# Lecture 13: Principal component and factor analyses

IST5573

統計方法 Statistical methods

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# Aspects of multivariate analysis

- Data include simultaneous measurements on many variables- multivariate analysis
- Multivariate methods include the following:
  1. Hypothesis construction and testing
  2. Investigation of the dependence among variables
  3. Data reduction or structure simplification (principal component and factor analysis)
  4. Sorting and grouping (clustering)
  5. Prediction (classification)

# PIXNET Hackathon 開放資料

https://developer.pixnet.pro/#!/doc/pixnetOpenData/index

## Datasets

### 1. 分類熱門照片（含 EXIF）

下載連結：JSON format | CSV format

資料格式：

ZIP 檔案內有 24 個 JSON 檔案，檔案名稱為 "相簿分類 ID"，分類名稱請參考頁面上方「資料使用須知」。所有的資料一定有 EXIF 與位置資訊。

### 2. 去識別化後的照片 EXIF 資訊

下載連結：JSON format | CSV format

資料格式：

ZIP 檔案內有 5 個 JSON 檔案，檔案名稱為 YYYY-W.json，每個檔案內含一週的資料，分類名稱請參考頁面上方「資料使用須知」。所有的資料一定有 EXIF 欄位。

### 3. 分類人氣部落格相關資料

下載連結：JSON format | CSV format

資料格式：

ZIP 檔案內有 41 個 JSON 檔案，檔案名稱為 "部落格分類ID"。部落格分類名稱請參考頁面上方「資料使用須知」。

### 4. 去識別化後的部落格訪客資料

下載連結：JSON format | CSV format

資料格式：

ZIP 檔案內有 1 個 JSON 檔案，檔案名稱為 `YYYY-mm.json`，表示該月份的訪客資訊。部落格文章分類名稱請參考頁面上方「資料使用須知」。

# Principal component analysis

# Principal component analysis (PCA)

- A PCA is concerned with explaining the variance-covariance structure of a set of variables through a few “linear” combinations of these variables.
- Objectives of a PCA:
  - data reduction: the total variability of $p$ variables can be accounted for by $k$ principle components, where $p>k$.
  - interpretation: can reveal relationship that were not previously suspected.

# PCA

- Principle components depend solely on the covariance matrix.
- Development of principle components dose **NOT** require a multivariate normal assumption.
- However, a multivariate normal assumption is useful for inference of the principle components.

# Principal components (PCs)

- Observed data: $\boldsymbol{X} = (X_1, X_2, \cdots, X_p)$
- $$\begin{aligned} Y_1 &= a_{11}X_1 + a_{12}X_2 + \cdots + a_{1p}X_p \\ Y_2 &= a_{21}X_1 + a_{22}X_2 + \cdots + a_{2p}X_p \\ &\vdots \\ Y_k &= a_{k1}X_1 + a_{k2}X_2 + \cdots + a_{kp}X_p \end{aligned}$$
- $k < p$

# PCs

- Find $a_{11}, a_{12}, \cdots, a_{1p}$ such that $\mathrm{Var}(Y_1)$ has the maximum variance among all linear combination of $\boldsymbol{X} \rightarrow Y_1$ is the 1st principal component
- Find $a_{21}, a_{22}, \cdots, a_{2p}$ such that $\mathrm{Var}(Y_2)$ has the maximum variance among all linear combination of $\boldsymbol{X}$ with $\mathrm{Cov}(Y_1, Y_2) = 0 \rightarrow Y_2$ is the 2nd principal component
- Find $a_{k1}, a_{k2}, \cdots, a_{kp}$ such that $\mathrm{Var}(Y_k)$ has the maximum variance among all linear combination of $\boldsymbol{X}$ with $\mathrm{Cov}(Y_i, Y_k) = 0\ \forall i < k \rightarrow Y_k$ is the *k*th principal component

# PCs (cont'd)

- $\mathrm{Var}(Y_1)$ = the largest eigenvalue of the covariance matrix $\mathrm{Cov}(\boldsymbol{X})$, and $(a_{11}, a_{12}, \cdots, a_{1p})$ is its corresponding eigenvector
- $\mathrm{Var}(Y_2)$ = the 2nd largest eigenvalue of the covariance matrix $\mathrm{Cov}(\boldsymbol{X})$, and $(a_{21}, a_{22}, \cdots, a_{2p})$ is its corresponding eigenvector
- $\mathrm{Var}(Y_k)$ = the *k*th largest eigenvalue of the covariance matrix $\mathrm{Cov}(\boldsymbol{X})$, and $(a_{k1}, a_{k2}, \cdots, a_{kp})$ is its corresponding eigenvector

# 分類熱門照片

| | A | B | C | D | E | F | G | H | I |
|---|---|---|---|---|---|---|---|---|---|
| 1 | 類別 | ISO | 光圈 | 快門 | 焦距 | 相機型號 | 上傳時間 | 累計人氣 | |
| 2 | 1 | 50 | 2.4 | 0.042 | 3 | 1 | 13.88202186 | 3876 | |
| 3 | 1 | 80 | 2.4 | 0.042 | 3 | 1 | 13.88202189 | 1650 | |
| 4 | 1 | 75 | 2.8 | 0.042 | 3 | 1 | 12.55760815 | 1184 | |
| 5 | 1 | 640 | 2.4 | 0.067 | 4 | 1 | 13.52986414 | 1178 | |
| 6 | 1 | 71 | 2.8 | 0.042 | 3 | 1 | 12.55760838 | 957 | |
| 7 | 1 | 73 | 2.8 | 0.059 | 3 | 1 | 12.55760834 | 913 | |
| 8 | 1 | 72 | 2.8 | 0.059 | 3 | 1 | 12.55760825 | 825 | |
| 9 | 1 | 74 | 2.8 | 0.05 | 3 | 1 | 12.5576083 | 805 | |
| 10 | 1 | 72 | 2.8 | 0.033 | 3 | 1 | 12.55760819 | 778 | |
| 11 | 1 | 1000 | 3.5 | 0.02 | 18 | 2 | 13.02962592 | 708 | |
| 12 | 1 | 79 | 2.8 | 0.05 | 3 | 1 | 12.65794278 | 594 | |
| 13 | 1 | 86 | 2.8 | 0.067 | 3 | 1 | 12.65794276 | 568 | |
| 14 | 1 | 220 | 2.8 | 0.067 | 3 | 1 | 12.65794273 | 405 | |
| 15 | 1 | 80 | 2.8 | 0.033 | 3 | 1 | 12.65794275 | 388 | |
| 16 | 1 | 1016 | 2.8 | 0.1 | 3 | 1 | 12.79276768 | 385 | |
| 17 | 1 | 640 | 2.8 | 0 | 28 | 2 | 12.55523557 | 358 | |

(RMD_example 13.1)

| Variable | Description |
|---|---|
| 類別 | 1=女生個人, 2=男生個人 |
| ISO | 照片的感光度，數值越高，對光越敏感 |
| 光圈 | 光圈值 |
| 快門 | 快門速度 (秒) |
| 焦距 | 毫米 (mm) |
| 相機型號 | 0, 1, 2 |
| 上傳時間 | UNIX 時間戳，與1970年1月1日00:00:00的秒差$\times 10^{-8}$ |
| 累計人氣 | Hits |

# 分類熱門照片 PC loadings

- $Y_1 = 0.97(\mathrm{ISO}) - 0.00015(\text{光圈}) + 0.000019(\text{快門}) + 0.000083(\text{焦距}) + 0.000001(\text{相機型號}) + 0.24(\text{上傳時間}) - 0.0095(\text{累積人氣})$
- $Y_2 = -0.24(\mathrm{ISO}) - 0.00040(\text{光圈}) - 0.000015(\text{快門}) - 0.00099(\text{焦距}) + 0.000035(\text{相機型號}) + 0.97(\text{上傳時間}) - 0.0070(\text{累積人氣})$

# PC loadings

Loadings:

| | Comp.1 | Comp.2 | Comp.3 | Comp.4 | Comp.5 |
|---|---|---|---|---|---|
| ISO | 0.9711254 | -0.2384491 | 0.0075776 | 0.0003176 | -0.0000632 |
| 光圈 | -0.0001543 | -0.0003978 | -0.0000032 | -0.0276181 | -0.9981672 |
| 快門 | 0.0000192 | -0.0000153 | 0.0000031 | 0.0006682 | -0.0038335 |
| 焦距 | 0.0000832 | -0.0009911 | 0.0002883 | -0.9996118 | 0.0273896 |
| 相機型號 | 0.0000015 | 0.0000354 | 0.0001029 | -0.0034608 | 0.0538259 |
| 上傳時間 | 0.2383799 | 0.9711294 | 0.0090343 | -0.0009512 | -0.0003986 |
| 累計人氣 | -0.0095131 | -0.0069668 | 0.9999304 | 0.0002946 | -0.0000126 |

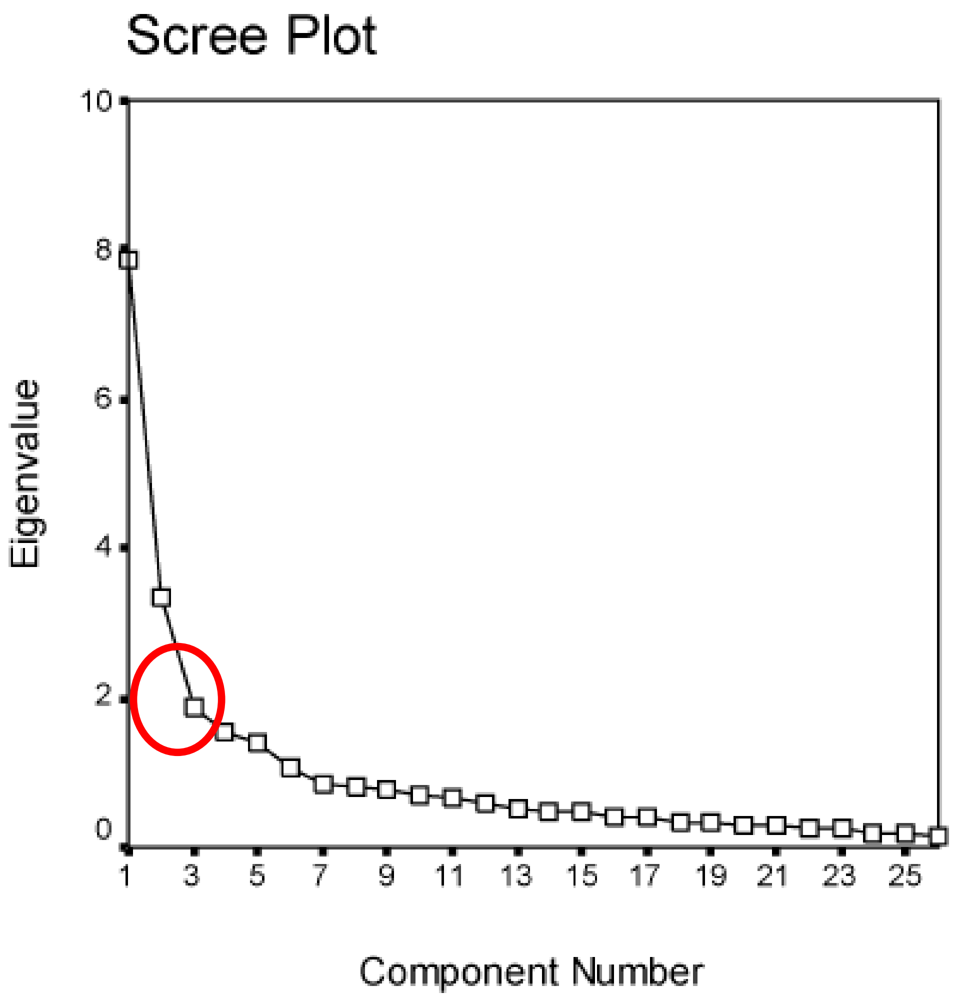
| | Comp.6 | Comp.7 |
|---|---|---|
| ISO | 0.0000109 | 0.0000227 |
| 光圈 | 0.0537373 | 0.0034113 |
| 快門 | -0.0073856 | -0.9999652 |
| 焦距 | -0.0049467 | -0.0007364 |
| 相機型號 | 0.9985155 | -0.0075836 |
| 上傳時間 | -0.0000176 | -0.0000093 |
| 累計人氣 | -0.0001011 | 0.0000040 |

(RMD_example 13.2)

# The number of PCs

- The amount of total variance explained
  - If most (e.g., 80% to 90%) of the total population variance can be explained by the first $k$ principle components ($k<p$), then these $k$ principle components can replace the original $p$ variables without much loss of information (total variance).
- The relative size of eigenvalues (variances)
  - Scree plot
- Subject-matter interpretation of the components

# Scree plot



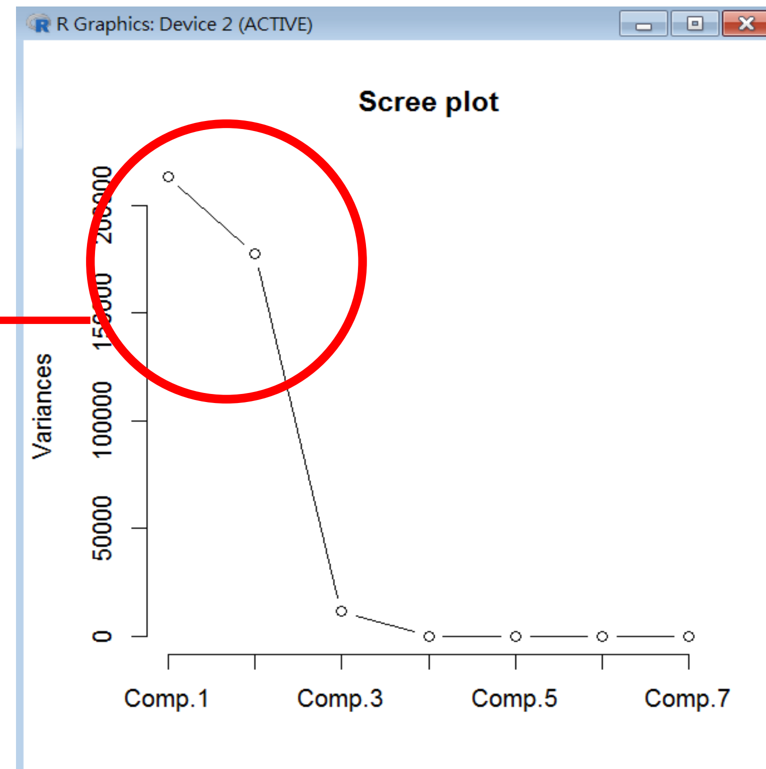

- The point at which the remaining eigenvalues are relatively small and all about the same size (an elbow (bend) in the scree plot).
- In the above plot, an elbow occurs at about $k$=3 → choose **TWO** principle components.

# 分類熱門照片:# of PCS

```
Importance of components:
                           Comp.1      Comp.2       Comp.3       Comp.4
Standard deviation     461.89174 421.5308688 106.98632088 5.857071e+00
Proportion of Variance   0.53003   0.4414473   0.02843653 8.522776e-05
Cumulative Proportion    0.53003   0.9714774   0.99991388 9.999991e-01
                             Comp.5       Comp.6       Comp.7
Standard deviation     5.228968e-01 2.88975e-01 3.199553e-02
Proportion of Variance 6.792850e-07 2.07463e-07 2.543307e-09
Cumulative Proportion  9.999998e-01 1.00000e+00 1.000000e+00
```

2 PCs with the amount of total variance explained > 90%

Scree plot with an elbow occurs at about *k*=3



# PCA from standardized variables

- Variables should probably be standardized if they are measures on scales with widely differing ranges.
- Example:

  $X_1$: annual sales in the \$10,000 to \$350,000 range

  $X_2$: the ratio (net annual income/total assets) that falls in the 0.01 to 0.6 range

  - No standardization: the 1st principle component will have a heavy weighting of $X_1$
  - Standardization: $X_2$ will play a larger role

# PCA from standardized variables

- Standardizing observed data:
  $Z_1 = \frac{X_1 - \mu_1}{\sigma_1}, Z_2 = \frac{X_2 - \mu_2}{\sigma_2}, \cdots$

- $$\begin{gathered} W_1 = b_{11}Z_1 + b_{12}Z_2 + \cdots + b_{1p}Z_p \\ W_2 = b_{21}Z_1 + b_{22}Z_2 + \cdots + b_{2p}Z_p \\ \vdots \\ W_k = b_{k1}Z_1 + b_{k2}Z_2 + \cdots + b_{kp}Z_p \end{gathered}$$

# PCA from standardized variables

- $\mathrm{Var}(W_1)$ = the largest eigenvalue of the correlation matrix $\mathrm{Cor}(\boldsymbol{X})$, and $(b_{11}, b_{12}, \cdots, b_{1p})$ is its corresponding eigenvector
- $\mathrm{Var}(W_2)$ = the 2nd largest eigenvalue of the correlation matrix $\mathrm{Cor}(\boldsymbol{X})$, and $(b_{21}, b_{22}, \cdots, b_{2p})$ is its corresponding eigenvector
- $\mathrm{Var}(W_k)$ = the $k$th largest eigenvalue of the correlation matrix $\mathrm{Cor}(\boldsymbol{X})$, and $(b_{k1}, b_{k2}, \cdots, b_{kp})$ is its corresponding eigenvector

# 分類熱門照片 standardized PCs

```
Importance of components:
                          Comp.1    Comp.2    Comp.3    Comp.4    Comp.5
Standard deviation     1.2154626 1.1551005 1.0297473 1.0079490 0.9408723
Proportion of Variance 0.2110499 0.1906082 0.1514828 0.1451373 0.1264630
Cumulative Proportion  0.2110499 0.4016581 0.5531409 0.6982782 0.8247412
                           Comp.6    Comp.7
Standard deviation     0.80580979 0.7599227
Proportion of Variance 0.09276134 0.0824975
Cumulative Proportion  0.91750250 1.0000000
```

```
Loadings:
        Comp.1     Comp.2     Comp.3     Comp.4     Comp.5
ISO     -0.0714726  0.6044901  0.4736265 -0.0812640 -0.1886824
光圈     0.6778339 -0.0083201 -0.0088570 -0.0707311 -0.0199902
快門     0.0633094  0.7067502  0.0454794  0.1313349  0.1457447
焦距     0.4731235 -0.1996835  0.4939576 -0.2235479 -0.4076155
相機型號 -0.0770545 -0.2603461  0.6730539  0.2121282  0.6414747
上傳時間 -0.5454875 -0.1516771  0.2716848 -0.1781902 -0.4716178
累計人氣  0.0639136 -0.0660834  0.0521810  0.9189236 -0.3777491
        Comp.6     Comp.7
ISO     -0.5171128 -0.3091128
光圈     0.3044372 -0.6650632
快門     0.5993112  0.3110681
焦距     0.0236462  0.5249793
相機型號  0.1026508 -0.0790929
上傳時間  0.5186529 -0.2871392
累計人氣 -0.0253233 -0.0326948
```

5 PCs

(RMD_example 13.3)

# Factor analysis

# Factor analysis

- The purpose of factor analysis is to describe the covariance relationships among many variables in terms of a few underlying, but unobservable, random quantities call factors.
- Factor analysis is motivated by
  - variables can be grouped by their correlation
  - all variables within a particular group are highly correlated among themselves
  - variables have relatively small correlations with variables in a different group

# Orthogonal factor model

- Observed data: $\boldsymbol{X} = (X_1, X_2, \cdots, X_p)$
- $X_1, X_2, \cdots, X_p$ are linearly dependent on a few unobservable random variables $F_1, F_2, \cdots, F_m$ (common factor)
- $p > m$

- $$\begin{aligned} X_1 - \mu_1 &= \ell_{11}F_1 + \ell_{12}F_2 + \cdots + \ell_{1m}F_m + \varepsilon_1 \\ X_2 - \mu_2 &= \ell_{21}F_1 + \ell_{22}F_2 + \cdots + \ell_{2m}F_m + \varepsilon_2 \\ &\vdots \\ X_p - \mu_p &= \ell_{p1}F_1 + \ell_{p2}F_2 + \cdots + \ell_{pm}F_p + \varepsilon_p \end{aligned}$$

  (in a matrix fom: $\boldsymbol{X} - \boldsymbol{\mu} = \boldsymbol{LF} + \boldsymbol{\varepsilon}$)

  $\mu_i$ = mean of variable *i*

  $\varepsilon_i$ = *i*th error

  $F_j$ = *j*th common factor

  $\ell_{ij}$ = loading of the *i*th variable on the *j*th factor
- Unobservable random vectors $F_j$'s and $\varepsilon_i$'s are mutually independent

# 分類熱門照片 ：factor analysis

```
Uniquenesses:
      ISO      光圈      快門      焦距   相機型號   上傳時間   累計人氣
0.0912872 0.4054439 0.7589743 0.6987590 0.9552639 0.7812365 0.9982685

Loadings:
         Factor1    Factor2    Factor3
ISO       0.9531224  0.0108353  0.0123782
光圈      -0.0684252  0.7676951 -0.0227622
快門       0.3126406  0.0768856 -0.3706365
焦距       0.0137846  0.4001137  0.3754566
相機型號  -0.0113459 -0.0559101  0.2036606
上傳時間   0.0454631 -0.3968105  0.2433759
累計人氣  -0.0336443  0.0209563 -0.0131131

                Factor1   Factor2   Factor3
SS loadings    1.0143859 0.9164991 0.3798918
Proportion Var 0.1449123 0.1309284 0.0542703
Cumulative Var 0.1449123 0.2758407 0.3301110
```

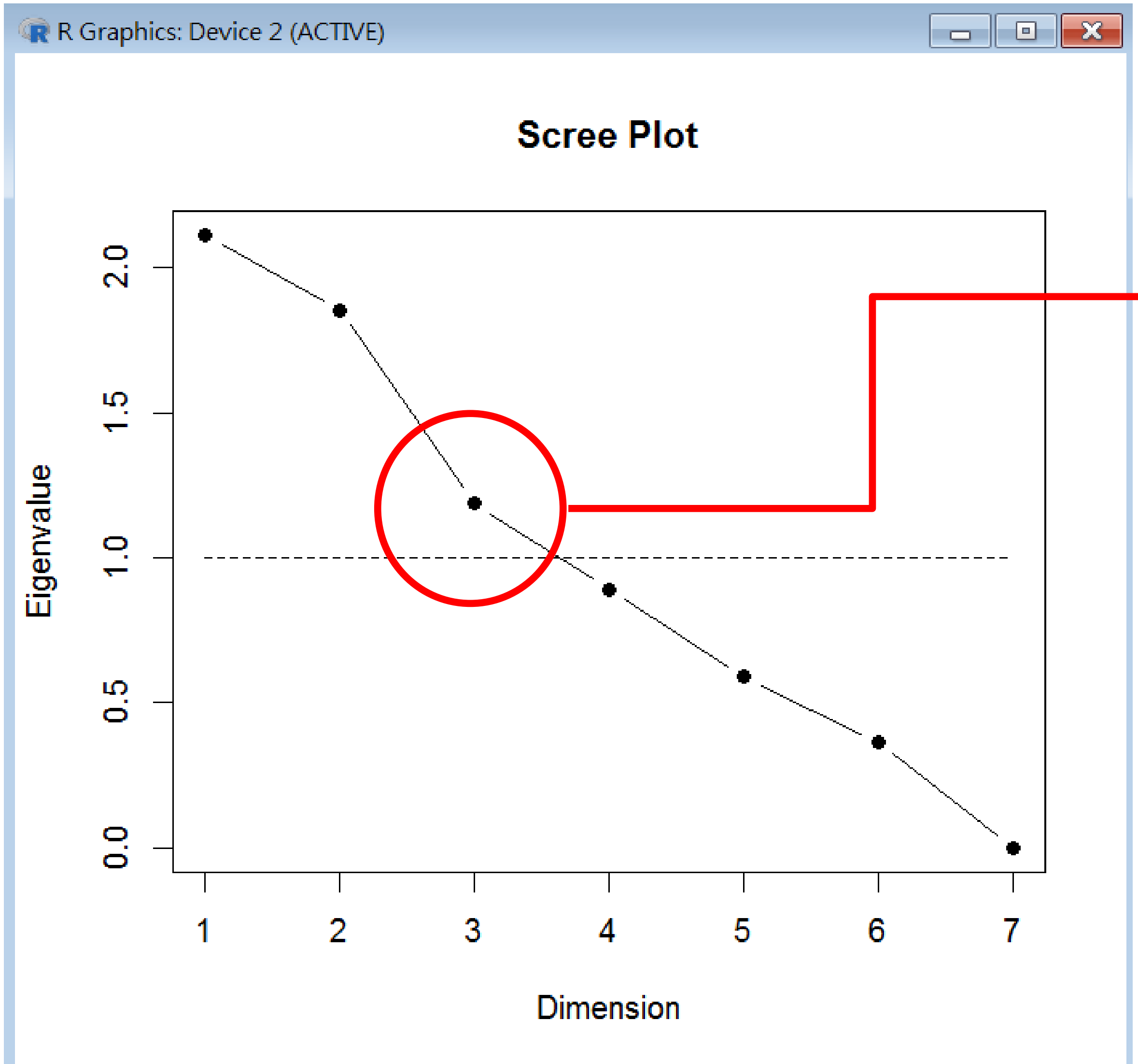
Factor loadings

(RMD_example 13.4)

# The number of factors

- Use criteria similar to those used in PCA
  - The amount of total variance explained until a suitable proportion
  - The relative size of eigenvalues (variances): scree plot of **the correlation matrix**
  - Set $m$ equal to **the number of eigenvalues of the correlation matrix greater than one**
  - Subject-matter interpretation of the factors

# 分類熱門照片：# of factors




The number of eigenvalues of the correlation matrix greater than one = 3

# Factor rotation

- Factor loadings $\boldsymbol{L}$ are determined only up to an orthogonal matrix $\boldsymbol{T}$ ($\boldsymbol{T}\boldsymbol{T}' = \boldsymbol{T}'\boldsymbol{T} = \boldsymbol{I}$):

$$\boldsymbol{X} - \boldsymbol{\mu} = \boldsymbol{L}\boldsymbol{F} + \boldsymbol{\varepsilon} = \boldsymbol{L}(\boldsymbol{T}\boldsymbol{T}')\boldsymbol{F} + \boldsymbol{\varepsilon} = \boldsymbol{L}^*\boldsymbol{F}^* + \boldsymbol{\varepsilon}$$

- $\boldsymbol{L}^* = \boldsymbol{L}\boldsymbol{T}$ (rotated loadings)

  $\boldsymbol{F}^* = \boldsymbol{T}'\boldsymbol{F}$ (rotated factors)

# Why factor rotation?

- Original loadings may not be readily interpretable, usual rotate them until a simpler structure is achieved.
- Ideally, we like to see a pattern of loadings such that each variable loads highly on a single factor and has small loadings on the remaining factors:

$$X_1 - \mu_1 = \underbrace{\ell_{11}}_{\text{large}} F_1 + \underbrace{\ell_{12}}_{\text{small}} F_2 + \cdots + \underbrace{\ell_{1m}}_{\text{small}} F_m + \varepsilon_1$$

$$X_2 - \mu_2 = \underbrace{\ell_{21}}_{\text{small}} F_1 + \underbrace{\ell_{22}}_{\text{large}} F_2 + \cdots + \underbrace{\ell_{2m}}_{\text{small}} F_m + \varepsilon_1$$

$$\vdots$$

$$X_p - \mu_p = \underbrace{\ell_{p1}}_{\text{small}} F_1 + \underbrace{\ell_{p2}}_{\text{small}} F_2 + \cdots + \underbrace{\ell_{pm}}_{\text{large}} F_p + \varepsilon_p$$

# Methods of factor rotation

- Varimax rotations
  - Select the orthogonal transformation $\boldsymbol{T}$ that maximizes the spreading out of the squares of the loadings in each factor.
  - We hope to find groups of large and negligible coefficients in any column of $\boldsymbol{L}^*$

- Oblique (non-orthogonal) rotations
  - Many investigators in social sciences consider the rotated factors are not necessarily to be independent.
  - Orthogonal rotations- a rigid rotation of the coordinate axes (factors) such that the rotated axes pass as closely the clusters of variables as possible.
  - Oblique rotation- a nonrigid rotation such that the rotated axes (no longer perpendicular) pass through the clusters of variables.

# 分類熱門照片：
# rotated vs. unrotated loadings

```
Loadings:
         Factor1    Factor2    Factor3
ISO       0.9325038  0.0598971  0.1885787
光圈     -0.1482474  0.7303608  0.1978678
快門      0.2281710 -0.0083560  0.4346206
焦距      0.0437581  0.4850338 -0.2531325
相機型號  0.0327628 -0.0007951 -0.2089456
上傳時間  0.1299696 -0.3160405 -0.3193487
累計人氣 -0.0374397  0.0151079  0.0106340
```

Rotated (varimax)

```
Loadings:
         Factor1    Factor2    Factor3
ISO       0.9531224  0.0108353  0.0123782
光圈     -0.0684252  0.7676951 -0.0227622
快門      0.3126406  0.0768856 -0.3706365
焦距      0.0137846  0.4001137  0.3754566
相機型號 -0.0113459 -0.0559101  0.2036606
上傳時間  0.0454631 -0.3968105  0.2433759
累計人氣 -0.0336443  0.0209563 -0.0131131
```

Unrotated

(RMD_example 13.4)

# Factor scores

- Estimated values of the common factors are called factor scores.
- Factor scores can be used for diagnostic purposes and inputs to a subsequent analysis.
- Factor scores are not estimates of unknown parameters. Factor scores are estimates of unobserved random factor vectors $F_1, F_2, \cdots, F_m$.

# 分類熱門照片 ：factor scores

```
> factfit$scores
          Factor1      Factor2       Factor3
 [1,] -0.744478512 -0.4390968203 -0.2421767848
 [2,] -0.572821108 -0.5262584971 -0.4302286198
 [3,] -0.843173384  0.2953278622  0.5238103500
 [4,]  0.514612877 -0.2920302012  0.0908727086
 [5,] -0.839981043  0.2847687444  0.5027908527
 [6,] -0.847735204  0.2585411098  0.6602863806
 [7,] -0.845381209  0.2545780777  0.6522816904
 [8,] -0.832918679  0.2673538481  0.5658902695
 [9,] -0.821629459  0.2905749951  0.4021470393
[10,]  1.266750889  1.9190923884 -0.7707859163
[11,] -0.795406138  0.2283314115  0.4833648686
[12,] -0.793919006  0.2040492470  0.6437493174
[13,] -0.514118004  0.2288582020  0.6643793857
[14,] -0.769122005  0.2446826331  0.3046530819
[15,]  1.096261264  0.3261509954  1.0949048259
[16,]  0.680574299  1.7287376488 -1.5034657744
[17,] -0.458116823  0.2322163316  0.6653574986
[18,]  1.100411881  0.3207546911  1.0836600315
[19,]  1.099298921  0.3235670407  1.0895351702
[20,] -0.526639685  0.2218586079  0.6519107506
[21,] -0.066986803  0.2568968261  0.6733340165
[22,]  0.072574391 -0.3867257670 -0.0505240060
[23,] -0.003387440  0.2635979134  0.6801051329
```

Every observation (picture) has scores on all 3 factors!

# Exploratory vs. confirmatory factor analysis

- EFA is a technique within factor analysis whose goal is to identify the underlying relationships between measured variables (i.e., identifying common factors).
- It should be used when the researcher has no a priori hypothesis about factors or patterns of measured variables.

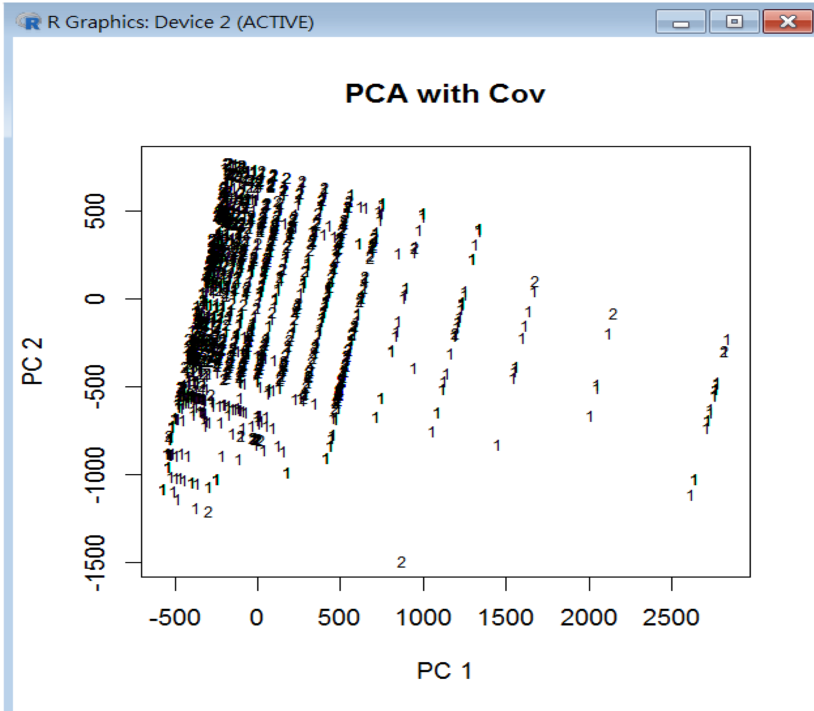
# Confirmatory factor analysis

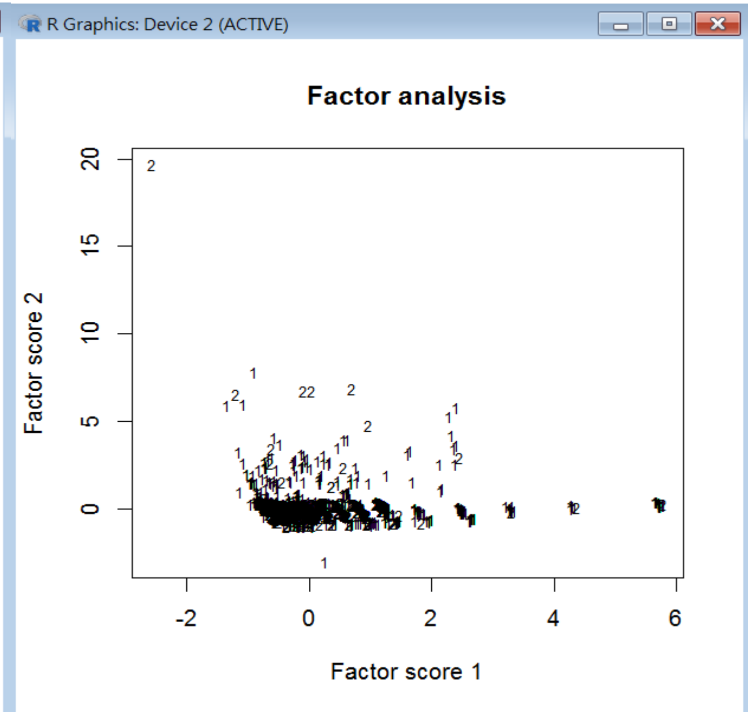
- Confirmatory factor analysis (CFA) is a special form of factor analysis, it is used to test whether measures of a construct are consistent with a researcher's understanding of the nature of that construct (or factor).

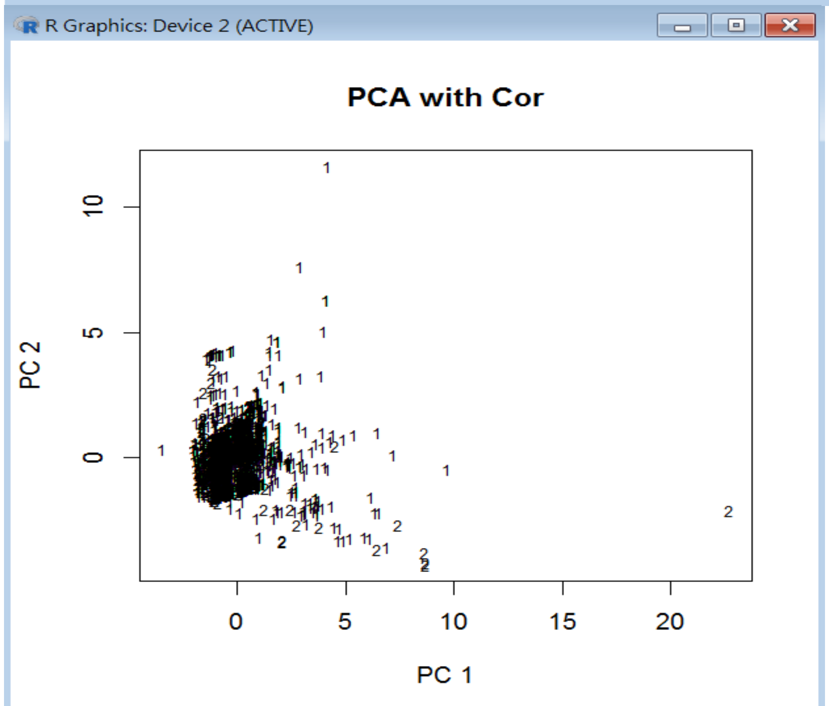
1. In CFA, first develop a hypothesis about what factors he believes are underlying the measures he has used.
2. Impose constraints (e.g., zero loadings) on the model based on these a priori hypotheses. By imposing these constraints, the researcher is forcing the model to be consistent with his theory.
3. **Model fit measures** could then be obtained to assess how well the proposed model captured the covariance between all the measures in the model.
   - If the constraints the researcher has imposed on the model are inconsistent with the sample data, then the results of statistical tests of model fit will indicate a poor fit, and the model will be rejected.

# Visualization of multivariate data

- Visualising and processing high-dimensional datasets, while still retaining as much of the variances in the data as possible.
- Can plot scores on the first two principal components or factors




# 分類熱門照片：visualization