Principal Components Analysis (part II)

Predictive Modeling & Statistical Learning

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Applying PCA

Painstaking PCA

In these slides I will show you how to perform what I consider a *full* / *exhaustive* Principal Components Analysis.

BTW: Most textbooks do not discuss all of the steps that I cover here. Sadly, most authors focus on just the decompositions, inspection of eigenvalues and loadings, scatterplot(s) of PCs, and the so-called biplot.

But you should know that there are more things to look at in a PCA.

Exhaustive PCA

Roadmap

- Determine **active** individuals and variables.
- Determine **supplementary** individuals and variables.
- Data transformation (e.g. usually standardized data).
- EVD or SVD of some data-based matrix.
- Computation of eigenvalues, loadings, and PCs.
- Determine how many dimensions (i.e. PCs) to retain.
- Interpretation tools:
  Plots, Quality measures, Contributions, stability, etc

PCA of NBA Team Stats

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`

Stats | Stats Home | Players | Teams | Advanced | Scores | Schedule | Hustle Stats

SEARCH FOR A PLAYER OR TEAM

Insights from SAP

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')

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"
```

Active and Supplementary Elements

Active vs Supplementary

Active

Selected individuals (rows) and variables (columns) that are used to compute eigenvalues, loadings and PCs.

Supplementary

Additional individuals and variables not used in the computation steps, but taken into account for interpretation purposes, and/or further data exploration.

Which Variables?

We are going to focus the analysis on the following **active** variables:

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

"Active" means these are the variables used to compute PCs.

Which Variables?

Supplementary Variables

Among the rest of the variables, we are going to consider three **supplementary** variables:

- `points3`
- `rebounds`
- `personal_fouls`

"Supplementary" means these variables are NOT used to compute PCs, but we will take them into account during the interpretation phase.

Which Individuals?

Active Individuals

All of the teams in season 2016-2017

Supplementary Individuals

Warriors and Cavaliers 2015-2016

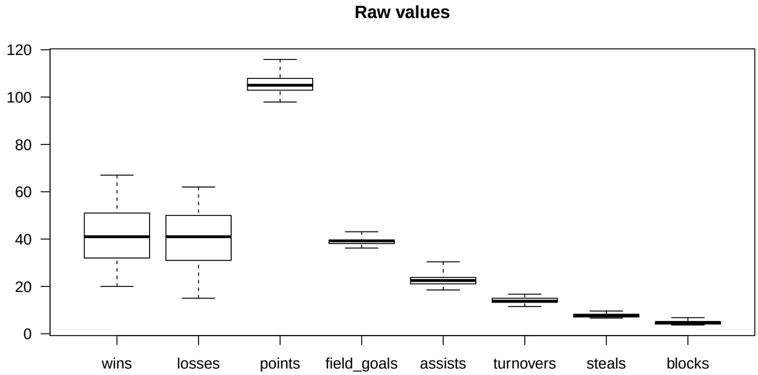
Transformation of Variables

Importance of Variables

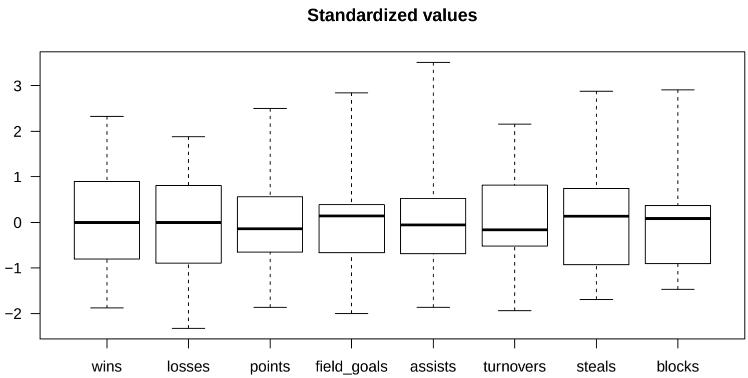
To standardize or not?

- A key issue has to do with the scale of the variables.
- If variables have different units of measurement, then we should standardize them to avoid variables with larger scales dominate the analysis.
- If variables have the same units:
  - you could leave them unstandardized
  - or you could standardize them (strongly suggested)

Regardless of the scaling decision, we operate on centered data.



If you use the raw scales, `wins` and `losses` will dominate the analysis due to their larger scales.



By standardizing the variables, they all play the same role.

PCA Basic Results (via EVD or SVD)

PCA via EVD

Let's work on the standardized data, denoted with matrix $\mathbf{X}$.

One way to obtain the basic results of PCA involves computing the eigenvalue decomposition of the (sample) correlation matrix $\mathbf{R} = \frac{1}{n-1}\mathbf{X}^\mathsf{T}\mathbf{X}$

$$\mathbf{R} = \mathbf{V}\mathbf{\Lambda}\mathbf{V}^\mathsf{T}$$

where:

- $\mathbf{V}$ is the matrix of eigenvectors
- $\mathbf{\Lambda}$ is the diagonal matrix of eigenvalues

PCA Essential Results

The core results of a PCA (via EVD) consists of:

- Eigenvalues: $\lambda_1, \lambda_2, \ldots, \lambda_r$
  where r is the rank of $\mathbf{X}$
- Loadings (i.e. $p \times r$ matrix of eigenvectors): $\mathbf{V}$
- Principal Components or Scores ($n \times r$ matrix): $\mathbf{Z}$

Essential Results: Eigenvalues

The eigenvalues $\lambda_1, \lambda_2, \dots, \lambda_r$ capture the projected inertia (i.e. variation) on each extracted dimension.

When $\mathbf{X}$ is standardized, the sum of eigenvalues equals the number of variables:

$$\sum_{k=1}^{r} \lambda_k = p \quad \longrightarrow \quad \text{total inertia}$$

and thus you can compute the proportion of of variation captured by each PC:

$$\lambda_k / p$$

Essential Results: PCs or Scores

The Principal Components (aka Scores), $\mathbf{Z}$, are obtained as:

$$\mathbf{Z} = \mathbf{X}\mathbf{V}$$

- Note that PCs are linear combinations of the variables.
- The coefficients are given by the eigenvectors $\mathbf{V}$, also referred to as Loadings in PCA terminology.
- The elements in a given loading $\mathbf{v_k} = \{v_{1k}, \ldots, v_{pk}\}$ reflect how much each variable X_j *loads* in the PC k.

How many PCs to retain?

Various criteria

Typical criteria used to determine the number of dimensions to retain:

- Screeplot (see if there's an "elbow")
- Predetermined amount of variation
- Kaiser rule
- Jollife rule

There's no universal agreement on which criterion is the best.

Table of Eigenvalues

The inspection of eigenvalues is done with a summary table like this:

	eigenvalues	proportion	cum_prop
comp1	3.68	46.01	46.01
comp2	1.62	20.22	66.23
comp3	1.02	12.73	78.96
comp4	0.62	7.77	86.73
comp5	0.47	5.90	92.63
comp6	0.46	5.77	98.40
comp7	0.13	1.60	100.00
comp8	0.00	0.00	100.00

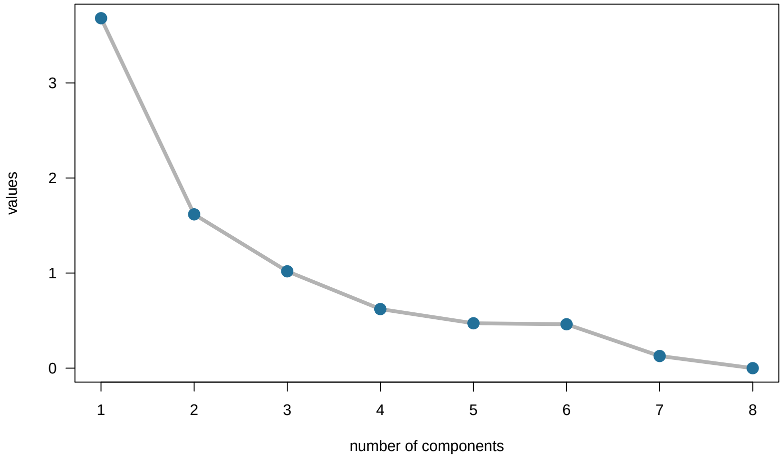
What's going on with eigenvalue of PC8?

Table of Eigenvalues

When working with standardized data, the total amount of variation (i.e. total inertia) is equal to the number of variables.

You can calculate the portion of variation captured by each PC, as well as the cumulative proportion.

Screeplot of eigenvalues



Look for an "elbow"

Predetermined amount of variation

One option to decide how many PCs to retain, consists of predefining a specified portion of variation: e.g. 60% or 70%

```
      eigenvalues proportion cum_prop
comp1      3.6806    46.0071  46.0071
comp2      1.6177    20.2214  66.2285
```

Kaiser's Rule

Another criterion to decide how many PCs to keep, is the so-called Kaiser's rule, which consists of retaining those PCs with eigenvalues $\lambda_k > 1$

```
      eigenvalues proportion cum_prop
comp1    3.680569   46.00711 46.00711
comp2    1.617713   20.22142 66.22853
comp3    1.018539   12.73174 78.96027
```

Jollife's Rule

An alternative to Kaiser's rule is the less known Jollife's rule, in which we retain those PCs with eigenvalues $\lambda_k > 0.7$

```
      eigenvalues proportion cum_prop
comp1    3.680569   46.00711 46.00711
comp2    1.617713   20.22142 66.22853
comp3    1.018539   12.73174 78.96027
```

Studying the Individuals

Studying the Individuals

When studying the individuals, we typically pay attention to:

- Scatterplots of PCs
- Quality of representation
- Individual Contributions to PCs

Principal Components

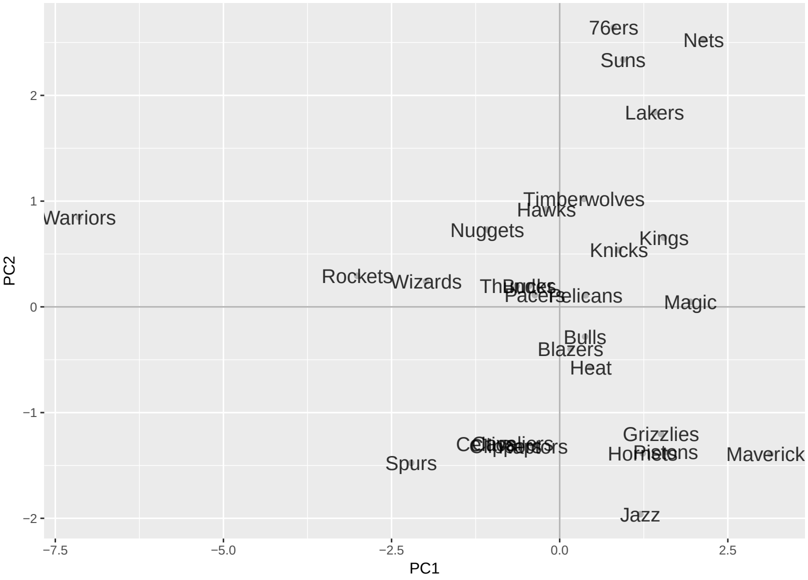
PCs are typically given by: $\mathbf{Z} = \mathbf{X}\mathbf{V}$, although it is possible to rescale them (e.g. variance = 1 or unit-norm)

The first 10 rows of each PC are given below:

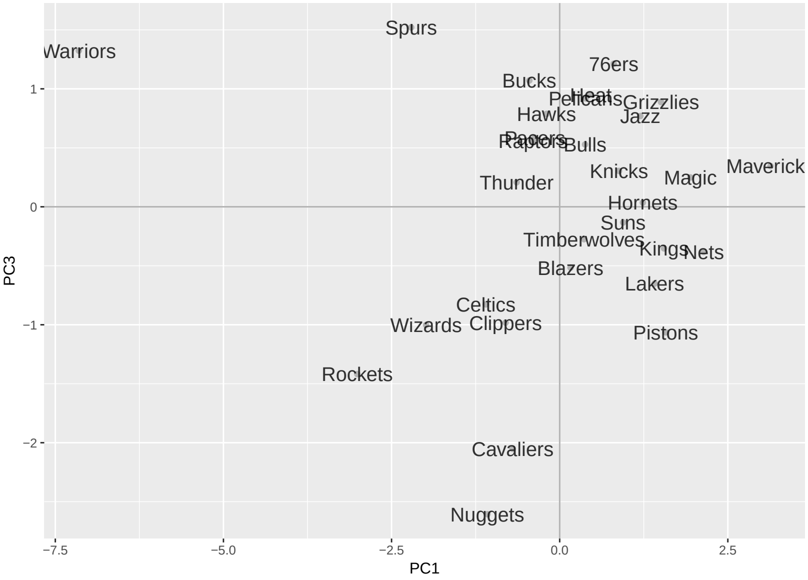
	PC1	PC2	PC3	PC4	PC5	PC6	PC7	PC8
Warriors	-7.150	0.848	1.324	0.369	-0.687	-0.606	-0.024	0
Spurs	-2.208	-1.475	1.521	0.186	0.086	0.546	0.261	0
Rockets	-3.010	0.294	-1.418	-0.842	0.194	0.454	-0.646	0
Celtics	-1.098	-1.298	-0.827	-0.875	-0.869	0.340	-0.257	0
Jazz	1.200	-1.961	0.770	0.147	0.341	1.686	0.295	0
Raptors	-0.394	-1.318	0.560	-0.162	2.078	-0.553	-0.401	0
Cavaliers	-0.699	-1.290	-2.052	0.398	0.059	0.848	0.018	0
Clippers	-0.805	-1.313	-0.982	-0.232	0.295	-0.071	-0.195	0
Wizards	-1.986	0.242	-1.002	-0.802	0.491	-0.878	0.492	0
Thunder	-0.640	0.197	0.208	-0.023	1.104	0.631	0.227	0

notice what happens with the last PC

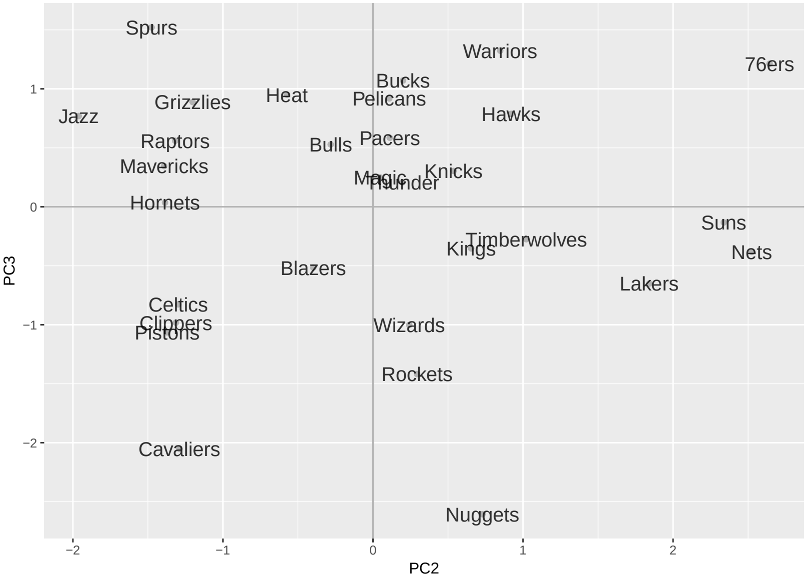
Scatterplot of individuals on PC1 and PC2



Scatterplot of individuals on PC1 and PC3

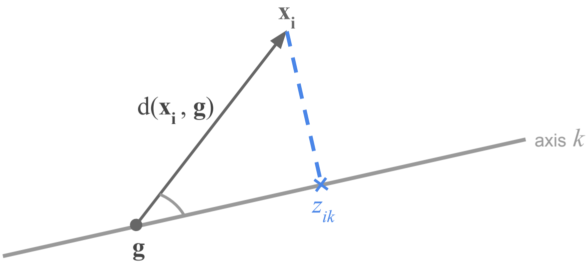


Scatterplot of individuals on PC2 and PC3



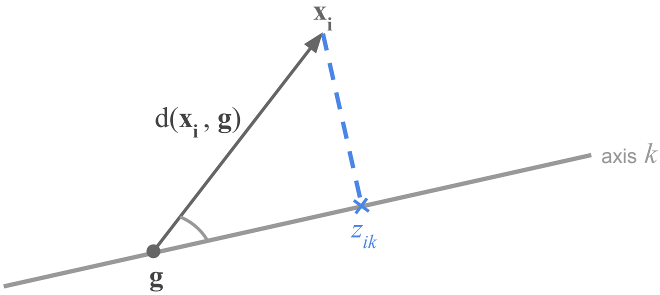
Quality of Representation

In addition to the PC plots, you can assess the quality of the individuals representation on a given dimension.



How good is the projection z_{ik} on axis k?

Quality of Representation



$$cos^2(i,k) = \frac{z_{ik}^2}{d^2(\mathbf{x_i}, \mathbf{g})}$$

Quality of Representation

$$cos^2(i,k) = \frac{z_{ik}^2}{d^2(\mathbf{x_i}, \mathbf{g})}$$

where:

- z_{ik} is the value of k-th PC for individual i
- $d^2(\mathbf{x_i}, \mathbf{g})$ is the squared distance of individual i to the centroig $\mathbf{g}$
- recall that with centered data, $\mathbf{g}$ is the origin

Cosine^2 equal to 1 indicates that individual i is exactly on axis Δ_k (angle zero). Conversely, a cosine^2 equal to 0 indicates that the individual i is on an orthogonal direction of axis Δ_k.

Quality of Representation

Adding the squared cosines over all principal axes for a given individual, we get:

$$\sum_{k=1}^{r} cos^2(i,k) = 1$$

This sum provides, in percentages, the "quality" of the representation of an individual on the subspace defined by the principal axes.

Quality of Representation

First 6 rows of $cos^2(i,k)$ for $k = 1, 2, 3, 4$

	PC1	PC2	PC3	PC4
Warriors	0.93682873	0.013170110	0.03212084	0.002495688
Spurs	0.49881739	0.222735807	0.23665382	0.003536342
Rockets	0.72317632	0.006904138	0.16053335	0.056596224
Celtics	0.22852854	0.319227201	0.12961118	0.144959032
Jazz	0.16098822	0.429843158	0.06618774	0.002415628
Raptors	0.02216717	0.247608673	0.04463893	0.003743516

Note that Warriors has a value close to 1 on PC1. On the other hand, Raptors has a value close to zero on PC1.

Quality of Representation

The squared cosine is used to evaluate the quality of the representation.

On a given PC, some distances between individuals will be well represented, while other distances will be highly distorted.

You can add the squared cosines of an individual over different axes, resulting in a “quality” measure of how well that individual is represented in that subspace.

Individual's Contributions

Another diagnostic tool involves assessing the importance of an observation for a given component by calculating what is known as **contribution**:

$$ctr(i, k) = \frac{m_i z_{ik}^2}{\lambda_k} \times 100$$

where:

- m_i is the mass or weight of individual i, in our case: $(\frac{1}{n-1})$
- z_{ik} is the value of k-th PC for individual i
- λ_k is the eigenvalue associated to k-th PC

Contributions

- $ctr(i, k)$ is the contribution of an individual to the construction of component k.
- The contribution is calculated as the percentage of inertia explained by the individual i on the component k
- The value of a contribution is between 0 and 100.
- For a given component, the sum of the contributions of all observations is equal to 100.
- The larger the value of the contribution, the more the individual contributes to the component.

Contributions

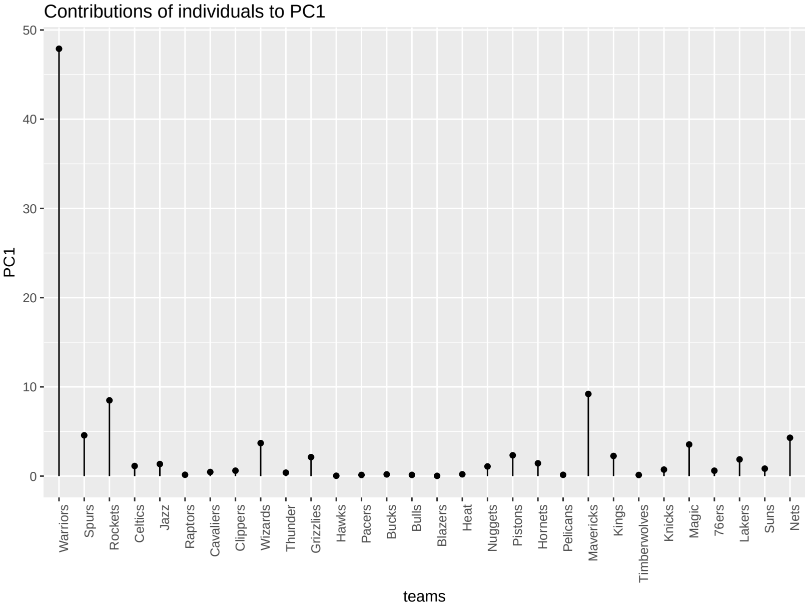
- A useful heuristic is to examine those contributions that are larger than the average contribution: larger than $\frac{100}{n-1}$
- If all individuals had a uniform contribution to a given PC, then they would have a contribution of $ctr(i,k) = \frac{100}{n-1}$.
- Outliers have an influence, and it is interesting to know to what extent their influence affects the construction of the components.
- Detecting those individuals that contribute to a given PC helps to assess the component's stability.

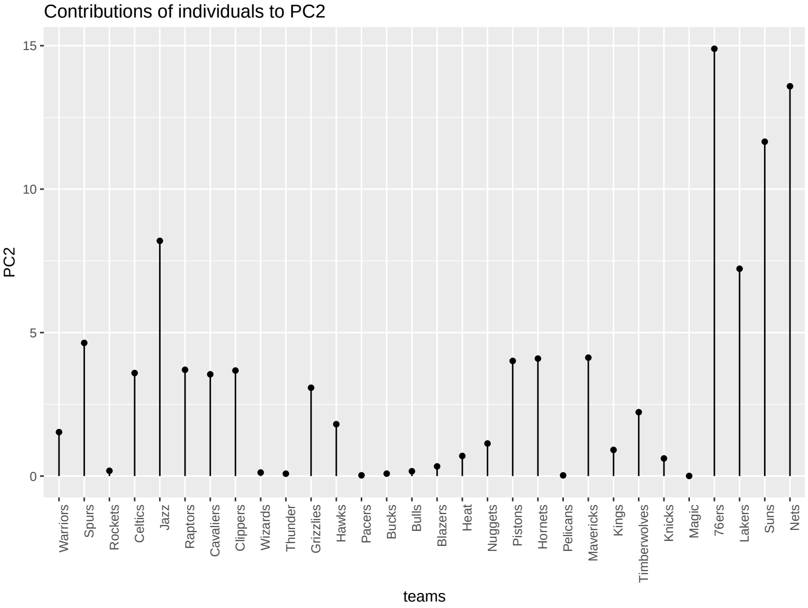
Contributions

First 6 rows of $ctr(i, k)$ for $k = 1, 2, 3, 4$

	PC1	PC2	PC3	PC4
Warriors	47.8979178	1.5320017	5.934452	0.7557724
Spurs	4.5678923	4.6406383	7.831142	0.1918107
Rockets	8.4869097	0.1843437	6.807819	3.9340253
Celtics	1.1297516	3.5905074	2.315380	4.2445545
Jazz	1.3495386	8.1981272	2.004962	0.1199404
Raptors	0.1457559	3.7042069	1.060638	0.1457941

Note that Warriors has a large contribution to PC1. On the other hand, Raptors has a value close to zero on PC1.


Contributions of individuals to PC1
PC1
teams
0
10
20
30
40
50
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


Contributions of individuals to PC2
15
10
5
0
PC2
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
teams

More about Contributions

The variance of $\mathbf{z_k}$ is equal to:

$$var(\mathbf{z_k}) = \sum_{i=1}^{n} m_i z_{ik}^2 = \lambda_k$$

which corresponds to the k-th eigenvalue.

Representing Supplementary Individuals

Supplementary Individuals?

The supplementary individuals are Warriors and Cavaliers 2015-2016, and the corresponding data is in the file `nba-teams-2016.csv`

```
# supplementary individuals
datsup <- read.csv('data/nba-teams-2016.csv')
```

Representing Supplementary Individuals

The representation of supplementary individuals is done by projecting them on the PCs.

With standardized data, you need to center and scale the supplementary individuals according the mean and standard deviation from the active individuals.

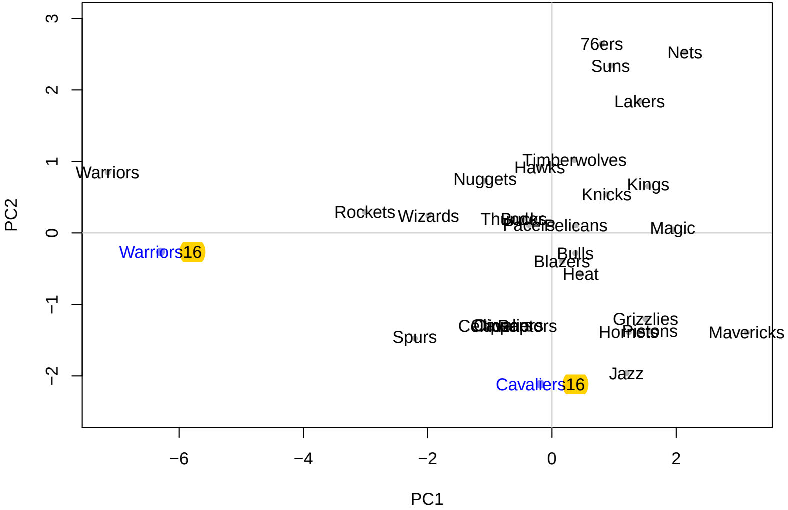
Representing Supplementary Individuals

Projecting supplementary individuals

- Let $\mathbf{v_k}$ be the k-th loading
- Let $\mathbf{x_{i^*}}$ represent the i-th supplementary individual
- Let $\hat{\mathbf{x}}_{\mathbf{i^*}}$ represent the projection of supplementary individual i onto the k-th PC

$$\hat{\mathbf{x}}_{\mathbf{i^*}} = \mathbf{x}_{\mathbf{i^*}}^{\top} \mathbf{v_k}$$

PCA plot with supplementary teams



Study of cloud of Variables

Studying the Variables

When studying the variables, we typically pay attention to:

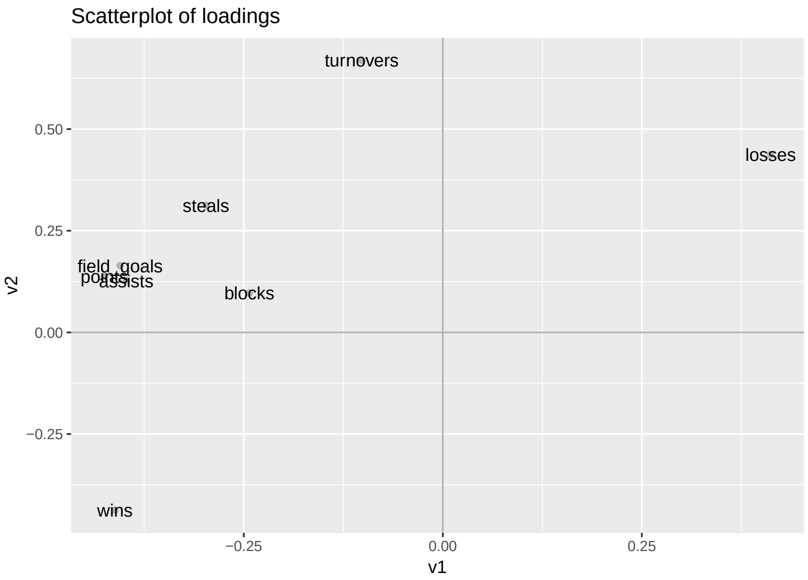
- Scatterplots of loadings (or some loading-based results)
- Quality of representation of variables
- Variables Contributions to PCs

Loadings (or eigenvectors)

	v1	v2	v3	v4	v5	v6	v7	v8
wins	-0.412	-0.4375	0.0541	-0.187	0.13813	0.2555	0.1291	7.07e-01
losses	0.412	0.4375	-0.0541	0.187	-0.13813	-0.2555	-0.1291	7.07e-01
points	-0.425	0.1378	-0.4490	0.160	0.16307	0.0476	-0.7379	0.00e+00
field_goals	-0.405	0.1642	-0.3302	0.412	0.20321	-0.3998	0.5734	1.67e-16
assists	-0.398	0.1270	-0.0301	-0.127	-0.89704	-0.0468	0.0422	-2.78e-17
turnovers	-0.102	0.6692	-0.0487	-0.191	0.14633	0.6489	0.2461	6.94e-17
steals	-0.297	0.3128	0.4178	-0.544	0.26045	-0.5119	-0.1176	0.00e+00
blocks	-0.243	0.0972	0.7111	0.622	-0.00466	0.1487	-0.1315	0.00e+00

Interpreting PCs

- Being linear combinations of the studied variables, PCs can sometimes being interpreted
- Analysts try to label them in some meaningful way
- This is useful, but not always possible
- You can look at the magnitude of the loadings
- You can also look at the correlations between variables and PCs

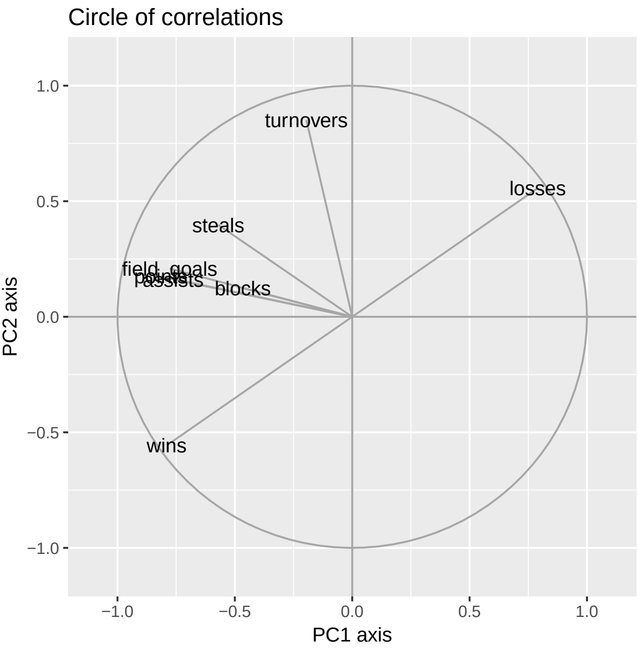

Scatterplot of loadings
turnovers
losses
steals
field_goals
points
assists
blocks
wins
0.50
0.25
0.00
−0.25
−0.25
0.00
0.25
v1
v2

Correlations between Variables and PCs

A more informative interpretation can be obtained by calculating the correlations between the Variables and PCs, and use them to plot a *Circle of Correlations*:

	PC1	PC2	PC3	PC4	PC5	PC6	PC7	PC8
wins	-0.790	-0.556	0.055	-0.148	0.095	0.174	0.046	-0.793
losses	0.790	0.556	-0.055	0.148	-0.095	-0.174	-0.046	0.793
points	-0.815	0.175	-0.453	0.126	0.112	0.032	-0.264	0.005
field_goals	-0.777	0.209	-0.333	0.325	0.140	-0.272	0.205	0.185
assists	-0.763	0.162	-0.030	-0.100	-0.616	-0.032	0.015	-0.155
turnovers	-0.195	0.851	-0.049	-0.150	0.101	0.441	0.088	0.531
steals	-0.571	0.398	0.422	-0.428	0.179	-0.348	-0.042	-0.047
blocks	-0.466	0.124	0.718	0.490	-0.003	0.101	-0.047	-0.126

These correlations are collinear with the loadings


Circle of correlations
turnovers
losses
steals
field goals
points
assists
blocks
wins
1.0
0.5
0.0
−0.5
−1.0
PC2 axis
−1.0
−0.5
0.0
0.5
1.0
PC1 axis

Squared Correlations

- The correlation between a component and a variable estimates the information they share.
- Note that the sum of the squared coefficients of correlation between a variable and all the components is equal to 1.
- As a consequence, the squared correlations are easier to interpret than the loadings.
- This is because the squared correlations give the proportion of the variance of the variables explained by the components.

Squared Correlations

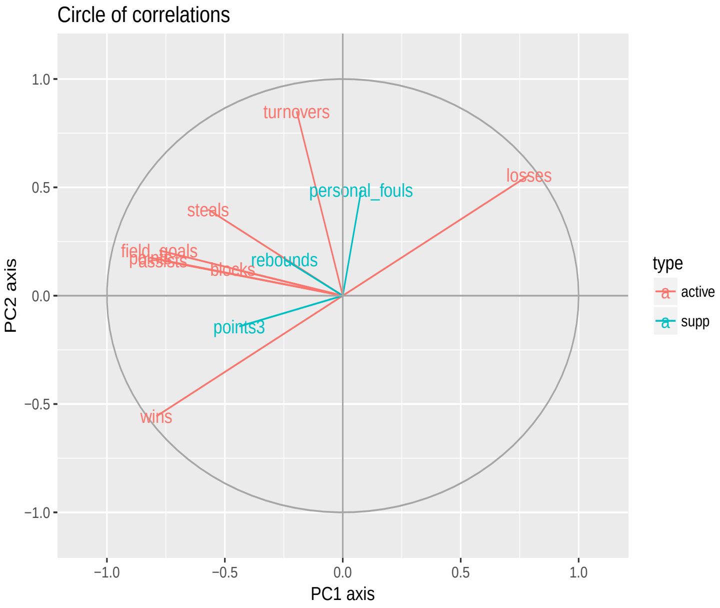
	PC1	PC2	PC3	PC4	PC5	PC6	PC7
wins	0.624	0.310	0.003	0.022	0.009	0.030	0.002
losses	0.624	0.310	0.003	0.022	0.009	0.030	0.002
points	0.665	0.031	0.205	0.016	0.013	0.001	0.070
field_goals	0.604	0.044	0.111	0.106	0.019	0.074	0.042
assists	0.582	0.026	0.001	0.010	0.380	0.001	0.000
turnovers	0.038	0.724	0.002	0.023	0.010	0.194	0.008
steals	0.326	0.158	0.178	0.184	0.032	0.121	0.002
blocks	0.217	0.015	0.515	0.240	0.000	0.010	0.002

Representing
Supplementary Variables

Correlations between all Variables and PCs

Correlations with all (active and supplementary) variables:

	PC1	PC2	PC3	PC4	PC5	PC6	PC7	type
wins	-0.790	-0.556	0.055	-0.148	0.095	0.174	0.046	active
losses	0.790	0.556	-0.055	0.148	-0.095	-0.174	-0.046	active
points	-0.815	0.175	-0.453	0.126	0.112	0.032	-0.264	active
field_goals	-0.777	0.209	-0.333	0.325	0.140	-0.272	0.205	active
assists	-0.763	0.162	-0.030	-0.100	-0.616	-0.032	0.015	active
turnovers	-0.195	0.851	-0.049	-0.150	0.101	0.441	0.088	active
steals	-0.571	0.398	0.422	-0.428	0.179	-0.348	-0.042	active
blocks	-0.466	0.124	0.718	0.490	-0.003	0.101	-0.047	active
points3	-0.439	-0.142	-0.353	-0.123	-0.233	0.369	-0.425	supp
rebounds	-0.247	0.168	-0.219	0.423	0.235	0.148	0.206	supp
personal_fouls	0.078	0.488	0.021	-0.148	0.474	-0.002	-0.153	supp


Circle of correlations
turnovers
losses
personal_fouls
steals
field_goals
points
assists
blocks
rebounds
points3
wins
1.0
0.5
0.0
−0.5
−1.0
PC2 axis
−1.0
−0.5
0.0
0.5
1.0
PC1 axis
type
active
supp

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