## STATISTICAL INFERENCE



FIGURE 8.3
Sample Estimators of Population Parameters

Main point: How to use the sample to conclude about unknown aspects of the population

Our first topic will be how to summarize the information included in a data collection (what is usually known as descriptive statistics or data exploratory analysis)

## Mains points to take into consideration:

- Location
- Variability
- Measures of the possible relationship among the variables in our data collection

Sometimes we have a large number of variables in our data collection and we need to summarize the information underlying a few main points. One of the possible techniques is Principal Components Analysis (PCA).

Some points to look at before initializing any analysis:

- Data Types - Categorical versus Numerical
- Level of measurement of each variable - Most of the time in actuarial problem we use quantitative variables measured in a ratio scale but ... there are exceptions


## Data Types - Categorical versus Numerical

## FIGURE 2.1

Data Types and Examples


How to determine the level of measurement (Doane and Seward)?

## FIGURE 2.3

Determining the Measurement Level


Location and variability measures (counterpart of population measures)

- Mean $\bar{x}=\frac{\sum_{i=1}^{n} x_{i}}{n}$
- Variance
$>$ Square of the variations around the mean $s^{2}=\frac{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)^{2}}{n-1}$
Why to divide by $n-1$ instead of $n$ (to be discussed later)?
$>$ Standard deviation $s=\sqrt{s^{2}}$
- Covariance $s_{x y}=\frac{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)\left(y_{i}-\bar{y}\right)}{n-1}$
same denominator as the variance
- Correlation coefficient $r_{x y}=\frac{s_{x y}}{s_{x} \times s_{y}}$

Association measures (counterpart of population measures)

- Covariance $s_{x y}=\frac{\sum_{i=1}^{n}\left(x_{i}-\bar{x}\right)\left(y_{i}-\bar{y}\right)}{n-1}$
same denominator as the variance
- Pearson's correlation coefficient $\quad r_{x y}=\frac{s_{x y}}{s_{x} \times s_{y}}$
- Spearman ${ }^{\text {s }}$ rank correlation coefficient, $r_{S}$

Replace each value $x_{i}$ by its rank, $r\left(x_{i}\right)$, and do the same to $y_{i}$, obtaining $r\left(y_{i}\right)$. Spearman's rank correlation coefficient is computed as Pearson's correlation between $r\left(x_{i}\right)$ and $r\left(y_{i}\right)$.

When there are no tied ranks, $r_{S}=1-\frac{6 \sum_{i=1}^{n} d_{i}^{2}}{n\left(n^{2}-1\right)}$

## Association and causation

- Association is different from causation
- Association - A relationship between two, or more, variables
- Correlation - Similar to association, depending on how correlation is computed. Pearson's correlation $\rightarrow$ linear association
- Causation - Changes in one variable causes changes in the other.


## Association Measures - Example

Manufacturers of perishable foods often use preservatives to retard spoilage. One concern is that too much preservative will change the flavor of the food. Suppose an experiment is conducted using samples of a food product with varying amounts of preservative added. Both length of time until the food shows signs of spoiling and a taste rating are recorded for each sample. The taste rating is the average rating for three tasters, each of whom rates each sample on a scale from 1 (good) to 5 (bad). Twelve sample measurements are shown in the following table.

|  | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
| :--- | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| $\mathrm{~N}^{\circ}$ Days | 30 | 47 | 26 | 94 | 67 | 83 | 36 | 77 | 43 | 109 | 56 | 70 |
| Taste | 4.3 | 3.6 | 4.5 | 2.8 | 3.3 | 2.7 | 4.2 | 3.9 | 3.6 | 2.2 | 3.1 | 2.9 |

Compute Pearson's and Spearman's correlation coefficient and comment.

## Association Measures - Example (solution)

```
> #### Correlation coefficients example
> x=c(30,47,26,94,67,83,36,77,43,109,56,70)
> y=c(4.3,3.6,4.5,2.8,3.3,2.7,4.2,3.9,3.6,2.2,3.1,2.9)
>
> # Pearson's coefficient
> cor.xy=cor(x,y) # Pearson's coefficient
>
> avg.x=mean(x); sd.x=sd(x)
> avg.y=mean(y); sd.y=sd(y)
> cbind(avg.x,avg.y,sd.x,sd.y,cor.xy)
    avg.x avg.y sd.x sd.y cor.xy
[1,] 61.5 3.425 26.29034 0.714938 -0.8771227
> # just to check formula
> cov.xy=cov(x,y)
> cov.xy/(sd.x*sd.y) # Pearson's coefficient
[1] -0.8771227
```


## Association Measures - Example (solution)

```
> # Spearman's coefficient
> cor(rank(x),rank(y)) # Spearman's coefficient
[1] -0.8791607
> rank(x); rank(y)
    [1] }20.
    [1] 11.0 7.5 12.0 3.0 6.0 2.0 10.0 9.0 7.5 1.0 5.0 4.0
> d=rank(x)-rank(y); n=12; 1-6*sum(d^2)/(n*(n^2-1)) # Approx value
since we have one tie
[1] -0.8758741
```

>

## PRINCIPAL COMPONENTE ANALYSIS (PCA)

Motivation: A financial analyst is interested in determining the financial health of firms in a given industry. Research studies have identified a number of financial ratios (say about 120) that can be used for such a purpose. Obviously, it would be extremely taxing to interpret the 120 pieces of information for assessing the financial health of firms. However, the analyst's task would be simplified if these 120 ratios could be reduced to a few indices (say about 3), which are linear combinations of the original 120 ratios.

Main purpose of PCA: To capture the main patterns explaining the variability in a data set using a small number of new variables that are uncorrelated linar combinations of the original variables keeping the loss of information under control.

## PCA - Introduction

- PCA is one of the multivariate exploratory data analysis techniques. It can be used by itself to reduce the dimension of a data set or as an auxiliary technique for other approaches.
- The new variables to be created are:
$>$ Linear combinations of the original variables
$>$ The linear combinations are uncorrelated with each other
$>$ The maximum number of new variables is equal to the number of original variables (assuming that there is no perfect correlation among the original variables)
- Let us first consider a very simple example: $p=2$ variables, $X_{1}$ and $X_{2}$ and $n=12$ observations for each variable (data are presented in Table 1)


## PCA - A simple example

Table1

| obs | 1 | 2 | 3 | 4 | 5 | 6 | 7 | 8 | 9 | 10 | 11 | 12 |
| :--- | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: | ---: |
| $X_{1}$ | 16 | 12 | 13 | 11 | 10 | 9 | 8 | 7 | 5 | 3 | 2 | 0 |
| $X_{2}$ | 8 | 10 | 6 | 2 | 8 | -1 | 4 | 6 | -3 | -1 | -3 | 0 |

Compute $S$, the covariance matrix between $X_{1}$ and $X_{2}$.

$$
S=\left[\begin{array}{ll}
s_{1}^{2}=s_{11} & s_{12} \\
s_{21} & s_{2}^{2}=s_{22}
\end{array}\right] \approx\left[\begin{array}{ll}
23.09091 & 16.45455 \\
16.45455 & 21.09091
\end{array}\right]
$$

$$
\text { using } \quad s_{i j}=\frac{\sum_{k=1}^{n}\left(x_{i k}-\bar{x}_{i}\right)\left(x_{j k}-\bar{x}_{j}\right)}{n-1} \text { and } \bar{x}_{i}=\frac{\sum_{k=1}^{n} x_{i k}}{n}
$$

- The total variance is then
$s_{1}^{2}+s_{2}^{2}=s_{11}+s_{22}=23.09091+21.09091=44.18182$
$s_{1}^{2}=23.09091$ (the variance of the first variable) represents $52.26 \%$ of this total while $s_{2}^{2}=21.09091$ represents $47.74 \%$.


## PCA - A simple example (cont)

- The first step is to replace the original variables, $X_{1}$ and $X_{2}$, by 2 linear combinations of them, $Y_{1}$ and $Y_{2}$, in such a way that the first one will cover must of the varability (most of the total variance).

$$
\left\{\begin{array} { l } 
{ Y _ { 1 } = e _ { 1 1 } X _ { 1 } + e _ { 1 2 } X _ { 2 } } \\
{ Y _ { 2 } = e _ { 2 1 } X _ { 1 } + e _ { 2 2 } X _ { 2 } }
\end{array} \text { and } \left\{\begin{array}{l}
s_{Y_{1}}^{2}=e_{11}^{2} s_{11}+e_{12}^{2} s_{22}+2 e_{11} e_{12} s_{12} \\
s_{Y_{2}}^{2}=e_{21}^{2} s_{11}+e_{22}^{2} s_{22}+2 e_{21} e_{22} s_{12}
\end{array}\right.\right.
$$

As it is obvious, if we multiply the coefficient $e_{i j}$ by a constant $k>1, s_{Y_{1}}^{2}$ and $s_{Y_{2}}^{2}$ will increase and then we need to introduce a constraint before maximizing. The constraint is $e_{i 1}^{2}+e_{i 2}^{2}=1$.

- The second step will be to discuss the data reduction: Is it acceptable to use less linear combinations ( $Y$ variables) than the original number of variables?

Let us, first, discuss the first step.

## PCA - A simple example (cont)

The problem: $\max _{Y_{1}}^{2}$ subject to $e_{i 1}^{2}+e_{i 2}^{2}=1$.
We need to maximize the Lagrangean function

$$
\begin{aligned}
L & =e_{11}^{2} s_{11}+e_{12}^{2} s_{22}+2 e_{11} e_{12} s_{12}-\lambda\left(e_{11}^{2}+e_{12}^{2}-1\right) \text { in order to } e_{11}, e_{12} \text { and } \lambda \\
& \left\{\begin{array}{l}
\frac{\partial L}{\partial e_{11}}=2 e_{11} s_{11}+2 e_{12} s_{12}-2 \lambda e_{11} \\
\frac{\partial L}{\partial e_{12}}=2 e_{12} s_{22}+2 e_{11} s_{12}-2 \lambda e_{12} \\
\frac{\partial L}{\partial \lambda}=-\left(e_{11}^{2}+e_{12}^{2}-1\right)
\end{array}\right.
\end{aligned}
$$

$$
\text { and then we must solve the system }\left\{\begin{array}{l}
e_{11} s_{11}+e_{12} s_{12}-\lambda e_{11}=0 \\
e_{12} s_{22}+e_{11} s_{12}-\lambda e_{12}=0 \\
-\left(e_{11}^{2}+e_{12}^{2}-1\right)=0
\end{array}\right.
$$

## PCA - A simple example (cont)

Using some matricial notation and defining $\mathbf{e}_{1}=\left[\begin{array}{l}e_{11} \\ e_{12}\end{array}\right], \mathbf{0}=\left[\begin{array}{l}0 \\ 0\end{array}\right], I$ as the identity matrix (size 2) and $S=\left[\begin{array}{ll}s_{11} & s_{12} \\ s_{21} & s_{22}\end{array}\right]$ we can rewrite the problem as

$$
\begin{aligned}
L= & \mathbf{e}_{1}^{T} S \mathbf{e}_{1}-\lambda\left(\mathbf{e}_{1}^{T} I \mathbf{e}_{1}-1\right)=\mathbf{e}_{1}^{T} S \mathbf{e}_{1}-\lambda\left(\mathbf{e}_{1}^{T} \mathbf{e}_{1}-1\right) \\
\frac{\partial L}{\partial \mathbf{e}_{1}} & =2 S \mathbf{e}_{1}-2 \lambda I \mathbf{e}_{1}=2(S-\lambda I) \mathbf{e}_{1} \\
\frac{\partial L}{\partial \lambda} & =-\lambda\left(\mathbf{e}_{1}^{T} \mathbf{e}_{1}-1\right)
\end{aligned}
$$

And then we must solve $(S-\lambda I) \mathbf{e}_{1}=\mathbf{0}$ knowing that $\mathbf{e}_{1}^{T} \mathbf{e}_{1}=1$ ( the same result can be obtained from the previous slide). This is a well known problem in linear algebra: Finding the eigenvalues and the eigen vectors of matrix $S$

## PCA - Eigenvalues and eigenvector of matrix $S$

Solve $(S-\lambda I) \mathbf{e}_{1}=\mathbf{0}$ subject to $\mathbf{e}_{1}^{T} \mathbf{e}_{1}=1$
As we have a homogeneous system of equations the trivial solution $\mathbf{e}_{1}=\mathbf{0}$ is always possible but irrelevant. So, we must guarantee that the determinant of the system is 0 , i.e., $|S-\lambda I|=0$.

This equation is a polynomial of order $k$ (the number of original variables) and therefore has $k$ roots (the eigenvalues of $S$ ), $\lambda_{1} \geq \lambda_{2} \geq \cdots \geq \lambda_{k}>0$, as $S$ is definite positive matrix (assuming that none of the variables is a linear combination of the others).

For each root $\lambda_{i}$ we get the corresponding eigenvector, $\mathbf{e}_{\mathbf{i}}$, normalized using $\mathbf{e}_{i}^{T} \mathbf{e}_{i}=1$.

## PCA - Eigenvalues and eigenvector of matrix $S$ (cont)

Let us consider the largest eigenvalue, $\lambda_{1}$. As it is a solution of the system we have

$$
\left\{\begin{array}{l}
\left(S-\lambda_{1} I\right) \mathbf{e}_{1}=\mathbf{0} \\
\mathbf{e}_{1}^{T} \mathbf{e}_{1}=1
\end{array}\right.
$$

Pre-multiplying the first equation by $\mathbf{e}_{1}^{T}$ originates
$\mathbf{e}_{1}^{T}\left(S-\lambda_{1} I\right) \mathbf{e}_{1}=\mathbf{e}_{1}^{T} \mathbf{0} \Leftrightarrow \mathbf{e}_{1}^{T} S \mathbf{e}_{1}-\mathbf{e}_{1}^{T} \lambda_{1} I \mathbf{e}_{1}=0 \Leftrightarrow \mathbf{e}_{1}^{T} S \mathbf{e}_{1}=\lambda_{1} \mathbf{e}_{1}^{T} \mathbf{e}_{1}=\lambda_{1}$
as $\mathbf{e}_{1}^{T} \mathbf{e}_{1}=1$.
We get $\mathbf{e}_{1}^{T} S \mathbf{e}_{1}=\lambda_{1}$ and if we repeat the process for the second largest eigenvalue we get $\mathbf{e}_{2}^{T} S \mathbf{e}_{2}=\lambda_{2}$ and so on. The variance of the $j$-th linear combination is equal to the $j$-th eigenvalue.

## PCA - A simple example (cont)

Back to our simple example we define the polynomial as

$$
\begin{aligned}
& \begin{aligned}
& \left.\begin{array}{rl}
23.09091-\lambda & 16.45455 \\
16.45455 & 21.09091-\lambda
\end{array} \right\rvert\,=0 \Leftrightarrow(23.09091-\lambda)(21.09091-\lambda)-16.45455^{2}=0 \\
& \Leftrightarrow \lambda^{2}-44.18182 \lambda+216.2561=0
\end{aligned} \\
& \left.\begin{array}{c}
\lambda=\frac{44.182 \pm \sqrt{44.182^{2}-4 \times 216.245}}{2}
\end{array}\right] \text { i.e., } \lambda_{1}=38.57582 \text { and } \lambda_{2}=5.606001 .
\end{aligned}
$$

The corresponding eigenvectors are given by
$\left\{\begin{array}{l}\left(23.09091-\lambda_{i}\right) e_{i 1}+16.45455 e_{i 2}=0 \\ e_{i 1}^{2}+e_{i 2}^{2}=1\end{array} \Leftrightarrow\left\{\begin{array}{l}e_{i 1}^{2}=\frac{1}{1+\left(\frac{23.09091-\lambda_{i}}{16.45455}\right)^{2}} \\ e_{i 2}=\left(\frac{23.09091-\lambda_{i}}{16.45455}\right) e_{i 1}\end{array}\right.\right.$

## PCA - A simple example (cont)

For each case (see slide we can choose the positive or the negative root to define $e_{i 1}$ as the results are equivalent. Let us choose the negative (to get the solution obtained using R)
$\lambda_{1}=38.57582 \quad(87.31 \%$ of total variance $) \quad \mathbf{e}_{1}^{T}=\left[\begin{array}{ll}-0.722388 & -0.685324\end{array}\right]$
$\lambda_{2}=5.606001$
$(12.69 \%$ of total variance $) \quad \mathbf{e}_{2}^{T}=\left[\begin{array}{ll}-0.685324 & 0.728238\end{array}\right]$
At this stage we are using all the information in a different way and we solve step 1.
Instead of representing (plotting) each observation using the original variables ( $X_{1}$ and $X_{2}$ ) we can use the principal components ( $\mathbf{e}_{1}$ and $\mathbf{e}_{2}$ ). For observation $i$ we get $\left[\begin{array}{l}Y_{1 i} \\ Y_{2 i}\end{array}\right]=\left[\begin{array}{ll}e_{11} & e_{12} \\ e_{21} & e_{22}\end{array}\right]\left[\begin{array}{l}X_{1 i} \\ X_{2 i}\end{array}\right]=\left[\begin{array}{ll}-0.722388 & 0.685324 \\ -0.685324 & 0.728238\end{array}\right]\left[\begin{array}{l}X_{1 i} \\ X_{2 i}\end{array}\right]$

## PCA - A simple example (cont)



- $1^{\text {st }}$ panel: observations (a to I), centering effect (dashed lines) and PC (red)
- $2^{\text {nd }}$ panel: centered observations (a to I), and PC (red) with unit and direction. The direction of each axis is arbitrary (remember that we can choose the negative or the positive root).
- 3rd panel: observations using the new axes system (PC).


## PCA

Two more definitions can be useful:

- Loadings: different definitions appear in the litterature but the most commom also called standardized loading - is the correlation coefficient between each PC and each original variable $l_{i j}=\frac{w_{i j}}{s_{j}} \sqrt{\lambda_{i}}$ where $l_{i j}$ stand for the loading of the $j$ th variable on $\mathrm{PC}_{i}$, $w_{i j}$ is the weight, $s_{j}$ the standard deviation of the $j$-th variable and $\lambda_{i}$ the eigenvalue (variance) associated to the $i$-th PC.
- Scores: the coordinates of each observation in terms of the principal components (see the right panel on previous slide)

Data reduction: Is the first PC (or how many PC are) enough to represent the data set? The answer depends on:

- How much variability (\% of total variability) is captured by the first PCs.
- How relevant is the loss of information for the problem under analysis.

Before addressing this point let's see how to use R to analyze the first example:

## PCA - Using R - A simple example

```
> x1=c(16,12,13,11,10,9,8,7,5,3,2,0)
> x2=c(8,10,6,2,8,-1,4,6,-3,-1,-3,0)
> x=cbind(x1,x2)
>
> ### Using eigenvalues and eigenvectors - centered only
> x1c=(x1-mean(x1)); x2c=(x2-mean(x2))
> Xc=cbind(x1c,x2c)
> S=(1/(length(xlc)-1))*(t(Xc)%*%Xc); S # covariance matrix
    x1c x2c
x1c 23.09091 16.45455
x2c 16.45455 21.09091
> out=eigen(S); out
eigen() decomposition
$`values`
[1] 38.575813 5.606005
```

\$vectors

$$
[, 1] \quad[, 2]
$$

$[1]-,0.7282381 \quad 0.6853242$
$[2]-0.6853242-$,

## PCA - Using R - A simple example

> cbind(out\$values[1]/sum(out\$values),out\$values[2]/sum(out\$values))
[,1] [,2]
[1,] 0.87311510 .1268849
$>$
> \#\#\# Using prcomp function (other sol are available in R)
$>$ out1=prcomp (x, center=T)
> out1 \# eigenvalues are the squares of st. dev.
Standard deviations (1, .., p=2):
[1] 6.2109432 .367700
Rotation $\underset{\text { PC1 }}{(\mathrm{n} \mathrm{x}} \mathrm{k})=\underset{\mathrm{PC} 2}{(2 \mathrm{x}} 2)$ :
$\begin{array}{lll}\mathrm{x} 1 & -0.7282381 & 0.6853242\end{array}$
x2 -0.6853242-0.7282381
> summary(out1)
Importance of components:

$$
\text { PC1 } \quad \mathrm{PC} 2
$$

Standard deviation 6.21092 .3677
Proportion of Variance 0.87310 .1269
Cumulative Proportion 0.87311 .0000

## PCA - Using R - A simple example

```
> out1$x # scores
    PC1 PC2
    [1,] -9.2525259 1.8414027
    [2,] -7.7102217 -2.3563703
    [3,] -5.6971632 1.2419065
    [4,] -1.4993902 2.7842106
    [5,] -4.8830971 -2.2705423
    [6,] 2.0130586 3.5982767
    [7,] -0.6853242 -0.7282381
    [8,] -1.3277344 -2.8700386
    [9,] 6.2966594 2.3134563
[10,] 6.3824874 -0.5136683
[11,] 8.4813738 0.2574838
[12,] 7.8818776 -3.2978790
> out1$rotation # weights, eigen vectors
    PC1 PC2
x1 -0.7282381 0.6853242
x2 -0.6853242 -0.7282381
```


## PCA - Using R - A simple example

```
> cor(x,out1$x)
        # loadings
    PC1
        PC2
    x1 -0.9412618 0.3376776
    x2 -0.9268425-0.3754503
```

or, using the formula, $l_{i j}=\frac{w_{i j}}{s_{j}} \sqrt{\lambda_{i}}$
> \# using the formula instead of the correlation
$>$ z.c=rbind(out1\$sdev,out1\$sdev)
$>$ sd.c=c(sd(x1),sd(x2)); sd.c=cbind(sd.c,sd.c)
> l=out1\$rotation*z.c/sd.c; l \# loadings
PC1 PC2
x1 -0.9412618 0.3376776
$x 2-0.9268425-0.3754503$

## PCA - Some issues

4 issues need to be briefly discussed:

1. In addition to centering (mean correct) should we scale the variables?
2. Number of principal components to extract
3. How to interpret principal components
4. Use of principal component scores

A new example - Food price index (Sharma) - will help to clarify these issues.
The average price (cents per pound - 1973) of five (just to keep things simple) food items are known for 23 US cities. Our main objective is to form a price index (like the Consumer Price Index) using PCA.

The data is presented in the R program: 5 food items and 23 cities
After reading the data set, our next task is to prerform a PCA as we did before

## PCA - Example 2 - Food price index

- First step $\rightarrow$ reading the data set

```
dta=read.csv("E:/Risk Models 2018/food price index.csv",header=T,sep=",")
> dta # Check input
                                City Bread Burger Milk Oranges Tomatoes
\begin{tabular}{lrrrrr}
1 & Atlanta & 24.5 & 94.5 & 73.9 & 80.1 \\
2 & Baltimore & 26.5 & 91.0 & 67.5 & 74.6 \\
3 & Boston & 29.7 & 100.8 & 61.4 & 104.0 \\
4 & Buffalo & 22.8 & 86.6 & 65.3 & 118.4 \\
5 & Chicago & 26.7 & 86.7 & 62.7 & 105.9 \\
6 & Cincinnati & 25.3 & 102.5 & 63.3 & 99.3 \\
7 & Cleveland & 22.8 & 88.8 & 52.4 & 110.9 \\
8 & Dallas & 23.3 & 85.5 & 62.5 & 117.9 \\
9 & Detroit & 24.1 & 93.7 & 51.5 & 109.7 \\
10 & Honolulu & 29.3 & 105.9 & 80.2 & 133.2 \\
11 & Houston & 22.3 & 83.6 & 67.8 & 108.6 \\
12 & Kansas City & 26.1 & 88.9 & 65.4 & 100.9 \\
13 & Los Angeles & 26.9 & 89.3 & 56.2 & 82.7 \\
14 & Milwaukee & 20.3 & 89.6 & 53.8 & 111.8 \\
15 & Minneapolis & 24.6 & 92.2 & 51.9 & 106.0 \\
16 & New York & 30.8 & 110.7 & 66.0 & 107.3 \\
17 & Philadelphia & 24.5 & 92.3 & 66.7 & 98.0 \\
18 & Pittsburgh & 26.2 & 95.4 & 60.2 & 117.1 \\
19 & St. Louis & 26.5 & 92.4 & 60.8 & 115.1 \\
20.9 & 62.6 \\
20 & San Diego & 25.5 & 83.7 & 57.0 & 92.8 \\
21 & San Francisco & 26.3 & 87.1 & 58.3 & 101.8 \\
22 & Seattle & 22.5 & 77.7 & 62.0 & 91.1 \\
23 & Washington DC & 24.2 & 93.8 & 66.0 & 81.6
\end{tabular}
```


## PCA - Example 2 - Food price index

- Second step $\rightarrow 1^{\text {st }}$ PCA using prcomp function (other solutions are available)

```
> attach(dta)
> x=cbind(Bread,Burger,Milk,Oranges,Tomatoes)
> outl=prcomp(x, center=T)
> out1
Standard deviations:
```

```
[1] 14.798604 9.577221
```

[1] 14.798604 9.577221
6.136994 4.561857
6.136994 4.561857
1.740468

```
1.740468
```

Rotation:

|  | PC1 | PC2 |  | PC3 |  |  |
| :---: | :---: | :---: | :---: | :---: | :---: | :---: |
| Bread | 0.02848905 | 653211 | -0.021 | 5748 | 189725 | -0.96 |
| Burger | 0.20012240 | . 6321849 | -0.25420 | 0475 | . 658624 | 0.2 |
| Milk | 0.04167230 | 421503 | 0.888 | 4949 - | 107659 | 0 |
| Oranges | 0.93885906-0 | 3143547 | 0.1213 | 5003 | 069046 | -0 |
| Tomatoes 0.275583890 .5279 > summary(out1) |  |  |  |  |  |  |
| Importance of components: |  |  |  |  |  |  |
|  |  | PC1 | PC2 | PC3 | PC4 | PC5 |
| Standard | deviation | 14.7986 | 9.5772 | 6.1370 | 4.56186 | 1.74047 |
| Proporti | n of Variance | 0.5884 | 0.2464 | 0.1012 | 0.05591 | 0.00814 |
| Cumulativ | e Proportion | 0.5884 | 0.8348 | 0.9359 | 0.99186 | 1.00000 |

## PCA - Scaling or not scaling the variables

As we can see PC1 is very much affected by the variable Oranges. This is partialy due to the fact that the variability associated with this variable is much higher than the variability associated with the other variables (see the satndard deviations).

If we do not want that the variability of each variable influences the output we can scale the variables (divide by the standard deviation) - we will analyze the correlation matrix instead of the covariance matrix.

The main point to think about before scaling or not scaling the variables is if we want to give the same (scale the variables) a priori weight to each variable or not.

To use scaled variables we can scale them before performing PCA or jus just replace outl=prcomp ( x , center=T) by outl=prcomp ( x, center=T,scale=T)

## PCA - Example 2 - Food price index

```
> out2=prcomp(x, center=T,scale=T)
> out2
Standard deviations:
[1] 1.5564279 1.0510352 0.8593489 0.7025748 0.4906784
```

Rotation:

|  | PC1 | PC2 | PC3 | PC4 | PC5 |
| :--- | ---: | ---: | ---: | ---: | ---: |
| Bread | 0.4961487 | -0.30861972 | 0.38639398 | 0.50930459 | -0.499898868 |
| Burger | 0.5757023 | -0.04380176 | 0.26247227 | -0.02813712 | 0.772635014 |
| Milk | 0.3395696 | -0.43080905 | -0.83463952 | 0.04910000 | 0.007882237 |
| Oranges | 0.2249898 | 0.79677694 | -0.29160659 | 0.47901574 | -0.005966796 |
| Tomatoes | 0.5064340 | 0.28702846 | 0.01226602 | -0.71270629 | -0.391201387 |

$>$ summary (out2)
Importance of components:

|  | PC1 | PC2 | PC3 | PC4 | PC5 |
| :--- | ---: | ---: | ---: | ---: | ---: | ---: |
| Standard deviation | 1.5564 | 1.0510 | 0.8593 | 0.70257 | 0.49068 |
| Proportion of Variance | 0.4845 | 0.2209 | 0.1477 | 0.09872 | 0.04815 |
| Cumulative Proportion | 0.4845 | 0.7054 | 0.8531 | 0.95185 | 1.00000 |

As we can see we get a different solution. Now, the weights for PC1 are more balanced. For the purpose of the example (CPI) this solution is probably better since we have no reason to give Oranges much more weight than for the other items.

## PCA - Number of PC to extract

Remember that the idea is to capture the main patterns explaining the variability in a data set using a small number of PC. Both topics ("main pattern" and "small number") are linked together and depend on the problem under analysis.

However there are some criteria that can be used when there is no clear answer to this question.

- Kaiser criterion - keep PC whose eigenvalues are greater than 1 (scaled data) or greater than the average of all eigenvalues (non-scaled data). Mainly used with scaled data.
- Scree-plot analysis - Plot the percent of variance accounted for by each PC and look for an elbow. Choose the value imidiately before the elbow (used with both scaled and non-scaled data) or use the second differences.
- Parallel analysis - Based on a simulation procedure (simulation will be discussed latter) that can be simplified using a table of constants (see sharma). More efficient but less used as it is more difficult to compute. In R we can use some packages to get a parallel analysis: paran or psych for instance.


## PCA - Example 2 - Food price index

- Kaiser criterion:
- Scaled data: retain the first 2 PC (remember that the eigenvalues are the square of the standard deviation of the principal components
- Non-scaled data: retain the first 2 PC

```
> lambda=out1$sdev^2; lambda
[1] 218.998679 91.723169 37.662690 20.810541 3.029229
> mean(lambda)
[1] 74.44486
```


## PCA - Example 2 - Food price index

- Scree plot: left panel for centered data and right panel for scaled (and centered) data


For non-scaled dat just replace out2 by out1
> \# scaled
> lambda=out2\$sdev^2
> plot (lambda,type="b")
> diff(lambda,lag=1,differences=2)
[1] 0.951598697 0.121325148-0.007976802
Both scree plots are similar and recommend the use of 2 PC

## PCA - Example 2 - Food price index

- Parallel analysis - Horn (1965)
- Using paran

```
> require(paran) # package paran must be installed before
> paran(x,iterations=100,graph=T)
Using eigendecomposition of correlation matrix.
Computing: 10% 20% 30% 40% 50% 60% 70% 80% 90% 100%
Results of Horn's Parallel Analysis for component retention
1 0 0 ~ i t e r a t i o n s , ~ u s i n g ~ t h e ~ m e a n ~ e s t i m a t e
```

| Component | Adjusted | Unadjusted | Estimated |
| :--- | :--- | :--- | :--- |
|  | Eigenvalue | Eigenvalue | Bias |

$1 \quad 1.791788 \quad 2.422467 \quad 0.630679$

Adjusted eigenvalues > 1 indicate dimensions to retain. (1components retained)

## PCA - Example 2 - Food price index

Parallel Analysis


## PCA - How to interpret principal components?

When possible retained PC can be interpreted using the loadings: The higher the loading (in absolute value) the more influence it had in the formation of the PC. But the main question is how high should the loading be before we can say that a given variable is influential in the formation of he PC. There are no clear answers to this question. In some applied work the value 0.5 or 0.6 for scaled data is used as a cutoff.

## PCA - Example 2 - Food price index

Back to the example, compute the loadings for each retained PC - assuming scaled variables and that 2 PC are retained

```
> cor(x,out2$x) # Loadings
\begin{tabular}{lrr} 
& PC1 & PC2 \\
Bread & 0.7722197 & -0.32437017 \\
Burger & 0.8960392 & -0.04603719 \\
Milk & 0.5285156 & -0.45279546 \\
Oranges & 0.3501804 & 0.83744058 \\
Tomatoes & 0.7882281 & 0.30167700
\end{tabular}
```

Using 0.5 as the cutoff value, PC1 is the "non-fruits" CPI (stricly speaking tomatoe is a fruit but is usually considered as a vegetable) and PC2 is the "fruit" CPI we can interpret PC1.

## PCA - Example 2 - Food price index

If non-scaled data is used, there interprteation is more puzzling

```
> cor(x,out1$x)
\begin{tabular}{lrr} 
& PC1 & PC2 \\
Bread & 0.16817616 & 0.6315875 \\
Burger & 0.39199944 & 0.8014061 \\
Milk & 0.08872954 & 0.6092695 \\
Oranges & 0.97573973 & -0.2114328 \\
Tomatoes & 0.53642447 & 0.6650256
\end{tabular}
```

PC1 linked to fruits (and vegetables) and PC2 linked to the remaining items.

## PCA - Use of principal component scores

PC scores can be plotted for further interpretting the results (but a clear interpretation is not guaranted).


Broadly speaking we can identify 5 groups:

- High fruit CPI and low non-fruit CPI: Milwaukee, Cleveland, Detroit, Buffalo, Minneapolis,Dallas;
- Avg fruit CPI and low non-fruit CPI : Houston, San Fr, Seattle, San Diego Kansas City;
- Avg fruit CPI and low non-fruit CPI : LA, Wash, Baltimore, Atlanta;
- Avg fruit CPI and avg non-fruit CPI : Pittsburgh, St Louis, Chicago, Philadelphia, Houston, Cincinanti;
- Avg fruit CPI and High non-fruit CPI : New-York, Honolulu,


