

Week 14 – Unsupervised Learning Principle Component Analysis (PCA)

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Unsupervised Learning

Unsupervised vs Supervised Learning:

- Most of this course focuses on *supervised learning* methods such as regression and classification.
- In that setting we observe both a set of features X_1, X_2, \dots, X_p for each object, as well as a response or outcome variable Y . The goal is then to predict Y using X_1, X_2, \dots, X_p .
- Here we instead focus on *unsupervised learning*, where we observe only the features X_1, X_2, \dots, X_p . We are not interested in prediction, because we do not have an associated response variable Y .

The Goals of Unsupervised Learning

- The goal is to discover interesting things about the measurements: is there an informative way to visualize the data? Can we discover subgroups among the variables or among the observations?
- We discuss two methods:
 - *principal components analysis*, a tool used for data visualization or data pre-processing before supervised techniques are applied, and
 - *clustering*, a broad class of methods for discovering unknown subgroups in data.

The Challenges of Unsupervised Learning

- Unsupervised learning is more subjective than supervised learning, as there is no simple goal for the analysis, such as prediction of a response.
- But techniques for unsupervised learning are of growing importance in a number of fields:
 - subgroups of breast cancer patients grouped by their gene expression measurements,
 - groups of shoppers characterized by their browsing and purchase histories,
 - movies grouped by the ratings assigned by movie viewers.

Advantages of Unsupervised Learning

- It is often easier to obtain *unlabeled data* — from a lab instrument or a computer — than *labeled data*, which can require human intervention.
- For example it is difficult to automatically assess the overall sentiment of a movie review: is it favorable or not?

Principle Components Analysis (PCA)

- PCA produces a low-dimensional representation of a dataset. It finds a sequence of linear combinations of the variables that have maximal variance, and are mutually uncorrelated.
- Apart from producing derived variables for use in supervised learning problems, PCA also serves as a tool for data visualization.

PCA (details)

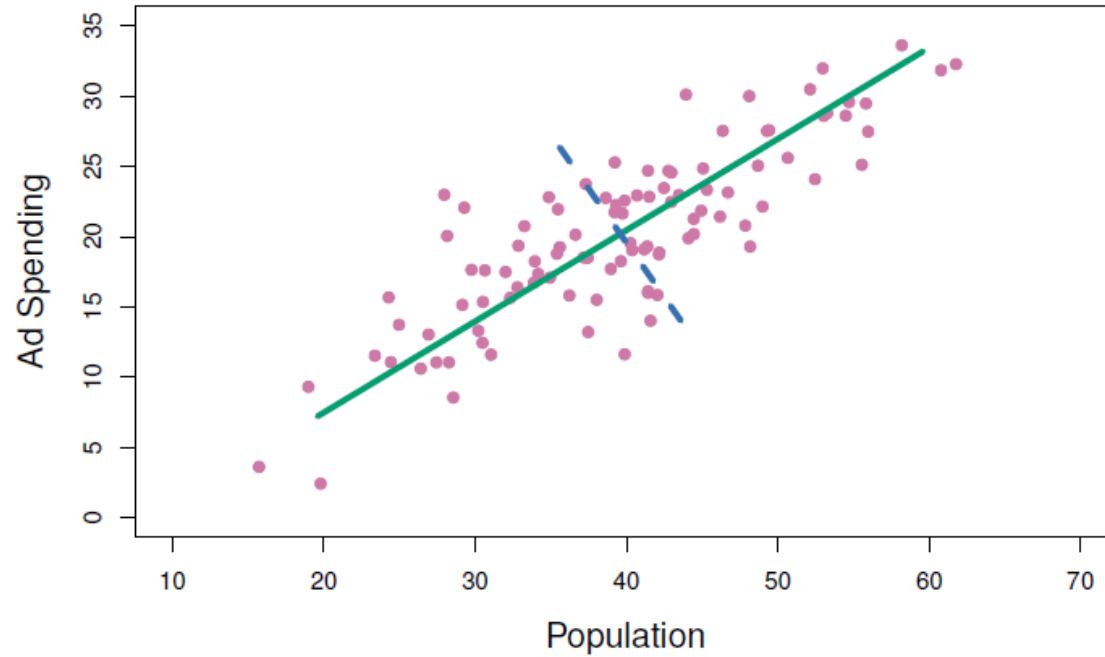
- The *first principal component* of a set of features X_1, X_2, \dots, X_p is the normalized linear combination of the features

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

that has the largest variance. By *normalized*, we mean that $\sum_{j=1}^p \phi_{j1}^2 = 1$.

- We refer to the elements $\phi_{11}, \dots, \phi_{p1}$ as the **loadings** of the first principal component; together, the loadings make up the principal component loading vector,
 $\phi_1 = (\phi_{11} \ \phi_{21} \ \dots \ \phi_{p1})^T$.
- We constrain the loadings so that their sum of squares is equal to one, since otherwise setting these elements to be arbitrarily large in absolute value could result in an arbitrarily large variance.

PCA Example



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 direction, and the blue dashed line indicates the second principal component direction.

PCA : Computation

- Suppose we have a $n \times p$ data set \mathbf{X} . Since we are only interested in variance, we assume that each of the variables in \mathbf{X} has been centered to have **mean zero** (that is, the column means of \mathbf{X} are zero).
- We then look for the linear combination of the sample feature values of the form

$$z_{i1} = \phi_{11}x_{i1} + \phi_{21}x_{i2} + \dots + \phi_{p1}x_{ip} \quad (1)$$

for $i = 1, \dots, n$ that has largest sample variance, subject to the constraint that $\sum_{j=1}^p \phi_{j1}^2 = 1$.

- Since each of the x_{ij} has **mean zero**, then so does z_{i1} (for any values of ϕ_{j1}). Hence the sample variance of the z_{i1} can be written as $\frac{1}{n} \sum_{i=1}^n z_{i1}^2$.

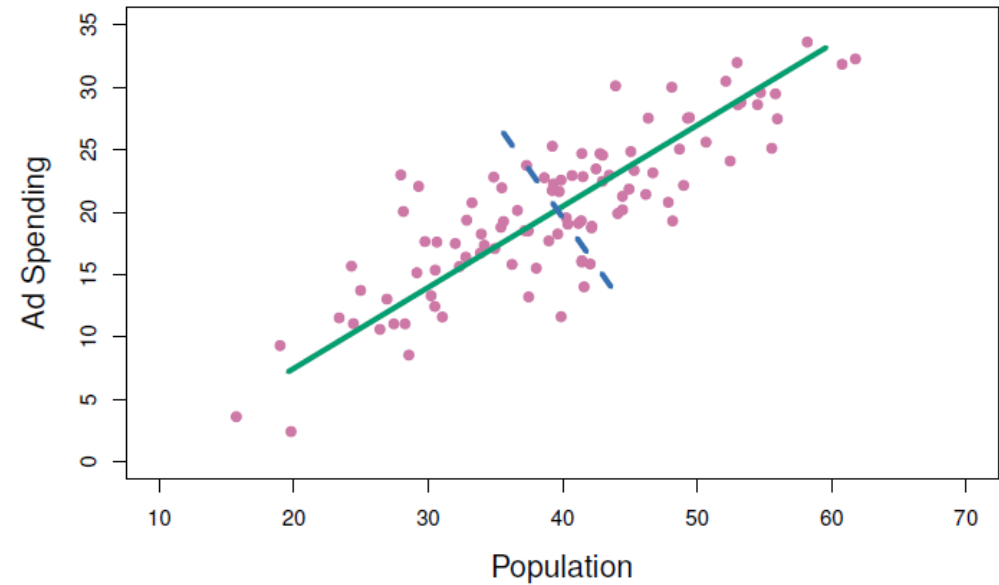
PCA : Computation (cont'd)

- Plugging in (1) the first principal component loading vector solves the optimization problem

$$\underset{\phi_{11}, \dots, \phi_{p1}}{\text{maximize}} \frac{1}{n} \sum_{i=1}^n \left(\sum_{j=1}^p \phi_{j1} x_{ij} \right)^2 \quad \text{subject to} \quad \sum_{j=1}^p \phi_{j1}^2 = 1.$$

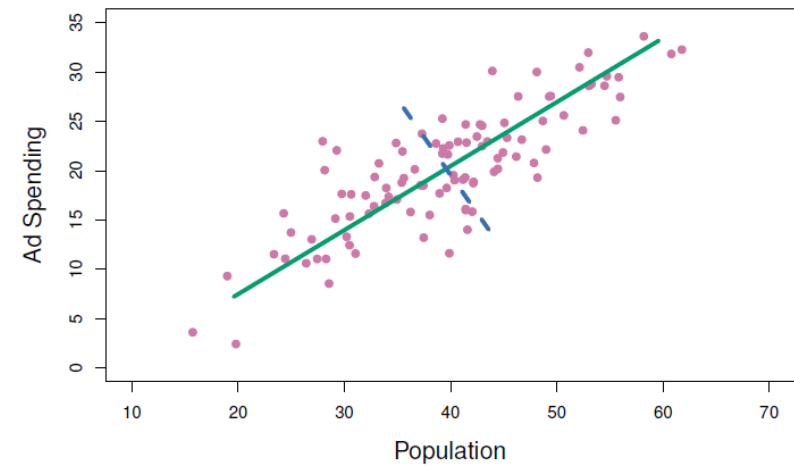
- This problem can be solved via a singular-value decomposition of the matrix \mathbf{X} , a standard technique in linear algebra.
- We refer to Z_1 as the first principal component, with realized values z_{11}, \dots, z_{n1}

PCA: Geometry



- The loading vector ϕ_1 with elements $\phi_{11}, \phi_{21}, \dots, \phi_{p1}$ defines a direction in feature space along which the data vary the most.
- If we project the n data points x_1, \dots, x_n onto this direction, the projected values are the principal component scores z_{11}, \dots, z_{n1} themselves.

PCA : Further components

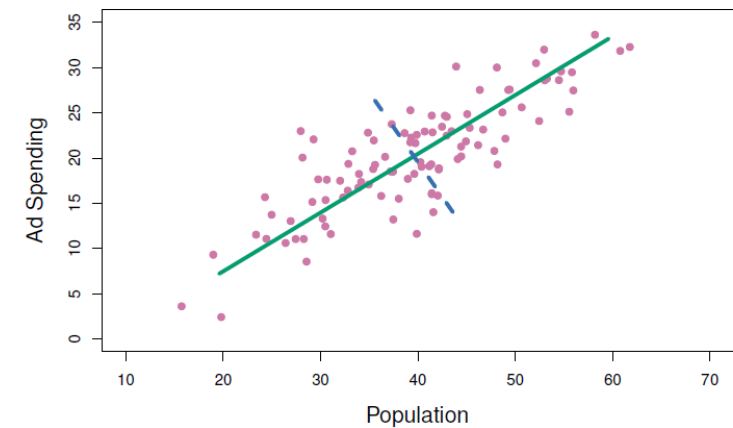


- The second principal component is the linear combination of X_1, \dots, X_p that has maximal variance among all linear combinations that are *uncorrelated* with Z_1 .
- The second principal component scores $z_{12}, z_{22}, \dots, z_{n2}$ take the form

$$z_{i2} = \phi_{12}x_{i1} + \phi_{22}x_{i2} + \dots + \phi_{p2}x_{ip},$$

where ϕ_2 is the second principal component loading vector, with elements $\phi_{12}, \phi_{22}, \dots, \phi_{p2}$.

PCA : Further components (cont'd)

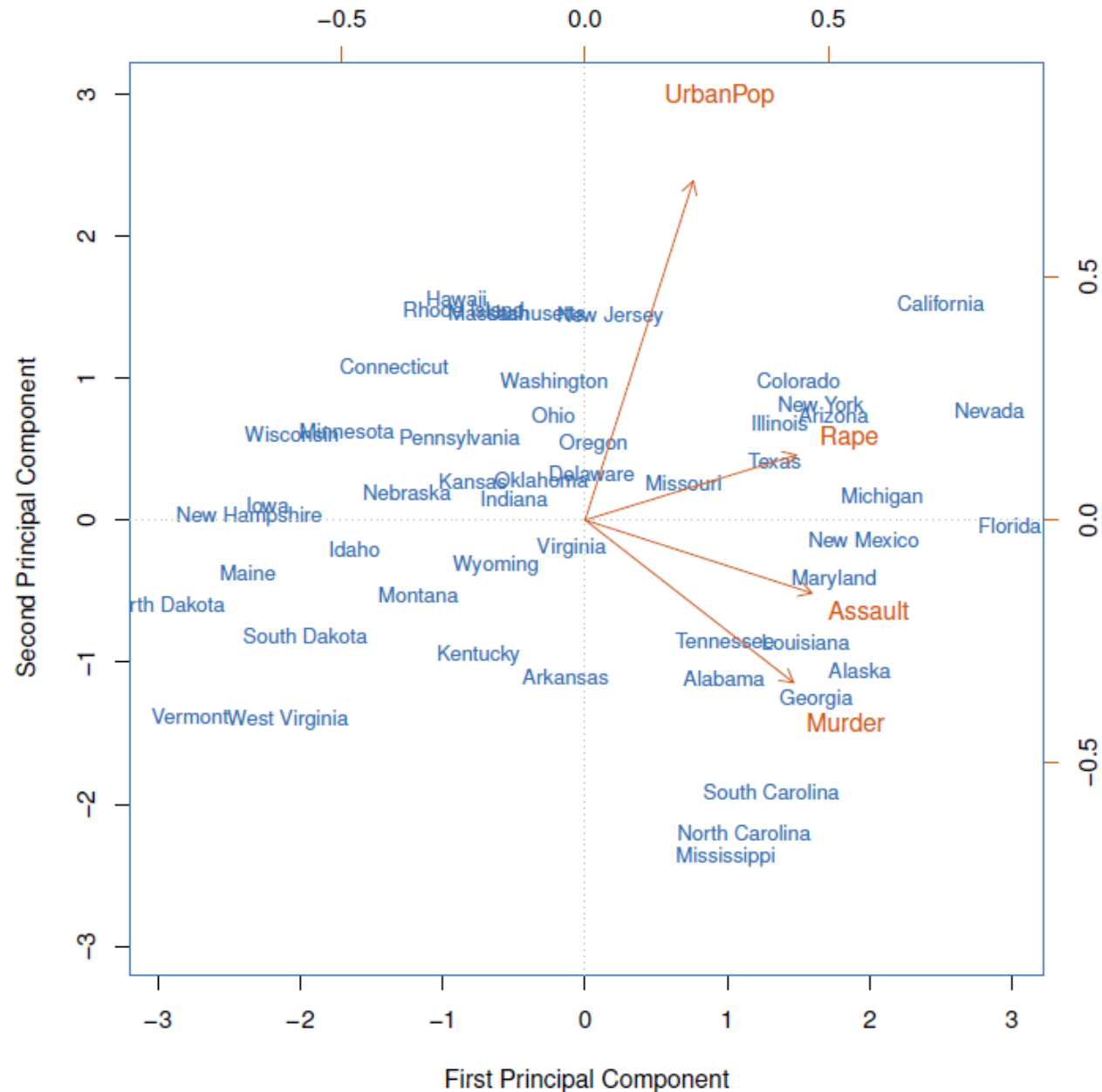


- It turns out that constraining Z_2 to be uncorrelated with Z_1 is equivalent to constraining the direction ϕ_2 to be **orthogonal** (perpendicular) to the direction ϕ_1 . And so on.
- The principal component directions $\phi_1, \phi_2, \phi_3, \dots$ are the ordered sequence of right singular vectors of the matrix \mathbf{X} , and the variances of the components are $\frac{1}{n}$ times the squares of the singular values. There are **at most** $\min(n - 1, p)$ principal components.

PCA: Numerical example

- **USAarrests** data: For each of the fifty states in the United States, the data set contains the number of arrests per 100,000 residents for each of three crimes: **Assault**, **Murder**, and **Rape**. We also record **UrbanPop** (the percent of the population in each state living in urban areas).
- The principal component score vectors have length $n = 50$, and the principal component loading vectors have length $p = 4$.
- PCA was performed after standardizing each variable to have mean zero and standard deviation one.

USA arrests data: PCA plot



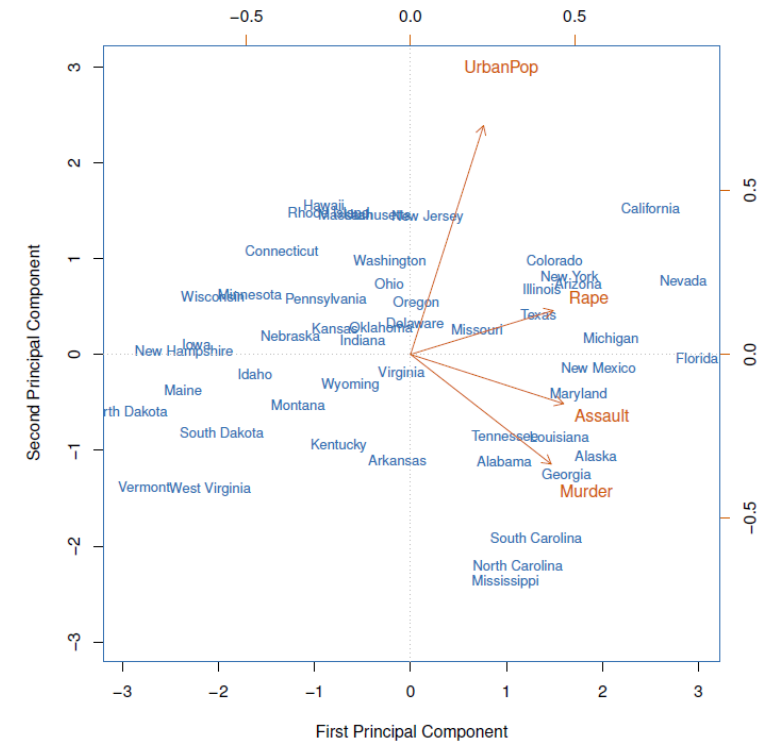
USA arrests data: PCA plot (details)

The first two principal components for the USArrests data.

- The **blue state** names represent the scores for the first two principal components.
- The **orange arrows** indicate the first two principal component loading vectors (with axes on the top and right). For example, the loading for **Rape** on the first component is 0.54, and its loading on the second principal component 0.17 [the word **Rape** is centered at the point (0.54, 0.17)].
- This figure is known as a *biplot*, because it displays both the principal component scores and the principal component loadings.

USA arrests data: PCA loadings

	PC1	PC2
Murder	0.5358995	-0.4181809
Assault	0.5831836	-0.1879856
UrbanPop	0.2781909	0.8728062
Rape	0.5434321	0.1673186

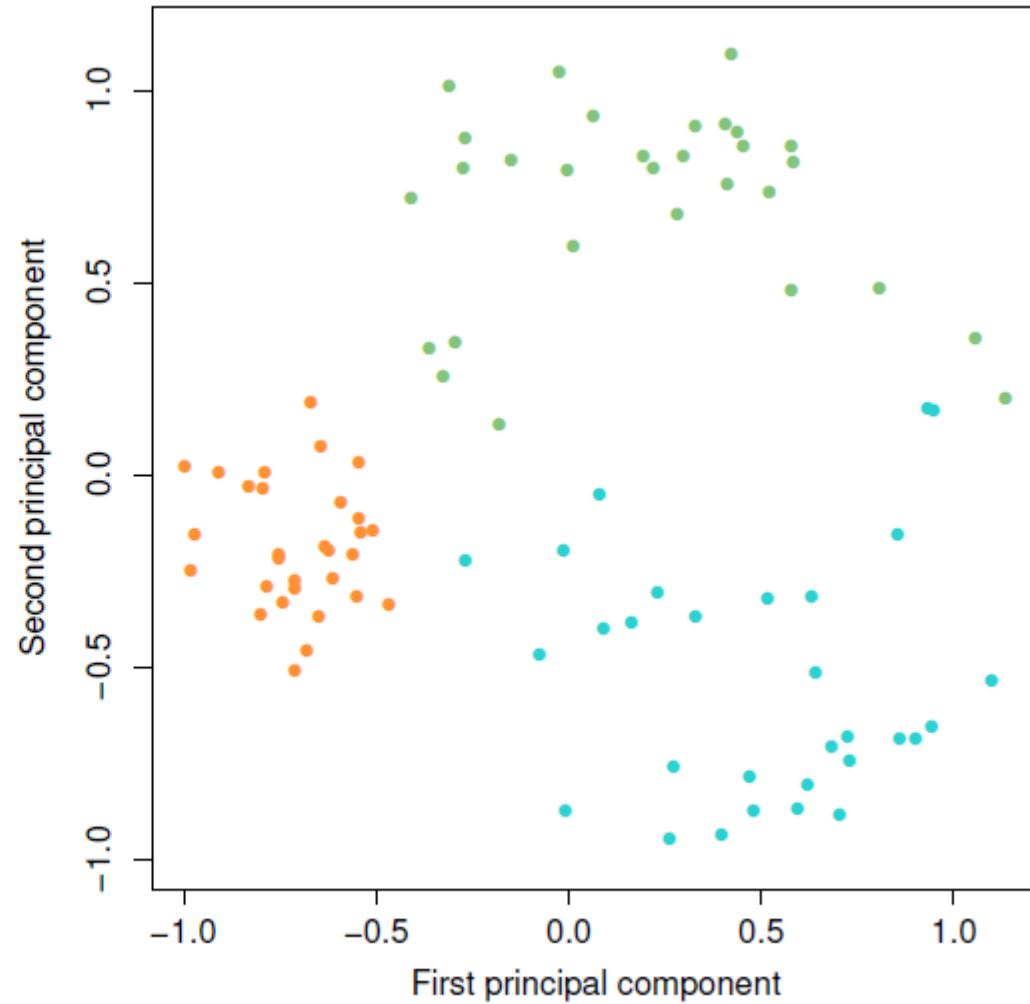
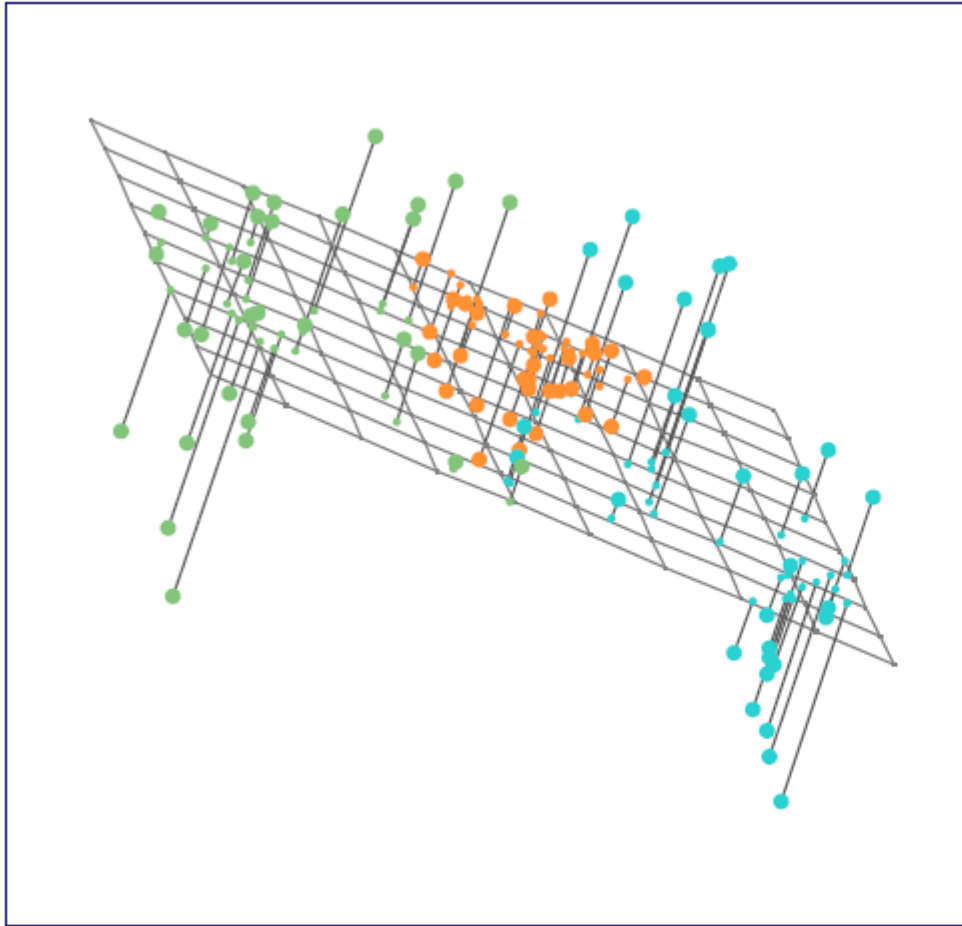


Another interpretation of PCA

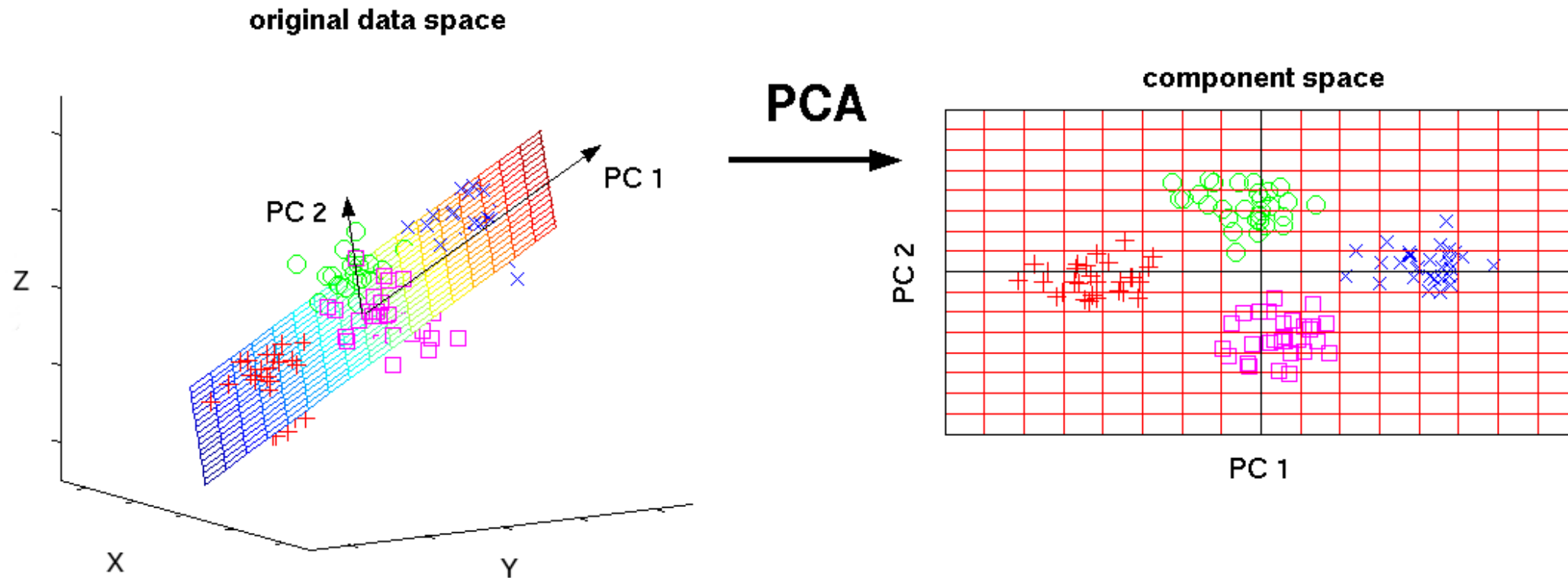
PCA find the hyperplane closest to the observations

- The first principal component loading vector has a very special property: it defines the line in p -dimensional space that is *closest* to the n observations (using average squared Euclidean distance as a measure of closeness)
- The notion of principal components as the dimensions that are closest to the n observations extends beyond just the first principal component.
- For instance, the first two principal components of a data set span the plane that is closest to the n observations, in terms of average squared Euclidean distance.

Another interpretation of PCA (cont'd)

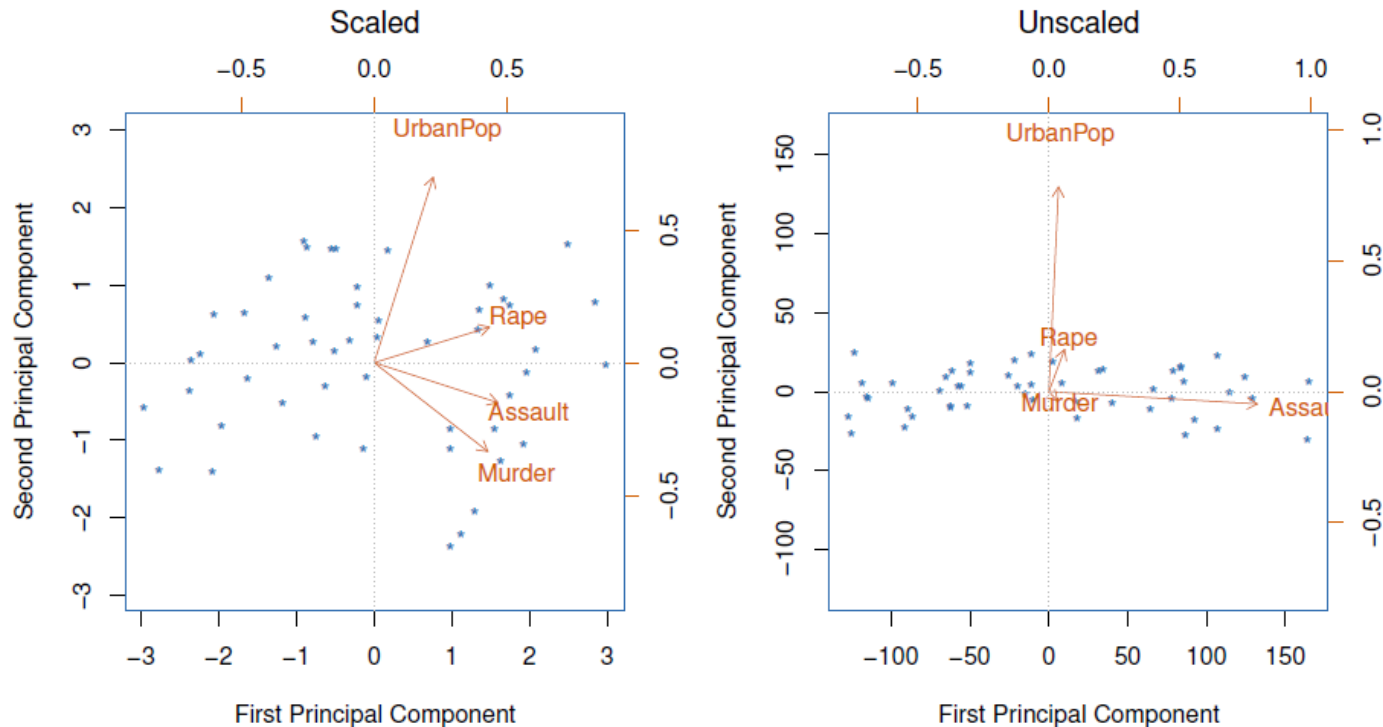


Another interpretation of PCA (cont'd)



PCA: Scaling matters

- If the variables are in different units, scaling each to have standard deviation equal to one is recommended.
- If they are in the same units, you might or might not scale the variables.



Proportion Variance Explained (PVE)

- To understand the strength of each component, we are interested in knowing the proportion of variance explained (PVE) by each one.
- The *total variance* present in a data set (assuming that the variables have been centered to have mean zero) is defined as

$$\sum_{j=1}^p \text{Var}(X_j) = \sum_{j=1}^p \frac{1}{n} \sum_{i=1}^n x_{ij}^2,$$

and the variance explained by the m th principal component is

$$\text{Var}(Z_m) = \frac{1}{n} \sum_{i=1}^n z_{im}^2.$$

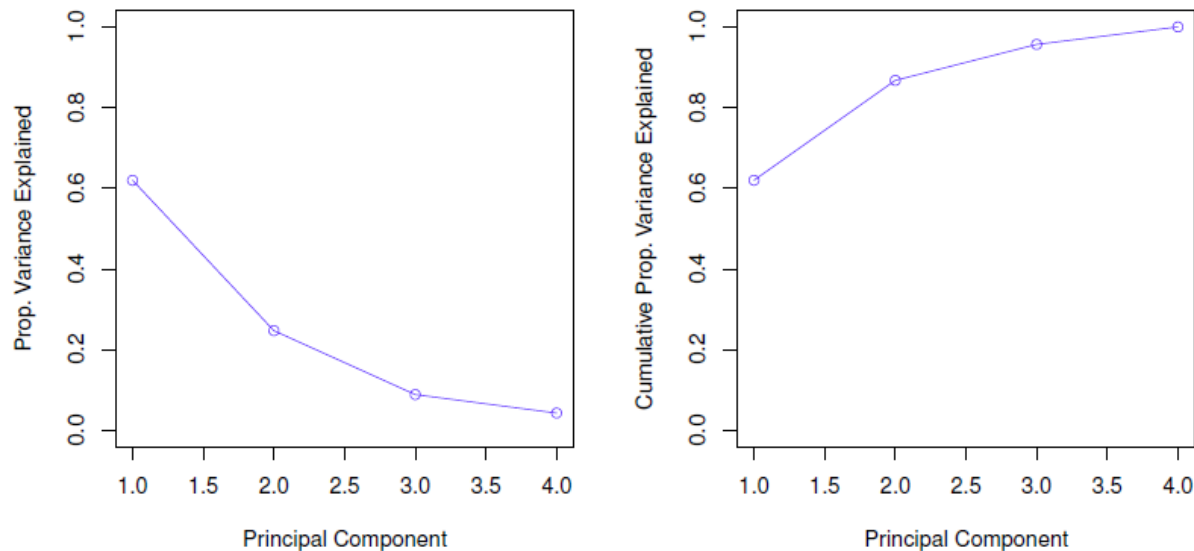
- It can be shown that $\sum_{j=1}^p \text{Var}(X_j) = \sum_{m=1}^M \text{Var}(Z_m)$, with $M = \min(n - 1, p)$.

Proportion Variance Explained (PVE)

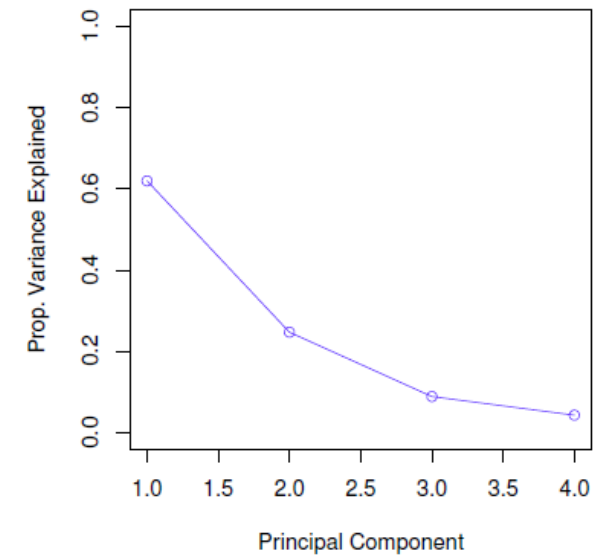
- Therefore, the PVE of the m th principal component is given by the positive quantity between 0 and 1

$$\frac{\sum_{i=1}^n z_{im}^2}{\sum_{j=1}^p \sum_{i=1}^n x_{ij}^2}.$$

- The PVEs sum to one. We sometimes display the cumulative PVEs.



Optimal number of Principle Components?



If we use principal components as a summary of our data, how many components are sufficient?

- No simple answer to this question, as cross-validation is not available for this purpose.
 - *Why not?*
 - When could we use cross-validation to select the number of components?
- the “scree plot” on the previous slide can be used as a guide: we look for an “elbow”.

Kernel PCA

Application:

What if we want to use a linear classifier (regressor) but the data is **non linearly separable**?

