Principal Component Analysis

McMaster University

Caitlin Simopoulos

2017-05-30

Principal Component Analysis:

- describes patterns in data
- is a way to reduce high dimensionality into fewer, linear components
- principal components = uncorrelated variables
- helpful when looking at data with a lot of features
- "goal is to explain the maximum amount of variance with the fewest number of principal components"
- commonly used in RNASeq QC, or for finding influencial genes
- This is a great visual explanation of PCA.

If this still isn't making any sense...

Read this if you like math.

Read this if you hate math.

An example of PCA with gene expression data...

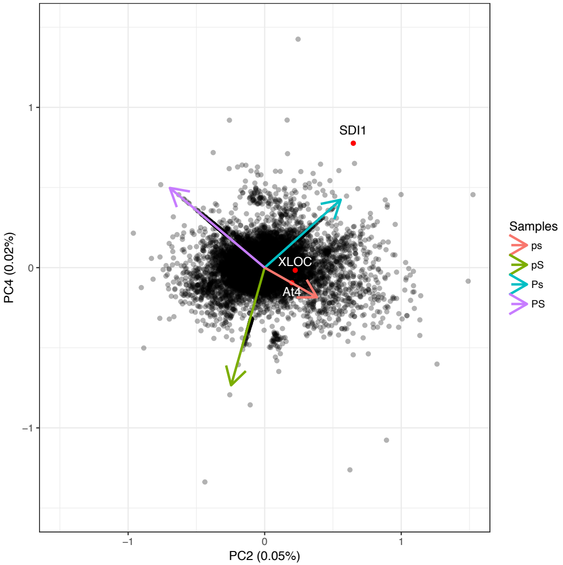


Figure 1:

Lots of features = difficult to interpret data

- visualizing data is one of the best ways to share and interpret data
- it's easy to plot and interpret 2D data...
- 3D is possible, but harder...
- 4D+ is very difficult, and will take a lot of time
- let's use PCA on 4D data

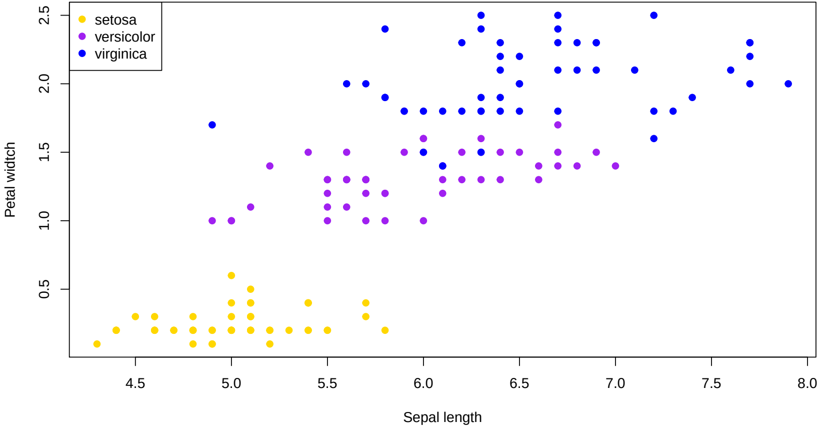
An example: iris data set

```r
data("iris")
table(iris$Species)
```

```
##
##     setosa versicolor  virginica
##         50         50         50
```

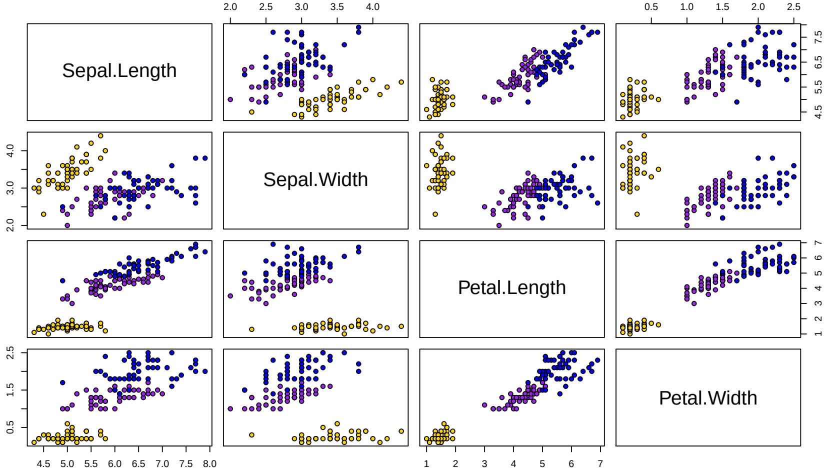
Plotting all features against each other would take a lot of time...

```r
plot.colors <- c("gold", "purple", "blue")
plot(iris$Sepal.Length, iris$Petal.Width, col=plot.colors[unclass(iris$Species)],
     ylab = "Petal widtch", xlab= "Sepal length", pch=19)
legend("topleft", pch=19, col=plot.colors, legend=unique(iris$Species))
```



Thankfully R has a built-in plotting feature for this

```
pairs(iris[,1:4], pch = 21,
      bg = plot.colors[unclass(iris$Species)])
```



Imagine doing this with more than 4 features...

Like with an RNASeq project with data from 30,000 genes and 50 different samples...yuck

Let’s do PCA instead

```
pca<- prcomp(iris[,1:4], center=TRUE, scale=TRUE)  # PCA with centering
pca$rotation  # The loadings are here
```

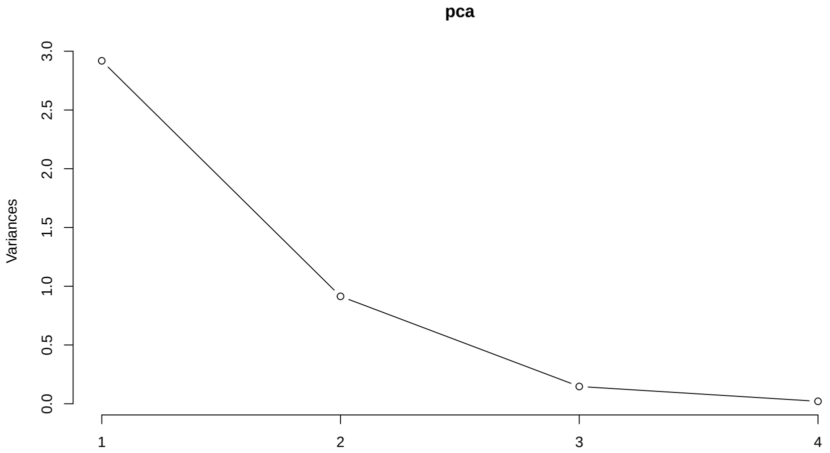
```
##                     PC1         PC2        PC3        PC4
## Sepal.Length  0.5210659 -0.37741762  0.7195664  0.2612863
## Sepal.Width  -0.2693474 -0.92329566 -0.2443818 -0.1235096
## Petal.Length  0.5804131 -0.02449161 -0.1421264 -0.8014492
## Petal.Width   0.5648565 -0.06694199 -0.6342727  0.5235971
```

```
summary(pca)
```

```
## Importance of components%s:
##                           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
```

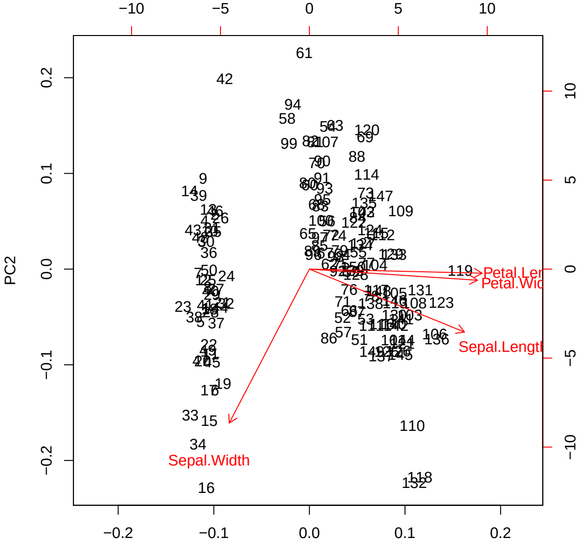
How much varience is described by each component?

```
plot(pca, type = "l")
```



Visualizing PC1 vs PC2

```
biplot(pca)
```



Hmm...

What do you think of this plot?

ggplot2 to the rescue!

- ggplot2 is a super flexible, super sleek plotting package for R
- used in combination with other packages of the “tidyverse”
- ggplot2 requires data in long format
    - 1 row per observation per feature

1. Make data.frame for PCA variables

```
#components
indVals<-data.frame(pca$x)
# variables
varVals<-data.frame(pca$rotation)
dim(indVals)
```

```
## [1] 150   4
```

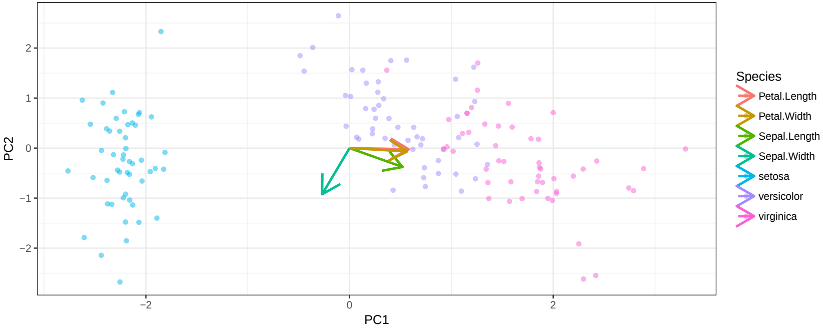
```
dim(varVals)
```

```
## [1] 4 4
```

```
## extrating all PCA data for ggplot
coords<-data.frame(X=rep(0, 4), Y=rep(0, 4), varVals,
                   feature = colnames(iris[1:4]))
indVals <- cbind(indVals, Species= iris$Species)
```

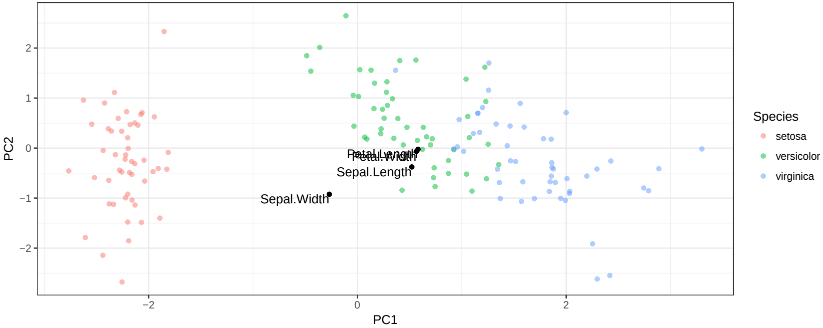
Plot PC1 vs PC2

```
library(ggplot2)
pc12plot <- ggplot(data = indVals, aes(x=PC1, y=PC2)) +
  geom_point(aes(color = Species), alpha=0.5) +
  geom_segment(data=coords, aes(x=X, y=Y, xend=PC1, yend=PC2,
  colour=colnames(iris[1:4])), arrow=arrow(), size=1) +
theme_bw()
print(pc12plot)
```



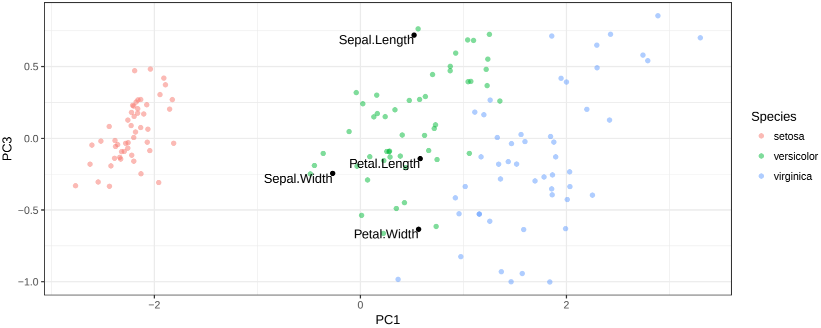
Plot PC1 vs PC2

```
pc12plot <- ggplot(data = indVals, aes(x=PC1, y=PC2)) +
   geom_point(aes(color = Species), alpha=0.5) +
   geom_point(data=coords, aes(x=PC1, y=PC2)) +
   geom_text(data = coords, aes(x=PC1, y=PC2,
   label=feature),hjust=1, vjust=1) +
   theme_bw()
print(pc12plot)
```



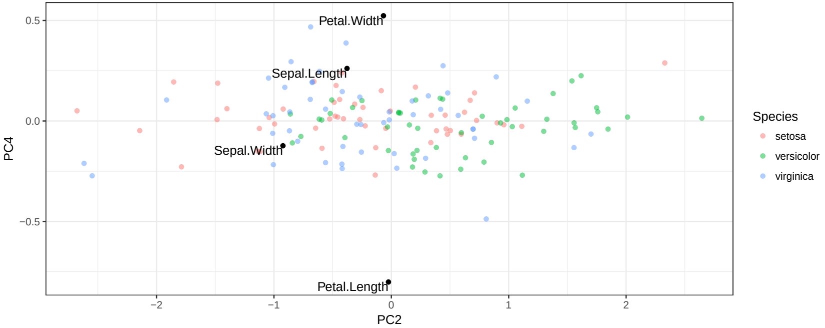
Plot PC1 vs PC3

```
pc12plot <- ggplot(data = indVals, aes(x=PC1, y=PC3)) +
   geom_point(aes(color = Species), alpha=0.5) +
   geom_point(data=coords, aes(x=PC1, y=PC3)) +
   geom_text(data = coords, aes(x=PC1, y=PC3,
   label=feature),hjust=1, vjust=1) +
   theme_bw()
print(pc12plot)
```



Plot PC2 vs PC4

```r
pc24plot <- ggplot(data = indVals, aes(x=PC2, y=PC4)) +
   geom_point(aes(color = Species), alpha=0.5) +
   geom_point(data=coords, aes(x=PC2, y=PC4)) +
   geom_text(data = coords, aes(x=PC2, y=PC4,
   label=feature),hjust=1, vjust=1) +
   theme_bw()
print(pc24plot)
```


Petal.Width
Sepal.Length
Sepal.Width
Petal.Length
PC4
PC2
Species
setosa
versicolor
virginica