Principal Component Analysis

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Overview

In this module, we focused on expanding principal component analysis (PCA) beyond a single principal component and applied it in datasets with more than two dimensions.

ISL 10.2 has a good breakdown of PCA.

Second Principal Component

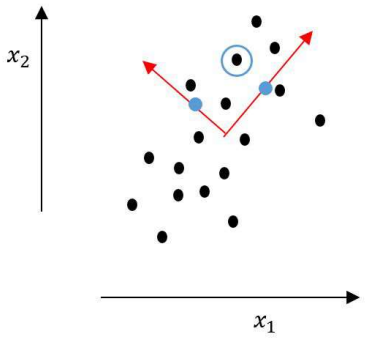
In a 2 dimesional dataset, a second principal component will always be perpendicular to the first. Once we add more dimensions, it will complicate this assumption.

In algebra terms:

original point (from first module on PCA): $x_i = (x_{i1}, x_{i2})$.

- With 1 principal component, we have an approximation of x_i.
  - $x_i \approx \alpha_i V$ where V is the first principal component and α is the score.
- With 2 principal compents, we have an exact equality.
  - $V_1 =$ first principal component
  - $V_2 =$ second principal component
  - $x_i = \alpha_{i1} V_1 + \alpha_{i2} V_2$
  - alphas are scores for x_i on those principal components

We can think of principal components as redefining the coordinate system.



Beyond 2 dimensions

As we expand beyond 2 dimensions, x_i is no longer defined by two coordinates. Instead, it is defined by some number, D, of coordinates.

$$x_i \epsilon \mathbb{R}^D$$

$$x_i = (x_{i1}, x_{i2}, \ldots, x_{iD})$$

Because we are working with more than 2 dimensions, two principal components will no longer explain all of the variation in our dataset.

Our first 2 dimensional vectors will look like this:

$V_1 =$ first principal component with scores α_{i1} $(\alpha_{i1} = x_1 \bullet v_1)$

$V_2 =$ second principal component with scores α_{i2} $(\alpha_{i2} = x_2 \bullet v_2)$

With these two vectors: $x_i = \alpha_{i1} V_1 + \alpha_{i2} V_2$.

As we include more vectors, we will explain more of the variation in x_i. When we reach D vectors, all of the variation will be explained, but this would be stupid in practice as the purpose of PCA is to compress the data. Having D vectors, would keep the same amount of data, but it would be more difficult to interpret. The goal is to explain a lot of the variation with significantly fewer variables.

NOTE: PCA in this context is meant to help us get a better understanding/summary/visualization/structure of the data.

Example 1 in R

For this example, we used pca_intro.R.

ggplot will help us create better plots:

```
library(ggplot2)
```

We will be using the iris dataset again.

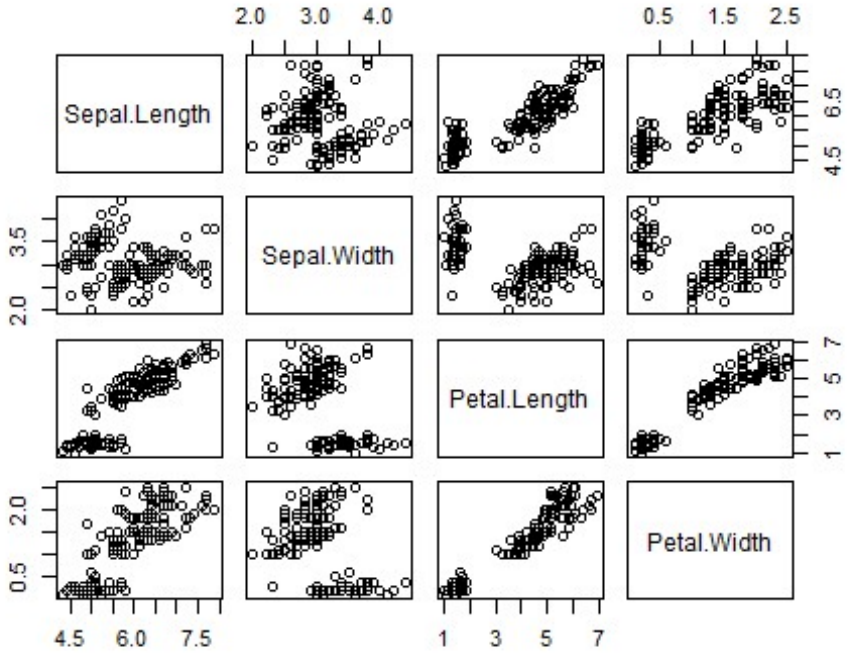
```
data(iris)
```

We want to use all of the flower structure predictors to build our principal components.

```
# Pick out the numerical columns from the data set (run ?iris for further info)
Z = iris[,1:4]
```

There is clearly a lot of correlation between these variables:

```
pairs(Z)
```



Now, we are going to run our principal component analysis.

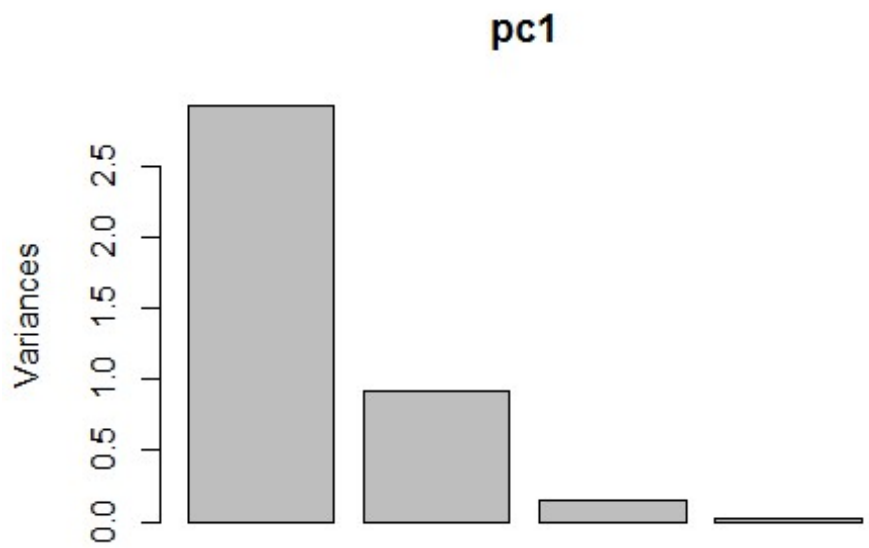
```
# Run PCA
pc1 = prcomp(Z, scale.=TRUE) #different from K-means, scaling may not be
necessary for PCA
```

Let's look at the principal components that were created.

```
# Look at the basic plotting and summary methods
pc1

## Standard deviations:
## [1] 1.7083611 0.9560494 0.3830886 0.1439265
##
## Rotation:
##                      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(pc1)

## 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
```

Which principal components are more powerful? A scree plot will summarize the variance of the original dataset captured by each component:

```
plot(pc1)
```

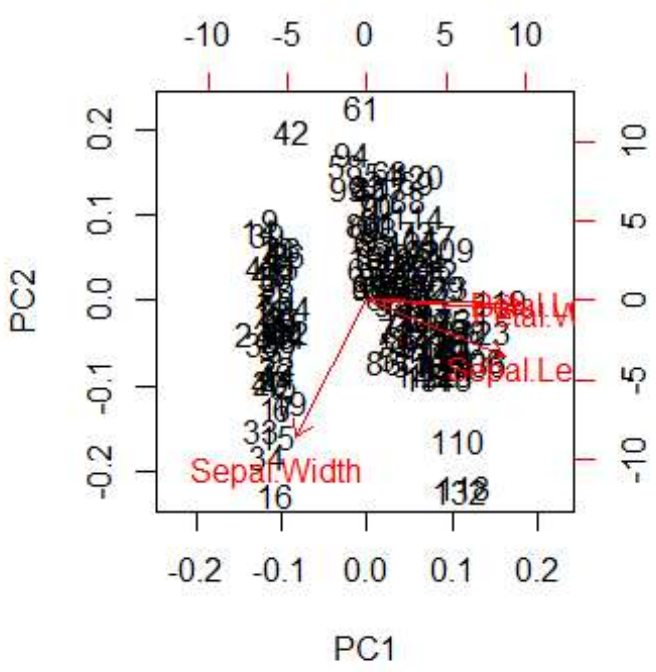


If we used all four of the components, we will capture all of the variation, but we can capture a significant portion of the variation if we just use 1 or 2 of the principal components.

*Note: The amount of variance captured by the principal components is entirely dependent on the nature of the variation in the original dataset. Highly correlated variables will allow more variation to be captured by the individual principals components.

A biplot will help us see the data points plotted within the new coordinate system created by the principal components.

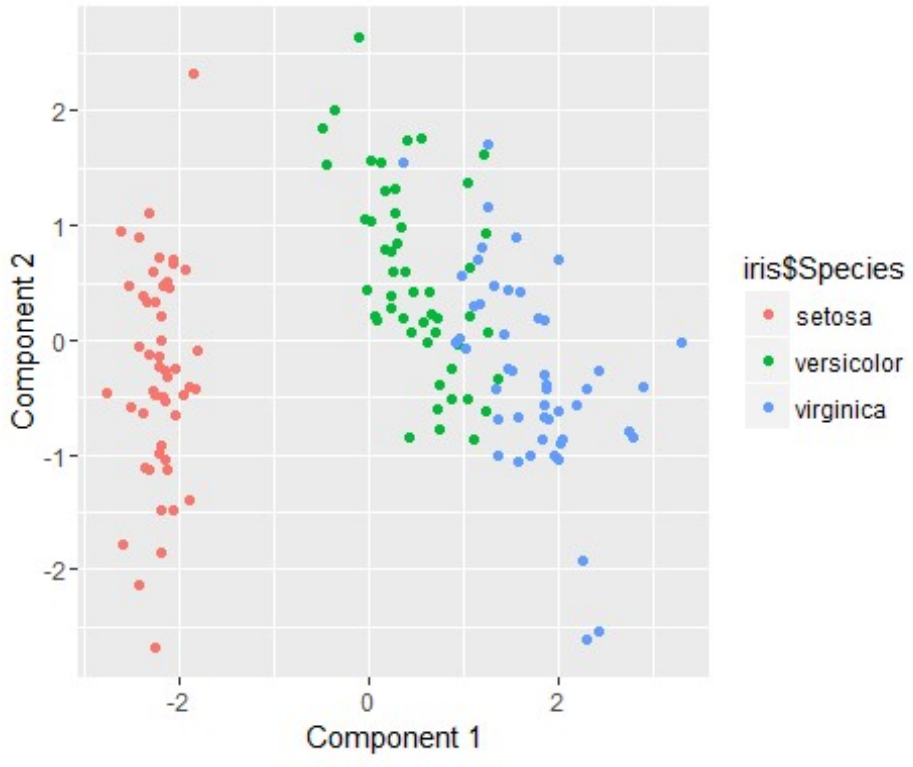
```
biplot(pc1)
```




```
#the points in the new coordinate space
```

Using ggplot, we can get a much more informative plot:

```
# A more informative biplot
loadings = pc1$rotation
scores = pc1$x
qplot(scores[,1], scores[,2], color=iris$Species, xlab='Component 1',
ylab='Component 2')
```



Notice that the axes represent the alphas given to each datapoint along that principal component.

A note about clusters: In this plot, we can see that PC1 separates the datapoints by species quite well. This is a side effect of our PCA and is related to the nature of the dataset. What it tells us is that the points' relative distances along these dimensions are highly related to their species. PCA is NOT a clustering method.

If we look at the loadings here, we can see what type of flowers will score well (get higher alphas) in the individual principal components.

```
#this is equal to pc1$rotation (see last code chunk)
loadings
```

```
##                     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
```

Example: On PC1, the flowers with the higher alphas have a higher sepal length, petal length, and pedal width than average. However, they have a lower sepal width than average.

Example 2 in R

A more complex dataset

The iris dataset is useful for understanding the essential concepts of PCA, but the value of the process is not evident on a dataset with only 4 predictors. To demonstrate this, we will need to look at a more complex dataset.

For this example, we will use a congressional data.

- The r script can be found here
- The datasets are
  - countdata
  - memberdata

```
countdata = read.csv("congress109.csv", header=TRUE, row.names=1)
memberdata = read.csv("congress109members.csv", header=TRUE, row.names=1)
```

Countdata tells us how many times certain members of congress evoke certain phrases in floor speeches. There are 1000 columns in this datase; we need compression, which is why PCA will be useful here. It will helps us find the underlying dimensions of the data.

Memberdata includes basic info about the member:

```
head(memberdata)

##                   party state chamber  repshare   cs1    cs2
## Chris Cannon          R    UT       H 0.7900621 0.534 -0.124
## Michael Conaway       R    TX       H 0.7836028 0.484  0.051
## Spencer Bachus        R    AL       H 0.7812933 0.369 -0.013
## Mac Thornberry        R    TX       H 0.7776520 0.493  0.002
## Randy Neugebauer      R    TX       H 0.7746633 0.506  0.070
## Nathan Deal           R    GA       H 0.7707892 0.474  0.058
```

Before we get started, we will want to normalize the frequencies.

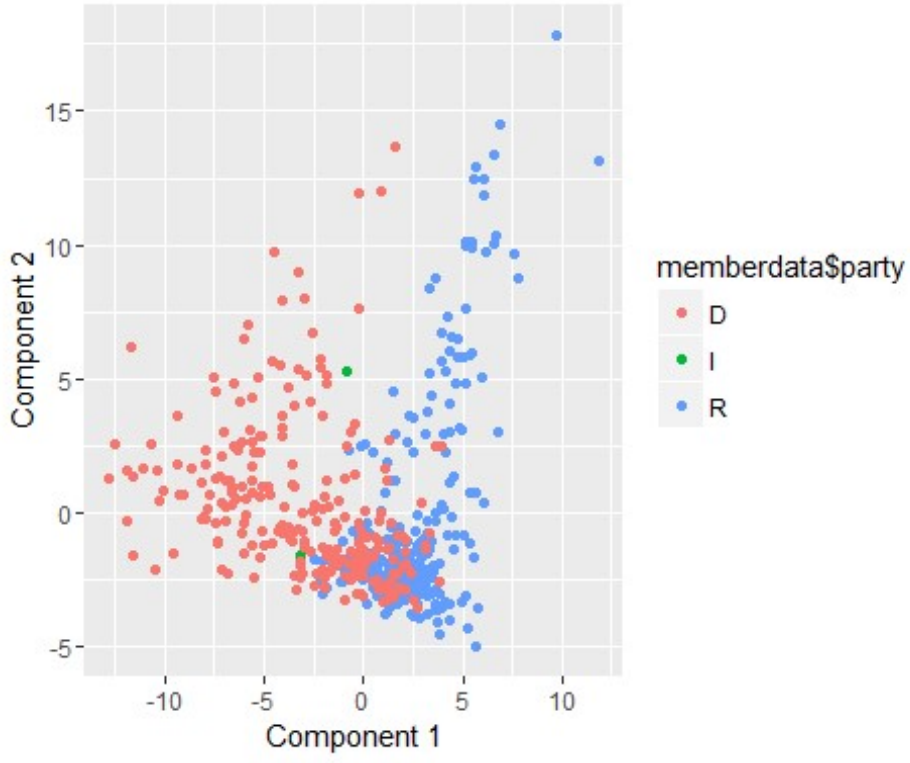
```
# Normalize phrase counts to phrase frequencies
Z = countdata/rowSums(countdata)
```

Then, we can run PCA. We will scale the data this time.

```
# PCA
pc2 = prcomp(Z, scale=TRUE)
#store the principals components
loadings = pc2$rotation
#store the alphas for each PC for each member
scores = pc2$x
```

If we look at a biplot of the data that is color coded according to the members party from the memberdata dataset, we can see that PC1 is a vector that divides the data by party:

```
#qplot is a part of ggplot2
qplot(scores[,1], scores[,2], color=memberdata$party, xlab='Component 1',
ylab='Component 2')
```



Members that are close to each other in this plot are evoking certain phrases in a relatively similar amount, meaning members who are concerned about similar issues will be close to each other on these principal components. This explains why the points are being divided up along party lines by PC1.*We have gone from 1000 features to 2 principal components and are already able to divide the data up reasonably well by party.*

We can look at the top words that affect a member's score (alpha) on PC1:

```
# The top words associated with each component
o1 = order(loadings[,1])

#what words contribute to negative on PC1
colnames(Z)[head(o1,25)]
```

```
##  [1] "private.account"              "cut.medicaid"
##  [3] "student.loan"                 "tax.cut.wealthy"
##  [5] "budget.cut"                   "child.support"
##  [7] "privatizing.social.security"  "privatize.social.security"
##  [9] "billion.tax.cut"              "cut.food.stamp"
## [11] "privatization.plan"           "president.plan"
## [13] "cut.student.loan"             "plan.privatize"
## [15] "tax.break"                    "care.cut"
## [17] "medicaid.cut"                 "cut.benefit"
```

```
## [19] "cut.social.security"           "plan.privatize.social"
## [21] "social.security.privatization" "president.social.security"
## [23] "education.cut"                 "live.poverty"
## [25] "pay.tax.cut"
```

These look like Republican phrases.

```
#what words contribute to positive on PC1
colnames(Z)[tail(o1,25)]
```

```
##  [1] "law.review"                "urban.affair"
##  [3] "housing.urban.affair"      "judge.john.robert"
##  [5] "chief.justice.william"     "committe.commerce.science"
##  [7] "date.time"                 "justice.william.rehnquist"
##  [9] "chief.justice"             "supreme.court.united"
## [11] "majority.vote"             "american.bar.association"
## [13] "partial.birth.abortion"    "partial.birth"
## [15] "birth.abortion"            "john.robert"
## [17] "committe.foreign.relation" "business.meeting"
## [19] "judicial.nomine"           "roe.wade"
## [21] "justice.supreme.court"     "court.judge"
## [23] "circuit.court.appeal"      "circuit.court"
## [25] "court.appeal"
```

And these look like democrat phrases. That matches our plot.

Note: The abundance of judicial phrases is related to the confirmation of Justice Roberts to the Supreme Court. He was a conservative judge, explaining the democrat's discussion of him.

Let's look at what affects a member's score on PC2:

```
#order the words
o2 = order(loadings[,2])
#what words contribute to negative on PC2
colnames(Z)[head(o2,25)]
```

```
##  [1] "strong.support"      "embryonic.stem.cel"  "embryonic.stem"
##  [4] "urge.support"        "stem.cel"            "cel.research"
##  [7] "death.tax"           "business.owner"      "adult.stem"
## [10] "adult.stem.cel"      "illegal.immigration" "pass.bil"
## [13] "repeal.death.tax"    "private.property"    "illegal.immigrant"
## [16] "border.security"     "stem.cel.line"       "cel.line"
## [19] "estate.tax"          "post.office"         "percent.growth"
## [22] "family.business"     "driver.license"      "sex.offender"
## [25] "oil.food"
```

```
#what words contribute to negative on PC2
colnames(Z)[tail(o2,25)]
```

```
##  [1] "minority.right"            "judge.robert"
##  [3] "final.minute"              "circuit.court.judge"
##  [5] "justice.supreme.court"     "john.robert"
```

```
##  [7] "committe.commerce.science" "circuit.court"
##  [9] "circuit.court.appeal"      "justice.priscilla.owen"
## [11] "majority.vote"             "change.senate.rule"
## [13] "supreme.court.united"      "banking.housing.urban"
## [15] "committe.foreign.relation" "nuclear.option"
## [17] "housing.urban.affair"      "american.bar.association"
## [19] "urban.affair"              "president.judicial.nomine"
## [21] "court.judge"               "circuit.judge"
## [23] "president.pro.tempore"     "court.appeal"
## [25] "judicial.nomine"
```

It is much less clear what PC2 is measuring. Subject area knowledge might help us to understand this.

A final note on PCA: The more you compress a feature (i.e. the fewer principal components you use) the more detail/variation from the original data will be lost. Think about a picture. If you compress it a lot, you lose clarity and detail from the image.