MONASH University

ETC3250

Business Analytics

Week 7
Principal Components Analysis

4 September 2017

Outline

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1	Introduction to business analytics & R	1	Souhaib
2	Statistical learning	2	Souhaib
3	Regression for prediction	3,7	Tas & David
4	Classification	4	Souhaib
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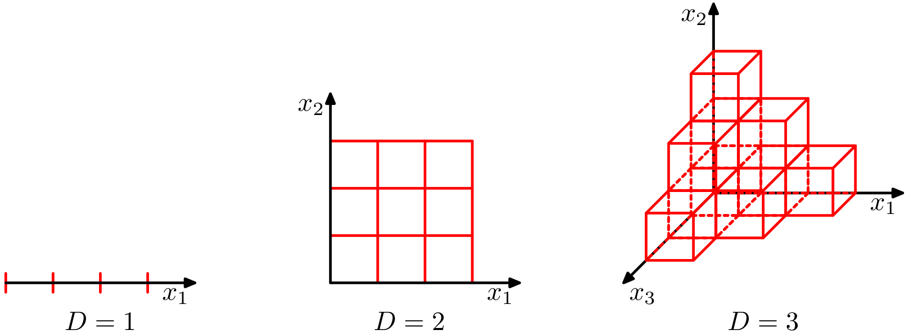
6	Model selection and resampling methods	5	Souhaib
7	**Dimension reduction**	6,10	Souhaib
	Principal Components Analysis		
	Advanced dimension reduction methods		
8	Advanced regression	6	Souhaib
9	Advanced learning methods	8	Souhaib
	Semester break		
10	Clustering	10	Souhaib
11	Visualization		Souhaib
12	Data wrangling		Souhaib

The curse of dimensionality



When the dimensionality increases, the volume of the space increases so fast that the available data become sparse.

The curse of dimensionality

Consider the **hyper-cube** $[-a, a]^d$ and the inscribed **hyper-sphere**. What does your intuition tell you about the relative sizes of these two objects?

1. volume of sphere $\approx$ volume of cube
2. volume of sphere $>>$ volume of cube
3. volume of sphere $<<$ volume of cube

The curse of dimensionality

$$s_d = \frac{\text{Volume(hyper-sphere)}}{\text{Volume(hyper-cube)}} = \frac{\frac{a^d \pi^{d/2}}{\Gamma(\frac{d}{2}+1)}}{(2a)^d} = \Bigg(\underbrace{\frac{\sqrt{\pi}}{2}}_{<1}\Bigg)^d \frac{1}{\Gamma(\frac{d}{2}+1)}$$

where $\Gamma(\cdot)$ is the Gamma function.

d	1	2	3	4	5	6
s_d	1	.785	.524	.308	.164	.080

- s_d does not depend on a, just on d!
- As the dimension increases the volume of the area between the cube and the sphere becomes larger
- High dimensional spaces are strange $\rightarrow$ never trust your intuition in high dimensions!

The curse of dimensionality

- Most data points are closer to the boundary of the sample space than to any other data point
- Prediction is much more difficult near the edges of the training sample: extrapolation vs interpolation

$\rightarrow$ Can we learn in high dimension?

The curse of dimensionality

- Most data points are closer to the boundary of the sample space than to any other data point
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$\rightarrow$ Can we learn in high dimension?

Yes!

- First, real data will often be confined to a region of the space having *lower intrinsic dimensionality*. The data *lives* in a low dimensional subspace.
- Second, real data will typically exhibit some smoothness properties (at least locally)

$\rightarrow$ Dimensionality reduction

Wy dimensionality reduction?

- Curse of dimensionality
- Intrinsic dimensionality
- Visualization
- Reduce computation and storage demand

We avoid unnecessary dimensions which can be measured in two ways:

- features are not useful
- features are not independent

Dimension reduction methods

- Feature selection vs feature extraction
- Unsupervised vs supervised
- Linear vs nonlinear

Principal components analysis (PCA) is an unsupervised linear feature extraction 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.
- We can **plot a small 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

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

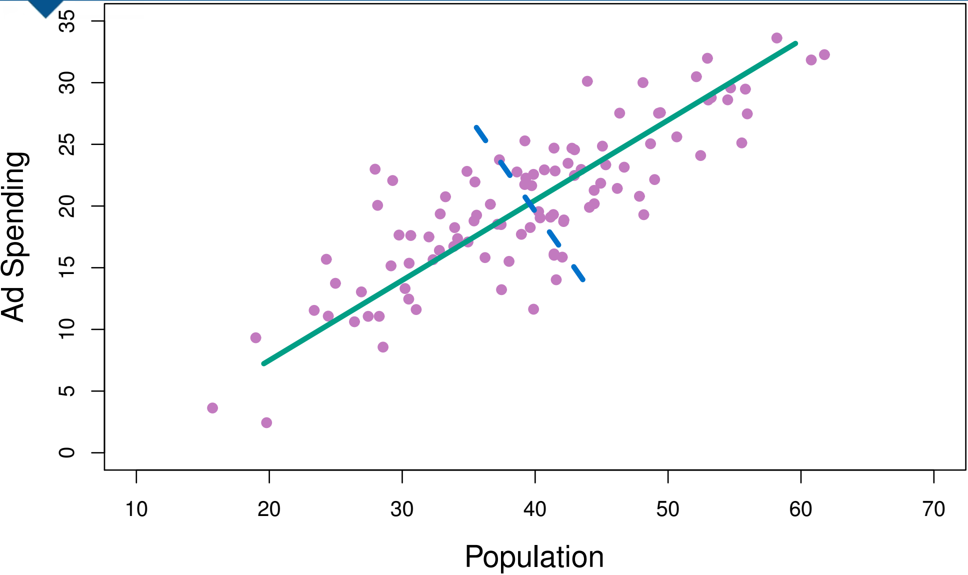
that has the largest variance such that $\sum_{j=1}^{p} \phi_{j1}^2 = 1$.

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

Geometry of PCA

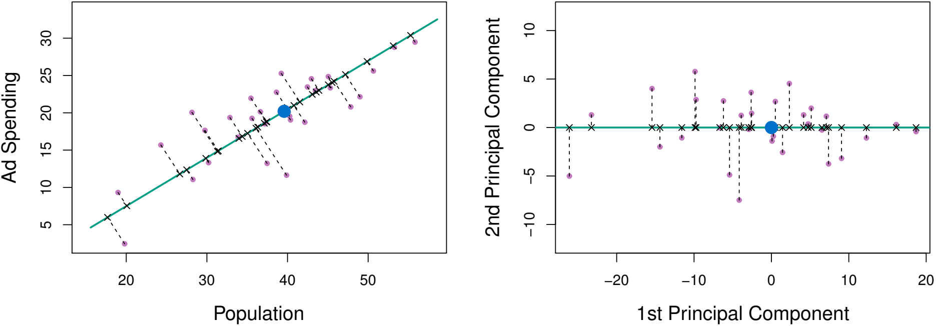
- The loading vector $\phi_1 = [\phi_{11}, \ldots, \phi_{p1}]'$ defines a direction in feature space along which the data vary the most.
- If we project the n data points $\boldsymbol{x}_1, \ldots, \boldsymbol{x}_n$ onto this direction, the projected values are the principal component scores $z_{11}, \ldots, z_{n1}$.
- 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.

PCA Example



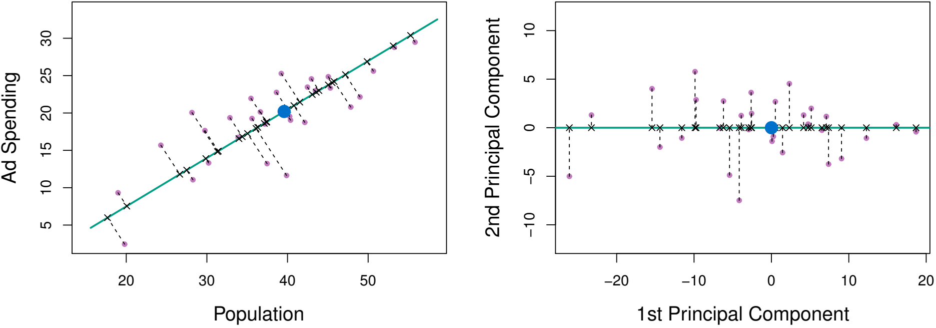
Green: first PC. Blue: second PC

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



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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 $\frac{1}{n}\sum_{i=1}^{n} z_{i1}^2$.

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

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:

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

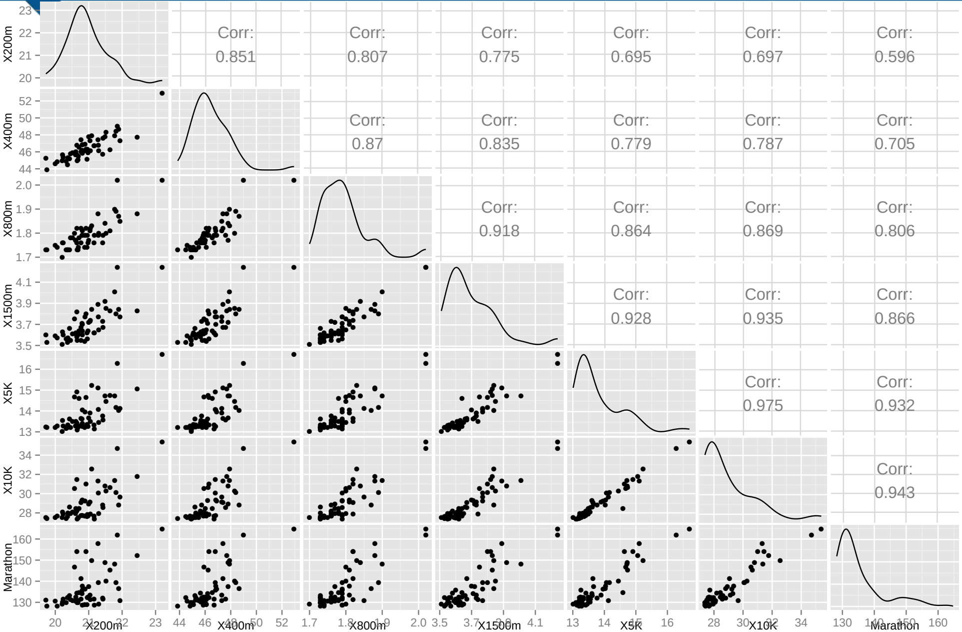
- Eigenvalues of $\boldsymbol{C}$ are squares of singular values of $\boldsymbol{X}$.
- Eigenvectors of $\boldsymbol{C}$ are right singular vectors of $\boldsymbol{X}$.
- The PC directions $\phi_1, \phi_2, \phi_3, \ldots$ are the right singular vectors of the matrix $\boldsymbol{X}$.

Example: National track records

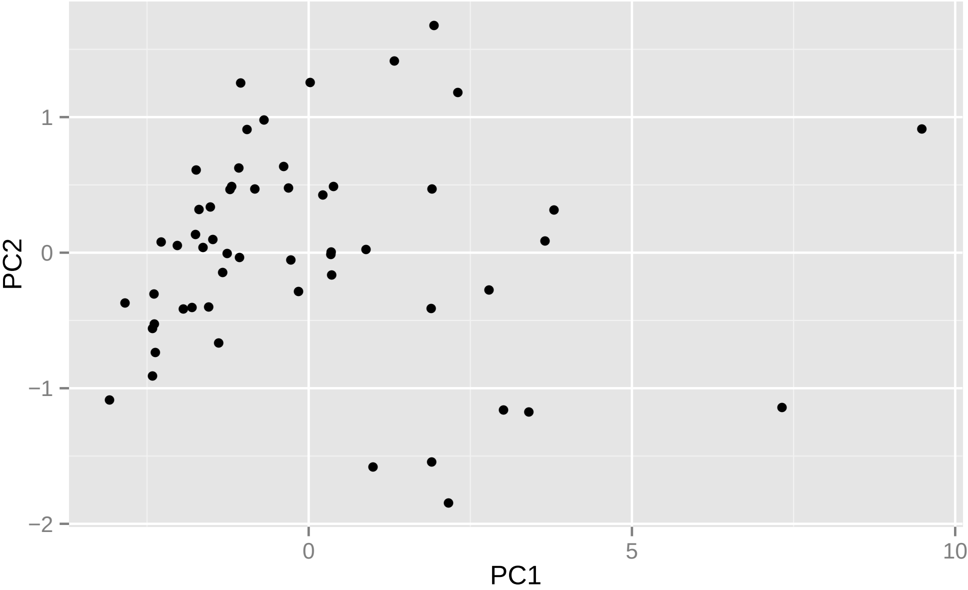
The data on national track records for men are listed in the following table (as at 1984):

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

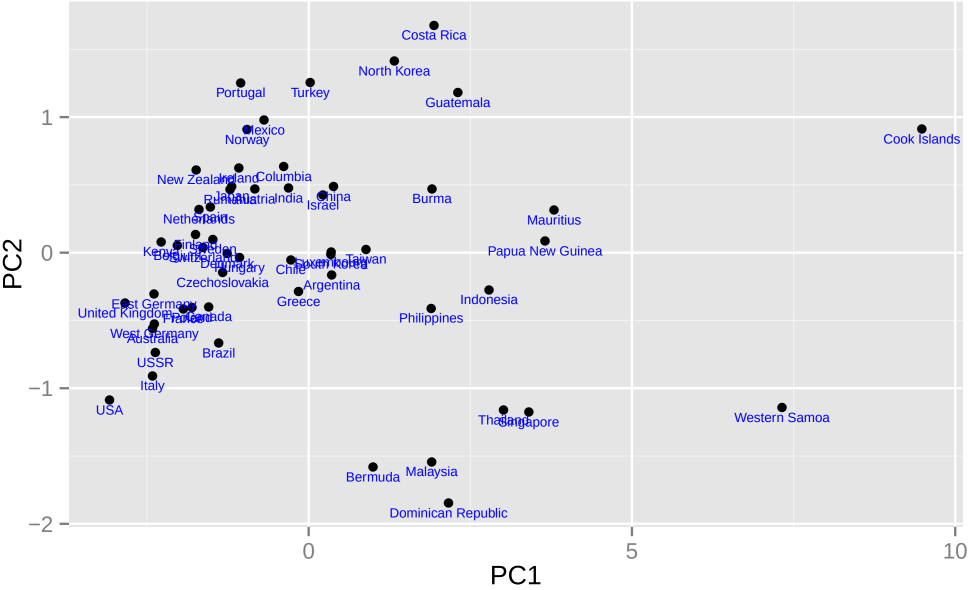
Example: National track records



Example: National track records



Example: National track records



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
```

Proportion of variance explained

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

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

Variance explained by mth PC:

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

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

Proportion of variance explained:

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

Scree plots and biplots

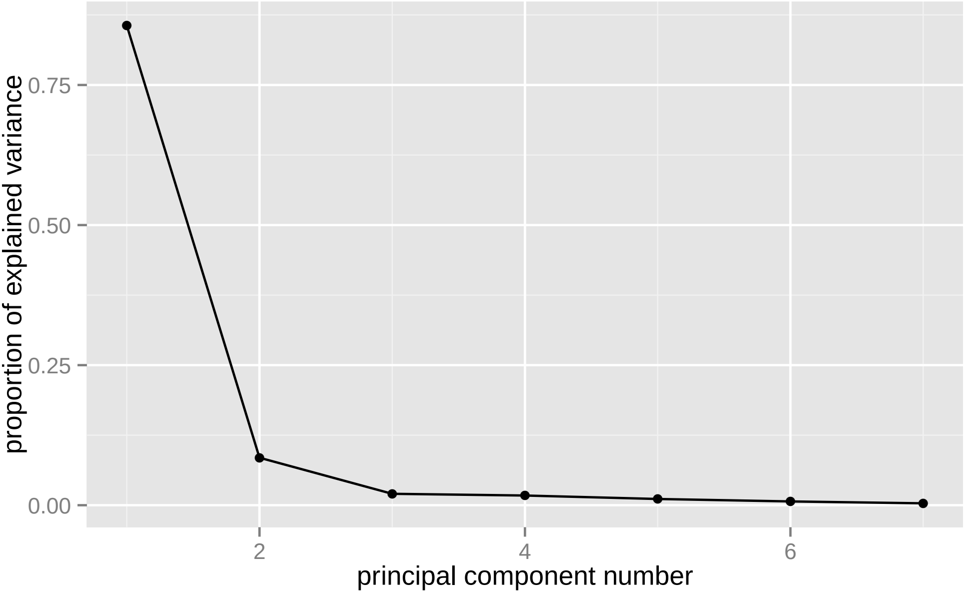
Scree plot

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

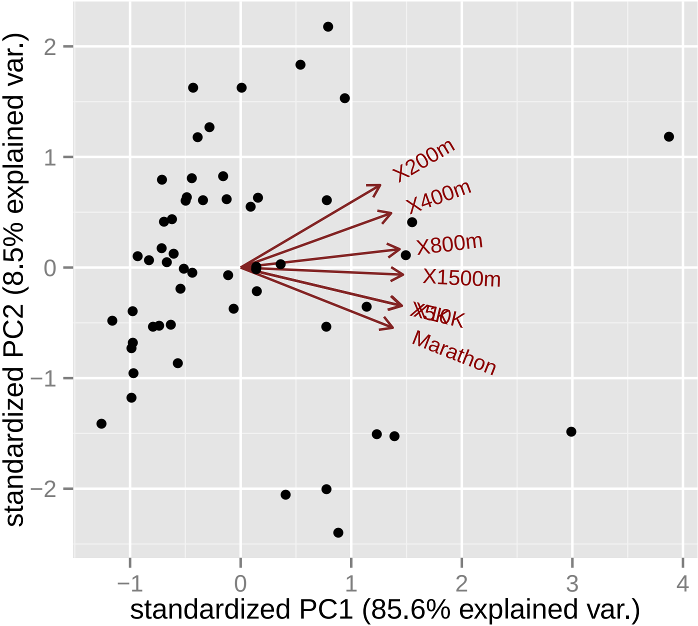
Biplot

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

Scree plot


0.75
0.50
0.25
0.00
proportion of explained variance
2
4
6
principal component number

Biplot



standardized PC2 (8.5% explained var.)
standardized PC1 (85.6% explained var.)
2
1
0
−1
−2
−1
0
1
2
3
4
X200m
X400m
X800m
X1500m
X5K
X10K
Marathon

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.