UNSUPERVISED LEARNING IN R

Introduction to PCA

Unsupervised learning

- Two methods of clustering — finding groups of homogeneous items
- Next up, dimensionality reduction
  - Find structure in features
  - Aid in visualization

Dimensionality reduction

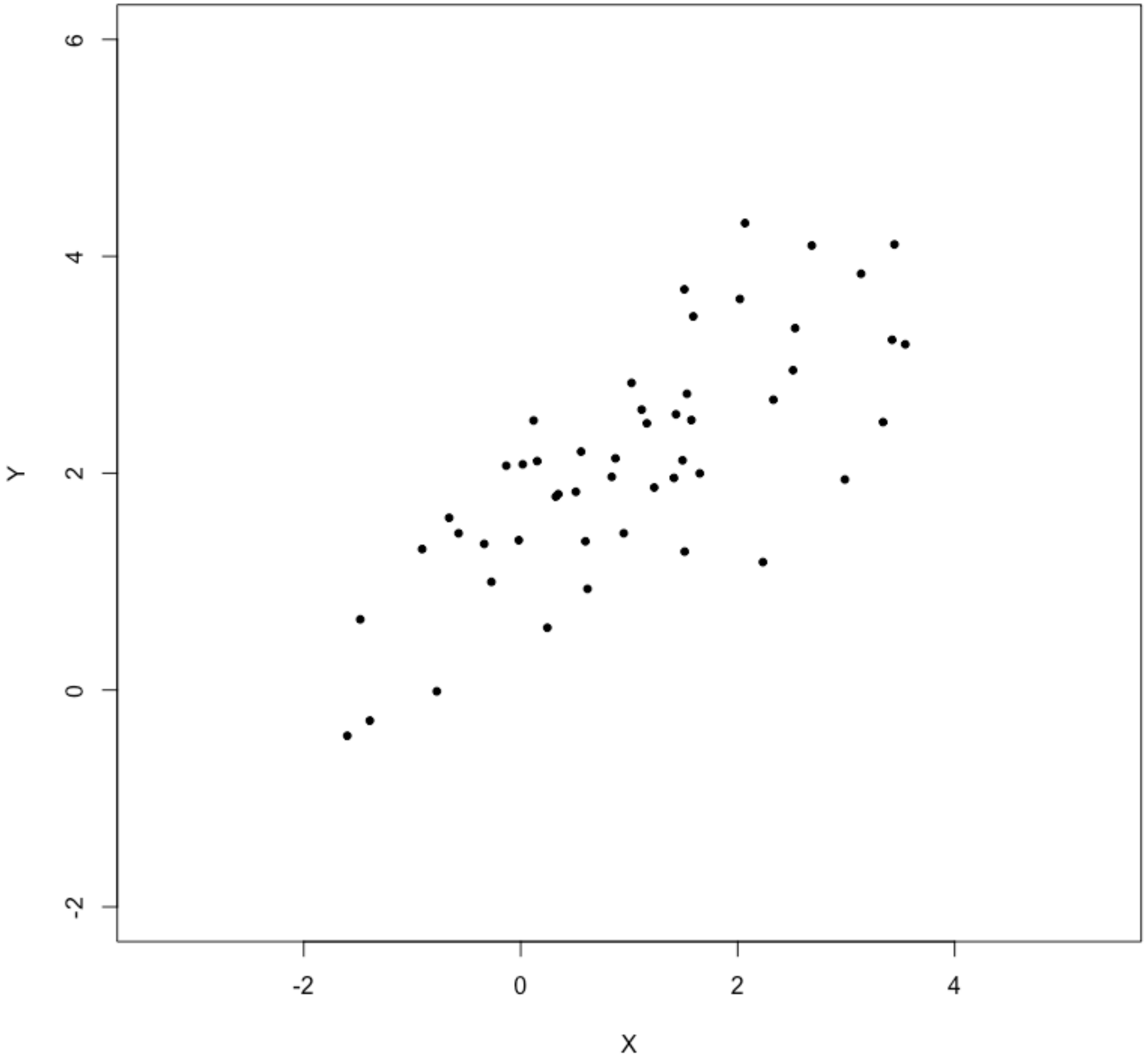
- A popular method is principal component analysis (PCA)
- Three goals when finding lower dimensional representation of features:
  - Find linear combination of variables to create principal components
  - Maintain most variance in the data
  - Principal components are uncorrelated (i.e. orthogonal to each other)

PCA intuition

2 dimensions:
x and y

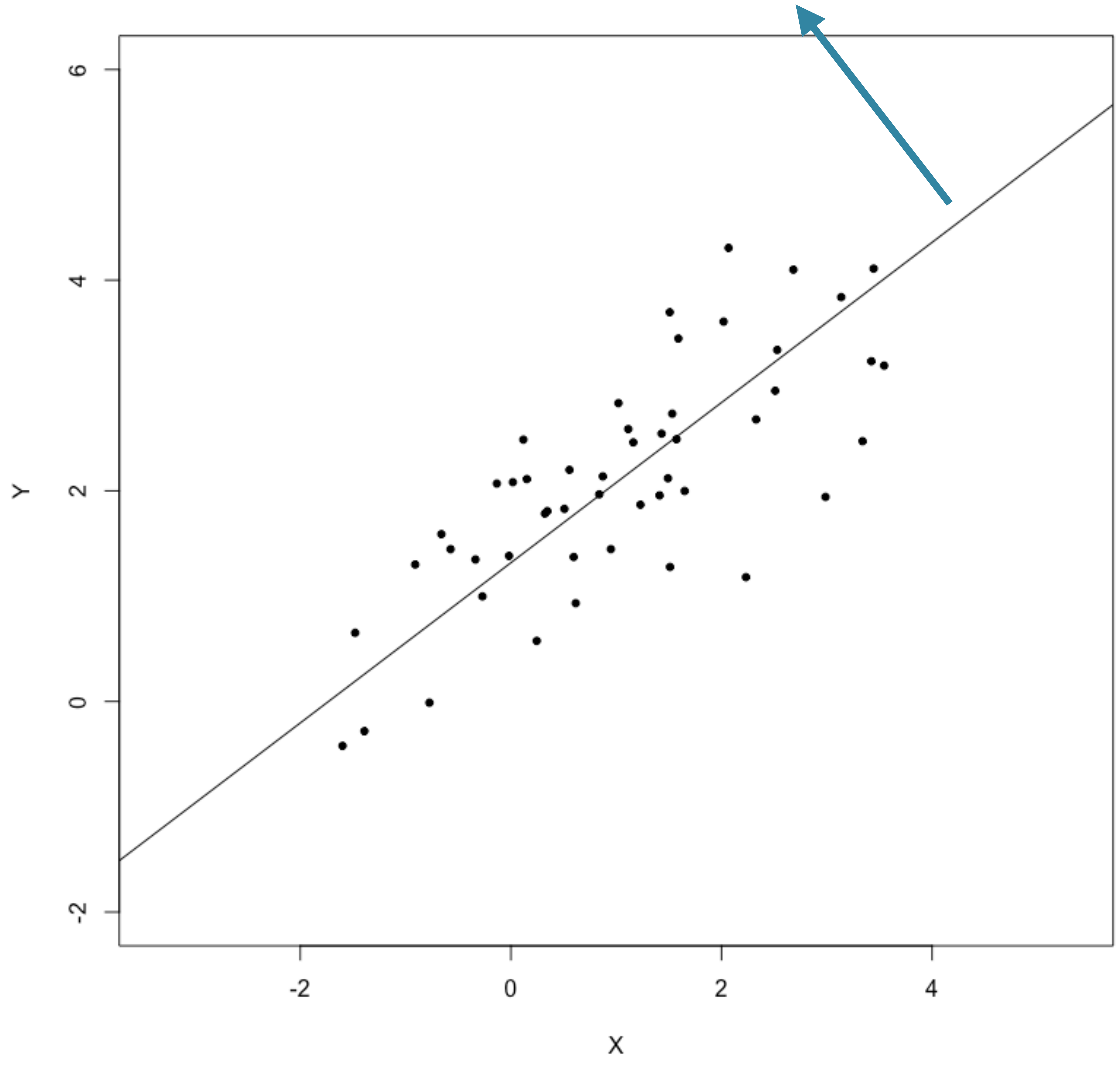
↓ PCA ↓

1 dimension:
One principal component



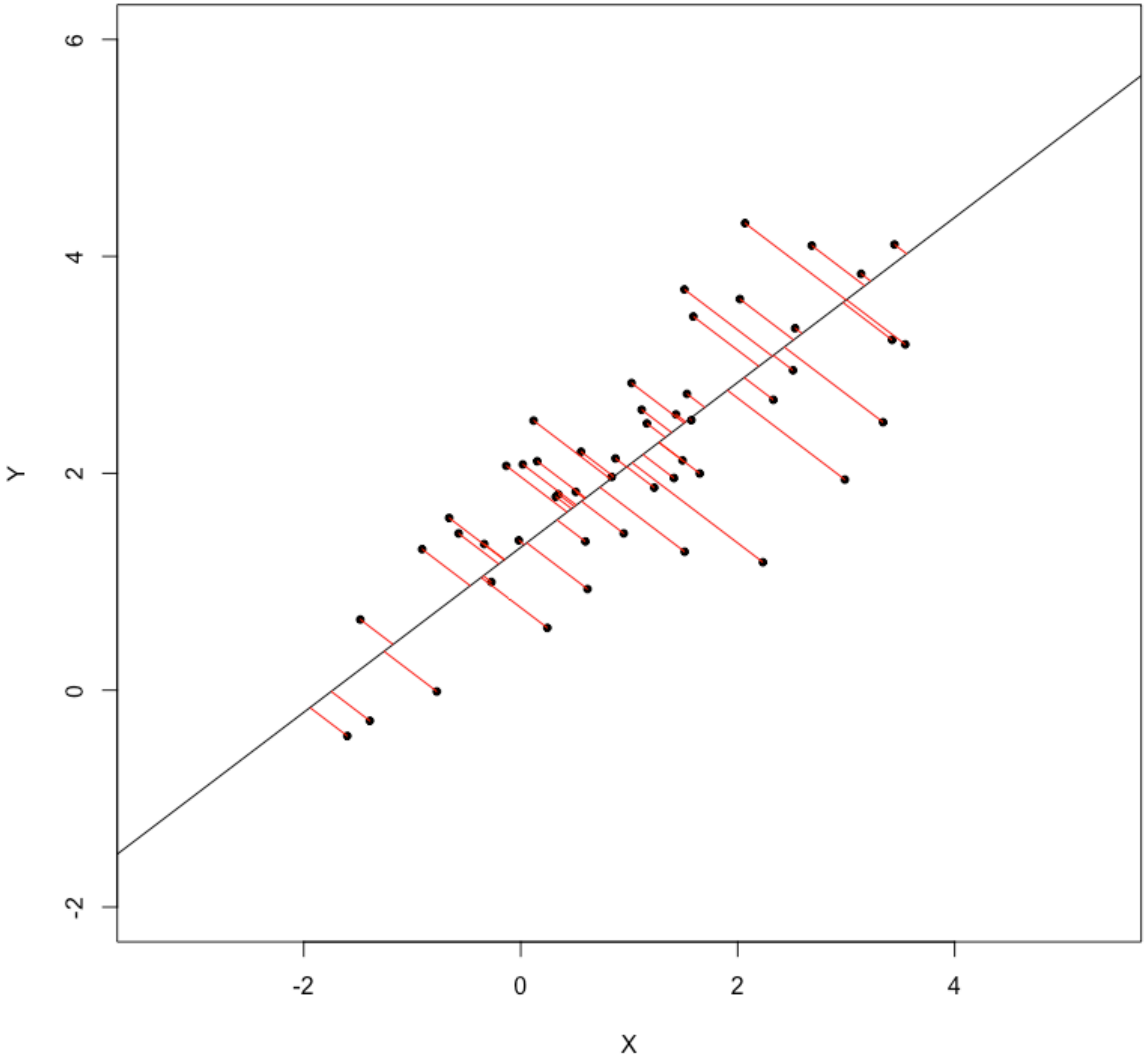
PCA intuition

Regression line represents the principal component

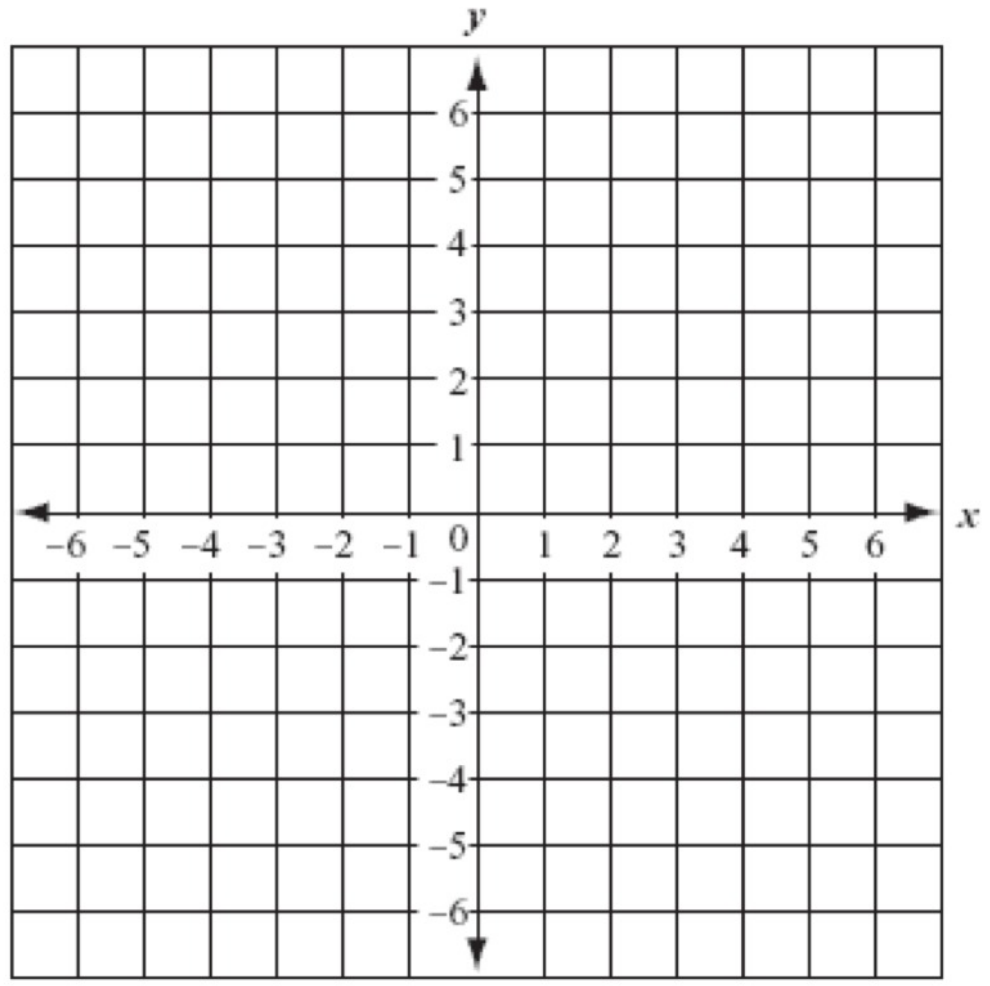


PCA intuition

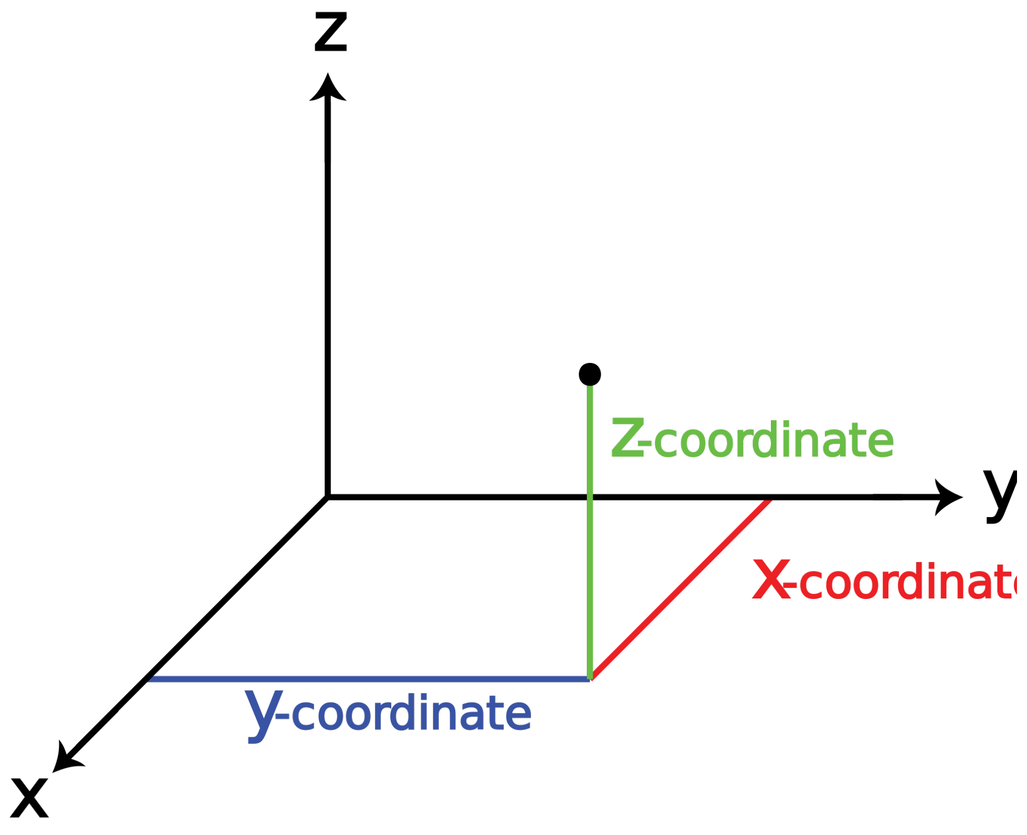
Projected values on principal component is called component scores or factor scores



Visualization of high dimensional data



Two-dimensional

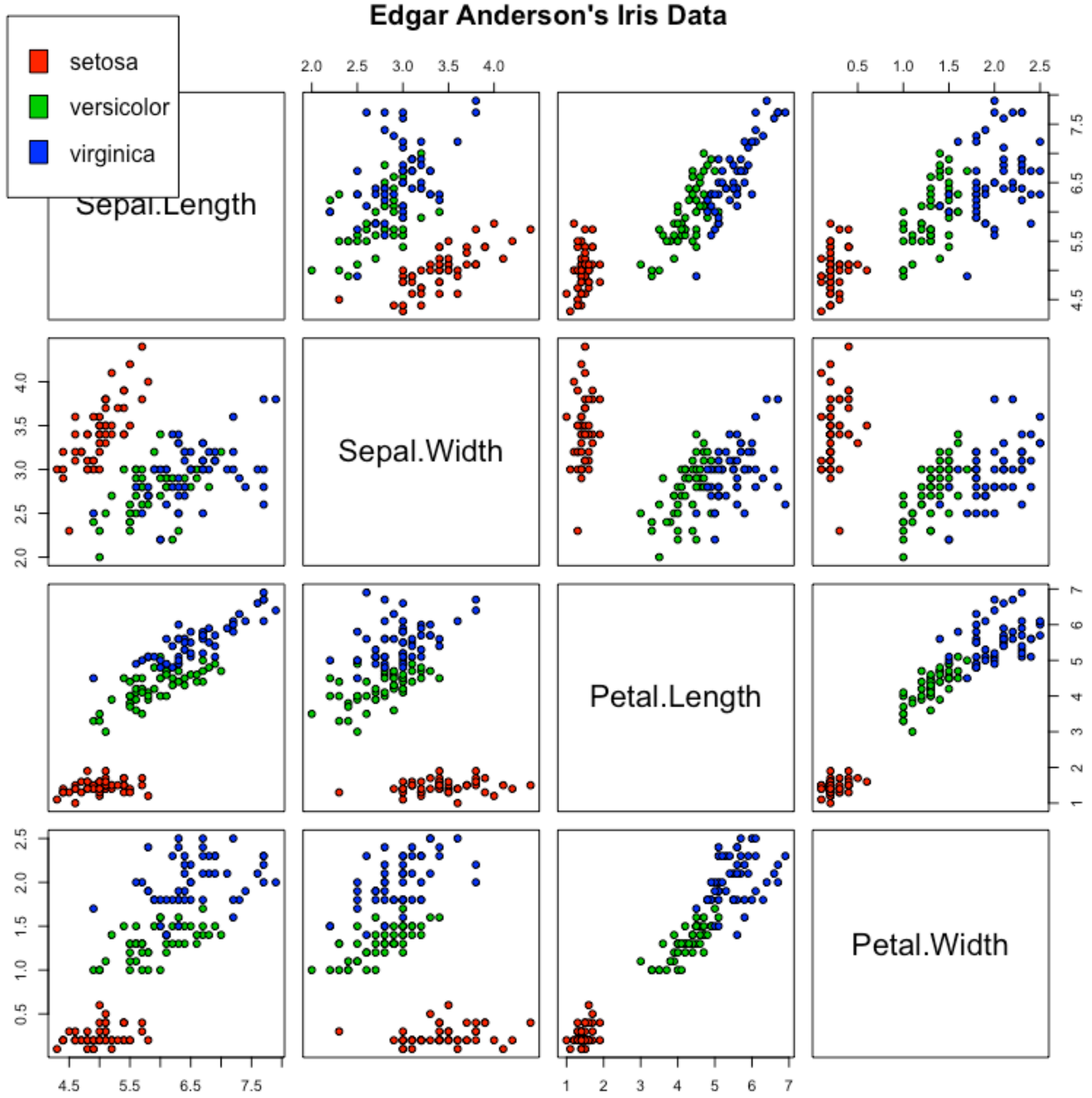


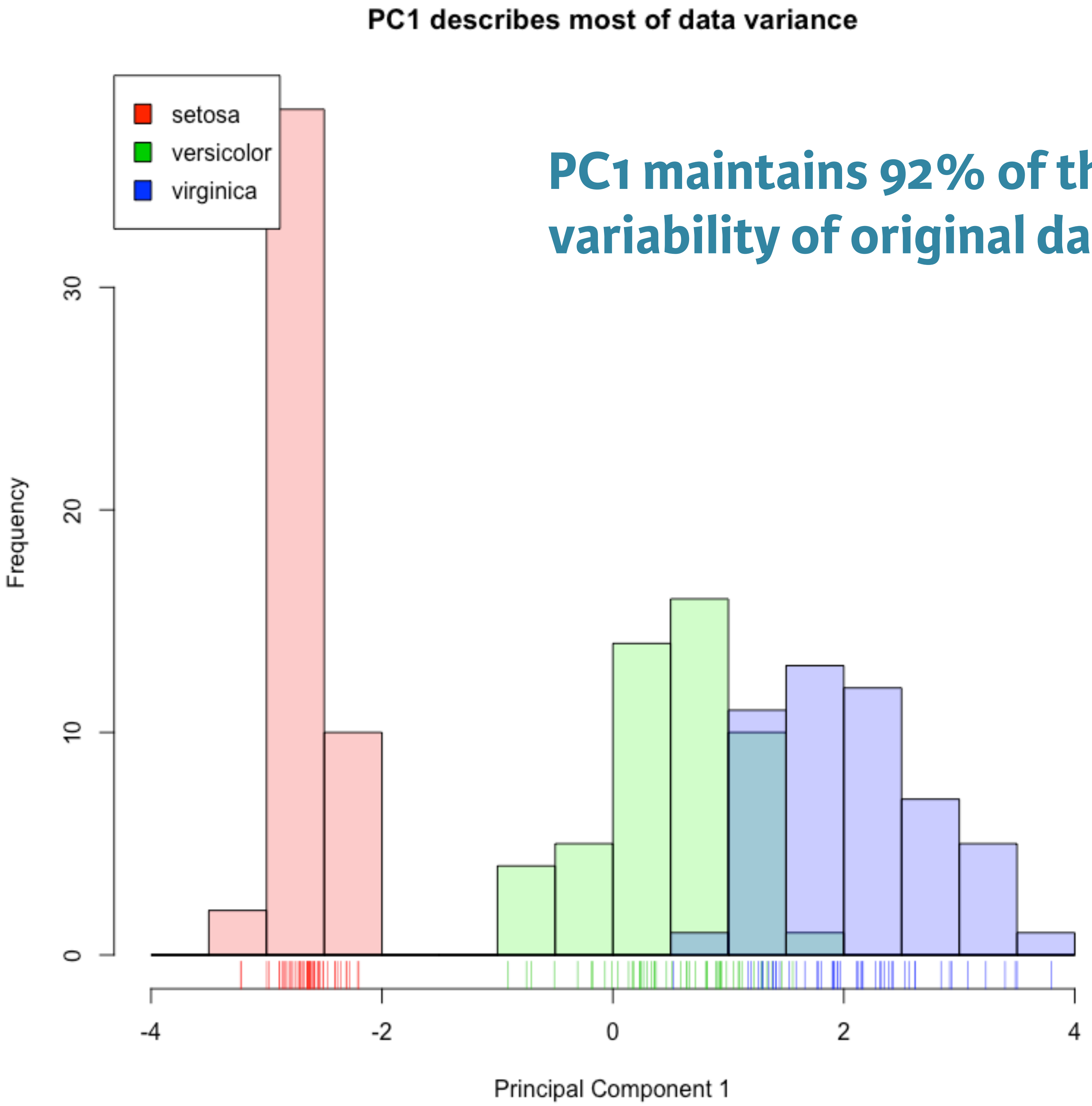
Three-dimensional

?

Four-dimensional

Visualization





PC1 maintains 92% of the variability of original data

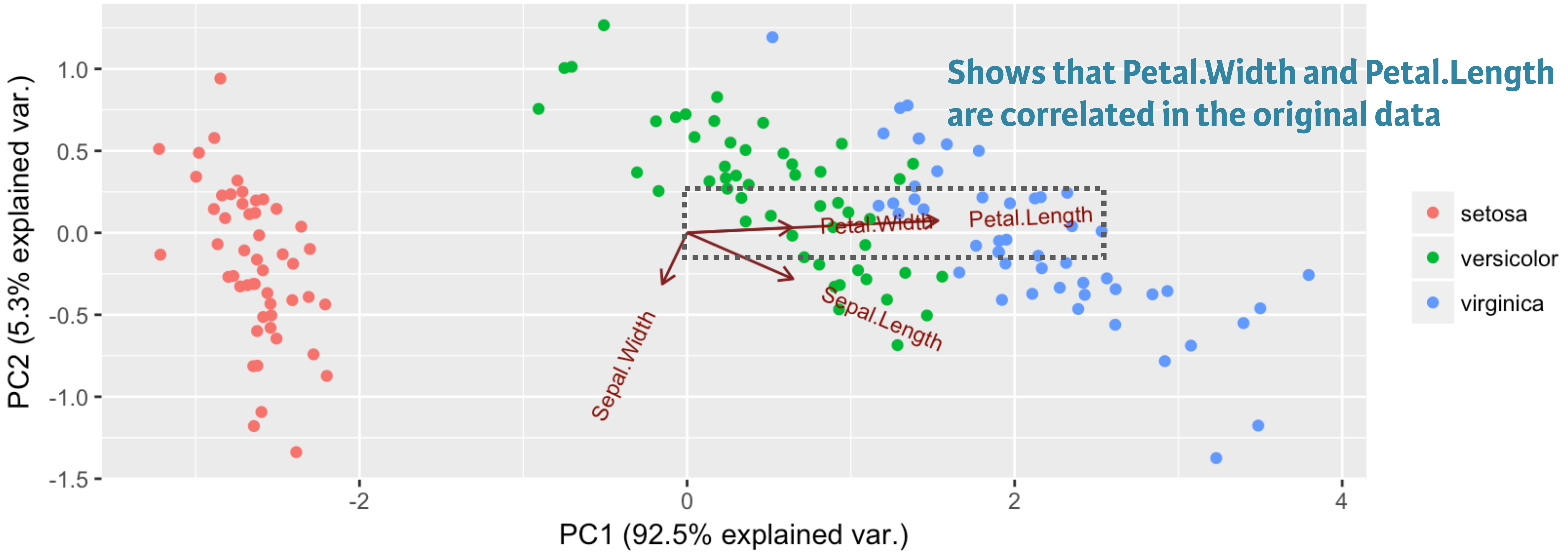
PCA in R

```
> pr.iris <- prcomp(x = iris[-5], scale = FALSE, center = TRUE)
> summary(pr.iris)
Importance of components:
                          PC1     PC2    PC3     PC4
Standard deviation     2.0563 0.49262 0.2797 0.15439
Proportion of Variance 0.9246 0.05307 0.0171 0.00521
Cumulative Proportion  0.9246 0.97769 0.9948 1.00000
```

Let’s practice!

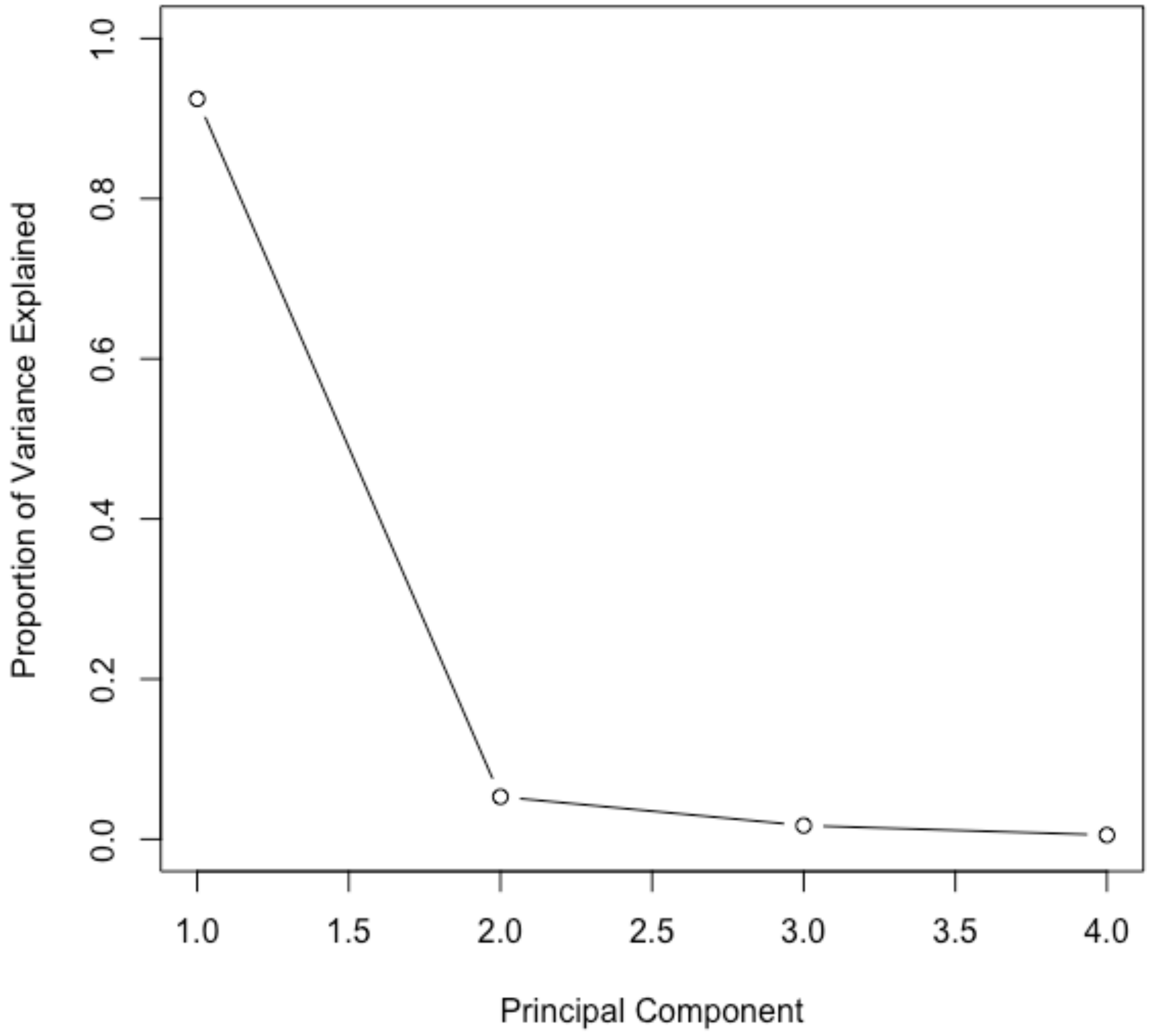
Visualizing and interpreting PCA results

Biplot

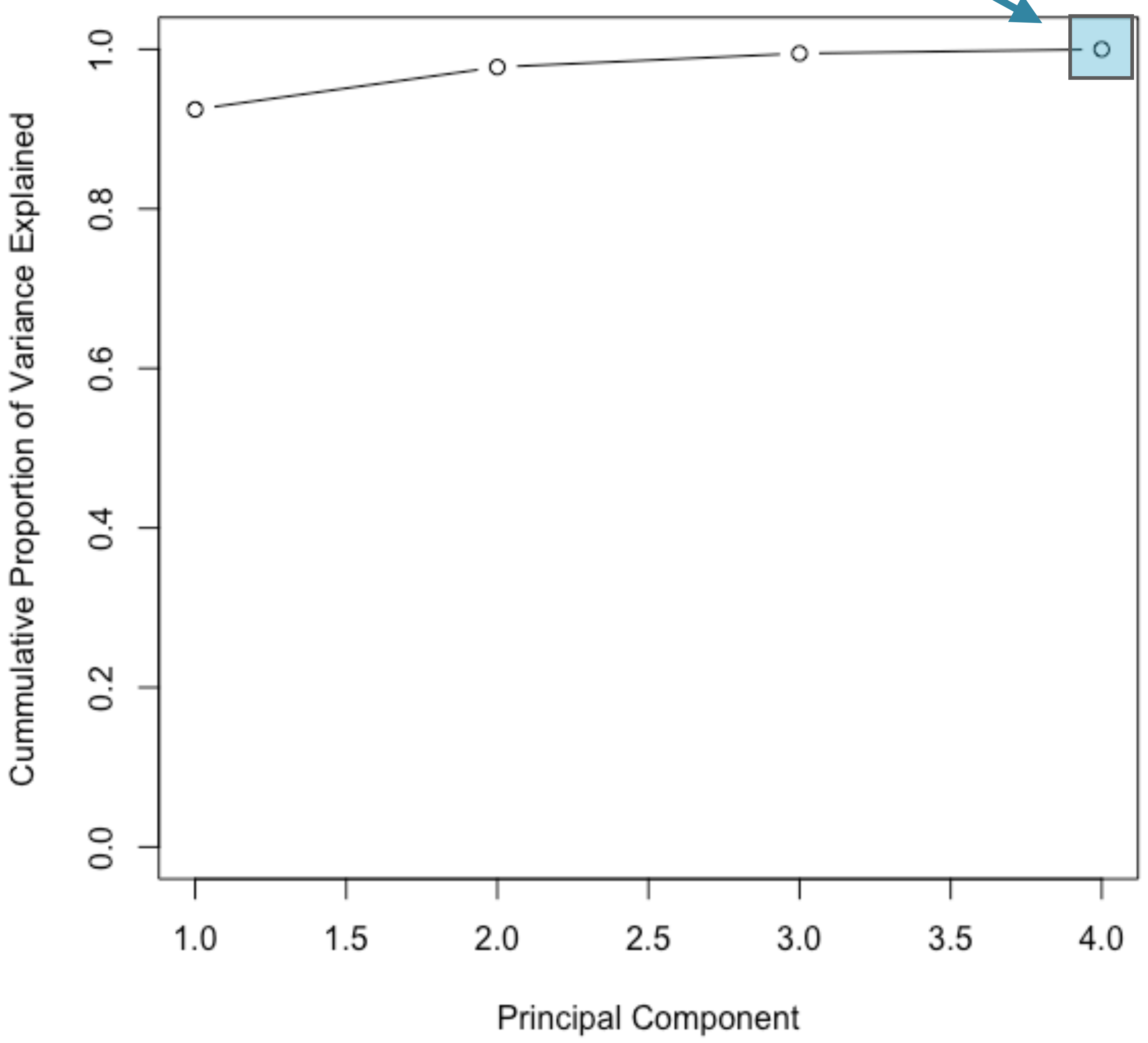


Shows that Petal.Width and Petal.Length are correlated in the original data

Scree plot



When number of PCs and number of original features are the same, the cumulative proportion of variance explained is 1

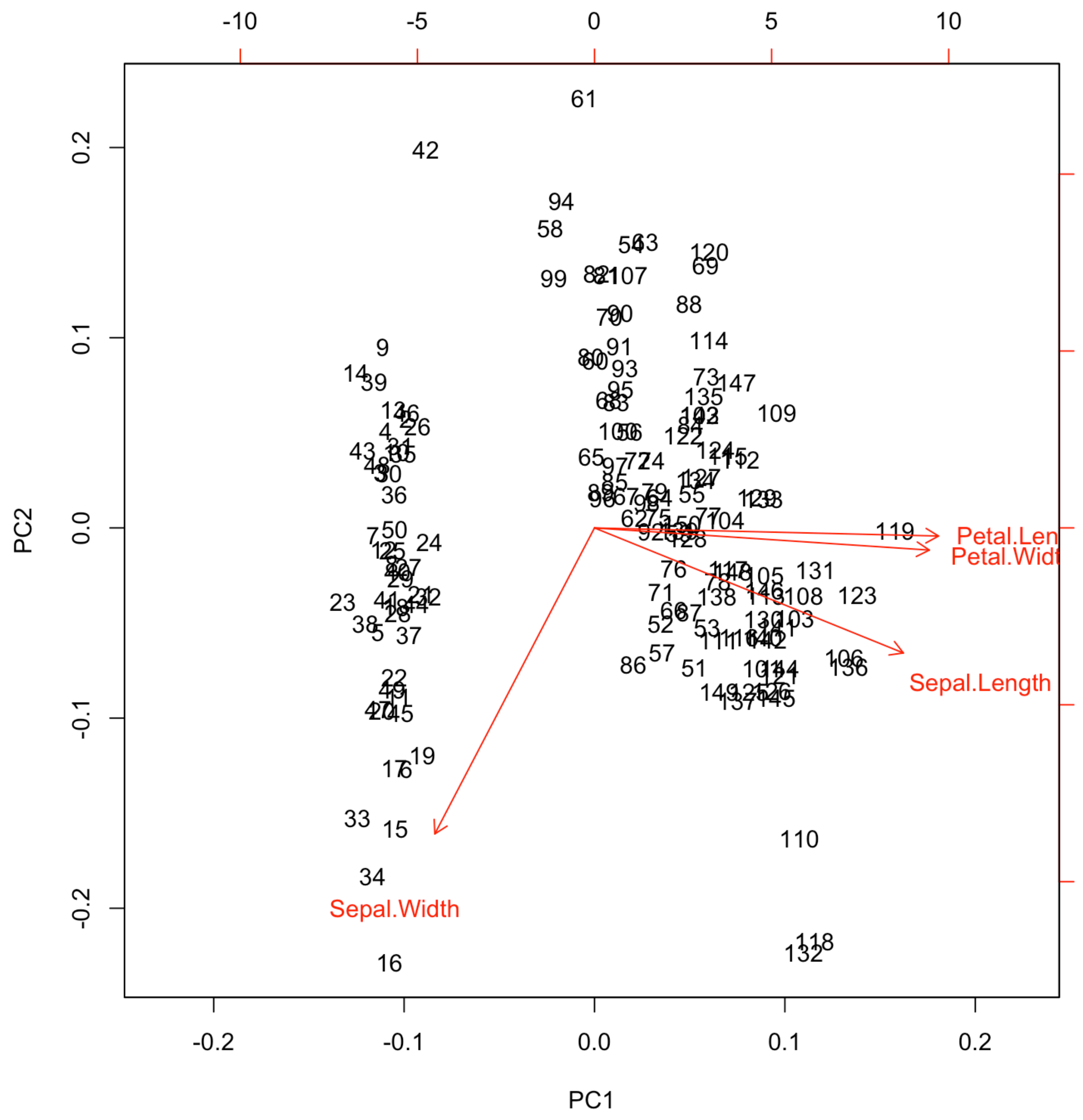


Biplots and scree plots in R

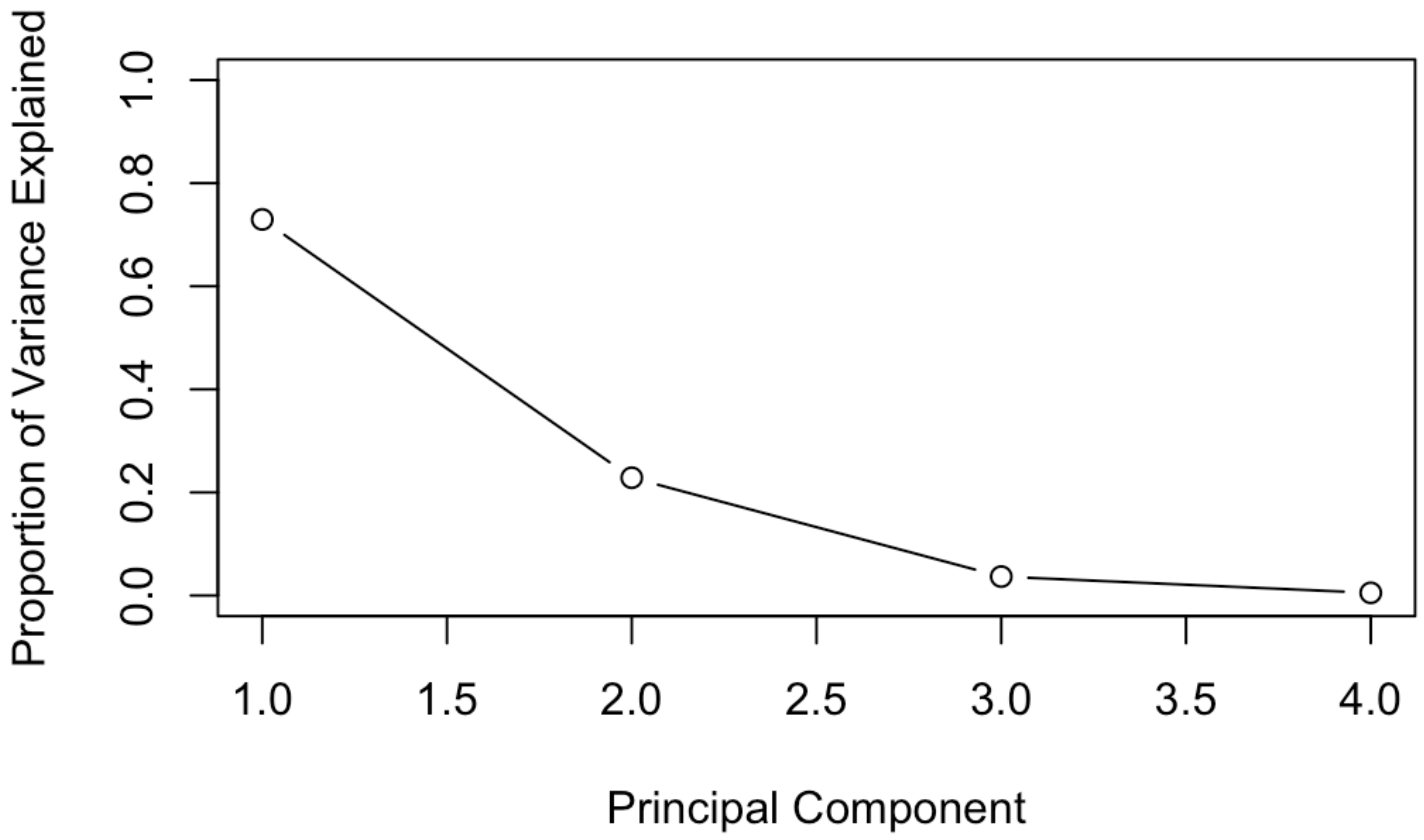
```
> # Creating a biplot
> pr.iris <- prcomp(x = iris[-5], scale = FALSE, center = TRUE)
> biplot(pr.iris)

> # Getting proportion of variance for a scree plot
> pr.var <- pr.iris$sdev^2
> pve <- pr.var / sum(pr.var)

> # Plot variance explained for each principal component
> plot(pve, xlab = "Principal Component",
       ylab = "Proportion of Variance Explained",
       ylim = c(0, 1), type = "b")
```

Biplots and scree plots in R

Biplot



Scree plot



Let’s practice!

Practical issues with PCA

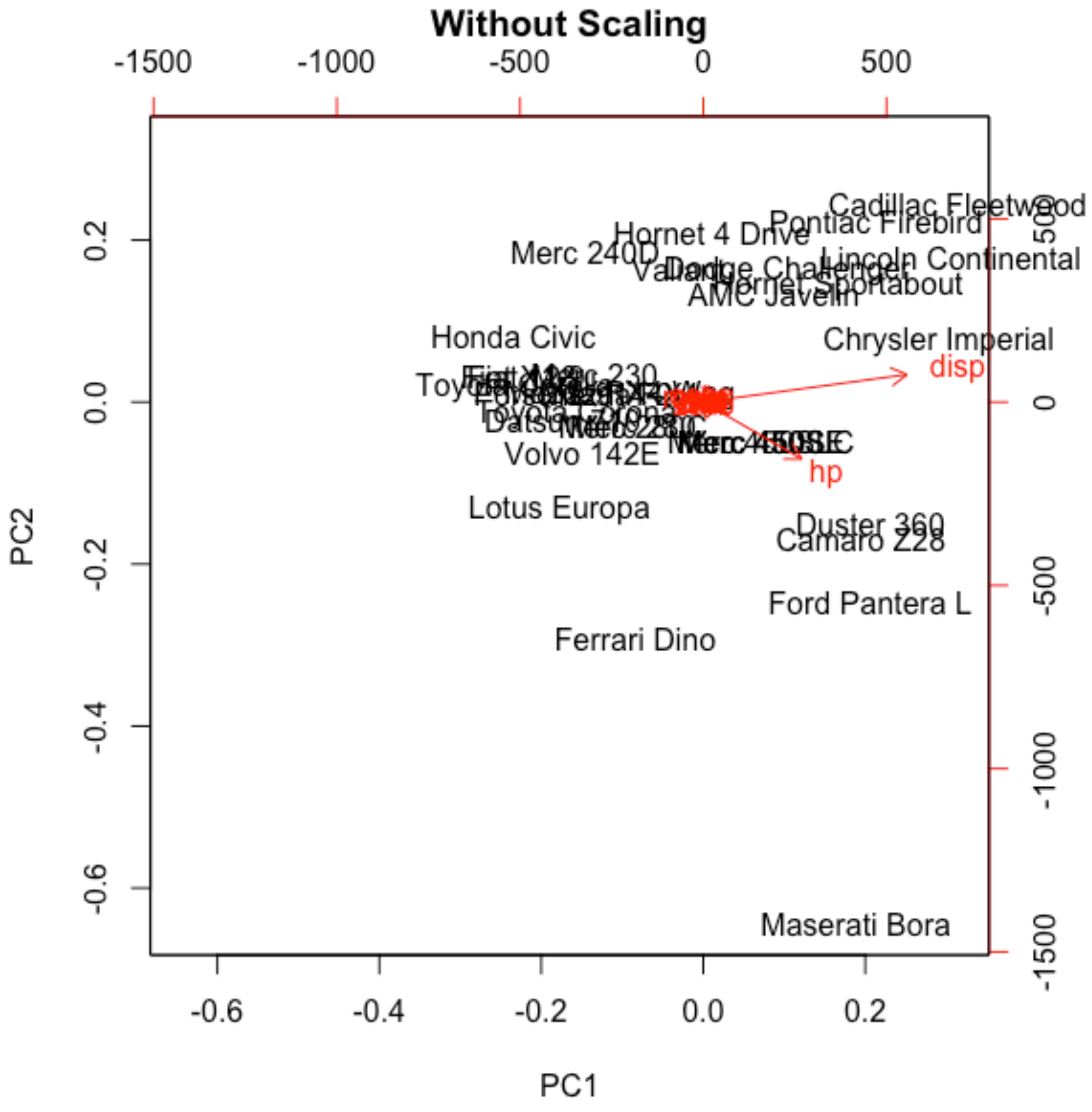
Practical issues with PCA

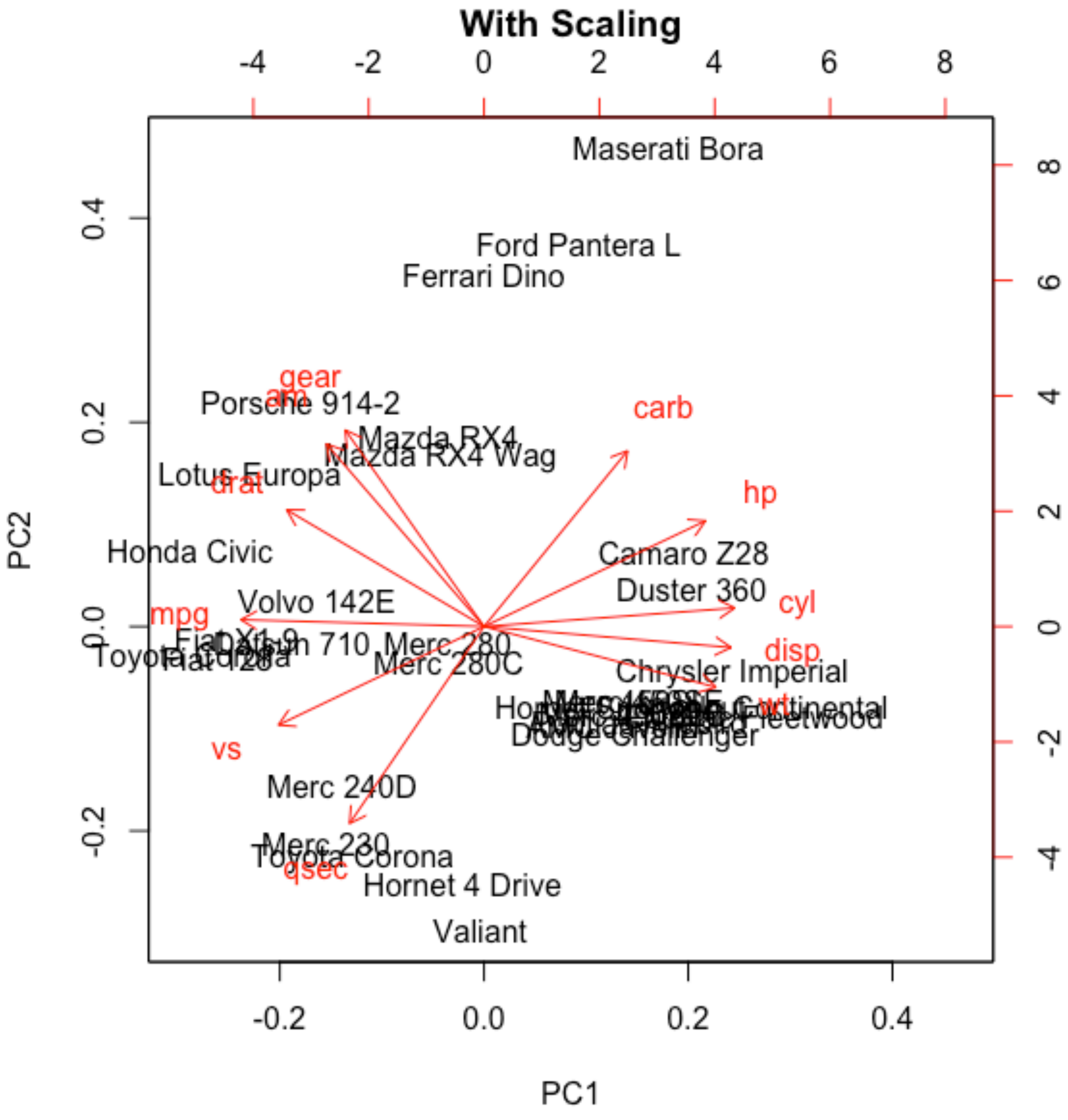
- Scaling the data
- Missing values:
  - Drop observations with missing values
  - Impute / estimate missing values
- Categorical data:
  - Do not use categorical data features
  - Encode categorical features as numbers

Scaling

```
> data(mtcars)
> head(mtcars)
                   mpg cyl disp  hp drat    wt  qsec vs am gear carb
Mazda RX4         21.0   6  160 110 3.90 2.620 16.46  0  1    4    4
Mazda RX4 Wag     21.0   6  160 110 3.90 2.875 17.02  0  1    4    4
Datsun 710        22.8   4  108  93 3.85 2.320 18.61  1  1    4    1
Hornet 4 Drive    21.4   6  258 110 3.08 3.215 19.44  1  0    3    1
Hornet Sportabout 18.7   8  360 175 3.15 3.440 17.02  0  0    3    2
Valiant           18.1   6  225 105 2.76 3.460 20.22  1  0    3    1

# Means and standard deviations vary a lot
> round(colMeans(mtcars), 2)
   mpg    cyl   disp     hp   drat     wt   qsec     vs     am   gear   carb
 20.09   6.19 230.72 146.69   3.60   3.22  17.85   0.44   0.41   3.69   2.81
> round(apply(mtcars, 2, sd), 2)
   mpg    cyl   disp     hp   drat     wt   qsec     vs     am   gear   carb
  6.03   1.79 123.94  68.56   0.53   0.98   1.79   0.50   0.50   0.74   1.62
```

Importance of scaling data





Scaling and PCA in R

```
> prcomp(x, center = TRUE, scale = FALSE)
```

Let’s practice!

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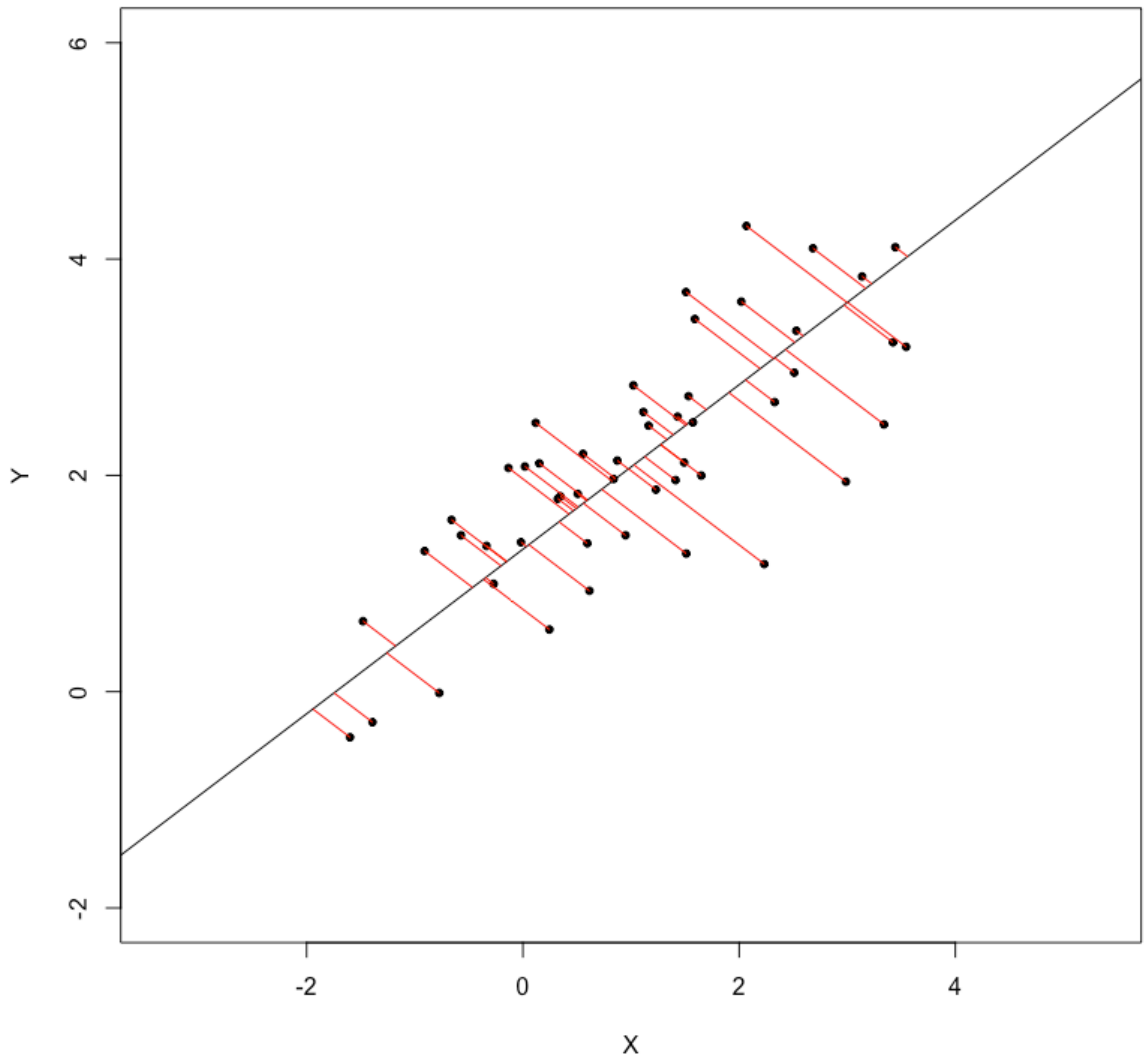
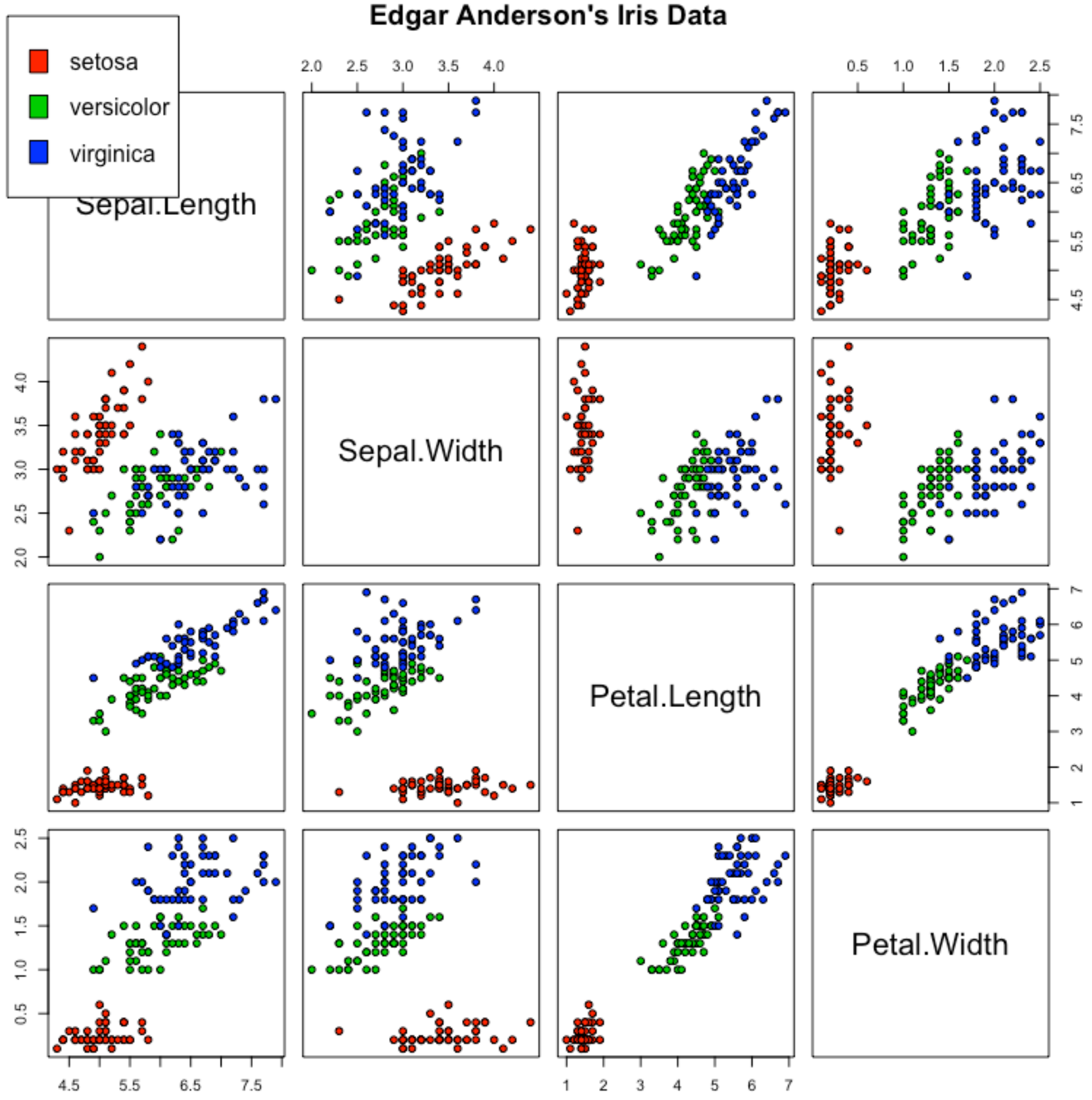
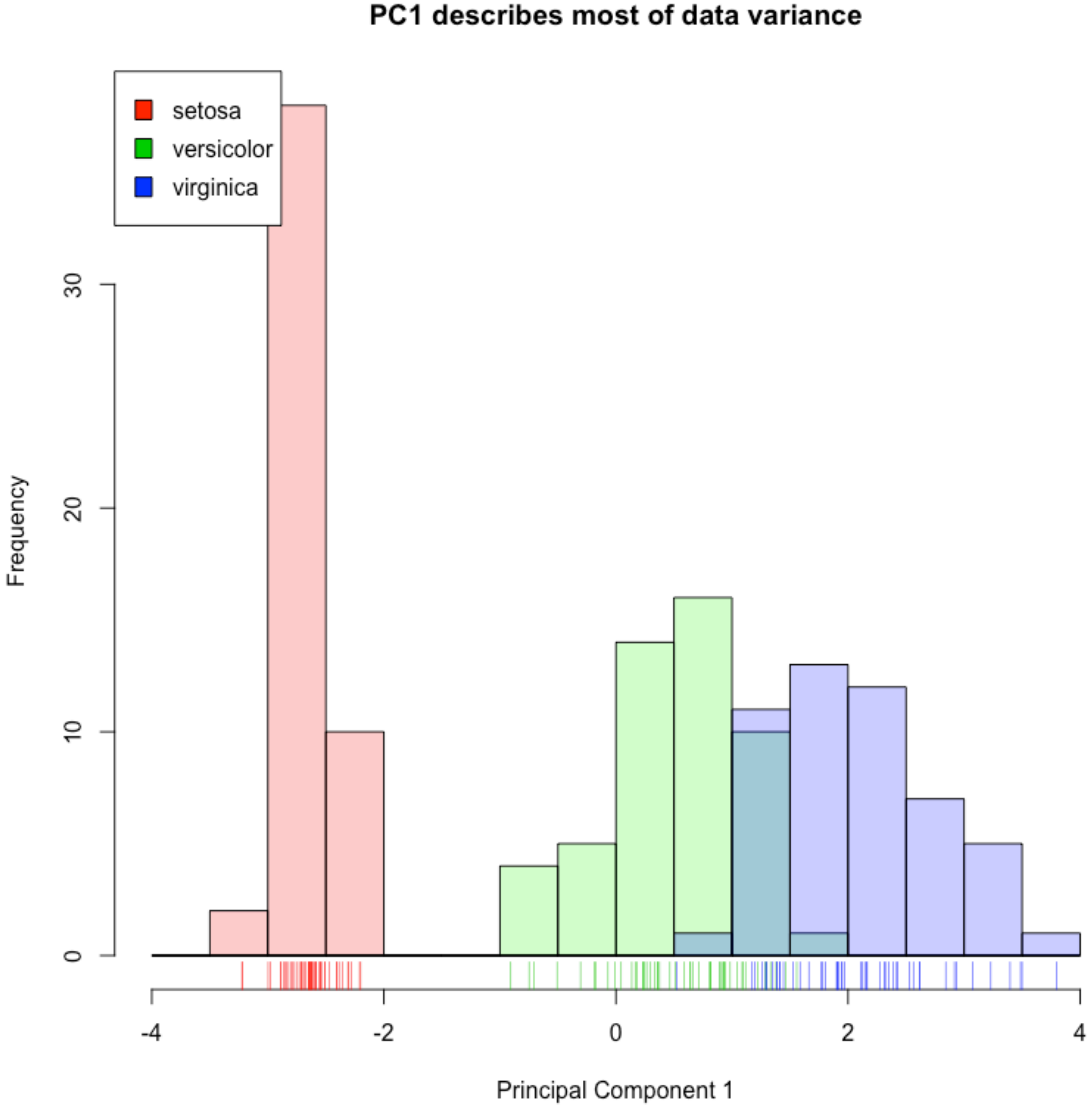
Additional uses of PCA and wrap-up

Dimensionality reduction

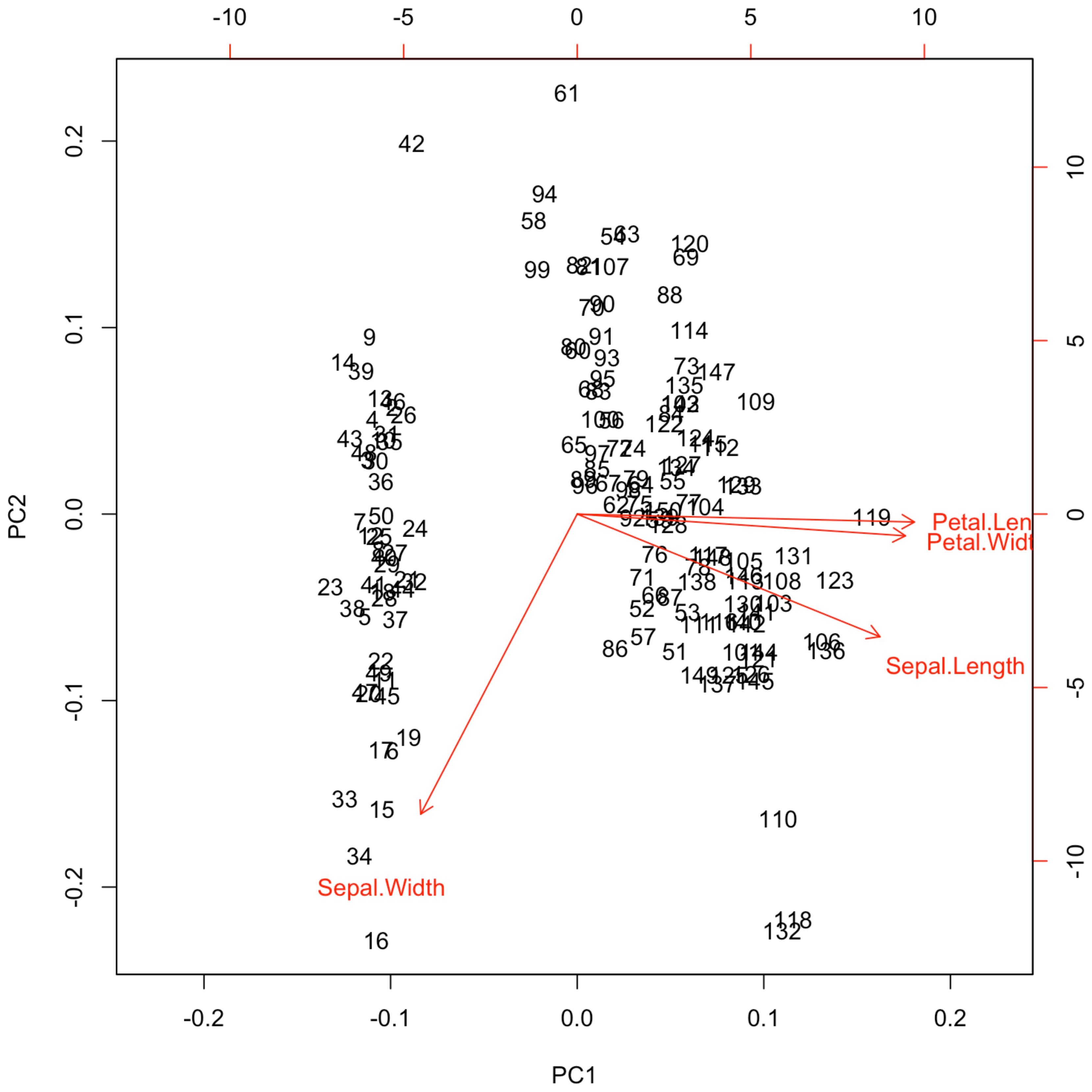


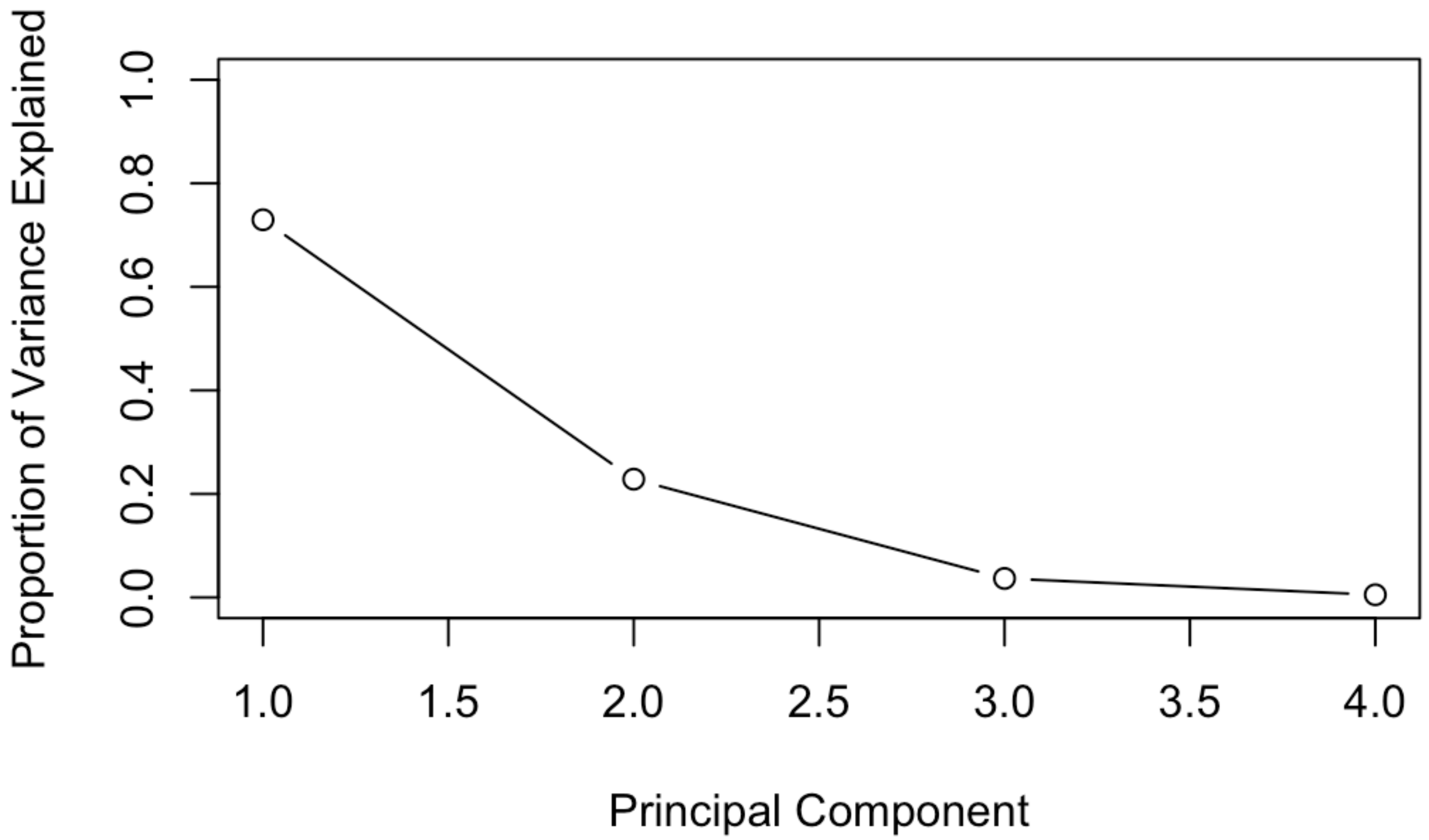
Data visualization



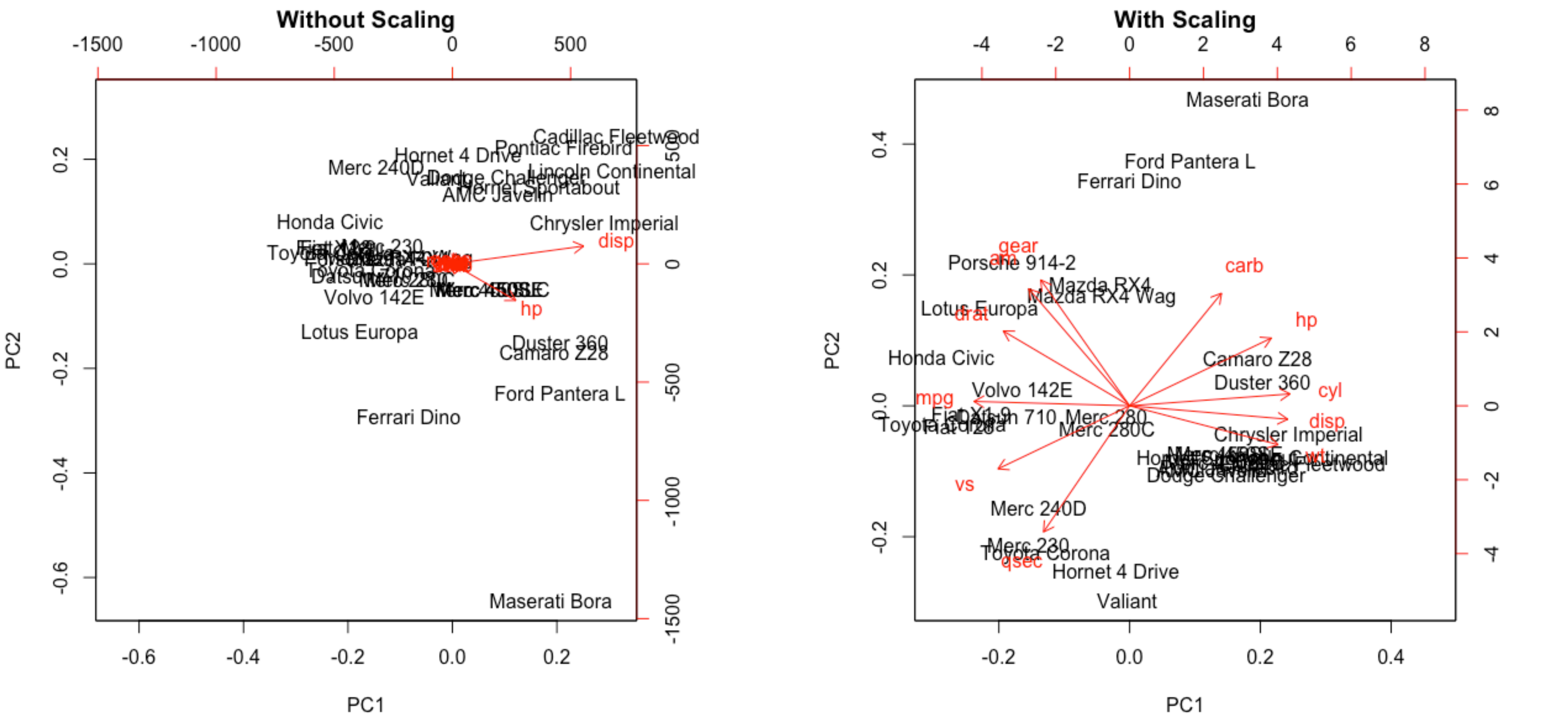


Interpreting PCA results





Importance of data scaling



Up next

```
# URL to cancer dataset hosted on DataCamp servers
> url <- "http://s3.amazonaws.com/assets.datacamp.com/production/
course_1903/datasets/WisconsinCancer.csv"

# Download the data: wisc.df
> wisc.df <- read.csv(url)
> wisc.data[1:6, 1:5]
         radius_mean texture_mean perimeter_mean area_mean smoothness_mean
842302         17.99        10.38         122.80    1001.0         0.11840
842517         20.57        17.77         132.90    1326.0         0.08474
84300903       19.69        21.25         130.00    1203.0         0.10960
84348301       11.42        20.38          77.58     386.1         0.14250
84358402       20.29        14.34         135.10    1297.0         0.10030
843786         12.45        15.70          82.57     477.1         0.12780
```

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