Dimension Reduction

Principal components analysis (PCA)

June 29th, 2021

What is the goal of dimension reduction?

We have p variables (columns) for n observations (rows) **BUT** which variables are **interesting**?

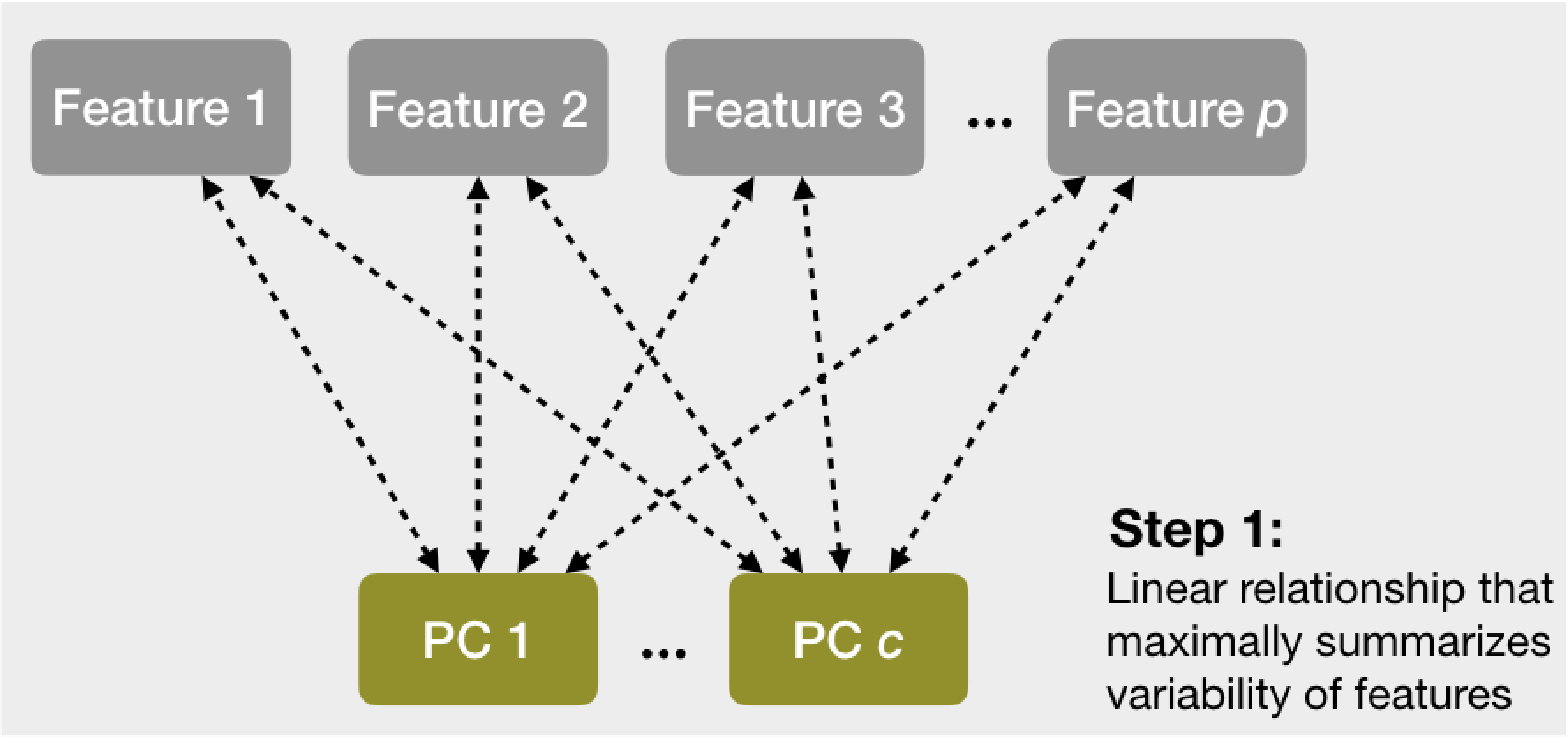
Can we find a smaller number of dimensions that captures the **interesting** structure in the data?

- Could examine all pairwise scatterplots of each variable - tedious, manual process
- Last week: clustered variables based on correlation
- Can we find a combination of the original p variables?

Dimension reduction:

- Focus on reducing the dimensionality of the feature space (i.e., number of columns),
- While **retaining** most of the information / **variability** in a lower dimensional space (i.e., reducing the number of columns)

Principal components analysis (PCA)



Principal components analysis (PCA)

- PCA explores the **covariance** between variables, and combines variables into a smaller set of **uncorrelated** variables called **principal components (PCs)**
- PCs are **weighted**, linear combinations of the original variables
    - Weights reveal how different variables are ***loaded*** into the PCs
- We want a **small number of PCs** to explain most of the information / variance in the data

First principal component:

$$Z_1 = \phi_{11}X_1 + \phi_{21}X_2 + \cdots + \phi_{p1}X_p$$

- ϕ_{j1} are the weights indicating the contributions of each variable $j \in 1, \ldots, p$
- Weights are normalized $\sum_{j=1}^{p} \phi_{j1}^2 = 1$
- $\phi_1 = (\phi_{11}, \phi_{21}, \ldots, \phi_{p1})$ is the **loading vector** for PC1
- Z_1 is a linear combination of the p variables that has the **largest variance**

Principal components analysis (PCA)

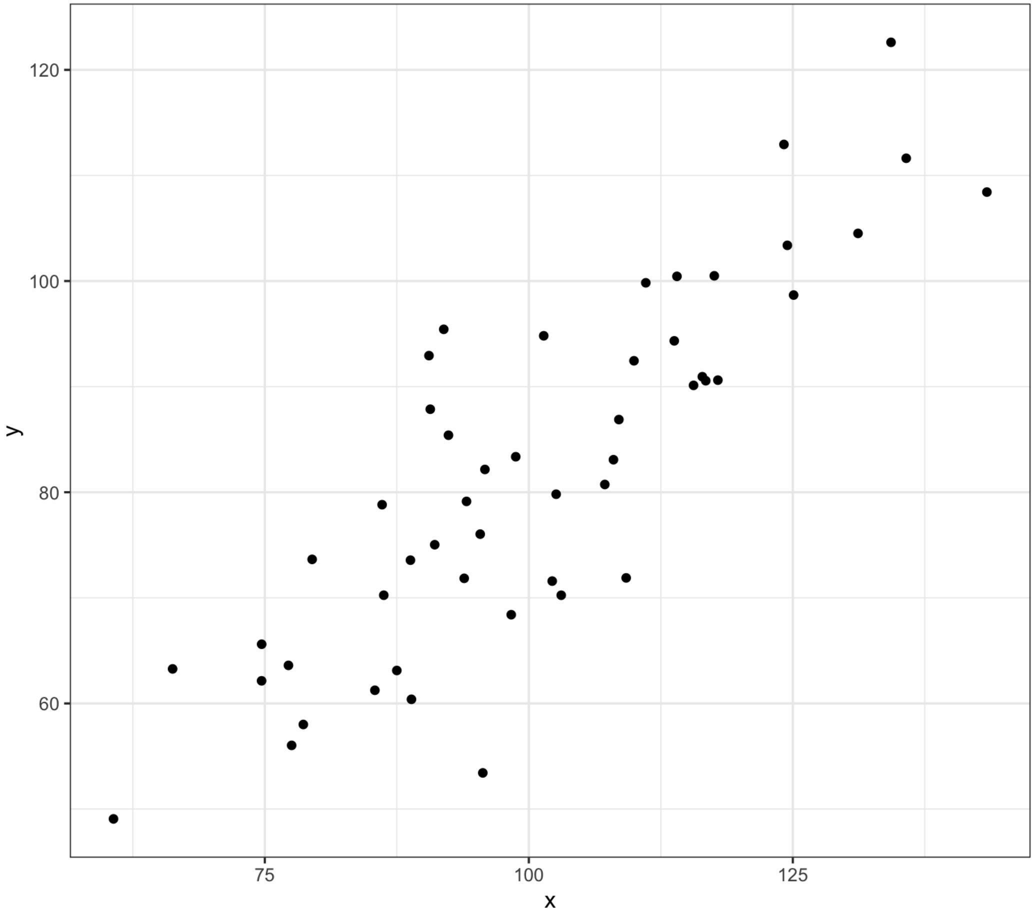
Second principal component:

$$Z_2 = \phi_{12} X_1 + \phi_{22} X_2 + \cdots + \phi_{p2} X_p$$

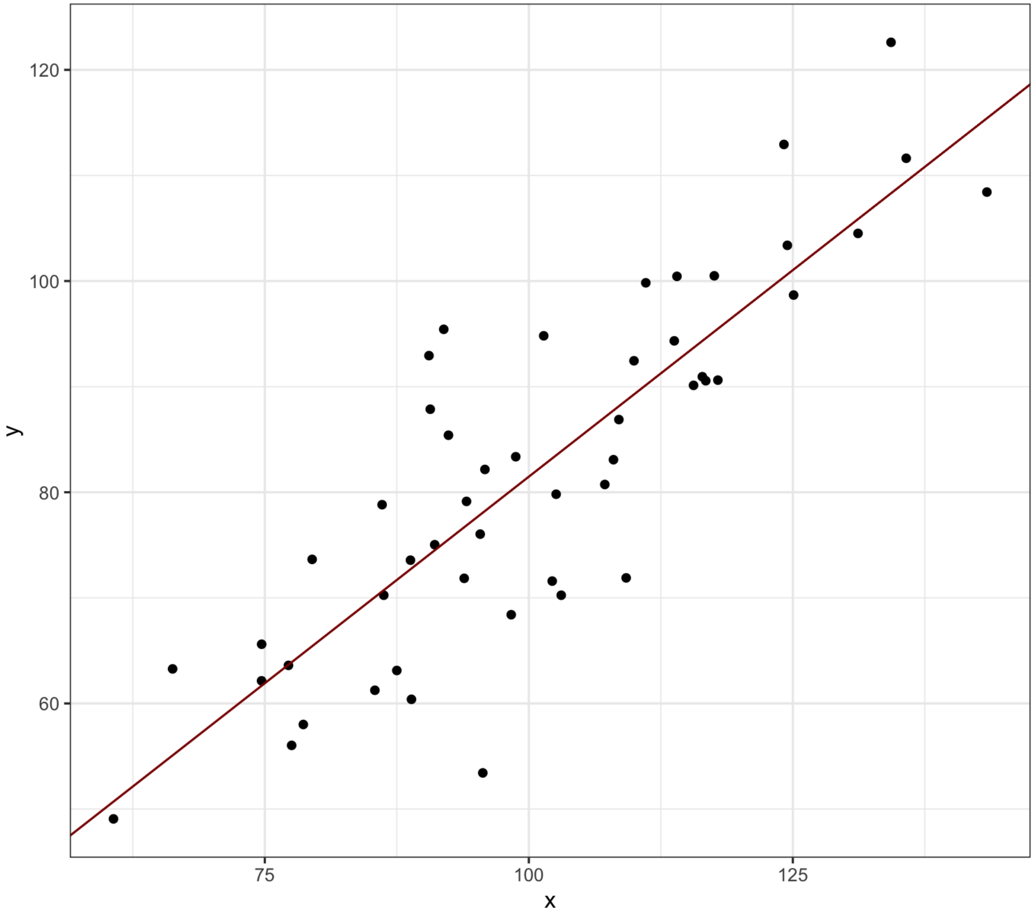
- ϕ_{j2} are the weights indicating the contributions of each variable $j \in 1, \ldots, p$
- Weights are normalized $\sum_{j=1}^p \phi_{j1}^2 = 1$
- $\phi_2 = (\phi_{12}, \phi_{22}, \ldots, \phi_{p2})$ is the **loading vector** for PC2
- Z_2 is a linear combination of the p variables that has the **largest variance**
    - **Subject to constraint it is uncorrelated with Z_1**

We repeat this process to create p principal components

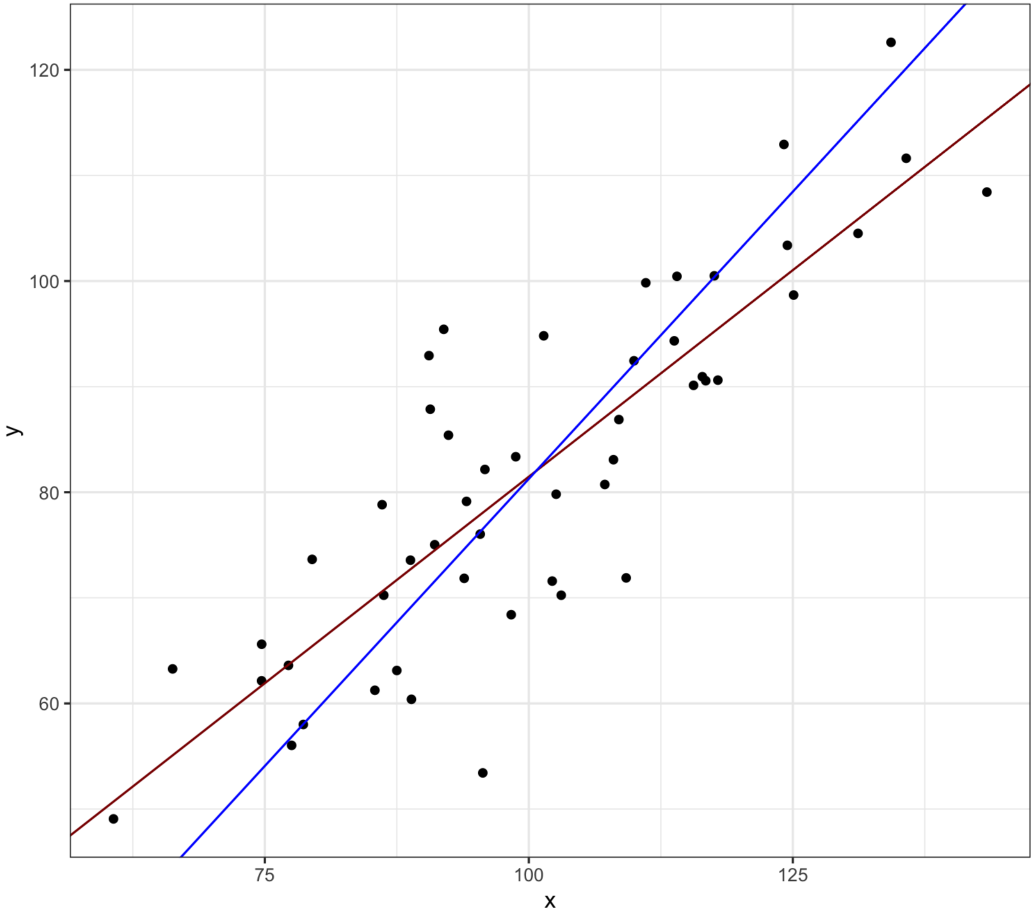
Visualizing PCA in two dimensions



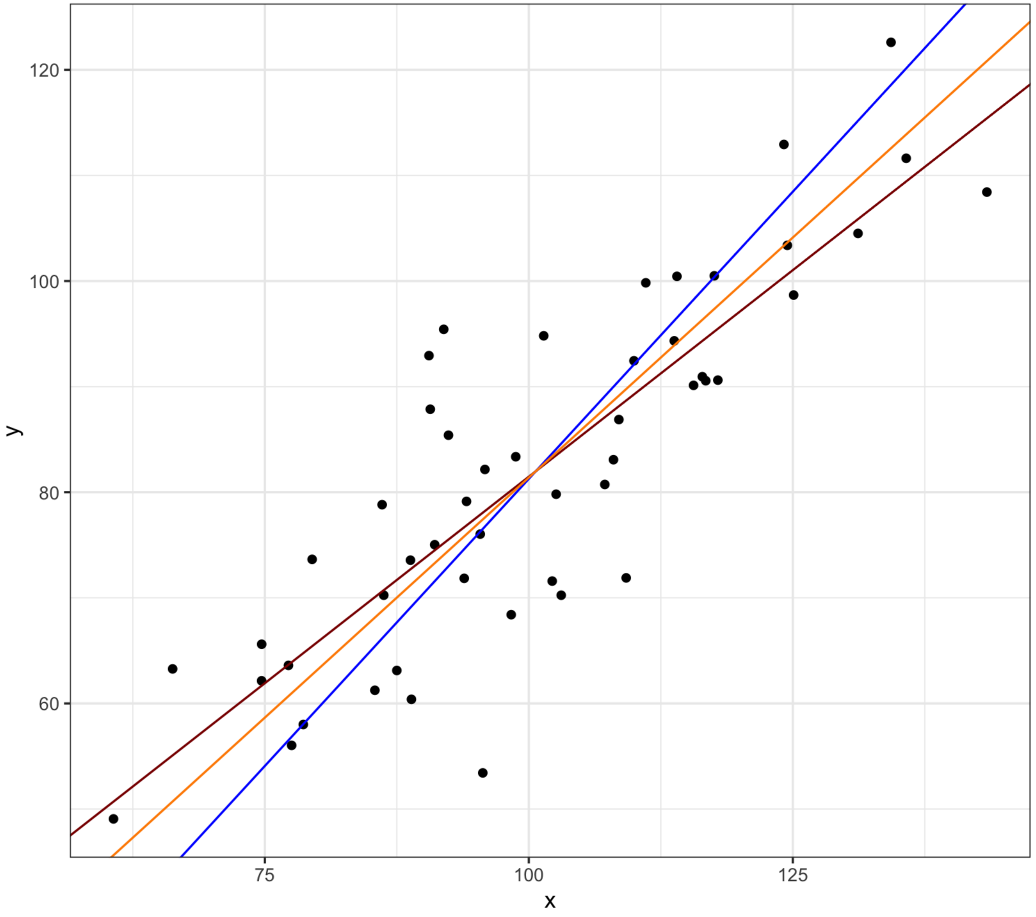
Visualizing PCA in two dimensions



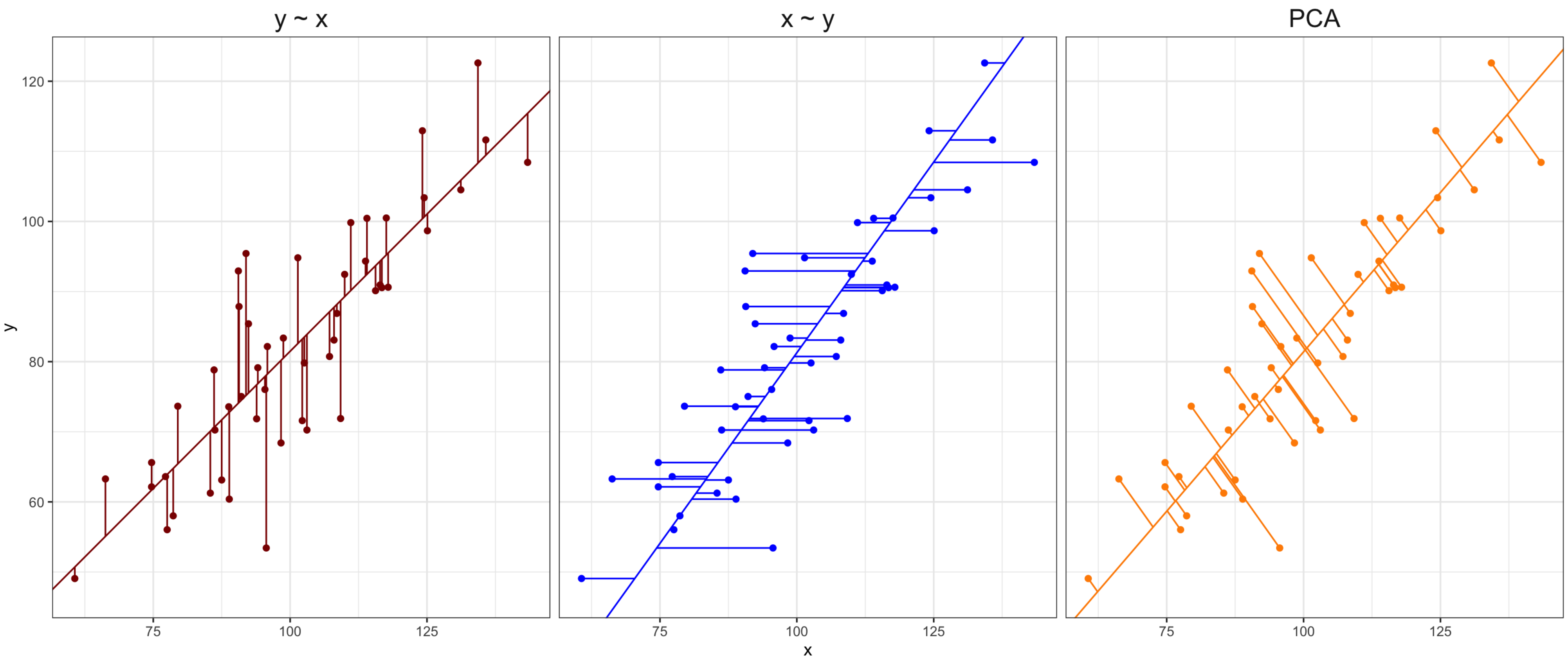
Visualizing PCA in two dimensions



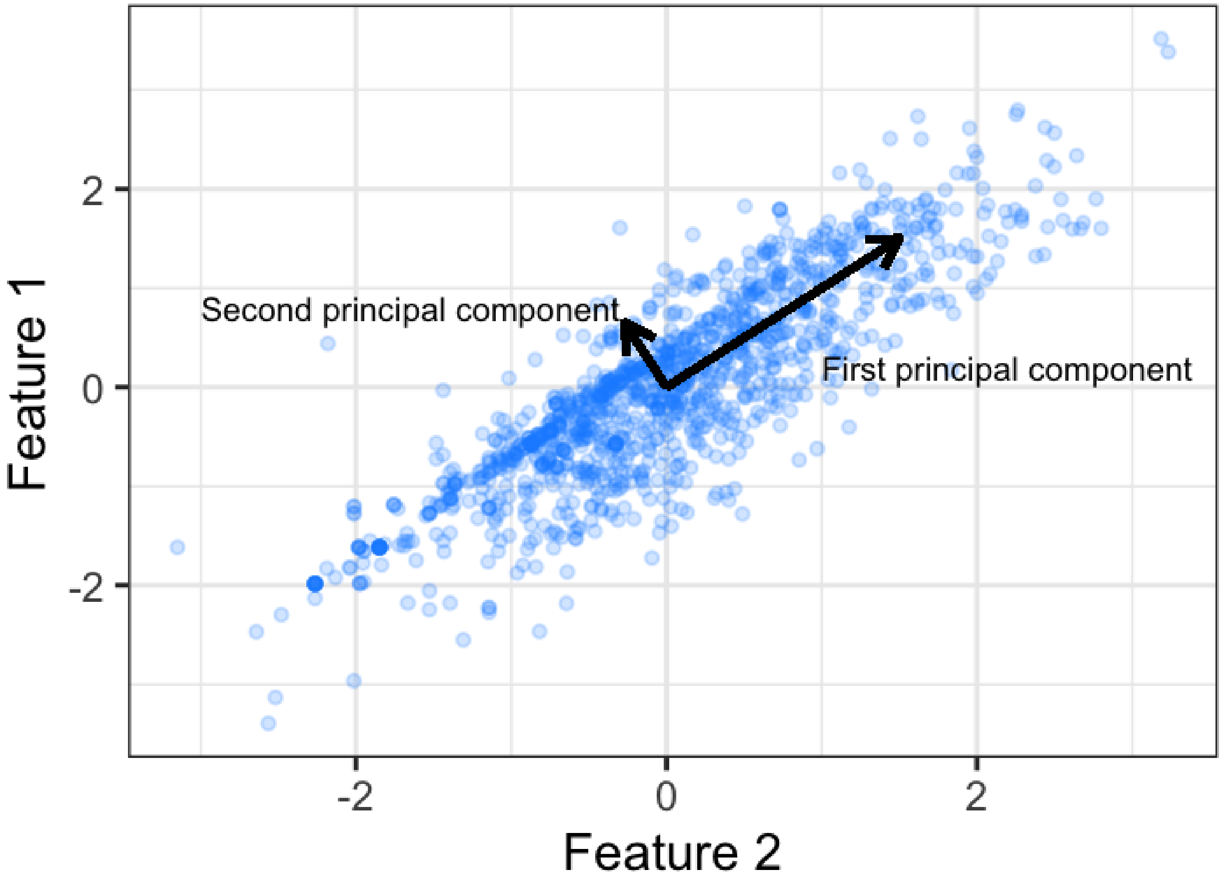
Visualizing PCA in two dimensions



Visualizing PCA in two dimensions



Searching for variance in orthogonal directions



PCA: singular value decomposition (SVD)

$$X = UDV^T$$

- Matrices U and V contain the left and right (respectively) **singular vectors of scaled matrix X**
- D is the diagonal matrix of the **singular values**
- SVD simplifies matrix-vector multiplication as **rotate, scale, and rotate again**

V is called the **loading matrix** for X with ϕ_j as columns,

- $Z = XV$ is the PC matrix

BONUS **eigenvalue decomposition** (aka spectral decomposition)

- V are the **eigenvectors** of X^TX (covariance matrix, ^{T} means *transpose*)
- U are the **eigenvectors** of XX^T
- The singular values (diagonal of D) are square roots of the **eigenvalues** of X^TX or XX^T
- Meaning that $Z = UD$

Eigenvalues solve time travel?

Probably not... but they guide dimension reduction

We want to choose $p^* < p$ such that we are explaining variation in the data

Eigenvalues λ_j for $j \in 1, \ldots, p$ indicate **the variance explained by each component**

- $\sum_j^p \lambda_j = p$, meaning $\lambda_j \geq 1$ indicates $\text{PC}j$ contains at least one variable's worth in variability
- λ_j / p equals proportion of variance explained by $\text{PC}j$
- Arranged in descending order so that λ_1 is largest eigenvalue and corresponds to PC1
- Can compute the cumulative proportion of variance explained (CVE) with p^* components:

$$\text{CVE}_{p^*} = \frac{\sum_j^{p*} \lambda_j}{p}$$

Can use **scree plot** to plot eigenvalues and guide choice for $p^* < p$ by looking for "elbow" (rapid to slow change)

Example data: NFL teams summary

Created dataset using `nflfastR` summarizing NFL team performances from 1999 to 2020

```
library(tidyverse)
nfl_teams_data <- read_csv("http://www.stat.cmu.edu/cmsac/sure/2021/materials/data/regression_pro
nfl_model_data <- nfl_teams_data %>%
  mutate(score_diff = points_scored - points_allowed) %>%
  # Only use rows with air yards
  filter(season >= 2006) %>%
  dplyr::select(-wins, -losses, -ties, -points_scored, -points_allowed, -season, -team)
```

NFL PCA example

Use the `prcomp` function (uses SVD) for PCA on **centered** and **scaled** data

```
model_x <- as.matrix(dplyr::select(nfl_model_data, -score_diff))
pca_nfl <- prcomp(model_x, center = TRUE, scale = TRUE)
summary(pca_nfl)
```

```
## Importance of components:
##                           PC1    PC2    PC3     PC4    PC5     PC6     PC7
## Standard deviation     3.2119 3.1086 2.3406 2.03961 1.5384 1.41243 1.33352
## Proportion of Variance 0.2149 0.2013 0.1141 0.08667 0.0493 0.04156 0.03705
## Cumulative Proportion  0.2149 0.4162 0.5304 0.61704 0.6663 0.70791 0.74495
##                            PC8     PC9    PC10    PC11    PC12    PC13   PC14
## Standard deviation     1.26070 1.15021 1.10316 1.01999 0.95873 0.93244 0.8314
## Proportion of Variance 0.03311 0.02756 0.02535 0.02167 0.01915 0.01811 0.0144
## Cumulative Proportion  0.77807 0.80563 0.83098 0.85265 0.87180 0.88992 0.9043
##                           PC15    PC16    PC17    PC18    PC19    PC20    PC21
## Standard deviation     0.82639 0.77427 0.65754 0.60286 0.58982 0.57864 0.53934
## Proportion of Variance 0.01423 0.01249 0.00901 0.00757 0.00725 0.00698 0.00606
## Cumulative Proportion  0.91855 0.93104 0.94004 0.94761 0.95486 0.96184 0.96790
##                           PC22    PC23    PC24    PC25    PC26    PC27    PC28
## Standard deviation     0.49402 0.47675 0.45810 0.41473 0.36075 0.33619 0.32284
## Proportion of Variance 0.00508 0.00474 0.00437 0.00358 0.00271 0.00235 0.00217
## Cumulative Proportion  0.97298 0.97772 0.98209 0.98567 0.98838 0.99074 0.99291
```

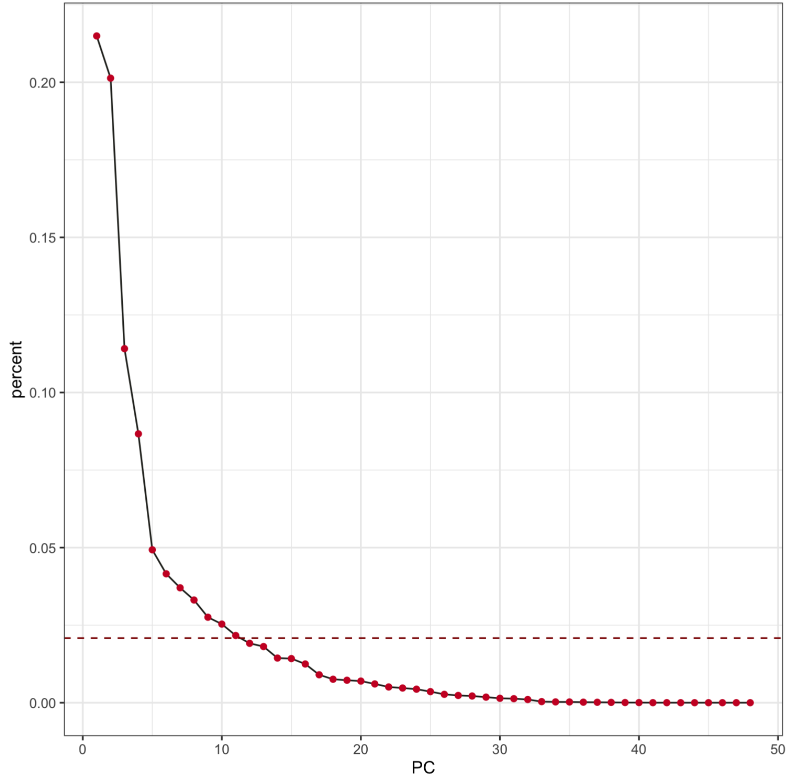
Proportion of variance explained

`prcomp$sdev` corresponds to the singular values, i.e., $\sqrt{\lambda_j}$, what is `pca_nfl$sdev^2 / ncol(model_x)`?

Can use the `broom` package easily tidy `prcomp` summary for plotting

```
library(broom)
pca_nfl %>%
  tidy(matrix = "eigenvalues") %>%
  ggplot(aes(x = PC, y = percent)) +
  geom_line() + geom_point() +
  geom_hline(yintercept = 1 / ncol(model_x),
             color = "darkred",
             linetype = "dashed") +
  theme_bw()
```

- Add reference line at $1/p$, *why*?



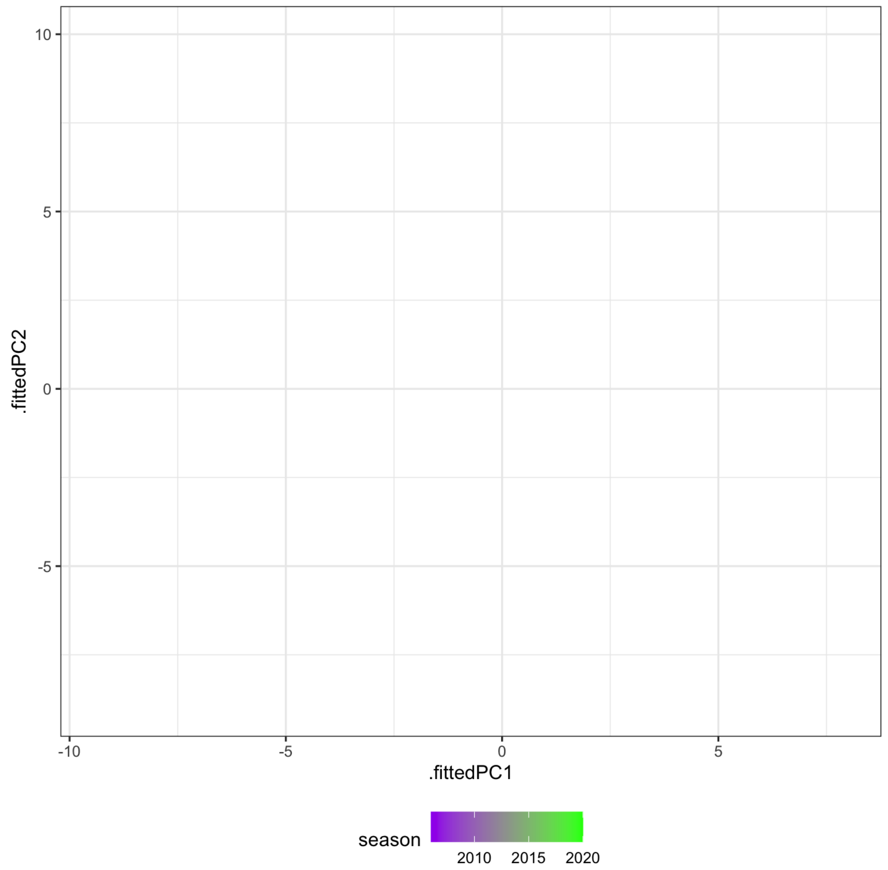
Display data in lower dimensions

`prcomp$x` corresponds to the matrix of **principal component scores**, i.e., $Z = XV$

Can augment dataset with PC scores for plotting

- Add team and season for context

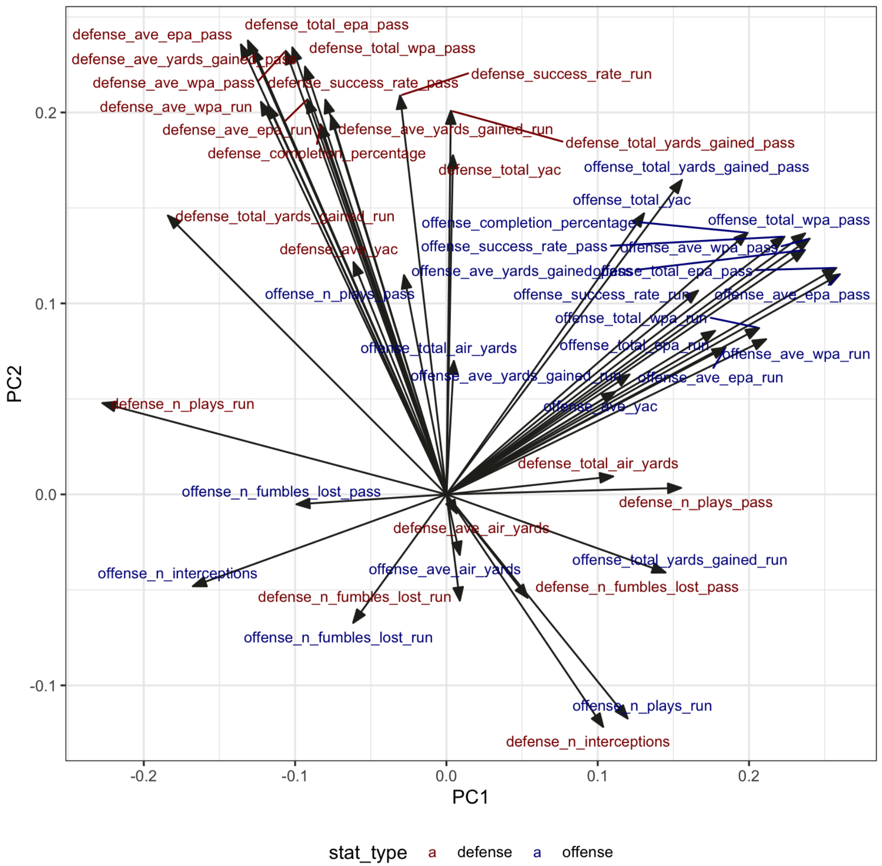
```
pca_nfl %>%
  augment(nfl_model_data) %>%
  bind_cols({
    nfl_teams_data %>%
      filter(season >= 2006) %>%
      dplyr::select(season, team)
  }) %>%
  unite("team_id", team:season, sep = "-",
        remove = FALSE) %>%
  ggplot(aes(x = .fittedPC1, y = .fittedPC2,
             color = season)) +
  geom_text(aes(label = team_id), alpha = 0.9
  scale_color_gradient(low = "purple", high =
  theme_bw() + theme(legend.position = "botto
```



What are the loadings of these dimensions?

`prcomp$rotation` corresponds to the **loading matrix**, i.e., V

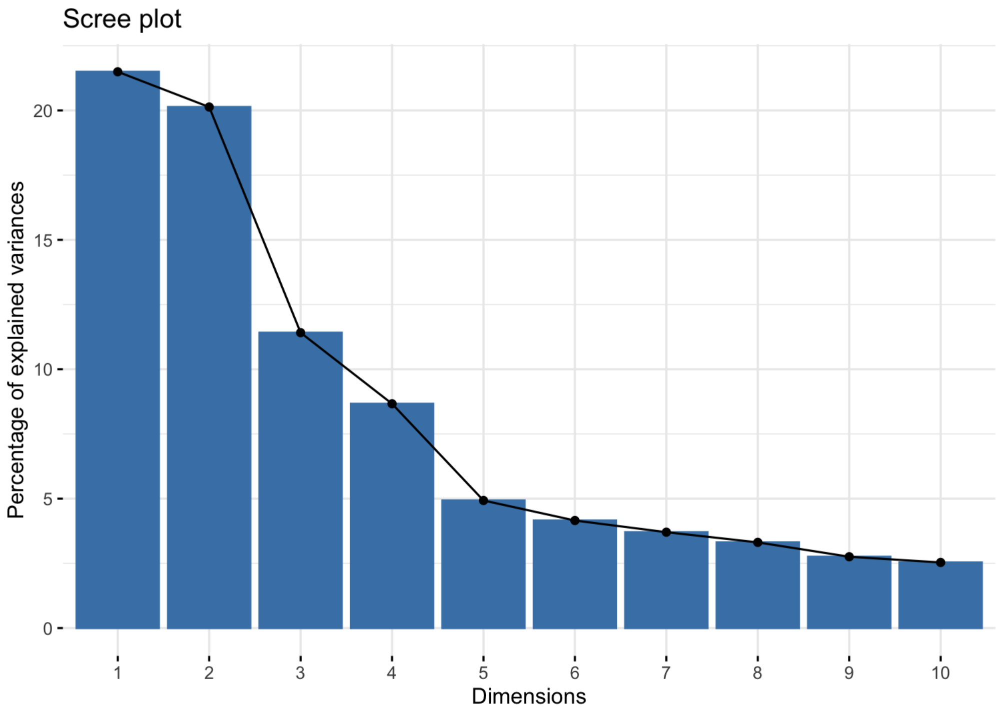
```
arrow_style <- arrow(
  angle = 20, ends = "first", type = "closed"
  length = grid::unit(8, "pt")
)
library(ggrepel)
pca_nfl %>%
  tidy(matrix = "rotation") %>%
  pivot_wider(names_from = "PC", names_prefix
              values_from = "value") %>%
  mutate(stat_type = ifelse(str_detect(column
                                "offense", "defen
  ggplot(aes(PC1, PC2)) +
  geom_segment(xend = 0, yend = 0, arrow = ar
  geom_text_repel(aes(label = column, color =
                   size = 3) +
  scale_color_manual(values = c("darkred", "d
  theme_bw() +
  theme(legend.position = "bottom")
```



PCA analysis with `factoextra`

Visualize the proportion of variance explained by each PC with `factoextra`

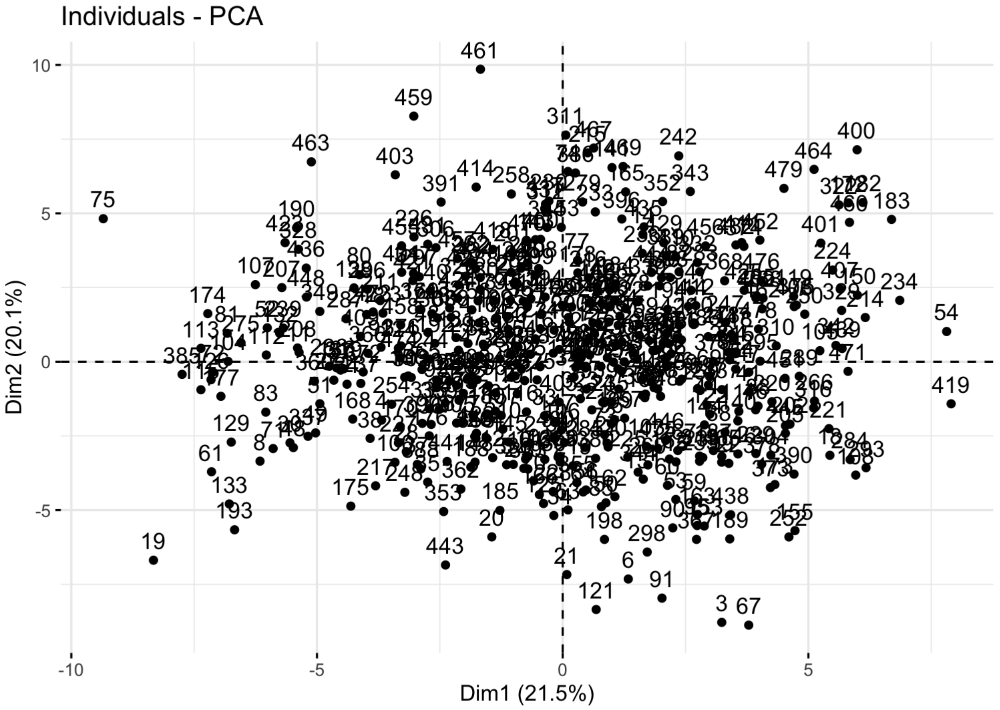
```
library(factoextra)
fviz_eig(pca_nfl)
```



PCA analysis with `factoextra`

Display observations with first two PC

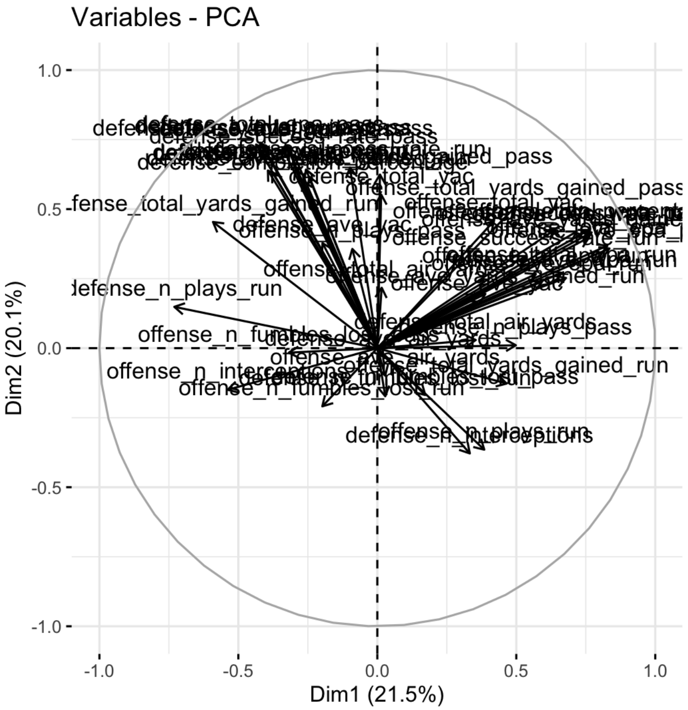
```
fviz_pca_ind(pca_nfl)
```



PCA analysis with `factoextra`

Projection of variables - angles are interpreted as correlations, where negative correlated values point to opposite sides of graph

```
fviz_pca_var(pca_nfl)
```



PCA analysis with `factoextra`

Biplot displays both the space of observations and the space of variables

- Arrows represent the directions of the original variables

```
fviz_pca_biplot(pca_nfl)
```