Introduction to Machine Learning for Economists and Business Analysts

Unsupervised Machine Learning

Anthony Strittmatter

Literature

- James, Witten, Hastie, and Tibshirani (2013): "An Introduction to Statistical Learning", Springer, Chapters 6.3.1, 10, download.
- Hastie, Tibshirani, and Friedman (2009): "Elements of Statistical Learning", 2nd ed., Springer, Chapters 14.2, 14.5, download.

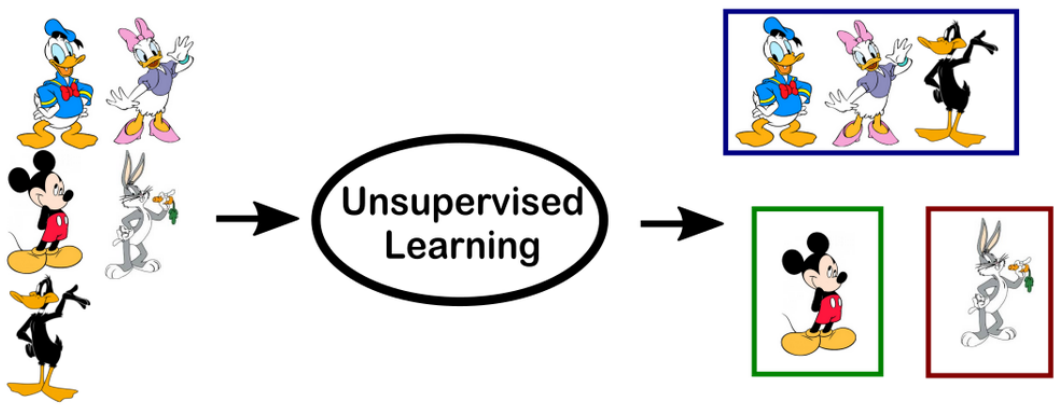
Supervised vs. Unsupervised Machine Learning

Supervised Machine Learning:

- We observe data on Y and X and want to learn the mapping $\widehat{Y} = \widehat{f}(X)$
- Classification when Y is discrete, regression when Y is continuous

Unsupervised Machine Learning:

- We observe only data on X and want to learn something about the data structure



Unsupervised Machine Learning

- Explorative data analysis.
- Discovering subgroups among observations or variables.
- No easy way to assess model accuracy.
- Visualization of X data.

$\Rightarrow$ We discuss **Principal Component Analysis (PCA)** and **K-Means Clustering**.

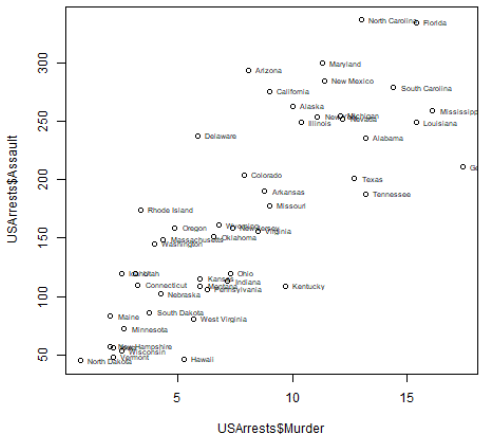
Violent Crime Rate by US States

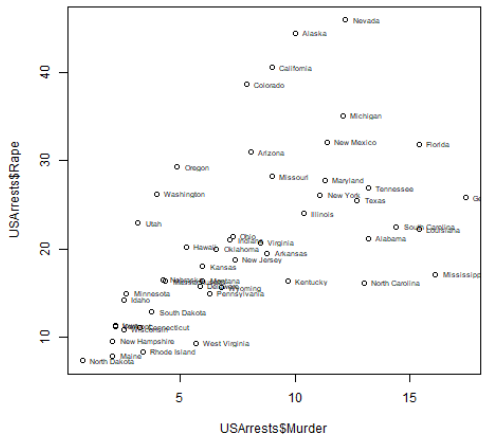
Variables:

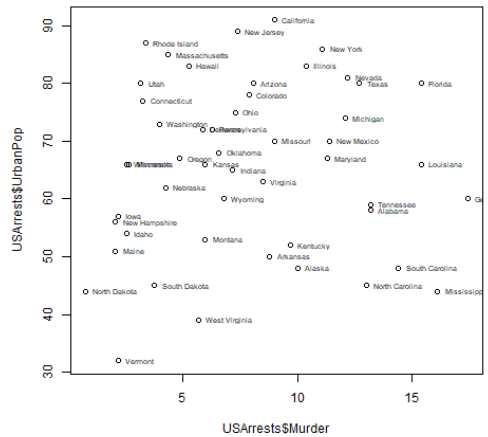
- Murder arrests (per 100,000)
- Assault arrests (per 100,000)
- Percent urban population (UrbanPop)
- Rape arrests (per 100,000)

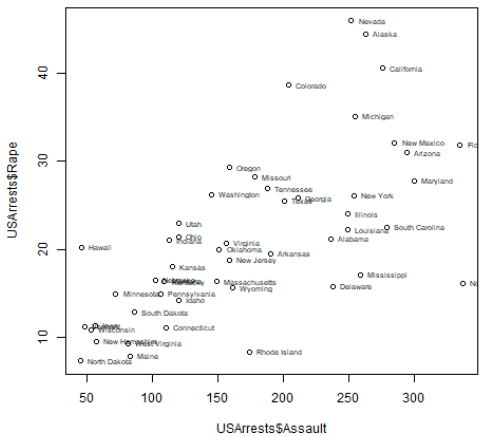
	Murder	Assault	UrbanPop	Rape
Alabama	13.2	236	58	21.2
Alaska	10	263	48	44.5
Arizona	8.1	294	80	31
Arkansas	8.8	190	50	19.5
California	9	276	91	40.6
Colorado	7.9	204	78	38.7
⋮	⋮	⋮	⋮	⋮

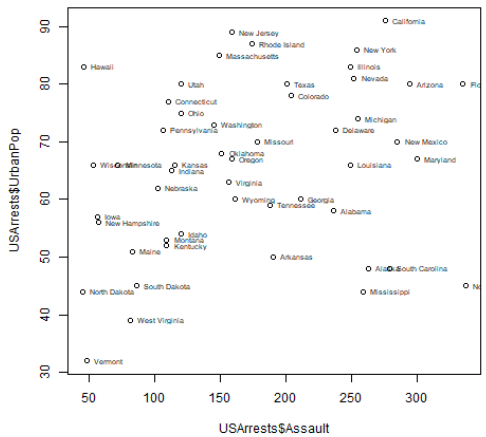
Scatterplots

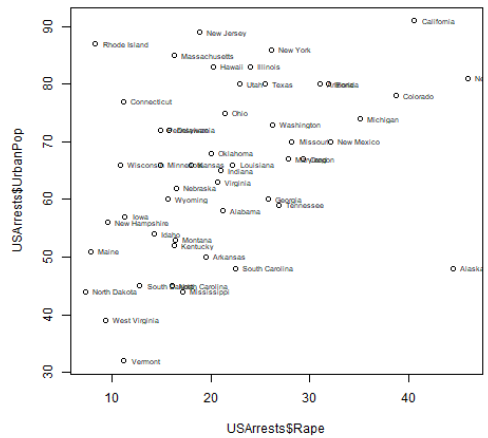












$\rightarrow$ PCA finds low dimensional representation of data that captures as much information as possible.

Principal Components

- We observe the features X_1, X_2, ..., X_p.
- Principal components are normalized linear combinations of the features

$$\begin{aligned} Z_1 &= \phi_{11}X_1 + \phi_{21}X_2 + ... + \phi_{p1}X_p, \\ Z_2 &= \phi_{12}X_1 + \phi_{22}X_2 + ... + \phi_{p2}X_p, \\ &\vdots \\ Z_p &= \phi_{1p}X_1 + \phi_{2p}X_2 + ... + \phi_{pp}X_p, \end{aligned}$$

  that maximize the variance of Z_1, Z_2, ... Z_p.
- The factor loadings of the principal component k are $\phi_k = \phi_{1k}, \phi_{2k}, ...\phi_{pk}$.
- Normalized means $\sum_{j=1}^{p} \phi_{jk}^2 = 1$ for all $k = 1, ..., p$.

Objective Function

- First Principal Component:

$$max_{\phi_{11},\ldots,\phi_{p1}} \left\{ \frac{1}{N} \sum_{i=1}^{N} \left(\sum_{j=1}^{p} \phi_{j1} x_{ij} \right)^2 \right\} \text{ s.t. } \sum_{j=1}^{p} \phi_{j1}^2 = 1.$$

- Second Principal Component:

$$max_{\phi_{12},\ldots,\phi_{p2}} \left\{ \frac{1}{N} \sum_{i=1}^{N} \left(\sum_{j=1}^{p} \phi_{j2} x_{ij} \right)^2 \right\} \text{ s.t. } \sum_{j=1}^{p} \phi_{j2}^2 = 1$$

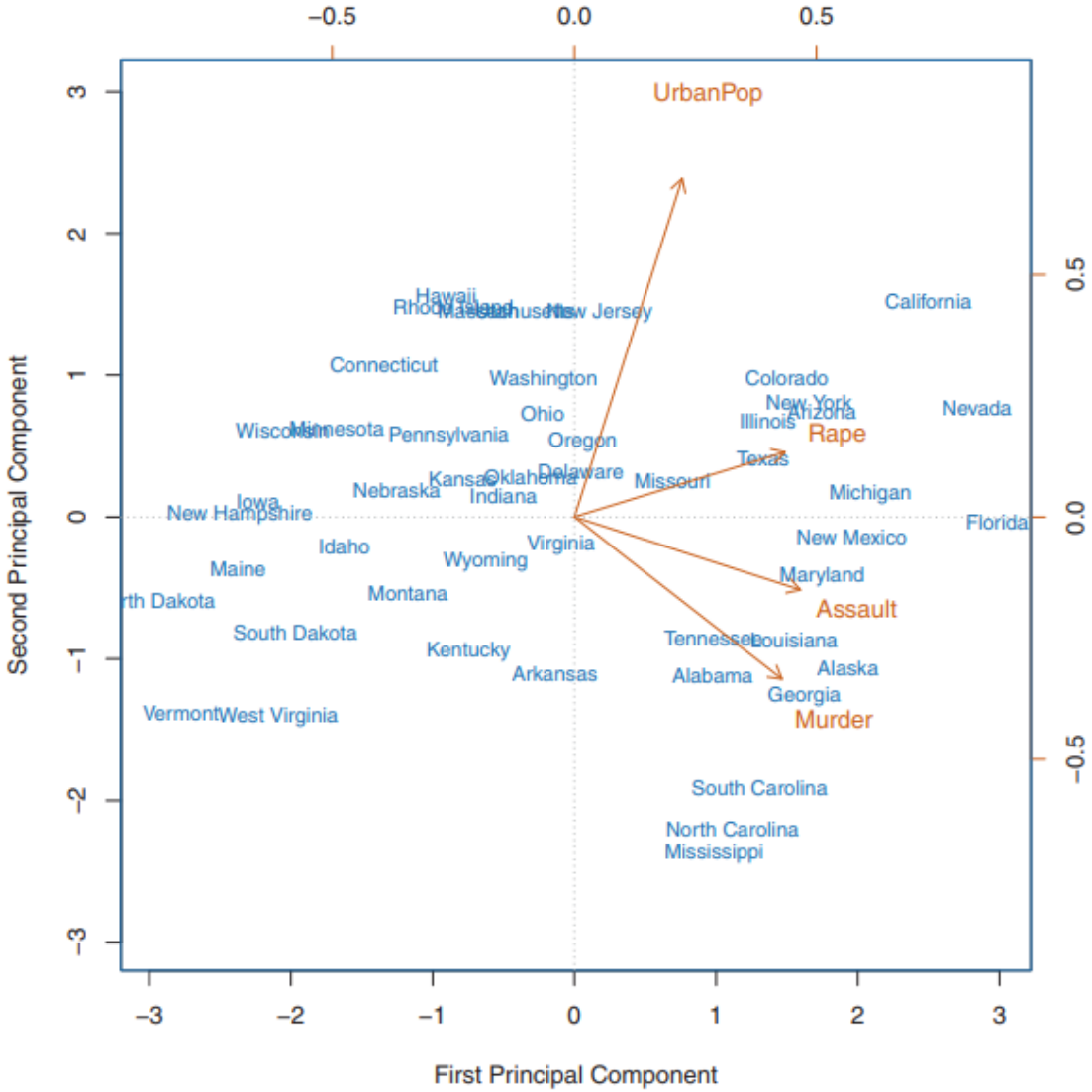
  and ϕ_2 is orthogonal to ϕ_1.

- etc.

Principal Component Loading Vectors

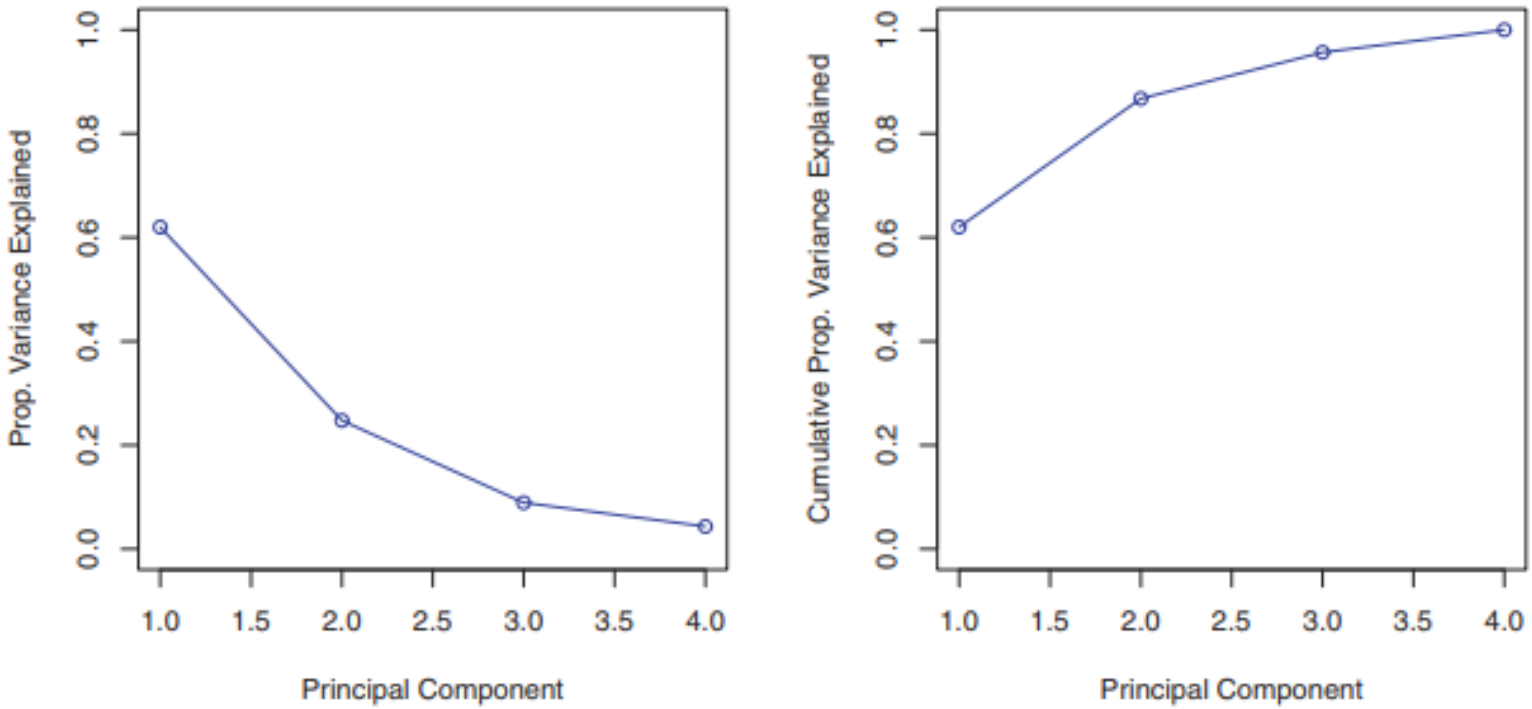
	Principal Component 1 ϕ_1	Principal Component 2 ϕ_2
Murder	0.536	-0.418
Assault	0.583	-0.188
Urban Population	0.278	0.873
Rape	0.543	0.167

Visualization of Principal Components



Source: James, Witten, Hastie, Tibshirani (2013)

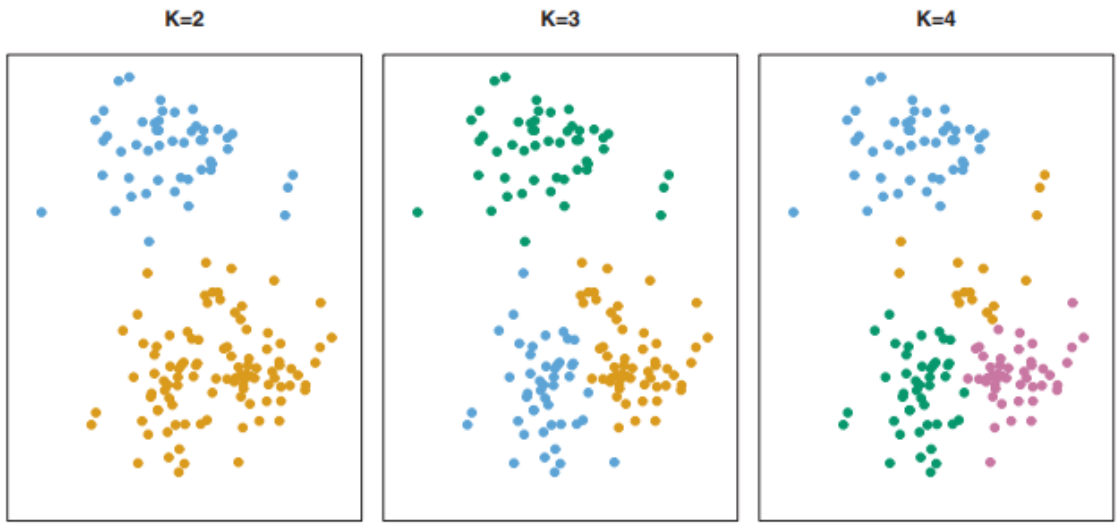
Proportion Variance Explained



Source: James, Witten, Hastie, Tibshirani (2013)

Difference between PCA and Clustering

- Principal Component Analysis (PCA) looks to find a low-dimensional representation of the observations that explain a good fraction of the variance.
- Clustering looks to find homogeneous subgroups among the observations.



Source: James, Witten, Hastie, Tibshirani (2013)

Objective Function K-means Clustering

- **Squared Euclidean distance:**

$$W(C_k) = \frac{1}{|C_k|} \sum_{i,i' \in C_k} \sum_{j=1}^{p} (x_{ij} - x_{i'j})^2$$

with $|C_k|$ being the number of observations in the kth cluster.

- **Optimization problem:**

$$\min_{C_1,\ldots,C_K} \left\{ \sum_{k=1}^{K} W(C_k) \right\}$$

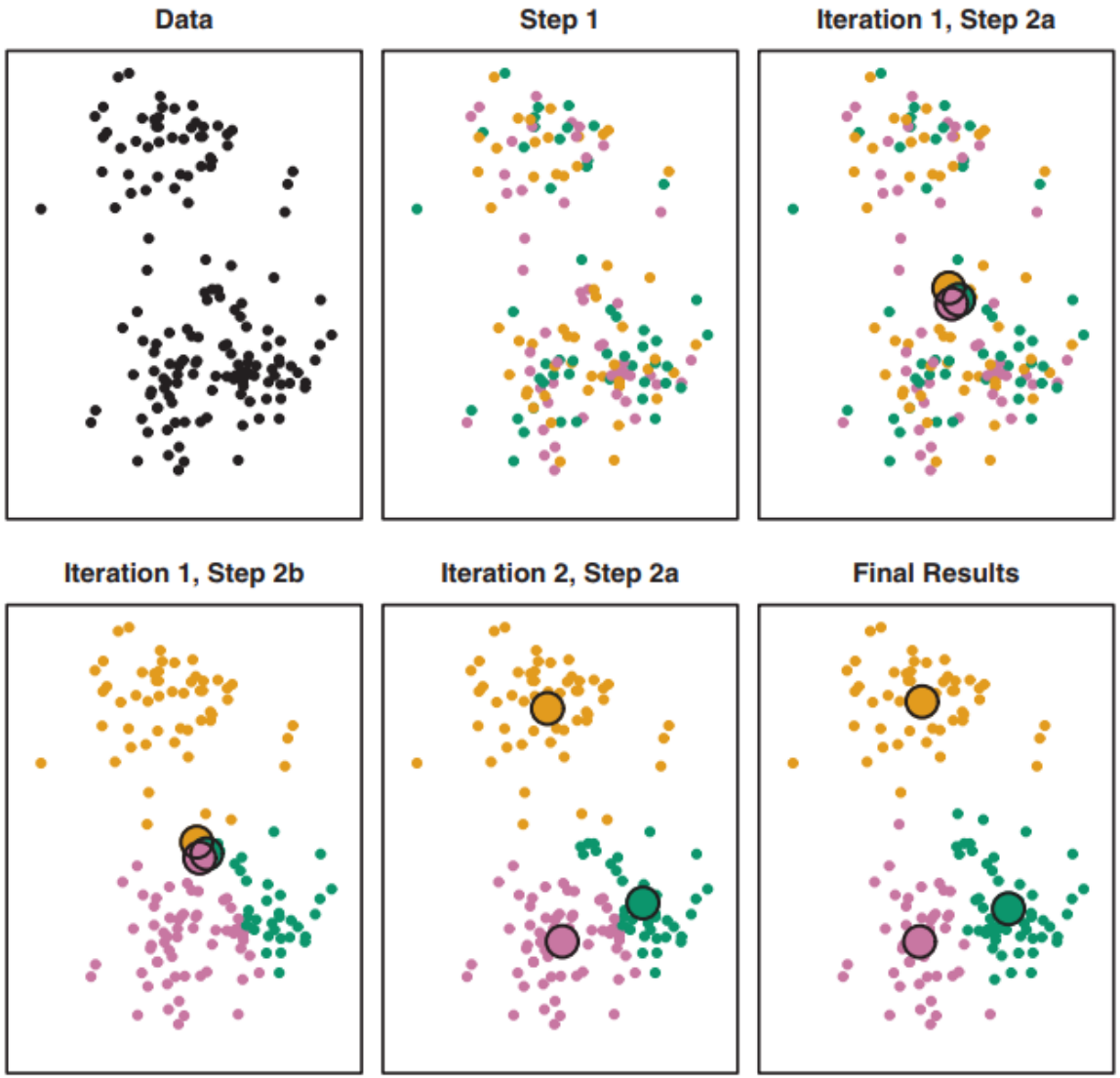
$\rightarrow$ Minimize the within cluster squared Euclidean distance.

Optimization Algorithm K-Means Clustering

Algorithm

1. Randomly assign a number, from 1 to K, to each of the observations. These serve as initial cluster assignments for the observations.
2. Iterate until the cluster assignments stop changing:
   - 2.1 For each of the K clusters, compute the cluster centroid. The kth cluster centroid is the vector of the p feature means for the observations in the kth cluster.
   - 2.2 Assign each observation to the cluster whose centroid is closest (where closest is defined by using the squared Euclidean distance)

Graphical Illustration of Optimization Algorithm



Source: James, Witten, Hastie, Tibshirani (2013)

Initialisation of the Algorithm (Step 1)

Source: James, Witten, Hastie, Tibshirani (2013)

4-Means Clustering for Crime Data

- **Cluster 1:** low crime
  Connecticut, Idaho, Indiana, Kansas, Kentucky, Montana, Nebraska, Ohio, Pennsylvania, Utah
- **Cluster 2:** very high crime
  Alabama, Alaska, Arizona, California, Delaware, Florida, Illinois, Louisiana, Maryland, Michigan, Mississippi, Nevada, New Mexico, New York, North Carolina, South Carolina
- **Cluster 3:** low pop, low crime
  Hawaii, Iowa, Maine, Minnesota, New Hampshire, North Dakota, South Dakota, Vermont, West Virginia, Wisconsin
- **Cluster 4:** high crime
  Arkansas, Colorado, Georgia, Massachusetts, Missouri, New Jersey, Oklahoma, Oregon, Rhode Island, Tennessee, Texas, Virginia, Washington, Wyoming

Descriptives by Cluster

	Mean			
	Cluster 1	Cluster 2	Cluster 3	Cluster 4
Murder	5.59	11.81	2.95	8.214
Assault	112.4	272.6	62.7	173.3
UrbanPop	65.6	68.31	53.9	70.64
Rape	17.27	28.38	11.51	22.84

Scatterplot of Clusters