Principal Components Analysis (part I)

Predictive Modeling & Statistical Learning

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Introduction

NBA Team Stats

- NBA Team Stats: regular season (2016-17)
- Github file: `data/nba-teams-2017.csv`
- Source: **stats.nba.com**
- http://stats.nba.com/teams/traditional/#!?sort=GP&dir=-1

SEASON **2016-17** | SEASON TYPE **Regular Season** | PER MODE **Per Game** | SEASON SEGMENT **All Games** | **Advanced Filters**

RECENT FILTERS GLOSSARY SHARE

	TEAM	GP	W	L	WIN%	MIN	PTS	FGM	FGA	FG%	3PM	3PA	3P%	FTM	FTA	FT%	OREB	DREB	REB	AST	TOV	STL	BLK	BLKA	PF	PFD	+/-
1	Miami Heat	82	41	41	.500	48.2	103.2	39.0	85.8	45.5	9.9	27.0	36.5	15.2	21.6	70.6	10.6	33.0	43.6	21.2	13.4	7.2	5.7	4.9	20.5	18.7	1.1
1	Atlanta Hawks	82	43	39	.524	48.5	103.2	38.1	84.4	45.1	8.9	26.1	34.1	18.1	24.9	72.8	10.3	34.1	44.3	23.6	15.8	8.2	4.8	5.2	18.2	21.6	-0.9
1	Brooklyn Nets	82	20	62	.244	48.2	105.8	37.8	85.2	44.4	10.7	31.6	33.8	19.4	24.6	78.8	8.8	35.1	43.9	21.4	16.5	7.2	4.7	5.6	21.0	20.4	-6.7
1	Charlotte Hornets	82	36	46	.439	48.4	104.9	37.7	85.4	44.2	10.0	28.6	35.1	19.4	23.8	81.5	8.8	34.8	43.6	23.1	11.5	7.0	4.8	5.5	16.6	19.9	0.2
1	Chicago Bulls	82	41	41	.500	48.2	102.9	38.6	87.1	44.4	7.6	22.3	34.0	18.0	22.5	79.8	12.2	34.1	46.3	22.6	13.6	7.8	4.8	4.6	17.7	18.8	0.4
1	Cleveland Cavaliers	82	51	31	.622	48.5	110.3	39.9	84.9	47.0	13.0	33.9	38.4	17.5	23.3	74.8	9.3	34.4	43.7	22.7	13.7	6.6	4.0	4.3	18.1	20.6	3.2
1	Dallas Mavericks	82	33	49	.402	48.2	97.9	36.2	82.3	44.0	10.7	30.2	35.5	14.8	18.5	80.1	7.9	30.7	38.6	20.8	11.9	7.5	3.7	3.4	19.1	19.4	-2.9
1	Denver Nuggets	82	40	42	.488	48.2	111.7	41.2	87.7	46.9	10.6	28.8	36.8	18.7	24.2	77.4	11.8	34.6	46.4	25.3	15.0	6.9	3.9	4.9	19.1	20.2	0.5
1	Detroit Pistons	82	37	45	.451	48.3	101.3	39.9	88.8	44.9	7.7	23.4	33.0	13.9	19.3	71.9	11.1	34.6	45.7	21.1	11.9	7.0	3.8	4.1	17.9	17.5	-1.1
1	Golden State Warriors	82	67	15	.817	48.2	115.9	43.1	87.1	49.5	12.0	31.2	38.3	17.8	22.6	78.8	9.4	35.0	44.4	30.4	14.8	9.6	6.8	3.8	19.3	19.4	11.6

```r
# variables
dat <- read.csv('data/nba-teams-2017.csv')
```

```r
dim(dat)
```

```
[1] 30 27
```

```r
names(dat)
```

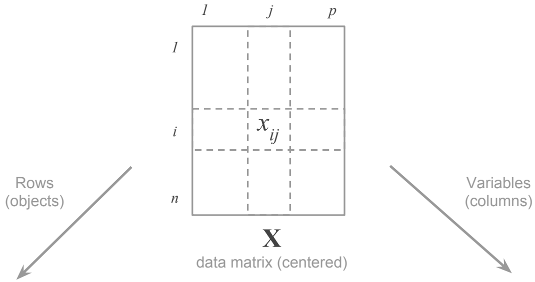
```
 [1] "team"                "games_played"          "wins"
 [4] "losses"              "win_prop"              "minutes"
 [7] "points"              "field_goals"           "field_goals_attempted"
[10] "field_goals_prop"    "points3"               "points3_attempted"
[13] "points3_prop"        "free_throws"           "free_throws_att"
[16] "free_throws_prop"    "off_rebounds"          "def_rebounds"
[19] "rebounds"            "assists"               "turnovers"
[22] "steals"              "blocks"                "block_fga"
[25] "personal_fouls"      "personal_fouls_drawn"  "plus_minus"
```

Exploratory Data Analysis

For illustration purposes, let's focus on the following variables:

- `wins`
- `losses`
- `points`
- `field_goals`
- `assists`
- `turnovers`
- `steals`
- `blocks`

EDA: Objects and Variables Perspectives

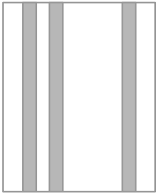


$\mathbf{X}$

data matrix (centered)

$\mathbf{X}\mathbf{X}^{\mathsf{T}}$

inner products of rows



$(1/n)\ \mathbf{X}^{\mathsf{T}}\mathbf{X}$

covariance matrix

EDA: Objects and Variables Perspectives

Data Perspectives

We are interested in analyzing a data set from both perspectives: **objects** and **variables**

At its simplest we are interested in 2 fundamental purposes:

- Study resemblance among individuals
  (resemblance among NBA teams)
- Study relationship among variables
  (relationship among team statistics)

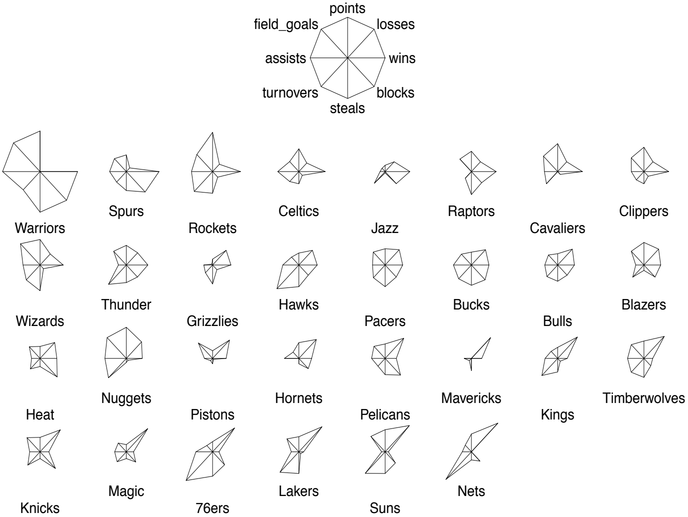
EDA

Exploration

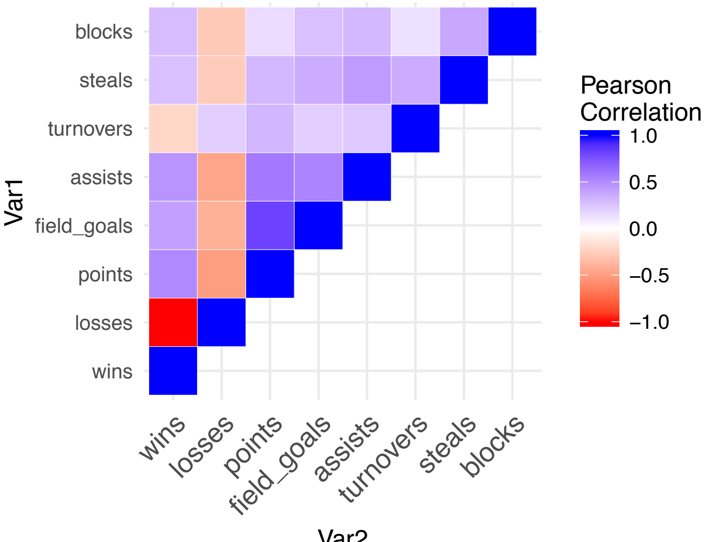
Likewise, we can explore variables at different stages:

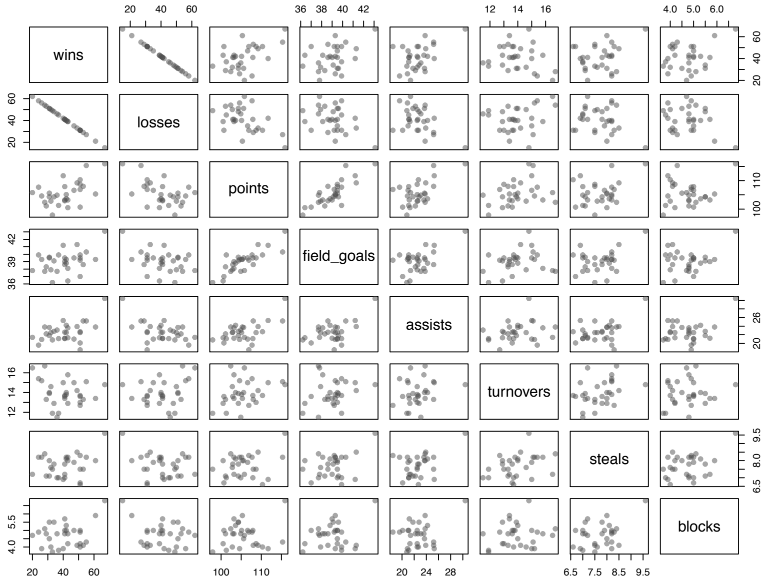
- Univariate: one variable at a time
- Bivariate: two variables simultaneously
- Multivariate: multiple variables

Let's see a shiny-app demo (see apps/ folder in github repo)

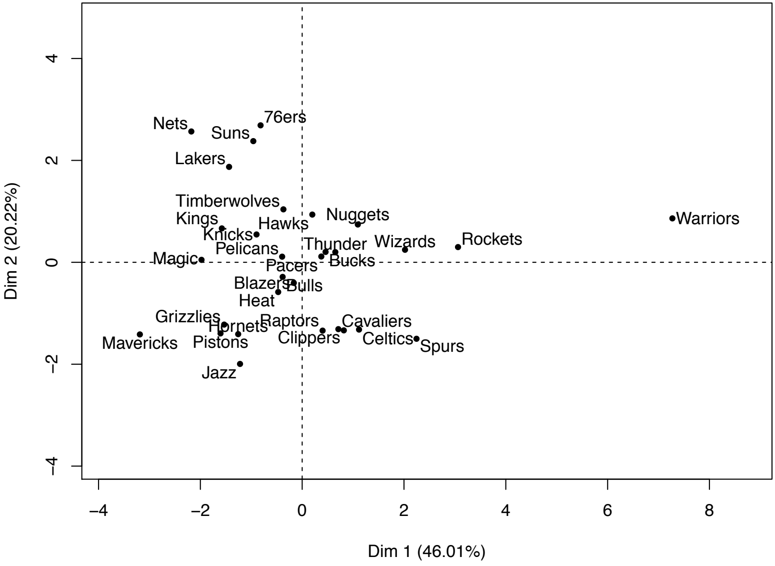

points
losses
wins
blocks
steals
turnovers
assists
field_goals
Warriors
Spurs
Rockets
Celtics
Jazz
Raptors
Cavaliers
Clippers
Wizards
Thunder
Grizzlies
Hawks
Pacers
Bucks
Bulls
Blazers
Heat
Nuggets
Pistons
Hornets
Pelicans
Mavericks
Kings
Timberwolves
Knicks
Magic
76ers
Lakers
Suns
Nets

Correlation heatmap

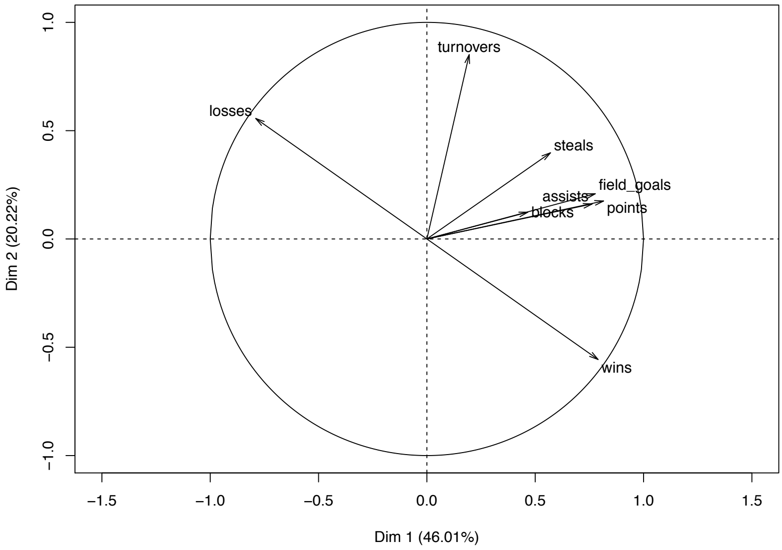



wins
losses
points
field_goals
assists
turnovers
steals
blocks
20
40
60
36
38
40
42
12
14
16
4.0
5.0
6.0
100
110
26
20
9.5
8.0
6.5
5.5
39
24
28
6.5
7.5
8.5

What if we could get a better low-dimensional summary of the data?



Nets
76ers
Suns
Lakers
Timberwolves
Kings
Hawks
Nuggets
Warriors
Knicks
Pelicans
Thunder
Wizards
Rockets
Magic
Pacers
Bucks
Blazers
Bulls
Heat
Grizzlies
Hornets
Raptors
Cavaliers
Mavericks
Pistons
Clippers
Celtics
Spurs
Jazz
Dim 2 (20.22%)
Dim 1 (46.01%)
4
2
0
−2
−4
−4
−2
0
2
4
6
8



turnovers
losses
steals
field_goals
assists
blocks
points
wins
Dim 1 (46.01%)
Dim 2 (20.22%)

About PCA

Data Structure

Principal Components Analysis (PCA) is a multivariate method that allows us to study and explore a set of quantitative variables measured on some objects.

Landmarks

- PCA was first introduced by Karl Pearson (1904)
  On lines and planes of closest fit to systems of points in space
- Further developed by Harold Hotelling (1933)
  Analysis of a complex of statistical variables into principal components
- Singular Value Decomposition (SVD) theorem by Eckart-Young (1936)
  The approximation of a matrix by another of a lower rank
- Computationally implemented in the 1960s

Core Idea

With PCA we seek to **reduce the dimensionality** (condense information in variables) of a data set while retaining as much as possible of the variation present in the data

PCA: Overall Goals

- Summarize a data set with the help of a small number of synthetic variables (i.e. the Principal Components).
- Visualize the position (resemblance) of individuals.
- Visualize how variables are correlated.
- Interpret the synthetic variables.

Applications

PCA can be used for

1. Dimension Reduction
2. Visualization
3. Feature Extraction
4. Data Compression
5. Smoothing of Data
6. Detection of Outliers
7. Preliminary process for further analyses

About PCA

Approaches:

PCA can be presented using various—different but equivalent—approaches. Each approach corresponds to a unique perspective and a way of thinking about data.

- Data dispersion from the individuals standpoint
- Data variability from the variables standpoint
- Data that follows a decomposition model

I will present PCA by mixing and connecting all of these approaches.

Geometric Approach

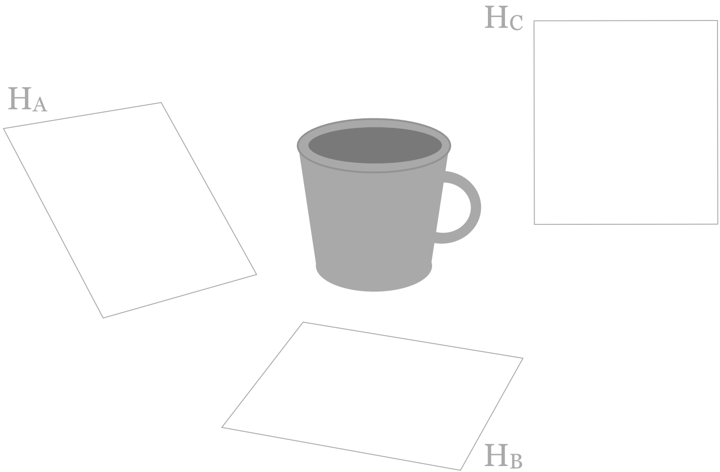
PCA for Data Visualization

One way to present PCA is based on a data visualization approach.

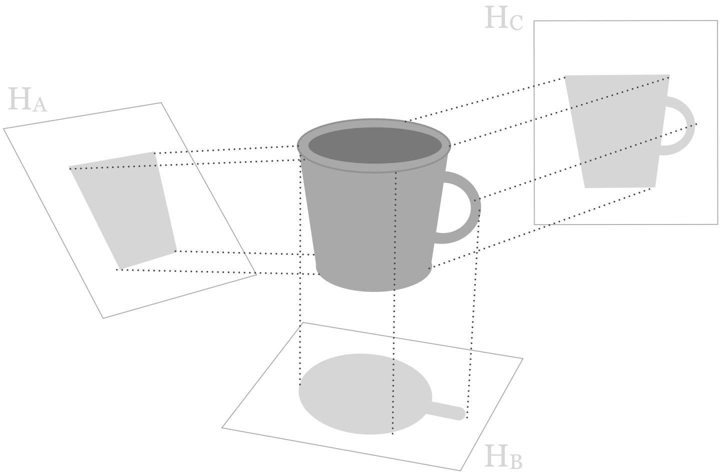
To help you understand the main idea of PCA from a geometric standpoint, I'd like to begin showing you my *mug-data* example.

Imagine a data set in a "high-dimensional space"

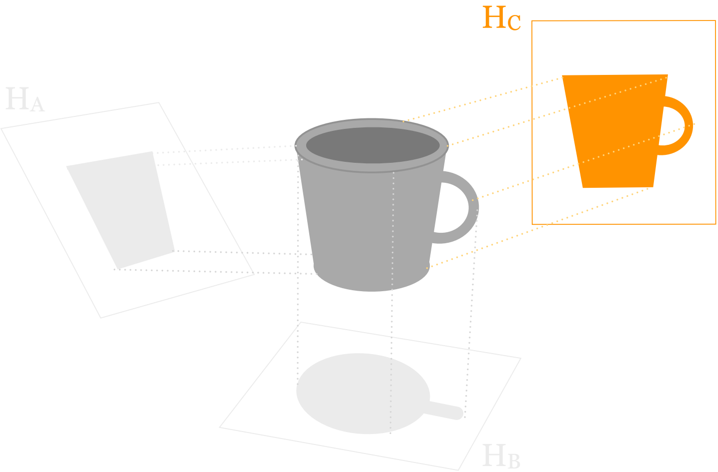
We are looking for Candidate Subspaces



with the best low-dimensional representation



Best low-dimensional projection



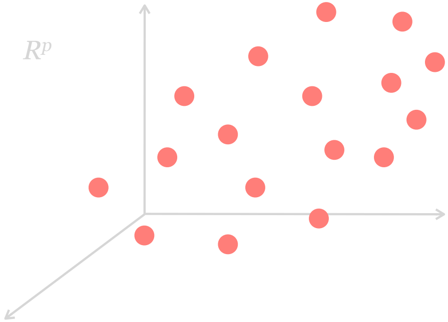
Geometric Idea

Looking at the cloud of points

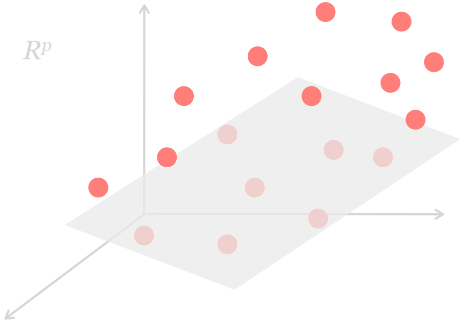
Under a purely geometric approach, PCA aims to represent the cloud of points in a space with reduced dimensionality in an "optimal" way.

We look for the "best" graphical representation that allows us to visualize the cloud of individuals in a low dimensional space (usually 2-dimensions).

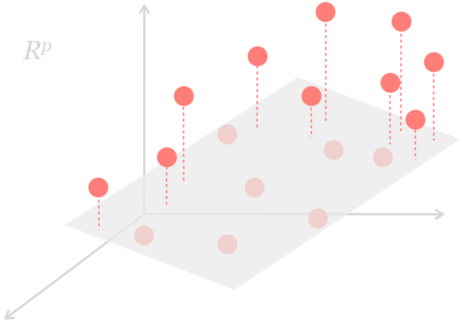
Objects in a high-dimensional space



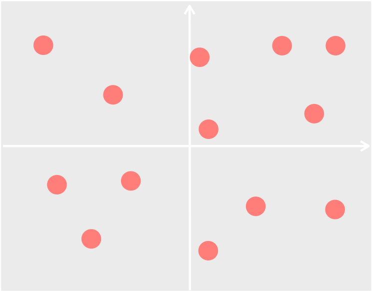
We look for a subspace such that



the projection of points on it



is the best low-dimensional representation



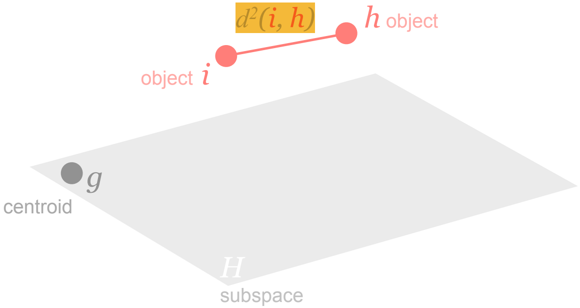
How do you find the associated axes?

Focus on Distances

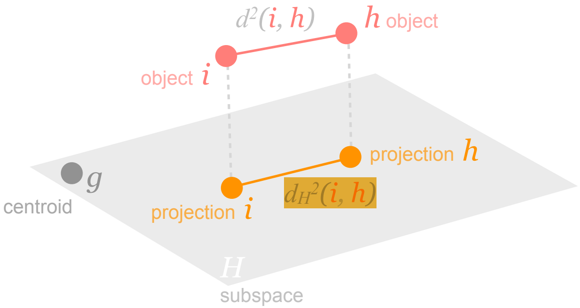
Distances between individuals

Looking for the best low-dimensional projection means that we want to find a subspace in which the projected distances among points are as much similar as possible to the original distances.

Focus on distances between objects



We want projected dists to preserve original dists



$d^2(i, h)$ as close as possible to $d_H{}^2(i, h)$

Focus on projected distances

The idea is to project the cloud of points on a plane (or a low-dim space) of $\mathbb{R}^p$, chosen in such a manner as to minimize distorting the distances between individuals as little as possible.

Distances and Dispersion

Dispersion of Data

Focusing on distances among all pairs of objects implicitly entails taking into account the **dispersion** or spread (i.e. variation) of the data.

Data Configuration

The reason to pay attention to distances and dispersion is to summarize in a quantitative way the original configuration of the data points.

How to measure dispersion? The concept of Inertia

Sum of Square Distances

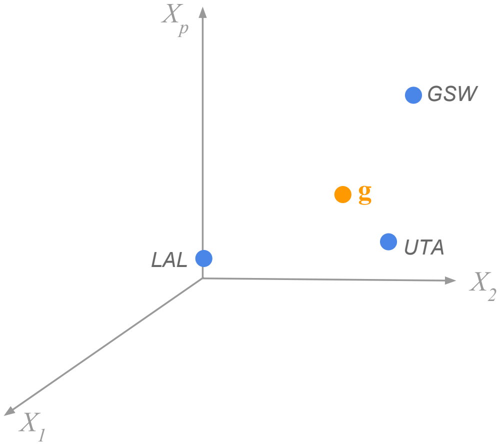
Pair-wise Square distances

One way to consider the dispersion of data (in a mathematical form) is by adding the square distances among all pairs of points.

Square distances from centroid

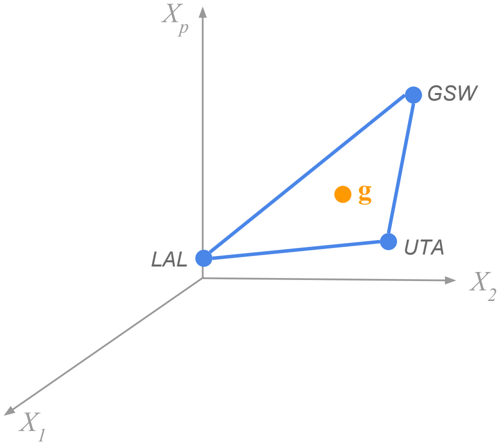
Another way to measure the dispersion of data is by considering the square distances of all points around the center of gravity (i.e. centroid)

Imagine 3 points and its centroid



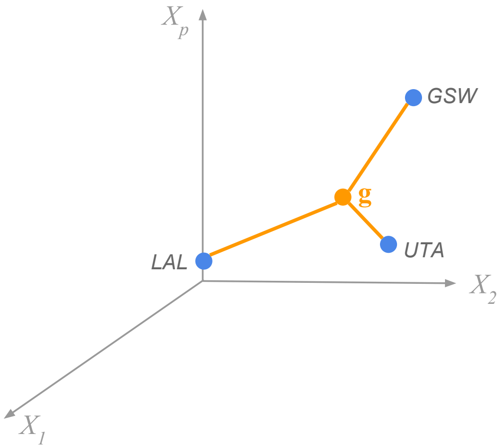
Centroid g is the “average” team.

Dispersion: Sum of square of all dists



$\text{SSD} = 2d^2(\text{LAL}, \text{GSW}) + 2d^2(\text{LAL}, \text{UTA}) + 2d^2(\text{GSW}, \text{UTA})$

Sum of 2n × square dists w.r.t. centroid



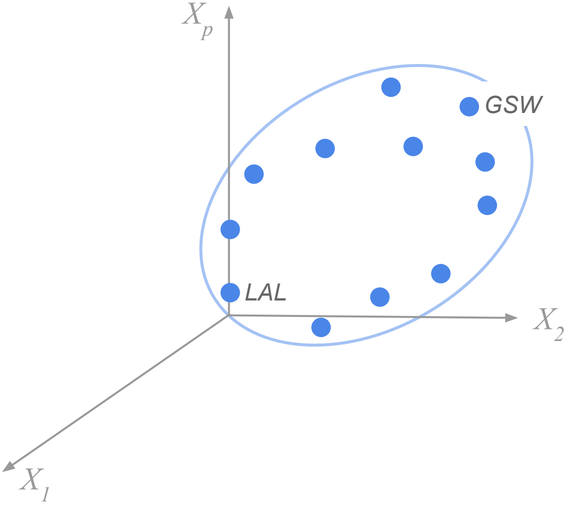
$$\mathsf{SSD} = (2 \times 3) \times \{d^2(\mathsf{LAL}, \mathbf{g}) + 2d^2(\mathsf{GSW}, \mathbf{g}) + 2d^2(\mathsf{UTA}, \mathbf{g})\}$$

Inertia

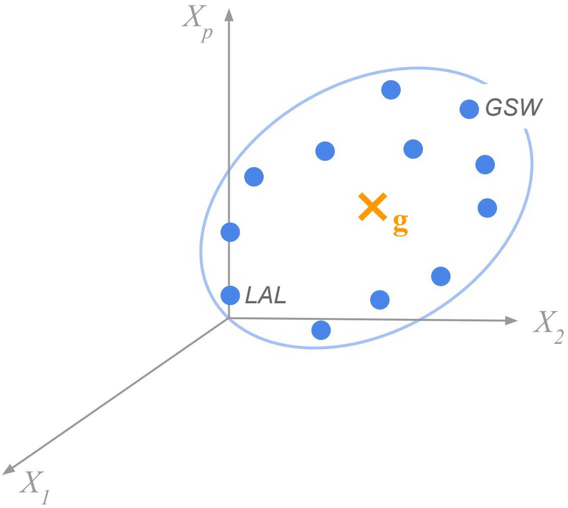
One way to take into account the dispersion of the data is with the concept of **Inertia**.

- Inertia is a term borrowed from the *moment of inertia* in mechanics (physics).
- This involves thinking about data as a rigid body (i.e. particles).
- We use the term Inertia to convey the idea of dispersion in the data.
- In multivariate methods, the term **Inertia generalizes the notion of variance**.
- Think of Inertia as a "multidimensional variance"

Cloud of teams in p-dimensional space



Centroid (i.e. the average team)

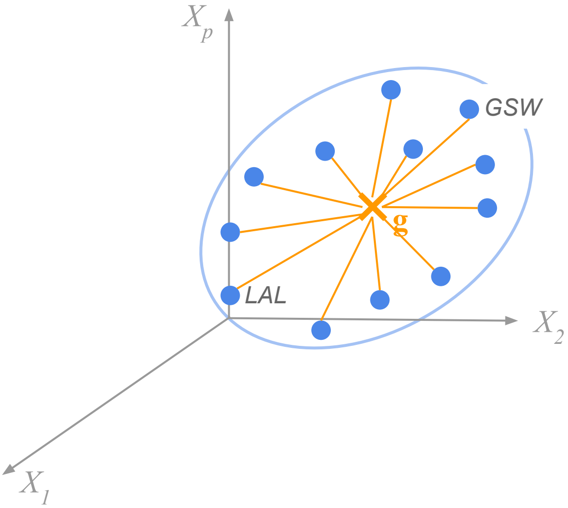


Formula of Total Inertia

The Total Inertia, I, is a weighted sum of square distances among all pairs of objects:

$$I = \frac{1}{2n^2} \sum_{i=1}^{n} \sum_{h=1}^{n} d^2(i, h)$$

Overall variation/spread (around centroid)



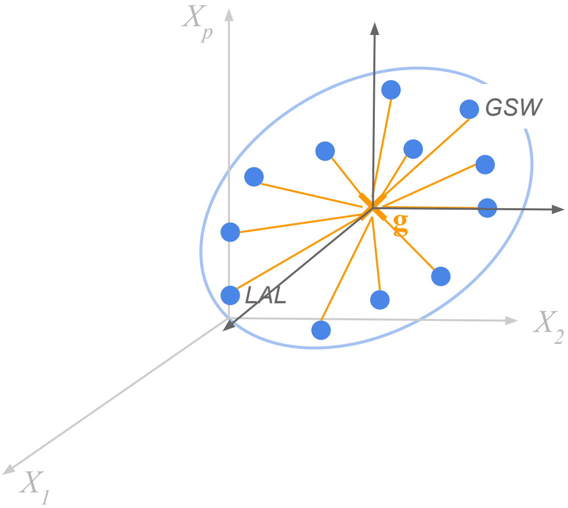
Formula of Total Inertia

Equivalently, the Total Inertia can be calculated in terms of the centoid $\mathbf{g}$:

$$I = \frac{1}{n} \sum_{i=1}^{n} d^2(\mathbf{x_i}, \mathbf{g})$$

The Inertia is an average sum of square distances around the centroid $\mathbf{g}$

Centered data: centroid is the origin



Computing Inertia

$$
\begin{aligned}
Inertia &= \sum_{i=1}^{n} m_i d^2(\mathbf{x_i}, \mathbf{g}) \\
&= \sum_{i=1}^{n} \frac{1}{n} (\mathbf{x_i} - \mathbf{g})^\mathsf{T} (\mathbf{x_i} - \mathbf{g}) \\
&= \frac{1}{n} tr(\mathbf{X}^\mathsf{T} \mathbf{X}) \\
&= \frac{1}{n} tr(\mathbf{X} \mathbf{X}^\mathsf{T})
\end{aligned}
$$

where m_i is the mass (i.e. weight) of individual i, usually $1/n$

Finding Principal Components

Inertia Concept

Inertia and PCA

In PCA we look for a low-dimensional subspace having Projected Inertia as close as possible to the Original Inertia.

Criterion

The criterion used for dimensionality reduction implies that the inertia of a cloud of points in the optimal subspace is maximum (but less than the inertia in the original space).

Criterion

Maximize Projected Inertia

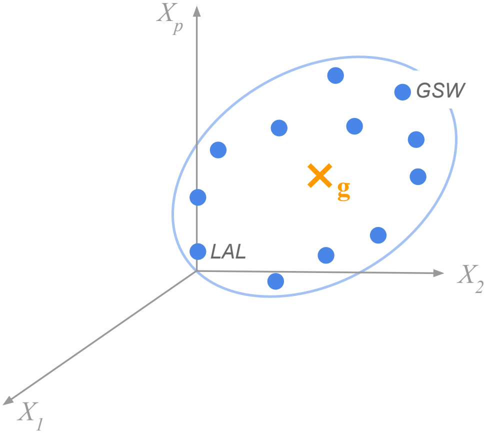
We want to maximize the Projected Inertia on subspace H:

$$max \ \text{projected} \sum_i d_H^2(\mathbf{x_i}, \mathbf{g})$$

Axis of Inertia

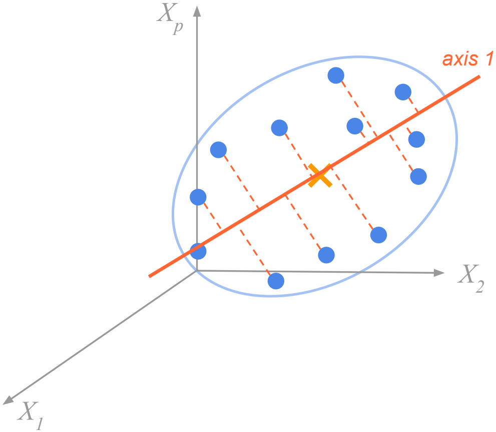
To find the subspace H we can look for each of its axes $\Delta_1, \Delta_2, \ldots, \Delta_k$ and its corresponding vectors $\mathbf{v_1}, \mathbf{v_2}, \ldots, \mathbf{v_k}$ $(k < p)$.

Looking for an axis 1



NBA teams in a p-dimensional space

1st axis



We want a 1st axis that retains most of the projected inertia

First Axis and Principal Component

Projection of object i on axis Δ_1 generated by vector $\mathbf{v_1}$

$$\mathbf{x_i}^\mathsf{T}\mathbf{v_1} = \sum_{j=1}^{p} x_{ij} v_{1j}$$

The 1st component $\mathbf{z_1}$ is the projection of all points on $\mathbf{v_1}$

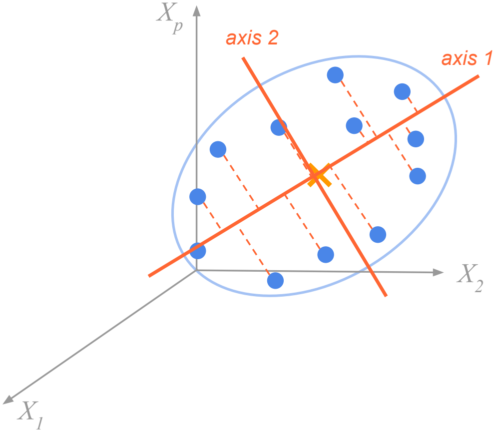
$$\mathbf{X}\mathbf{v_1} = \mathbf{z_1}$$

we don't really manipulate the axis Δ_1, but its associated vector $\mathbf{v_1}$

First Axis and Principal Component

- The axis Δ_1 passes through the centroid $\mathbf{g}$ (with centered data, $\mathbf{g}$ is the origin)
- The axis Δ_1 is created by the unit-norm vector $\mathbf{v_1}$, eigenvector of $\frac{1}{n}\mathbf{X}^\mathsf{T}\mathbf{X}$, associated to the largest eigenvalue λ_1
- The explained inertia by the axis Δ_1 is equal to λ_1
- With standardized data, the proportion of explained inertia by Δ_1 is λ_1/p

2nd axis



We want a 2nd axis, orthogonal to Δ_1, that retains most of the remaining projected inertia

Second Axis and Principal Component

Projection of object i on axis Δ_2 generated by vector $\mathbf{v_2}$

$$\mathbf{x_i}^\mathsf{T} \mathbf{v_2} = \sum_{j=1}^{p} x_{ij} v_{2j}$$

The 2nd component $\mathbf{z_2}$ is the projection of all points on $\mathbf{v_2}$

$$\mathbf{X v_2} = \mathbf{z_2}$$

we don't really manipulate the axis Δ_2, but its associated vector $\mathbf{v_2}$

Second Axis and Principal Component

- The axis Δ_2 passes through the centroid $\mathbf{g}$ and it is perpendicular to Δ_1
- The axis Δ_2 is created by the unit-norm vector $\mathbf{v_2}$, eigenvector of $\frac{1}{n}\mathbf{X}^\mathsf{T}\mathbf{X}$, associated to the second largest eigenvalue λ_2
- The explained inertia by the axis Δ_2 is equal to λ_2
- With standardized data, the proportion of explained inertia by Δ_2 is λ_2/p

Computational note

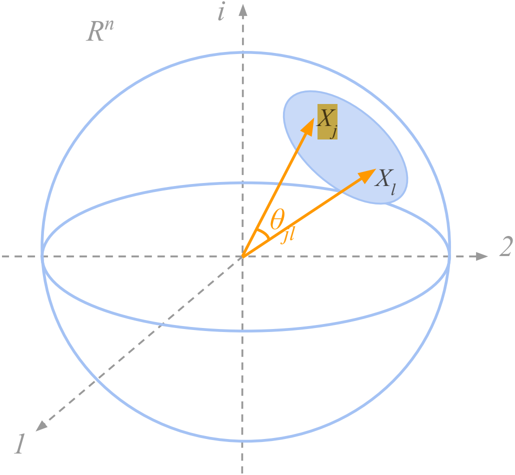
In practice, most software routines for PCA don't really work with the *population covariance* matrix $\frac{1}{n}\mathbf{X}^\top\mathbf{X}$.

Instead, most programs work with the sample covariance matrix: $\frac{1}{n-1}\mathbf{X}^\top\mathbf{X}$

Notice that with standardized data, $\frac{1}{n-1}\mathbf{X}^\top\mathbf{X} = \mathbf{R}$, is the (sample) correlation matrix.

Looking at Variables

Looking at the cloud of standardized variables



Looking at the cloud of standardized variables

- With standardized data, the p variables are located within a hypersphere of radius 1 in an n-dimensional space..
- We represent them graphically as vectors.
- The scalar product between two variables X_j and X_l is:

$$\langle X_j, X_l \rangle = \sum_{i=1}^{n} x_{ij} x_{il} = \|\mathbf{x_j}\| \, \|\mathbf{x_l}\| \, cos(\theta_{jl})$$

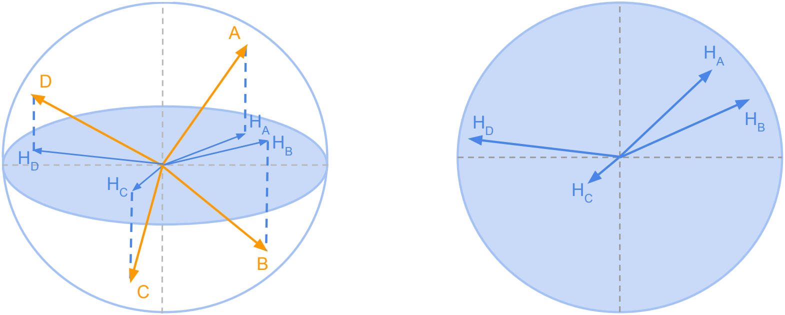
- Notice that:

$$cos(\theta_{jl}) = \frac{\mathbf{x_j}^\mathsf{T} \mathbf{x_l}}{\|\mathbf{x_j}\| \, \|\mathbf{x_l}\|} = cor(X_j, X_l)$$

Projecting the cloud of standardized variables

- The property $cos(\theta_{jl}) = cor(X_j, X_l)$ is essential in PCA
- A representation of the cloud of variables can be used to visualize the correlations (through the angles between variables)
- The cloud of variables is also projected onto a low dimensional space.
- In this case, the distance between two variables is computed with inner products.

Projection of best subspace



Projection of the scatterplot of variables on the main plane of variability

Projecting the cloud of standardized variables

The projection of variable j onto an axis k, is equal to the cosine of the angle θ_{jk}.

The criterion maximizes:

$$\sum_{j=i}^{p} cos^2(\theta_{jk}) = \sum_{j=1}^{p} cor^2(\mathbf{x_j}, \mathbf{z_k})$$

where $\mathbf{z_k}$ is the new variable which is the most correlated with all of the original variables.

Finding subspace for variables

Projection of variable j on axis H_1 generated by vector $\mathbf{u_1}$

$$\mathbf{x_j}^\mathsf{T}\mathbf{u_1} = \sum_{i=1}^{n} x_{ij} u_{i1}$$

The synthetic variable $\mathbf{u_1}$ can be used to obtain a factor $\mathbf{q_1}$

$$\mathbf{X}^\mathsf{T}\mathbf{u_1} = \mathbf{q_1}$$

we don't really manipulate the axis H_1, but its associated vector $\mathbf{u_1}$

Finding subspace for variables

Solution: $\mathbf{u_1}$ is the first eigenvector of $\frac{1}{n}\mathbf{X}\mathbf{X}^\mathsf{T}$, the matrix of inner products between individuals

$$\frac{1}{n}\mathbf{X}\mathbf{X}^\mathsf{T}\mathbf{u_1} = \lambda_1 \mathbf{u_1}$$

The subsequent dimensions are the other eigenvectors $\mathbf{u_2}, \mathbf{u_3}, \ldots$

And the corresponding variable factors are given by:

$$\mathbf{Q} = \mathbf{X}^\mathsf{T}\mathbf{U}$$

Finding subspace for variables

It can be shown that the PCs can also be obtained as:

$$\mathbf{Z} = \frac{1}{\sqrt{n}}\mathbf{U}\mathbf{\Lambda}^{\mathbf{1/2}}$$

where:

- $\mathbf{\Lambda}$ is the diagonal matrix of eigenvectors of $\frac{1}{n}\mathbf{X}\mathbf{X}^{\mathsf{T}}$
- $\mathbf{U}$ is the matrix of eigenvectors of $\frac{1}{n}\mathbf{X}\mathbf{X}^{\mathsf{T}}$

But keep in mind that PCs can be rescaled.

Note that most PCA programs work with $n-1$ instead of n.

Relationship between the representations of Individuals and Variables

Link between representations

$$\text{SVD of:} \quad \frac{1}{\sqrt{n-1}}\mathbf{X} = \mathbf{U}\mathbf{D}\mathbf{V}^\mathsf{T}$$

$$\mathbf{Z} = \mathbf{X}\mathbf{V} = \frac{1}{\sqrt{n-1}}\mathbf{X}\mathbf{Q}\mathbf{D}^{\mathbf{-1}} \quad \Rightarrow \quad \mathbf{V} = \frac{1}{\sqrt{n-1}}\mathbf{Q}\mathbf{D}^{\mathbf{-1}}$$

$$\mathbf{Q} = \mathbf{X}^\mathsf{T}\mathbf{U} = \frac{1}{\sqrt{n-1}}\mathbf{X}^\mathsf{T}\mathbf{Z}\mathbf{D}^{\mathbf{-1}} \quad \Rightarrow \quad \mathbf{U} = \frac{1}{\sqrt{n-1}}\mathbf{Z}\mathbf{D}^{\mathbf{-1}}$$

Link between representations

Principal Components or Scores

$$z_{ik} = \frac{1}{\sqrt{n-1}} \times \frac{1}{\sqrt{\lambda_k}} \times \sum_{j=1}^{p} x_{ij} q_{jk}$$

Factors for Variables

$$q_{jk} = \frac{1}{\sqrt{n-1}} \times \frac{1}{\sqrt{\lambda_k}} \times \sum_{i=1}^{n} x_{ij} z_{ik}$$

Principal Components?

Meaning of *Principal*

The term **Principal**, as used in PCA, has to do with the notion of **principal axis** from geometry and linear algebra

Principal Axis

A *principal axis* is a certain line in a Euclidean space associated to an ellipsoid or hyperboloid, generalizing the major and minor axes of an ellipse

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