Principal Component Analysis (PCA)

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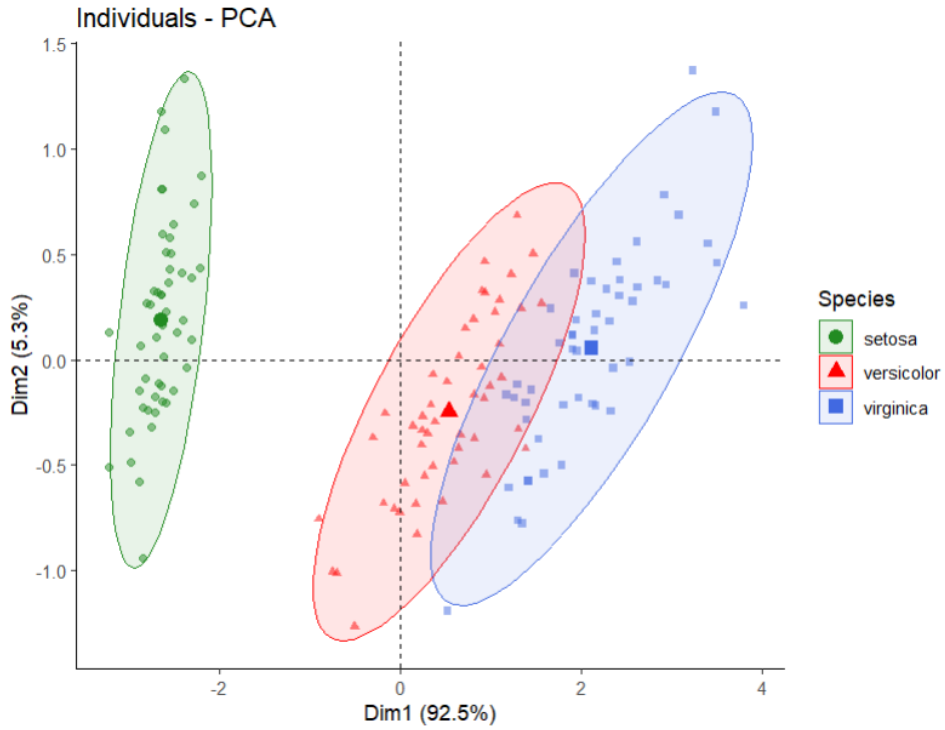
Data sets are often complex, with multiple variables to consider

Making multiple comparisons between all these variables can reach a point of impossibility!

What if there was a way to reduce this complexity, and look at overall patterns in the data?

This is what a PCA does

PCAs transform data by means of "dimension reductions"



Let's have a look at the Iris dataset

```
head(iris_data)
  sepal_length sepal_width petal_length petal_width species
1          5.1         3.5          1.4         0.2  setosa
2          4.9         3.0          1.4         0.2  setosa
3          4.7         3.2          1.3         0.2  setosa
4          4.6         3.1          1.5         0.2  setosa
5          5.0         3.6          1.4         0.2  setosa
6          5.4         3.9          1.7         0.4  setosa
```

We have three species and four morphological measurements

Iris Versicolor | Iris Setosa | Iris Virginica

After removing the non-numeric column (species), and checking for NA values, we can run a PCA on the data frame:

```
pca_iris = prcomp(iris_data_clean, scale = TRUE)
```

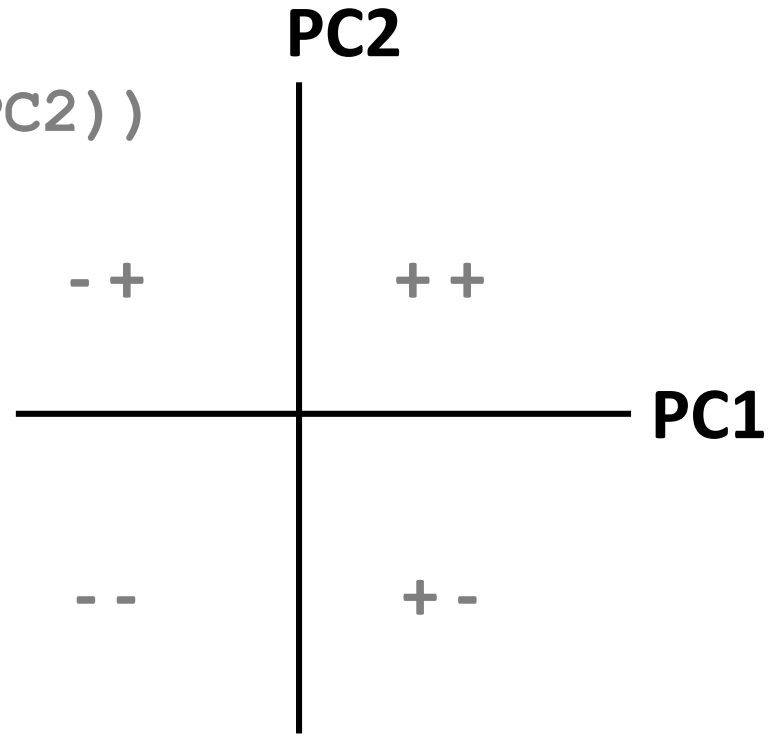
```
> summary(pca_iris)
Importance of components:
                          PC1    PC2     PC3     PC4
Standard deviation     1.7084 0.9560 0.38309 0.14393
Proportion of Variance 0.7296 0.2285 0.03669 0.00518
Cumulative Proportion  0.7296 0.9581 0.99482 1.00000
```

PC1 accounts for 73% of the variation in the data, and PC2 accounts for 23%

Let's look at the loadings:

```
pca_loadings_iris = pca_iris$rotation %>%
as.data.frame() %>%  dplyr::select(c(PC1, PC2))

> pca_loadings_iris
                    PC1         PC2
sepal_length  0.5210659 -0.37741762
sepal_width  -0.2693474 -0.92329566
petal_length  0.5804131 -0.02449161
petal_width   0.5648565 -0.06694199
```

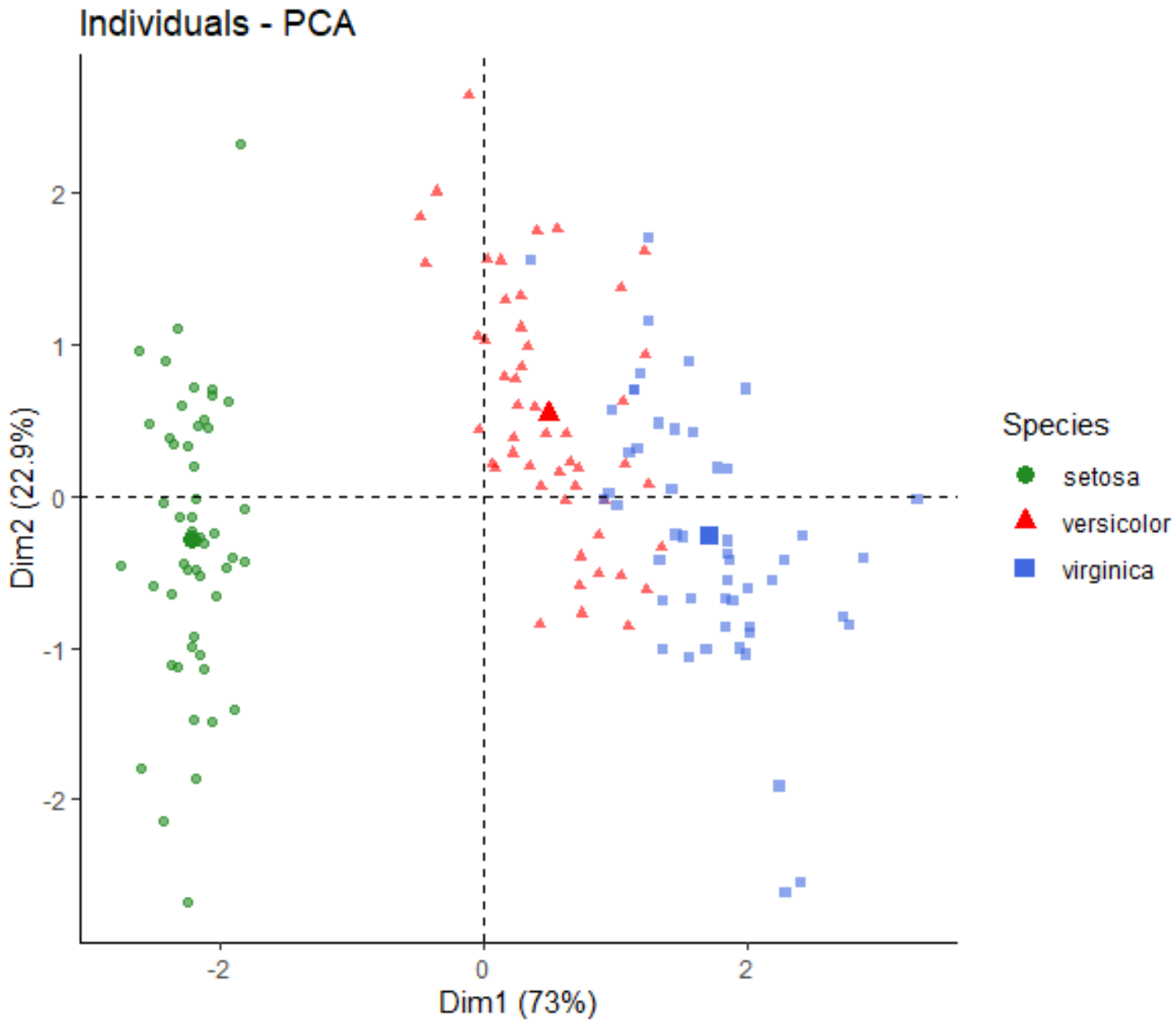


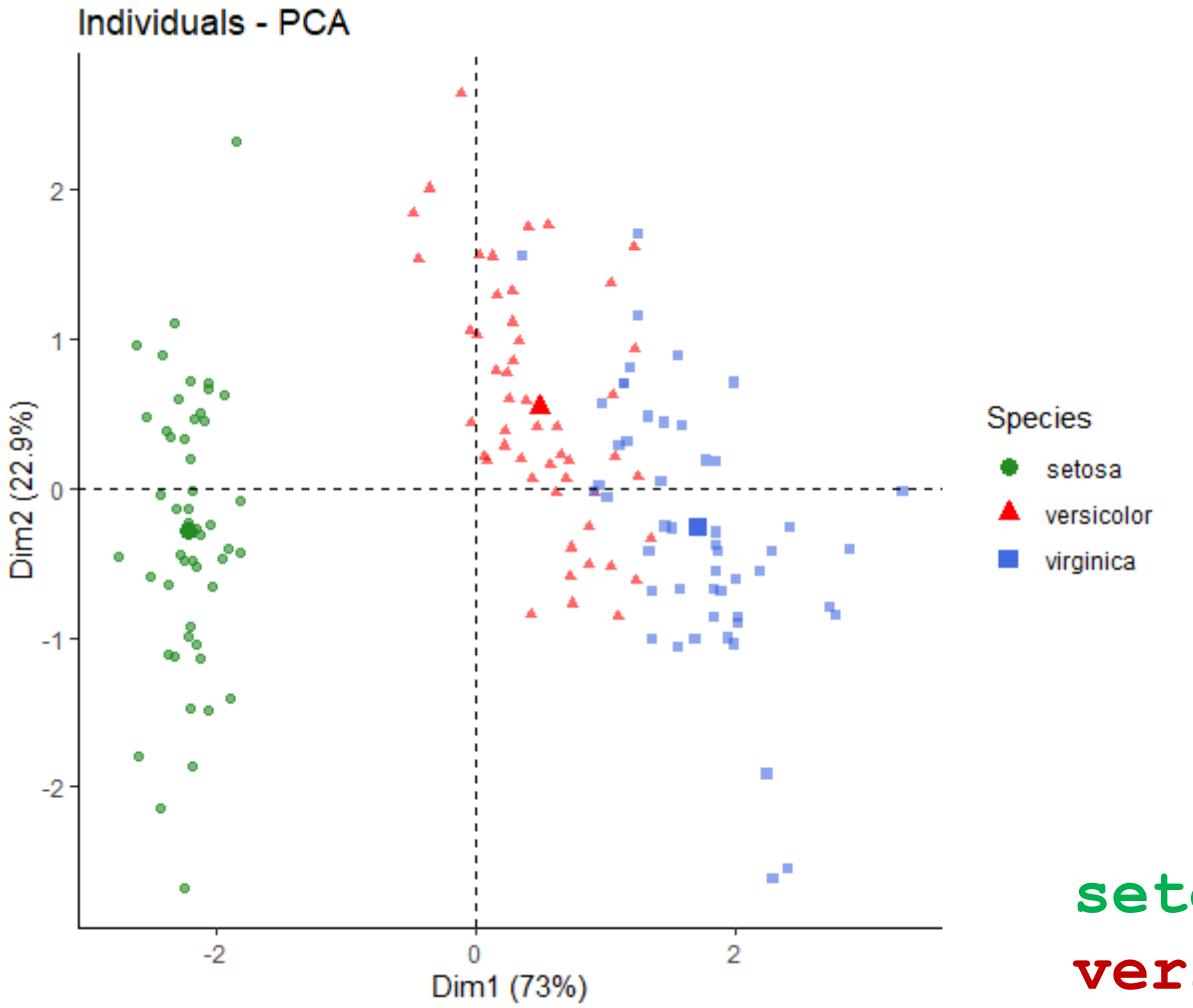
Sepal length, petal length, and petal width all increase along the + side of the PC1 axis, while sepal width increases on the – side of the PC1 axis

Plot using ggplot:

```
factoextra::fviz_pca_ind(pca_iris, geom = "point",
col.ind = iris_data$species,
palette = c("forestgreen", "red", "royalblue"),
legend.title = "Species", alpha.ind = 0.6) +
scale_shape_manual(values=c(19, 17, 15)) +
theme_classic()
```

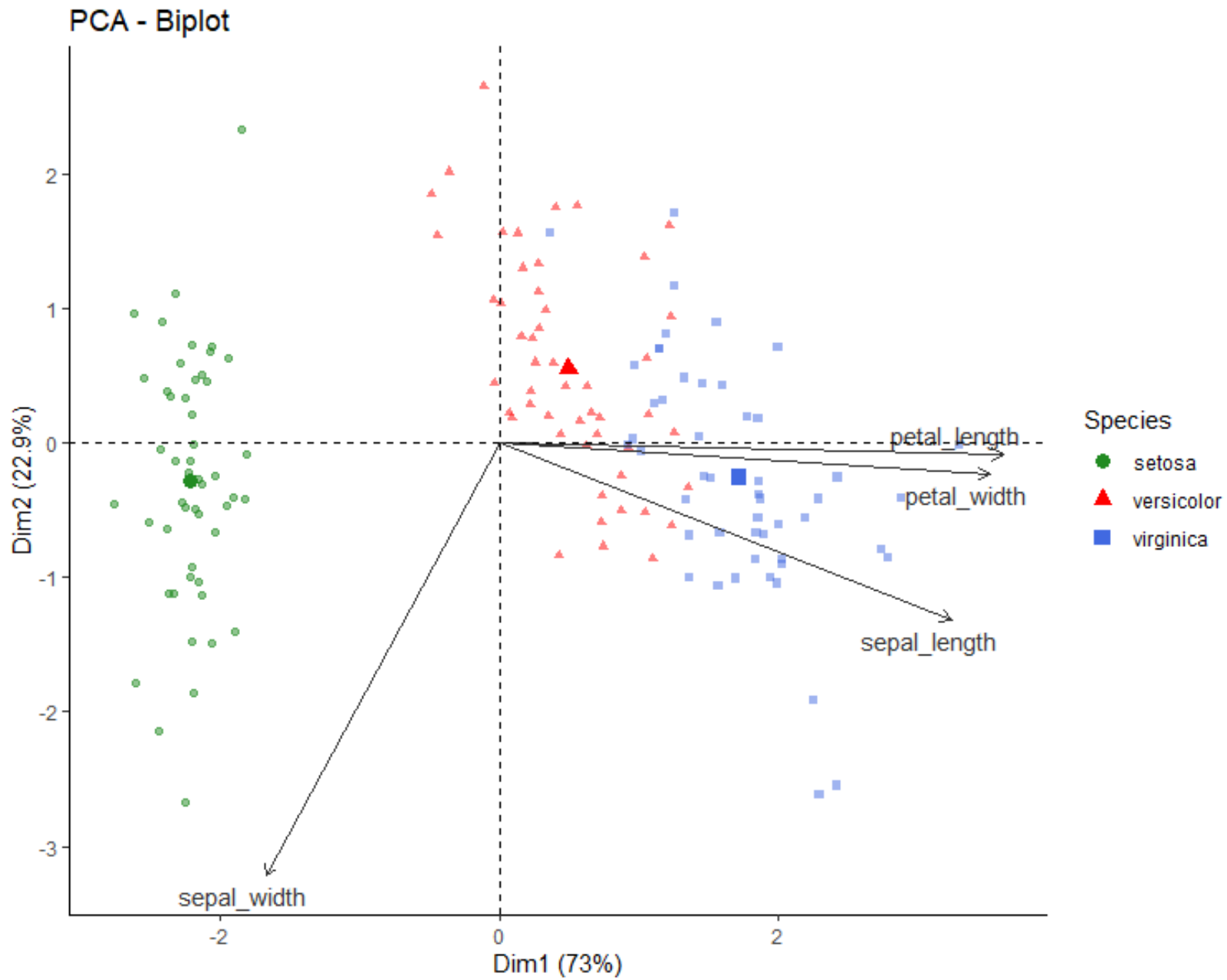
We're specifying three colours and shape values for each of the three Iris species, and we'll use the `fviz_pca_ind()` function in the `factoextra` package


Individuals - PCA
Dim2 (22.9%)
Dim1 (73%)
2
1
0
-1
-2
-2
0
2
Species
setosa
versicolor
virginica

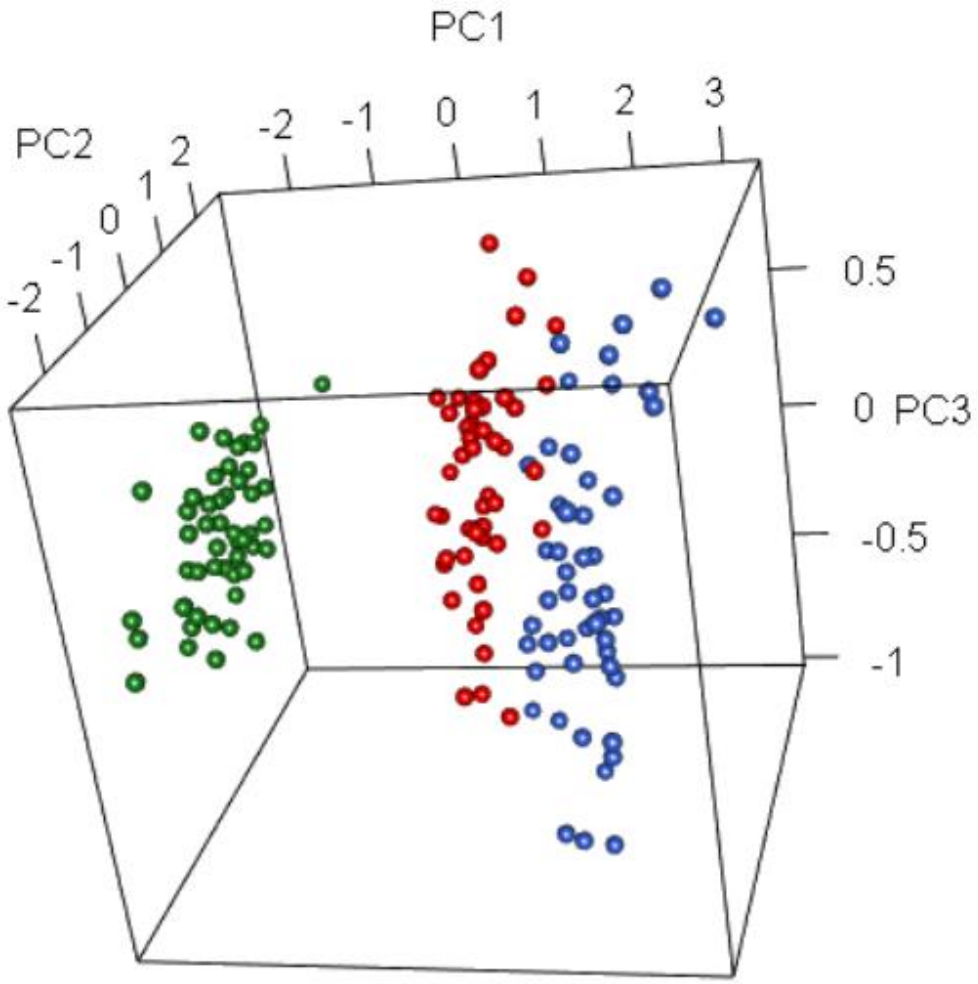


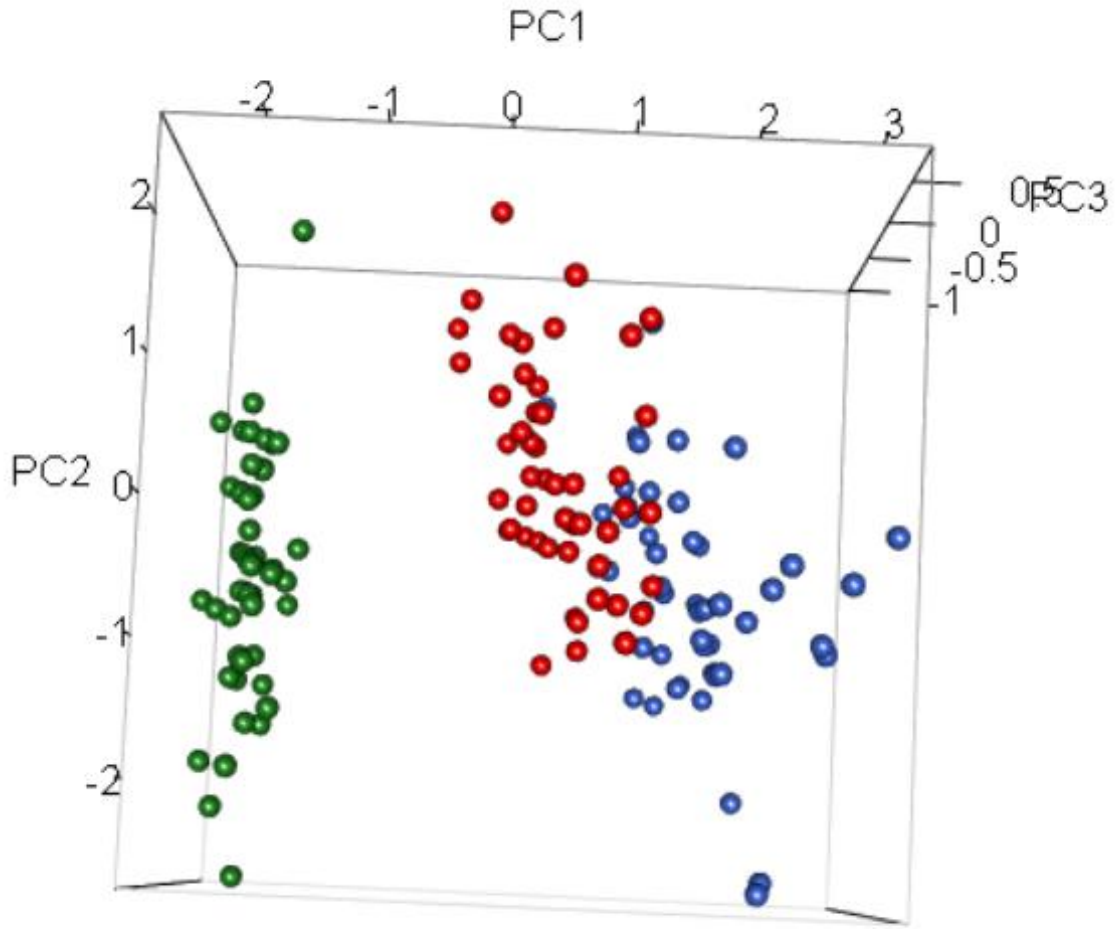

```
> pca_loadings_iris
                     PC1         PC2
sepal_length   0.5210659 -0.37741762
sepal_width   -0.2693474 -0.92329566
petal_length   0.5804131 -0.02449161
petal_width    0.5648565 -0.06694199
```

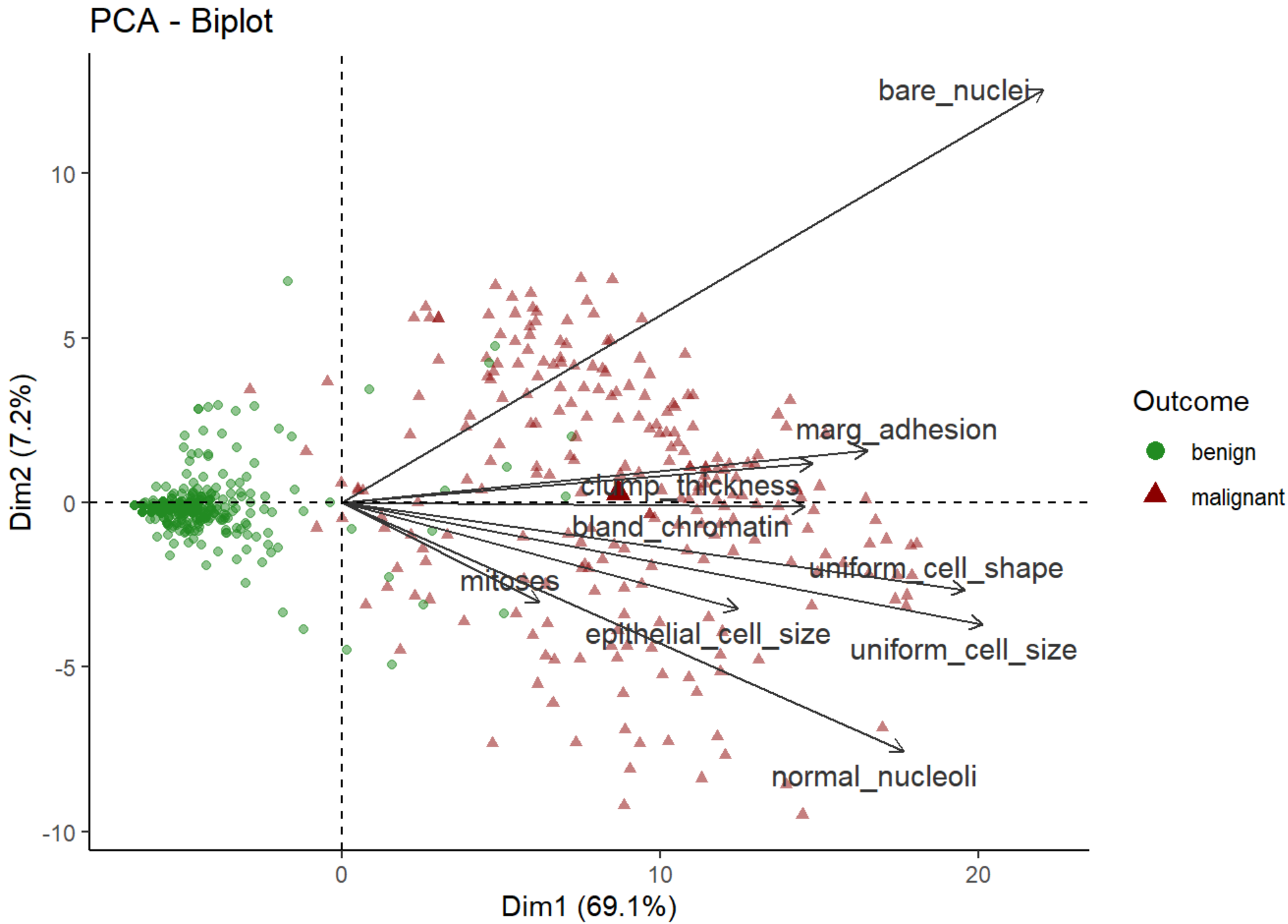
setosa has larger sepal widths than versicolor and virginica, but versicolor and viriginica have larger sepal lengths, and petal lengths and widths than setosa


PCA - Biplot
Dim2 (22.9%)
Dim1 (73%)
2
1
0
-1
-2
-3
-2
0
2
petal_length
petal_width
sepal_length
sepal_width
Species
setosa
versicolor
virginica

The `rgl` package offers 3D plots to explore your data






PCA - Biplot
bare_nuclei
marg_adhesion
clump_thickness
bland_chromatin
uniform_cell_shape
mitoses
epithelial_cell_size
uniform_cell_size
normal_nucleoli
Outcome
benign
malignant
Dim2 (7.2%)
Dim1 (69.1%)
10
5
0
-5
-10
0
10
20