Clustering and PCA

```r
library(ISLR)
library(factoextra)
library(gridExtra)
library(corrplot)
library(RColorBrewer)
library(gplots)
```

The dataset we use contains data on 166 first generation Pokemon, including their names and basic stats: HP, Attack, Defense, Special Attack, Special Defense, and Speed. The data is from Kaggle (https://www.kaggle.com/abcsds/pokemon). We will apply unsupervised learning methods on this data. The list of Pokemon can be found at (https://pokemondb.net/pokedex/national).

```r
dat <- read.csv("Pokemon.csv")
dat1 <- dat[,2:7]
dat1 <- scale(dat1)
rownames(dat1) <- dat[,1]
```

K means clustering

Partitioning methods such as k-means clustering require the users to specify the number of clusters to be generated. The function `fviz_nbclust()` determines and visualizes the optimal number of clusters using different methods: within cluster sums of squares, average silhouette and gap statistics. We use average silhouette, and the greater the silhouette value the better.

```r
fviz_nbclust(dat1,
             FUNcluster = kmeans,
             method = "silhouette")
```
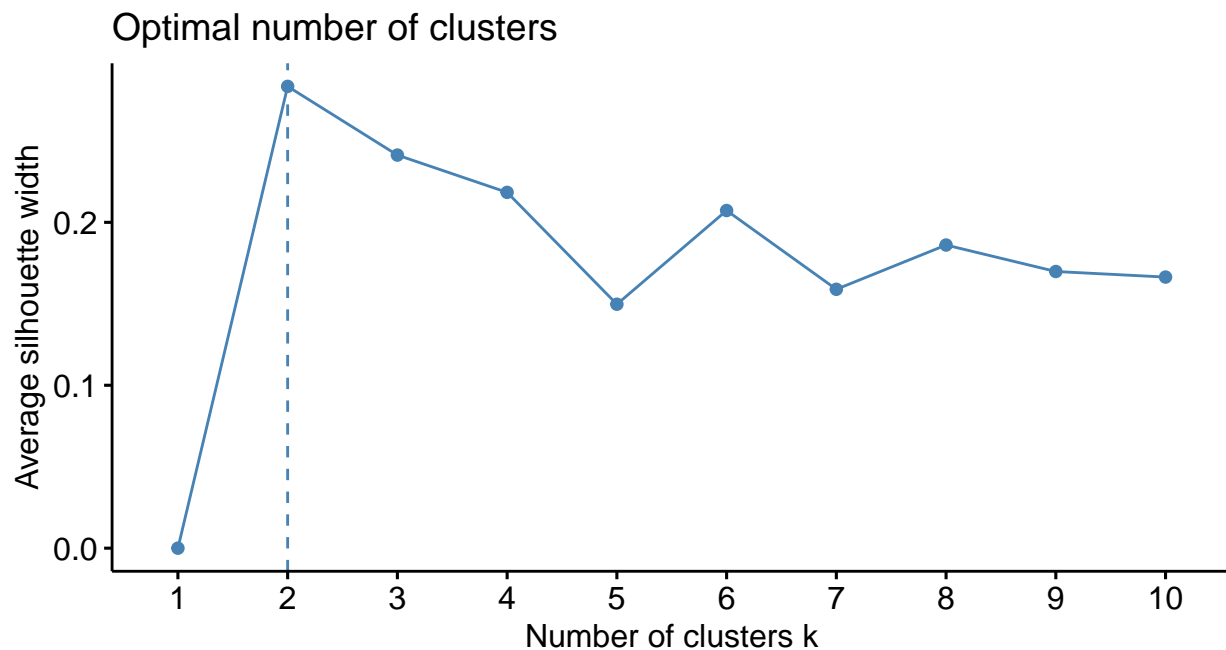
```
set.seed(1)
km <- kmeans(dat1, centers = 2, nstart = 20)
```

The function `fviz_cluster()` provides ggplot2-based visualization of partitioning methods including K means. Observations are represented by points in the plot, using principal components if $p > 2$. An ellipse is drawn around each cluster.

```
km_vis <- fviz_cluster(list(data = dat1, cluster = km$cluster),
                       ellipse.type = "convex",
                       geom = c("point","text"),
                       labelsize = 5,
                       palette = "Dark2") + labs(title = "K-means")

km_vis
```
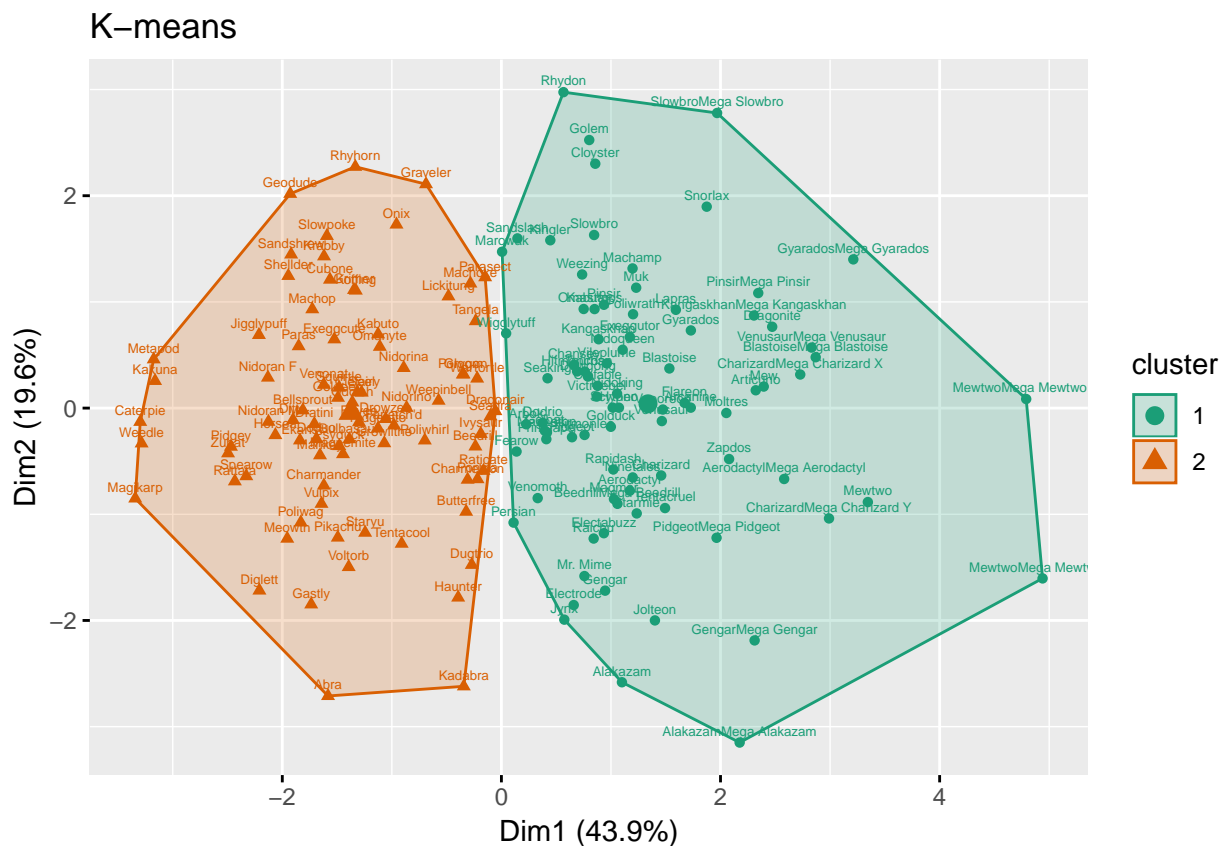

Hierarchical clustering

We can also apply hierarchical clustering on this data. Here we use the Euclidean distance and different types of linkage.

```
hc.complete <- hclust(dist(dat1), method = "complete")
hc.average  <- hclust(dist(dat1), method = "average")
hc.single   <- hclust(dist(dat1), method = "single")
hc.centroid <- hclust(dist(dat1), method = "centroid")
```

The function `fviz_dend()` can be applied to visualize the dendrogram.

```r
fviz_dend(hc.complete, k = 4,
          cex = 0.3,
          palette = "jco",
          color_labels_by_k = TRUE,
          rect = TRUE, rect_fill = TRUE, rect_border = "jco",
          labels_track_height = 2.5)
```

Cluster Dendrogram
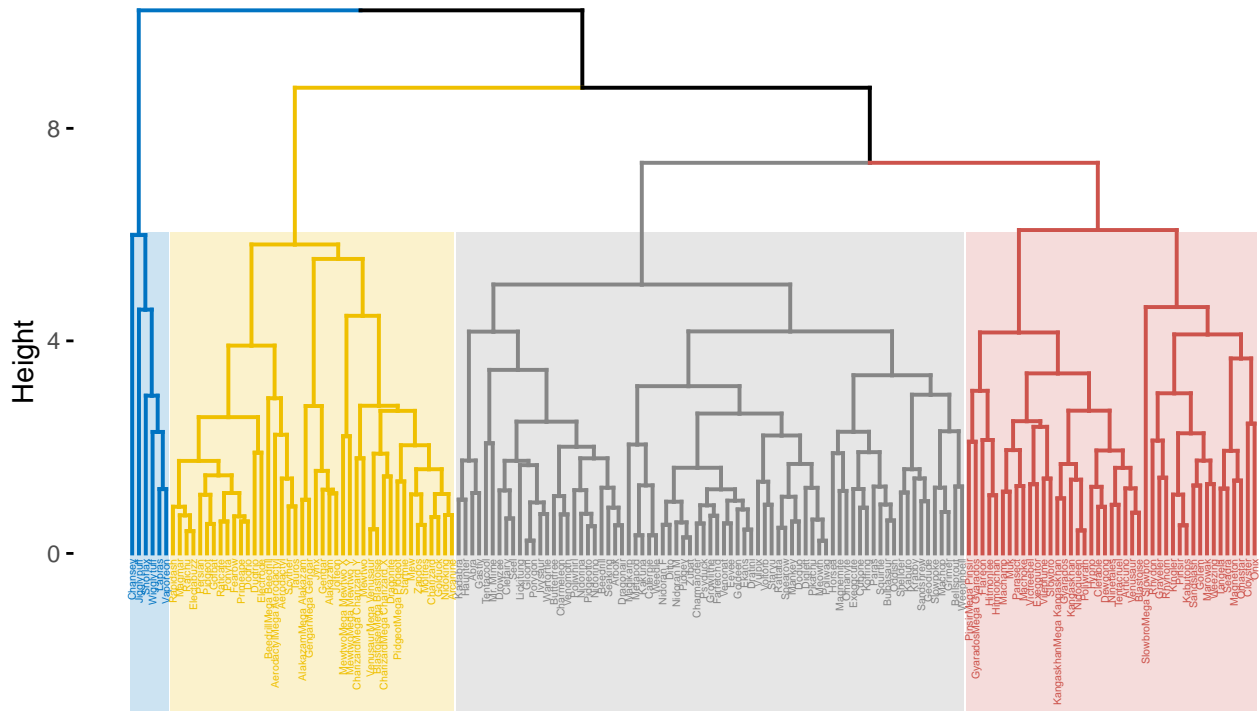

```r
ind4.complete <- cutree(hc.complete, 4)

# Who are in the fourth cluster?
dat[ind4.complete == 4,]
```

```
##               Name HitPoints Attack Defense SpecialAttack SpecialDefense Speed
## 45      Jigglypuff       115     45      20            45             25    20
## 46      Wigglytuff       140     70      45            85             50    45
## 122        Chansey       250      5       5            35            105    50
## 143         Lapras       130     85      80            85             95    60
## 146        Vaporeon       130     65      60           110             95    65
## 156         Snorlax       160    110      65            65            110    30
##       Legendary
## 45        FALSE
## 46        FALSE
## 122       FALSE
## 143       FALSE
## 146       FALSE
## 156       FALSE
```

To display more details, we show the heatmap of the data.

```
#display.brewer.all(n=NULL, type="all", select=NULL, exact.n=TRUE)
col1 <- colorRampPalette(brewer.pal(9, "GnBu"))(100)
col2 <- colorRampPalette(brewer.pal(3, "Spectral"))(2)

heatmap.2(t(dat1),
          col = col1, keysize=.8, key.par = list(cex=.5),
          trace = "none", key = TRUE, cexCol = 0.75,
          labCol = as.character(dat[,1]),
          ColSideColors = col2[as.numeric(dat[,"Legendary"])+1],
          margins = c(10, 10))
```
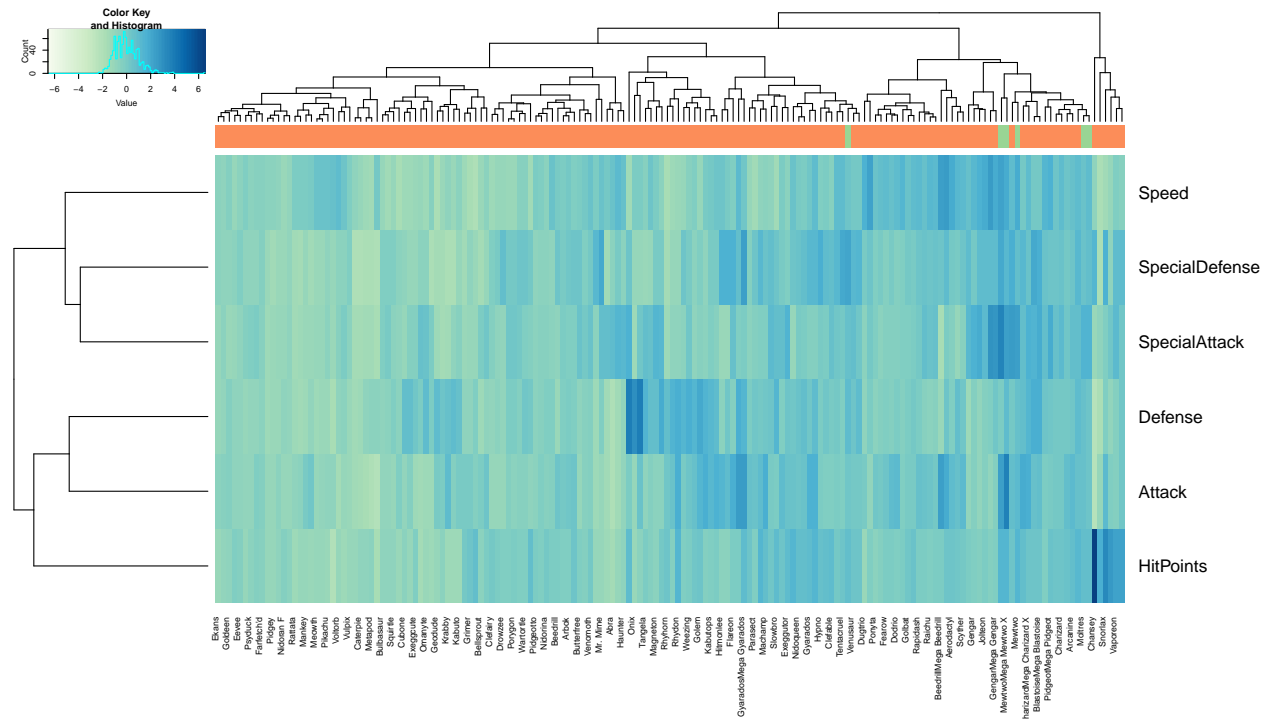

PCA

The function prcomp() can be used to perform PCA.

```
pca <- prcomp(dat1)
pca$rotation
```

```
##                     PC1        PC2         PC3          PC4         PC5
## HitPoints      0.3638022  0.2862972 -0.72425610  0.078135517 -0.42663445
## Attack         0.4363956  0.3149994  0.27779372  0.573757403 -0.12333177
## Defense        0.3031184  0.5812622  0.48929801 -0.361032760  0.03453292
## SpecialAttack  0.4378985 -0.3119077  0.03743076 -0.654754892 -0.29724064
## SpecialDefense 0.5204254 -0.1331800 -0.25037584  0.006718302  0.80453025
## Speed          0.3503261 -0.6049135  0.30786700  0.324966961 -0.25682461
##                      PC6
## HitPoints      -0.27020899
## Attack          0.53736079
## Defense        -0.44643458
```
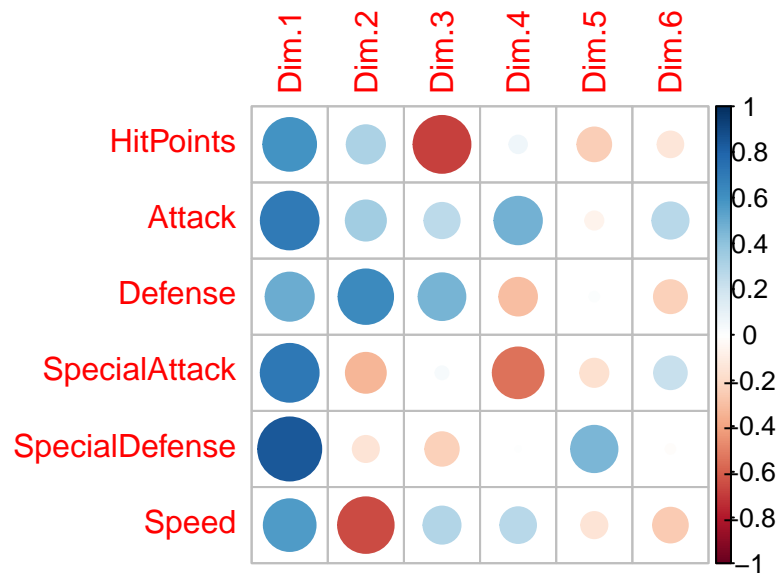
4

```
## SpecialAttack    0.43874986
## SpecialDefense -0.03766086
## Speed          -0.49498168
```

```
pca$sdev
```

```
## [1] 1.6238460 1.0848056 0.9487926 0.8345883 0.5670204 0.5177487
```
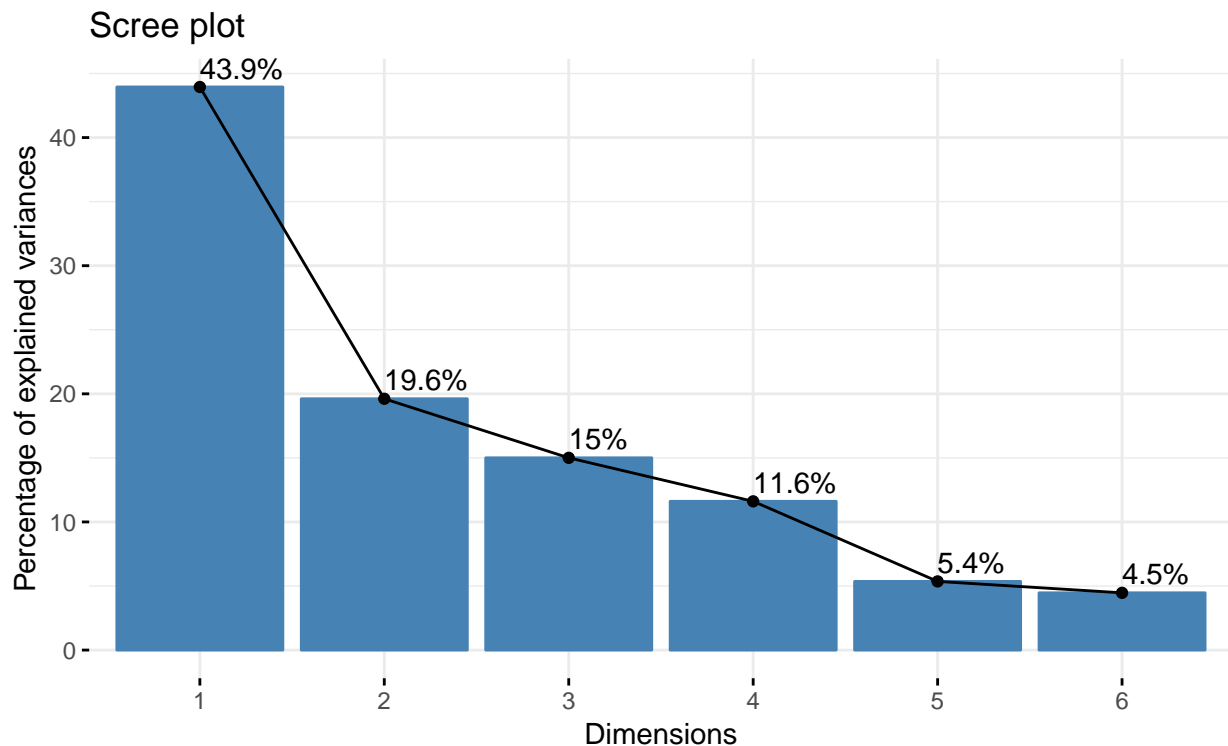
```
var <- get_pca_var(pca)
corrplot(var$cor)
```
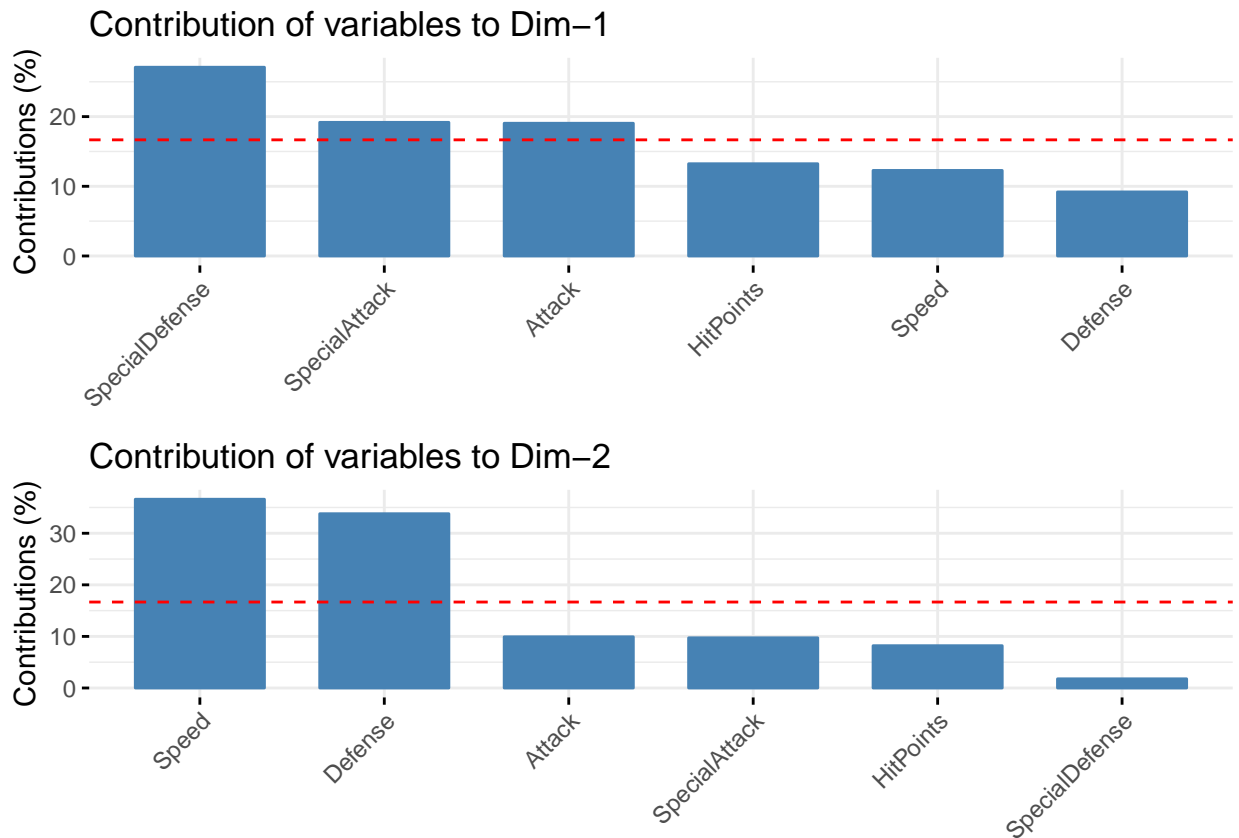

The function `fviz_eig()` plots the eigenvalues/variances against the number of dimensions.

```
fviz_eig(pca, addlabels = TRUE)
```

The function `fviz_contrib()` can be used to visualize the contribution of variables from the results of PCA.

```
a <- fviz_contrib(pca, choice = "var", axes = 1)
b <- fviz_contrib(pca, choice = "var", axes = 2)
grid.arrange(a, b, nrow = 2)
```
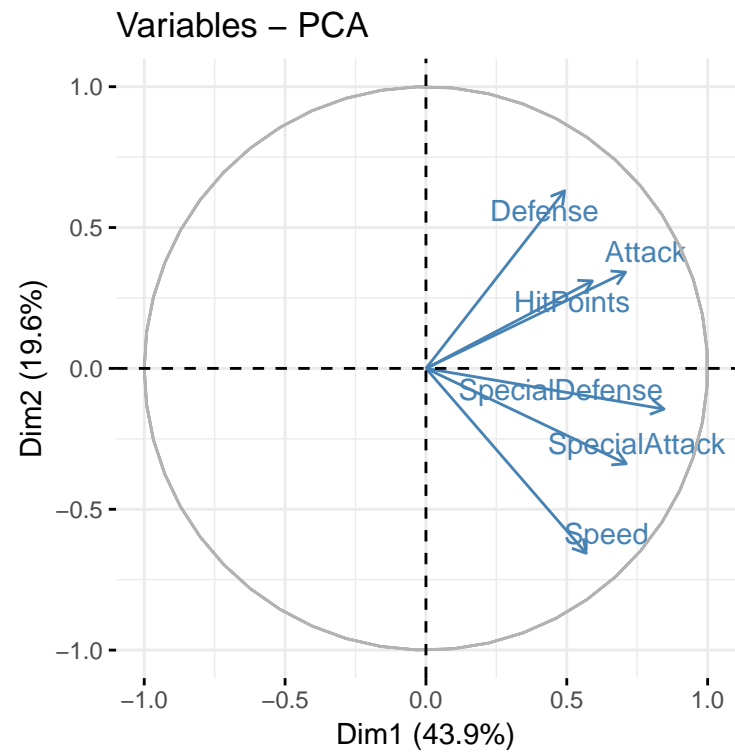

The function `fviz_pca_biplot()` can be used to obtain the biplot of individuals and variables.

```
fviz_pca_biplot(pca, axes = c(1,2),
                habillage = ifelse(dat$Legendary==TRUE, "Legendary","Not legendary"),
                label = c("var"),
                addEllipses = TRUE)
```

PCA – Biplot
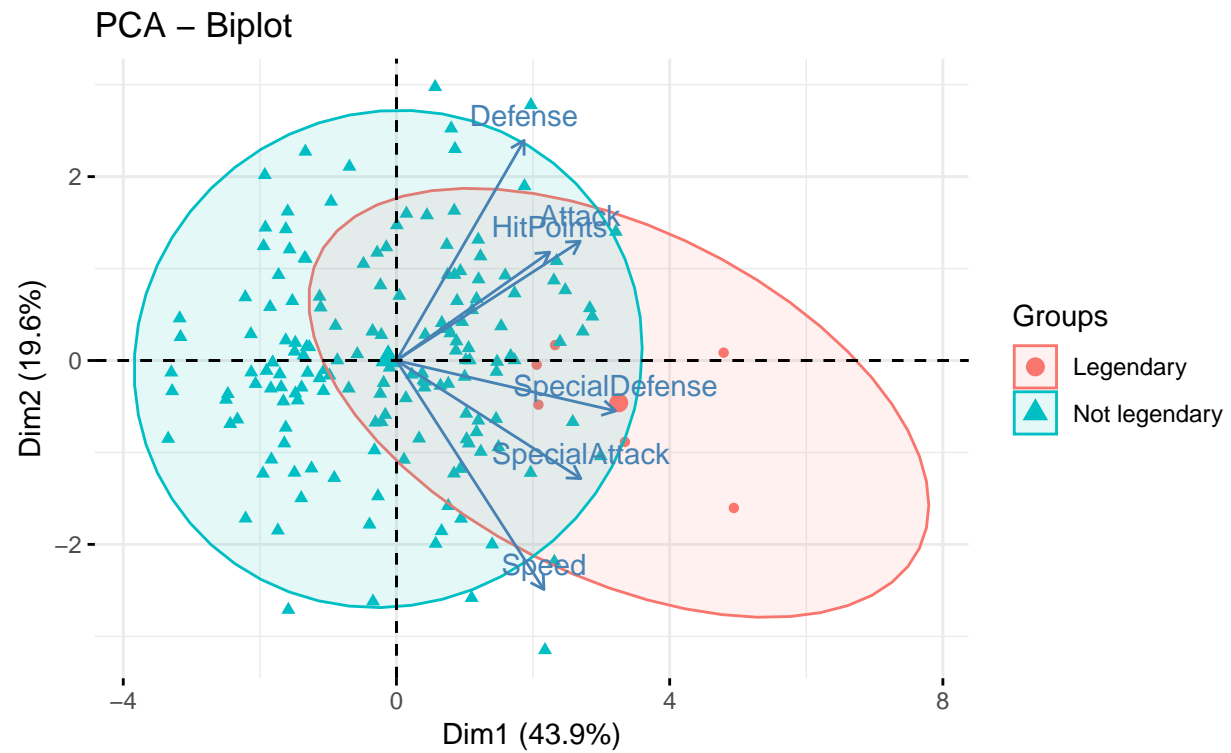
```
fviz_pca_var(pca, col.var = "steelblue", repel = TRUE)
```


Variables – PCA

```
fviz_pca_ind(pca,
             habillage = ifelse(dat$Legendary==TRUE,"Legendary","Not legendary"),
             label = "none",
             addEllipses = TRUE)
```