ETC3250: Dimension reduction

Semester 1, 2019

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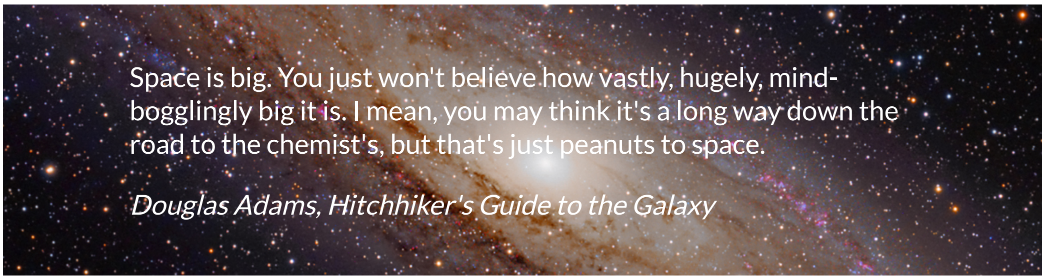
Econometrics and Business Statistics
Monash University

Week 4 (a)



Outline

- High dimensions
  - Definition

Remember, our data can be denoted as:

$$\mathcal{D} = \{(x_i, y_i)\}_{i=1}^{N}, \quad \text{where } x_i = (x_{i1}, \dots, x_{ip})^T$$

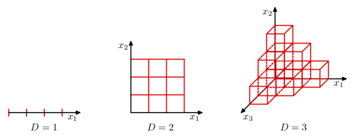
then

Dimension of the data is p, the number of variables.

Outline

- High dimensions
  - Definition
  - Cubes and spheres

Space expands exponentially with dimension:



As dimension increases the volume of a sphere of same radius as cube side length becomes much smaller than the volume of the cube:

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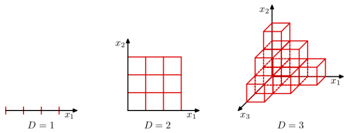

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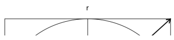

Outline

Data will often be confined to a region of the space having lower intrinsic dimensionality. The data lives in a low-dimensional subspace.

SO, reduce dimensionality, to the subspace containing the data.

Outline

- High dimensions
  - Definition
  - Cubes and spheres
  - Sub-spaces

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SO, reduce dimensionality, to the subspace containing the data.

Outline

- High dimensions
- PCA
  - Definition

Principal component 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. It is an unsupervised learning method.

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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First principal component

The first principal component of a set of variables $x_1, x_2, \ldots, x_p$ 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.

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Outline

- The loading vector $\phi_1 = [\phi_{11}, \ldots, \phi_{p1}]'$ defines direction in feature space along which data vary most.
- If we project the n data points $x_1, \ldots, x_n$ 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.

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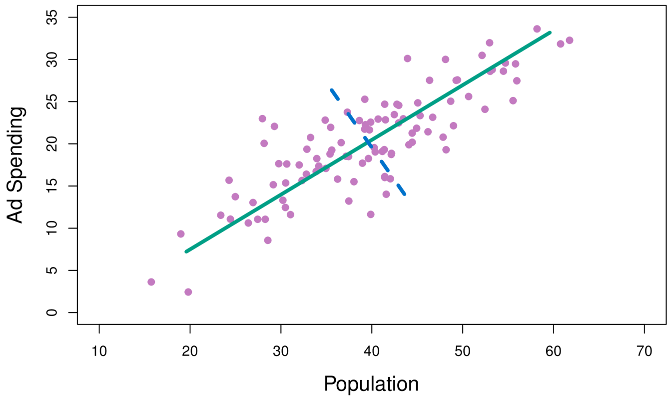
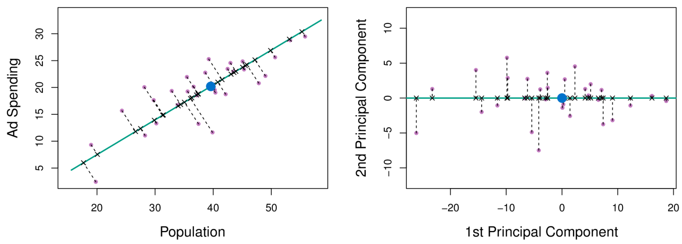
Outline



First PC; second PC

Outline



If you think of the first few PCs like a linear model fit, and the others as the error, it is like regression, except that errors are orthogonal to model.

(Chapter6/6.15.pdf)

Outline

PCA can be thought of as fitting an n-dimensional ellipsoid to the data, where each axis of the ellipsoid represents a principal component. The new variables produced by principal components correspond to rotating and scaling the ellipse into a circle.

Outline

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

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

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

Outline

1. Compute the covariance matrix (after scaling the columns of X)

$$C = X'X$$

2. Find eigenvalues and eigenvectors:

$$C = VDV'$$

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

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

Outline

Singular Value Decomposition

$$X = U\Lambda V'$$

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

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

Outline

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

Relationship with covariance:

$$C = X'X = V\Lambda U'U\Lambda V' = V\Lambda^2 V' = VDV'$$

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

Outline

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

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

If variables are standardised, TV=number of variables!

Variance explained by m'th PC:

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

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

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  - Example
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Outline

Proportion of variance explained:

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

Choosing the number of PCs that adequately summarises the variation in X, is achieved by examining the cumulative proportion of variance explained.

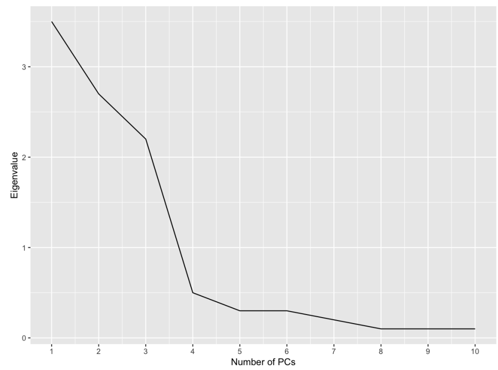
Cumulative proportion of variance explained:

$$\mathrm{CPVE}_k = \sum_{m=1}^{k} \frac{V_m}{TV}$$

and also by a scree plot.

Outline

Scree plot: Plot of variance explained by each component vs number of component.



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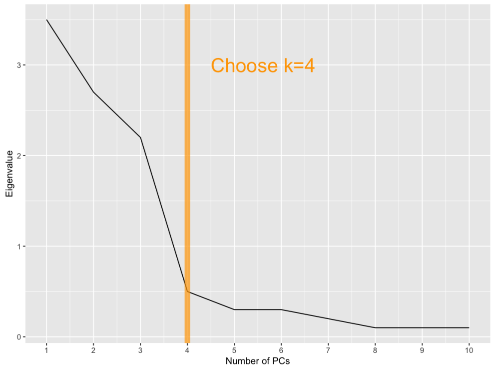


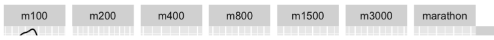
Outline

The data on national track records for women (as at 1984).

```
## Observations: 55
## Variables: 8
## $ m100     <dbl> 11.61, 11.20, 11.43, 11.41, 11.46, 11.31, 12.14, 1
## $ m200     <dbl> 22.94, 22.35, 23.09, 23.04, 23.05, 23.17, 24.47, 2
## $ m400     <dbl> 54.50, 51.08, 50.62, 52.00, 53.30, 52.80, 55.00, 5
## $ m800     <dbl> 2.15, 1.98, 1.99, 2.00, 2.16, 2.10, 2.18, 2.00, 2.
## $ m1500    <dbl> 4.43, 4.13, 4.22, 4.14, 4.58, 4.49, 4.45, 4.06, 4.
## $ m3000    <dbl> 9.79, 9.08, 9.34, 8.88, 9.81, 9.77, 9.51, 8.81, 9.
## $ marathon <dbl> 178.52, 152.37, 159.37, 157.85, 169.98, 168.75, 19
## $ country  <chr> "argentin", "australi", "austria", "belgium", "ber
```

Source: Johnson and Wichern, Applied multivariate analysis

Outline



Outline


```
track_pca <- prcomp(track[,1:7], center=TRUE, scale=TRUE)
track_pca
```

```
## Standard deviations (1, .., p=7):
## [1] 2.41 0.81 0.55 0.35 0.23 0.20 0.15
##
## Rotation (n x k) = (7 x 7):
##           PC1   PC2    PC3    PC4    PC5     PC6    PC7
## m100     0.37  0.49 -0.286  0.319  0.231  0.6198  0.052
## m200     0.37  0.54 -0.230 -0.083  0.041 -0.7108 -0.109
## m400     0.38  0.25  0.515 -0.347 -0.572  0.1909  0.208
## m800     0.38 -0.16  0.585 -0.042  0.620 -0.0191 -0.315
## m1500    0.39 -0.36  0.013  0.430  0.030 -0.2312  0.693
## m3000    0.39 -0.35 -0.153  0.363 -0.463  0.0093 -0.598
## marathon 0.37 -0.37 -0.484 -0.672  0.131  0.1423  0.070
```

Outline

Summary of the principal components:

	PC1	PC2	PC3	PC4	PC5	PC6	PC7
Variance	5.81	0.65	0.30	0.13	0.05	0.04	0.02
Proportion	0.83	0.09	0.04	0.02	0.01	0.01	0.00
Cum. prop	0.83	0.92	0.97	0.98	0.99	1.00	1.00

Increase in variance explained large until $k = 3$ PCs, and then tapers off. A choice of 3 PCs would explain 97% of the total variance.

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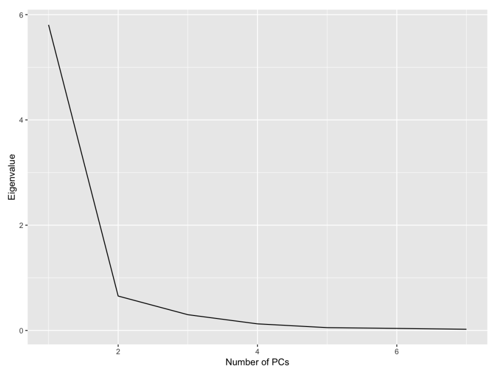
  - Data
  - Explore
  - Compute
  - Assess

Scree plot: Where is the elbow?



At $k = 2$, thus the scree plot suggests 2 PCs would be

Outline

Visualise model using a biplot: Plot the principal component scores, and also the contribution of the original variables to the principal component.

Outline

Explain and interpret: using the coefficients of the principal components.

- PC1 measures overall magnitude, the strength of the athletics program. High positive values indicate poor programs with generally slow times across events.
- PC2 measures the contrast in the program between short and long distance events. Some countries have relatively stronger long distance atheletes, while others have relatively stronger short distance athletes.
- There are several outliers visible in this plot, `wsamoa`, `cookis`, `dpkorea`. PCA, because it is computed using the

variance in the data, can be affected by outliers. It may be

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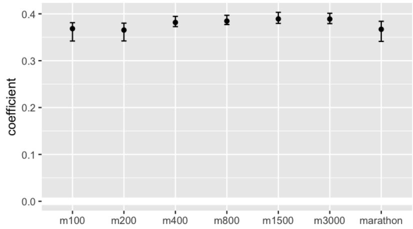
Outline

Bootstrap can be used to assess whether the coefficients of a PC are significantly different from 0. The 95% bootstrap confidence intervals are:



All of the coefficients on PC1 are significantly different from 0, and positive, approximately equal, not significantly different from each other.

🧑‍💻 Made by a human with a computer

Slides at https://monba.dicook.org.

Code and data at https://github.com/dicook/Business_Analytics.

Created using R Markdown with flair by **xaringan**, and **kunoichi** (female ninja) style.