Unsupervised Learning

Principal Components Analysis

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Program

Morning session

Principal Components Analysis

Principal components analysis (PCA) is a data reduction technique. It's aim is to capture the information present in a large number of variables in a much smaller number of principal components. For example, a personality test may consist 5 groups of 10 questions each, with each group measuring a different personality trait. If the test is constructed well, the PCA will identify 5 principal components that each measure a different personality trait. By saving the indivdual scores on these principal components the dimension of the data is reduced from 50 to 5 variables, and the 5 variables can be used to make individual personality profiles.

Course materials

- Lecture sheets
- R lab
- R Markdown lab template

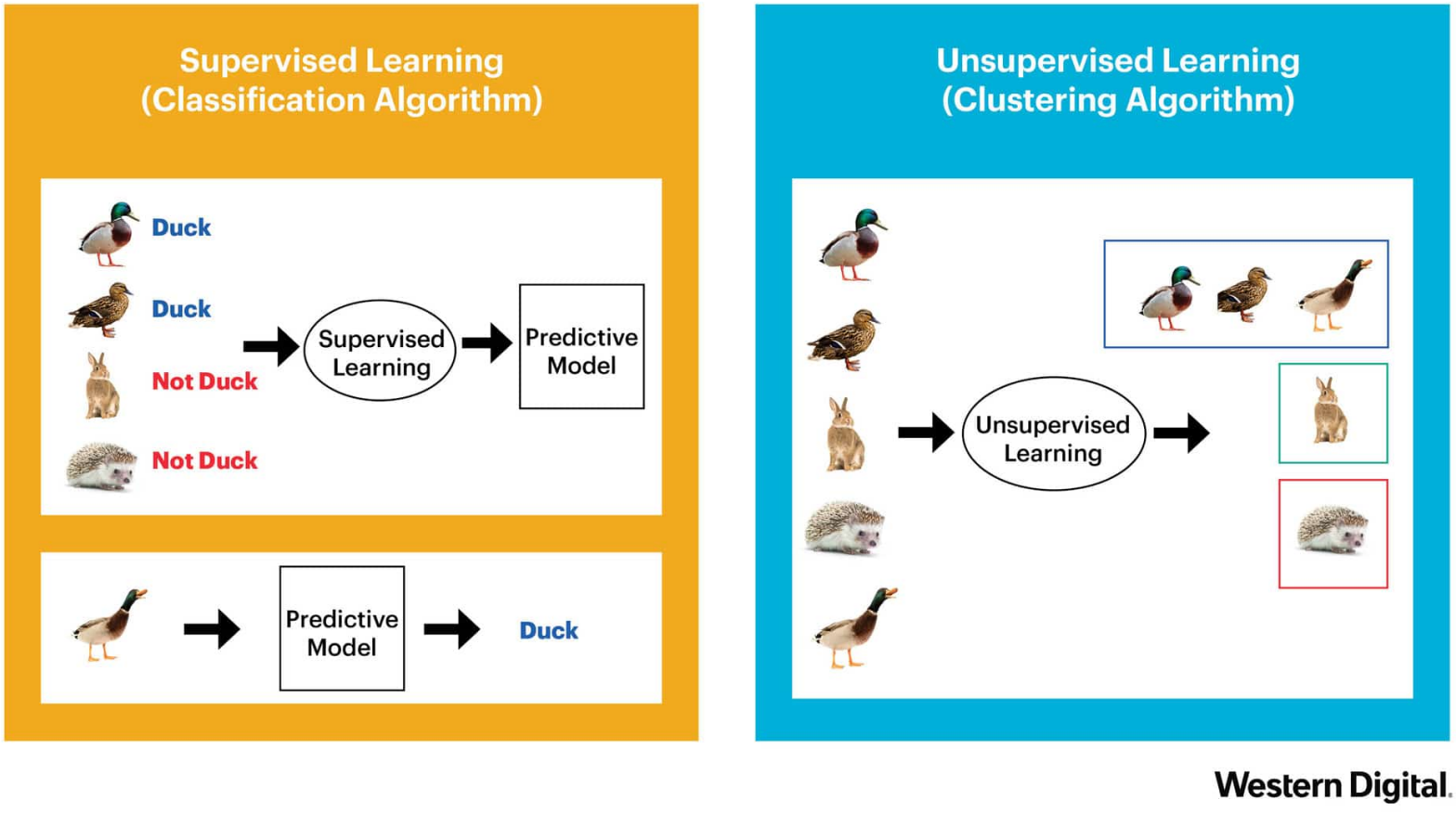
Content

1. Unsupervised learning
2. Principal components analysis
3. Iris data

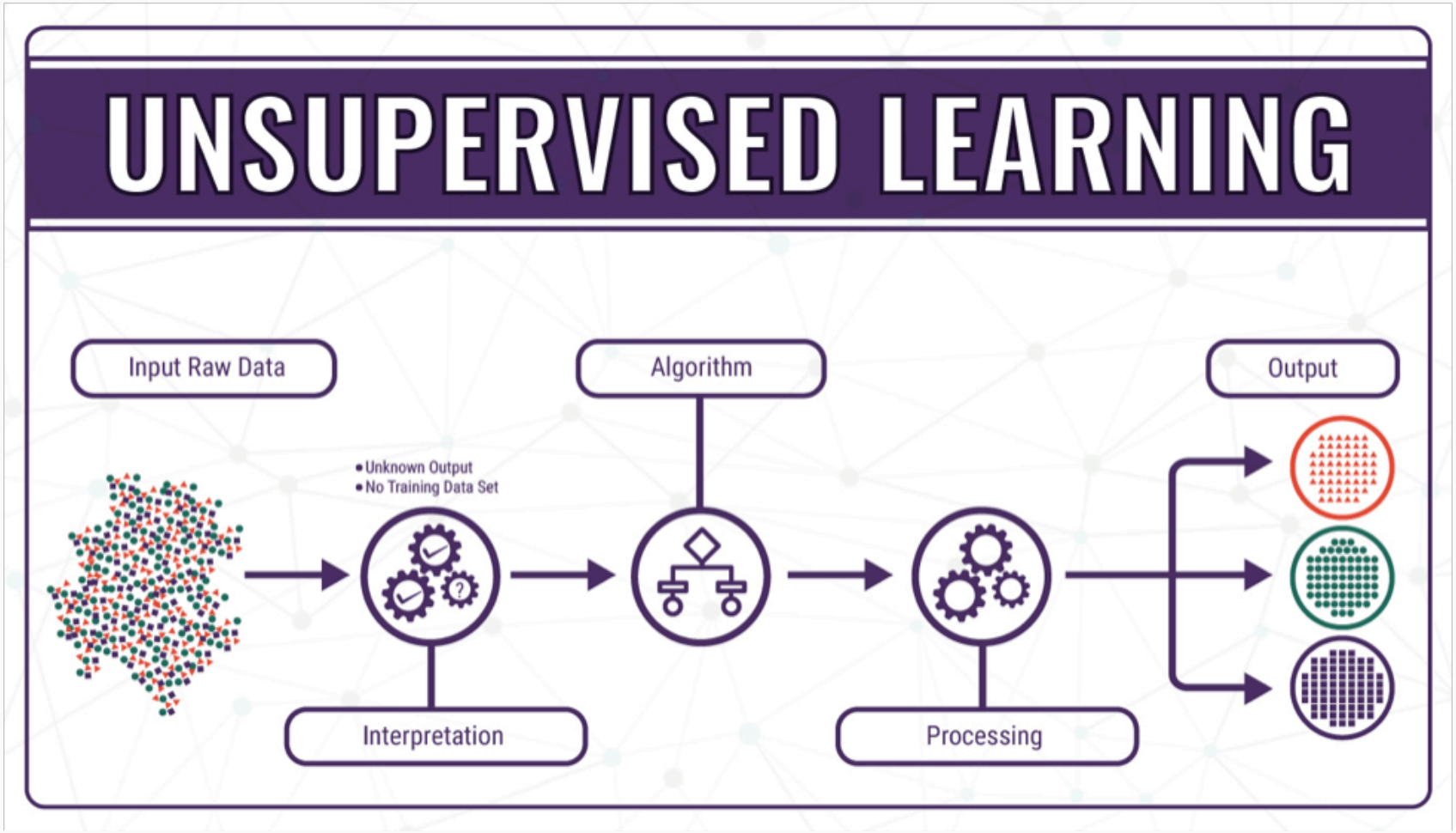
Supervised vs unsupervised

Known outcome

Unknown outcome



Unsupervised learning



Principal Components Analysis

How to make customer profiles?

Profiles of bought products

- many products but only a few profiles

What is Principal Components Analysis

Data of high dimension

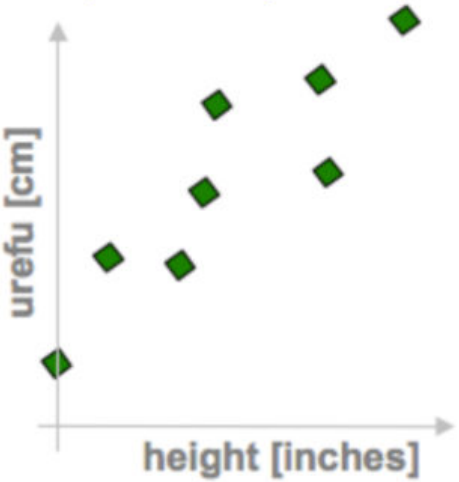
- many features containing different information
- high correlations within groups of features
- low correlations between groups of features

Dimension reduction

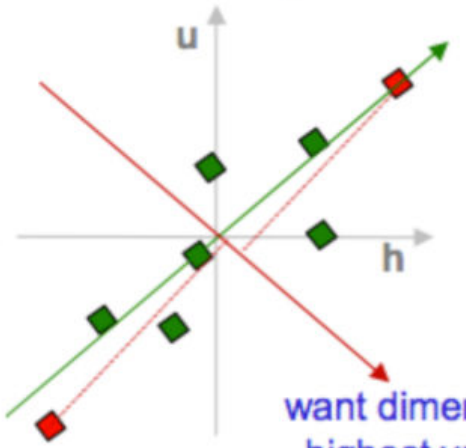
- groups of correlated features form a single principal component
- different groups form different principal components

PCA in a nutshell

1. correlated hi-d data
("urefu" means "height" in Swahili)



2. center the points



want dimension of highest variance

3. compute covariance matrix

	h	u
h	2.0	0.8
u	0.8	0.6

$$\text{cov}(h,u) = \frac{1}{n}\sum_{i=1}^{n} h_i u_i$$

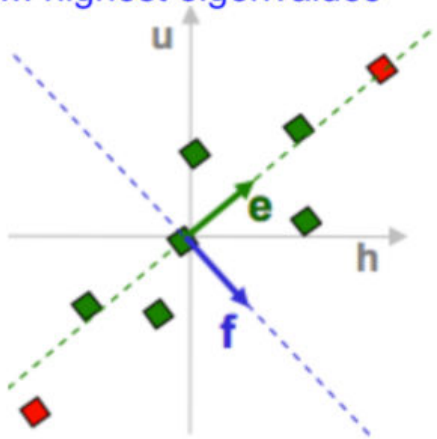
4. eigenvectors + eigenvalues

$$\begin{pmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{pmatrix} \begin{pmatrix} e_h \\ e_u \end{pmatrix} = \lambda_e \begin{pmatrix} e_h \\ e_u \end{pmatrix}$$

$$\begin{pmatrix} 2.0 & 0.8 \\ 0.8 & 0.6 \end{pmatrix} \begin{pmatrix} f_h \\ f_u \end{pmatrix} = \lambda_f \begin{pmatrix} f_h \\ f_u \end{pmatrix}$$

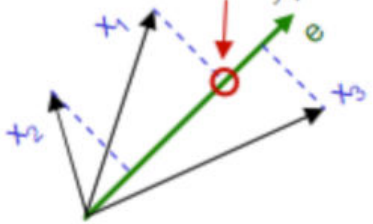
`eig(cov(data))`

5. pick m<d eigenvectors
w. highest eigenvalues

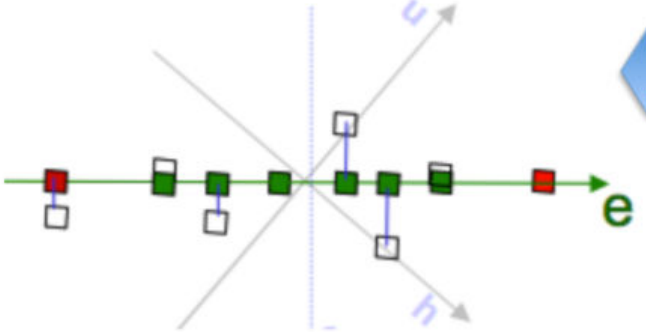


6. project data points to those eigenvectors

$$x_e' = x^T e = \sum_{j=1}^{d} x_{ij} e_j$$



7. uncorrelated low-d data



Principal components

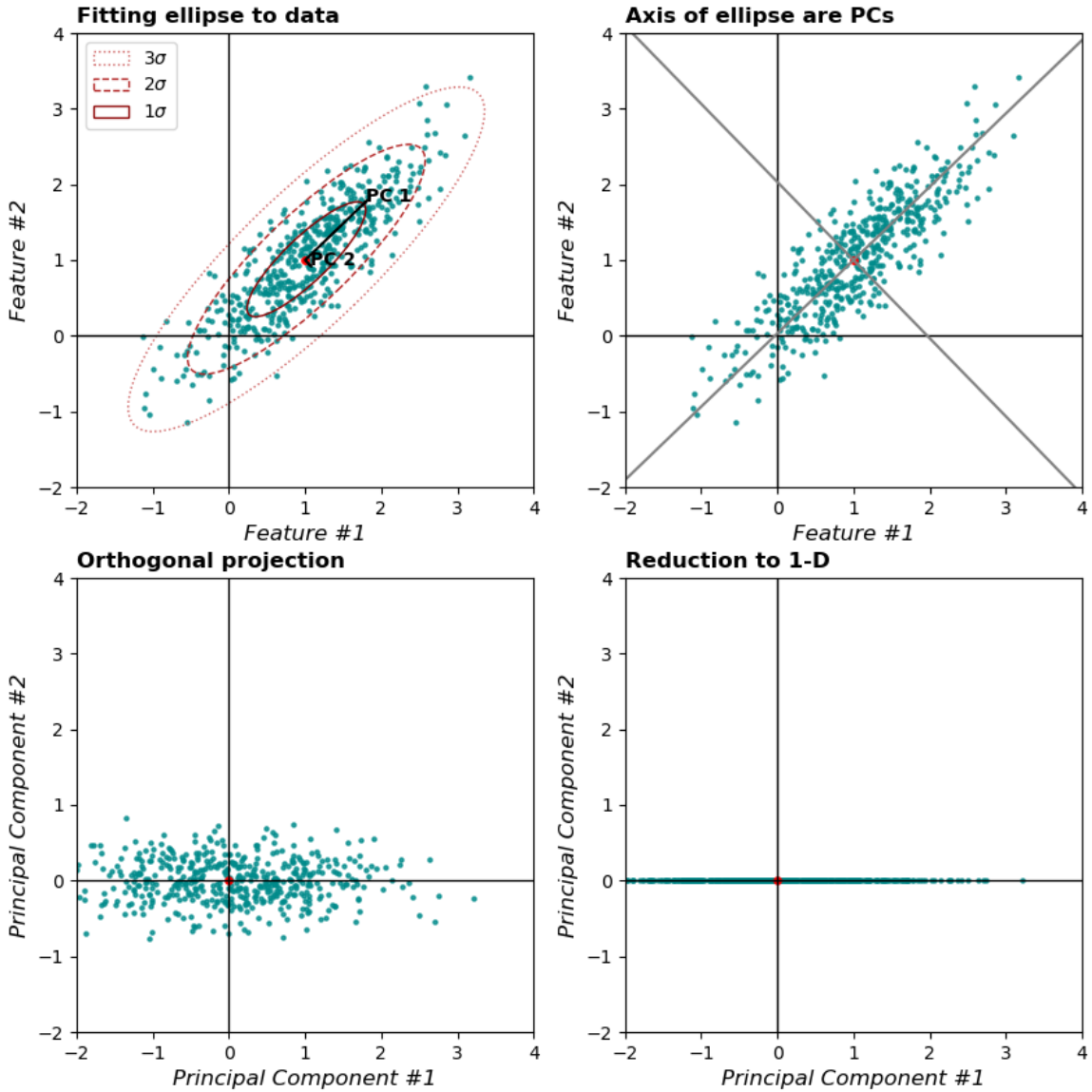
The p principal component Z_j are computed as:

$$Z_j = \phi_{1j} X_1 + ... + \phi_{pj} X_p, \qquad j = 1, ..., p$$

- Z_j is weighted sum of the features
- ϕ_{1j} is loading of X_1 on Z_J (like a correlation)

The $Z_1, ..., Z_p$ are ordered in terms of explained variance

PCA in two-dimensional space



PCA in high-dimensional space

Properties of principal components (PCs)

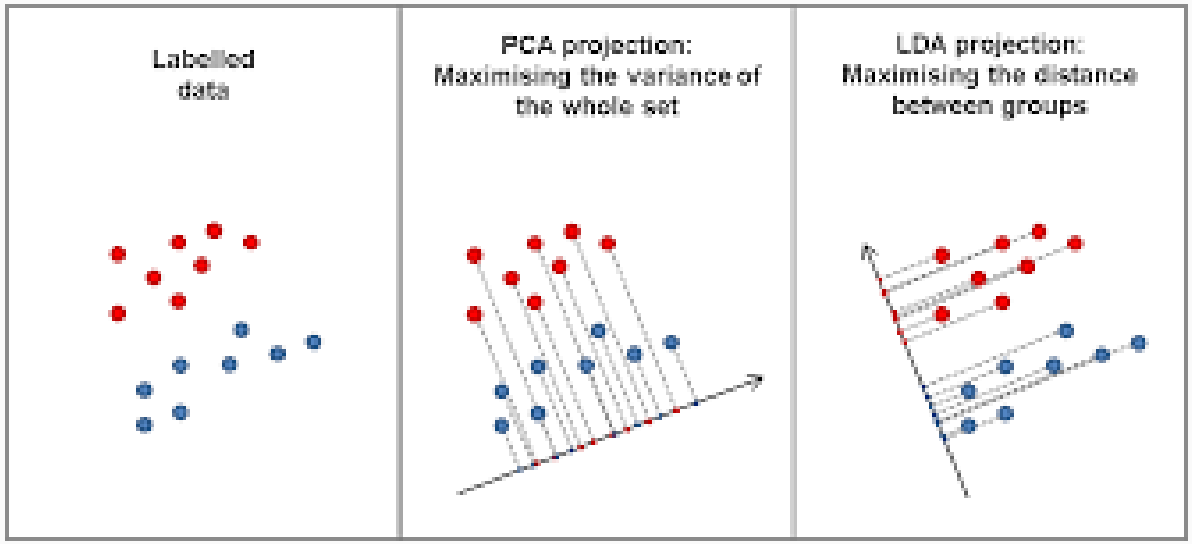
- explained variance is expressed in *eigenvalues*
- sum of eigenvalues is p (number of features)
- PCs with eigenvalues > 1 are considered informative
- PCs with eigenvalues < 1 are considered noise

Dimension reduction criteria, retain PC's

- with eigenvalues > 1
- above the elbow in scree plot

PCA vs LDA

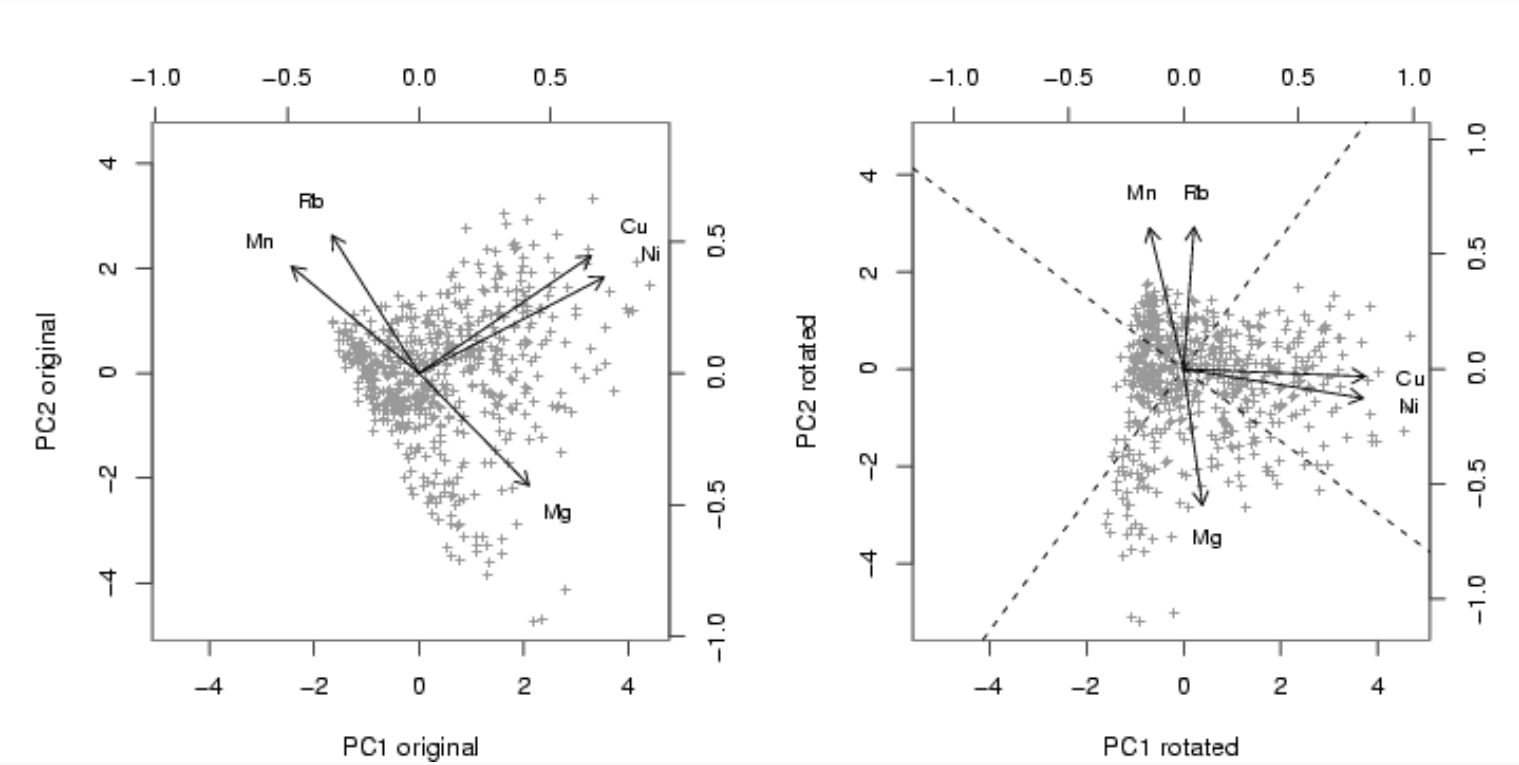
- PCA maximizes variance between data points
- LDA maximizes variance between groups



Rotation

Facilitates interpretation of PC's

- maximizes loading on one PC
- minimizes loadings on others

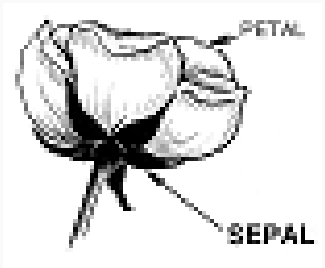


Iris data

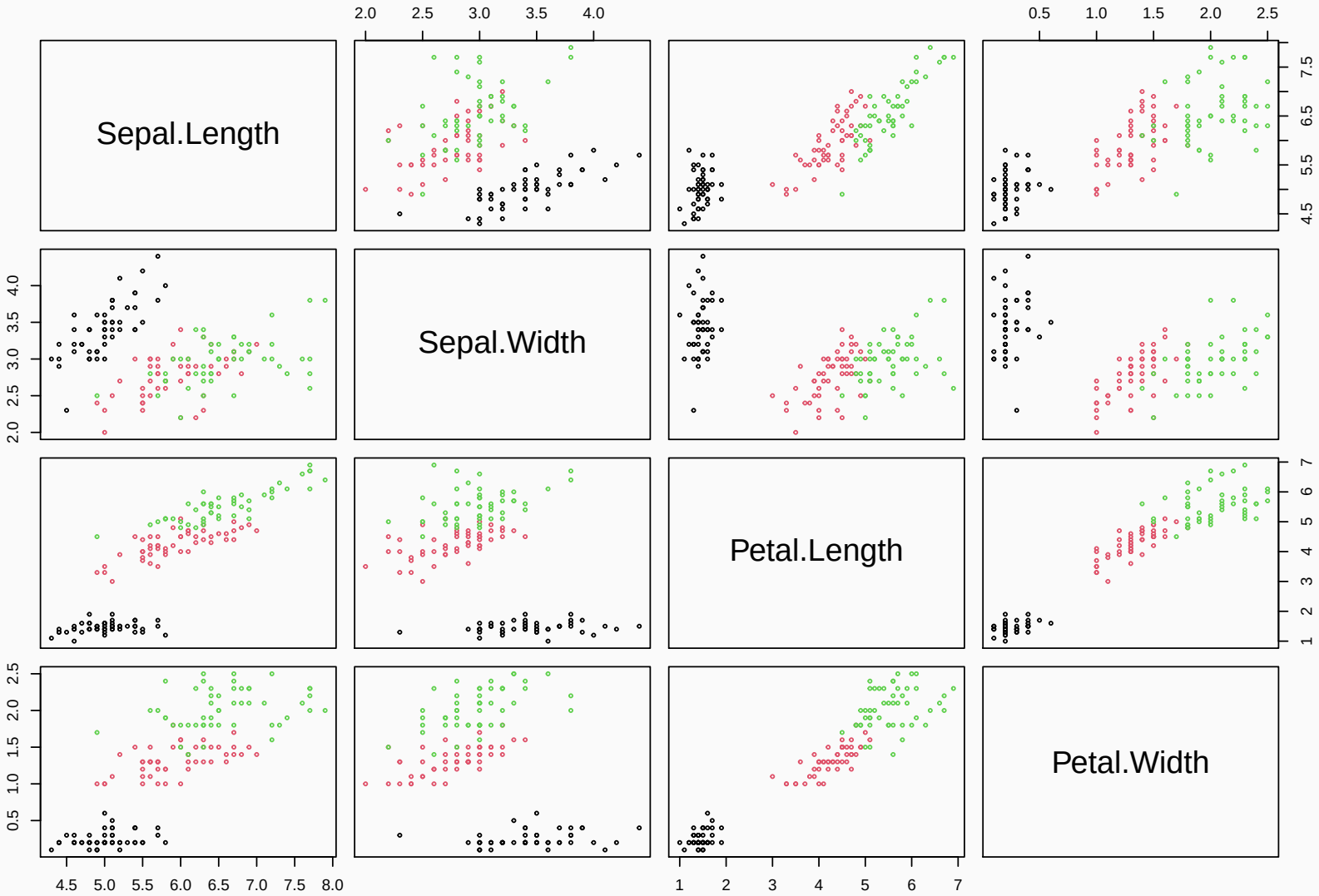
Example iris data

4-dimensional data:

- 150 Iris flowers (3 species)
- 4 features
  - petal length
  - petal width
  - sepal length
  - sepal width



Feature structure in 4 dimensions



PCA solution with 4 components

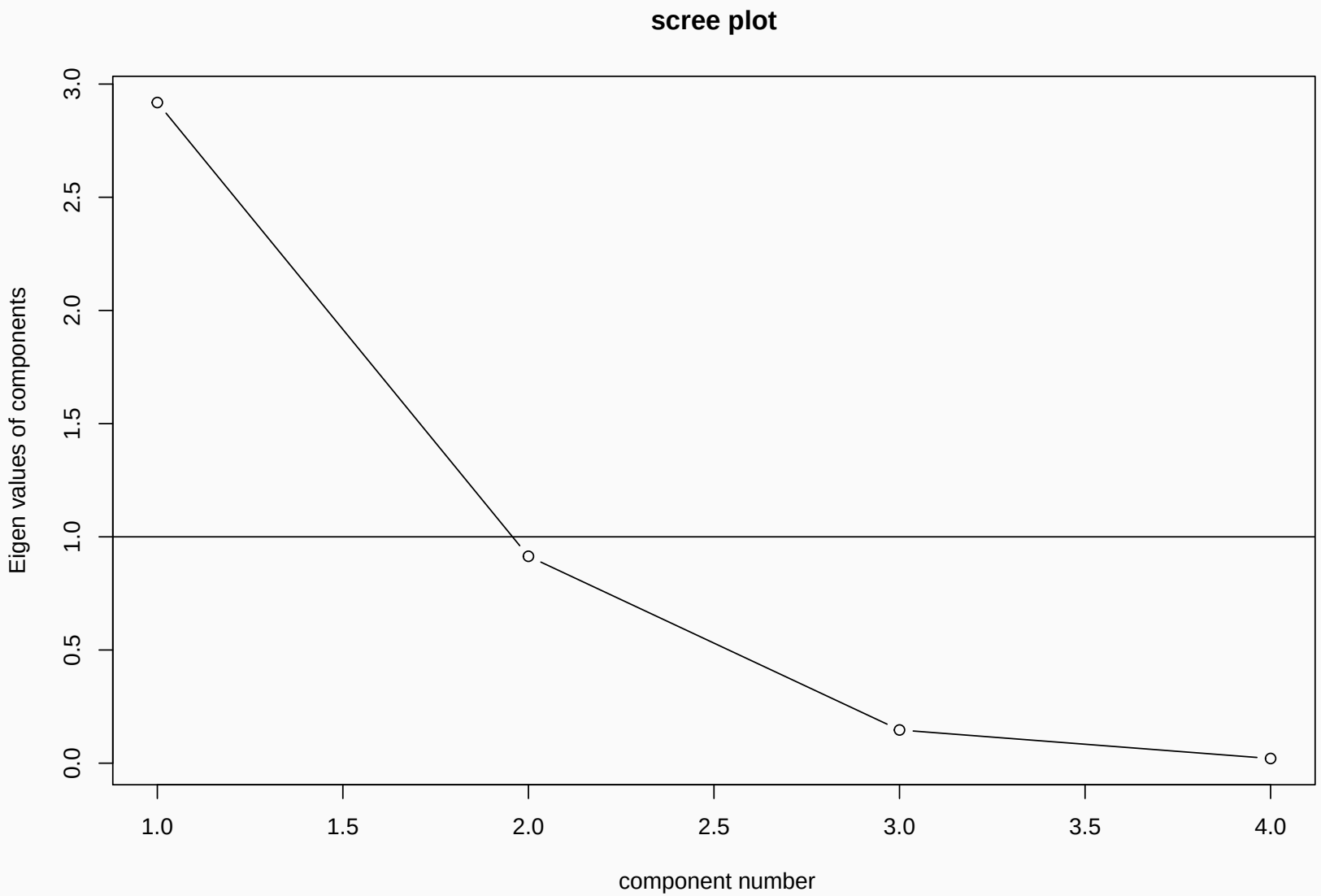
```r
pc4 <- principal(iris[, 1:4], nfactors = 4, rotate = "none")

print(loadings(pc4), cutoff = .1)
```

```
Loadings:
             PC1    PC2    PC3    PC4
Sepal.Length  0.890  0.361 -0.276
Sepal.Width  -0.460  0.883
Petal.Length  0.992                0.115
Petal.Width   0.965         0.243

                 PC1   PC2   PC3   PC4
SS loadings    2.918 0.914 0.147 0.021
Proportion Var 0.730 0.229 0.037 0.005
Cumulative Var 0.730 0.958 0.995 1.000
```

Elbow criterion

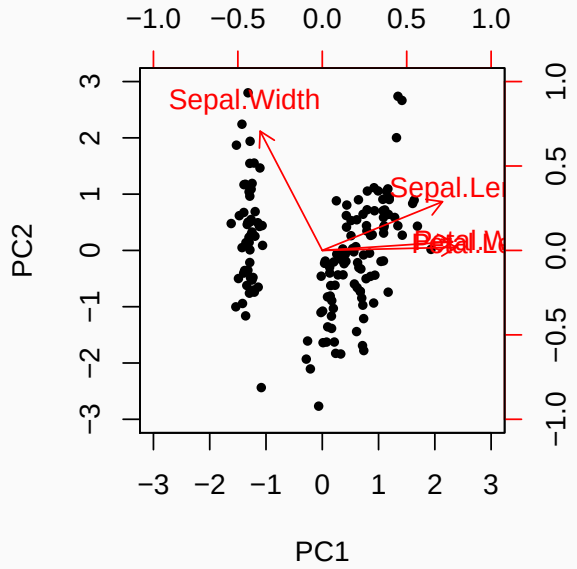


Conclusion: Extract one or two PCs (elbow is unclear)

Unrotated loadings

```
pc2 <- principal(iris[, -5], nfactors = 2, rotate = "none")
round(loadings(pc2)[1:4, 1:2], 2)
```

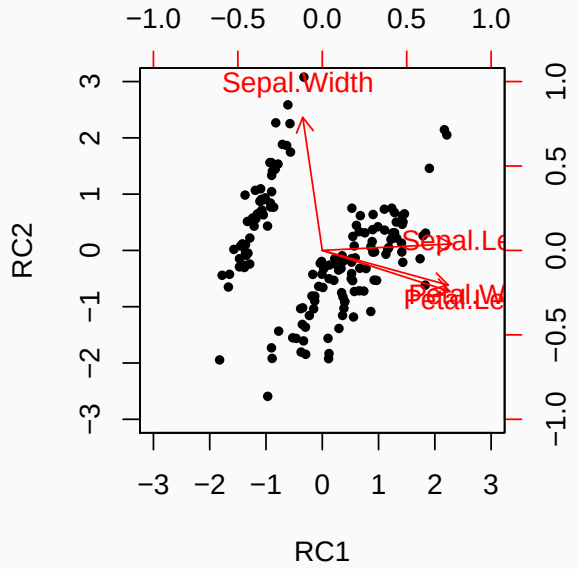
```
              PC1  PC2
Sepal.Length  0.89 0.36
Sepal.Width  -0.46 0.88
Petal.Length  0.99 0.02
Petal.Width   0.96 0.06
```



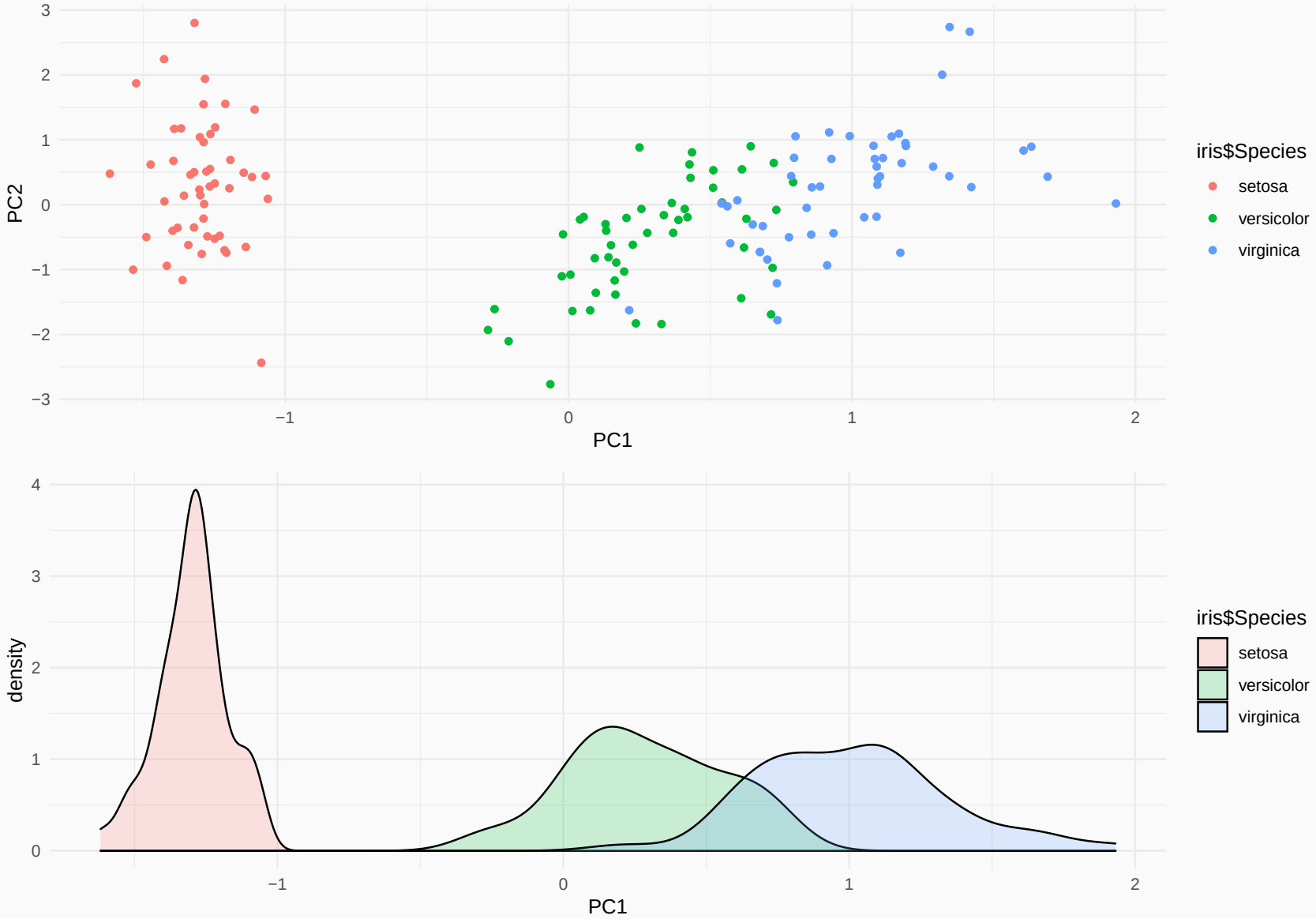
Rotated loadings

```
pc2rot <- principal(iris[, -5], nfactors = 2, rotate = "varimax")
round(loadings(pc2rot)[1:4, 1:2], 2)
```

```
                RC1   RC2
Sepal.Length   0.96  0.05
Sepal.Width   -0.14  0.98
Petal.Length   0.94 -0.30
Petal.Width    0.93 -0.26
```



PC scores with species in 1 and 2 dimensions



Large data sets

Function `prcomp()` handles data with $p > n$

```
pc2 <- prcomp(x = iris[, -5])
```

We need this function in the lab for some exercises.