MONASH University

ETC3250

Business Analytics

Week 5

Principal Components Analysis

24 August 2015

Principal components analysis

Unsupervised vs Supervised Learning

- In **supervised learning** methods, we observe a set of features $x_1, x_2, \ldots, x_p$ as well as a response or outcome variable y. The goal is to predict y using $x_1, x_2, \ldots, x_p$.
- In **unsupervised learning**, we observe only the features $x_1, x_2, \ldots, x_p$. We are not interested in prediction.
- **Principal components analysis** is an unsupervised learning method.

Principal components analysis

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.

Why?

- We may have too many predictors for a regression. Instead, we can use the first few principal components.
- Understanding relationships between variables.
- Data visualization. We can plot a small number of variables more easily than a large number of variables.

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Principal components analysis

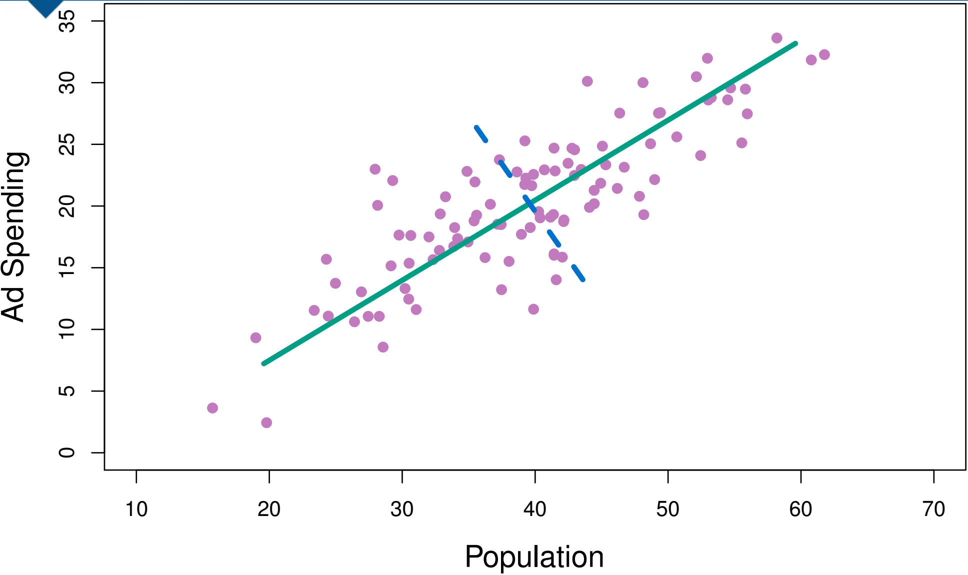
The first principal component of a set of features $x_1, x_2, \ldots, x_p$ is the linear combination

$$z_1 = \phi_{11}x_1 + \phi_{21}x_2 + \cdots + \phi_{p1}x_p$$

that has the largest variance such that $\sum_{j=1}^{p} \phi_{j1}^2 = 1$.

- The elements $\phi_{11}, \ldots, \phi_{p1}$ are the **loadings** of the first principal component.

PCA Example

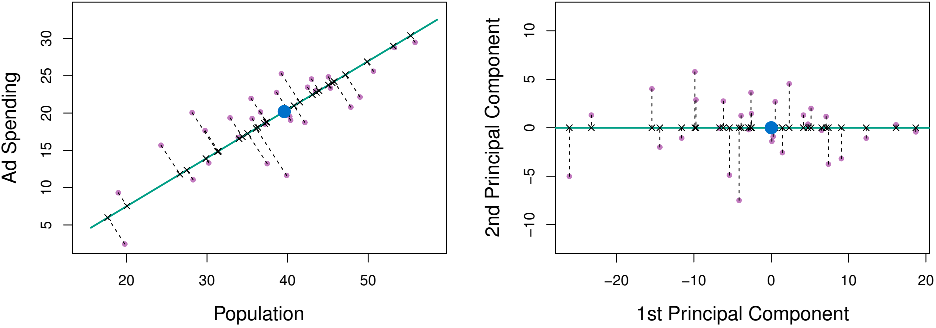


Green: first PC. Blue: second PC

Geometry of PCA

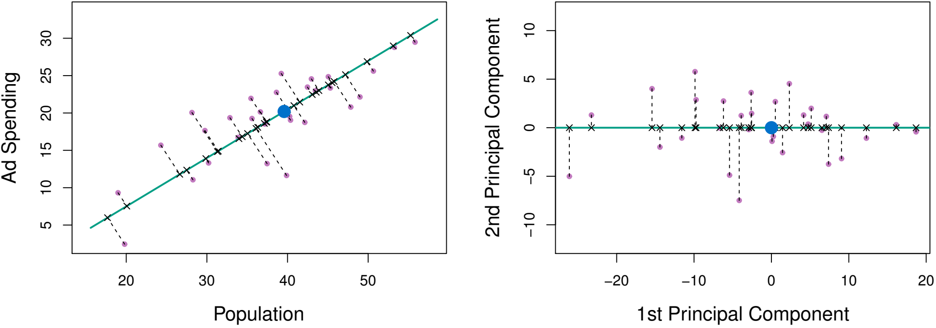
- The loading vector $\phi_1 = [\phi_{11}, \ldots, \phi_{p1}]'$ defines a direction in feature space along which the data vary the most.
- If we project the n data points $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n$ onto this direction, the projected values are the principal component scores $z_{11}, \ldots, z_{n1}$.
- The second principal component is the linear combination $z_{i2} = \phi_{12}x_{i1} + \phi_{22}x_{i2} + \cdots + \phi_{p2}x_{ip}$ that has maximal variance among all linear combinations that are *uncorrelated* with z_1.
- Equivalent to constraining ϕ_2 to be orthogonal (perpendicular) to ϕ_1. And so on.
- There are at most $\min(n-1, p)$ PCs.

Further principal components



PCA can be thought of as fitting an *n*-dimensional ellipsoid to the data, where each axis of the ellipsoid represents a principal component.

Further principal components



PCA can be thought of as fitting an *n*-dimensional ellipsoid to the data, where each axis of the ellipsoid represents a principal component.

Computation of PCs

Suppose we have a $n \times p$ data set $\boldsymbol{X} = [x_{ij}]$.

- Centre each of the variables to have mean zero (i.e., the column means of $\boldsymbol{X}$ are zero).
- $z_{i1} = \phi_{11}x_{i1} + \phi_{21}x_{i2} + \cdots + \phi_{p1}x_{ip}$
- Sample variance of z_{i1} is $\displaystyle\frac{1}{n}\sum_{i=1}^{n} z_{i1}^2$.

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

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Computation of PCs

1. Compute the covariance matrix (after scaling the columns of $\boldsymbol{X}$)

$$\boldsymbol{C} = \boldsymbol{X}'\boldsymbol{X}$$

2. Find eigenvalues and eigenvectors:

$$\boldsymbol{C} = \boldsymbol{V}\boldsymbol{D}\boldsymbol{V}'$$

   where columns of $\boldsymbol{V}$ are orthonormal (i.e., $\boldsymbol{V}'\boldsymbol{V} = \boldsymbol{I}$)

3. Compute PCs: $\Phi = \boldsymbol{V}$. $\boldsymbol{Z} = \boldsymbol{X}\Phi$.

Computation of PCs

Singular Value Decomposition

$$\boldsymbol{X} = \boldsymbol{U}\Lambda\boldsymbol{V}'$$

- $\boldsymbol{X}$ is $n \times p$ matrix
- $\boldsymbol{U}$ is $n \times r$ matrix with orthonormal columns ($\boldsymbol{U}'\boldsymbol{U} = \boldsymbol{I}$)
- Λ is $r \times r$ diagonal matrix with non-negative elements.
- $\boldsymbol{V}$ is $p \times r$ matrix with orthonormal columns ($\boldsymbol{V}'\boldsymbol{V} = \boldsymbol{I}$).

It is always possible to uniquely decompose a matrix in this way.

Computation of PCs

1. Compute SVD: $\boldsymbol{X} = \boldsymbol{U}\Lambda\boldsymbol{V}'$.
2. Compute PCs: $\Phi = \boldsymbol{V}$. $\boldsymbol{Z} = \boldsymbol{X}\Phi$.

Relationship with covariance:

$$\boldsymbol{C} = \boldsymbol{X}'\boldsymbol{X} = \boldsymbol{V}\Lambda\boldsymbol{U}'\boldsymbol{U}\Lambda\boldsymbol{V}' = \boldsymbol{V}\Lambda^2\boldsymbol{V}' = \boldsymbol{V}\boldsymbol{D}\boldsymbol{V}'$$

- Eigenvalues of $\boldsymbol{C}$ are squares of singular values of $\boldsymbol{X}$.
- Eigenvectors of $\boldsymbol{C}$ are right singular vectors of $\boldsymbol{X}$.
- The PC directions $\phi_1, \phi_2, \phi_3, \ldots$ are the right singular vectors of the matrix $\boldsymbol{X}$.
- The variances of the components are $1/n$ times the eigenvalues of $\boldsymbol{C}$.

Computation of PCs

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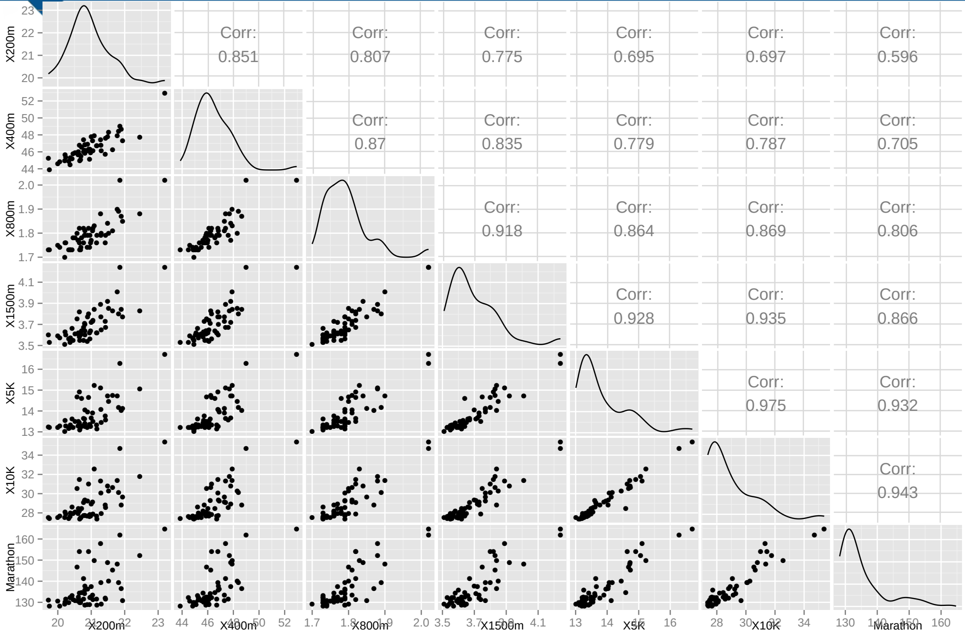
Example: National track records

The data on national track records for men are listed in the following table (as at 1984):

Country	100m *(s)*	200m *(s)*	400m *(s)*	800m *(min)*	1500m *(min)*	5000m *(min)*	10000m *(min)*	Marathon *(min)*
Argentina	10.39	20.81	46.84	1.81	3.70	14.04	29.36	137.72
Australia	10.31	20.06	44.84	1.74	3.57	13.28	27.66	128.30
Austria	10.44	20.81	46.82	1.79	3.60	13.26	27.72	135.90
Belgium	10.34	20.68	45.04	1.73	3.60	13.22	27.45	129.95
Bermuda	10.28	20.58	45.91	1.80	3.75	14.68	30.55	146.62
Brazil	10.22	20.43	45.21	1.73	3.66	13.62	28.62	133.13
⋮								
Turkey	10.71	21.43	47.60	1.79	3.67	13.56	28.58	131.50
USA	9.93	19.75	43.86	1.73	3.53	13.20	27.43	128.22
USSR	10.07	20.00	44.60	1.75	3.59	13.20	27.53	130.55
W.Samoa	10.82	21.86	49.00	2.02	4.24	16.28	34.71	161.83

Example: National track records



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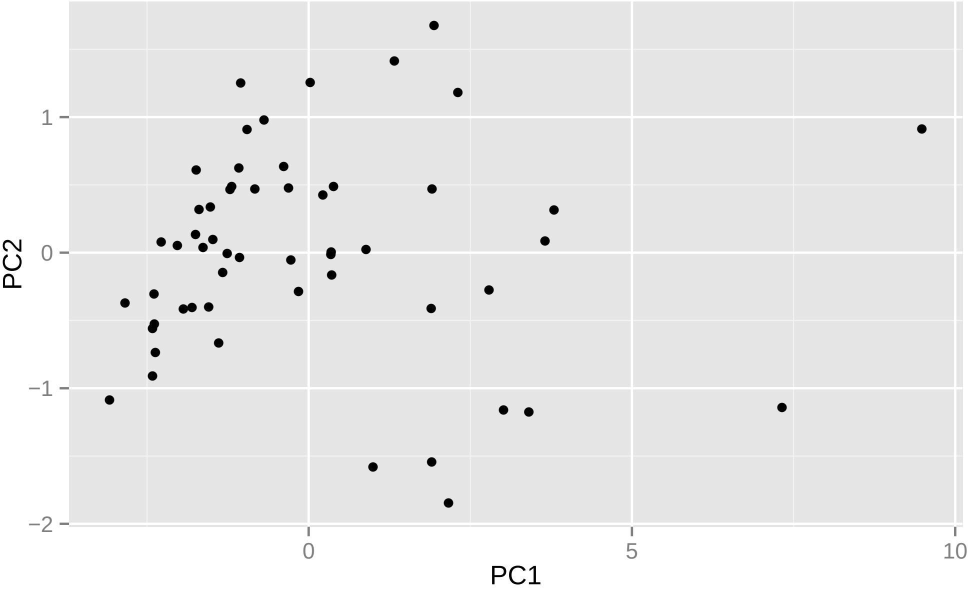

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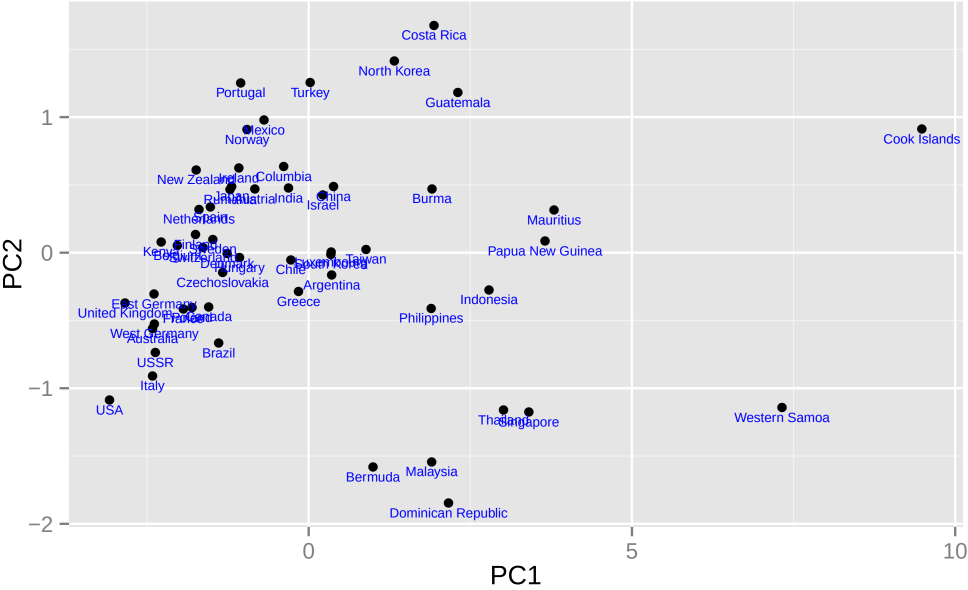
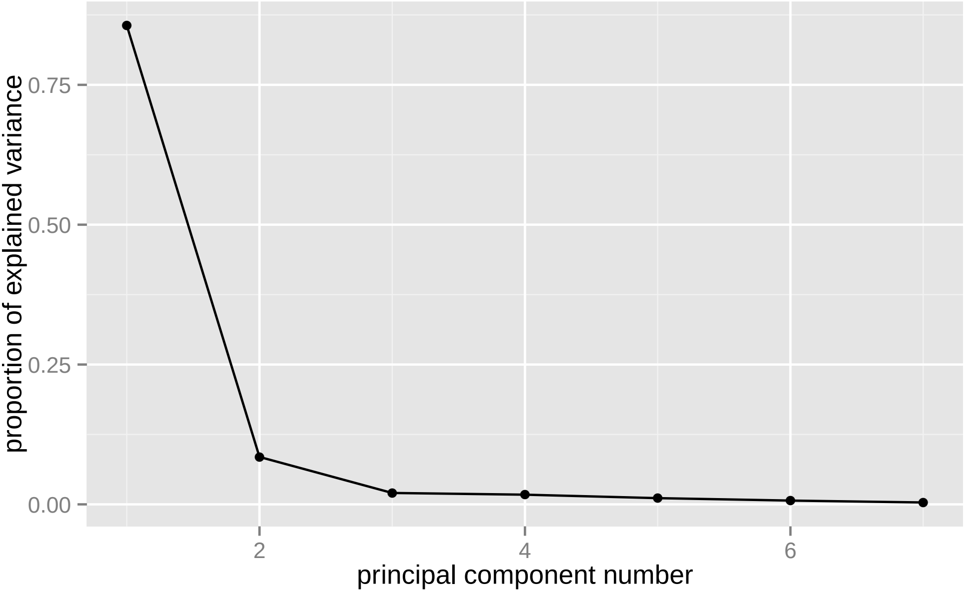


Example: National track records

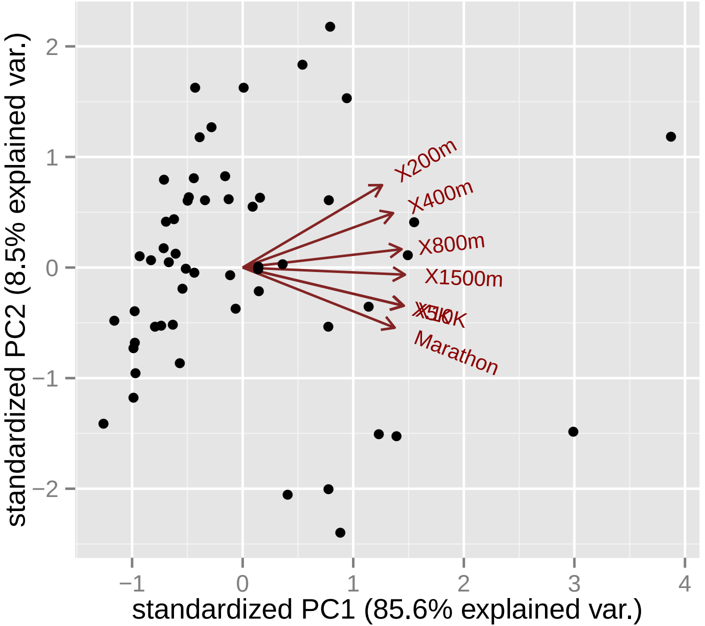
```
> pca
Standard deviations:
[1] 2.573 0.937 0.399 0.352 0.283 0.261 0.215 0.150

Rotation:
           PC1     PC2    PC3     PC4    PC5     PC6      PC7       PC8
X100m    0.318  0.5669  0.332 -0.1276  0.263 -0.5937  0.13624 -0.105542
X200m    0.337  0.4616  0.361  0.2591 -0.154  0.6561 -0.11264  0.096054
X400m    0.356  0.2483 -0.560 -0.6523 -0.218  0.1566 -0.00285  0.000127
X800m    0.369  0.0124 -0.532  0.4800  0.540 -0.0147 -0.23802  0.038165
X1500m   0.373 -0.1398 -0.153  0.4045 -0.488 -0.1578  0.61001 -0.139291
X5K      0.364 -0.3120  0.190 -0.0296 -0.254 -0.1413 -0.59130 -0.546697
X10K     0.367 -0.3069  0.182 -0.0801 -0.133 -0.2190 -0.17687  0.796795
Marathon 0.342 -0.4390  0.263 -0.2995  0.498  0.3153  0.39882 -0.158164
```

Scree plots and biplots



Scree plots and biplots



Scree plots and biplots

Scree plot

Plot of variance explained by each component vs number of component.

Biplot

Plot of PC2 vs PC1, overlaid with directions of the loading vectors (ϕ_{j1}, ϕ_{j2}).

Scaling

- 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 of variance explained

Total variance in data (assuming variables centered at 0):

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

Variance explained by mth PC:

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

$$\text{TV} = \sum_{m=1}^{M} V_m \qquad \text{where } M = \min(n-1, p).$$

Proportion of variance explained:

$$\text{PVE}_m = V_m / TV$$