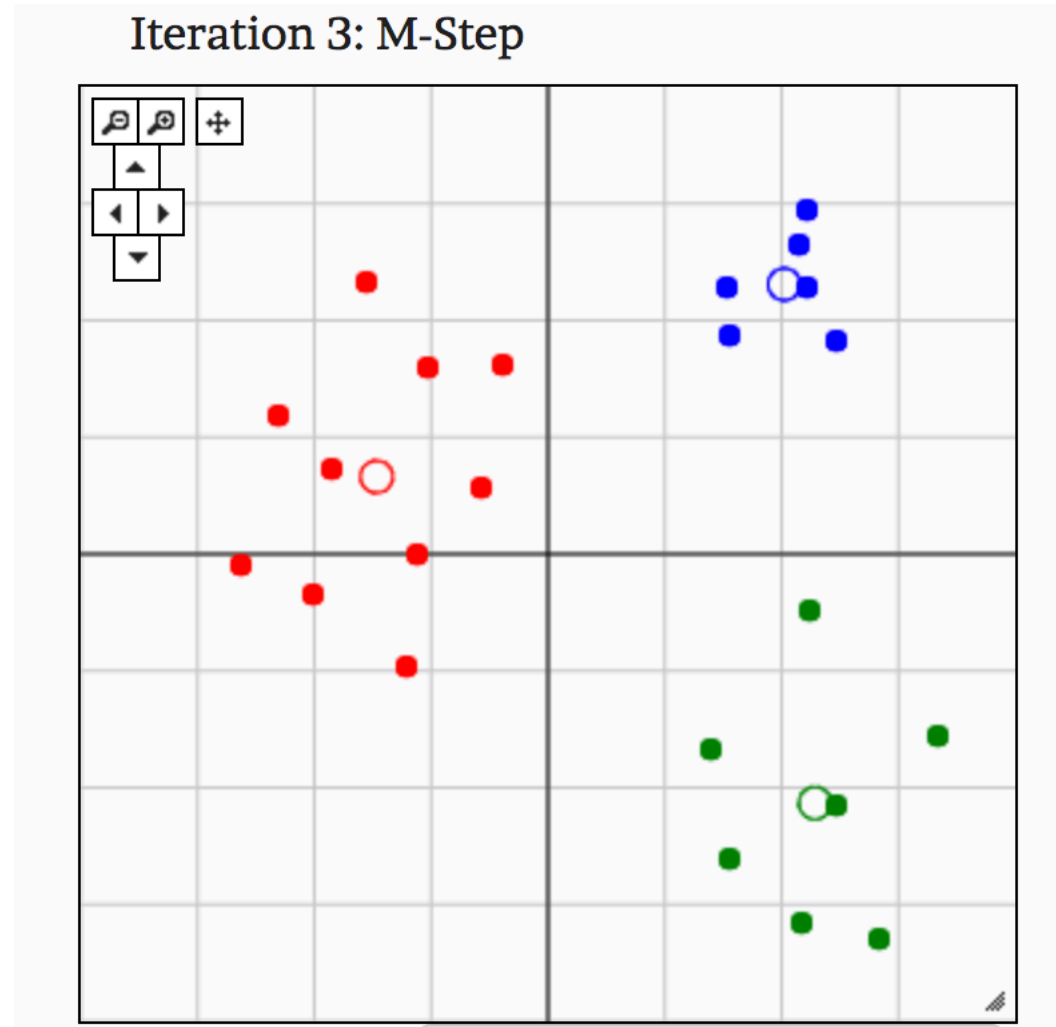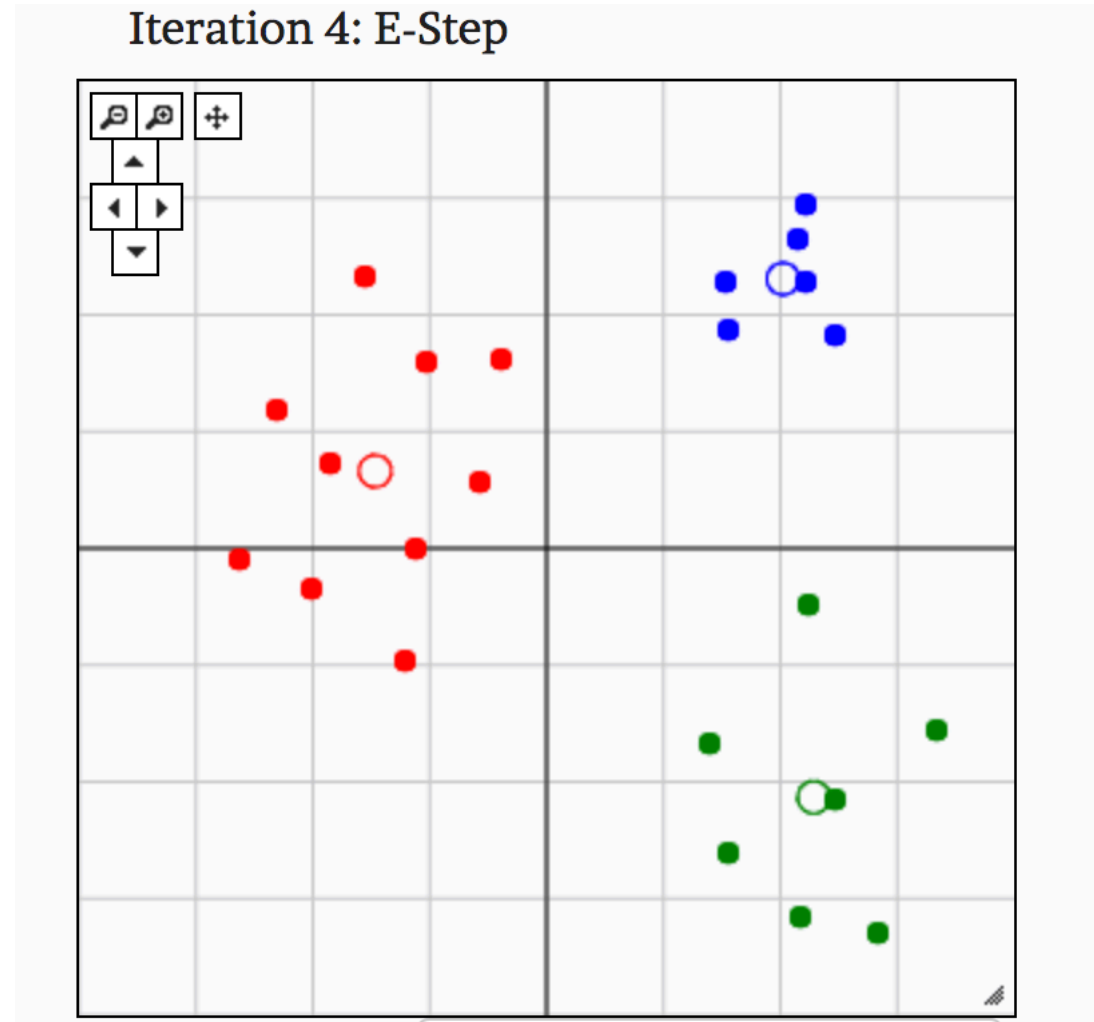
Examples of clustering: Customer Segmentation
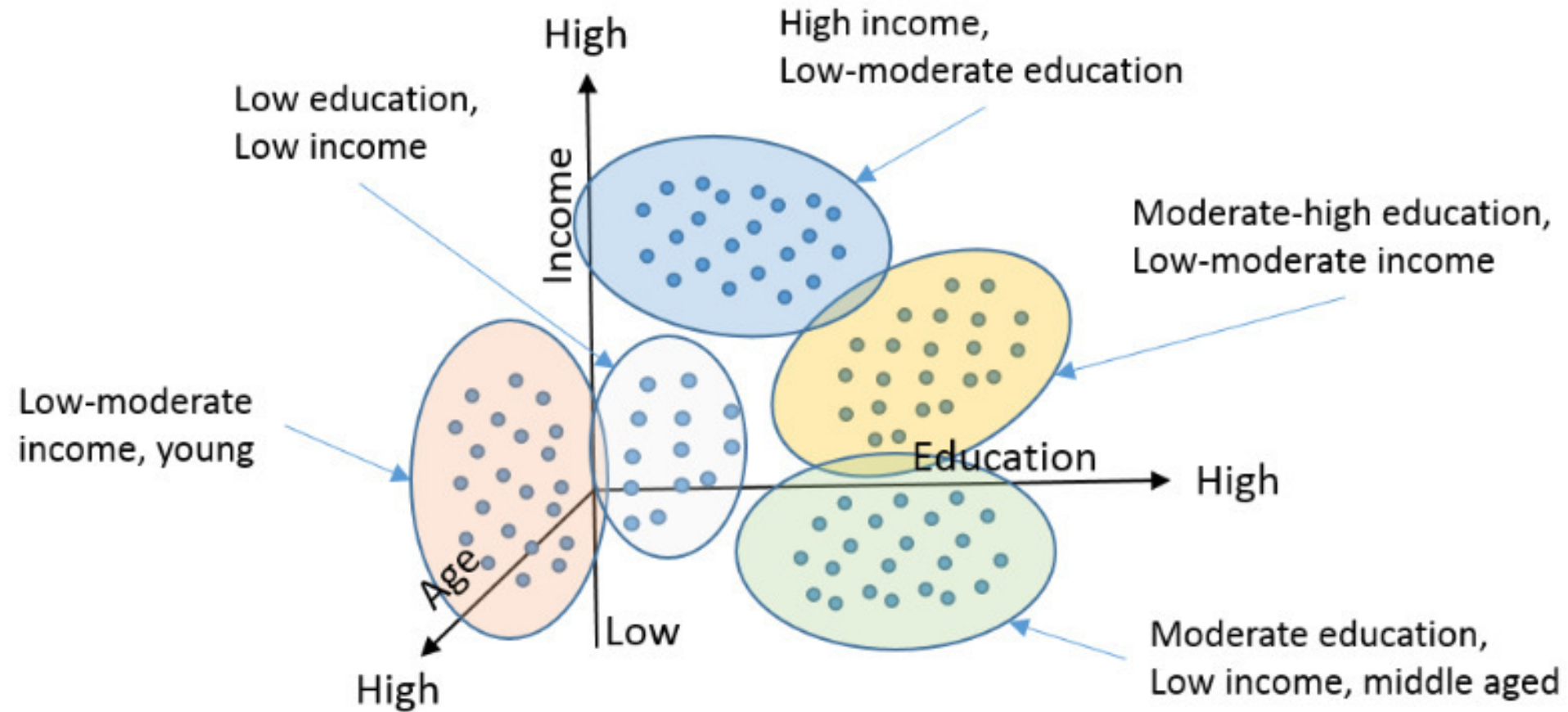
Examples of clustering: Clustering Wide Receivers

Using k-means clustering to find similar players

Wed 23 September 2015

Most of the posts so far have focused on what data scientists call *supervised* methods -- you have some outcome you're trying to predict and you use a combination of predictor variables to do so. Another important class of methods are called *unsupervised*. In this case, you might not know what exactly you're looking for or what metric you want to optimize for, but you want to explore the data and identify similarities among cases. For example, you might want to identify a list of "similar" players for your fantasy draft. This is a little late for the start of fantasy season, but with the rise of daily fantasy sports, perhaps not. However, maybe you don't know what "similar" means in this case or you don't have a single number or index that you want to match on. Perhaps you just want to find players with similar production to hedge against bye weeks or injuries.

This is where unsupervised methods come in. We'll be focusing on a popular unsupervised method called *clustering*. You'll see these kinds of methods used on a number of sports sites. Boris Chen, a data scientist at the New York Times, uses a kind of clustering to produce his fantasy football player tiers. Krishna Narsu recently used a kind of clustering to redefine the defensive positions in the NBA.

One popular method is called *k-means clustering*. (Note, this isn't the same k as in k-fold cross-validation, k is just a common stand-in for an unknown integer value.) I'll be working through an example clustering wide receivers using their 2013 statistics. K-means is really beautifully simple. The basic idea is that we want to take our entire data set and divide the observations into k sections and have each of the observations be as similar to each other as possible (and potentially as dissimilar to every other cluster as possible). Each cluster has what's known as a 'center' or 'centroid', which is the point against which all of the observations in that cluster are compared. You can think of it as the "ideal" or "prototypical" observation that typifies each cluster.

EDIT: As always, code for this example is up on GitHub.

- From: http://thespread.us/clustering.html

Examples of clustering: Clustering Wide Receivers

Cluster	Targets	Receptions	Yards	TDs	Fumbles	Fantasy Points
0	-0.84	-0.82	-0.81	-0.72	-0.4	-0.82
1	0.49	0.47	0.43	0.41	-0.38	0.45
2	1.74	1.82	1.9	1.72	0.47	1.93
3	0.21	0.12	0.08	-0.07	2.46	0.01

Player	cluster
A.Hawkins	0
A.Robinson	0
B.Golden	0
C.Johnson	2
E.Bennett	0
E.Weems	0
J.Boyce	0
J.Criner	1
J.Ebert	0
K.Allen	2
K.Martin	0
L.Brazill	1
L.Hankerson	1
L.Moore	1
R.Shepard	0
R.Shepard	0
R.Woods	1
R.Woods	1
S.Smith	1
V.Jackson	2

- From: http://thespread.us/clustering.html

Plan for Today

- What topics to cover for Data Management?
  - Merging data
  - Dplyr basics
  - What else?
- No problem set 11 (is that okay?)
- Signup for presentations
  - Monday, Dec 3rd
  - Wednesday, Dec 5th
- Hierarchical clustering

- K-means code
- PCA
- PCA code

Hierarchical clustering algorithm

1. Begin with *n* observations and calculate all of the pairwise dissimilarities. Treat each observation as its own cluster

2. For *i = n, n − 1, . . . , 2* :
   - Examine all pairwise inter-cluster dissimilarities among the *i* clusters and identify the clusters that are most similar. Fuse these two clusters.
   - Compute the new pairwise inter-cluster dissimilarities among the *i − 1* remaining clusters
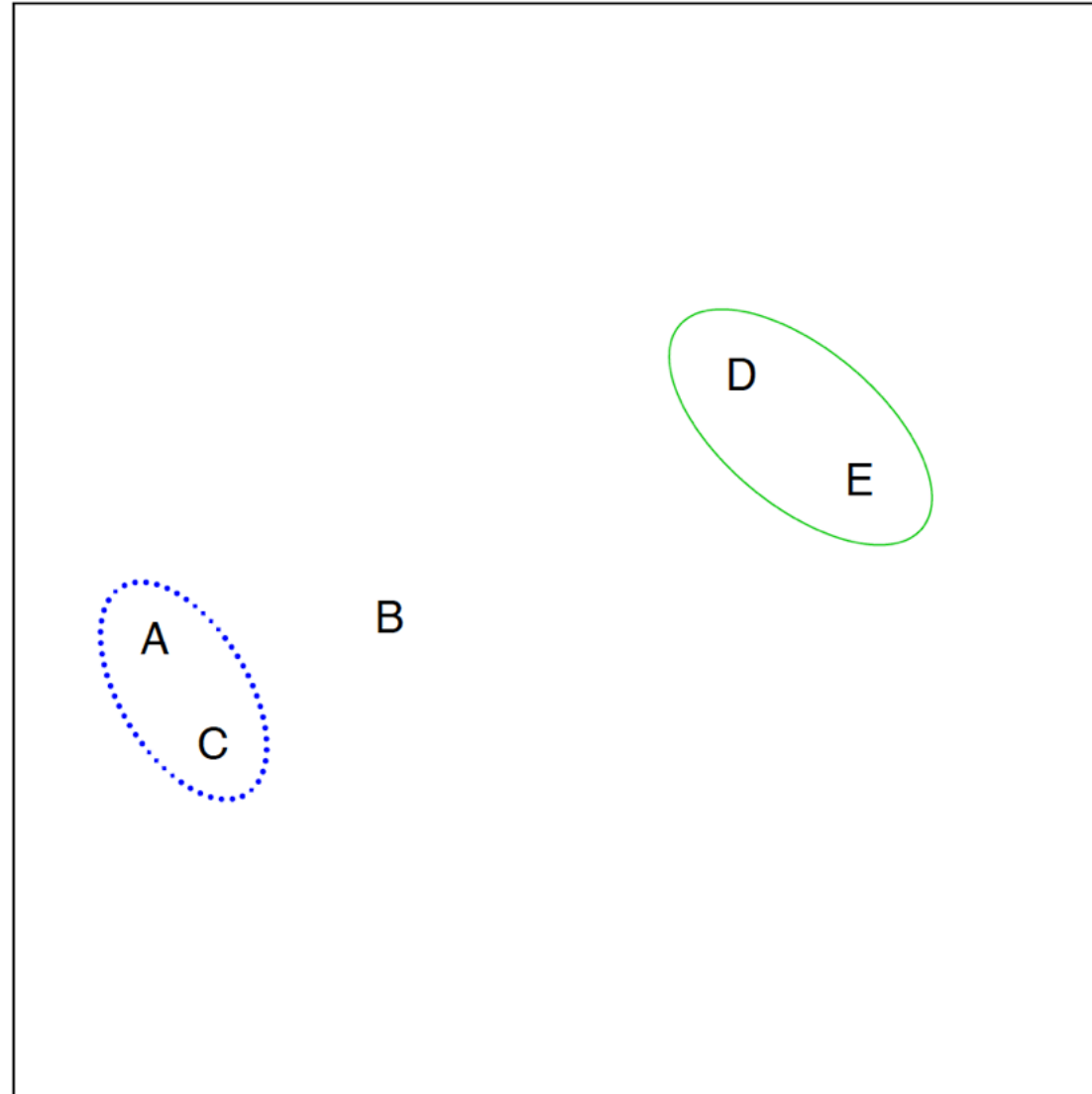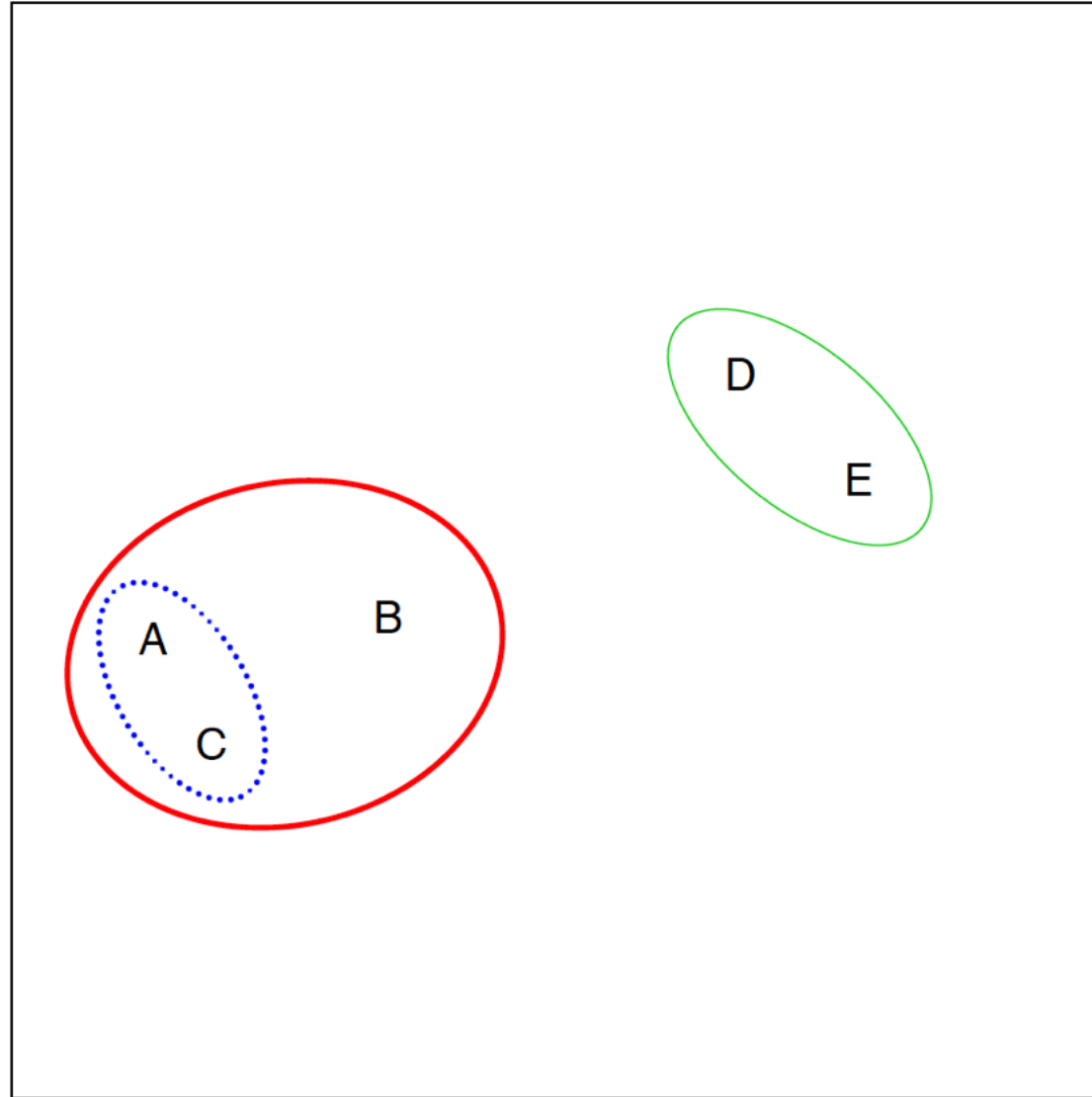
Hierarchical clustering in action
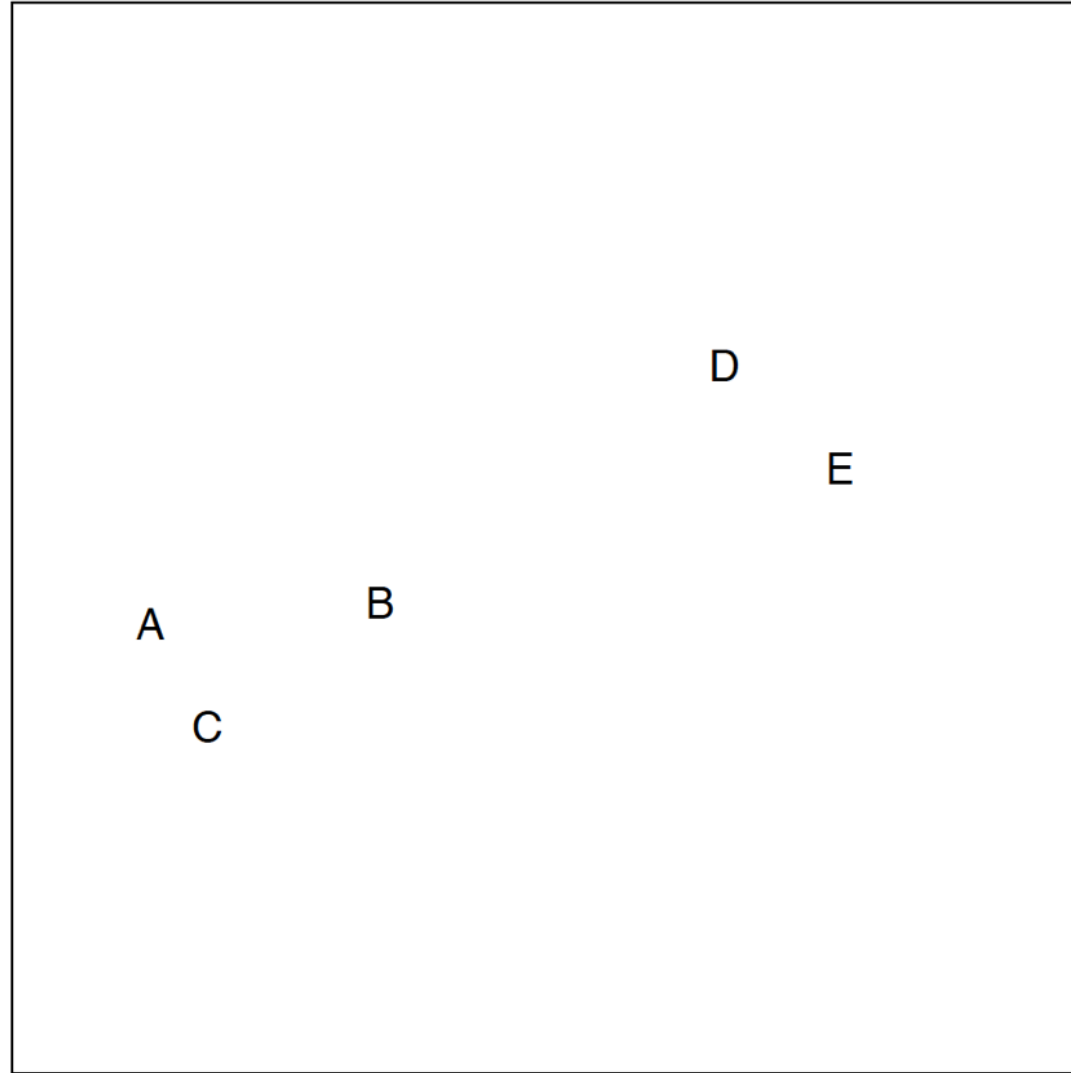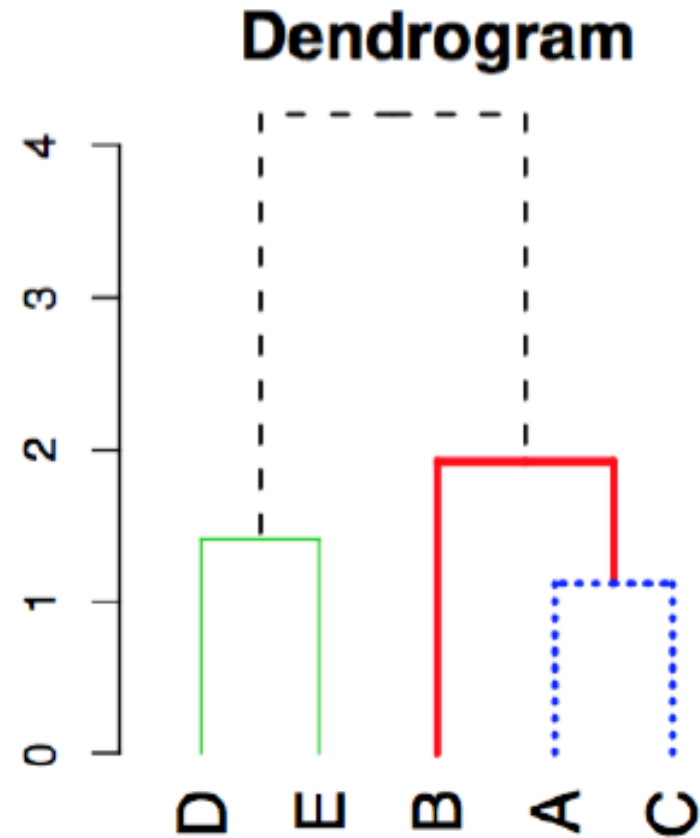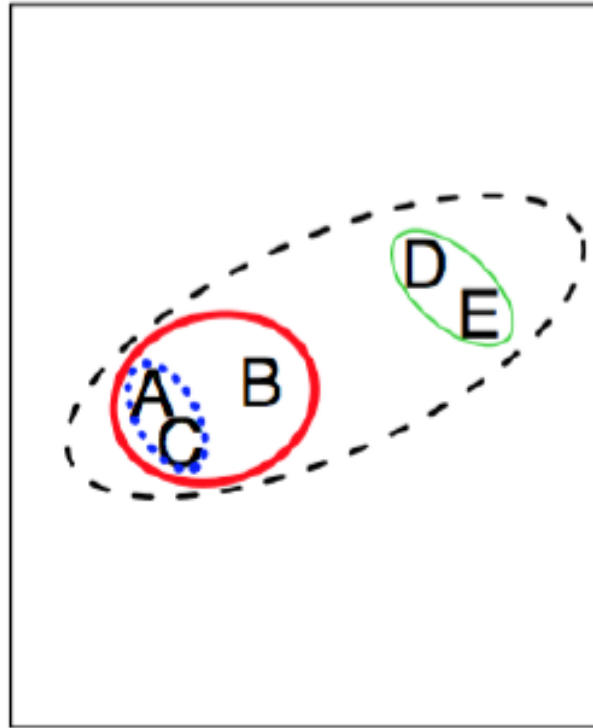
Hierarchical clustering in action
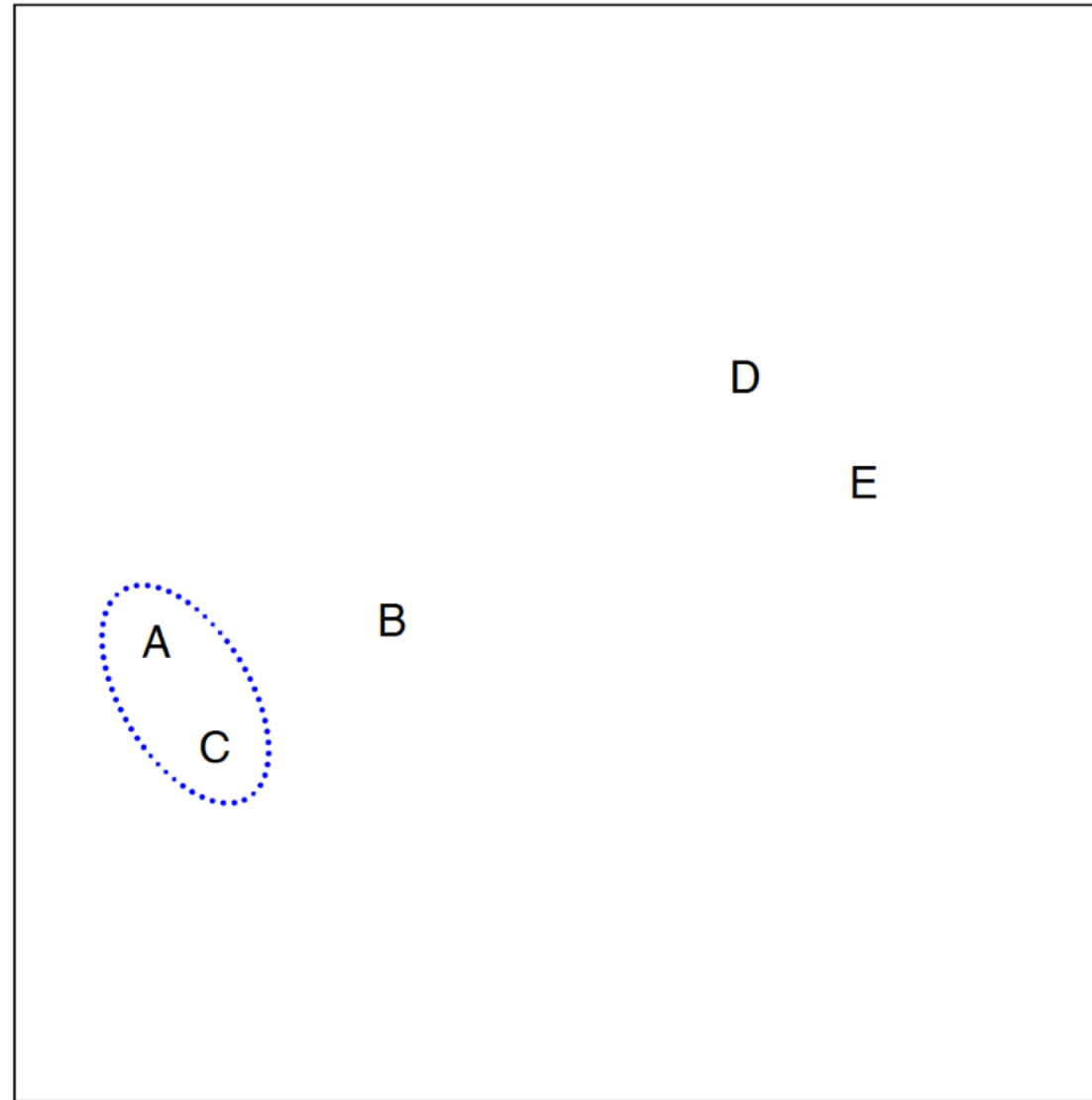
Hierarchical clustering in action

Hierarchical clustering in action

Connection to "dendrograms"

K-means in R

```r
library('ISLR')
library('factoextra')
library('cluster')
data("USArrests")
kmeans3 <- kmeans(USArrests, centers = 3, nstart = 25)
str(kmeans3)
kmeans3
```

K-means in R

```
> kmeans3
K-means clustering with 3 clusters of sizes 14, 20, 16

Cluster means:
     Murder   Assault UrbanPop      Rape
1  8.214286 173.2857 70.64286 22.84286
2  4.270000  87.5500 59.75000 14.39000
3 11.812500 272.5625 68.31250 28.37500
```
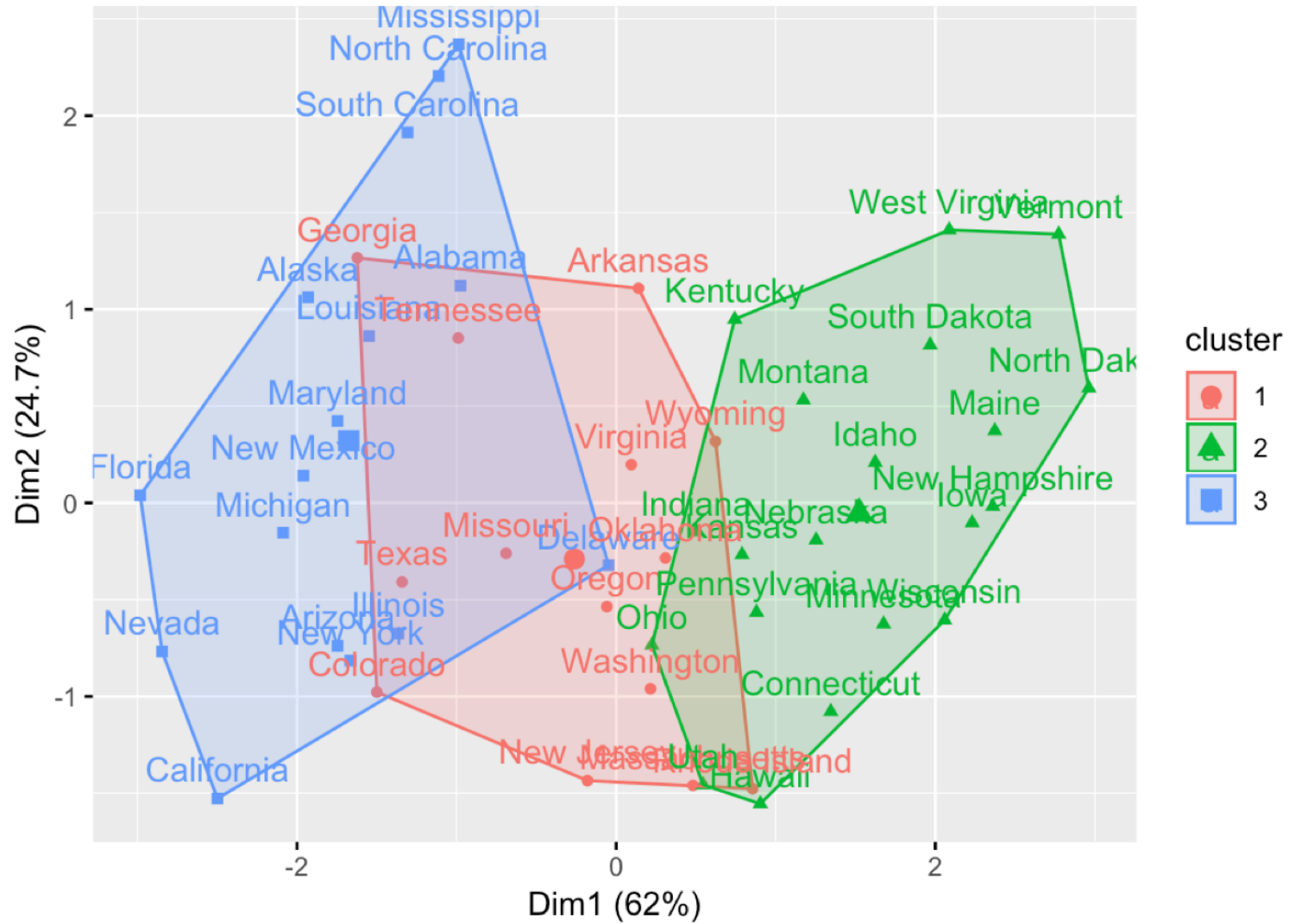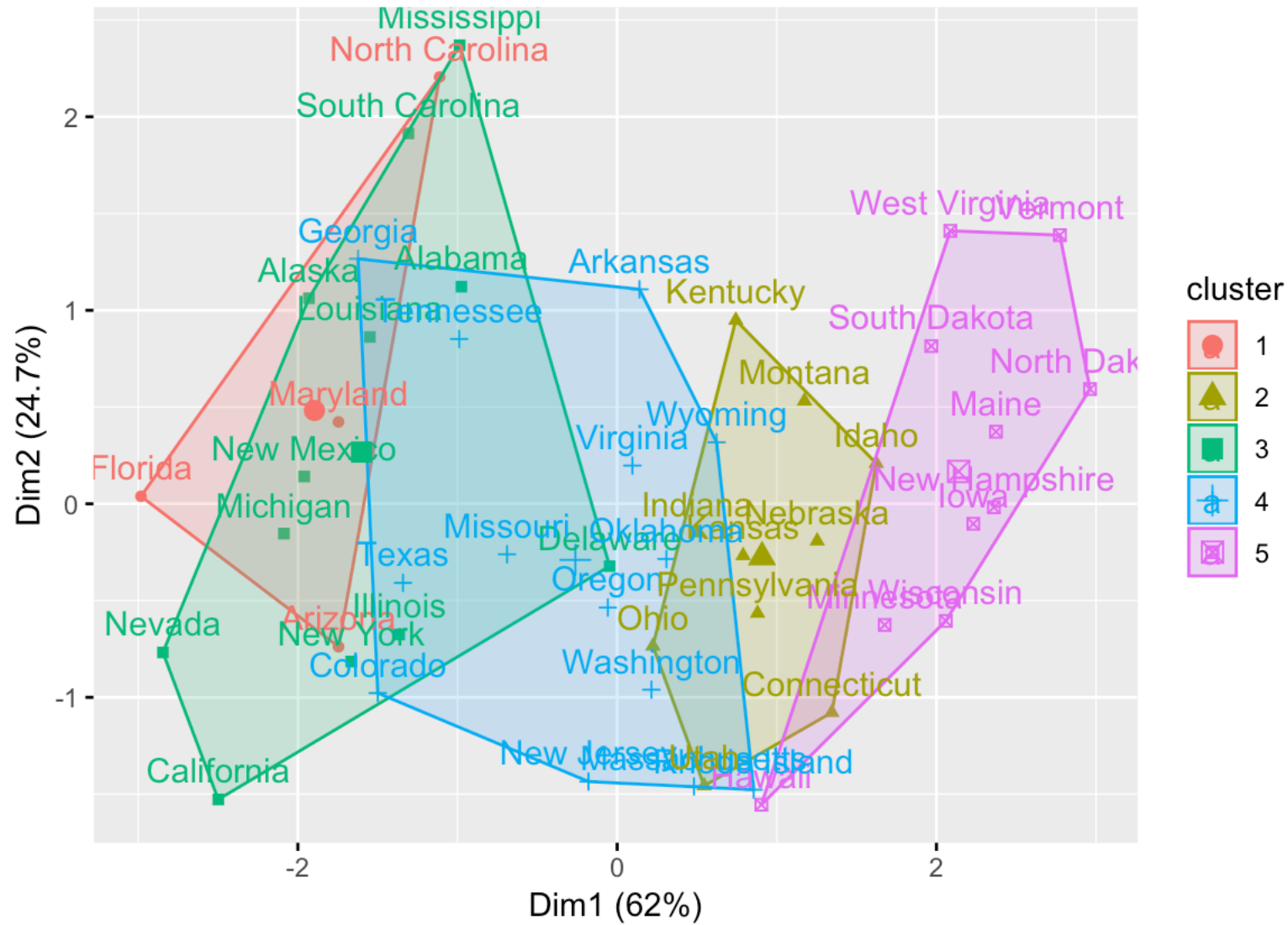
```
Within cluster sum of squares by cluster:
[1]  9136.643 19263.760 19563.863
 (between_SS / total_SS =  86.5 %)
```

K=3 means clustering

```
fviz_cluster(kmeans3, data = USArrests, main = "K=3 means clustering")
```

K=5 means clustering


```
kmeans5 <- kmeans(USArrests, centers = 5, nstart = 25)
fviz_cluster(kmeans5, data = USArrests, main = "K=5 means clustering")
```

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How to pick k? "Elbow Method"

- Plot explained variance by # of clusters
- Look for the "bend" in the plot

```r
# how many clusters? Elbow method
wss <- function(k){
  kmeans(USArrests, k, nstart = 25)$tot.withinss
}
wss_values <- map_dbl(1:15, wss)
plot(1:15, wss_values,
     type = "b", pch = 19, frame = FALSE,
     xlab = "Number of clusters K",
     ylab = "Total within-cluster sum of squares")
```

Within-cluster sum of squares by # of clusters
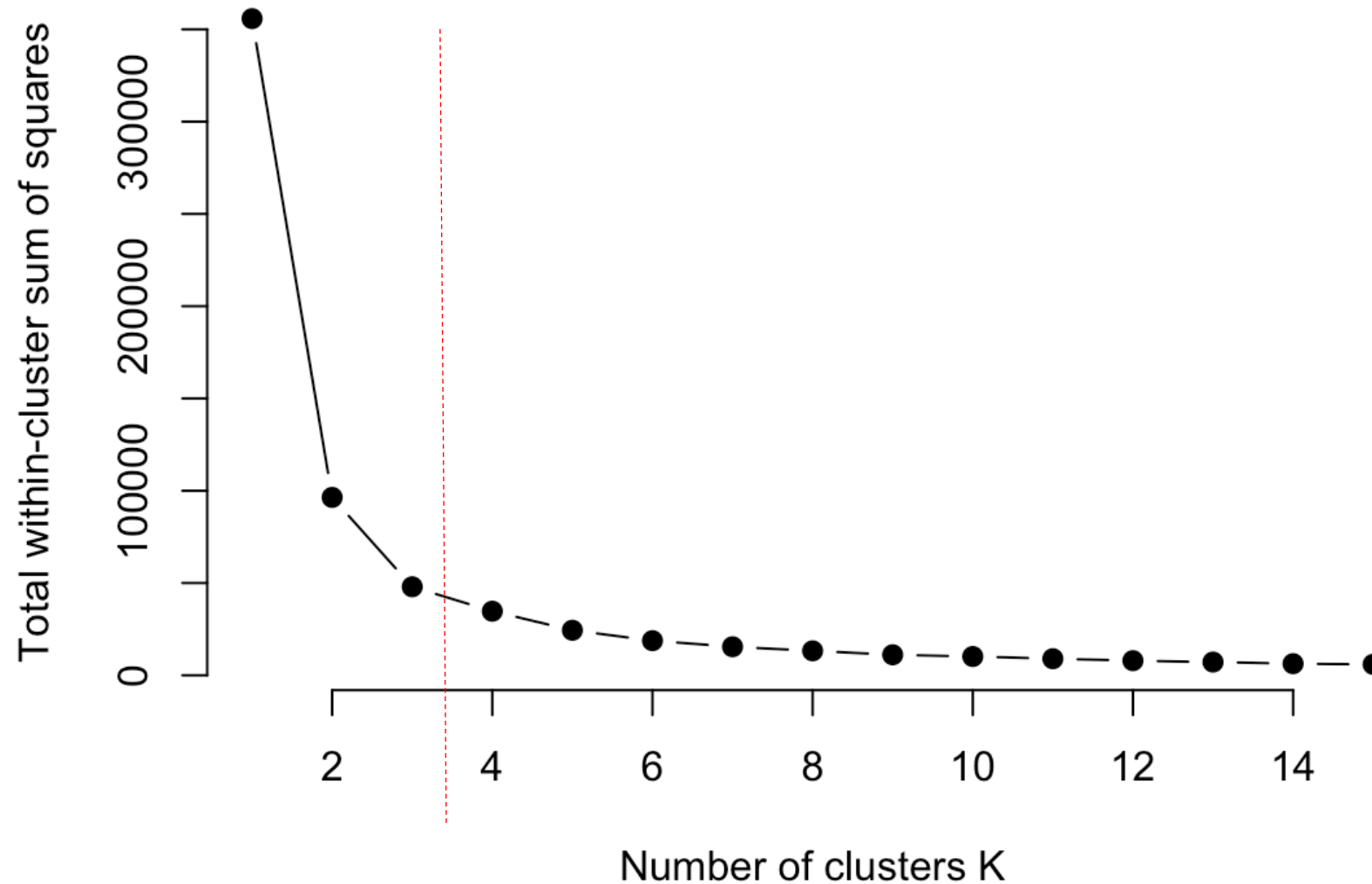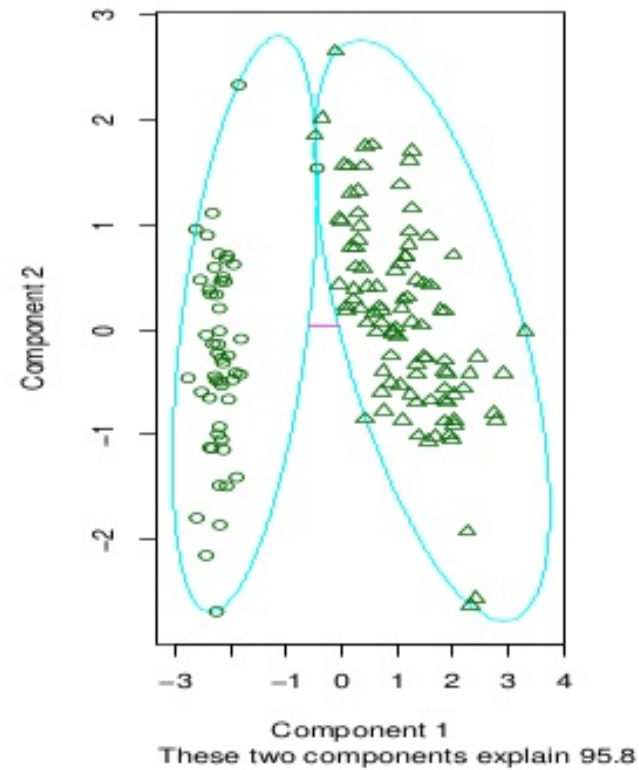
How to pick k?

Silhouette score:

- $a_i =$ measure of dissimilarity between point i and other observations in its cluster.
    - 1 = good match with cluster
    - -1 = really bad match
- $b_i =$ measure of dissimilarity between i and all other points in any cluster
- $s_i = \dfrac{b_i - a_i}{\max\{a_i, b_i\}}$

Silhouette Score

```
layout(matrix(c(1, 2), 1, 2))   # 2 graphs per page
plot(pamk.result$pamobject)
```


clusplot(pam(x = sdata, k = k, diss = d

Silhouette plot of pam(x = sd

n = 150

2 clusters C_j

$j : n_j \mid ave_{i \in C_j} s_i$

1 : 51 | 0.81

2 : 99 | 0.62

Component 1
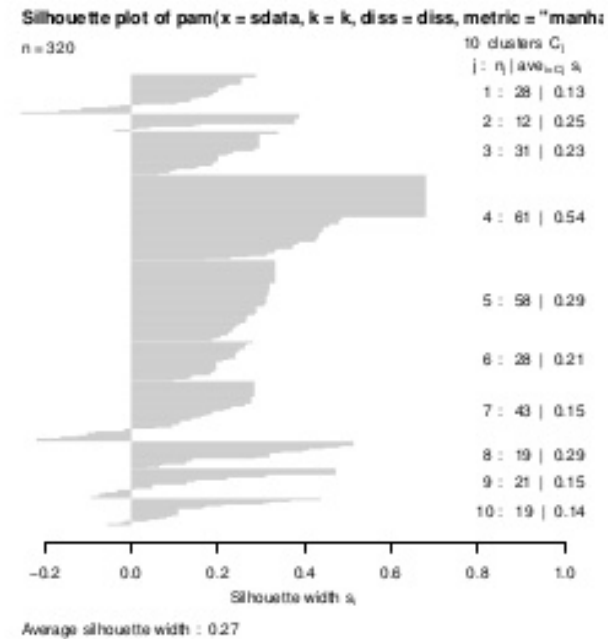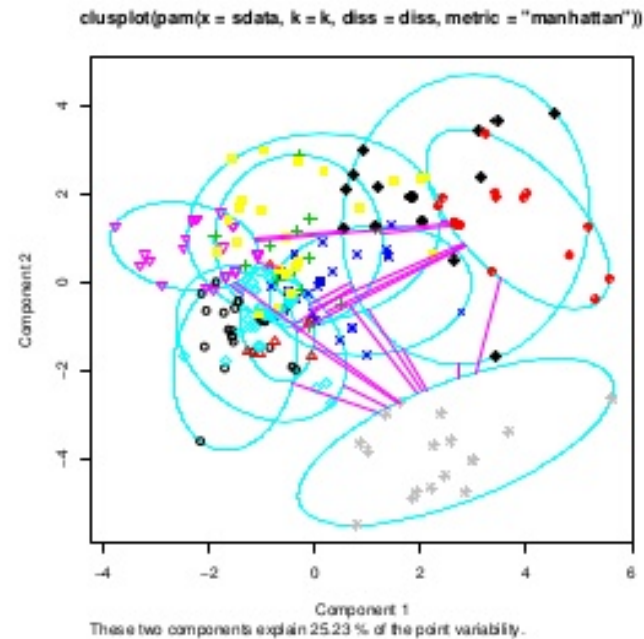These two components explain 95.8

Silhouette width s_i

Average silhouette width : 0.69
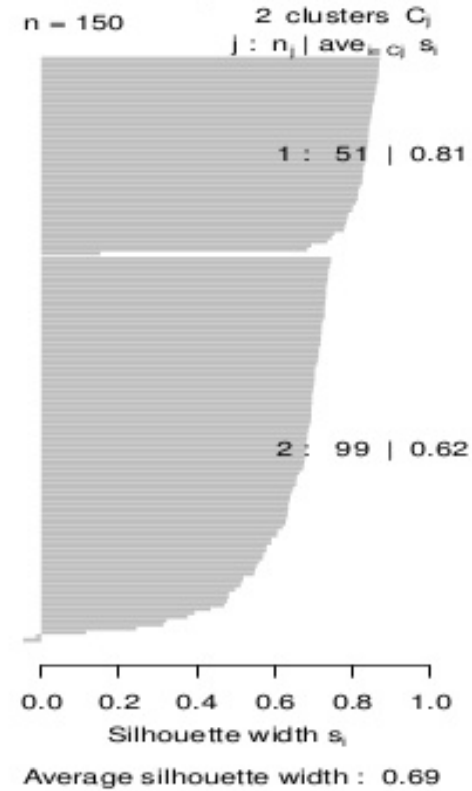
```
layout(matrix(1))   # change back to one graph per page
```

Silhouette Score

```
# plot clustering result
layout(matrix(c(1, 2), 1, 2))  # set to two graphs per page
plot(pamResult, col.p = pamResult$clustering)
```



```
layout(matrix(1))  # change back to one graph per page
```

Motivation for Dimension Reduction 1

- Suppose we want to visualize n observations that have p variables, $X_1, \ldots, X_n$

- We could examine every two-dimensional sub-plot

- However, that would be $(how\ many)$ subplots?
  - $\binom{p}{2} = \frac{p(p-1)}{2}$

- How do we visualize data to see how "far apart" certain observations are from one another?

Motivation for Dimension Reduction 2

- Sometimes in a regression setting, we care about controlling for many characteristics, but don't care about interpreting those characteristics.

- We can take those control variables, project them down into a lower dimensional subspace, then control for only those lower dimensional variables

- E.g. take 100 controls variables, project down to 2 dimensions, and only control for those 2 variables

Enter Principal Component Analysis

- **PCA produces a low-dimensional representation of a dataset**.

- It does so by finding directions of maximal variance that are mutually orthogonal

- In other words it asks the question

If I had to pick a set of direction such that if I projected the data onto those directions, and then computed the variance of the points, which directions would maximize explained variance?

First Principal Component

- PCA finds sequence of linear combinations of the variables that maximize variance and are mutually uncorrelated

- The first principal component of a set of features $X_1, X_2, \ldots, X_p$ is the normalized linear combination of the features

$$Z_1 = \phi_{11}X_1 + \phi_{21}X_2 + \cdots + \phi_{p1}X_p$$

    That have the largest variance

- Normalized here means $\sum_{j=1}^{p} \phi_{j1}^2 = 1$

- $\boldsymbol{\phi_1} = \left(\phi_{11}\phi_{21}\ldots\phi_{p1}\right)^T$ is the vector of factor loadings of the first principal component
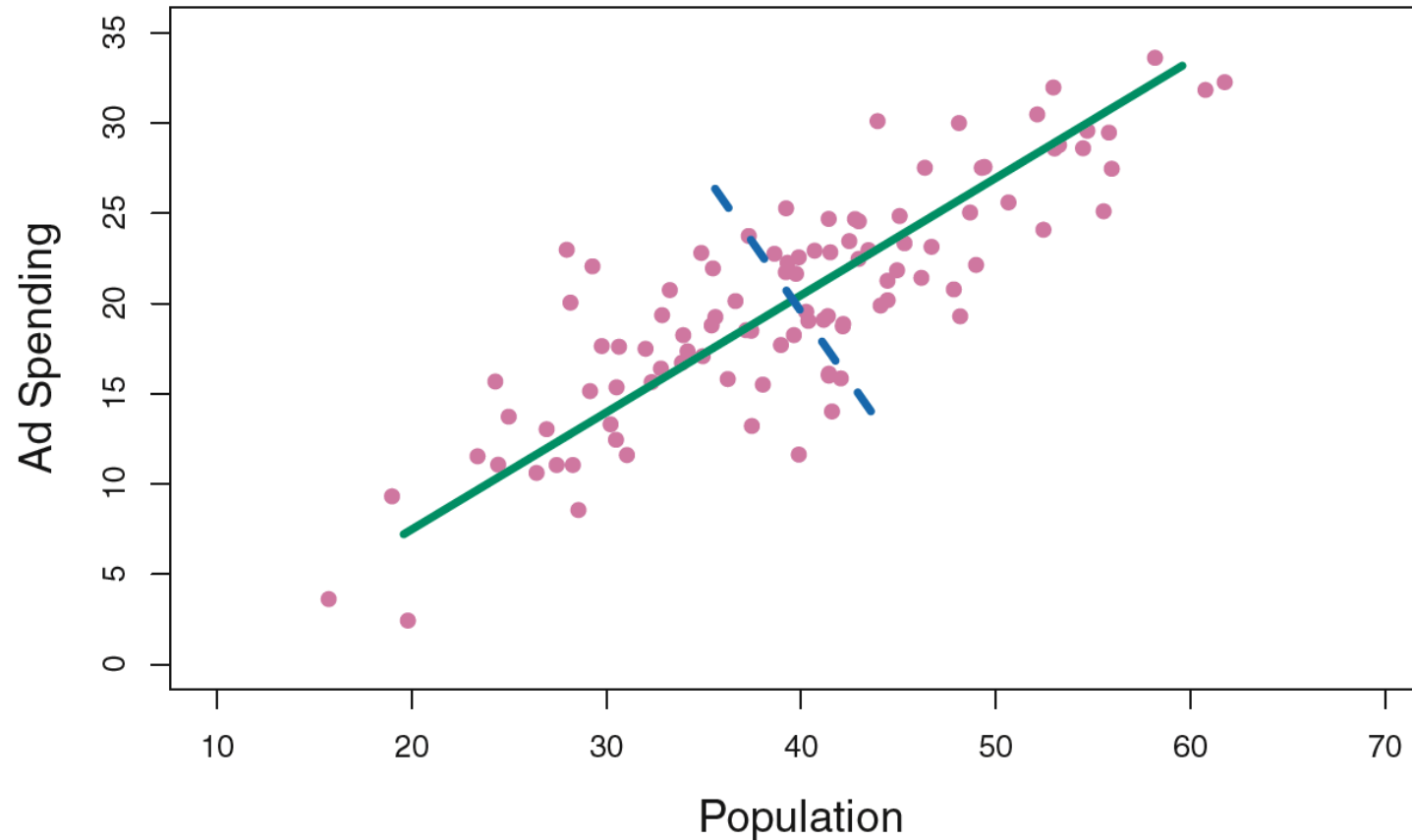
First Principal Component

FIGURE 6.14. *The population size (*pop*) and ad spending (*ad*) for* 100 *different cities are shown as purple circles. The green solid line indicates the first principal component, and the blue dashed line indicates the second principal component.*

Second Principal Component

- After we have calculated the first principal component, Z_1, the second principle component is the linear combination of $X_1, \cdots, X_p$ that has maximal variance out of all linear combinations that are uncorrelated with Z_1

- The second principal component takes the form

$$Z_2 = \phi_{12}X_1 + \phi_{22}X_2 + \cdots + \phi_{p2}X_p$$

$\boldsymbol{\phi_2} = \left(\phi_{12}\phi_{22}\dots\phi_{p2}\right)^T$ is the vector of factor loadings of the second principal component

- Constraining Z_2 to be uncorrelated with Z_1 is equivalent to constraining X_1 to be orthogonal (perpendicular) to X_2
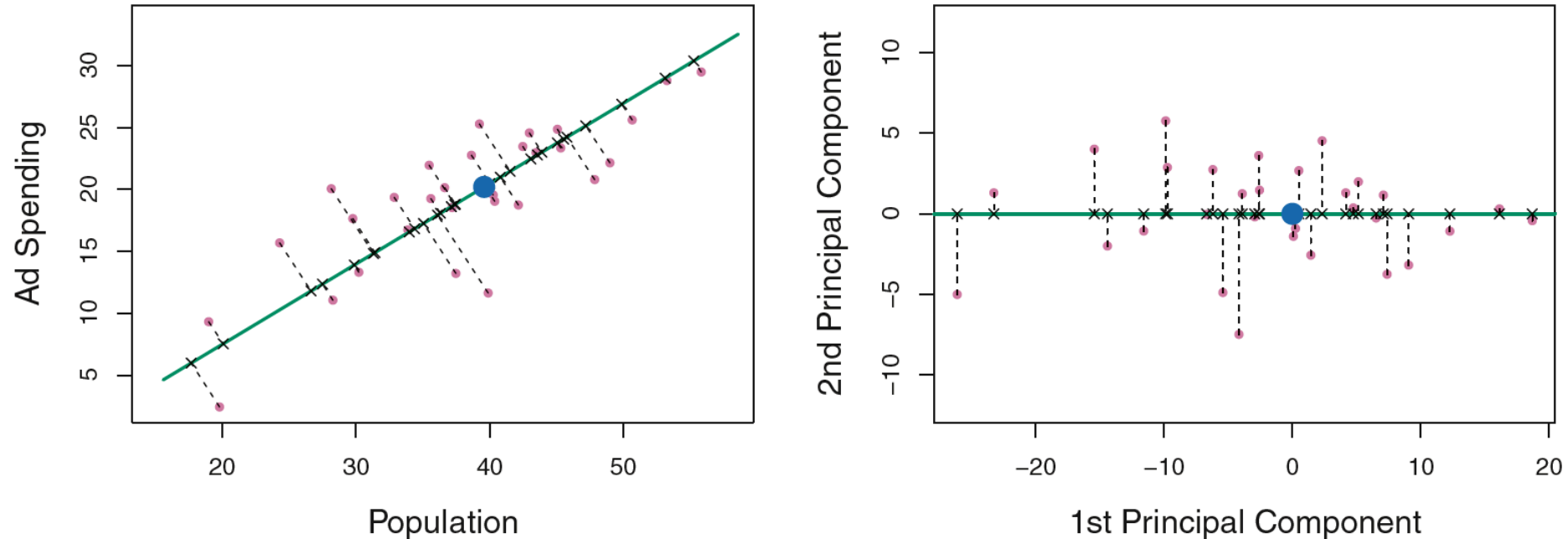
Second Principal Component

FIGURE 6.15. *A subset of the advertising data. The mean* pop *and* ad *budgets are indicated with a blue circle.* Left: *The first principal component direction is shown in green. It is the dimension along which the data vary the most, and it also defines the line that is closest to all n of the observations. The distances from each observation to the principal component are represented using the black dashed line segments. The blue dot represents* $(\overline{\text{pop}}, \overline{\text{ad}})$. Right: *The left-hand panel has been rotated so that the first principal component direction coincides with the x-axis.*
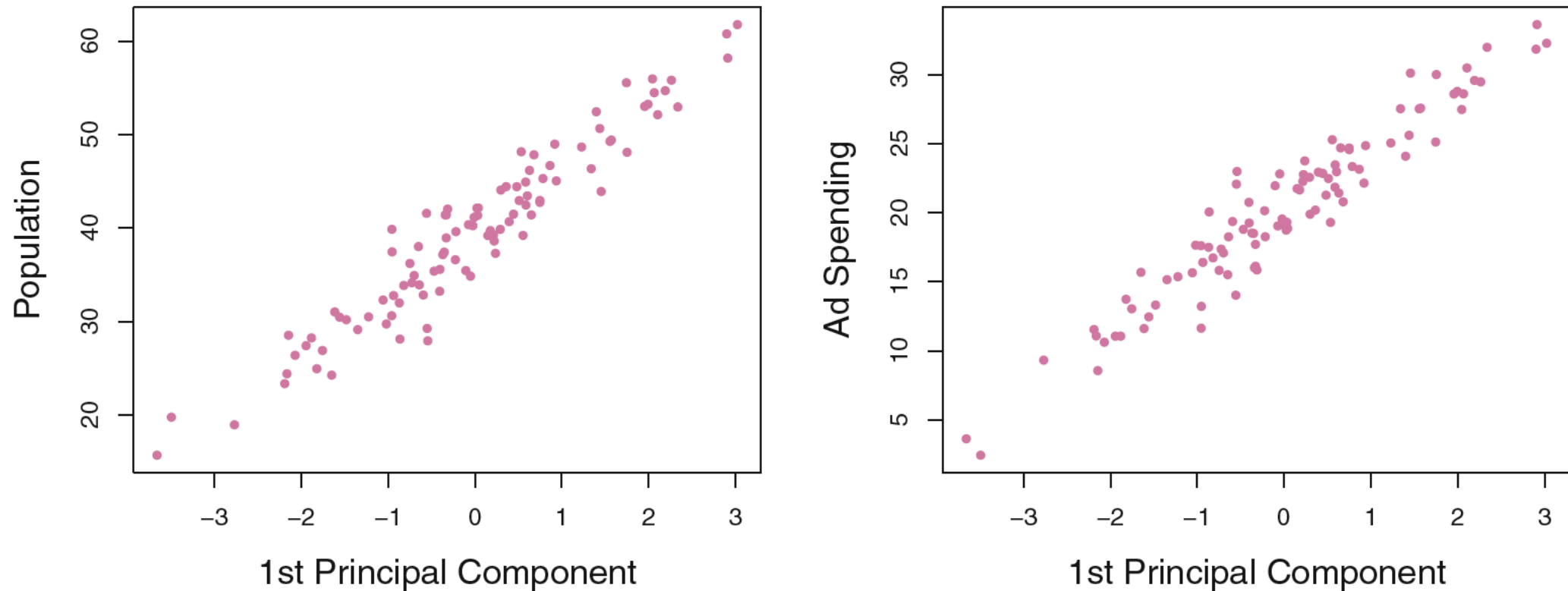
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Second Principal Component

FIGURE 6.16. *Plots of the first principal component scores z_{i1} versus* pop *and* ad. *The relationships are strong.*

PCA Illustration

- USAarrests data: For each 50 state in the US, number of arrests per 100,000 residents for each of the three crimes: assault, murder, and rape. Also record UrbanPop.

- Principal component score vectors have a length of n = 50, and loading vectors have length p = 4

- PCA was performed after standardizing variables to have a mean of 0 and standard deviation of 1.

PCA Illustration

```r
require('ISLR')
dimnames(USArrests)
apply(USArrests,2,mean)
apply(USArrests,2,var)

## Standardize the variables and PCA the vars
pca.out <- prcomp(USArrests, scale=TRUE)
pca.out
```
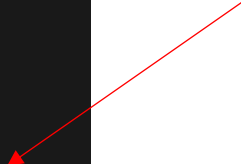
PCA Illustration

```
> pca.out
Standard deviations (1, .., p=4):
[1] 1.5748783 0.9948694 0.5971291 0.4164494

Rotation (n x k) = (4 x 4):
                   PC1          PC2          PC3          PC4
Murder     -0.5358995   0.4181809  -0.3412327   0.64922780
Assault    -0.5831836   0.1879856  -0.2681484  -0.74340748
UrbanPop   -0.2781909  -0.8728062  -0.3780158   0.13387773
Rape       -0.5434321  -0.1673186   0.8177779   0.08902432
```
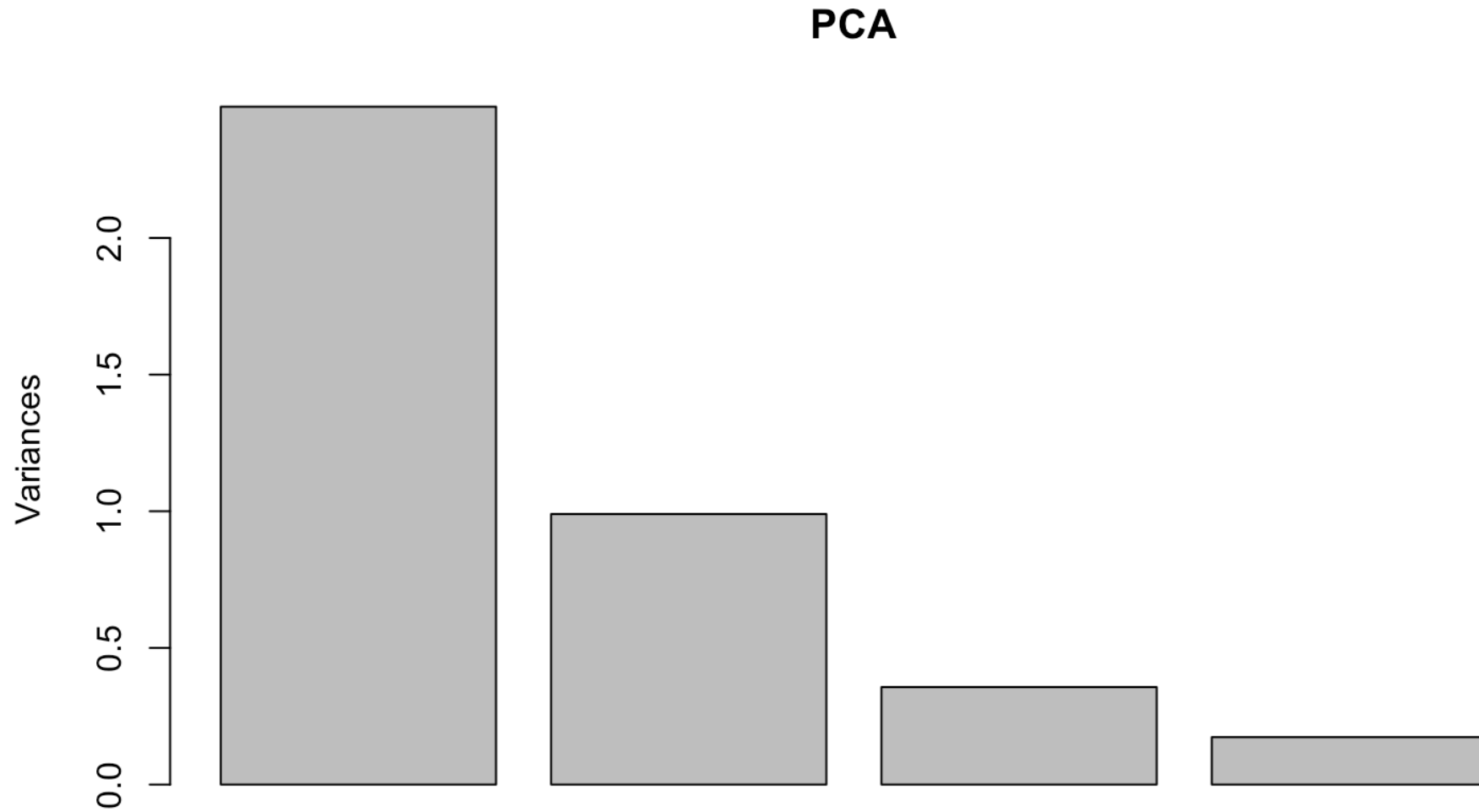
Factor loadings

How many PCAs to use? "Elbow Method" from "Skree" plot

PCA

Plotting PC1 and PC2

- As promised, we can now use the 1st and 2nd principal component to visualize the P-dimensional data on a 2-dimensional plot

- This is called "projecting" our data in 2 dimensions

```r
# boring biplot plot
biplot(pca.out)

# ggplot biplot
library('ggfortify')
autoplot(prcomp(USArrests), data = USArrests,
         loadings = TRUE, loadings.colour = 'blue',
         loadings.label = TRUE, loadings.label.size = 5,
         label = TRUE) + theme_bw()
```

PCA "Biplot"