## STATISTICAL INFERENCE



Source: Doane and Seward - Applied Statistics in Business and Economics

# 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** 



Source: Doane and Seward - Applied Statistics in Business and Economics

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#### How to determine the level of measurement?

#### FIGURE 2.3 Determining the Measurement Level



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Location and variability measures

#### (counterpart of population measures)

- Mean  $\overline{x} = \frac{\sum_{i=1}^{n} x_i}{n}$
- Median
- Variance

Square of the variations around the mean  $s^2 = \frac{\sum_{i=1}^{n} (x_i - \overline{x})^2}{n-1}$ 

Why to divide by n-1 instead of n (to be discussed later)?

> Standard deviation  $s = \sqrt{s^2}$ 

Association measures (counterpart of population measures)

• Covariance  $s_{xy} = \frac{\sum_{i=1}^{n} (x_i - \overline{x})(y_i - \overline{y})}{n-1}$ 

same denominator as the variance

- Pearson's correlation coefficient  $r_{xy} = \frac{S_{xy}}{S_x \times S_y}$
- Spearman's rank correlation coefficient,  $r_s$

Replace each value  $x_i$  by its rank,  $r(x_i)$ , and do the same to  $y_i$ , obtaining  $r(y_i)$ . Spearman's rank correlation coefficient is computed as Pearson's correlation between  $r(x_i)$  and  $r(y_i)$ .

When there are no tied ranks, 
$$r_s = 1 - \frac{6\sum_{i=1}^n d_i^2}{n(n^2 - 1)}$$
 where  $d_i = r(x_i) - r(y_i)$ 

#### 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 → 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
Nº 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] 2 5 1 11 7 10 3 9 4 12 6 8
[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
> # Alternative computation - Approximate value since we have one
tie
> d=rank(x)-rank(y); n=12; 1-6*sum(d^2)/(n*(n^2-1))
[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
$\overline{X}_2$	8	10	6	2	8	-1	4	6	-3	-1	-3	0

Compute S, the covariance matrix between  $X_1$  and  $X_2$ .

$$S = \begin{bmatrix} s_1^2 = s_{11} & s_{12} \\ s_{21} & s_2^2 = s_{22} \end{bmatrix} \approx \begin{bmatrix} 23.09091 & 16.45455 \\ 16.45455 & 21.09091 \end{bmatrix}$$
  
using  $s_{ij} = \frac{\sum_{k=1}^{n} (x_{ik} - \overline{x}_i)(x_{jk} - \overline{x}_j)}{n-1}$  and  $\overline{x}_i = \frac{\sum_{k=1}^{n} x_{ik}}{n}$ 

• 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%.



• 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 most of the varability (most of the total variance).

$$\begin{cases} Y_1 = e_{11} X_1 + e_{12} X_2 \\ Y_2 = e_{21} X_1 + e_{22} X_2 \end{cases} \text{ and } \begin{cases} s_{Y_1}^2 = e_{11}^2 s_{11} + e_{12}^2 s_{22} + 2 e_{11} e_{12} s_{12} \\ s_{Y_2}^2 = e_{21}^2 s_{11} + e_{22}^2 s_{22} + 2 e_{21} e_{22} s_{12} \end{cases}$$

As it is obvious, if we multiply all the coefficients  $e_{ij}$  by a constant k > 1,  $s_{Y_1}^2$  and  $s_{Y_2}^2$  will increase (and if k < 1 both will decrease). So to keep the scale constant, we need to introduce a scale constraint before maximizing. The constraint is  $e_{i1}^2 + e_{i2}^2 = 1$ .

- 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.

The problem:  $max s_{Y_1}^2$  subject to  $e_{i1}^2 + e_{i2}^2 = 1$ .

We need to maximize the Lagrangean function  $L = e_{11}^2 s_{11} + e_{12}^2 s_{22} + 2 e_{11} e_{12} s_{12} - \lambda (e_{11}^2 + e_{12}^2 - 1)$  in order to  $e_{11}$ ,  $e_{12}$  and  $\lambda$  $\begin{cases} \frac{\partial L}{\partial e_{11}} = 2 e_{11} s_{11} + 2 e_{12} s_{12} - 2\lambda e_{11} \\\\ \frac{\partial L}{\partial e_{12}} = 2 e_{12} s_{22} + 2 e_{11} s_{12} - 2\lambda e_{12} \\\\ \frac{\partial L}{\partial \lambda} = -(e_{11}^2 + e_{12}^2 - 1) \end{cases}$  $e_{11}s_{11} + e_{12}s_{12} - \lambda e_{11} = 0$ and then we must solve the system  $\begin{cases} e_{12} s_{22} + e_{11} s_{12} - \lambda e_{12} = 0\\ -(e_{11}^2 + e_{12}^2 - 1) = 0 \end{cases}$ 

Using some matricial notation and defining  $\mathbf{e}_1 = \begin{bmatrix} e_{11} \\ e_{12} \end{bmatrix}$ ,  $\mathbf{0} = \begin{bmatrix} 0 \\ 0 \end{bmatrix}$ , I as the identity matrix (size 2) and  $S = \begin{bmatrix} s_{11} & s_{12} \\ s_{21} & s_{22} \end{bmatrix}$  with  $s_{12} = s_{21}$  we get  $Y_1 = \mathbf{e}_1^T X \qquad s_{Y_1}^2 = \mathbf{e}_1^T S \mathbf{e}_1 \qquad \mathbf{e}_1^T \mathbf{e}_1 = \mathbf{e}_{11}^2 + \mathbf{e}_{12}^2$ 

and se can rewrite the problem as

 $\max L = \mathbf{e}_1^T S \mathbf{e}_1 - \lambda \left( \mathbf{e}_1^T I \mathbf{e}_1 - 1 \right) = \mathbf{e}_1^T S \mathbf{e}_1 - \lambda \left( \mathbf{e}_1^T \mathbf{e}_1 - 1 \right)$ 



PCA – A simple example (cont)

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

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 without matrix notation). This is a well known problem in linear algebra: Finding the eigenvalues and the eigenvectors of matrix *S* 

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 $\ensuremath{\mathsf{PCA}}$  – 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.,  $|S - \lambda I| = 0$ , to get a relevant solution.

This equation is a polynomial of order k (the number of original variables) and therefore has k roots (the eigenvalues of S),  $\lambda_1 \ge \lambda_2 \ge L \ge \lambda_k > 0$ , as S is positive definite matrix (assuming that none of the variables is a linear combination of the others).

For each root  $\lambda_i$  we get the corresponding eigenvector,  $\mathbf{e}_i$ , 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

$$\begin{cases} (S - \lambda_1 I) \mathbf{e}_1 = \mathbf{0} \\ \mathbf{e}_1^T \mathbf{e}_1 = 1 \end{cases}$$

Pre-multiplying the first equation by  $\mathbf{e}_1^T$  originates

$$\mathbf{e}_{1}^{T}(S - \lambda_{1}I)\mathbf{e}_{1} = \mathbf{e}_{1}^{T}\mathbf{0} \Leftrightarrow \mathbf{e}_{1}^{T}S\mathbf{e}_{1} - \mathbf{e}_{1}^{T}\lambda_{1}I\mathbf{e}_{1} = \mathbf{0} \Leftrightarrow \mathbf{e}_{1}^{T}S\mathbf{e}_{1} = \lambda_{1}\mathbf{e}_{1}^{T}\mathbf{e}_{1} = \lambda_{1}$$
  
as  $\mathbf{e}_{1}^{T}\mathbf{e}_{1} = 1$ .

We get  $\mathbf{e}_1^T S \mathbf{e}_1 = \lambda_1$  (remember that  $s_{Y_1}^2 = \mathbf{e}_1^T S \mathbf{e}_1$ ) 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.



Back to our simple example we define the polynomial as

$$\begin{vmatrix} 23.09091 - \lambda & 16.45455 \\ 16.45455 & 21.09091 - \lambda \end{vmatrix} = 0 \Leftrightarrow (23.09091 - \lambda)(21.09091 - \lambda) - 16.45455^2 = 0 \\ \Leftrightarrow \lambda^2 - 44.18182 \lambda + 216.2561 = 0 \\ \lambda = \frac{44.182 \pm \sqrt{44.182^2 - 4 \times 216.245}}{2}, \text{ i.e., } \lambda_1 = 38.57582 \text{ and } \lambda_2 = 5.606001. \end{aligned}$$

The corresponding eigenvectors are given by

$$\begin{cases} (23.09091 - \lambda_i) e_{i1} + 16.45455 e_{i2} = 0 \\ e_{i1}^2 + e_{i2}^2 = 1 \end{cases} \Leftrightarrow \begin{cases} e_{i1}^2 = \frac{1}{1 + \left(\frac{23.09091 - \lambda_i}{16.45455}\right)^2} \\ e_{i2} = -\left(\frac{23.09091 - \lambda_i}{16.45455}\right) e_{i1} \end{cases}$$



For each eigenvalue we can choose the positive or the negative root to define  $e_{i1}$  as the results are equivalent.

 $1^{st}$  eigenvalue  $\rightarrow \lambda_1 = 38.57582$  (87.31% of total variance)

 $e_1^T = [0.722388 0.685324]$  positive root or

 $e_1^T = [-0.722388 - 0.685324]$  negative root

 $2^{nd}$  eigenvalue  $\rightarrow \lambda_2 = 5.606001$  (12.69% of total variance)

 $e_2^T = [0.685324 - 0.722388]$  positive root or

 $e_2^T = [-0.685324 \quad 0.722388]$  negative root

To get the solution obtained using R, let us choose the negative root for the  $1^{st}$  eigen value and the positive root for the  $2^{nd}$  eigen value



At this stage step 1 is solved and the principal components (the linear combinations of the original variables  $X_1$  and  $X_2$ ) are found.

For observation *i* we get

$$\begin{bmatrix} Y_{1i} \\ Y_{2i} \end{bmatrix} = \begin{bmatrix} e_{11} & e_{12} \\ e_{21} & e_{22} \end{bmatrix} \begin{bmatrix} X_{1i} \\ X_{2i} \end{bmatrix} = \begin{bmatrix} -0.722388 & -0.685324 \\ 0.685324 & -0.728238 \end{bmatrix} \begin{bmatrix} X_{1i} \\ X_{2i} \end{bmatrix}$$

$$\begin{cases} Y_{1i} = -0.722388 X_{1i} - 0.685324 X_{2i} \\ Y_{2i} = & 0.685324 X_{1i} - 0.722388 X_{2i} \end{cases}$$

Instead of representing (plotting) each observation using the original variables  $(X_1 \text{ and } X_2)$  we can use the principal components ( $\mathbf{e}_1$  and  $\mathbf{e}_2$ ) as the new coordinates.

PCA – A simple example (cont)



- 1<sup>st</sup> panel: observations (a to I), centering effect (dashed lines) and PC (red)
- 2<sup>nd</sup> 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 loadings is the correlation coefficient between each PC and each original variable  $l_{ij} = \frac{W_{ij}}{s_j} \sqrt{\lambda_i}$  where  $l_{ij}$  stand for the loading of the jth variable on PC<sub>i</sub>,  $w_{ij}$  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:

```
> x1=c(16,12,13,11,10,9,8,7,5,3,2,0)
> x^2=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(x1c)-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
                 [,2]
           [, 1]
[1,] -0.7282381 0.6853242
```

```
[2,] -0.6853242 -0.7282381
```

```
> cbind(out$values[1]/sum(out$values),out$values[2]/sum(out$values))
          [,1] [,2]
[1,] 0.8731151 0.1268849
>
> ### Using prcomp function (other solutions are available in R)
> out1=prcomp(x,center=T)
> out1 # eigenvalues are the squares of st. dev.
Standard deviations (1, ..., p=2):
[1] 6.210943 2.367700
Rotation (n \times k) = (2 \times 2):
          PC1
                     PC2
x1 -0.7282381 0.6853242
x2 -0.6853242 -0.7282381
> summary(out1)
Importance of components:
                          PC1
                                 PC2
Standard deviation 6.2109 2.3677
Proportion of Variance 0.8731 0.1269
Cumulative Proportion 0.8731 1.0000
```

> out1\$x # scores PC2 PC1 [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 > outl\$rotation # weights, eigen vectors PC2 PC1 x1 -0.7282381 0.6853242 x2 -0.6853242 -0.7282381

or, using the formula, 
$$l_{ij} = \frac{W_{ij}}{S_j} \sqrt{\lambda_i}$$

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

## • First step $\rightarrow$ reading the data set

> (	dta=read.csv("B	E:/Ris]	k Models	s 2018	B/food pi	rice	<pre>index.csv",header=T,sep=",")</pre>
> (	dta # Checł	k input	L L				
	City	Bread	Burger	Milk	Oranges	Toma	toes
1	Atlanta	24.5	94.5	73.9	80.1		41.6
2	Baltimore	26.5	91.0	67.5	74.6		53.3
3	Boston	29.7	100.8	61.4	104.0		59.6
4	Buffalo	22.8	86.6	65.3	118.4		51.2
5	Chicago	26.7	86.7	62.7	105.9		51.2
6	Cincinnati	25.3	102.5	63.3	99.3		45.6
7	Cleveland	22.8	88.8	52.4	110.9		46.8
8	Dallas	23.3	85.5	62.5	117.9		41.8
9	Detroit	24.1	93.7	51.5	109.7		52.4
10	Honolulu	29.3	105.9	80.2	133.2		61.7
11	Houston	22.3	83.6	67.8	108.6		42.4
12	Kansas City	26.1	88.9	65.4	100.9		43.2
13	Los Angeles	26.9	89.3	56.2	82.7		38.4
14	Milwaukee	20.3	89.6	53.8	111.8		53.9
15	Minneapolis	24.6	92.2	51.9	106.0		50.7
16	New York	30.8	110.7	66.0	107.3		62.6
17	Philadelphia	24.5	92.3	66.7	98.0		61.7
18	Pittsburgh	26.2	95.4	60.2	117.1		49.3
19	St. Louis	26.5	92.4	60.8	115.1		46.2
20	San Diego	25.5	83.7	57.0	92.8		35.4
21	San Francisco	26.3	87.1	58.3	101.8		41.5
22	Seattle	22.5	77.7	62.0	91.1		44.9
23	Washington DC	24.2	93.8	66.0	81.6		46.2

• Second step  $\rightarrow$  PCA using prcomp function (other solutions are available)

```
> attach(dta)
> x=cbind(Bread,Burger,Milk,Oranges,Tomatoes)
> out1=prcomp(x, center=T)
> out1
Standard deviations:
[1] 14.798604 9.577221 6.136994 4.561857 1.740468
Rotation:
               PC1
                          PC2
                                      PC3
                                                  PC4
                                                             PC5
        0.02848905 0.1653211 -0.02135748 0.18972574 -0.96716354
Bread
Burger
       0.20012240 0.6321849 -0.25420475 0.65862454 0.24877074
        0.04167230 0.4421503 0.88874949 -0.10765906 0.03606094
Milk
Oranges 0.93885906 -0.3143547 0.12135003 0.06904699 -0.01521357
Tomatoes 0.27558389 0.5279160 -0.36100184 -0.71684022 -0.03429221
> summary(out1)
Importance of components:
                                       PC3
                          PC1
                                 PC2
                                                PC4
                                                       PC5
Standard deviation
                     14.7986 9.5772 6.1370 4.56186 1.74047
Proportion of Variance 0.5884 0.2464 0.1012 0.05591 0.00814
Cumulative 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 standard 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 a priori weight to each variable or not. If so, scale the variables.

To use scaled variables we can scale them before performing PCA or just replace out1=prcomp(x,center=T) by out1=prcomp(x,center=T,scale=T)

```
> out2=prcomp(x, center=T,scale=T)
```

> out2

Standard deviations:

[1] 1.5564279 1.0510352 0.8593489 0.7025748 0.4906784

Rotation:

	PC1	PC2	2	PC3	E	PC4	PC5	
Bread	0.4961487	-0.30861972	2 0.38	639398	0.509304	159 -0.49	99898868	
Burger	0.5757023	-0.0438017	6 0.262	247227	-0.028137	712 0.77	72635014	
Milk	0.3395696	-0.4308090	5 -0.83	463952	0.049100	0.00	7882237	
Oranges	0.2249898	0.7967769	4 -0.293	160659	0.479015	574 -0.00	)5966796	
Tomatoes	0.5064340	0.2870284	6 0.012	226602 ·	-0.712706	529 -0.39	91201387	
> summary	> summary(out2)							
Importanc	Importance of components:							
		PC1	PC2	PC3	PC4	PC5		
Standard	deviation	1.5564	1.0510	0.8593	0.70257	0.49068		
Proportio	on of Varia	ance 0.4845	0.2209	0.1477	0.09872	0.04815		
Cumulativ	ve Proporti	on 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 much more weight to Oranges than to the other food 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 immediately 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.



- Kaiser criterion:
  - Scaled data: retain the first 2 PC (remember that the eigenvalues are the square of the standard deviation of the principal components
  - $\,\circ\,$  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
```



• 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

• 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 100 iterations, using the mean estimate

Component	Adjusted	Unadjusted	Estimated
	Eigenvalue	Eigenvalue	Bias
1	1.791788	2.422467	0.630679

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



Parallel Analysis

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#### 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.



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

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.



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

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).



