# The curse of dimensionality

DIMENSIONALITY REDUCTION IN R

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# Curse of dimensionality

- **Dimensions:** Columns in the dataset that represent features of the row points
- **Dimensionality**: Number of features/columns characterizing the dataset

# Curse of dimensionality

The `iris` dataset:

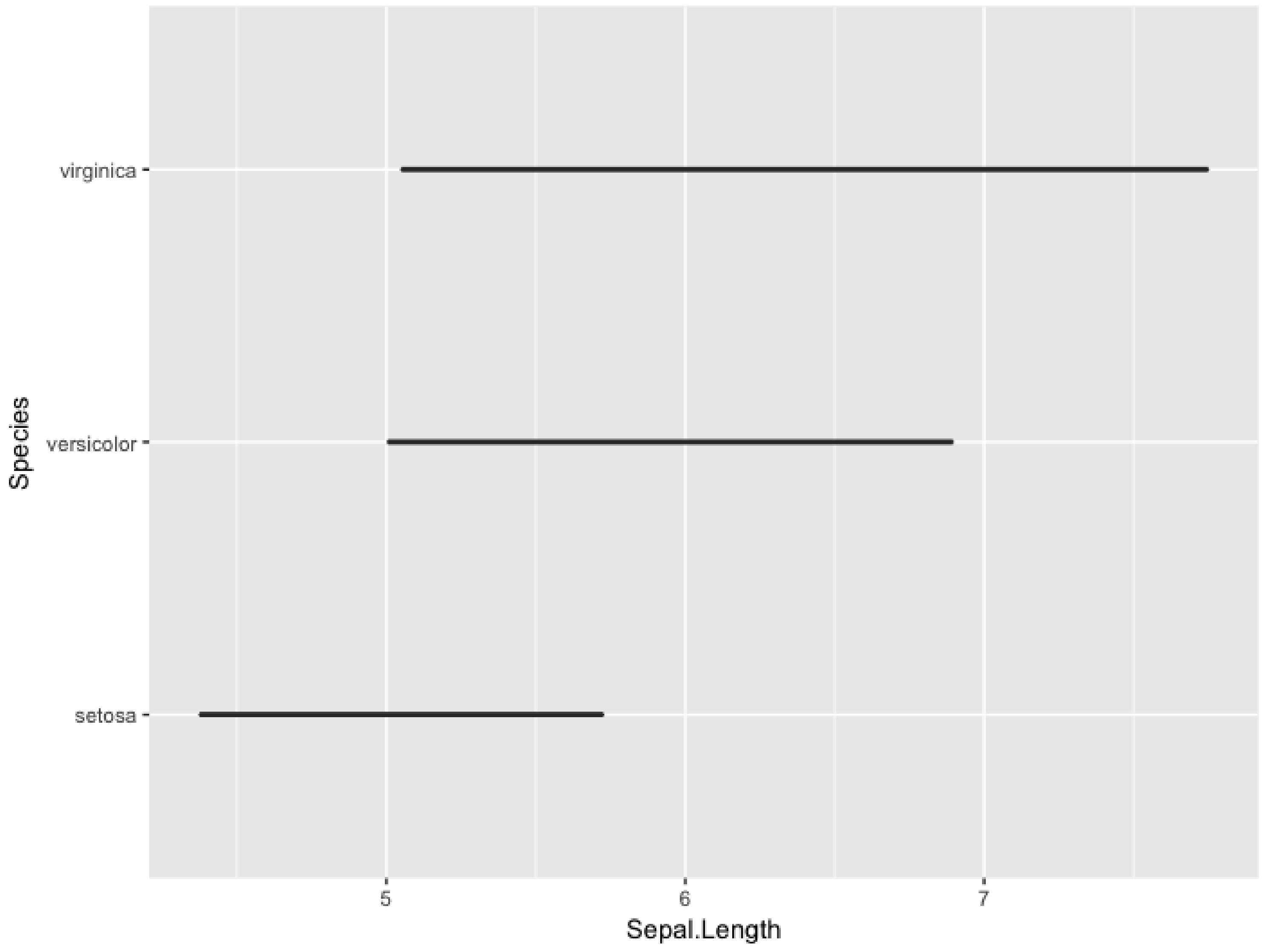
```
dim(iris)
```

```
150   5
```

5 columns: **4 features/dimensions** + 1 class

| ID | Sepal.Length | Sepal.Width | Petal.Length | Petal.Width |
|---|---|---|---|---|
| 1 | 5.1 | 3.5 | 1.4 | 0.2 |
| 2 | 4.9 | 3.0 | 1.4 | 0.2 |
| 3 | 4.7 | 3.2 | 1.3 | 0.2 |
| ... | ... | ... | ... | ... |

# 1 Dimension: Sepal.Length

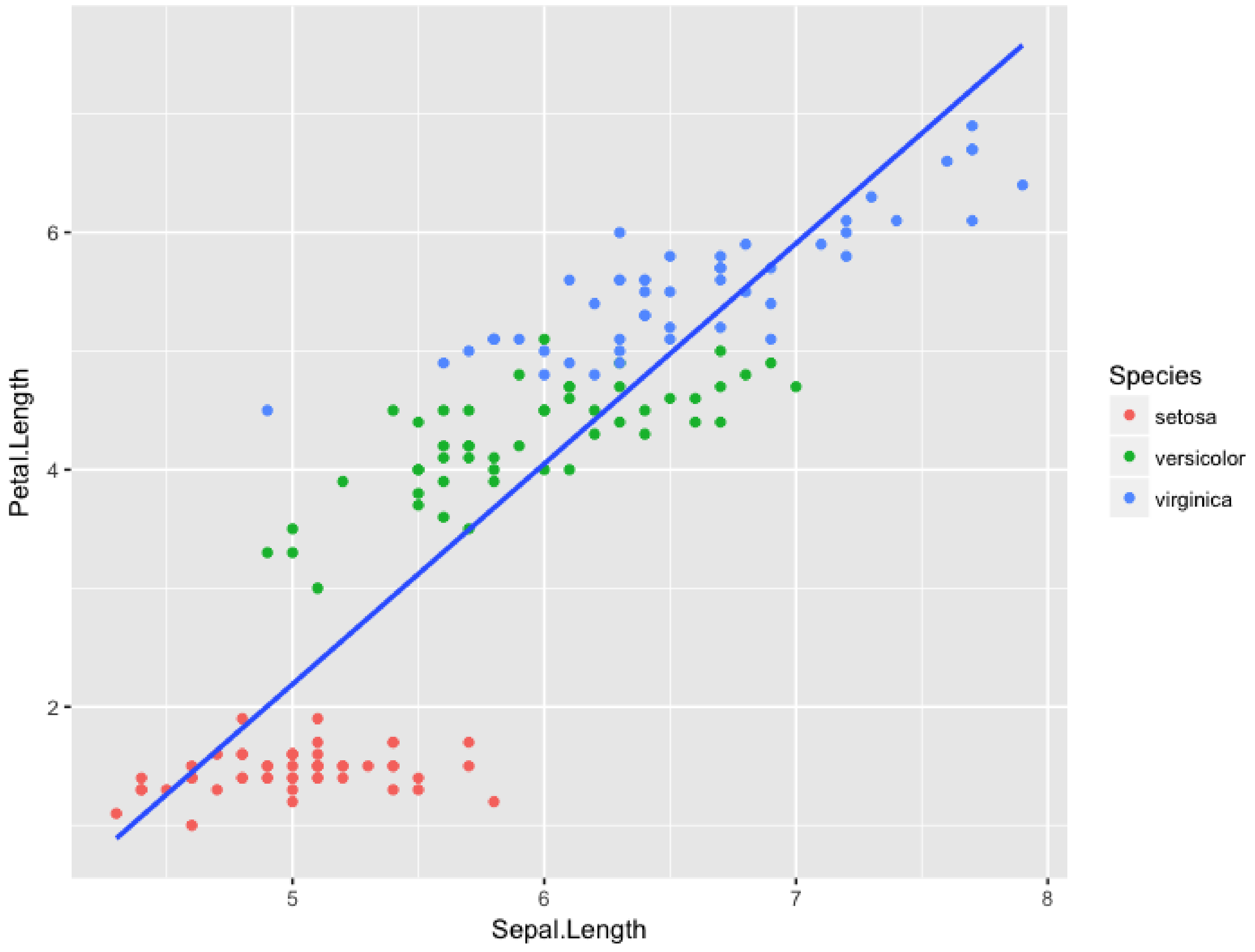



```
range(iris$Sepal.Length)
```

```
4.3 7.9
```

- Feature space filled within **4** units of measurement.
- Data density: 150/4 = **37.5** samples/interval.

# 2 Dimensions: Sepal.Length, Petal.Length

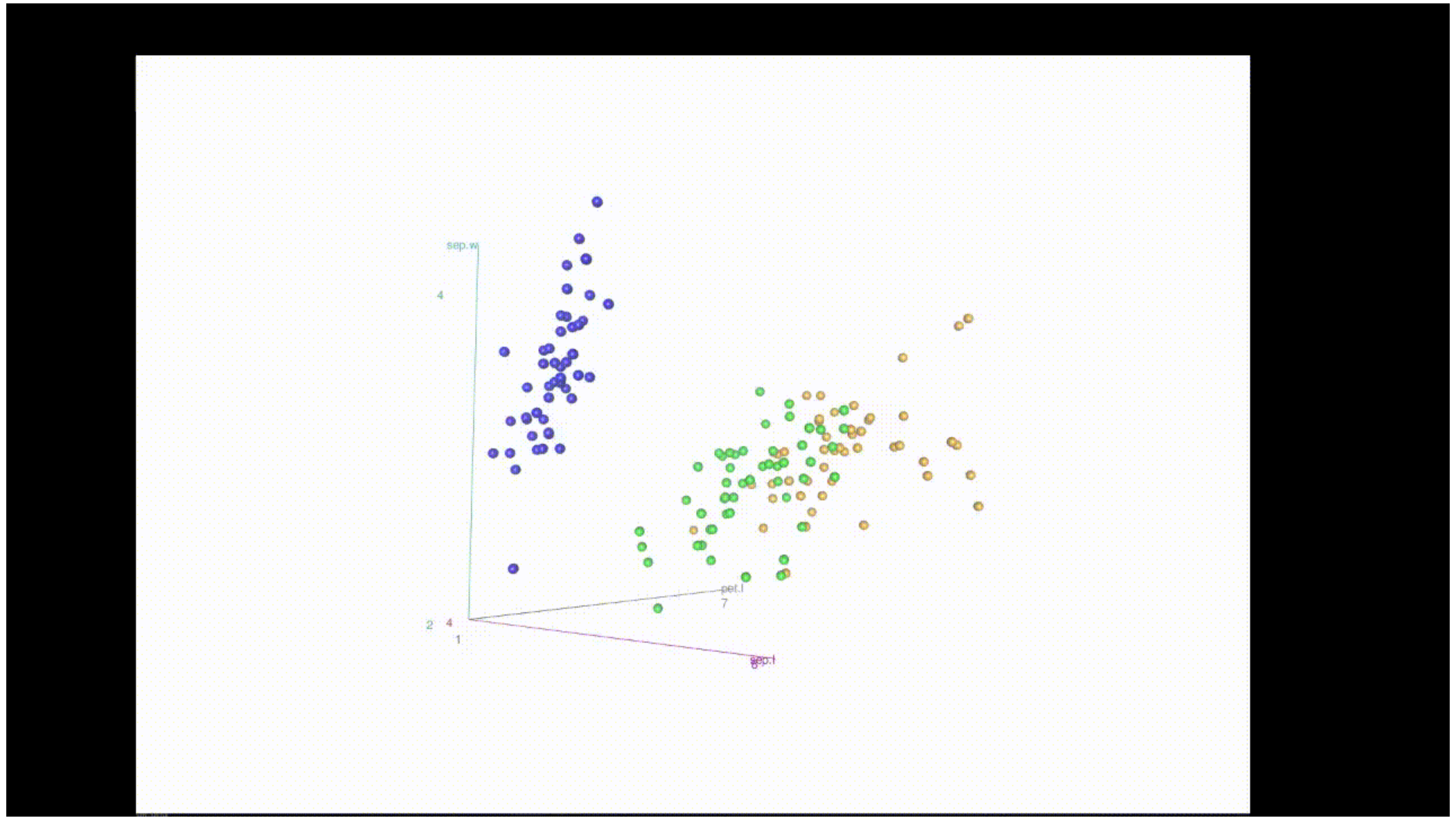



```
range(iris$Petal.Length)
```

```
1.0 6.9
```

- Feature space: filled within **24 [4*6]** possible combinations of unit measurements.
- Data density: 150/24 = **6.25** samples/interval

# 3 Dimensions: Sepal.Length, Petal.Length, Sepal.Width



```
range(iris$Sepal.Width)
```

```
2.0 4.4
```

- Feature space: filled within **72 [4*6*3]** possible combinations of unit measurements.
- Data density: 150/72 = **2.083333** samples/interval

# What is this curse all about?

- **As the dimensionalities of the data grow, the feature space grows rapidly.**

Why even bother?

- **Big computational cost** to handle high-dimensional data.
- **Estimation accuracy** decreases.
- **Difficult interpretation** of the data.

# The mtcars dataset

```
dim(mtcars)
```

```
32 11
```

- Most of the dimensions could probably be reduced due to a small set of latent dimensions, such as:
  - the size of the car or
  - the country of origin or
  - the construction year
- **Observed vs True Dimensionality:** observed features obscure the true or *intrinsic* dimensionality of the data.

# Exploring correlation

How do we trace correlation patterns?

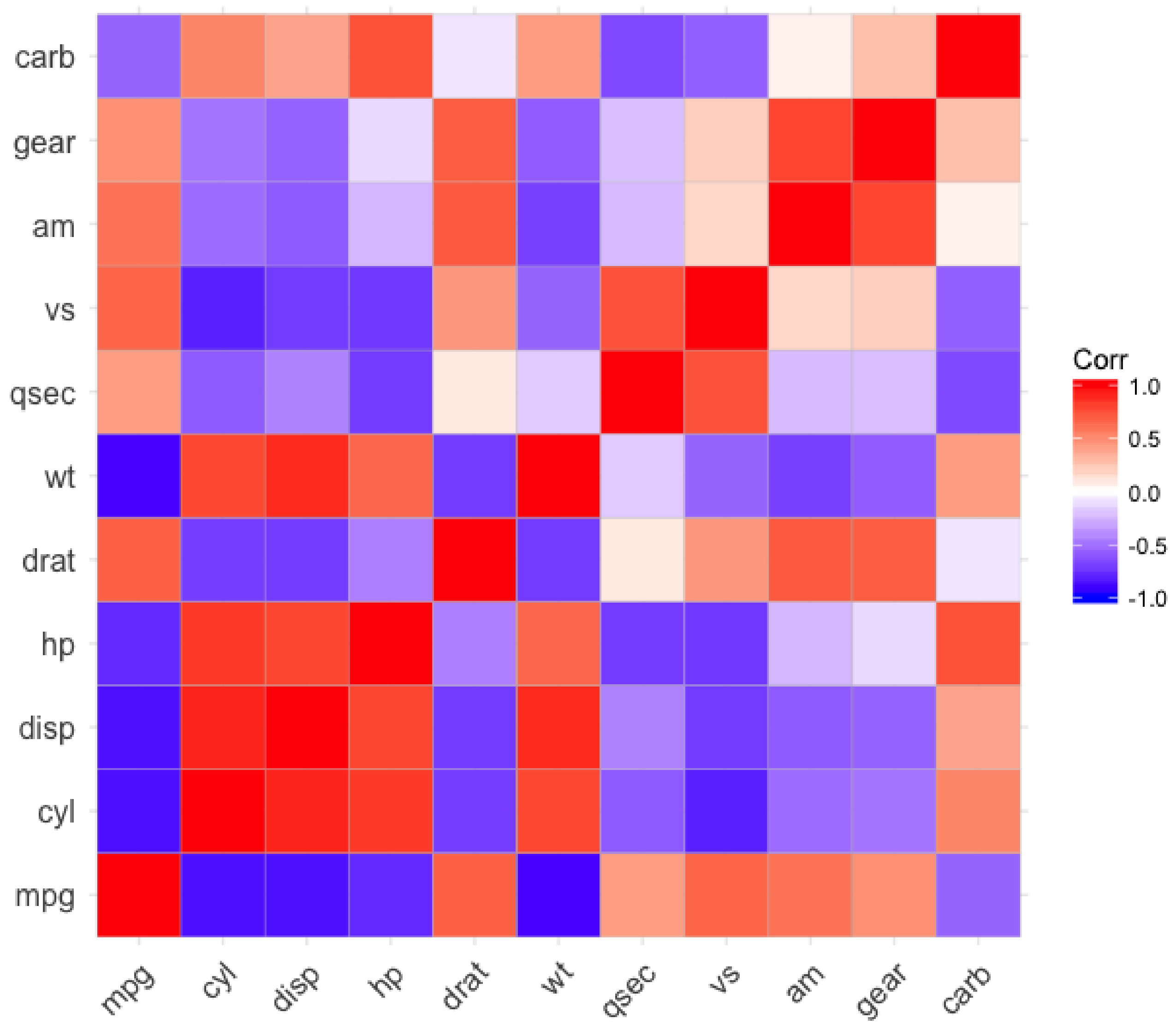
- **Correlation matrix** is a matrix of correlation coefficients.
- Smaller number of dimensions translates to less complex correlation matrix.

```
mtcars$cyl <- as.numeric(as.character(mtcars$cyl))
mtcars_correl <- cor(mtcars, use = "complete.obs")
```

| | mpg | cyl | disp | hp | drat | wt | qsec | vs | am | gear | carb |
|---|---|---|---|---|---|---|---|---|---|---|---|
| mpg | 1.0000000 | -0.8521620 | -0.8475514 | -0.7761684 | 0.68117191 | -0.8676594 | 0.41868403 | 0.6640389 | 0.59983243 | 0.4802848 | -0.55092507 |
| cyl | -0.8521620 | 1.0000000 | 0.9020329 | 0.8324475 | -0.69993811 | 0.7824958 | -0.59124207 | -0.8108118 | -0.52260705 | -0.4926866 | 0.52698829 |
| disp | -0.8475514 | 0.9020329 | 1.0000000 | 0.7909486 | -0.71021393 | 0.8879799 | -0.43369788 | -0.7104159 | -0.59122704 | -0.5555692 | 0.39497686 |
| hp | -0.7761684 | 0.8324475 | 0.7909486 | 1.0000000 | -0.44875912 | 0.6587479 | -0.70822339 | -0.7230967 | -0.24320426 | -0.1257043 | 0.74981247 |
| drat | 0.6811719 | -0.6999381 | -0.7102139 | -0.4487591 | 1.00000000 | -0.7124406 | 0.09120476 | 0.4402785 | 0.71271113 | 0.6996101 | -0.09078980 |
| wt | -0.8676594 | 0.7824958 | 0.8879799 | 0.6587479 | -0.71244065 | 1.0000000 | -0.17471588 | -0.5549157 | -0.69249526 | -0.5832870 | 0.42760594 |
| qsec | 0.4186840 | -0.5912421 | -0.4336979 | -0.7082234 | 0.09120476 | -0.1747159 | 1.00000000 | 0.7445354 | -0.22986086 | -0.2126822 | -0.65624923 |
| vs | 0.6640389 | -0.8108118 | -0.7104159 | -0.7230967 | 0.44027846 | -0.5549157 | 0.74453544 | 1.0000000 | 0.16834512 | 0.2060233 | -0.56960714 |
| am | 0.5998324 | -0.5226070 | -0.5912270 | -0.2432043 | 0.71271113 | -0.6924953 | -0.22986086 | 0.1683451 | 1.00000000 | 0.7940588 | 0.05753435 |
| gear | 0.4802848 | -0.4926866 | -0.5555692 | -0.1257043 | 0.69961013 | -0.5832870 | -0.21268223 | 0.2060233 | 0.79405876 | 1.0000000 | 0.27407284 |
| carb | -0.5509251 | 0.5269883 | 0.3949769 | 0.7498125 | -0.09078980 | 0.4276059 | -0.65624923 | -0.5696071 | 0.05753435 | 0.2740728 | 1.00000000 |

# Visualising correlation patterns with ggcorrplot

```
library(ggcorrplot)
ggcorrplot(mtcars_correl)
```



# How do we deal with the Curse of Dimensionality?

Two solutions:

- Feature Engineering: Requires domain knowledge
- **Remove redundancy**

# Reduction methods we will explore

- **Principal Components Analysis [PCA]**
- Non-Negative Matrix Factorization [N-NMF]
- Exploratory Factor Analysis [EFA]

# Let's practice!

DIMENSIONALITY REDUCTION IN R

# Getting PCA to work with FactoMineR

DIMENSIONALITY REDUCTION IN R

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# PCA: What does it do?

Conceptually:

1. Removes correlation.
2. Extracts new dimensions (=*principal components*).
3. Reveals the true dimensionality of the data.

Practically:

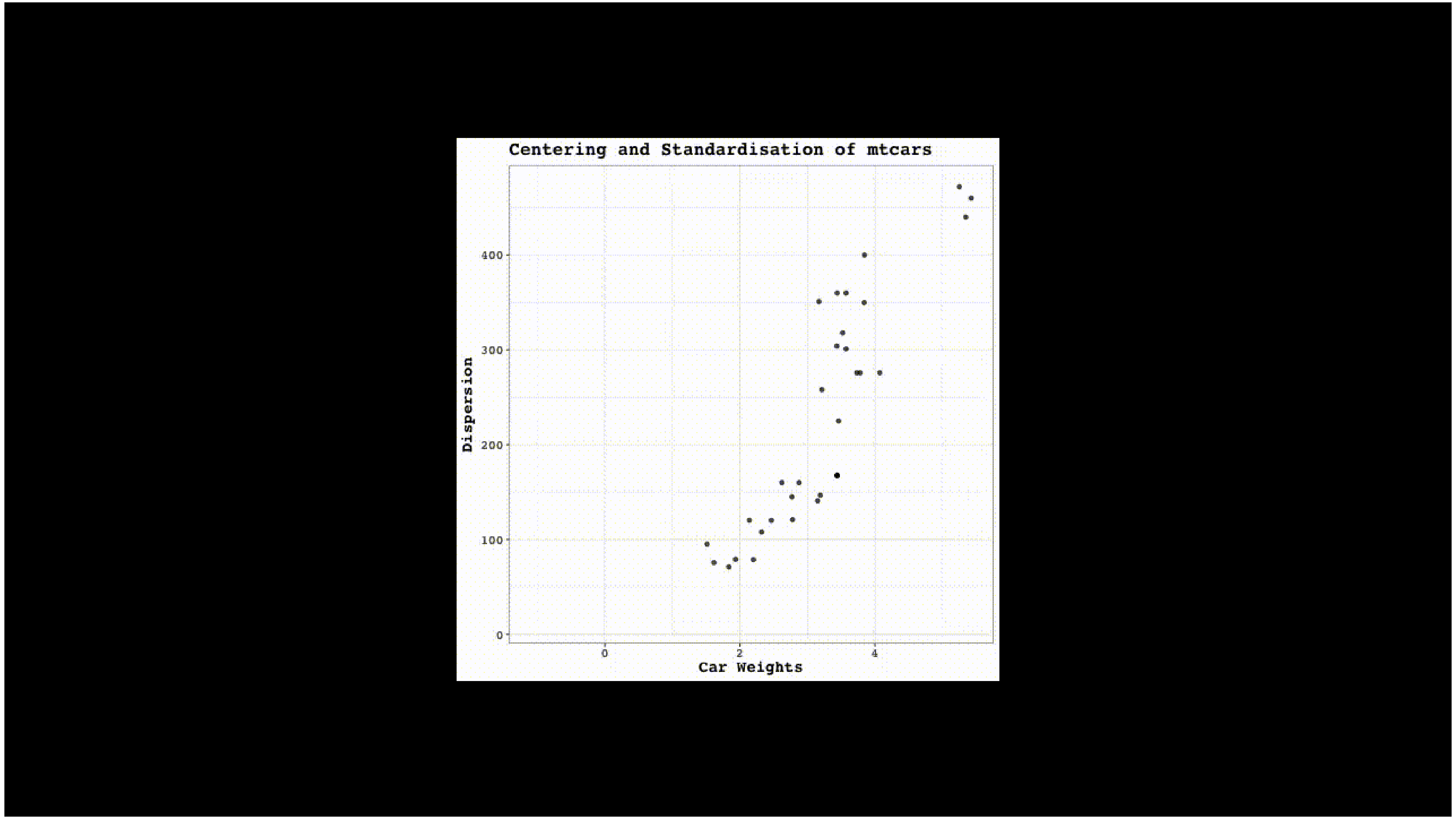
1. Decomposes the correlation matrix.
2. Changes the coordinate system.
3. Helps reduce the number of dimensions.

# PCA: The five steps to perform

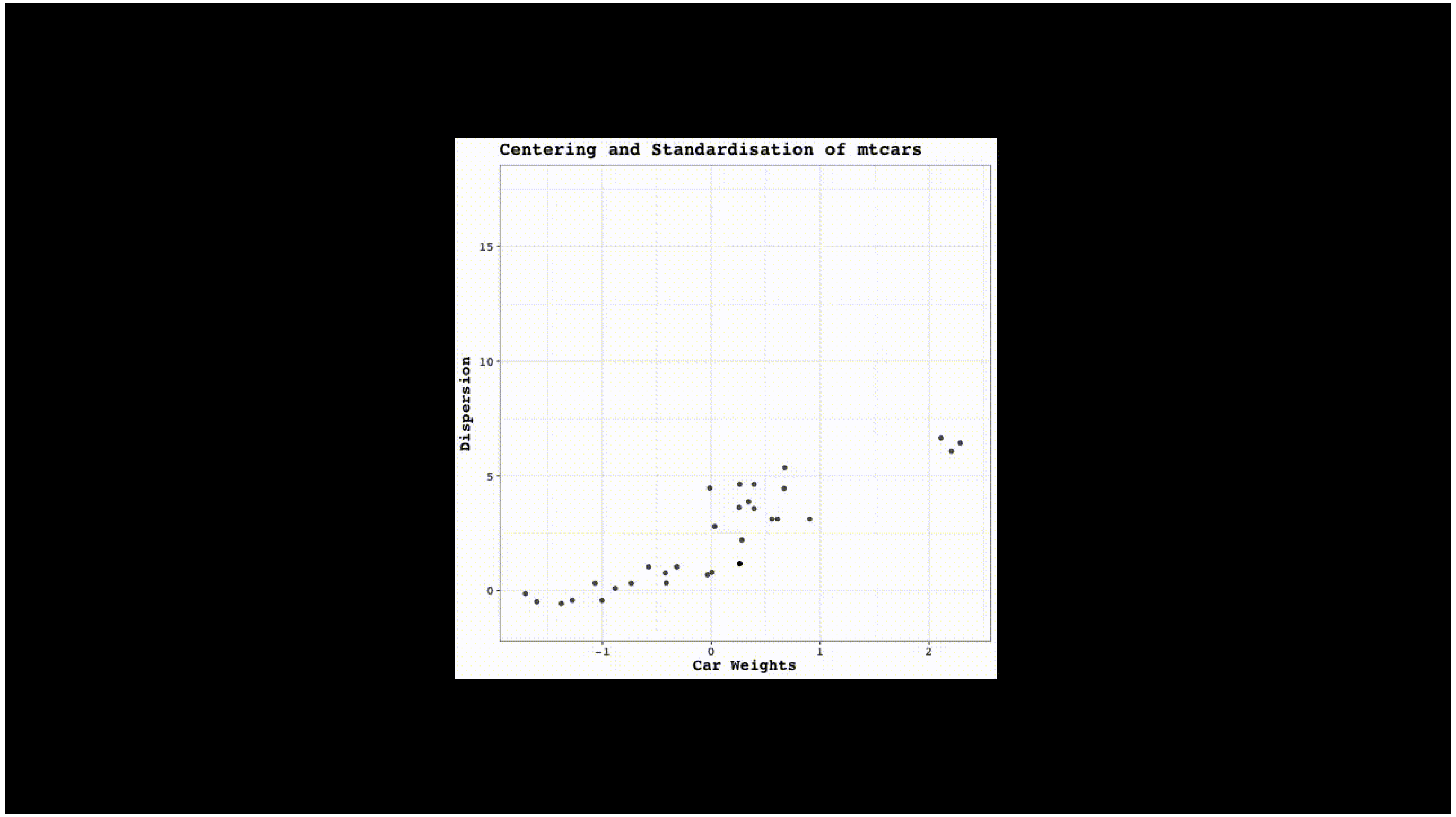
1. Pre-processing steps
2. Change of coordinate system
3. Explained variance

- Centering
- Standardisation
- Rotation
- Projection
- Reduction

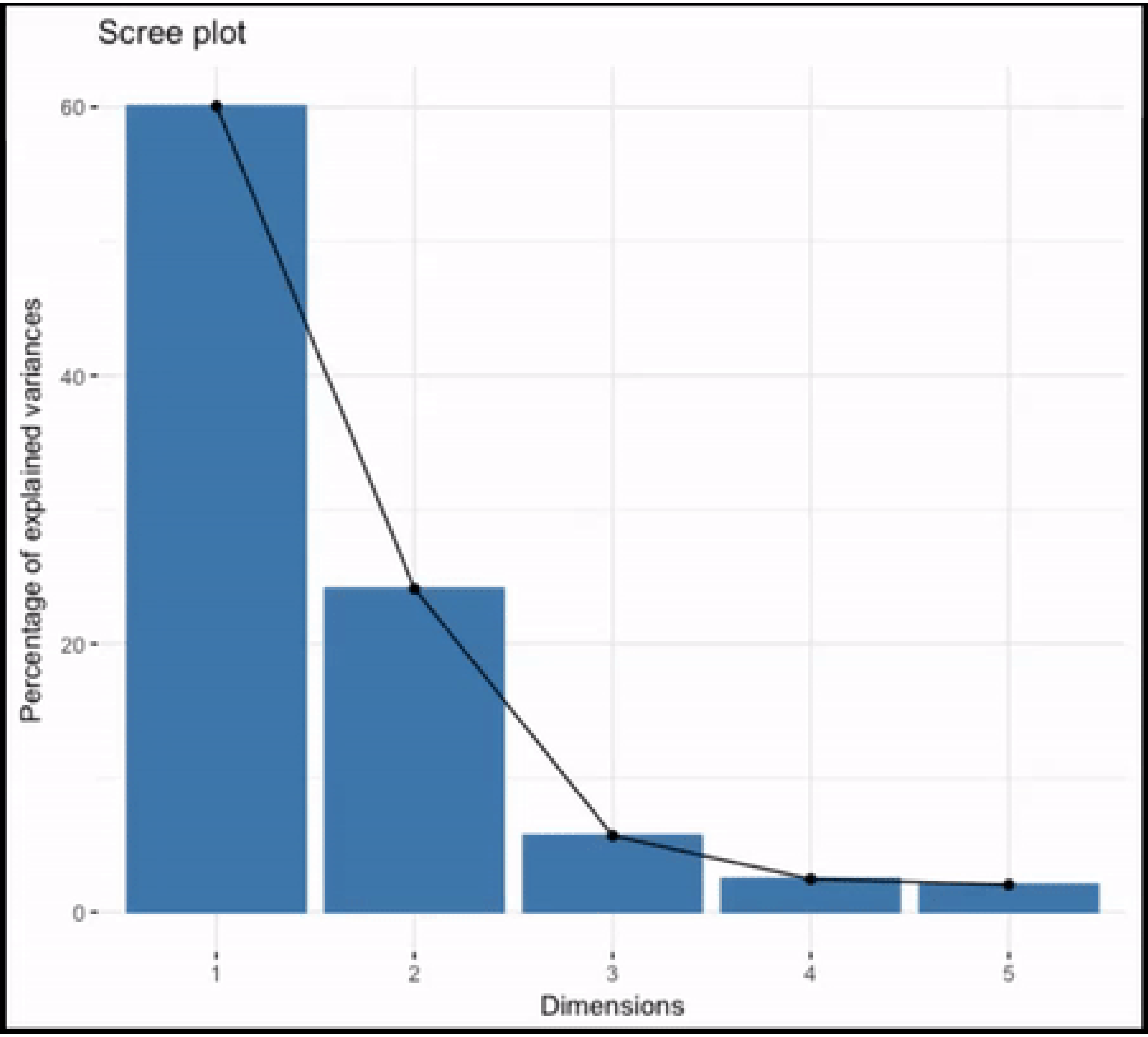
# Pre-processing steps: Data Centering and Standardisation



# Change of coordinate system: Rotation and Projection



# Reduction: Screeplot and the explained variance



# PCA with base R's prcomp()

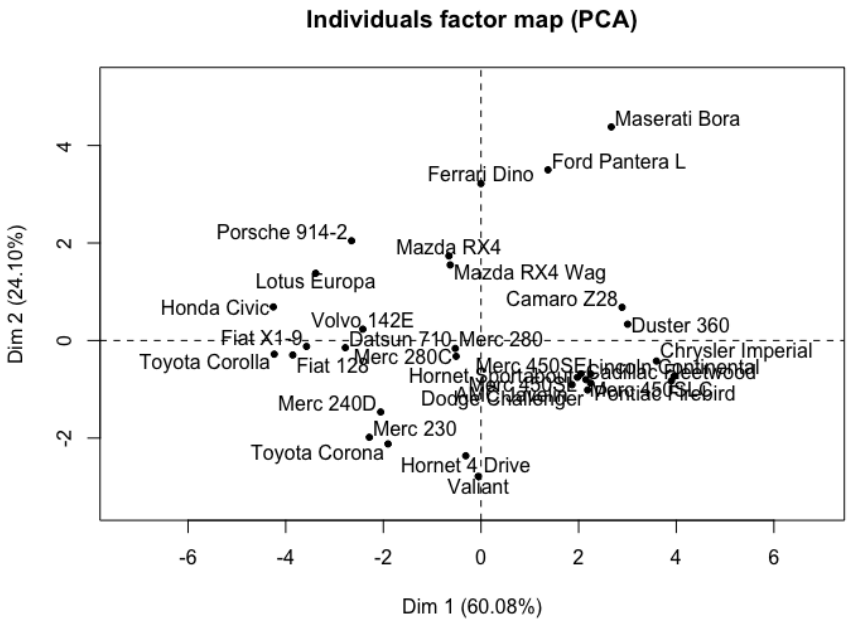
```r
mtcars_pca <- prcomp(mtcars)
```

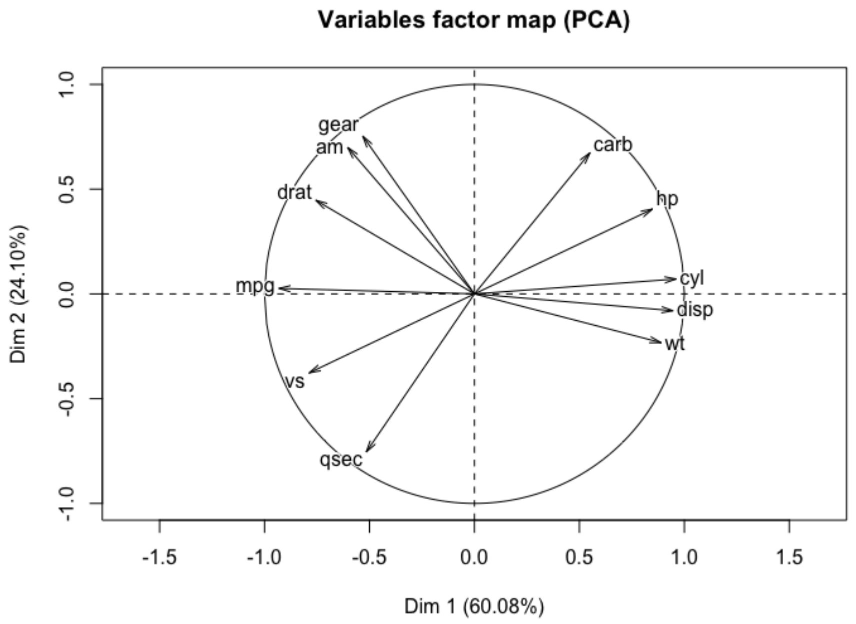
```
Standard deviations (1, .., p=11):
 [1] 136.5330479  38.1480776   3.0710166   1.3066508   0.9064862   0.6635411   0.3085791   0.2859604   0.2506973   0.2106519   0.1984238

Rotation (n x k) = (11 x 11):
              PC1          PC2          PC3          PC4         PC5          PC6          PC7           PC8          PC9         PC10          PC11
mpg  -0.038118199  0.009184847  0.982070847  0.047634784 -0.08832843 -0.143790084 -0.039239174  2.271040e-02 -0.002790139  0.030630361 -0.0158569365
cyl   0.012035150 -0.003372487 -0.063483942 -0.227991962  0.23872590 -0.793818050  0.425011021 -1.890403e-01  0.042677206  0.131718534  0.1454453628
disp  0.899568146  0.435372320  0.031442656 -0.005086826 -0.01073597  0.007424138  0.000582398 -5.841464e-04  0.003532713 -0.005399132  0.0009420262
hp    0.434784387 -0.899307303  0.025093049  0.035715638  0.01655194  0.001653685 -0.002212538  4.748087e-06 -0.003734085  0.001862554 -0.0021526102
drat -0.002660077 -0.003900205  0.039724928 -0.057129357 -0.13332765  0.227229260  0.034847411 -9.385817e-01 -0.014131110  0.184102094 -0.0973818815
wt    0.006239405  0.004861023 -0.084910258  0.127962867 -0.24354296 -0.127142296 -0.186558915  1.561907e-01 -0.390600261  0.829886844 -0.0198581635
qsec -0.006671270  0.025011743 -0.071670457  0.886472188 -0.21416101 -0.189564973  0.254844548 -1.028515e-01 -0.095914479 -0.204240658  0.0110677880
vs   -0.002729474  0.002198425  0.004203328  0.177123945 -0.01688851  0.102619063 -0.080788938 -2.132903e-03  0.684043835  0.303060724  0.6256900918
am   -0.001962644 -0.005793760  0.054806391 -0.135658793 -0.06270200  0.205217266  0.200858874 -2.273255e-02 -0.572372433 -0.162808201  0.7331658036
gear -0.002604768 -0.011272462  0.048524372 -0.129913811 -0.27616440  0.334971103  0.801625551  2.174878e-01  0.156118559  0.203540645 -0.1909325849
carb  0.005766010 -0.027779208 -0.102897231 -0.268931427 -0.85520810 -0.283788381 -0.165474186  3.972219e-03  0.127583043 -0.239954748  0.0557957968
```

# PCA with FactoMineR's PCA()

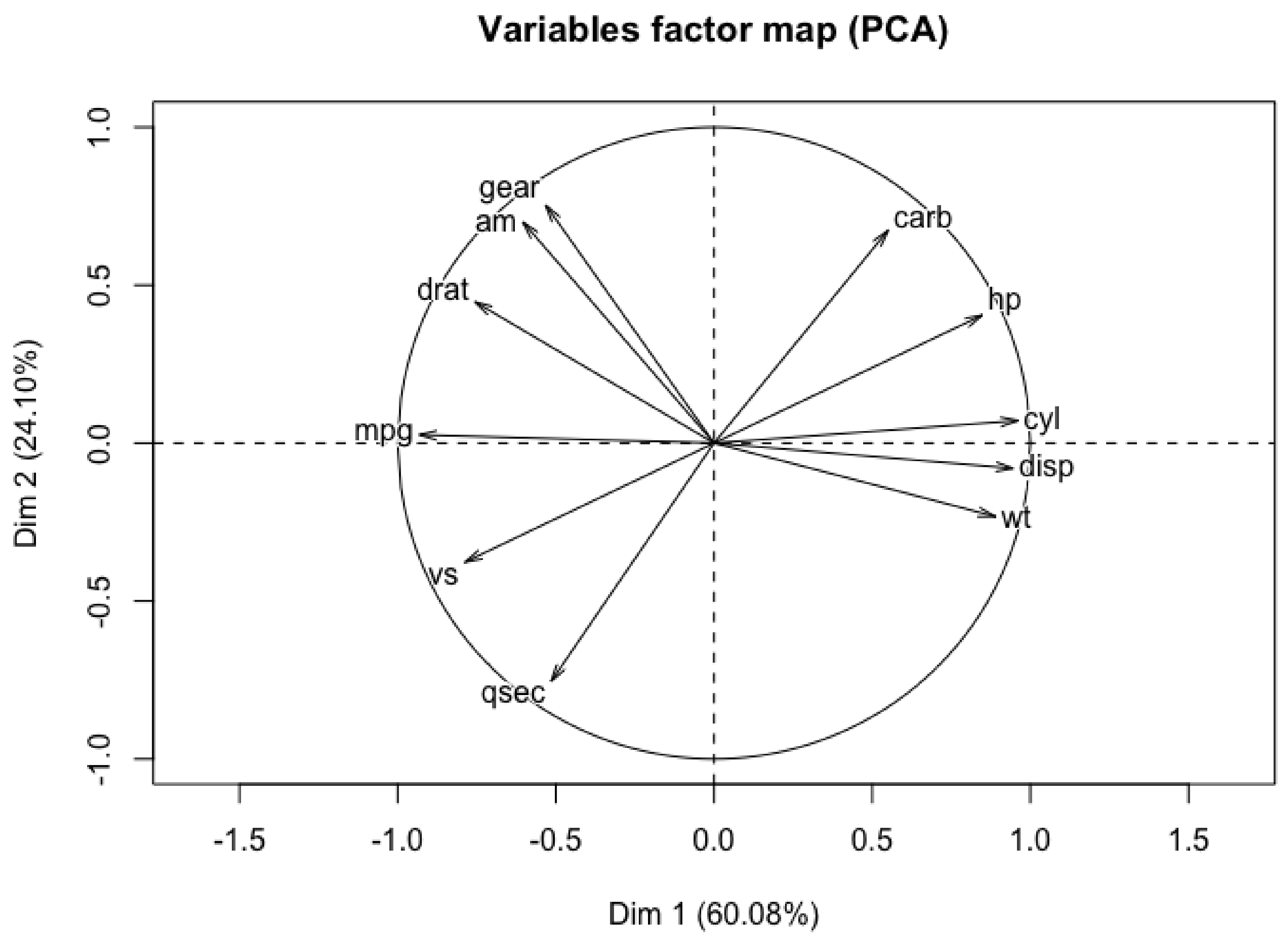
```r
library(FactoMineR)
mtcars_pca <- PCA(mtcars)
```

```
**Results for the Principal Component Analysis (PCA)**
The analysis was performed on 32 individuals, described by 11 variables
*The results are available in the following objects:

   name               description
1  "$eig"             "eigenvalues"
2  "$var"             "results for the variables"
3  "$var$coord"       "coord. for the variables"
4  "$var$cor"         "correlations variables - dimensions"
5  "$var$cos2"        "cos2 for the variables"
6  "$var$contrib"     "contributions of the variables"
7  "$ind"             "results for the individuals"
8  "$ind$coord"       "coord. for the individuals"
9  "$ind$cos2"        "cos2 for the individuals"
10 "$ind$contrib"     "contributions of the individuals"
11 "$call"            "summary statistics"
12 "$call$centre"     "mean of the variables"
13 "$call$ecart.type" "standard error of the variables"
14 "$call$row.w"      "weights for the individuals"
15 "$call$col.w"      "weights for the variables"
```



# Variables' factor map



# Digging into PCA()

```
mtcars_pca$eig
```

```
mtcars_pca$var$cos2
```

| | eigenvalue | percentage of variance | cumulative percentage of variance |
|---|---|---|---|
| comp 1 | 6.60840025 | 60.0763659 | 60.07637 |
| comp 2 | 2.65046789 | 24.0951627 | 84.17153 |
| comp 3 | 0.62719727 | 5.7017934 | 89.87332 |
| comp 4 | 0.26959744 | 2.4508858 | 92.32421 |
| comp 5 | 0.22345110 | 2.0313737 | 94.35558 |
| comp 6 | 0.21159612 | 1.9236011 | 96.27918 |
| comp 7 | 0.13526199 | 1.2296544 | 97.50884 |
| comp 8 | 0.12290143 | 1.1172858 | 98.62612 |
| comp 9 | 0.07704665 | 0.7004241 | 99.32655 |
| comp 10 | 0.05203544 | 0.4730495 | 99.79960 |
| comp 11 | 0.02204441 | 0.2004037 | 100.00000 |

| | Dim.1 | Dim.2 | Dim.3 | Dim.4 | Dim.5 |
|---|---|---|---|---|---|
| mpg | 0.8685312 | 0.0006891117 | 0.031962249 | 1.369725e-04 | 0.0023634487 |
| cyl | 0.9239416 | 0.0050717032 | 0.019276287 | 1.811054e-06 | 0.0007642822 |
| disp | 0.8958370 | 0.0064482423 | 0.002370993 | 1.775235e-02 | 0.0346868281 |
| hp | 0.7199031 | 0.1640467049 | 0.012295659 | 1.234773e-03 | 0.0651697911 |
| drat | 0.5717921 | 0.1999959326 | 0.016295731 | 1.970035e-01 | 0.0013361275 |
| wt | 0.7916038 | 0.0542284172 | 0.073281663 | 1.630161e-02 | 0.0012578888 |
| qsec | 0.2655437 | 0.5690984542 | 0.101947952 | 1.249426e-03 | 0.0060588455 |
| vs | 0.6208539 | 0.1422249798 | 0.115330572 | 1.244460e-02 | 0.0803189801 |
| am | 0.3647715 | 0.4887450097 | 0.026555457 | 2.501834e-04 | 0.0018011675 |
| gear | 0.2829342 | 0.5665806069 | 0.052667265 | 1.888829e-02 | 0.0005219259 |
| carb | 0.3026882 | 0.4533387304 | 0.175213444 | 4.333912e-03 | 0.0291718181 |

# Digging into PCA()

```
mtcars_pca$var$contrib
```

```
        Dim.1      Dim.2      Dim.3        Dim.4      Dim.5
mpg  13.142837  0.02599962  5.0960440 5.080631e-02  1.0577029
cyl  13.981320  0.19135124  3.0734010 6.717622e-04  0.3420355
disp 13.556034  0.24328694  0.3780299 6.584761e+00 15.5232297
hp   10.893757  6.18934888  1.9604134 4.580062e-01 29.1651238
drat  8.652504  7.54568403  2.5981826 7.307322e+01  0.5979507
wt   11.978751  2.04599412 11.6839894 6.046647e+00  0.5629370
qsec  4.018275 21.47162226 16.2545274 4.634414e-01  2.7114861
vs    9.394919  5.36603293 18.3882452 4.615993e+00 35.9447677
am    5.519816 18.43995209  4.2339880 9.279888e-02  0.8060678
gear  4.281433 21.37662593  8.3972408 7.006107e+00  0.2335750
carb  4.580356 17.10410194 27.9359384 1.607550e+00 13.0551238
```

```
dimdesc(mtcars_pca)
```

```
$Dim.1
$Dim.1$quanti
      correlation      p.value
cyl     0.9612188 2.471950e-18
disp    0.9464866 2.804047e-16
wt      0.8897212 9.780198e-12
hp      0.8484710 8.622043e-10
carb    0.5501711 1.105272e-03
qsec   -0.5153093 2.542578e-03
gear   -0.5319156 1.728737e-03
am     -0.6039632 2.520665e-04
drat   -0.7561693 5.575736e-07
vs     -0.7879428 8.658012e-08
mpg    -0.9319502 9.347042e-15
```

# Let's practice!

DIMENSIONALITY REDUCTION IN R

# Interpreting and visualising PCA models with factoextra

DIMENSIONALITY REDUCTION IN R

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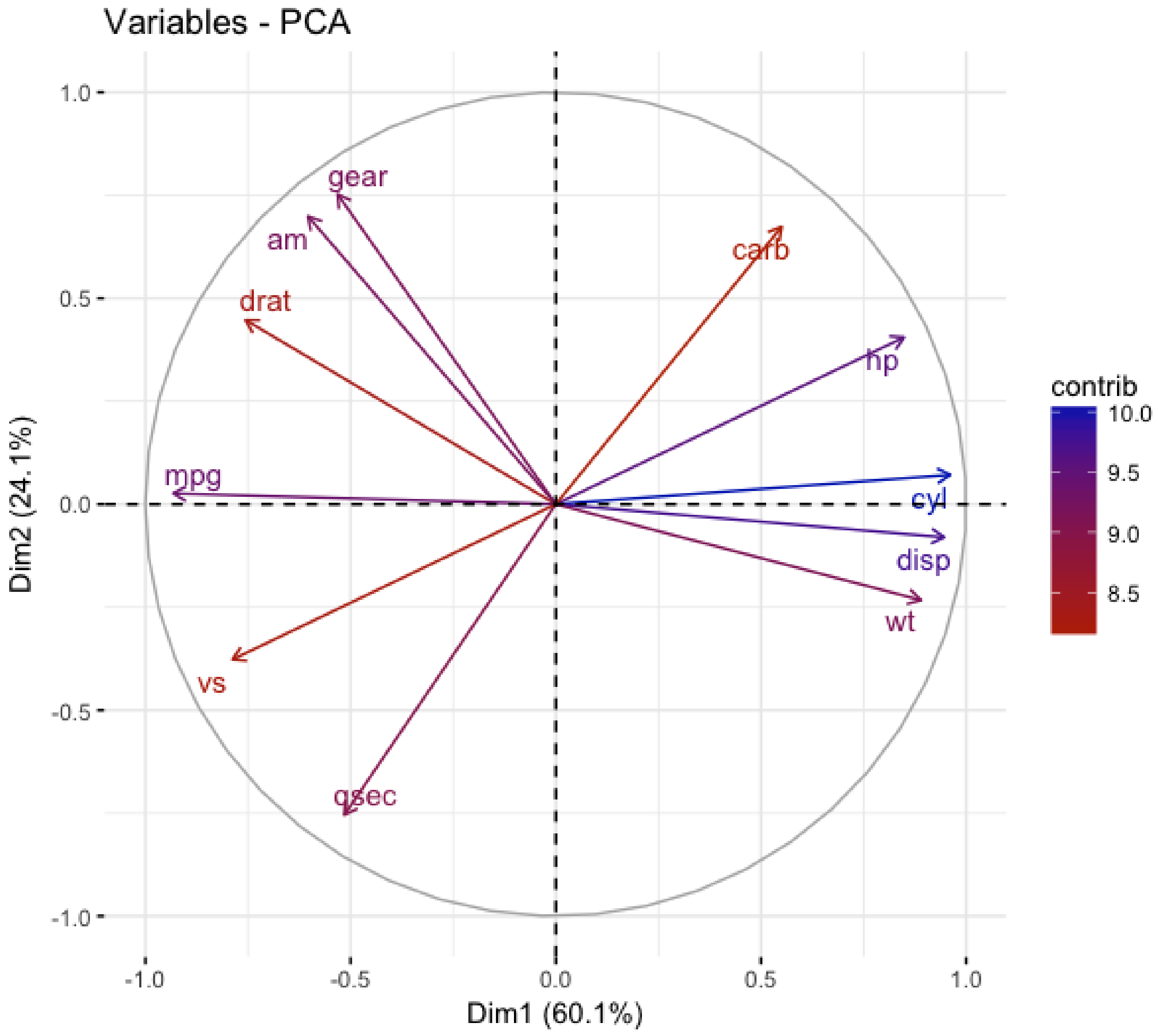
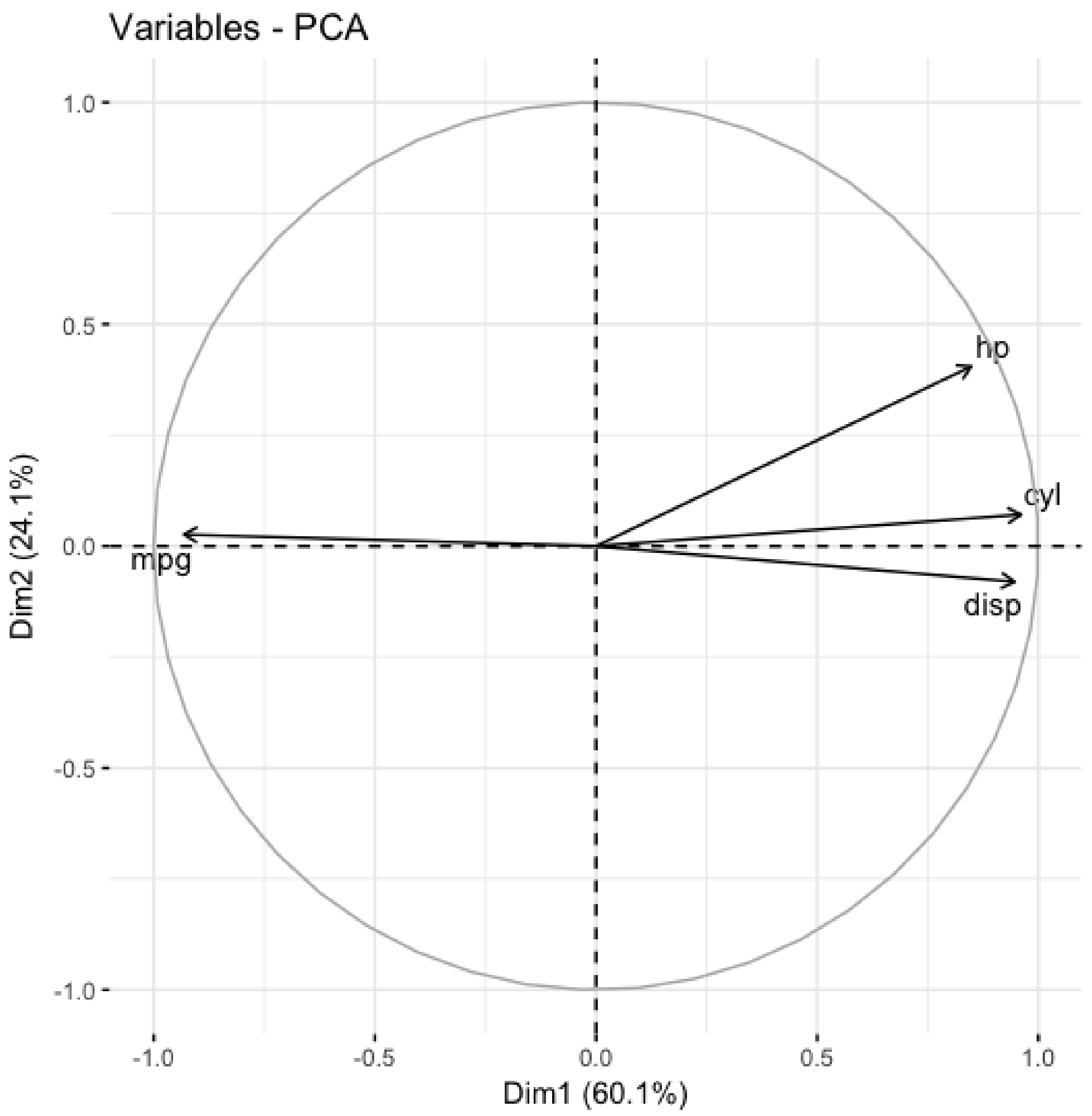
# Plotting contributions of variables

```
fviz_pca_var(mtcars_pca,
 col.var = "contrib",
 gradient.cols = c("#bb2e00", "#002bbb"),
 repel = TRUE)
```



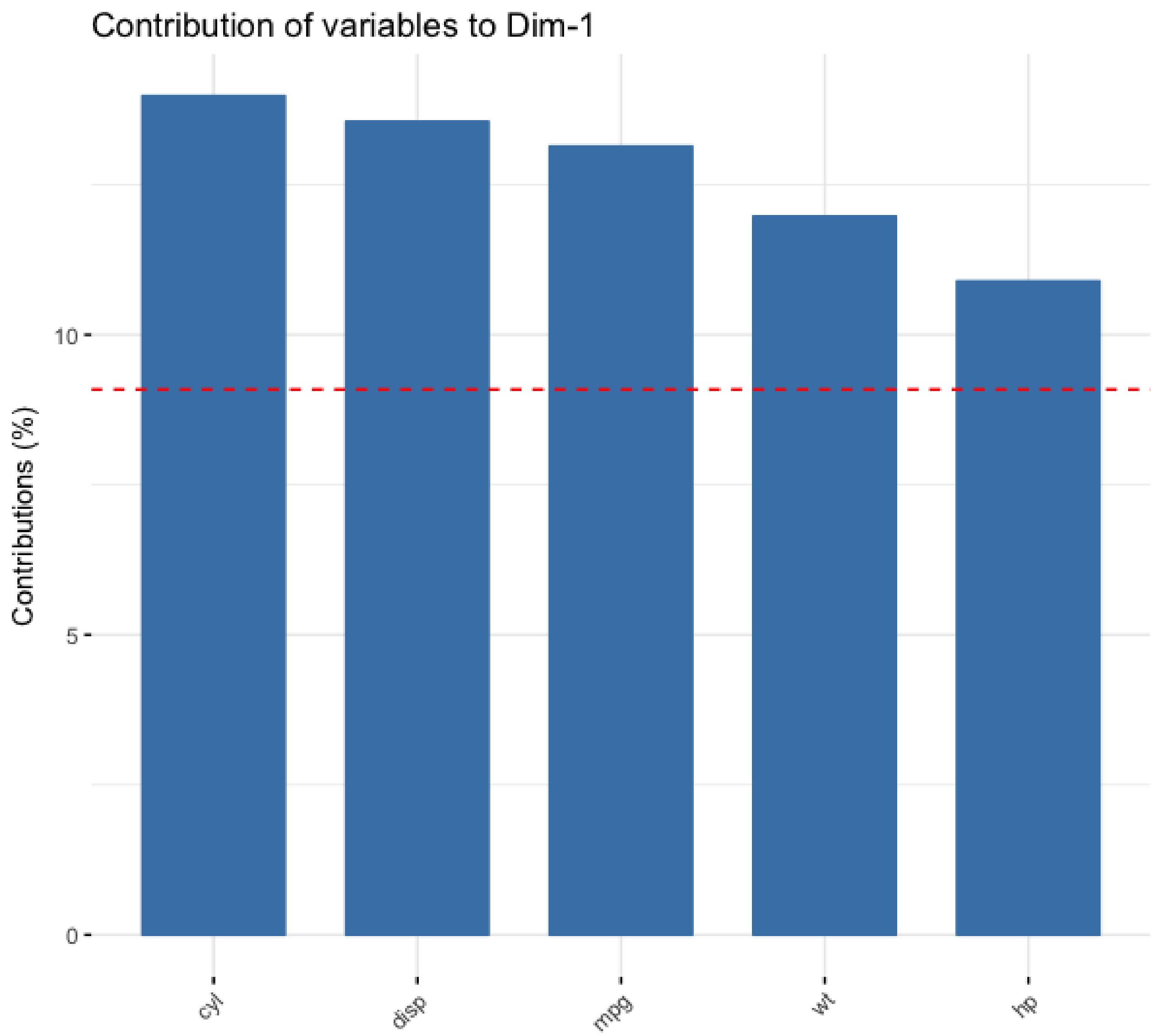
# Plotting contributions of selected variables

```
fviz_pca_var(mtcars_pca,
 select.var = list(contrib = 4),
 repel = TRUE)
```



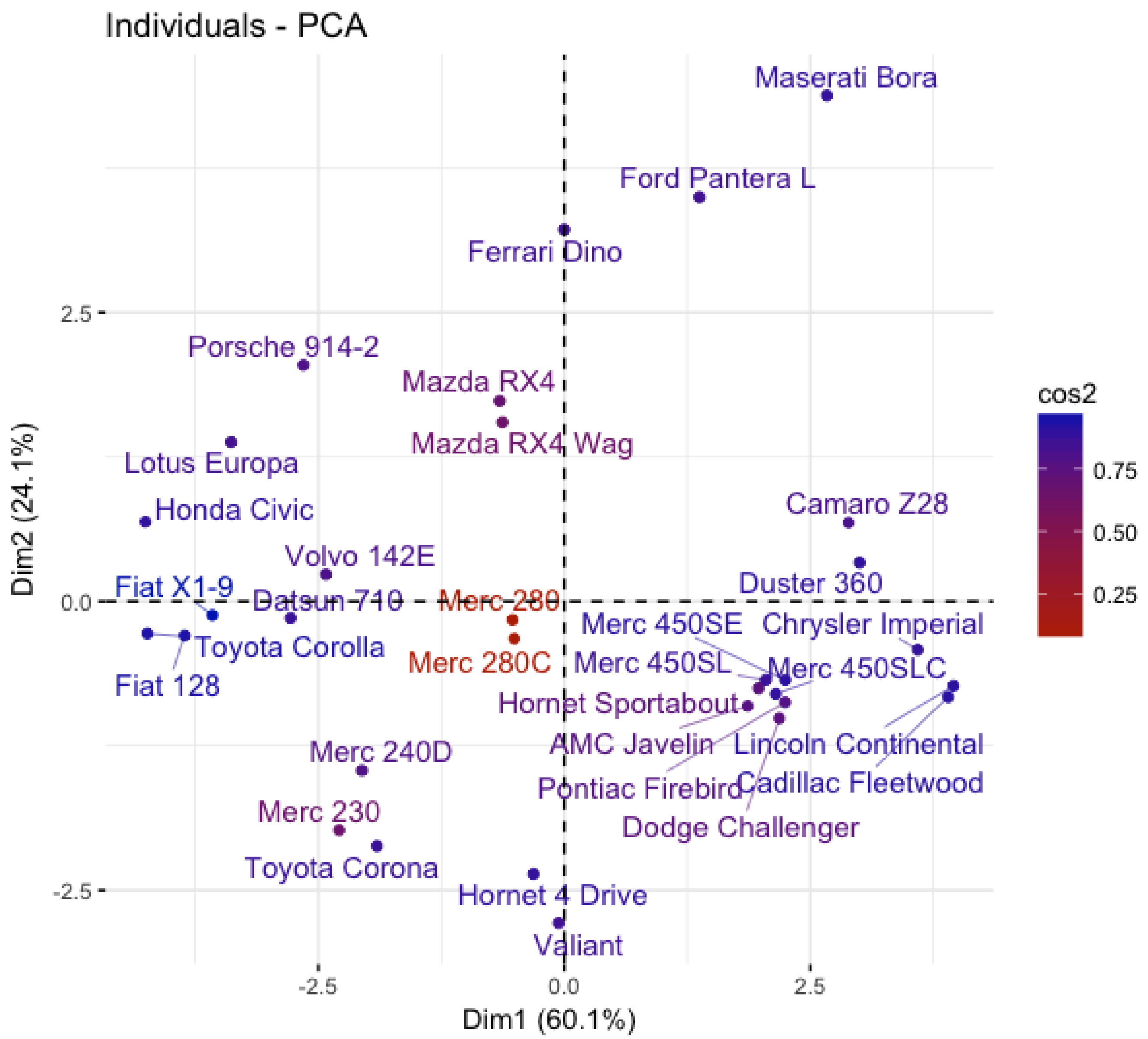
# Barplotting the contributions of variables

```
fviz_contrib(mtcars_pca,
    choice = "var",
    axes = 1,
    top = 5)
```



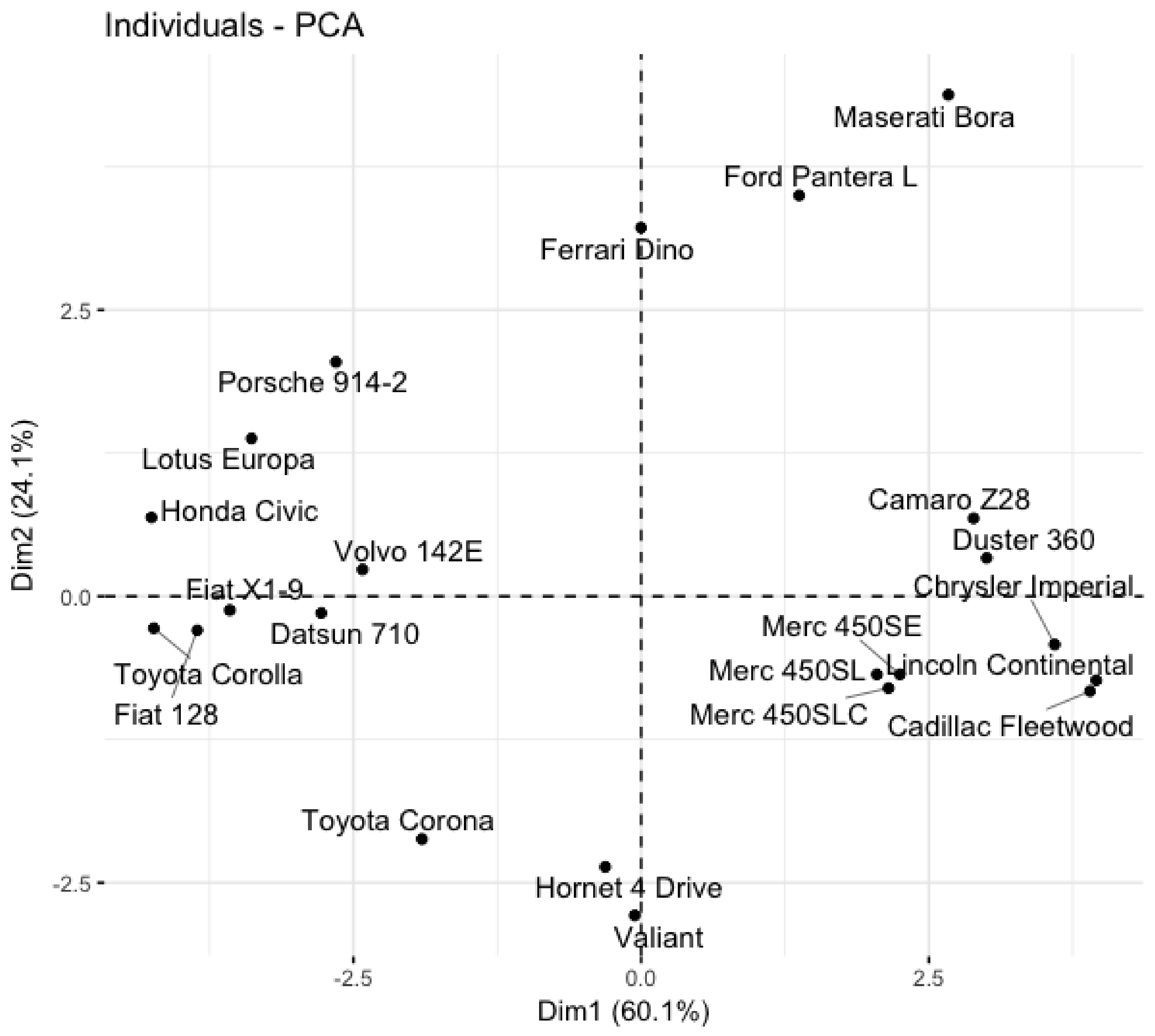
# Plotting cos2 for individuals

```
fviz_pca_ind(mtcars_pca,
    col.ind="cos2",
    gradient.cols = c("#bb2e00", "#002bbb"),
    repel = TRUE)
```



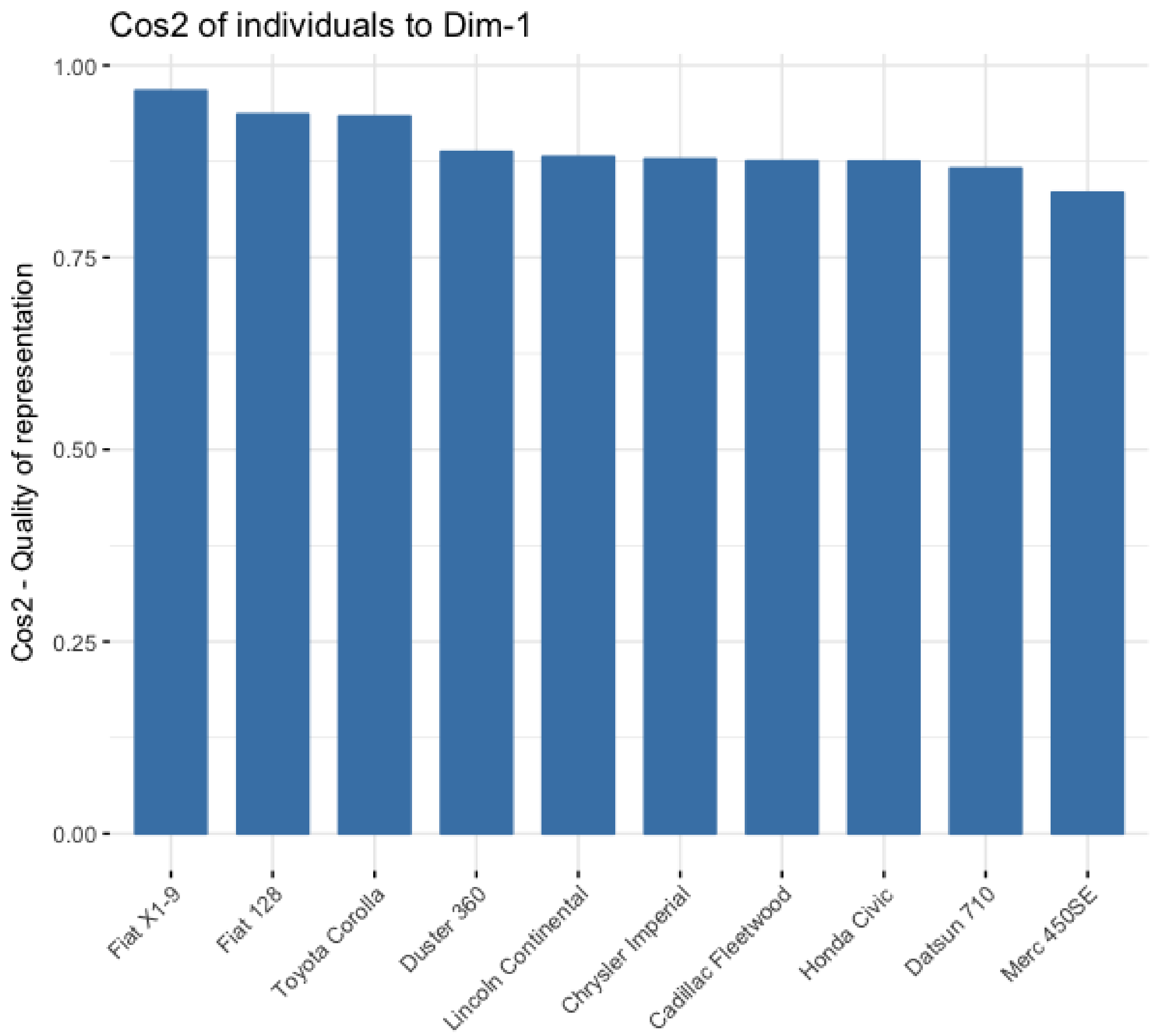
# Plotting cos2 for selected individuals

```
fviz_pca_ind(mtcars_pca,
    select.ind = list(cos2 = 0.8),
    gradient.cols = c("#bb2e00", "#002bbb"),
    repel = TRUE)
```



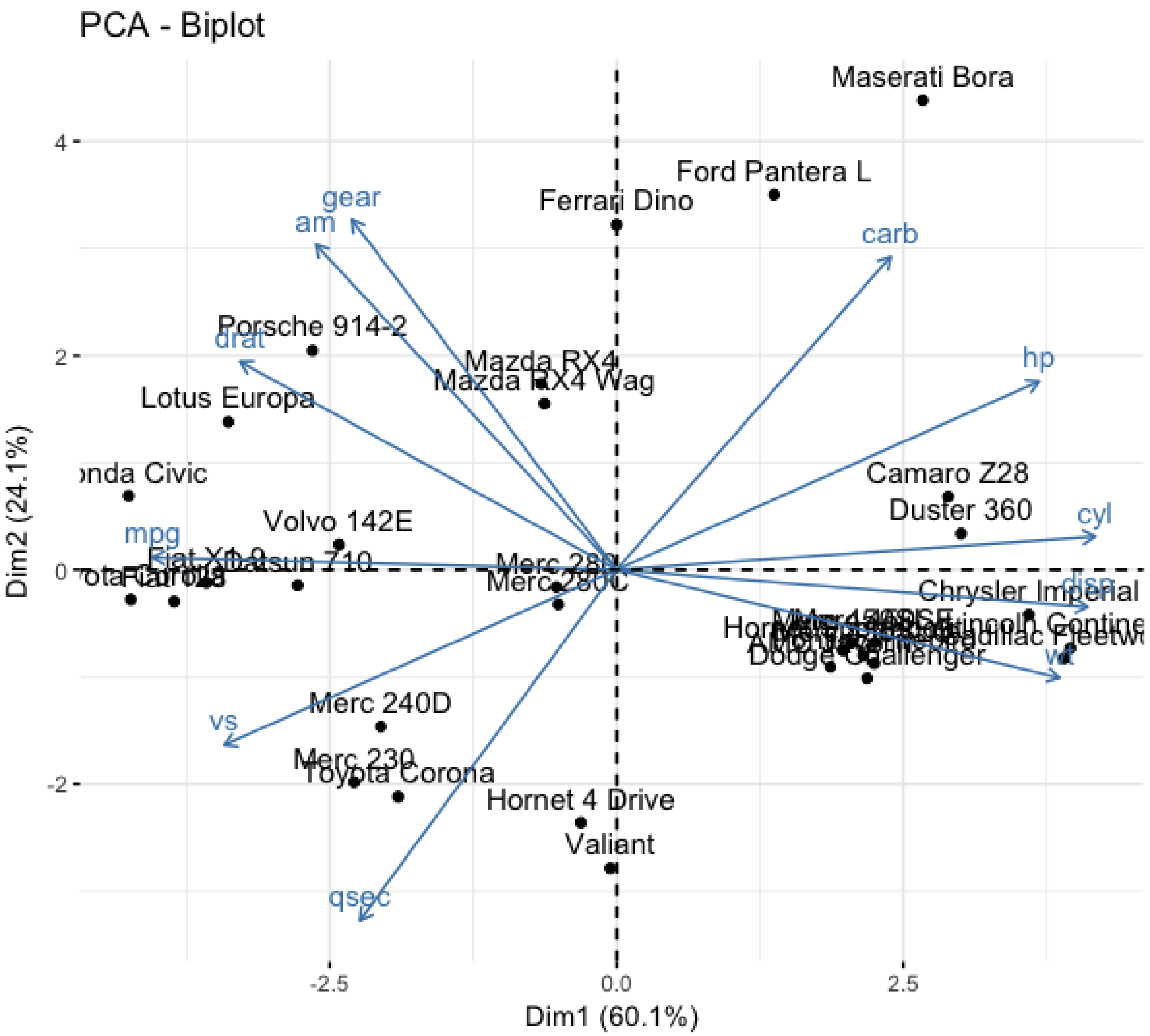
# Barplotting cos2 for individuals

```
fviz_cos2(mtcars_pca,
    choice = "ind",
    axes = 1,
    top = 10)
```



# Biplots

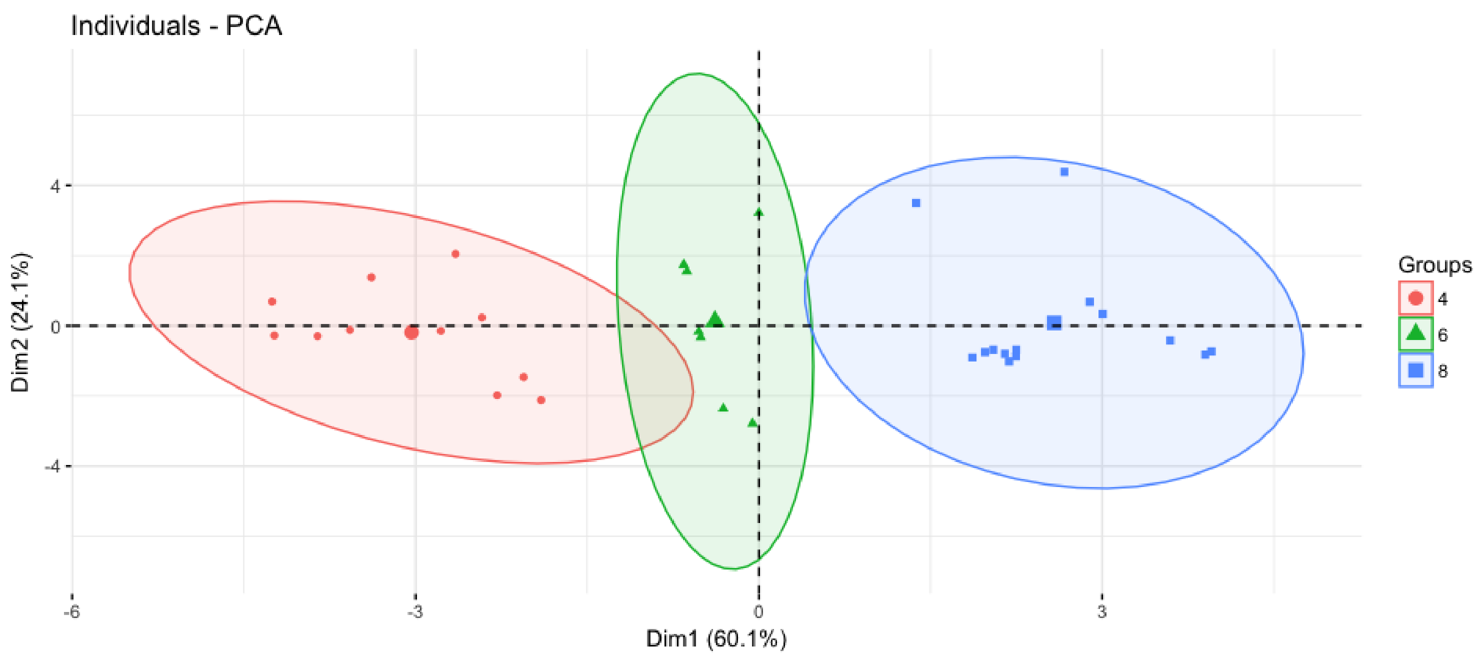
```
fviz_pca_biplot(mtcars_pca)
```



# Adding ellipsoids

```
mtcars$cyl <- as.factor(mtcars$cyl)
```

```
fviz_pca_ind(mtcars_pca,
    label="var",
    habillage=mtcars$cyl,
    addEllipses=TRUE)
```



# Let's practice!

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