Statistical Computing with R: Masters in Data Sciences 503 (S25) Second Batch, SMS, TU, 2023

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Review Preview: Unsupervised models

- Dimension reduction
  - Principal component analysis
  - Principal axis factoring
  - Multi-dimensional scaling
- Clustering
  - K-means clustering
  - Hierarchical clustering
- Association rules
- Monte Carlo simulations

Unsupervised learning:

- Dependent variable is not available for this type of learning
- We need to work with the independent variables **ONLY**
- We can form a composite score using all the independent variables (dimension reduction)
- Dimension = variables = features
- We can group a independent variables with similar characteristics (clustering)
- In both cases, correlation and distance measures plays very important role so this is known and multivariate exploratory analysis in statistics

You need to read Chapter 12: Unsupervised Learning (page 503 of PDF file) of the book “An Introduction to Statistical Learning” shared to you in the MS Team few days back. It contains the theory + lab works!

IBM: Unsupervised learning

- Unsupervised learning, also known as unsupervised machine learning, uses machine learning algorithms to analyze and cluster unlabeled datasets.
- **These algorithms discover hidden patterns or data groupings without the need for human intervention.**
- Its ability to discover similarities and differences in information make it the ideal solution for **exploratory data analysis**, cross-selling strategies, customer segmentation, and image recognition.

Alternatively:

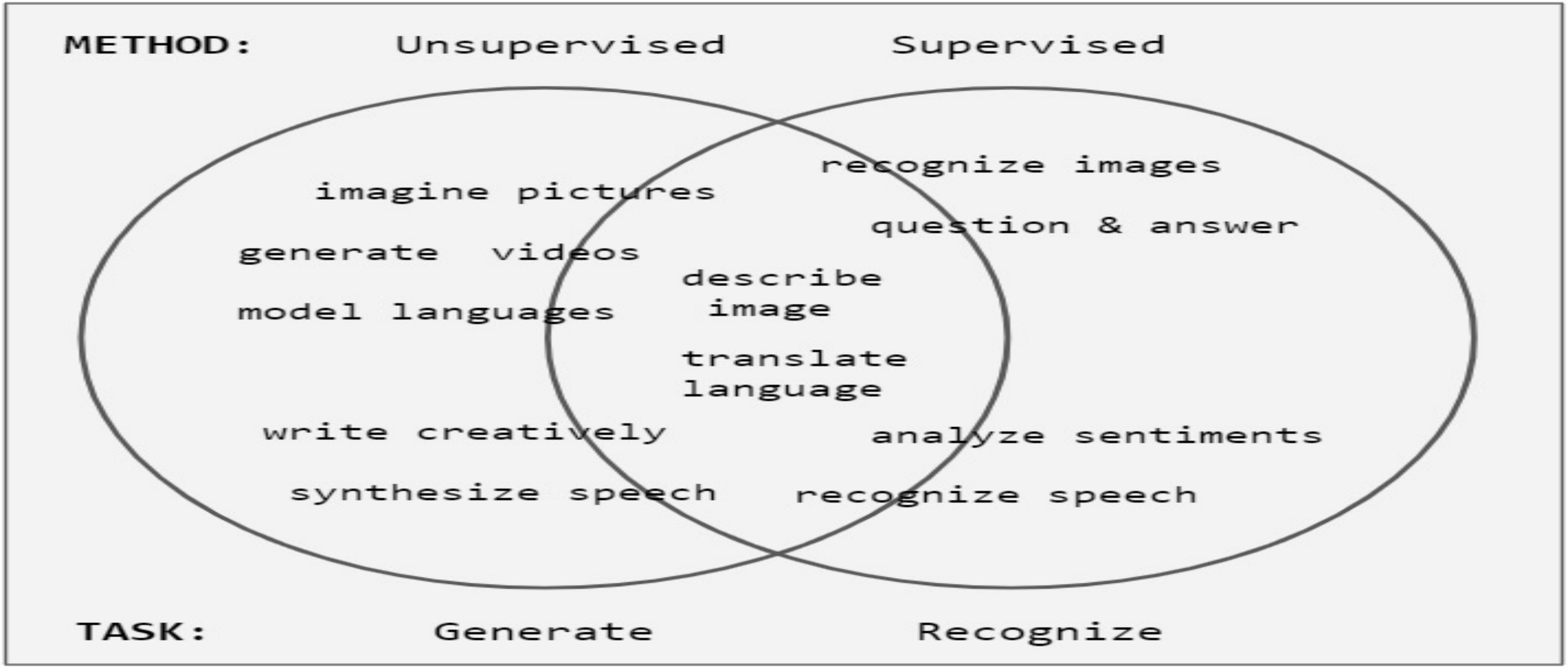
https://en.wikipedia.org/wiki/Unsupervised_learning

- **Unsupervised learning** is a type of machine learning in which the algorithm is not provided with any pre-assigned labels or scores for the training data.

- As a result, unsupervised learning algorithms must first self-discover any naturally occurring patterns in that training data set.

- Common examples include **clustering**, where the algorithm automatically groups its training examples into categories with similar features, and **principal component analysis**, where the algorithm finds ways to compress the training data set by identifying which features are most useful for discriminating between different training examples, and discarding the rest.

Unsupervised vs Supervised learning and overlapping:



https://en.wikipedia.org/wiki/Unsupervised_learning

Application of unsupervised learning: https://www.ibm.com/cloud/learn/unsupervised-learning

- **Computer vision**
  - Unsupervised learning algorithms are used for visual perception tasks, such as object recognition.
- **Medical imaging**
  - Unsupervised machine learning provides essential features to medical imaging devices, such as image detection, classification and segmentation, used in radiology and pathology to diagnose patients quickly and accurately.
- **Anomaly detection**
  - Unsupervised learning models can comb through large amounts of data and discover atypical data points within a dataset. These anomalies can raise awareness around faulty equipment, human error, or breaches in security.
- **Customer personas**
  - Defining customer personas makes it easier to understand common traits and business clients' purchasing habits. Unsupervised learning allows businesses to build better buyer persona profiles, enabling organizations to align their product messaging more appropriately.
- **Recommended Engines**
  - Using past purchase behavior data, unsupervised learning can help to discover data trends that can be used to develop more effective cross-selling strategies. This is used to make relevant add-on recommendations to customers during the checkout process for online retailers.

Unsupervised Learning-Dimension Reduction: https://www.ibm.com/cloud/learn/unsupervised-learning

- While more data generally yields more accurate results, it can also impact the performance of machine learning algorithms (e.g. overfitting) and it can also make it difficult to visualize datasets.
- **Dimensionality reduction is a technique used when the number of features, or dimensions, in a given dataset is too high.**
- It reduces the number of data inputs to a manageable size while also preserving the integrity of the dataset as much as possible.
- It is commonly used in the preprocessing data stage i.e. before fitting a model, and there are a few different dimensionality reduction methods that can be used, such as:
    - Principal Component Analysis
    - Singular Value Decomposition (**ISLR Chapter 12 has example of this method!**)
    - Autoencoder (neural networks)
- **PCA is used to classify households poverty level with "wealth quintiles" in surveys and find components of a questionnaire with large number of items based on their correlations**

Principal Component Analysis (PCA) for Dimension Reduction: Read ISLR Chapter 12!

- Dimensionality reduction is a technique used when the number of features, or variables, in a given dataset is too high. It reduces the number of data inputs to a manageable size while also preserving the integrity of the dataset as much as possible.

- **Principal component analysis (PCA) is a type of dimensionality reduction algorithm which is used to reduce redundancies and to compress datasets through feature extraction**. This method uses a linear transformation to create a new data representation, yielding a set of "principal components."

- The first principal component is the direction which maximizes the variance of the dataset. While the second principal component also finds the maximum variance in the data, **it is completely uncorrelated to the first principal component**, yielding a direction that is perpendicular, or orthogonal, to the first component.

- This process repeats based on the number of dimensions, where a next principal component is the direction orthogonal to the prior components with the most variance.

- **We can use Kaiser's rule or Scree plot or both to extract components after PCA is applied to the data**

Let's use PCA: The ISLR Chapter 12 explains PCA with USArrests data too!

#We will use the built-in USArrests data

- head(USArrests)

	Murder	Assault	UrbanPop	Rape
• Alabama	13.2	236	58	21.2
• Alaska	10.0	263	48	44.5
• Arizona	8.1	294	80	31.0
• Arkansas	8.8	190	50	19.5
• California	9.0	276	91	40.6
• Colorado	7.9	204	78	38.7

- We need to combine the murder, assault and rape variables and create a latent variable i.e. "criminality" score using these three variables

"An Introduction to Statistical Learning" book chapter 12 uses all these variables to fit the PCA so I strongly suggest you to read and compare the result with the one we will get now onwards.

Fit a PCA in the data without the 3rd feature:

#Getting **criminality scale** after removing 3rd column i.e. Urban Population and scaling them

- library(dplyr)
- USArrests.1 <- USArrests[,-3] %>% scale

#Fitting PCA in the new data:

- pca.1 <- prcomp(USArrests.1)
- summary(pca.1)

#It can also be done directly:
pca.2 <- prcomp(USArrests[,-3], scale = TRUE)
summary(pca.2)

- Importance of components:

	PC1	PC2	PC3
SD:	**1.5358**	0.6768	0.42822
Prop. Var	0.7862	0.1527	0.06112
Cum. Prop.	0.7862	0.9389	1.00000

PC1 explained around 79% of variance whereas PC2 explained around 15% and PC3 explained around 6% of variance with the latent variable i.e. criminality score.

As per Kaiser's rule, PC with Eigenvalue >= 1 (SD-square) must be used/retained for the latent variable.

We can say that we need only one component to create the latent variable as it explains 79% variance and SD^2>=1.

Alternative, we can use “psych” package:

#Alternative

- library(psych)
- fa.1 <- psych::principal(USArrests.1, nfactors = 3, rotate = "none")
- fa.1

- **Standardized loadings** (pattern matrix) based upon correlation matrix

	PC1	PC2	PC3	h2	u2 com
Murder	**0.89**	-0.36	0.26	1	-2.2e-16 1.5
Assault	**0.93**	-0.14	-0.33	1	-2.2e-16 1.3
Rape	**0.83**	0.55	0.09	1	4.4e-16 1.8

The correlation of murder, assault and rape is very high with PC1 so variance explained by PC1 is also high!

#Sum of square and variance explained:

SS loading = Eigenvalue = SD-square

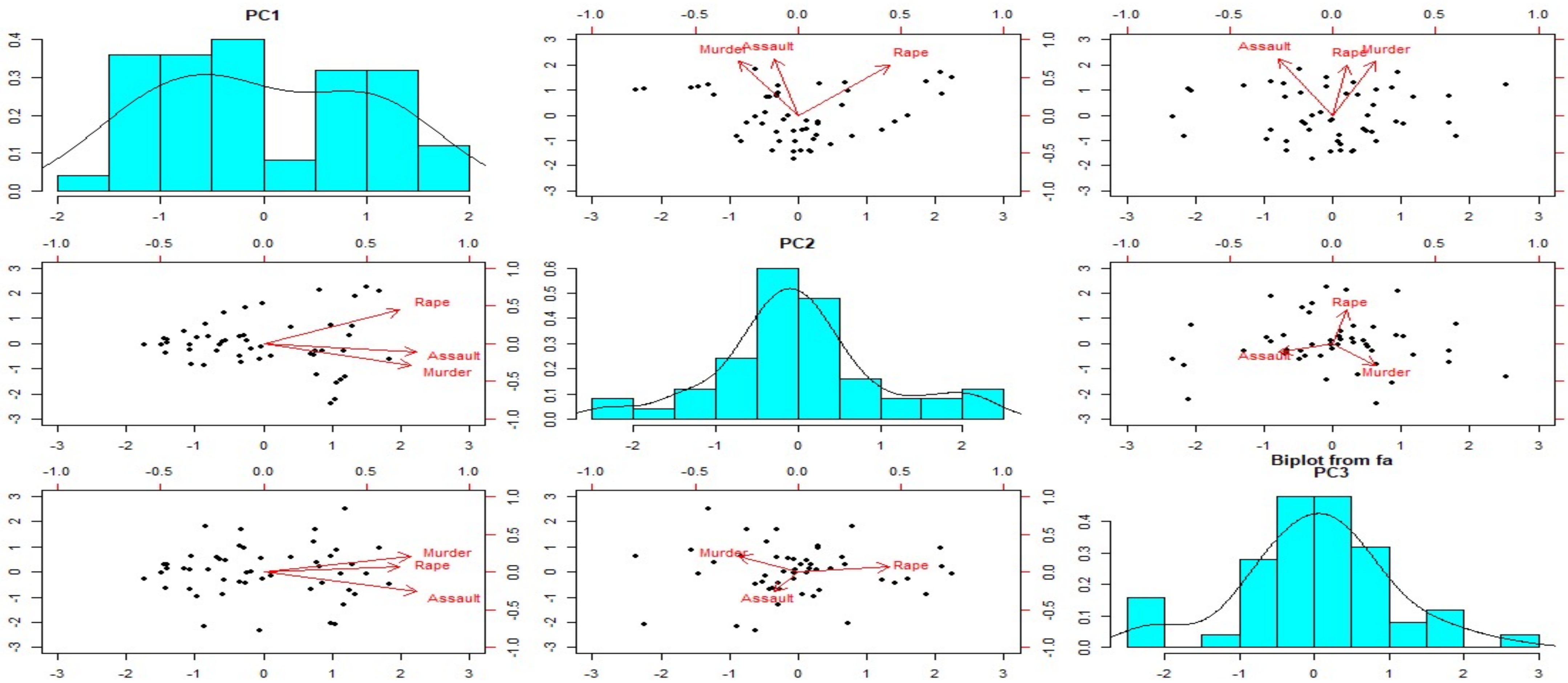
	PC1	PC2	PC3
SS loadings	2.36	0.46	0.18
Proportion Var	**0.79**	**0.15**	**0.06**
Cumulative Var	0.79	0.94	1.00

- Prop. Explained 0.79 0.15 0.06
- Cum. Proportion 0.79 0.94 1.00

Proportion variance explained by PC1 = 79%, PC2=15% and PC3 = 6%.
SS loadings = Eigenvalues (check with squared SD)

Bi-plot using "psych" package: Interpretation?

biplot(fa.1, labels = rownames(USArrests.1))



Getting eigen values from “FactoMineR”:

- library(factoextra)
- library(FactoMineR)

- str(USArrests)
- pca.data <- USArrests[,-3]
- head(pca.data)

- res.pca <- PCA(pca.data, graph=F)
- res.pca$eig

	eigenvalue
comp 1	**2.3585802**
comp 2	0.4580513
comp 3	0.1833685

	percentage of variance
comp 1	78.619340
comp 2	15.268378
comp 3	6.112282

Eigenvalue > 1 = Only 1 component

Principal Component Analysis in R Tutorial

https://www.datacamp.com/tutorial/pca-analysis-r

- This tutorial show how the PCA are derived from the correlation matrix ~ covariance matrix
- The correlation matrix is used to get covariance matrix, which is then used to get eigenvectors and eigenvalues
- Eigenvalue is used to select the principal components

- Five steps for PCA:

1. Data Normalization
2. Covariance matrix
3. Eigenvectors and eigenvalues
4. Selection of principal components with criteria
5. Data transformation in new dimensional space

Can we improve the PCA?
We can try PCA with "VARIMAX" rotation!

- #Rotated PCA with variance maximization
- fa.2 <- psych::principal(USArrests.1, nfactors = 3, rotate = "varimax")
- summary(fa.2)

	RC2	RC3	RC1
• Murder	0.26	**0.89**	0.37
• Assault	0.36	0.45	**0.82**
• Rape	**0.93**	0.24	0.27

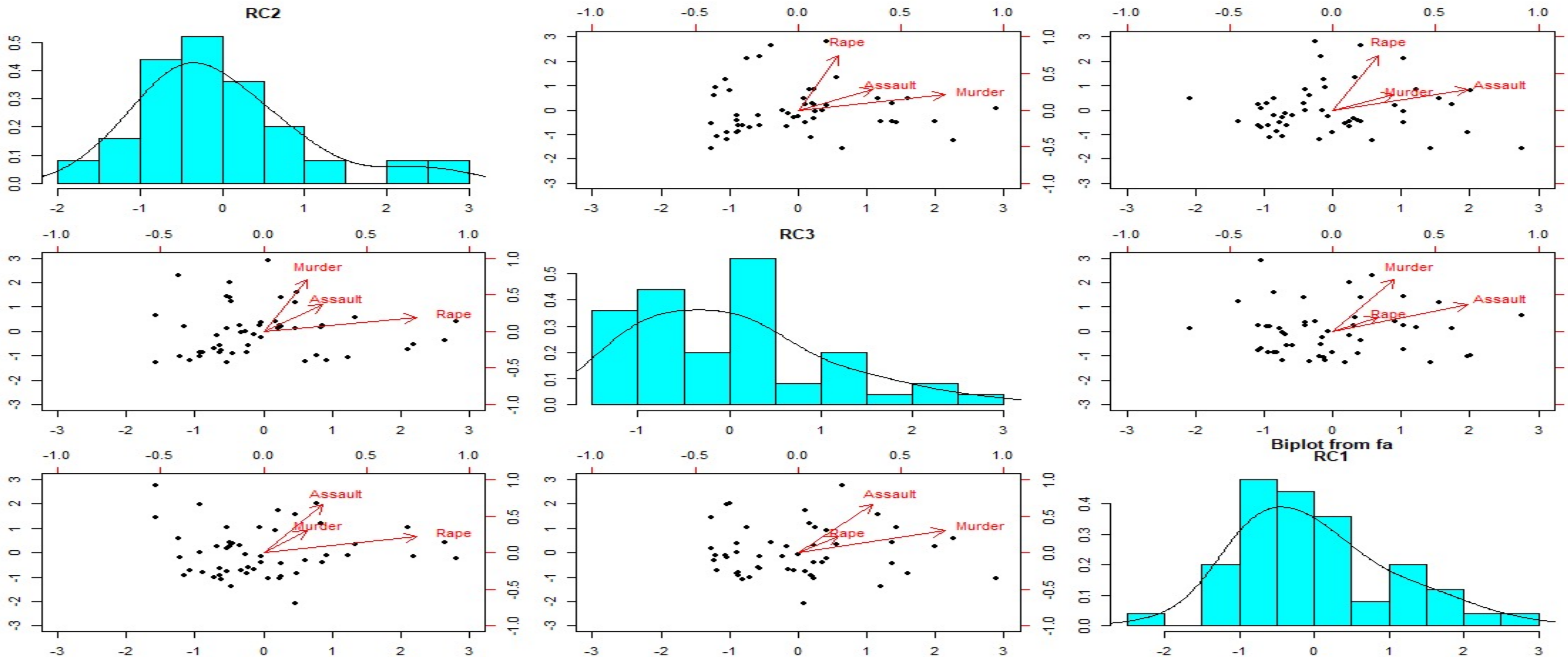
	RC2	RC3	RC1
• SS loadings	1.06	1.05	0.88
• Proportion Var	**0.35**	**0.35**	**0.29**
• Cumulative Var	0.35	0.71	1.00
• Proportion Explained	0.35	0.35	0.29
• Cumulative Proportion	0.35	0.71	1.00

Did it improve the PCA?

What happened? **Is this a "data reduction"!**

Why?

Biplot: **How to interpret these bi-plots?**
biplot(fa.2, labels = rownames(USArrests.1))



Note:

- PCA must be used to produce "orthogonal" components
- PCA with "varimax" rotation also produced "orthogonal" components
- PCA with "varimax" rotation cannot be interpreted as a "true" PCA, why?

- If we need to get a **latent variable** with "correlated" components then we must use other **oblique** rotation methods and PCA not longer applies here
- Thus, we must use principal axis factoring (PFA) or factor analysis in such situations
- The common oblique rotation are:
  - Promax
  - Equimax etc.

I strongly suggest to use FactoMineR package to fit PCA and other factor analysis methods in R.
Methods: http://factominer.free.fr/factomethods/index.html
Example of PCA with this package here: http://www.sthda.com/english/wiki/wiki.php?id_contents=7851

PAC with varimax: Is it really a PCA? Discussion: https://stats.stackexchange.com/questions/612/is-pca-followed-by-a-rotation-such-as-varimax-still-pca

- From: Abdi & Williams, 2010, Principal component analysis
- After the number of components has been determined, and in order to facilitate the interpretation, the analysis often involves a rotation of the components that were retained [see, e.g., Ref 40 and 67, for more details].
- Two main types of rotation are used: orthogonal when the new axes are also orthogonal to each other, and oblique when the new axes are not required to be orthogonal. Because the rotations are always performed in a subspace, the new axes will always explain less inertia than the original components (which are computed to be optimal).
- However, the part of the inertia explained by the total subspace after rotation is the same as it was before rotation (only the partition of the inertia has changed). It is also important to note that because rotation always takes place in a subspace (i.e., the space of the retained components), the choice of this subspace strongly influences the result of the rotation.
- Therefore, it is strongly recommended to try several sizes for the subspace of the retained components in order to assess the robustness of the interpretation of the rotation. When performing a rotation, the term loadings almost always refer to the elements of matrix Q.

So, how many components to retain?

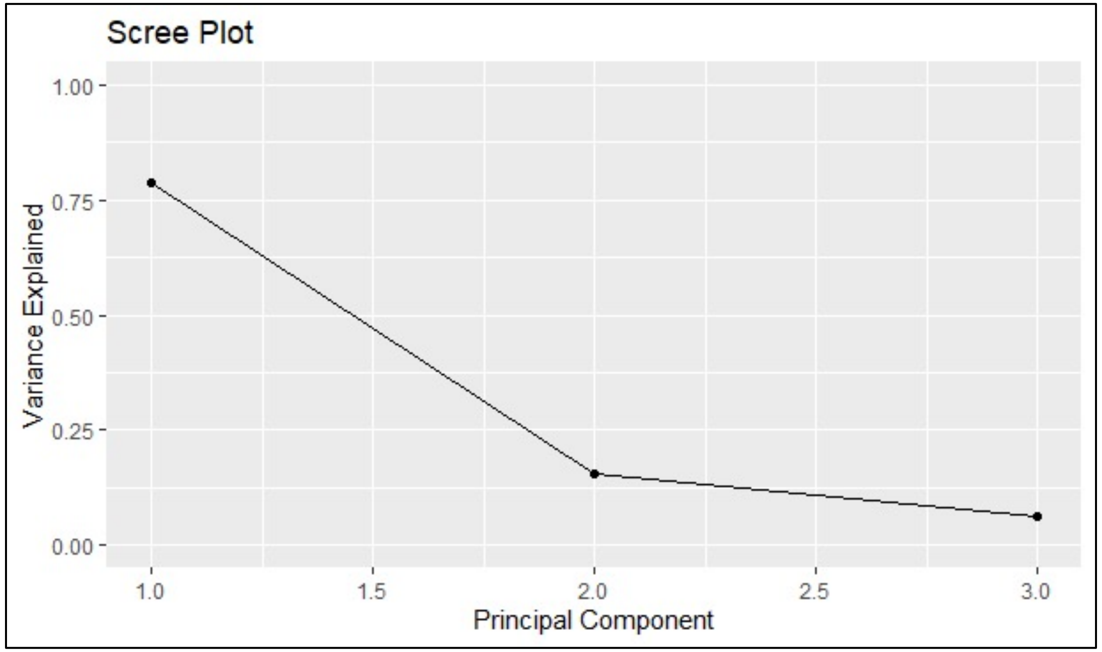
We need scree plot of pca.1 model!

#calculate total variance explained by each principal component

- var_explained = pca.1$sdev^2 / sum(pca.1$sdev^2)

#create scree plot

- library(ggplot2)
- qplot(c(**1:3**), var_explained) +
- geom_line() +
- xlab("Principal Component") +
- ylab("Variance Explained") +
- ggtitle("Scree Plot") +
- ylim(0, 1)



pca.1$sdev^2 = pca.1 (sdev-square) = pca.1 (eigenvalue)

It will be wise to use Kaiser's rule and Scree plot to decide how to many components to retain for the problem in hand! We can use scree plot's suggestion for now: 2

Final model: PCA with 2-components?

If only 1-component is retained, it will be “unidimensional”!

#Final DRM: Unrotated PCA with 2 components

- fa.3 <- psych::principal(USArrests.1, nfactors = 2, rotate = "none")
- fa.3

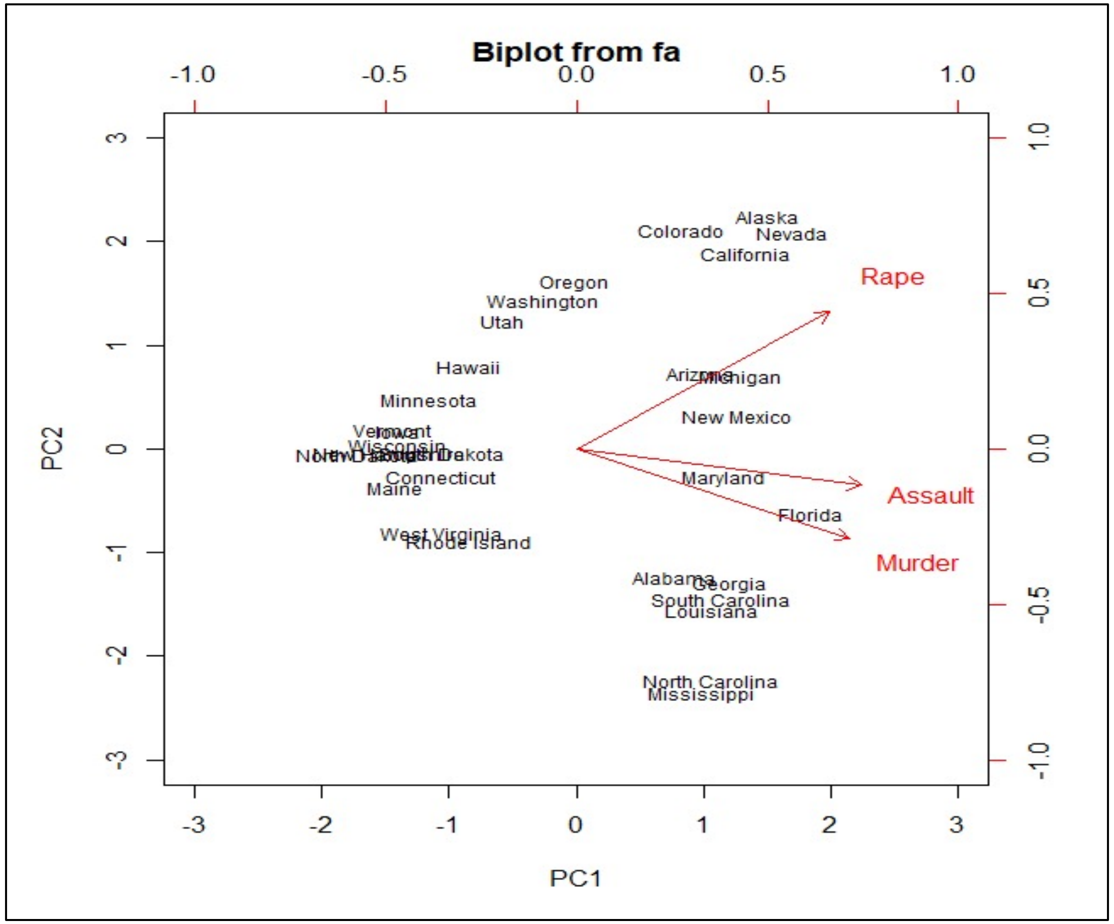
	PC1	PC2
• SS loadings	2.36	0.46
• Proportion **Var**	**0.79**	**0.15**
• Cumulative Var	0.79	0.94
• Prop. Explained	0.84	0.16
• Cum. Proportion	0.84	1.00

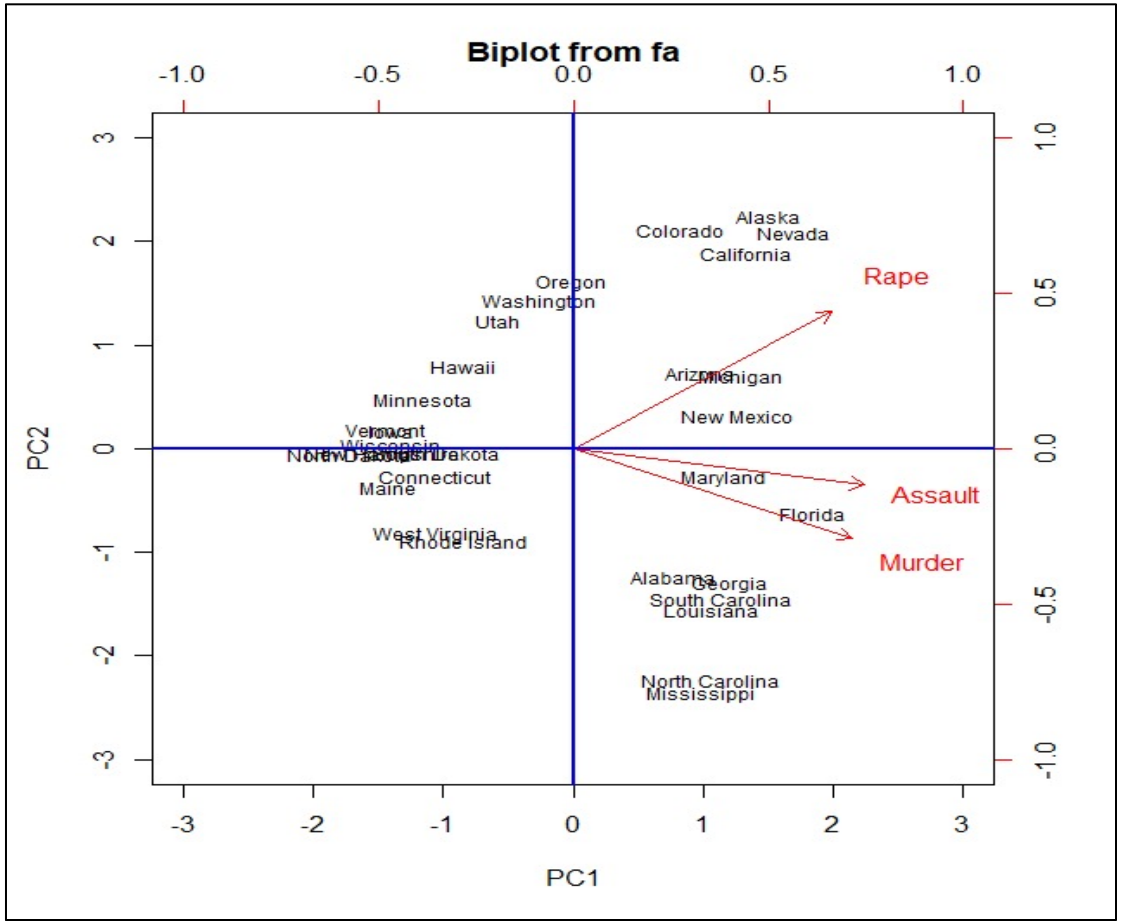
Latent variable = criminality score can be created using two variables.

These two variables explains around 94% of the variance in the latent variable!

Bi-plot: https://statisticsglobe.com/biplot-pca-explained

biplot(fa.3, labels = rownames(USArrests.1))





Final components:

- PC1 and PC2 components using Scree plot

- This is “suggestive”

- PC1 = Single component using Kaiser’s criteria of EV > 1

- This is “confirmative”

- So, it is better to use PC1 as the “criminality score” to represent 3 features/variables using PCA method in the USArrests data

Question/queries?

- Next class

Unsupervised learning with:

- Classical MDS
- Clustering
  - K-means cluster analysis
  - HCA cluster analysis

Thank you!

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