Tut 8: PCA Dimensional Reduction

June 2023

When variances Var$(x_{\cdot j})$ for features/columns $x_{\cdot j}$ differ a lot, we need to perform scaling:

`pca$scale`: $\sqrt{\frac{\sum_i (x_{ij} - \overline{x}_{\cdot j})^2}{n-1}}$

However, you do not need to scale the data unless it is stated in the question.

Original data: X; Data shifted to centre: $\widetilde{X}$

`pca$center`: $\overline{x}_{\cdot j}$

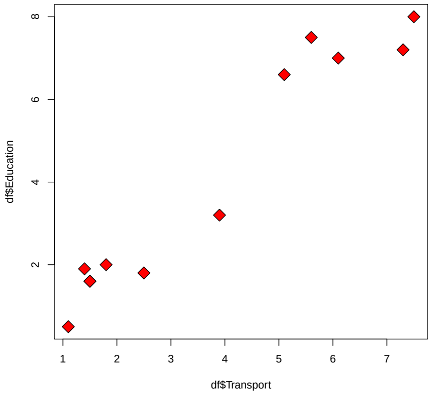
`pca$sdev`: $\sqrt{\lambda_i}$

`pca$rotation`: $[\boldsymbol{e}_1, \boldsymbol{e}_2, \cdots]$

`pca$x`: $[\widetilde{X}\boldsymbol{e}_1, \widetilde{X}\boldsymbol{e}_2, \cdots]$

1. You are given 12 communities that were rated according to transportation and education — the higher the score the better. For example, a better transportation system will score higher. Higher education facilities will score higher as well. The table below shows the score for 12 communities in the two criteria:

Obs	Transportation	Education
1	1.1	0.5
2	3.9	3.2
3	1.5	1.6
4	5.6	7.5
5	2.5	1.8
6	7.3	7.2
7	1.4	1.9
8	6.1	7.0
9	1.5	1.6
10	5.1	6.6
11	1.8	2.0
12	7.5	8.0



(a) Use a computer software (e.g. R or Excel) to plot the above scatterplot which is based on the above table.

Solution. A simple R script:

```
d.f = data.frame(
        Transport = c(1.1,3.9,1.5,5.6,2.5,7.3,1.4,6.1,1.5,5.1,1.8,7.5),
        Education = c(0.5,3.2,1.6,7.5,1.8,7.2,1.9,7.0,1.6,6.6,2.0,8.0)
)
plot(d.f$Transport,d.f$Education,type=’p’,pch=23,bg="red",cex=2)
```

□

(b) Generate two principal components for the data.

Solution. Calculating using R script:

```
Transport = c(1.1,3.9,1.5,5.6,2.5,7.3,1.4,6.1,1.5,5.1,1.8,7.5)
Education = c(0.5,3.2,1.6,7.5,1.8,7.2,1.9,7.0,1.6,6.6,2.0,8.0)
X = data.frame(Transport, Education)
PC = prcomp(X)
print(PC)
```

```
Standard deviations:
[1] 3.7504618 0.4861164

Rotation:
                PC1        PC2
Transport 0.6429319 -0.7659234
Education 0.7659234  0.6429319
```

Manual calculation:

i. Shift $\boldsymbol{X}$ to centre, i.e. find $\mu_1 = 3.775$, $\mu_2 = 4.075$ and generate table $\boldsymbol{X}^*$ below.

x_1	-2.675	0.125	-2.275	1.825	-1.275	3.525	-2.375
			2.325	-2.275	1.325	-1.975	3.725
x_2	-3.575	-0.875	-2.475	3.425	-2.275	3.125	-2.175
			2.925	-2.475	2.525	-2.075	3.925

ii. Calculate the covariance matrix for $\boldsymbol{X}^*$, i.e.

$$C = \frac{1}{12-1}(\boldsymbol{X}^*)^T\boldsymbol{X}^* = \begin{bmatrix} 5.952955 & 6.810227 \\ 6.810227 & 8.349318 \end{bmatrix}$$

iii. Find the eigenvalues and eigenvectors of C which characterises the "variance" of the data $\boldsymbol{X}^*$, i.e.

$$|C - \lambda I| = (5.952955 - \lambda)(8.349318 - \lambda) - 6.810227^2 = \lambda^2 - 14.302273\lambda + 3.323923 = 0$$

Using calculator, we obtain

$$\lambda_1 = 14.065963, \ \lambda_2 = 0.236310$$

iv. We then find the eigenvalues for λ_1 and λ_2:

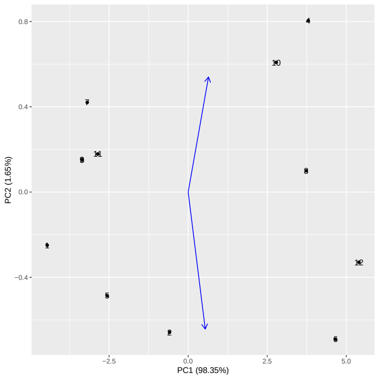
$$\boldsymbol{e}_1 = \frac{1}{\sqrt{6.810227^2 + (8.113008)^2}} \begin{bmatrix} 6.810227 \\ -(5.952955 - 14.065963) \end{bmatrix} = \begin{bmatrix} 0.6429319 \\ 0.765923 \end{bmatrix}$$

$$\boldsymbol{e}_2 = \frac{1}{\sqrt{6.810227^2 + (-5.716645)^2}} \begin{bmatrix} 6.810227 \\ -(5.952955 - 0.236310) \end{bmatrix} = \begin{bmatrix} 0.765923 \\ -0.6429319 \end{bmatrix}$$

Observe that when $\boldsymbol{e}_1 = [a, b]$ and $\boldsymbol{e}_1 \cdot \boldsymbol{e}_2 = 0$, $\boldsymbol{e}_2 = [b, -a]$ is an answer.
Note: $\boldsymbol{e}_1$ and $\boldsymbol{e}_2$ correspond to `PC1` and `PC2` in the `Rotation` of `prcomp`.

v. Calculate the "principal components":
$PC_1 = \sum_{i=1}^{2} e_{i1}(X_i - \mathbb{E}(X_i)) = 0.6429319x_1^* + 0.7659234x_2^*$
$PC_2 = \sum_{i=1}^{2} e_{i2}(X_i - \mathbb{E}(X_i)) = 0.7659234x_1^* - 0.6429319x_2^*$

PC_1	PC_2
-4.4580188	-0.24963649
-0.5898165	-0.65830582
-3.3583304	0.15121924
3.7966382	0.80423156
-2.5622138	-0.48611775
4.6598454	-0.69071771
-3.1928465	0.42069114
3.7351425	0.09980394
-3.3583304	0.15121924
2.7858412	0.60855455
-2.8590814	0.17861498
5.4011705	-0.32955688



By rotating the “principal components” and shift it to the centre (μ_1, μ_2), we can “recover” the original data. □

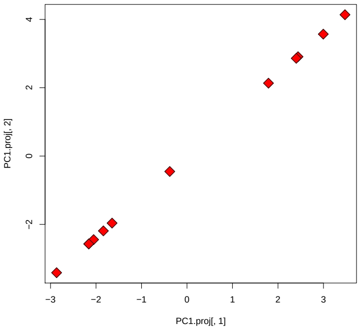
(c) Choose one suitable principal component to represent the data.

Solution. It must be the first principal component, i.e. PC_1. □

(d) Plot your data with the principal component you chose in (c).

Solution. Projecting the centred data $\boldsymbol{X}^*$ to the space span by PC1:

$x_1^{\#}$	$x_2^{\#}$
-2.8662	-3.4145
-0.3792	-0.4518
-2.1592	-2.5722
2.4410	2.9079
-1.6473	-1.9625
2.9960	3.5691
-2.0528	-2.4455
2.4014	2.8608
-2.1592	-2.5722
1.7911	2.1337
-1.8382	-2.1898
3.4726	4.1369



□

(e) With the eigenvalues computed in (b), calculate the proportion of variance explained by each component and the cumulative proportion.

Solution. `print(summary(PC))`

```
                         PC1      PC2
Standard deviation      3.7505 0.48612
Proportion of Variance 0.9835 0.01652
Cumulative Proportion  0.9835 1.00000
```

Manual calculation:

	Eigenvalue	PVE	Cumulative PVE
PC1	14.0660	$\frac{14.0660}{14.3023} = 0.9835$	0.9835
PC2	0.2363	$\frac{0.2363x}{14.3023} = 0.0165$	1
$\lambda_1 + \lambda_2$	14.3023		

□

(f) With a targeted explained variation of 95%, how many principal components should be considered? State the total variation explained.

Solution. One principal component, PC1. Total variance explained is 98.35%. □

2. (May 2020 Final Q4(a)) Given the following data with 8 observations in Table 4.1:

Table 4.1: Data with 2 features.

Obs	x	y
A	5.51	5.35
B	20.82	24.03
C	-0.77	-0.57
D	19.30	19.39
E	14.24	12.77
F	9.74	9.68
G	11.59	12.06
H	-6.08	-5.22

Find the first principle component and project the data $(5.51, 5.35)$ to the space span by the first principal component. (4 marks)

Solution. First, we need to find the mean: $\overline{x} = 9.29375$, $\overline{y} = 9.68625$ .... [0.5 mark]

and shift the data to centre at the mean:

$X=$

Obs	x	y
A	-3.78375	-4.33625
B	11.52625	14.34375
C	-10.06375	-10.25625
D	10.00625	9.70375
E	4.94625	3.08375
F	0.44625	-0.00625
G	2.29625	2.37375
H	-15.37375	-14.90625

.... [0.5 mark]

Form the covariant matrix and

$$\frac{1}{8-1}X^T X = \begin{bmatrix} 614.8648 & 631.9173 \\ 631.9173 & 661.2402 \end{bmatrix} = \begin{bmatrix} 87.83783 & 90.27390 \\ 90.27390 & 94.46288 \end{bmatrix} \qquad [0.5 \text{ mark}]$$

By solving the eigenvalue problem

$$\begin{vmatrix} 87.83783-\lambda & 90.27390 \\ 90.27390 & 94.46288-\lambda \end{vmatrix} = \lambda^2 - 182.3007\lambda + 148.0374 = 0 \qquad [1 \text{ mark}]$$

leads to the eigenvalues 181.4850, 0.8157

The first principle component corresponds $\boldsymbol{v}$ to the linear algebra problem of the eigenvalue 181.4850

$$\begin{bmatrix} 87.83783-181.4850 & 90.27390 \\ 90.27390 & 94.46288-181.4850 \end{bmatrix} \boldsymbol{v} = \boldsymbol{0}$$

i.e.

$$\boldsymbol{v} = \frac{1}{\sqrt{90.27390^2 + 93.64717^2}} \begin{bmatrix} 90.27390 \\ 93.64717 \end{bmatrix} = \begin{bmatrix} 0.69402 \\ 0.71995 \end{bmatrix} \qquad [0.5 \text{ mark}]$$

The projection of (5.51, 5.35) to the first principle component space is

$$(-3.78375, -4.33625)\cdot(0.69402, 0.71995)\begin{bmatrix}0.69402\\0.71995\end{bmatrix} + \begin{bmatrix}9.29375\\9.68625\end{bmatrix} = \begin{bmatrix}5.3046\\5.5481\end{bmatrix} \qquad \text{[1 mark]}$$

□

3. (Jan 2021 Final Q3(a)) Given the following data with 11 observations in Table 3.1:

Table 3.1: Data with two features.

Obs	x	y
1	-5.79	4.91
2	-3.73	4.87
3	-3.25	3.98
4	-2.61	4.09
5	-2.76	4.90
6	2.81	-5.34
7	2.92	-6.15
8	1.97	-4.51
9	5.17	-5.29
10	2.66	-7.10
11	3.47	-4.70

Find the proportions of variance and the principle components. (5 marks)

Solution. First, we need to find the mean: $\overline{x} = 0.07818182$, $\overline{y} = -0.94$ . . . . [0.5 mark]

and shift the data to centre at the mean:

$X=$

Obs	x	y
1	-5.868182	5.85
2	-3.808182	5.81
3	-3.328182	4.92
4	-2.688182	5.03
5	-2.838182	5.84
6	2.731818	-4.40
7	2.841818	-5.21
8	1.891818	-3.57
9	5.091818	-4.35
10	2.581818	-6.16
11	3.391818	-3.76

. . . . [0.5 mark]

Form the covariant matrix and

$$\frac{1}{11-1}X^TX = \begin{bmatrix}138.5108 & -187.3119\\-187.3119 & 281.8462\end{bmatrix} = \begin{bmatrix}13.85108 & -18.73119\\-18.73119 & 28.18462\end{bmatrix}. \qquad \text{[1 mark]}$$

By solving the eigenvalue problem

$$\begin{vmatrix}13.85108-\lambda & -18.73119\\-18.73119 & 28.18462-\lambda\end{vmatrix} = \lambda^2 - 42.0357\lambda + 39.52995 = 0$$

leads to the eigenvalues 41.073275, 0.962425 . . . . [1 mark]

The proportions of variance are

$$\frac{41.073275}{41.073275+0.962425}=0.977105, \quad \frac{0.962425}{41.073275+0.962425}=0.022895 \qquad [0.5 \text{ mark}]$$

The first principle component corresponds $\boldsymbol{v}$ to the linear algebra problem of the eigenvalue 41.073275

$$\begin{bmatrix} 13.85108-41.073275 & -18.73119 \\ -18.73119 & 28.18462-41.073275 \end{bmatrix} \boldsymbol{v}=\mathbf{0}$$

i.e.

$$\boldsymbol{v}=\frac{1}{\sqrt{(-18.73119)^2+(27.222195)^2}}\begin{bmatrix} -18.73119 \\ 27.222195 \end{bmatrix}=\begin{bmatrix} -0.566856 \\ 0.823817 \end{bmatrix} \qquad [1 \text{ mark}]$$

The second principle component is orthogonal to the first principle component:

$$\begin{bmatrix} 0.823817 \\ 0.566856 \end{bmatrix} \qquad [0.5 \text{ mark}]$$

□

4. (Final Exam Jan 2023, Q3(a)) Given the two-dimensional data in Table 3.1.

x_1	x_2
6.0	9.5
2.5	7.5
6.4	10.4
2.1	8.7
5.6	8.7
7.3	8.1

Table 3.1: Two-dimensional data.

Suppose the covariance matrix of the data is

$$\begin{bmatrix} 4.6537 & 0.9623 \\ 0.9623 & 1.0497 \end{bmatrix},$$

find the eigenvalues and normalised eigenvectors of the covariance matrix of the two-dimensional data and write down the principal components of the data in Table 3.1. (8 marks)

Solution. By solving the quadratic equation

$$\begin{vmatrix} 4.6537-\lambda & 0.9623 \\ 0.9623 & 1.0497-\lambda \end{vmatrix}=\lambda^2-5.7034\lambda+3.958968=0 \qquad [3 \text{ marks}]$$

we obtain the eigenvalues of the covariance matrix C:

$$\lambda=4.8945,\ 0.8089 \qquad [1 \text{ mark}]$$

The eigenvectors are obtained by solving linear algebra problems and using the spectral theorem:

The normal eigenvector corresponding to $\lambda = 4.8945$ is

$$\begin{bmatrix} 4.6537 - 4.8945 & 0.9623 \\ 0.9623 & 1.0497 - 4.8945 \end{bmatrix} \mathbf{x}_1 = \mathbf{0} \Rightarrow \mathbf{x}_1 = \frac{1}{\sqrt{(0.9623^2 + 0.2408^2}} \begin{bmatrix} 0.9623 \\ 0.2408 \end{bmatrix} = \begin{bmatrix} 0.970089 \\ 0.242749 \end{bmatrix} \quad \text{[2 marks]}$$

By orthogonality, the normal eigenvector corresponding to $\lambda = 0.8089$ is

$$\mathbf{x}_2 = \begin{bmatrix} 0.242749 \\ -0.970089 \end{bmatrix} \quad \text{[1 mark]}$$

The principal components are

$$\begin{aligned} PC1 &= 0.970089(x_1 - \overline{x_1}) + 0.242749(x_2 - \overline{x_2}) \\ PC2 &= 0.242749(x_1 - \overline{x_1}) - 0.970089(x_2 - \overline{x_2}) \end{aligned} \quad \text{[1 mark]}$$

Average: 6.32 / 8 marks in Jan 2023; 10% below 4 marks.

□

5. (Final Exam Jan 2023, Q3(b)) Given the five-dimensional data in Table 3.2.

Obs.	x_1	x_2	x_3	x_4	x_5
A	5.2	7.8	4.9	3.6	3.3
B	7.1	6.4	3.6	4.6	3.9
C	1.3	6.6	2.5	7.3	0.8
D	8.0	7.4	3.3	-0.8	0.9
E	2.7	9.5	2.4	6.6	1.0
F	2.9	10.8	-2.2	3.8	-0.3

Table 3.2: Five-dimensional data.

Suppose the output of the principal component analysis by R is as follows.

```
Centres (1, ..., p=5):
[1] 4.5333 8.0833 2.4167 4.1833 1.6000

Standard deviations (1, .., p=5):
[1] 3.9593 2.9483 1.1729 0.9856 0.4294

Rotation (n x k) = (5 x 5):
         PC1     PC2     PC3      PC4     PC5
[1,] -0.6499 -0.1170 -0.4415 -0.19537 -0.5752
[2,]  0.2283 -0.3966 -0.3836  0.78791 -0.1505
[3,] -0.3866  0.5944  0.3845  0.56568 -0.1714
[4,]  0.5678  0.5815 -0.3444 -0.12603 -0.4527
[5,] -0.2315  0.3709 -0.6257  0.07177  0.6420
```

Find the **proportions of variance explained, PVEs**, of the principal component analysis. Then, calculate the PC1 for the point A in Table 3.2. (4 marks)

Solution. The PVEs are

$$\begin{aligned} PVE_i &= \frac{(3.9593^2, 2.9483^2, 1.1729^2, 0.9856^2, 0.4294^2)}{3.9593^2 + 2.9483^2 + 1.1729^2 + 0.9856^2 + 0.4294^2} \\ &= \frac{(15.6761, 8.6925, 1.3757, 0.9714, 0.1844)}{26.90002} && \text{[2 marks]} \\ &= (0.5828, 0.3231, 0.0511, 0.0361, 0.0069) \end{aligned}$$

The PC1 for point A is

$$\begin{aligned} PC1(A) = &-0.6499 * (5.2 - 4.5333) + 0.2283 * (7.8 - 8.0833) \\ &- 0.3866 * (4.9 - 2.4167) + 0.5678 * (3.6 - 4.1833) && \text{[2 marks]} \\ &- 0.2315 * (3.3 - 1.6000) = -2.182757 \end{aligned}$$

Average: 1.10 / 4 marks in Jan 2023; 66% below 2 marks.

Reason for low marks: Not much pay attention in practical class to relate theory to the output of the R command `prcomp`. Check out page 1 of this tutorial. □