

Homework 3 - Principal Component Analysis

Daniel Carpenter

August 2022

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Packages

```
library(tidyverse) # get tidverse for piping
library(skimr)
library(knitr)
library(scales)
require(lubridate)

library(mlbench) # Glass data
library(ggbiplot) # biplots
library(corrplot)
library(caret) # preProcess for centering and z score scaling
library(MASS) # Linear discreiminant analysis with lda

library(HSAUR2) # olympic data
library(outliers) # grubbs.test
library(DescTools) # for the %like% operator
```

1. Glass Data

Get and Clean Data

```
data(Glass)

# Remove duplicates
Glass <- Glass[!duplicated(Glass), ]
```

1 (a) Mathematics of PCA

i. Create the correlation matrix of all the numerical attributes in the `Glass` data and store the results in a new object `corMat`

```
skimmed <- skim(Glass)

# Notice one factor data, for variable `type`
skimmed$skim_type
```

```
[1] "factor" "numeric" "numeric" "numeric" "numeric" "numeric" "numeric"
[8] "numeric" "numeric" "numeric"
```

```
# Get only numeric data
GlassNumeric <- Glass %>% dplyr::select(where(is.numeric))

# Create correlation matrix using only numeric data type
corMat <- cor(GlassNumeric)
```

ii. Compute the eigenvalues and eigenvectors of `corMat`.

Eigenvalues

```
# prcomp(corMat)
eigenValues = eigen(corMat)$values
eigenValues
```

```
[1] 2.510152168 2.058169337 1.407484057 1.144693344 0.914768873 0.528593040
[7] 0.370262639 0.064267543 0.001608997
```

Eigenvectors

```
eigenVectors = eigen(corMat)$vectors
eigenVectors
```

```
      [,1]      [,2]      [,3]      [,4]      [,5]      [,6]
[1,] 0.5432231 -0.28911804 -0.08849541 0.1479796 0.07670808 -0.11455615
[2,] -0.2676141 -0.26909913 0.36710090 0.5010669 -0.14626769 0.55790564
[3,] 0.1093261 0.59215502 -0.02295318 0.3842440 -0.11610001 -0.30585293
[4,] -0.4269512 -0.29636272 -0.32602906 -0.1488756 -0.01720068 0.02014091
[5,] -0.2239232 0.15874450 0.47979931 -0.6394962 -0.01763694 -0.08850787
[6,] -0.2156587 0.15305116 -0.66349177 -0.0733491 0.30154622 0.24107648
[7,] 0.4924367 -0.34678973 0.01380151 -0.2743430 0.18431431 0.14957911
[8,] -0.2516459 -0.48262056 -0.07649040 0.1299431 -0.24970936 -0.65986429
[9,] 0.1912640 0.06089167 -0.27223834 -0.2252596 -0.87828176 0.24066617
      [,7]      [,8]      [,9]
[1,] -0.08223530 0.75177166 -0.02568051
[2,] -0.15419352 0.12819398 0.31188932
[3,] 0.20691746 0.07799332 0.57732740
[4,] 0.69982052 0.27334224 0.19041178
[5,] -0.20945417 0.38077660 0.29747147
```

```
[6,] -0.50515516  0.11064442  0.26075531
[7,]  0.09984144 -0.39885229  0.57999243
[8,] -0.35043794 -0.14497643  0.19853265
[9,] -0.07120579  0.01650505  0.01459278
```

iii. Use `prcomp` to compute the principal components of the `Glass` attributes (make sure to use the `scale` option).

```
# Using only numeric data
pc.glass <- prcomp(GlassNumeric, scale = TRUE)
pc.glass
```

Standard deviations (1, ..., p=9):

```
[1] 1.58434597 1.43463213 1.18637433 1.06990343 0.95643550 0.72704404 0.60849210
[8] 0.25351044 0.04011231
```

Rotation (n x k) = (9 x 9):

	PC1	PC2	PC3	PC4	PC5	PC6
RI	-0.5432231	0.28911804	-0.08849541	-0.1479796	0.07670808	-0.11455615
Na	0.2676141	0.26909913	0.36710090	-0.5010669	-0.14626769	0.55790564
Mg	-0.1093261	-0.59215502	-0.02295318	-0.3842440	-0.11610001	-0.30585293
Al	0.4269512	0.29636272	-0.32602906	0.1488756	-0.01720068	0.02014091
Si	0.2239232	-0.15874450	0.47979931	0.6394962	-0.01763694	-0.08850787
K	0.2156587	-0.15305116	-0.66349177	0.0733491	0.30154622	0.24107648
Ca	-0.4924367	0.34678973	0.01380151	0.2743430	0.18431431	0.14957911
Ba	0.2516459	0.48262056	-0.07649040	-0.1299431	-0.24970936	-0.65986429
Fe	-0.1912640	-0.06089167	-0.27223834	0.2252596	-0.87828176	0.24066617

	PC7	PC8	PC9
RI	-0.08223530	-0.75177166	-0.02568051
Na	-0.15419352	-0.12819398	0.31188932
Mg	0.20691746	-0.07799332	0.57732740
Al	0.69982052	-0.27334224	0.19041178
Si	-0.20945417	-0.38077660	0.29747147
K	-0.50515516	-0.11064442	0.26075531
Ca	0.09984144	0.39885229	0.57999243
Ba	-0.35043794	0.14497643	0.19853265
Fe	-0.07120579	-0.01650505	0.01459278

iv. Compare the results from (ii) and (iii) - Are they the same? Different? Why?

- The eigenvalues differ

- The eigenvectors are the same in absolute value, but the signs are the opposite within each value of the vectors
- Why do they differ? Past `ii` uses the correlation matrix; the principal component analysis (`ii`) uses the covariance matrix, which is a scaled, or *normalized*, version of the correlation matrix.

v. Using R demonstrate that principal components 1 and 2 from (`iii`) are orthogonal. (Hint: the inner product between two vectors is useful in determining the angle between the two vectors)

- The dot product the two vectors is nearly 0, so we can assume orthogonal

```
df.pc.glass <- data.frame(pc.glass$x)

#Orthogonal because they dot product is practically 0
df.pc.glass$PC2 %*% df.pc.glass$PC1
```

```
      [,1]
[1,] -1.723066e-13
```

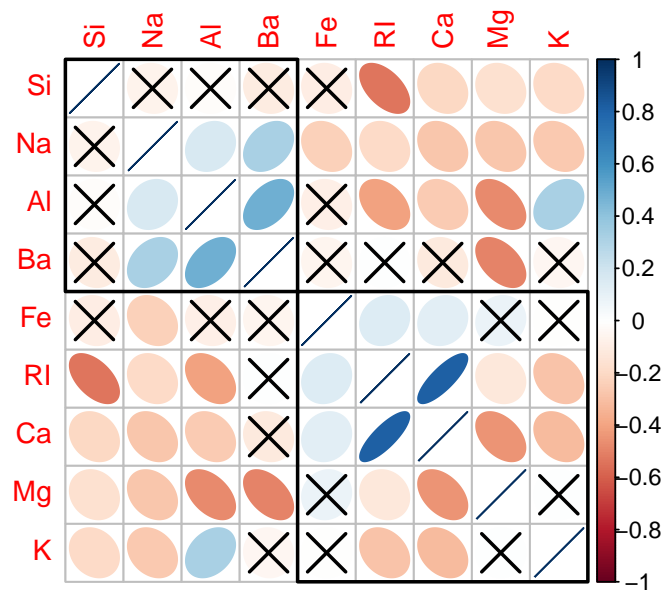
1 (b) Applications of PCA

i. Create a visualization of the corMat correlation matrix (i.e., a heatmap or variant).

- `corrplot` options.

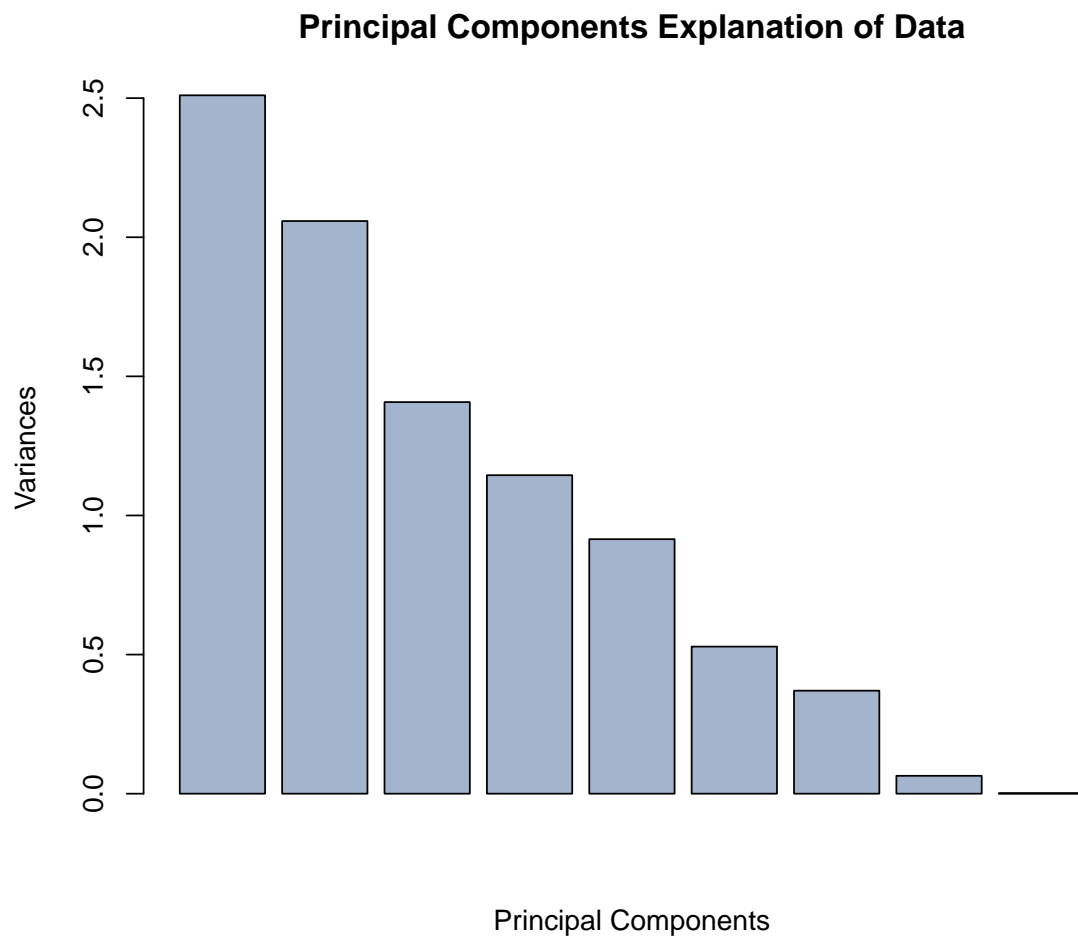
```
testRes = cor.mtest(GlassNumeric, conf.level = 0.90)

# Correlation matrix to show spread and significance
corrplot(corMat,
  p.mat      = testRes$p, # Significance 'x' marks
  sig.level  = 0.10,      # ""          levels
  order      = 'hclust',  # Clustering
  addrect    = 2,
  method     = 'ellipse') # Show spread and direction
```



- ii. Provide visualizations of the principal component analysis results from the Glass data. Consider incorporating the glass type to group and color your biplot.

```
# First show the spread of the components
plot(pc.glass,
     main = 'Principal Components Explanation of Data',
     xlab = 'Principal Components',
     col = 'lightsteelblue3'
)
```



```

# NExt show the biplots
ggbiplot(pc.glass,
  obs.scale = 1,
  var.scale = 1,
  varname.size = 4,
  labels.size = 10,
  circle = TRUE,
  group = Glass$Type#,
  # ellipse = TRUE
) +

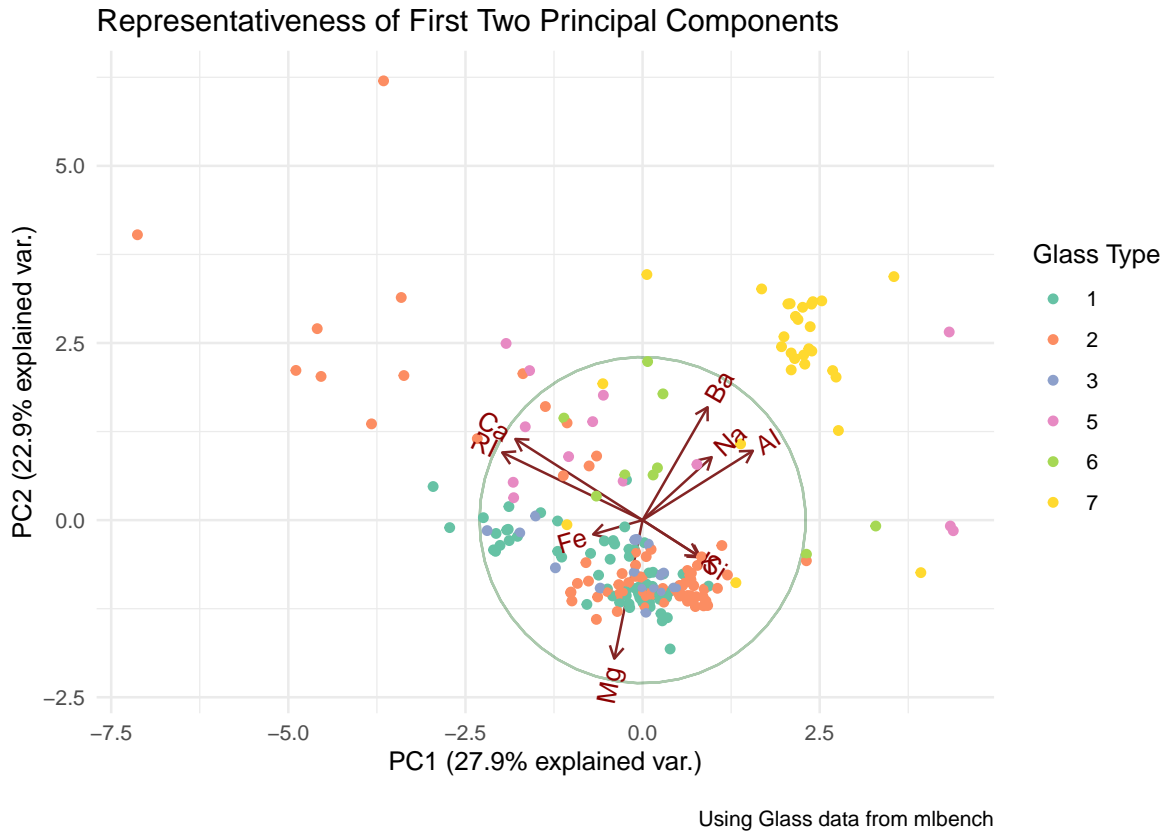
# Titles and caption
labs(title = 'Representativeness of First Two Principal Components',
  caption = '\nUsing Glass data from mlbench') +

# Add color to points by glass type
geom_point(aes(colour=Glass$Type), size = 1) +

# Categorical palette on glass type
scale_color_brewer(name = 'Glass Type',
  palette = 'Set2', type = 'qual') +

theme_minimal() # the theme

```

iii. Provide an interpretation of the first two principal components of the Glass data.

- Both PC1 and PC2 represent roughly half (50%) of the cumulative proportion of variance (see summary below)
- PC1 best explains Fe, K, and Si glass types, since they lie closest to parallel with the x axis
- PC2 best represents Ba, and Mg, since they lie close to parallel with the y axis.
- Other variables appear to be explained by both principal components, since they are near a 45 degree angle.

Summary of cumulative proportion located here

```
summary(pc.glass)
```

Importance of components:

	PC1	PC2	PC3	PC4	PC5	PC6	PC7
--	-----	-----	-----	-----	-----	-----	-----

Standard deviation	1.5843	1.4346	1.1864	1.0699	0.9564	0.72704	0.60849
Proportion of Variance	0.2789	0.2287	0.1564	0.1272	0.1016	0.05873	0.04114
Cumulative Proportion	0.2789	0.5076	0.6640	0.7912	0.8928	0.95154	0.99268
	PC8	PC9					
Standard deviation	0.25351	0.04011					
Proportion of Variance	0.00714	0.00018					
Cumulative Proportion	0.99982	1.00000					

- iv. Based on the PCA results, do you believe that you can effectively reduce the dimension of the data? If so, to what degree? If not, why?
- Given the cumulative proportions above, it is clear that the first two principal components capture only half (~50%) of the variation in the original data. We could compare that to a coin flip, or a random chance.
 - However, the *first four* PC's capture roughly 80%. This cuts the number of variables in half, which is impressive.
 - Note that if your q threshold was set to 95%, then this analysis would not perform well, since all but one of the PC's capture 95% of the variation in the actual data.

1 (c) Application of LDA

- i. Since the `Glass` data is grouped into various labeled glass types we can consider linear discriminant analysis (LDA) as another form of dimension reduction. Use the `lda` method from the `MASS` package to reduce the `Glass` data dimensionality.

```
preproc.param <- Glass %>% preProcess(method = c("center", "scale"))

# Transform the data using the estimated parameters
# Apply centering and scaling to the dataset
transformed <- preproc.param %>% predict(Glass)

# Fit the model , '.' means *
lda.model <- lda(Type ~ ., data = transformed)
lda.model
```

Call:

```
lda(Type ~ ., data = transformed)
```

Prior probabilities of groups:

	1	2	3	5	6	7
	0.32394366	0.35680751	0.07981221	0.06103286	0.04225352	0.13615023

Group means:

	RI	Na	Mg	Al	Si	K
1	0.10586803	-0.21529537	0.6021709	-0.55566964	-0.03051835	-0.07127292
2	0.08928758	-0.35801082	0.2236651	-0.08333047	-0.07370057	0.03395576
3	-0.12668032	0.04037692	0.5986928	-0.50069475	-0.32346915	-0.14146475
5	0.19121411	-0.70579005	-1.3197807	1.17832829	-0.37327809	1.48675612
6	-0.29416453	1.52153712	-0.9514821	-0.16699477	0.71265830	-0.76375492
7	-0.40605128	1.27100801	-1.4829529	1.35761437	0.40154052	-0.26592900

	Ca	Ba	Fe
1	-0.11782012	-0.32708816	0.005626553
2	0.08387772	-0.25209570	0.230146481
3	-0.12002632	-0.33526691	-0.002235610
5	0.82037781	0.02373083	0.035785004
6	0.28233912	-0.35297613	-0.586918470
7	-0.32450463	1.73435095	-0.449113729

Coefficients of linear discriminants:

	LD1	LD2	LD3	LD4	LD5
RI	0.94568441	0.07527438	1.0863607	-0.818100075	2.3954624

Na	1.93653461	2.56835550	0.3710009	-5.620203296	-2.1990082
Mg	1.06291733	4.27171386	2.2661557	-9.823318476	-4.4675280
Al	1.65414159	0.83192958	1.1005447	-3.192430110	-0.6006326
Si	1.89406393	2.29624206	1.3286024	-5.857566773	-0.9918384
K	1.02248031	1.19667679	0.8324237	-5.232631319	-2.0664499
Ca	1.42618954	3.35575714	0.9098493	-9.431977031	-5.6893657
Ba	1.14918330	1.69975242	1.2850261	-3.150403464	-2.3353652
Fe	-0.04927568	0.01955888	0.1195656	-0.002693645	0.1268396

Proportion of trace:

	LD1	LD2	LD3	LD4	LD5
	0.8145	0.1168	0.0417	0.0158	0.0111

ii. How would you interpret the first discriminant function, LD1?

- Within the coefficient matrix, you can see that LD1's top 3 coefficients contain Na, Si, and Al, which shows that there are greater levels of separation
- Additionally, LD1 holds 81% of the discriminatory power. This value holds an important role in between group discrimination.

iii. Use the `ldahist` function from the MASS package to visualize the results for LD1 and LD2. Comment on the results.

- Please see below on my best ability to use `ldahist()`
- For the most part the predictions do well, although you can see that there is a spread from the average by type from reviewing the original and centered data

```
# -----

# Predict the values
predictions <- lda.model %>% predict(transformed)

# Tried below and did not work, which is everything that I found online
# https://www.r-bloggers.com/2018/03/discriminant-analysis-statistics-all-the-way/
# https://www.andreaperlato.com/mlpost/linear-discriminant-analysis/
# ldahist(data=predictions$x[, 1], g = Type)

# Recreating the ldahist to the best of my ability in ggplot2...

# Get LD1 and type from the predicted data, combine into single dataset
LD1 <- predictions$x[, 1]
```

```

Type = predictions$class

predictedLD1 <- data.frame(Type, LD1)

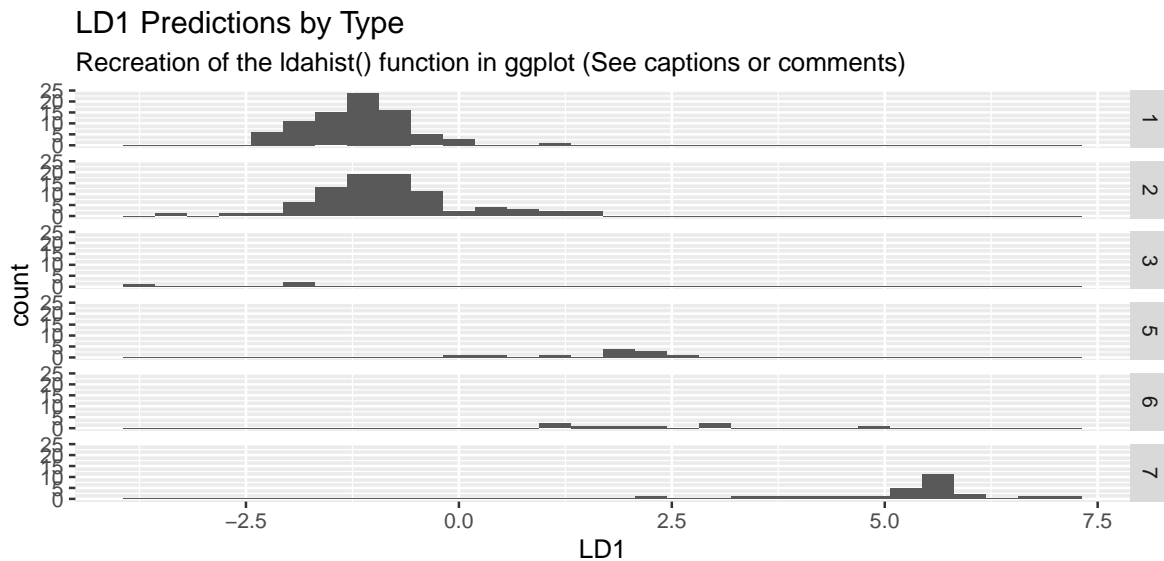
# Recreate the ldahist() output
predictedLD1 %>%
  ggplot(aes(x = LD1)) +

  # Create a histogram
  geom_histogram() +

  # Facet on type
  facet_grid(Type ~ .) +
  labs(title = 'LD1 Predictions by Type',
       subtitle = 'Recreation of the ldahist() function in ggplot (See captions or comments)',
       caption = paste0('\nTried ldahist() (see above) and did not work, Sources attempted: ',
                        '\nhttps://www.r-bloggers.com/2018/03/discriminant-analysis-statistics-all-the-way/, ',
                        '\nhttps://www.andreaperlato.com/mlpost/linear-discriminant-analysis/'))
  )

```

`stat_bin()` using `bins = 30`. Pick better value with `binwidth`.



Tried ldahist() (see above) and did not work, Sources attempted:
<https://www.r-bloggers.com/2018/03/discriminant-analysis-statistics-all-the-way/>
<https://www.andreaperlato.com/mlpost/linear-discriminant-analysis/>

2. Principal components for dimension reduction

2 (a) Remove outlier

- Launa from PNG is the outlier. She is an outlier in highjump, longjump, run800m, and hurdles. See image below.
- Notice that Joyner is an outlier too, but not removed since problem does not specify

```
data(heptathlon)

grubbs.test(heptathlon$score)
```

Grubbs test for one outlier

```
data: heptathlon$score
G = 2.68194, U = 0.68781, p-value = 0.04618
alternative hypothesis: lowest value 4566 is an outlier
```

```
# Who is the outlier?
heptathlon[heptathlon$score==outlier(heptathlon$score),]
```

	hurdles	highjump	shot	run200m	longjump	javelin	run800m	score
Launa (PNG)	16.42	1.5	11.78	26.16	4.88	46.38	163.43	4566

```
# To show the outlier
heptathlonPivot <- heptathlon %>%

# Get the competitor name as own col
mutate(competitor = rownames(heptathlon) ) %>%

pivot_longer(cols = hurdles:score,
              names_to = 'event',
              values_to = 'eventScore')

# Create a plot of each event
heptathlonPivot %>%

ggplot(aes(x = 1,
           y = eventScore)) +
```

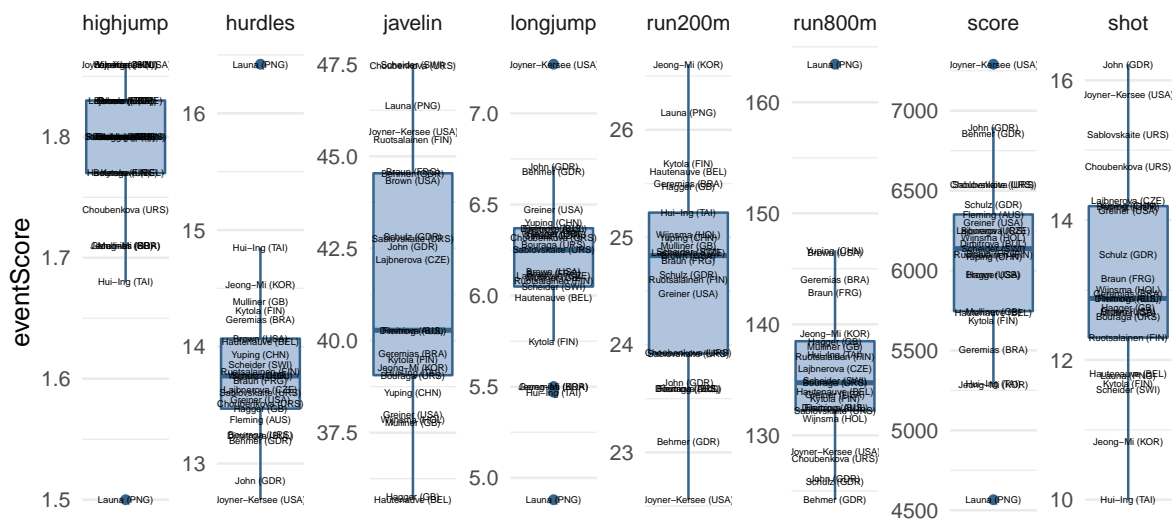
```
# To see the distribution
geom_boxplot(color = 'steelblue4', fill = 'lightsteelblue') +

# Display the olympians
geom_text(label = heptathlonPivot$competitor, size = 1.5) +

facet_wrap(. ~ event, nrow = 1, scales = 'free') +

# Aesthetics
ggtitle('Distribution of Event Scores from the Heptathlon') +
theme_minimal() + theme(axis.text.x = element_blank(),
                        axis.title.x = element_blank(),
                        panel.grid.major.x = element_blank(),
                        panel.grid.minor.x = element_blank())
```

Distribution of Event Scores from the Heptathlon



```
# Remove outlier from data set
heptathlon <- heptathlon[heptathlon$score!=outlier(heptathlon$score),]
```

2 (b)

Transform the running events (hurdles, run200m, run800m) so that large values are good.

```
heptathlon.goodBad <- heptathlon %>%  
  mutate(hurdles = max(hurdles) - hurdles,  
         run200m = max(run200m) - run200m,  
         run800m = max(run800m) - run800m  
  )
```

2 (c)

Perform PCA and store in Hpca

```
Hpca <- prcomp(heptathlon.goodBad,  
              center = TRUE, # Mean centered  
              scale = TRUE # Z-Score standardized  
              )
```

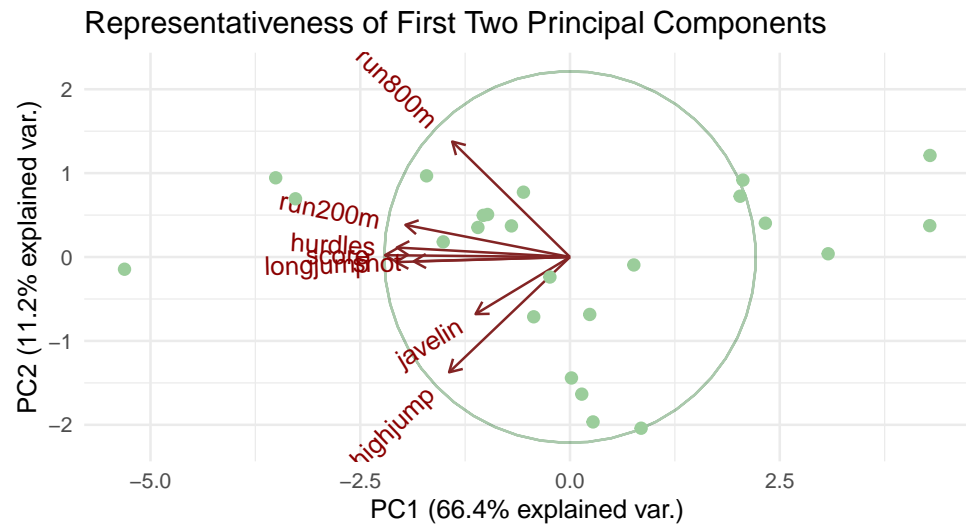
2 (d)

Visualize first two principal components

```
# Create the biplot  
ggbiplot(Hpca,  
         obs.scale = 1,  
         var.scale = 1,  
         varname.size = 4,  
         labels.size = 10,  
         circle = TRUE  
         ) +  
  
# Titles and caption  
labs(title = 'Representativeness of First Two Principal Components',  
     caption = '\nUsing scaled and centered heptathlon data from HSAUR2') +  
  
# Add color to points by glass type
```



```
geom_point(color = 'darkseagreen3', size = 2) +  
theme_minimal() # the theme
```



Using scaled and centered heptathlon data from HSAUR2

Interpretation of Results

PC1:

- Explains 66% of the variation in the data
- Explains all variables very well (*except for run800m, javelin, and highjump*)

PC2:

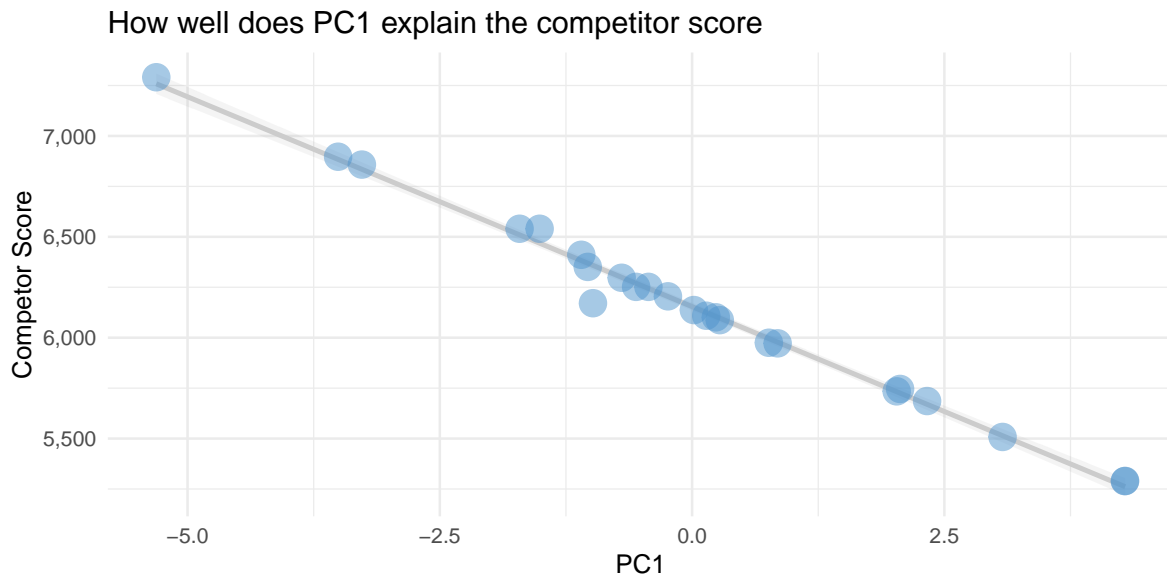
- Explains 11% of the variation in the data
- Explains some of run800m, javelin, and highjump. Since the angles are nearly 45 degrees, you can tell that the explanatory power splits between PC1 and PC2

2 (e)

Plot the heptathlon score against the principal component 1 projections

```
heptathlon %>%  
  
  # Add PC1 to dataset  
  mutate(PC1 = Hpca$x[, 1]) %>%  
  
  # Using PC1 and score  
  ggplot(aes(y = score,  
             x = PC1  
             ) ) +  
  
  # Add OLS  
  geom_smooth(method = lm, color = 'grey80', alpha = 0.10) +  
  
  # Add points  
  geom_point(color = 'steelblue3',  
            alpha = 0.5,  
            size = 5) +  
  
  # Labels and colors  
  labs(  
    title = 'How well does PC1 explain the competitor score',  
    y = 'Competor Score'  
  ) +  
  
  scale_y_continuous(labels = comma) +  
  
  theme_minimal()
```

`geom_smooth()` using formula 'y ~ x'



Interpretation of Score ~ PC1

- You can see that PC1 explains the competitor score extremely well just by this simple visual.

3. Housing data dimension reduction and exploration

Read and Clean data

```
# Read data
housingData <- read_csv('housingData.csv')
```

Rows: 1000 Columns: 74

-- Column specification -----

Delimiter: ","

chr (38): MSZoning, Alley, LotShape, LandContour, LotConfig, LandSlope, Neig...

dbl (36): Id, MSSubClass, LotFrontage, LotArea, OverallQual, OverallCond, Ye...

i Use `spec()` to retrieve the full column specification for this data.

i Specify the column types or set `show_col_types = FALSE` to quiet this message.

```
hd <- housingData %>%

# selects only numeric columns
select_if(is.numeric) %>%

# creates new variables age, ageSinceRemodel, and ageofGarage, and
dplyr::mutate(age = YrSold - YearBuilt,
              ageSinceRemodel = YrSold - YearRemodAdd,
              ageofGarage = ifelse(is.na(GarageYrBlt), age, YrSold - GarageYrBlt)) %>%

# removes a few columns that are not needed
dplyr::select(!c(Id, MSSubClass, LotFrontage, GarageYrBlt,
                 MiscVal, YrSold, MoSold, YearBuilt,
                 YearRemodAdd, MasVnrArea))
```

Correlation Analysis

Please see interpretation of correlation analysis below:

- You can see that there are many variables within the data set that are highly correlated
- Some variables do not show high correlation
- Please see correlation plot in depth for variable specific correlations.

```

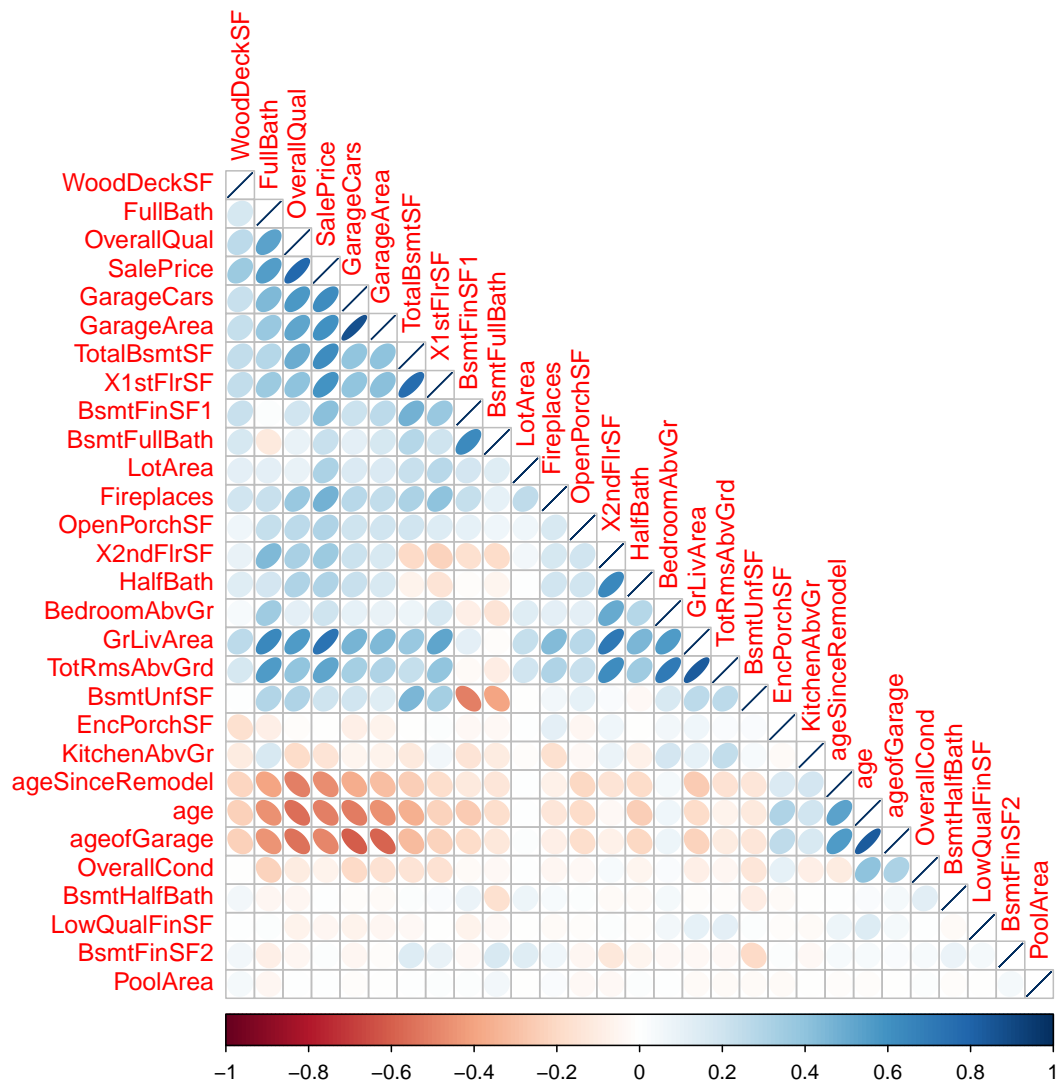
# Parameters
numericData = hd
confInt      = 0.90

# Create correlation matrix
corMatHouse <- cor(numericData)

testRes = cor.mtest(numericData, conf.level = confInt)

# Correlation matrix to show spread and significance
corrplot(corMatHouse,
          order      = 'hclust', # Clustering
          addirect    = 2,
          method      = 'ellipse', # Show spread and direction
          type        = 'lower')

```



Principal Component Analysis

Cumulative Proportions

Please see interpretation of cumulative proportions below:

- The first two principal components explain ~36% of the variation in the data, so we would need to use more than just those
- If our q threshold for variation kept within the data was around 95%, then we could keep only the first 20 principal components while removing 10 columns from the original data set.
- If we were satisfied with retaining 80% of the variation via these PC's, we could remove 18 variables from the data set.
- Note that there are 30 numeric variables within the dataset

```
ncol(hd) # Number of columns in the dataset
```

```
[1] 29
```

```
# Perform PCA while centering and scaling data
pc.house <- prcomp(hd,
                   center = TRUE, # Mean centered
                   scale  = TRUE # Z-Score standardized
                   )
```

```
# See first 10 cumulative proportions
pc.house.summary <- summary(pc.house)
pc.house.summary$importance[, 1:6]
```

	PC1	PC2	PC3	PC4	PC5	PC6
Standard deviation	2.685852	1.809361	1.516124	1.391959	1.174618	1.096403
Proportion of Variance	0.248750	0.112890	0.079260	0.066810	0.047580	0.041450
Cumulative Proportion	0.248750	0.361640	0.440900	0.507720	0.555290	0.596740

```
# Create a data frame for ggplot
pc.hd.cumProportion <- data.frame(cumProp = pc.house.summary$importance['Cumulative Proportion', 1:6])

# See how Individual PC's perform
pc.hd.cumProportion %>%
```

```

# Create the plot with x summarizing the PC's as only their number
ggplot(aes(x = reorder(1:nrow(pc.hd.cumProportion), cumProp),
            group = 1,
            y = cumProp)
) +

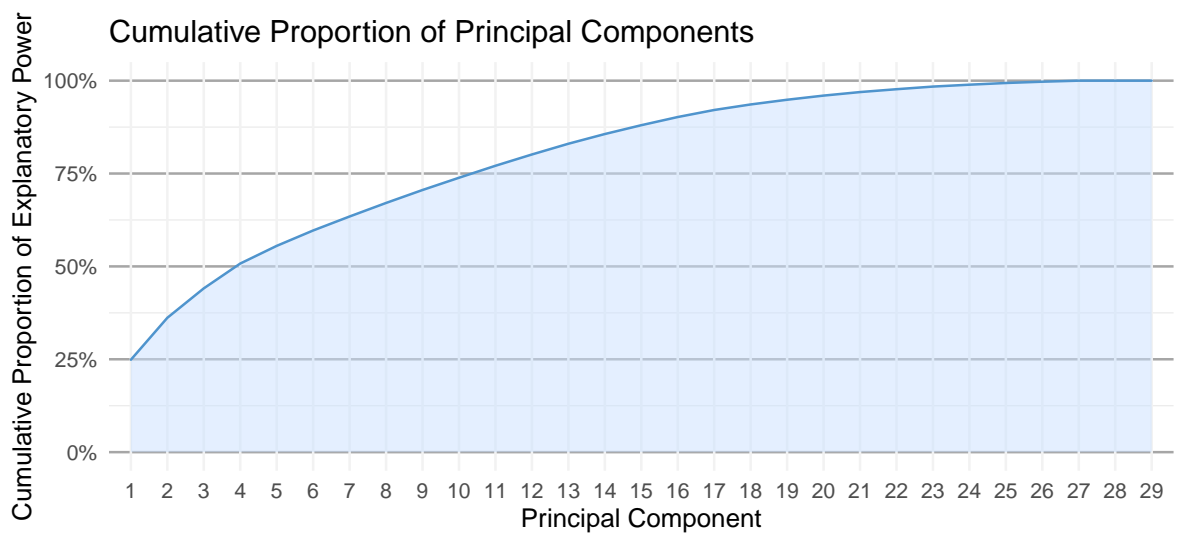
# Area chart
geom_area(alpha = 0.5,
          color = 'steelblue3',
          fill = 'lightsteelblue1'
) +

# Labels, scales, and colors
labs(title = 'Cumulative Proportion of Principal Components',
      x = 'Principal Component',
      y = 'Cumulative Proportion of Explanatory Power',
      caption = '\nUsing housing dataset. Data centered and scaled.'
) +

scale_y_continuous(labels = percent) +

theme_minimal() + theme(panel.grid.major.x = element_line(color = 'grey95'),
                        panel.grid.major.y = element_line(color = 'grey65'))

```



Using housing dataset. Data centered and scaled.

Bi-Plots

- Since there are so many variables, it can be difficult to interpret all of the results
- However, you can see that there are not many outliers affecting the analysis
- Some variables that PC1 contains well: Fireplaces, OverallQual, GarageCars.
- Some variables that PC2 contains well: BsmtFullBath, BsmtFinSF1, EncPorchSF

```
ggbiplot(pc.house,  
  obs.scale = 1,  
  var.scale = 1,  
  varname.size = 3,  
  labels.size = 10,  
  circle = TRUE,  
  alpha = 0.1  
) +  
  
# Titles and caption  
labs(title = 'Representativeness of First Two Principal Components',  
  caption = '\nUsing housing dataset. Data centered and scaled.') +  
  
theme_minimal() # the theme
```

