Introduction to Principal Component Analysis and other multivariate statistics

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Load in `ggplot2` for making graphs

```
library(ggplot2)
```

If needed, `install.packages("ggrepel")` Load in `ggrepel`, for making labels on your ggplots

```
library(ggrepel)
```

If needed, `install.packages("ggdendro")` Load in `ggdendro`, for making nice dendrograms out of your hierarchical clustering results

```
library(ggdendro)
```

If needed, `install.packages("ape")` Load in ape, for making nice dendrograms out of your hierarchical clustering results

```
library(ape)
```

Principal Component Analysis (PCA)

Let's read in the dataset for the nutrition labels for our 75 candy types to learn how to do Principal Component Analysis (PCA) in R

```
data <- read.table("./candy_nutrition.txt", header=TRUE)
```

Check the names of our data

```
names(data)
```

```
##  [1] "id"                "name"              "company"
##  [4] "class"             "serving_size_g"    "calories"
##  [7] "calories_fat"      "total_fat_g"       "saturated_fat_g"
## [10] "cholesterol_mg"    "sodium_mg"         "total_carb_g"
## [13] "dietary_fiber_g"   "sugars_g"          "protein_g"
## [16] "primary_ingredient"
```

The dataset includes names of the candies, the company that made them, their general class, calories, serving size, and a number of nutritional values, in addition to primary ingredient

Let's first normalize the nutritional values by dividing them by `serving_size_g`. We'll create new variables

```
data$total_fat_per_serv <- data$total_fat_g/data$serving_size_g
data$saturated_fat_per_serv <- data$saturated_fat_g/data$serving_size_g
data$cholesterol_per_serv <- data$cholesterol_mg/data$serving_size_g
data$sodium_per_serv <- data$sodium_mg/data$serving_size_g
data$total_carb_per_serv <- data$total_carb_g/data$serving_size_g
data$dietary_fiber_per_serv <- data$dietary_fiber_g/data$serving_size_g
data$sugars_per_serv <- data$sugars_g/data$serving_size_g
data$protein_per_serv <- data$protein_g/data$serving_size_g
```

Now, let's perform a PCA using the `prcomp()` function. PCA is a dimension-reduction technique that reorients the axes of your data so that they explain the maximum amount of variance in the fewest number of dimensions. One way to think about PCAs is that if you measure your data using variables x, y, z in 3D, then imagine reorienting the angle of a camera to take a 2D photo that maximizes the viewable variance in the photo (that is, 2D). PCA is a lot like this, except often it is performed on much higher dimensional data than just 3 dimensions. To get a feeling for how PCAs work, try rotaing the 3D dataset in this http://setosa.io/ev/principal-component-analysis/ to see how the data remains fundamentally the same, but is now described by axes that explain greater amounts of variance.

Let's now perform a PCA using the `prcomp` function. Check out `?prcomp`. `prcomp` requires input data, but also the variables `center` and `scale.` to be specified. Let's set `center` to `TRUE` and `scale.` to `TRUE` as well. This is because the nutritional information is collected in different units

N.B.: You could manually scale your data if you wanted to. For example, you could use the `scale()` function, which sets the mean of a data column to 0 and the variance to 1. You would create an object, `scaled_data <- scale(data[17:24])` and could use that as the input into the PCA as well.

Make sure that the column numbers correspond to the new normalized traits we created! This should be columns 17-24 `?prcomp`

```
pca <- prcomp(data[17:24], center=TRUE, scale.=TRUE)
```

Now that we've done our PCA, let's look at some of the outputs, which you can look up with ?prcomp

But first, let's do a summary to see the percent variance explained by each PC

```
summary(pca)
```

```
## Importance of components:
##                           PC1    PC2     PC3     PC4     PC5     PC6
## Standard deviation     2.2679 1.0742 0.77439 0.72721 0.49683 0.48787
## Proportion of Variance 0.6429 0.1442 0.07496 0.06611 0.03086 0.02975
## Cumulative Proportion  0.6429 0.7872 0.86215 0.92826 0.95911 0.98886
##                           PC7     PC8
## Standard deviation     0.25479 0.15547
## Proportion of Variance 0.00811 0.00302
## Cumulative Proportion  0.99698 1.00000
```

Nice! The first four PCs explain >90% of variance in our data. PCs 1 and 2 explain >75%!

What do these PCs mean? What combination of our variables consitute each of the PCs? To figure this out, we look at the loadings, which you can find using the rotation output

```
pca$rotation
```

```
##                                PC1         PC2        PC3         PC4
## total_fat_per_serv     -0.4236773  0.13269577 -0.1568617  0.05851302
## saturated_fat_per_serv -0.3922951  0.23421654 -0.2184548 -0.10138886
## cholesterol_per_serv   -0.2925627  0.50479458 -0.0466282 -0.61129836
## sodium_per_serv        -0.2281962 -0.58836586 -0.7210734 -0.09112375
## total_carb_per_serv     0.4232201  0.09612676 -0.1627624  0.03660121
## dietary_fiber_per_serv -0.3677174  0.15269038  0.0145450  0.52409455
## sugars_per_serv         0.2688428  0.53504086 -0.5411732  0.41511592
## protein_per_serv       -0.3772636 -0.08785818  0.2932223  0.39493205
##                                PC5        PC6         PC7          PC8
## total_fat_per_serv     -0.1942906  0.2400786  0.09644378  0.818640342
## saturated_fat_per_serv -0.4346917  0.4720047 -0.29859715 -0.482015890
## cholesterol_per_serv    0.3838829 -0.3527579 -0.10883972  0.008904835
## sodium_per_serv         0.1990342 -0.1631544 -0.06810743 -0.051275071
## total_carb_per_serv    -0.1003685 -0.1016358 -0.82985714  0.273398215
## dietary_fiber_per_serv -0.2888437 -0.6830207 -0.06725374 -0.110053733
## sugars_per_serv         0.2998563  0.1441395  0.24303059 -0.080692914
## protein_per_serv        0.6347403  0.2662573 -0.36442260 -0.037556471
```

The contribution of a variable to a PC is proportional to the absolute value of the loading, and positively or negatively contributes towards the PC based on its sign. For example, `total_fat_per_serv` is negatively associated with PC1 and `total_carb_per_serv` is postively associated

Now, let's get the PC scores

```
scores <- as.data.frame(pca$x)
head(scores)
```

```
##         PC1        PC2        PC3        PC4        PC5         PC6
## 1 -1.360340  1.2253820 -0.2491928 -0.2812836  0.2172947  0.34206721
## 2  0.483663 -1.6948183  1.3240001 -0.8875114 -0.2790751 -0.28996199
## 3  2.292019  0.5537819  0.2028140  0.4763461  0.2948282  0.07010778
## 4  2.350462 -0.2731776 -1.5442805  0.1312974  0.2260422 -0.41877992
## 5  1.259095 -0.6934915  0.3911153 -0.1329304  0.2391956 -0.11518484
## 6 -1.326783  1.0001694 -0.4836604 -0.7715705  0.2412477  1.10978569
##          PC7         PC8
## 1  0.1100176 -0.05937806
## 2  0.3795090 -0.02460115
## 3 -0.3638014  0.11301354
## 4 -0.3298129  0.09024576
## 5  0.3493761 -0.18264299
## 6  0.1913661  0.13902258
```

That's nice, but it would be better if the scores also had the associated data from the original dataset linked to the PC scores. Let's use `cbind()` to combine these columns into a single dataset

```
pca_scores <- cbind(data, scores)
head(pca_scores)
```

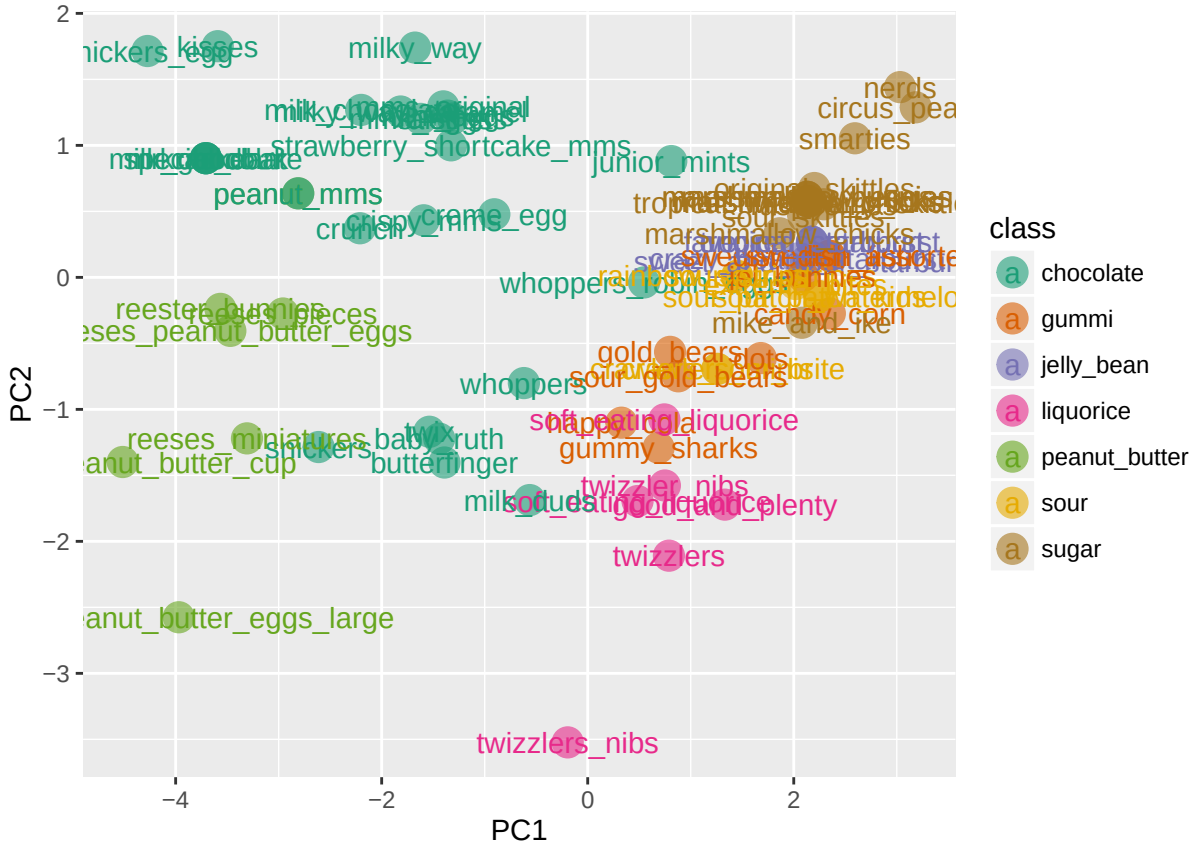
```
##     id                     name     company     class serving_size_g
## 1 id_1                mini_eggs     cadbury chocolate             40
## 2 id_2    soft_eating_liquorice darrell_lea liquorice             42
## 3 id_3              raspberries      haribo     sugar             39
```

```
## 4 id_4               candy_corn        nice     gummi             41
## 5 id_5           crawlers_minis      trolli      sour             40
## 6 id_6 strawberry_shortcake_mms        mars chocolate             42
##   calories calories_fat total_fat_g saturated_fat_g cholesterol_mg
## 1      190          70           8               5              5
## 2      140          10           1               0              0
## 3      140           0           0               0              0
## 4      160         160           0               0              0
## 5      130           0           0               0              0
## 6      210         100          10               6              5
##   sodium_mg total_carb_g dietary_fiber_g sugars_g protein_g
## 1        30           28             0.5       27         2
## 2        40           30             0.0       16         1
## 3         0           36             0.0       29         1
## 4        75           39             0.0       32         0
## 5        35           31             0.0       24         1
## 6        40           29             0.0       28         2
##   primary_ingredient total_fat_per_serv saturated_fat_per_serv
## 1          chocolate         0.20000000              0.1250000
## 2              syrup         0.02380952              0.0000000
## 3              sugar         0.00000000              0.0000000
## 4              sugar         0.00000000              0.0000000
## 5              syrup         0.00000000              0.0000000
## 6          chocolate         0.23809524              0.1428571
##   cholesterol_per_serv sodium_per_serv total_carb_per_serv
## 1            0.1250000        0.750000           0.7000000
## 2            0.0000000        0.952381           0.7142857
## 3            0.0000000        0.000000           0.9230769
## 4            0.0000000        1.829268           0.9512195
## 5            0.0000000        0.875000           0.7750000
## 6            0.1190476        0.952381           0.6904762
##   dietary_fiber_per_serv sugars_per_serv protein_per_serv       PC1
## 1                 0.0125       0.6750000       0.05000000 -1.360340
## 2                 0.0000       0.3809524       0.02380952  0.483663
## 3                 0.0000       0.7435897       0.02564103  2.292019
## 4                 0.0000       0.7804878       0.00000000  2.350462
## 5                 0.0000       0.6000000       0.02500000  1.259095
## 6                 0.0000       0.6666667       0.04761905 -1.326783
##          PC2        PC3        PC4        PC5         PC6        PC7
## 1  1.2253820 -0.2491928 -0.2812836  0.2172947  0.34206721  0.1100176
## 2 -1.6948183  1.3240001 -0.8875114 -0.2790751 -0.28996199  0.3795090
## 3  0.5537819  0.2028140  0.4763461  0.2948282  0.07010778 -0.3638014
## 4 -0.2731776 -1.5442805  0.1312974  0.2260422 -0.41877992 -0.3298129
## 5 -0.6934915  0.3911153 -0.1329304  0.2391956 -0.11518484  0.3493761
## 6  1.0001694 -0.4836604 -0.7715705  0.2412477  1.10978569  0.1913661
##           PC8
## 1 -0.05937806
## 2 -0.02460115
## 3  0.11301354
## 4  0.09024576
## 5 -0.18264299
## 6  0.13902258
```

That's better. Now we can visualize our PCA results to see how it separates different candy types by their

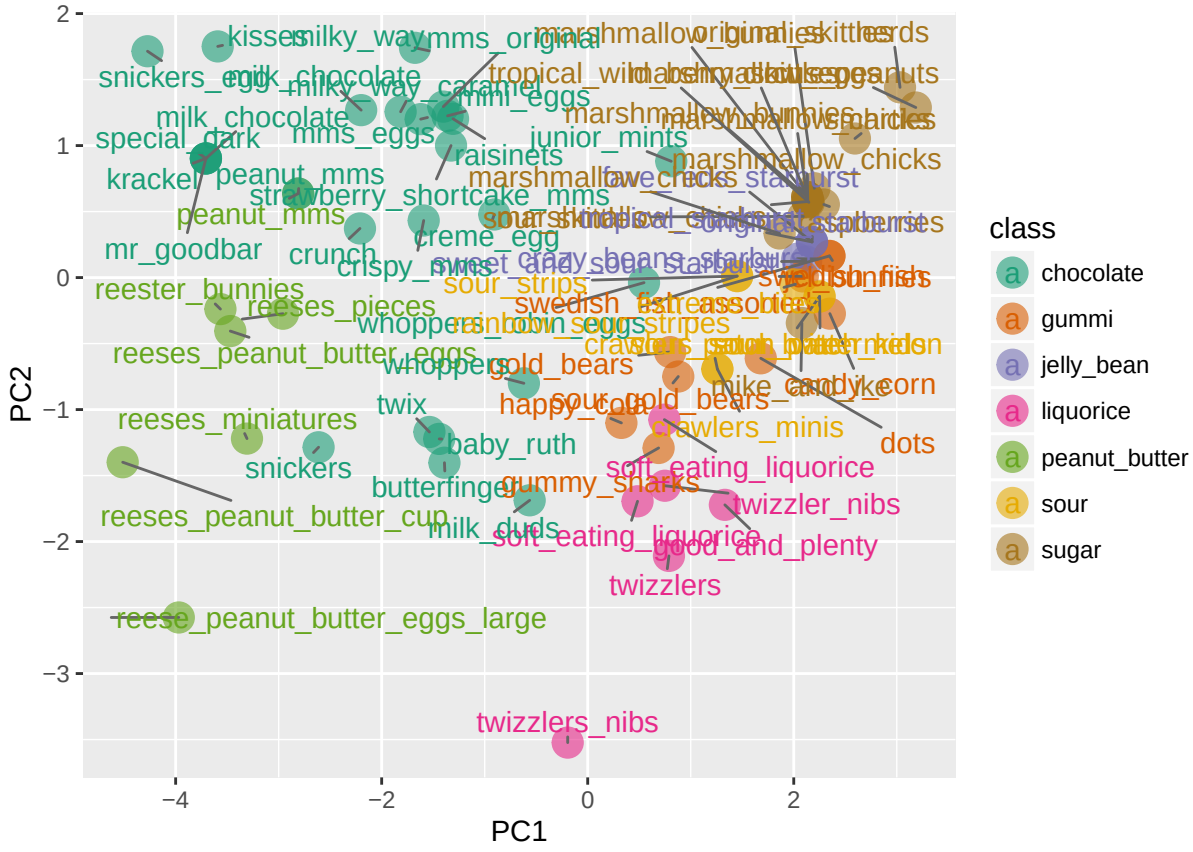
nutritional lable information

```
p <- ggplot(pca_scores, aes(PC1, PC2, colour=class))
p + geom_point(size=5, alpha=0.6) + geom_text(data=pca_scores, aes(x=PC1, y=PC2, label=name)) + scale_c
```



The overlap of the labels with the data isn't good, so let's use ggrepel to fix that

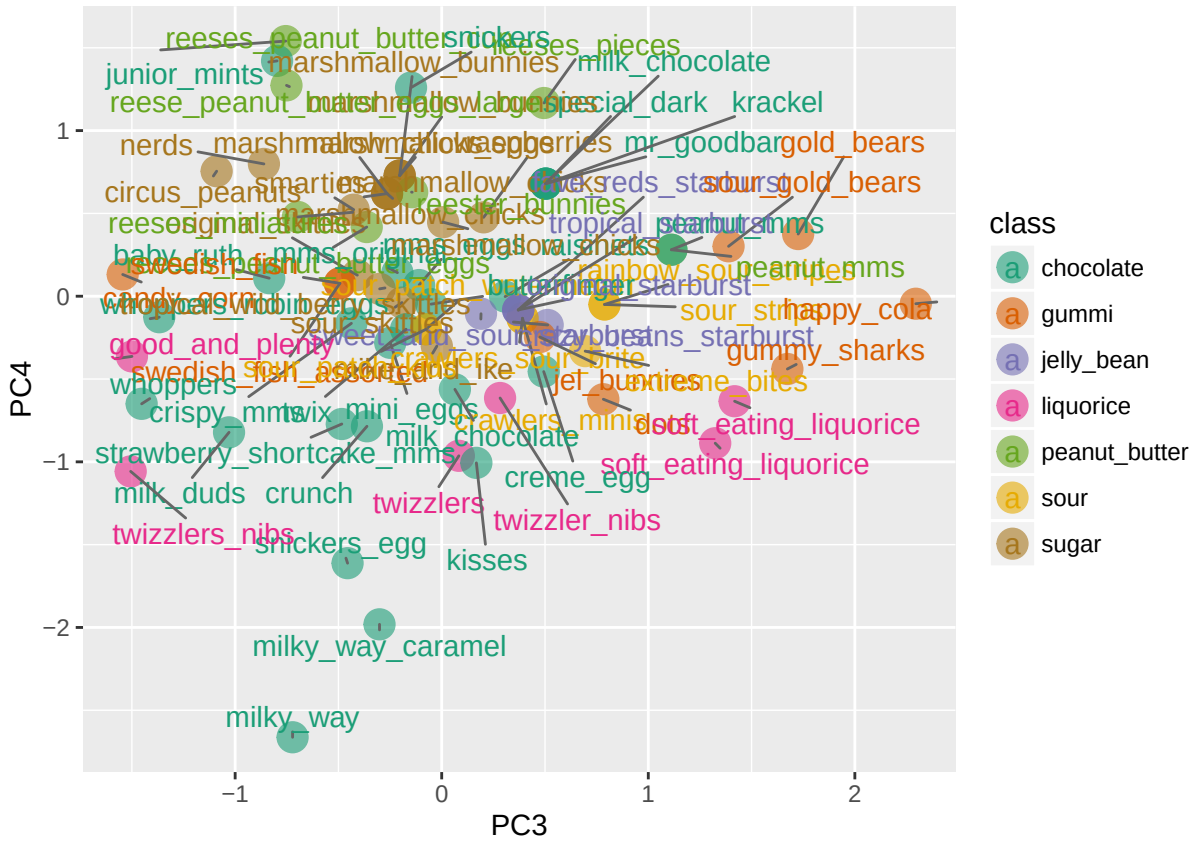
```
p <- ggplot(pca_scores, aes(PC1, PC2, colour=class))
p + geom_point(size=5, alpha=0.6) + geom_text_repel(data=pca_scores, aes(x=PC1, y=PC2, label=name)) + s
```



Nice! The PCA does a good job of separating by groups we know to exist, like chocolate, peanut butter, gummi, helly bean, liquorice, sour, and sugar candies.

We can also see what PC3 and PC4 look like too

```
p <- ggplot(pca_scores, aes(PC3, PC4, colour=class))
p + geom_point(size=5, alpha=0.6) + geom_text_repel(data=pca_scores, aes(x=PC3, y=PC4, label=name)) + s
```



Hierarchical Clustering

As mentioned above, it is important to scale our data (column means=0 and variance=1) so that scaling effects are not detected, just patterns of variance between variables. Let's use the scale function here to scale our data before performing hierarchical clustering. The column names in the object data currently correspond to nutrition information. So, the samples to be clustered will be the nutrition informtion itself. But after scaling the nutrition information, let's transpose that dataset and analyze a scaled matrix where the candies are the columns, so that we will cluster by candy type. We will analyze the two datasets, `scaled_nutrition` and `scaled_candies` in parallel.

```
scaled_nutrition <- scale(data[17:24])
scaled_candies <- scale(t(scaled_nutrition))
colnames(scaled_candies) <- as.matrix(data[2])

head(scaled_nutrition)
```

```
##      total_fat_per_serv saturated_fat_per_serv cholesterol_per_serv
## [1,]          0.7634841              0.9663872            1.1503643
## [2,]         -0.6883584             -0.9029575           -0.5626088
## [3,]         -0.8845533             -0.9029575           -0.5626088
## [4,]         -0.8845533             -0.9029575           -0.5626088
## [5,]         -0.8845533             -0.9029575           -0.5626088
## [6,]          1.0773960              1.2334364            1.0687941
##      sodium_per_serv total_carb_per_serv dietary_fiber_per_serv
## [1,]     -0.22223971         -0.59177589              0.2390135
```

```
## [2,]     -0.01984752         -0.47038623             -0.6266729
## [3,]     -0.97228137          1.30377031             -0.6266729
## [4,]      0.85708852          1.54290566             -0.6266729
## [5,]     -0.09723277          0.04551981             -0.6266729
## [6,]     -0.01984752         -0.67270233             -0.6266729
##      sugars_per_serv protein_per_serv
## [1,]       0.4539947        0.4125308
## [2,]      -1.8929612       -0.3875676
## [3,]       1.0014472       -0.3316167
## [4,]       1.2959509       -1.1149298
## [5,]      -0.1446216       -0.3511995
## [6,]       0.3874818        0.3397946
```

```
head(scaled_candies)
```

```
##                         mini_eggs soft_eating_liquorice raspberries
## total_fat_per_serv      0.6247621            0.01015079  -0.7143345
## saturated_fat_per_serv  0.9701606           -0.38152273  -0.7349530
## cholesterol_per_serv    1.2833416            0.23966130  -0.3536552
## sodium_per_serv        -1.0532188            1.23027675  -0.8126176
## total_carb_per_serv    -1.6822740            0.40798048   1.7372779
## dietary_fiber_per_serv -0.2680353            0.12273539  -0.4254271
##                        candy_corn crawlers_minis strawberry_shortcake_mms
## total_fat_per_serv     -0.7657406     -1.2313422                0.9686218
## saturated_fat_per_serv -0.7826166     -1.2823811                1.1759707
## cholesterol_per_serv   -0.4705286     -0.3385209                0.9571914
## sodium_per_serv         0.8312848      0.9520672               -0.4894129
## total_carb_per_serv     1.4601555      1.3479508               -1.3569368
## dietary_fiber_per_serv -0.5292732     -0.5161844               -1.2957722
##                        milk_chocolate  milk_duds marshmallow_chicks
## total_fat_per_serv          0.6900816  0.5508796         -0.7670138
## saturated_fat_per_serv      0.6346596  0.6135935         -0.7880509
## cholesterol_per_serv        0.2653056 -0.5088880         -0.3990132
## sodium_per_serv            -0.6119204  2.0490322         -0.4590349
## total_carb_per_serv        -1.5293963 -0.6148121          1.0939546
## dietary_fiber_per_serv      1.4187958 -0.5806734         -0.4722420
##                        crazy_beans_starburst  creme_egg   mms_eggs
## total_fat_per_serv                -0.58098095  0.7934789  0.7089045
## saturated_fat_per_serv            -0.61223115  1.2553936  0.7024987
## cholesterol_per_serv              -0.03432204  0.5928605  1.0226337
## sodium_per_serv                   -0.72994244 -0.9790771 -1.1962131
## total_carb_per_serv                1.71969022 -0.9963272 -1.5514798
## dietary_fiber_per_serv            -0.14310228 -1.1330215  0.9447997
##                        gold_bears original_skittles crawlers_sour_brite
## total_fat_per_serv     -0.6517637        -0.4290930          -1.2313422
## saturated_fat_per_serv -0.6761136        -0.1649326          -1.2823811
## cholesterol_per_serv   -0.2258115        -0.4144500          -0.3385209
## sodium_per_serv        -0.7678333        -0.5951565           0.9520672
## total_carb_per_serv     0.8021868         1.7164702           1.3479508
## dietary_fiber_per_serv -0.3105722        -0.4869597          -0.5161844
##                        reeses_pieces milky_way_caramel  raisinets
## total_fat_per_serv         0.4032352         0.3556871  0.4621047
## saturated_fat_per_serv     1.2972586         0.6664809  0.7496776
## cholesterol_per_serv      -0.8213735         1.9782369  1.0744053
```

```
## sodium_per_serv           -0.2495609        -0.2344105 -1.5043053
## total_carb_per_serv       -1.3540784        -1.0780661 -1.2759934
## dietary_fiber_per_serv     0.5113097        -0.9672375  0.9974636
##                         circus_peanuts sweet_and_sour_starburst
## total_fat_per_serv         -0.5940916               -0.6433016
## saturated_fat_per_serv     -0.6072432               -0.6711654
## cholesterol_per_serv       -0.3640293               -0.1558821
## sodium_per_serv            -0.4687186               -0.3976031
## total_carb_per_serv         1.4367796                1.7296733
## dietary_fiber_per_serv     -0.4098097               -0.2528743
##                         reeses_peanut_butter_cup whoppers_robin_eggs
## total_fat_per_serv                   0.39908807        -0.002694724
## saturated_fat_per_serv              -0.06731952         1.184399770
## cholesterol_per_serv                -0.43154124        -1.026618608
## sodium_per_serv                      0.94956668         0.730947067
## total_carb_per_serv                 -1.66084978         0.774338434
## dietary_fiber_per_serv               0.99689223        -1.119259034
##                          twizzlers      nerds sour_patch_watermelon
## total_fat_per_serv     -0.3837281 -0.5516585            -0.6601577
## saturated_fat_per_serv -0.5319207 -0.5653804            -0.6832339
## cholesterol_per_serv   -0.1164805 -0.3116231            -0.2564865
## sodium_per_serv         1.9774459 -0.6170669             0.0135461
## total_carb_per_serv     0.8851214  1.1448908             2.1041687
## dietary_fiber_per_serv -0.1946791 -0.3593880            -0.3368135
##                          crispy_mms snickers_egg swedish_fish_assorted
## total_fat_per_serv      0.04211436    0.3177629           -0.69934765
## saturated_fat_per_serv  0.46741840    0.3185124           -0.72065503
## cholesterol_per_serv    1.21379022    1.7602410           -0.32661819
## sodium_per_serv         0.21708791   -0.1153662            0.02609201
## total_carb_per_serv    -1.48693012   -1.6140235            1.65399497
## dietary_fiber_per_serv  1.11976952    0.3798587           -0.40078802
##                         sour_skittles rainbow_sour_stripes peanut_mms
## total_fat_per_serv         -0.4058366           -0.3878780  0.7742583
## saturated_fat_per_serv     -0.1181373           -0.2933576  0.2556515
## cholesterol_per_serv       -0.3898887           -0.3615561  0.5893067
## sodium_per_serv            -0.5866977           -1.1950542 -0.8239140
## total_carb_per_serv         1.9309141            2.1723185 -1.5315691
## dietary_fiber_per_serv     -0.4688596           -0.4918975  0.5472760
##                           baby_ruth junior_mints marshmallow_bunnies
## total_fat_per_serv       0.72913244   -0.6840201          -0.7898629
## saturated_fat_per_serv   0.72312786   -0.2966324          -0.8101718
## cholesterol_per_serv    -0.92908588   -1.0685705          -0.4346016
## sodium_per_serv          1.61547265   -0.6264816          -0.5418110
## total_carb_per_serv     -1.31973972    0.8249680           1.1741231
## dietary_fiber_per_serv  -0.04697188    1.0970156          -0.5052954
##                         fave_reds_starburst reeses_peanut_butter_eggs
## total_fat_per_serv               -0.5786255                 0.9417943
## saturated_fat_per_serv           -0.6056776                 0.7235978
## cholesterol_per_serv             -0.1054048                -0.2183600
## sodium_per_serv                  -0.7075755                 0.4499203
## total_carb_per_serv               1.7252235                -1.8671754
## dietary_fiber_per_serv           -0.1995715                 0.5027051
##                         butterfinger milk_chocolate special_dark mr_goodbar
## total_fat_per_serv         0.8437179      1.0226564    0.6900816  0.6900816
```

```
## saturated_fat_per_serv    0.6282753      1.3720806    0.6346596  0.6346596
## cholesterol_per_serv     -0.8273575      0.7798505    0.2653056  0.2653056
## sodium_per_serv           1.1768329     -0.9247076   -0.6119204 -0.6119204
## total_carb_per_serv      -0.5964164     -1.4965845   -1.5293963 -1.5293963
## dietary_fiber_per_serv    0.1828065     -0.1775223    1.4187958  1.4187958
##                            snickers       twix marshmallow_chicks
## total_fat_per_serv      0.573977821  1.1608674         -0.7670138
## saturated_fat_per_serv  0.005825866  0.9295415         -0.7880509
## cholesterol_per_serv   -0.866524822 -0.7619254         -0.3990132
## sodium_per_serv         0.864832622  0.8592227         -0.4590349
## total_carb_per_serv    -1.515933517 -0.9116942          1.0939546
## dietary_fiber_per_serv  0.891065641 -0.8327969         -0.4722420
##                        marshmallow_bunnies   whoppers twizzlers_nibs
## total_fat_per_serv              -0.7898629  0.4020778    -0.35114768
## saturated_fat_per_serv          -0.8101718  1.6240890    -0.37555585
## cholesterol_per_serv            -0.4346016 -0.7732742    -0.27563274
## sodium_per_serv                 -0.5418110  1.2932608     2.38867861
## total_carb_per_serv              1.1741231 -0.2884618    -0.01790401
## dietary_fiber_per_serv          -0.5052954 -0.8426784    -0.31735953
##                        swedish_fish        dots twizzler_nibs jel_bunnies
## total_fat_per_serv      -0.69934765 -0.55235711    -0.4879646 -0.59022754
## saturated_fat_per_serv  -0.72065503 -0.59081639    -0.5526435 -0.61940310
## cholesterol_per_serv    -0.32661819  0.12041018    -0.2878586 -0.07986019
## sodium_per_serv          0.02609201  0.04799853     1.8098892 -0.54495639
## total_carb_per_serv      1.65399497  2.27905434     1.1283863  2.03543739
## dietary_fiber_per_serv  -0.40078802 -0.01346450    -0.3984298 -0.18141873
##                        gummy_sharks good_and_plenty mike_and_ike
## total_fat_per_serv      -0.49588358      -0.7564517   -0.6852924
## saturated_fat_per_serv  -0.52780342      -0.7740060   -0.7109985
## cholesterol_per_serv     0.06248932      -0.4493752   -0.2356156
## sodium_per_serv          0.15869446       2.0214855    0.2397959
## total_carb_per_serv      1.00582544       0.9411548    2.0973638
## dietary_fiber_per_serv  -0.04862190      -0.5104807   -0.3250973
##                        sour_patch_kids sour_strips     kisses    krackel
## total_fat_per_serv          -0.6601577  -0.3878780  0.5640830  0.6900816
## saturated_fat_per_serv      -0.6832339  -0.2933576  0.6564900  0.6346596
## cholesterol_per_serv        -0.2564865  -0.3615561  1.5044583  0.2653056
## sodium_per_serv              0.0135461  -1.1950542 -0.6715016 -0.6119204
## total_carb_per_serv          2.1041687   2.1723185 -1.6024616 -1.5293963
## dietary_fiber_per_serv      -0.3368135  -0.4918975  0.2151779  1.4187958
##                        reester_bunnies marshmallow_chicks  happy_cola
## total_fat_per_serv           0.9502916         -0.7670138 -0.37560637
## saturated_fat_per_serv       0.5426627         -0.7880509 -0.39881442
## cholesterol_per_serv        -0.1726143         -0.3990132  0.03037146
## sodium_per_serv              0.2429543         -0.4590349 -0.48623306
## total_carb_per_serv         -1.8418005          1.0939546  0.26147177
## dietary_fiber_per_serv       0.6384235         -0.4722420 -0.05041450
##                        mms_original   smarties soft_eating_liquorice
## total_fat_per_serv        0.3826890 -0.5466747          -0.091906779
## saturated_fat_per_serv    0.7450218 -0.5639333          -0.189137192
## cholesterol_per_serv      1.1055817 -0.2447711           0.155368005
## sodium_per_serv          -1.3934494 -0.6289418           0.144791434
## total_carb_per_serv      -1.4125001  0.9800433           1.284414721
## dietary_fiber_per_serv    1.0179193 -0.3048472          -0.004264772
```

```
##                         tropical_wild_berry_skittles sour_gold_bears
## total_fat_per_serv                         -0.4190331      -0.7622266
## saturated_fat_per_serv                     -0.1428986      -0.7873358
## cholesterol_per_serv                       -0.4037264      -0.3229913
## sodium_per_serv                            -0.5926242      -0.3827465
## total_carb_per_serv                         1.8237862       1.1358232
## dietary_fiber_per_serv                     -0.4795229      -0.4103952
##                         peanut_mms extreme_bites     crunch   milky_way
## total_fat_per_serv       0.7742583  -0.542000238  0.9290599  0.04530828
## saturated_fat_per_serv   0.2556515  -0.573287073  1.1363936  0.42777271
## cholesterol_per_serv     0.5893067   0.005299495  0.8974378  2.23277955
## sodium_per_serv         -0.8239140  -0.691136354  0.1140189 -0.11943278
## total_carb_per_serv     -1.5315691   2.122498274 -1.5621533 -0.79349944
## dietary_fiber_per_serv   0.5472760  -0.103608265 -0.2493862 -0.85756236
##                         marshmallow_eggs tropical_starburst
## total_fat_per_serv           -0.7898629         -0.5786255
## saturated_fat_per_serv       -0.8101718         -0.6056776
## cholesterol_per_serv         -0.4346016         -0.1054048
## sodium_per_serv              -0.5418110         -0.7075755
## total_carb_per_serv           1.1741231          1.7252235
## dietary_fiber_per_serv       -0.5052954         -0.1995715
##                         reeses_miniatures reese_peanut_butter_eggs_large
## total_fat_per_serv              0.7648285                       0.5073612
## saturated_fat_per_serv          0.1521519                      -0.1210199
## cholesterol_per_serv           -0.3197383                      -0.6691984
## sodium_per_serv                 1.1163536                       1.3244299
## total_carb_per_serv            -1.7301019                      -1.4970192
## dietary_fiber_per_serv          0.2747974                       0.4352581
##                         original_starburst marshmallow_chicks
## total_fat_per_serv             -0.5786255         -0.8113357
## saturated_fat_per_serv         -0.6056776         -0.8373981
## cholesterol_per_serv           -0.1054048         -0.3554263
## sodium_per_serv                -0.7075755         -0.4297861
## total_carb_per_serv             1.7252235          0.9211802
## dietary_fiber_per_serv         -0.1995715         -0.4461482
```

The way similarity between variables is calculated is through correlation. Let's use the cor function to create a pairwise correlation matirx for our data, the correlation of all variable to each other. Let's be conservative and instead of using a parametric correlation parameter like "pearson", we'll use a non-parametric one, like "spearman", which makes no assumptions about the distributions of our data

```
corell_nutrition <- cor(scaled_nutrition, method="spearman")
corell_candies <- cor(scaled_candies, method="spearman")

head(corell_nutrition)
```

```
##                         total_fat_per_serv saturated_fat_per_serv
## total_fat_per_serv               1.0000000              0.9368297
## saturated_fat_per_serv           0.9368297              1.0000000
## cholesterol_per_serv             0.7231604              0.7391776
## sodium_per_serv                  0.5766610              0.5181643
## total_carb_per_serv             -0.8333848             -0.7492149
## dietary_fiber_per_serv           0.8152061              0.7129886
```

```
##                         cholesterol_per_serv sodium_per_serv
## total_fat_per_serv                 0.7231604       0.5766610
## saturated_fat_per_serv             0.7391776       0.5181643
## cholesterol_per_serv               1.0000000       0.2921460
## sodium_per_serv                    0.2921460       1.0000000
## total_carb_per_serv               -0.6637718      -0.5644365
## dietary_fiber_per_serv             0.6441498       0.4431272
##                         total_carb_per_serv dietary_fiber_per_serv
## total_fat_per_serv               -0.8333848              0.8152061
## saturated_fat_per_serv           -0.7492149              0.7129886
## cholesterol_per_serv             -0.6637718              0.6441498
## sodium_per_serv                  -0.5644365              0.4431272
## total_carb_per_serv               1.0000000             -0.7332656
## dietary_fiber_per_serv           -0.7332656              1.0000000
##                         sugars_per_serv protein_per_serv
## total_fat_per_serv          -0.5303592        0.7249913
## saturated_fat_per_serv      -0.4071991        0.6302843
## cholesterol_per_serv        -0.2347752        0.5786847
## sodium_per_serv             -0.5220287        0.4196859
## total_carb_per_serv          0.7290826       -0.8234517
## dietary_fiber_per_serv      -0.3983687        0.7196518
```

```
head(corell_candies)
```

```
##                           mini_eggs soft_eating_liquorice raspberries
## mini_eggs                  1.0000000           -0.54761905 -0.21428571
## soft_eating_liquorice     -0.5476190            1.00000000 -0.07142857
## raspberries               -0.2142857           -0.07142857  1.00000000
## candy_corn                -0.4523810            0.04761905  0.40476190
## crawlers_minis            -0.7142857            0.54761905  0.50000000
## strawberry_shortcake_mms   0.9047619           -0.57142857 -0.40476190
##                           candy_corn crawlers_minis
## mini_eggs                 -0.45238095     -0.7142857
## soft_eating_liquorice      0.04761905      0.5476190
## raspberries                0.40476190      0.5000000
## candy_corn                 1.00000000      0.7380952
## crawlers_minis             0.73809524      1.0000000
## strawberry_shortcake_mms -0.52380952     -0.7380952
##                           strawberry_shortcake_mms milk_chocolate
## mini_eggs                                9.0047619      0.4523810
## soft_eating_liquorice                   -0.5714286     -0.2857143
## raspberries                             -0.4047619     -0.5476190
## candy_corn                              -0.5238095     -0.6666667
## crawlers_minis                          -0.7380952     -0.8809524
## strawberry_shortcake_mms                 1.0000000      0.4047619
##                           milk_duds marshmallow_chicks
## mini_eggs                 0.1666667         -0.3571429
## soft_eating_liquorice     0.1904762          0.1666667
## raspberries              -0.9047619          0.8333333
## candy_corn               -0.1904762          0.5952381
## crawlers_minis           -0.3571429          0.8095238
## strawberry_shortcake_mms  0.3333333         -0.5000000
##                           crazy_beans_starburst  creme_egg   mms_eggs
## mini_eggs                           -0.07142857  0.6904762  0.7142857
```

```
## soft_eating_liquorice              -0.38095238 -0.2380952 -0.3095238
## raspberries                         0.64285714 -0.2380952 -0.2619048
## candy_corn                          0.76190476 -0.7142857 -0.5000000
## crawlers_minis                      0.30952381 -0.5476190 -0.7619048
## strawberry_shortcake_mms           -0.26190476  0.8333333  0.4761905
##                           gold_bears original_skittles crawlers_sour_brite
## mini_eggs                -0.14285714        0.09523810          -0.7142857
## soft_eating_liquorice     0.26190476       -0.54761905           0.5476190
## raspberries               0.80952381        0.47619048           0.5000000
## candy_corn               -0.02380952        0.59523810           0.7380952
## crawlers_minis            0.28571429        0.14285714           1.0000000
## strawberry_shortcake_mms -0.40476190        0.07142857          -0.7380952
##                          reeses_pieces milky_way_caramel  raisinets
## mini_eggs                   0.30952381         0.8809524  0.7142857
## soft_eating_liquorice      -0.07142857        -0.1428571 -0.3809524
## raspberries                -0.57142857        -0.4523810 -0.1190476
## candy_corn                 -0.92857143        -0.5714286 -0.4761905
## crawlers_minis             -0.73809524        -0.6190476 -0.7619048
## strawberry_shortcake_mms    0.42857143         0.8571429  0.4523810
##                          circus_peanuts sweet_and_sour_starburst
## mini_eggs                    -0.1904762               -0.2857143
## soft_eating_liquorice        -0.2380952               -0.1190476
## raspberries                   0.5476190                0.5714286
## candy_corn                    0.9047619                0.9285714
## crawlers_minis                0.5238095                0.5714286
## strawberry_shortcake_mms     -0.3809524               -0.4761905
##                          reeses_peanut_butter_cup whoppers_robin_eggs
## mini_eggs                               -0.1666667         -0.02380952
## soft_eating_liquorice                    0.3333333         -0.38095238
## raspberries                             -0.6428571         -0.04761905
## candy_corn                              -0.5238095          0.42857143
## crawlers_minis                          -0.3095238          0.09523810
## strawberry_shortcake_mms                -0.1190476          0.19047619
##                           twizzlers       nerds sour_patch_watermelon
## mini_eggs                -0.5476190  0.02380952           -0.45238095
## soft_eating_liquorice     0.8571429 -0.50000000            0.04761905
## raspberries              -0.0952381  0.61904762            0.40476190
## candy_corn                0.3809524  0.73809524            1.00000000
## crawlers_minis            0.5476190  0.26190476            0.73809524
## strawberry_shortcake_mms -0.6428571 -0.16666667           -0.52380952
##                           crispy_mms snickers_egg swedish_fish_assorted
## mini_eggs                 0.52380952    0.6666667           -0.45238095
## soft_eating_liquorice    -0.02380952   -0.1666667            0.04761905
## raspberries              -0.59523810   -0.4285714            0.40476190
## candy_corn               -0.35714286   -0.5476190            1.00000000
## crawlers_minis           -0.59523810   -0.7619048            0.73809524
## strawberry_shortcake_mms  0.33333333    0.4523810           -0.52380952
##                          sour_skittles rainbow_sour_stripes peanut_mms
## mini_eggs                   0.09523810         -0.04761905  0.4761905
## soft_eating_liquorice      -0.54761905         -0.23809524  0.1190476
## raspberries                 0.47619048          0.83333333 -0.2380952
## candy_corn                  0.59523810          0.23809524 -0.8333333
## crawlers_minis              0.14285714          0.33333333 -0.5714286
## strawberry_shortcake_mms    0.07142857         -0.07142857  0.4047619
```

```
##                           baby_ruth junior_mints marshmallow_bunnies
## mini_eggs                 0.04761905   -0.4285714         -0.33333333
## soft_eating_liquorice     0.11904762   -0.4761905          0.07142857
## raspberries              -0.85714286    0.2380952          0.90476190
## candy_corn               -0.50000000    0.4761905          0.54761905
## crawlers_minis           -0.35714286    0.1904762          0.71428571
## strawberry_shortcake_mms  0.35714286   -0.3571429         -0.52380952
##                          fave_reds_starburst reeses_peanut_butter_eggs
## mini_eggs                       -0.07142857                 0.4047619
## soft_eating_liquorice           -0.38095238                -0.1666667
## raspberries                      0.64285714                -0.6428571
## candy_corn                       0.76190476                -0.8809524
## crawlers_minis                   0.30952381                -0.8095238
## strawberry_shortcake_mms        -0.26190476                 0.5952381
##                          butterfinger milk_chocolate special_dark
## mini_eggs                  -0.1428571      0.8571429    0.4523810
## soft_eating_liquorice       0.3571429     -0.4523810   -0.2857143
## raspberries                -0.8095238     -0.4285714   -0.5476190
## candy_corn                 -0.4523810     -0.7857143   -0.6666667
## crawlers_minis             -0.2619048     -0.9285714   -0.8809524
## strawberry_shortcake_mms    0.1666667      0.8809524    0.4047619
##                          mr_goodbar    snickers       twix
## mini_eggs                 0.4523810 -0.09523810  0.3571429
## soft_eating_liquorice    -0.2857143  0.38095238  0.0952381
## raspberries              -0.5476190 -0.47619048 -0.7857143
## candy_corn               -0.6666667 -0.71428571 -0.6666667
## crawlers_minis           -0.8809524 -0.30952381 -0.5952381
## strawberry_shortcake_mms  0.4047619 -0.04761905  0.5952381
##                          marshmallow_chicks marshmallow_bunnies
## mini_eggs                       -0.3571429         -0.33333333
## soft_eating_liquorice            0.1666667          0.07142857
## raspberries                      0.8333333          0.90476190
## candy_corn                       0.5952381          0.54761905
## crawlers_minis                   0.8095238          0.71428571
## strawberry_shortcake_mms        -0.5000000         -0.52380952
##                             whoppers twizzlers_nibs swedish_fish
## mini_eggs                 0.07142857    -0.61904762  -0.45238095
## soft_eating_liquorice    -0.19047619     0.97619048   0.04761905
## raspberries              -0.57142857    -0.02380952   0.40476190
## candy_corn                0.14285714     0.21428571   1.00000000
## crawlers_minis           -0.14285714     0.61904762   0.73809524
## strawberry_shortcake_mms  0.38095238    -0.64285714  -0.52380952
##                                dots twizzler_nibs jel_bunnies gummy_sharks
## mini_eggs                -0.3571429   -0.61904762  -0.2857143  -0.52380952
## soft_eating_liquorice     0.3095238    0.97619048  -0.1190476   0.92857143
## raspberries               0.2380952   -0.02380952   0.5714286   0.21428571
## candy_corn                0.8333333    0.21428571   0.9285714  -0.02380952
## crawlers_minis            0.5714286    0.61904762   0.5714286   0.52380952
## strawberry_shortcake_mms -0.5476190   -0.64285714  -0.4761905  -0.59523810
##                          good_and_plenty mike_and_ike sour_patch_kids
## mini_eggs                     -0.6190476  -0.45238095     -0.45238095
## soft_eating_liquorice          0.4761905   0.04761905      0.04761905
## raspberries                    0.2619048   0.40476190      0.40476190
## candy_corn                     0.8571429   1.00000000      1.00000000
```

```
## crawlers_minis                 0.9047619   0.73809524      0.73809524
## strawberry_shortcake_mms      -0.6904762  -0.52380952     -0.52380952
##                          sour_strips     kisses    krackel reester_bunnies
## mini_eggs                -0.04761905  0.8571429  0.4523810       0.2380952
## soft_eating_liquorice    -0.23809524 -0.1666667 -0.2857143       0.0000000
## raspberries               0.83333333 -0.4523810 -0.5476190      -0.5000000
## candy_corn                0.23809524 -0.6904762 -0.6666667      -0.8571429
## crawlers_minis            0.33333333 -0.7857143 -0.8809524      -0.6666667
## strawberry_shortcake_mms -0.07142857  0.7619048  0.4047619       0.3571429
##                          marshmallow_chicks happy_cola mms_original
## mini_eggs                        -0.3571429 -0.1428571    0.7619048
## soft_eating_liquorice             0.1666667  0.5000000   -0.4761905
## raspberries                       0.8333333  0.4523810   -0.2619048
## candy_corn                        0.5952381 -0.2619048   -0.3809524
## crawlers_minis                    0.8095238  0.0952381   -0.7619048
## strawberry_shortcake_mms         -0.5000000 -0.3333333    0.5238095
##                             smarties soft_eating_liquorice
## mini_eggs                 0.02380952            -0.4523810
## soft_eating_liquorice    -0.50000000             0.8333333
## raspberries               0.61904762             0.3571429
## candy_corn                0.73809524             0.1190476
## crawlers_minis            0.26190476             0.5238095
## strawberry_shortcake_mms -0.16666667            -0.5952381
##                          tropical_wild_berry_skittles sour_gold_bears
## mini_eggs                                  0.09523810      -0.4523810
## soft_eating_liquorice                     -0.54761905       0.7857143
## raspberries                                0.47619048       0.5238095
## candy_corn                                 0.59523810       0.1666667
## crawlers_minis                             0.14285714       0.6666667
## strawberry_shortcake_mms                   0.07142857      -0.6428571
##                          peanut_mms extreme_bites     crunch  milky_way
## mini_eggs                 0.4761905   -0.07142857  0.7142857  0.8095238
## soft_eating_liquorice     0.1190476   -0.38095238 -0.1666667 -0.2142857
## raspberries              -0.2380952    0.64285714 -0.7619048 -0.4523810
## candy_corn               -0.8333333    0.76190476 -0.6428571 -0.2142857
## crawlers_minis           -0.5714286    0.30952381 -0.7619048 -0.4285714
## strawberry_shortcake_mms  0.4047619   -0.26190476  0.8333333  0.8333333
##                          marshmallow_eggs tropical_starburst
## mini_eggs                     -0.33333333        -0.07142857
## soft_eating_liquorice          0.07142857        -0.38095238
## raspberries                    0.90476190         0.64285714
## candy_corn                     0.54761905         0.76190476
## crawlers_minis                 0.71428571         0.30952381
## strawberry_shortcake_mms      -0.52380952        -0.26190476
##                          reeses_miniatures reese_peanut_butter_eggs_large
## mini_eggs                      -0.09523810                     -0.09523810
## soft_eating_liquorice           0.47619048                      0.47619048
## raspberries                    -0.69047619                     -0.69047619
## candy_corn                     -0.57142857                     -0.57142857
## crawlers_minis                 -0.19047619                     -0.19047619
## strawberry_shortcake_mms        0.07142857                      0.07142857
##                          original_starburst marshmallow_chicks
## mini_eggs                      -0.07142857         -0.3571429
## soft_eating_liquorice          -0.38095238          0.1666667
```

```
## raspberries                  0.64285714          0.8333333
## candy_corn                   0.76190476          0.5952381
## crawlers_minis               0.30952381          0.8095238
## strawberry_shortcake_mms    -0.26190476         -0.5000000
```

Next, let's create a distance matrix using the as.dist funciton, which assigns distances between our samples using the correlation matrix we just calculated. There are many different methods to calculate distance, and the default is Eucledian, which we'll be using. We will take the absolute value of the correlation matirx (because strong negative as well as positive correlations indicate similarity) and also subtract that value from 1, as strong correlation (e.g., rho=1) means a closer distance (e.g., 0)

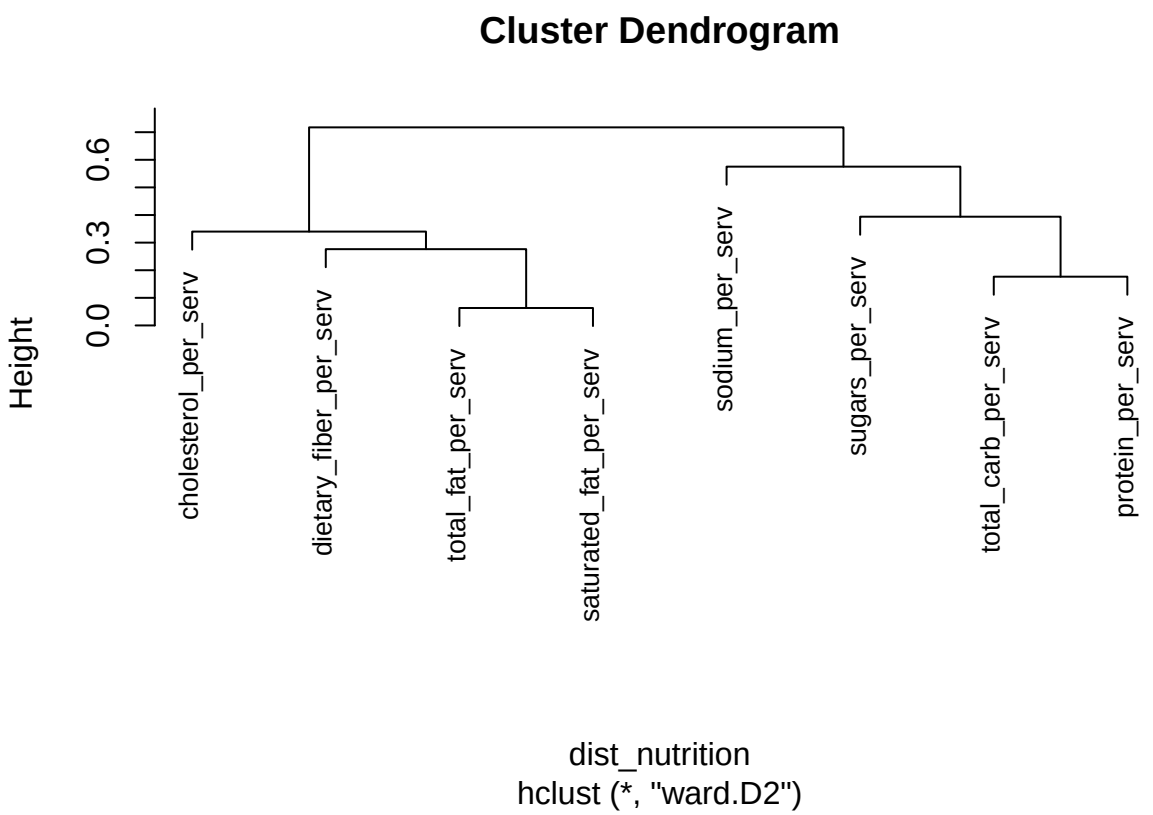
```
dist_nutrition <- as.dist(1-abs(corell_nutrition))
dist_candies <- as.dist(1-abs(corell_candies))
```

Finally, using our distance matrix, let's convert it to a dendrogram using the hclust function. Check out `?hclust`, as there are many different methods by which to cluster your results. For this example, we'll start by using the method `ward.D`

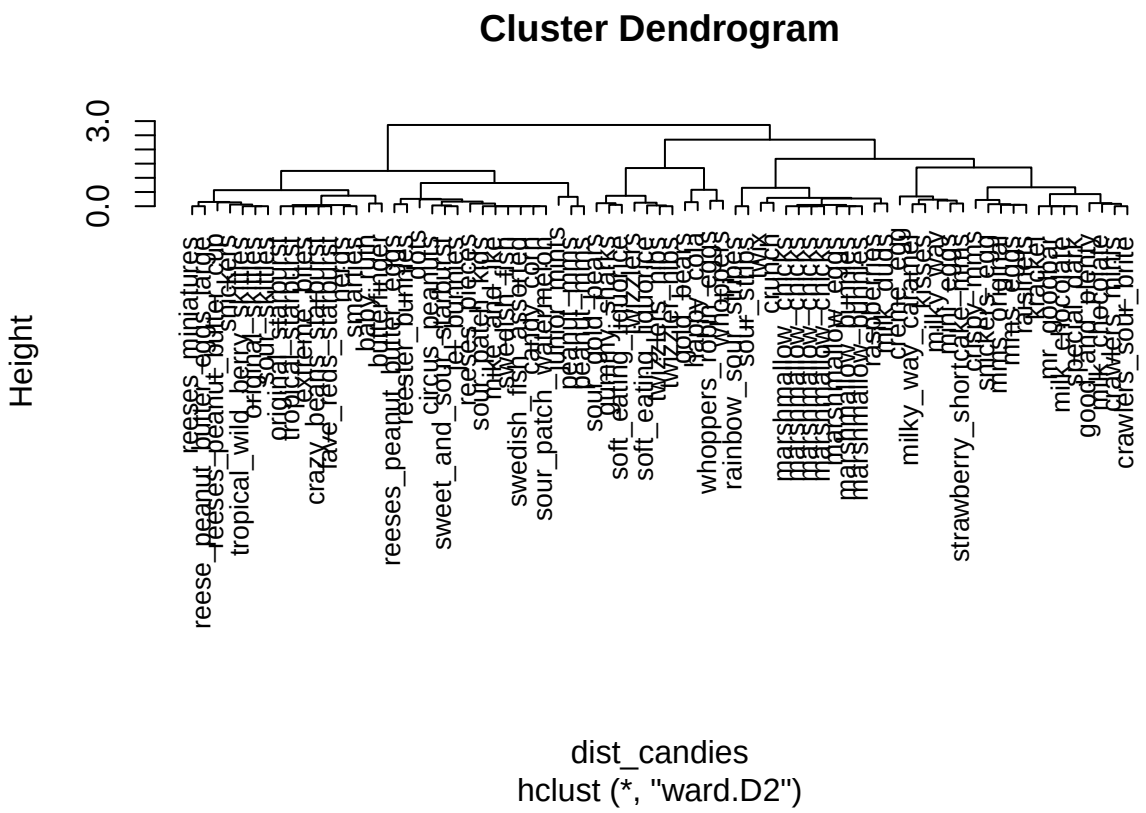
```
hc_nutrition <- hclust(dist_nutrition, method="ward.D2")
hc_candies <- hclust(dist_candies, method="ward.D2")
```

Let's plot out our dendrograms!

```
plot(hc_nutrition, cex=0.8)
```

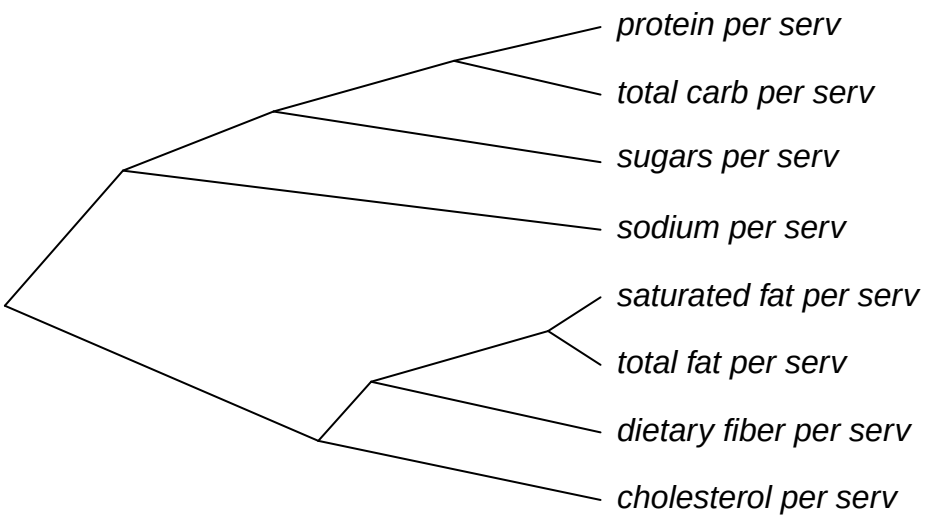


```
plot(hc_candies, cex=0.8)
```

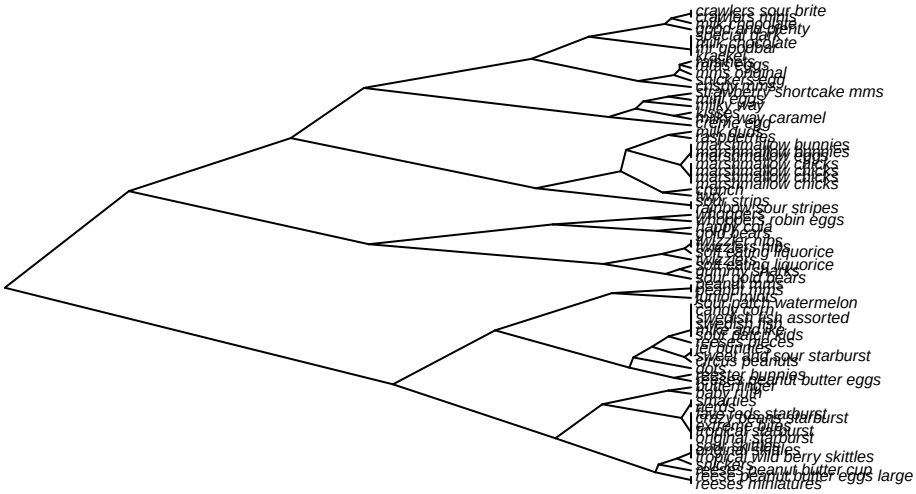


Using the packages ggdendro and ape you can plot out nicer looking dendrograms if you like. Use the "cex" option to change the size of the text if you need to

```
plot(as.phylo(hc_nutrition), type="cladogram", label.offset=0.01)
```




```
plot(as.phylo(hc_candies), type="cladogram", label.offset=0.01, cex=0.5)
```



Shape descriptors and allometry

Let's read in a datafile with basic shape information about individual candy pieces

```
shape_desc <- read.table("./shape_descriptors.txt", header=TRUE)
names(shape_desc)
```

```
## [1] "label"    "id"       "candy_no" "area"     "cm2"      "circ"
## [7] "ar"       "round"    "solid"
```

```
head(shape_desc)
```

```
##          label    id candy_no area       cm2  circ    ar round solid
## 1 ID_52_22.jpg id_52       22 5721 0.8362881 0.563 2.881 0.347 0.947
## 2 ID_18_15.jpg id_18       15 5964 0.8718095 0.824 1.451 0.689 0.973
## 3 ID_52_12.jpg id_52       12 7036 1.0285130 0.697 2.242 0.446 0.970
## 4 ID_52_14.jpg id_52       14 7239 1.0581873 0.663 2.267 0.441 0.954
## 5 ID_52_07.jpg id_52        7 7383 1.0792370 0.714 2.197 0.455 0.962
## 6 ID_71_10.jpg id_71       10 7433 1.0865459 0.828 1.579 0.633 0.973
```

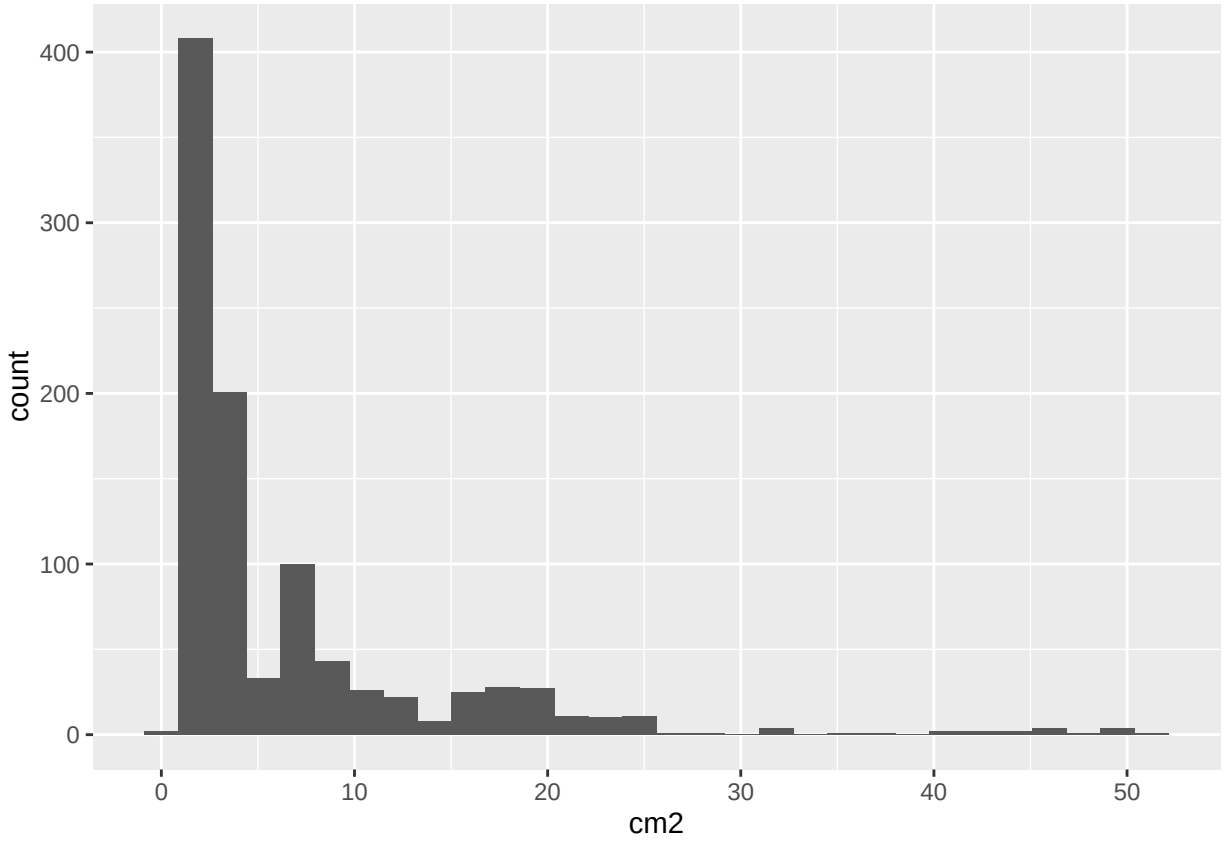
The variables in this dataset are:

- label: the name of the file measured
- id: the candy ID
- candy_no: for a given candy ID, the individual candy piece in question
- area: area in pixels
- cm2: area in cm^2
- circ: circularity, which is 4pi(area/perimeter^2). More lanky, jagged things have smaller circ values. More smoother, rounder things have higher circ values
- ar: aspect ratio. The ratio of the major to minor axes of the best fitted ellipse. Longer things have higher aspect ratios
- round: inversely related to ar
- solidity: the ratio of the area to convex area. More jagged things have lower solidity values

Let's first look at the distribution of cm2 values using a histogram

```
p <- ggplot(shape_desc, aes(x=cm2))
p + geom_histogram()
```

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

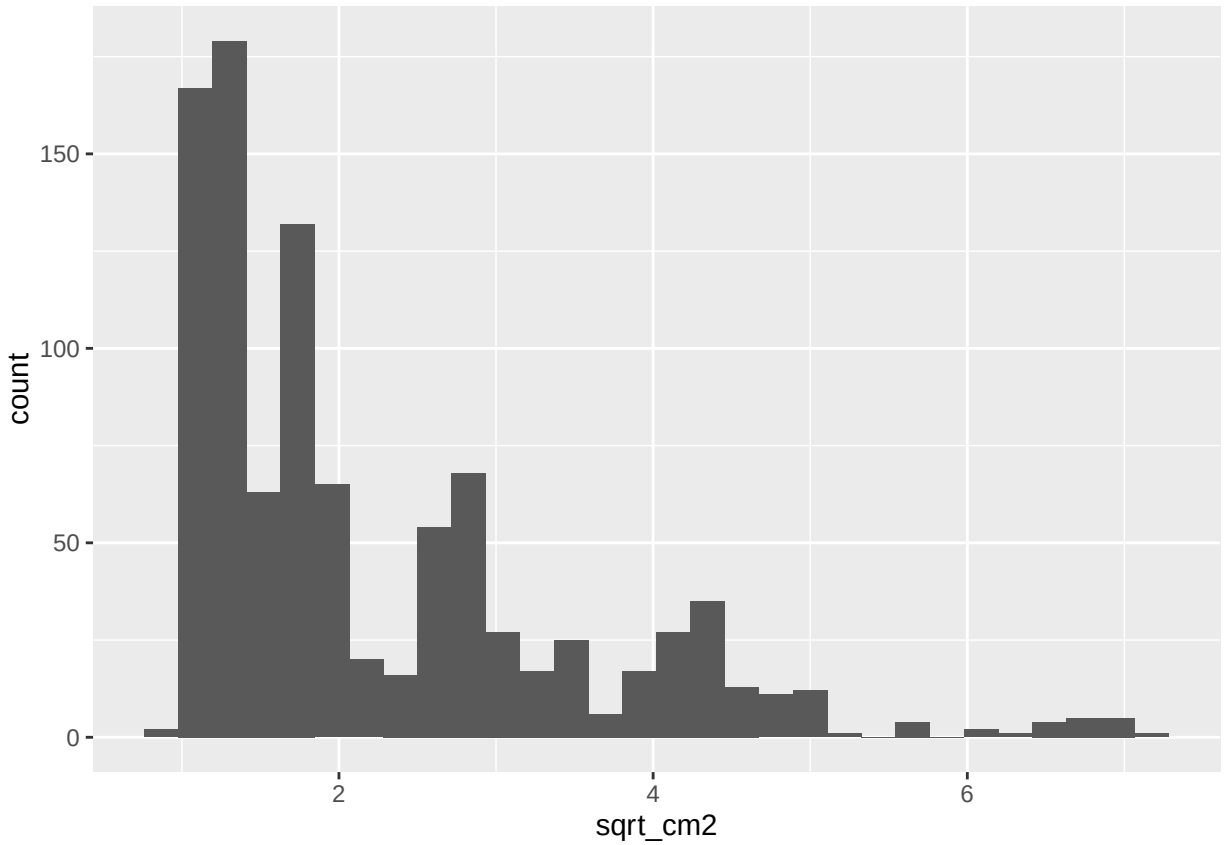


As is typical for area, the distribution is skewed. Let's create a transformed value for area by taking the square root and see how that looks

```
shape_desc$sqrt_cm2 <- sqrt(shape_desc$cm2)

p <- ggplot(shape_desc, aes(x=sqrt_cm2))
p + geom_histogram()
```

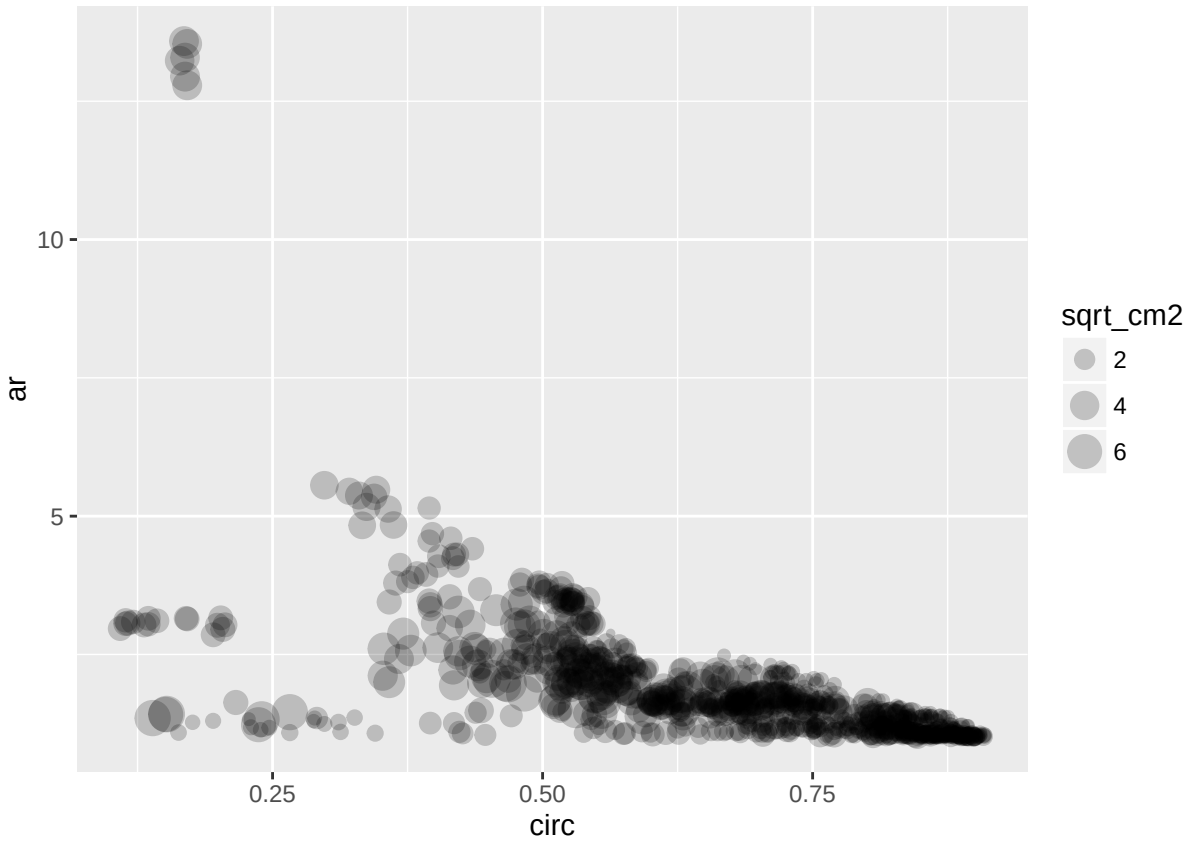
```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```



That's a little more normal looking, assuming discrete populations in our data (which there are). Let's use this square root value in the future.

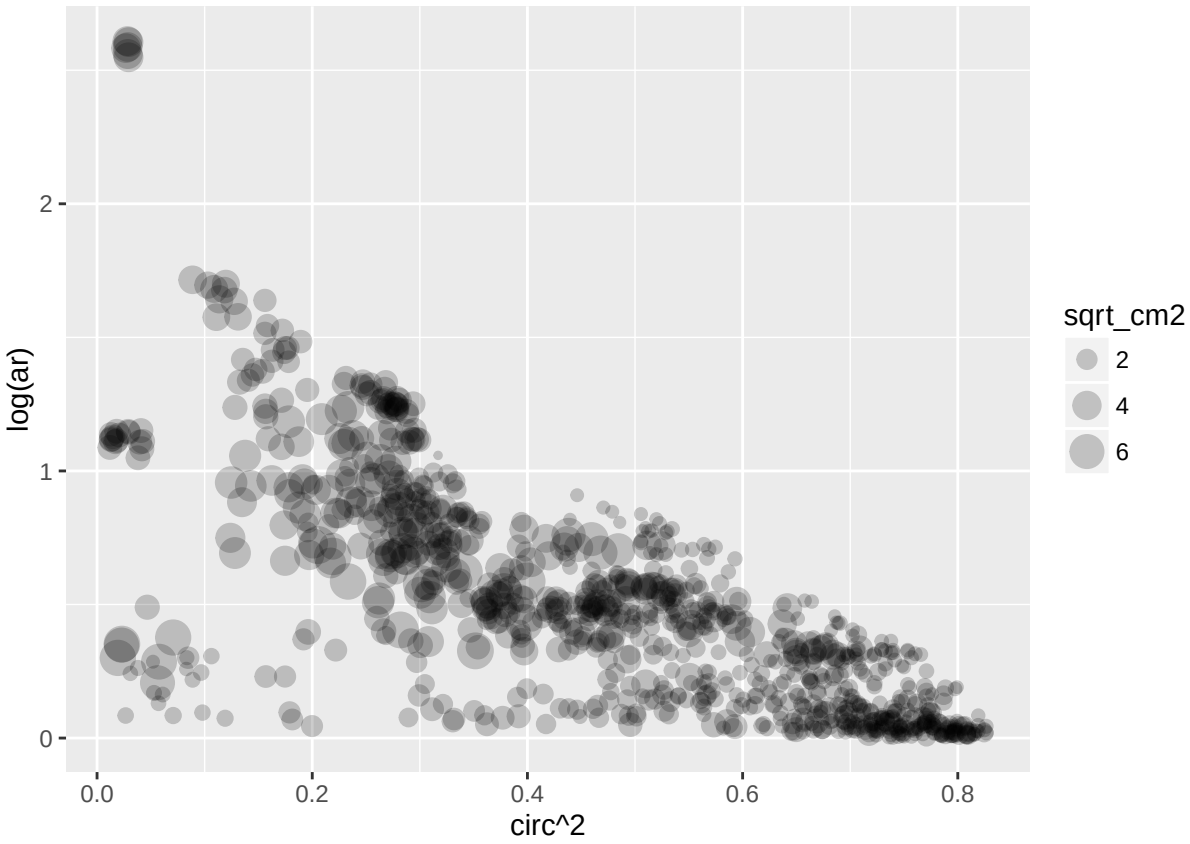
Let's get an idea for how our data looks and plot aspect ratio vs. circularity, making the size of the points `sqrt_cm2`

```
p <- ggplot(shape_desc, aes(x=circ, y=ar, size=sqrt_cm2))
p + geom_point(alpha=0.2)
```



Interesting! Let's get a little more separation and transform our variables. I tried squaring circ and taking the log of ar, but you can try your own transformations!

```
p <- ggplot(shape_desc, aes(x=circ^2, y=log(ar), size=sqrt_cm2))
p + geom_point(alpha=0.2)
```



Wouldn't it be nice if we had the other information for the candies associated with this dataset? Let's use the merge function to merge our nutritional label dataset with the shape descriptor dataset

Check out `?merge`

But the gist is that you input an `x` dataset that will be merged with a `y` dataset. Using `by.x` and `by.y` you can specify the columns by which to merge in each dataset. `all.x` or `all.y` or all set to `TRUE` will insure that every row specifed by `all` is included in the merge, even if there is no corresponding data in the other dataset to merge with. Let's merge our shape descriptor individual candy dataset `shape_desc` with the nutritional information for each of our candy types, `data`

```
mdata <- merge(x=shape_desc, y=data, by.x="id", by.y="id", all.x=TRUE)
summary(mdata)
```

```
##        id               label        candy_no          area
##  id_16  : 50   ID_01_01.jpg:  1   Min.   : 1.00   Min.   :  5721
##  id_14  : 30   ID_01_02.jpg:  1   1st Qu.: 5.00   1st Qu.: 10825
##  id_52  : 30   ID_01_03.jpg:  1   Median : 9.00   Median : 20989
##  id_64  : 28   ID_01_04.jpg:  1   Mean   :10.73   Mean   : 44678
##  id_05  : 27   ID_01_05.jpg:  1   3rd Qu.:15.00   3rd Qu.: 53384
##  id_20  : 25   ID_01_06.jpg:  1   Max.   :50.00   Max.   :356531
##  (Other):789   (Other)     :973
##       cm2              circ              ar             round
##  Min.   : 0.8363   Min.   :0.1090   Min.   : 1.003   Min.   :0.0740
##  1st Qu.: 1.5824   1st Qu.:0.5490   1st Qu.: 1.137   1st Qu.:0.4860
##  Median : 3.0681   Median :0.7120   Median : 1.513   Median :0.6610
##  Mean   : 6.5310   Mean   :0.6737   Mean   : 1.817   Mean   :0.6624
##  3rd Qu.: 7.8035   3rd Qu.:0.8270   3rd Qu.: 2.058   3rd Qu.:0.8785
```

```
##  Max.   :52.1172   Max.   :0.9090   Max.   :13.587   Max.   :0.9970
##
##      solid           sqrt_cm2                                 name
##  Min.   :0.7120   Min.   :0.9145   reeses_pieces               : 50
##  1st Qu.:0.9200   1st Qu.:1.2579   good_and_plenty            : 30
##  Median :0.9560   Median :1.7516   original_skittles          : 30
##  Mean   :0.9385   Mean   :2.2339   tropical_wild_berry_skittles: 28
##  3rd Qu.:0.9720   3rd Qu.:2.7935   mms_original               : 25
##  Max.   :0.9880   Max.   :7.2192   (Other)                    :689
##                                    NA's                       :127
##       company              class     serving_size_g     calories
##  hershey  :215   chocolate    :217   Min.   : 7.00   Min.   : 25.0
##  wrigley  :167   sugar        :135   1st Qu.:40.00   1st Qu.:140.0
##  mars     : 99   gummi        :123   Median :40.00   Median :150.0
##  haribo   : 62   jelly_bean   :109   Mean   :39.22   Mean   :158.7
##  just_born: 60   peanut_butter:101   3rd Qu.:41.00   3rd Qu.:190.0
##  (Other)  :249   (Other)      :167   Max.   :45.00   Max.   :220.0
##  NA's     :127   NA's         :127   NA's   :127     NA's   :127
##   calories_fat     total_fat_g     saturated_fat_g cholesterol_mg
##  Min.   :  0.00   Min.   : 0.000   Min.   :0.000   Min.   : 0.000
##  1st Qu.:  0.00   1st Qu.: 0.000   1st Qu.:0.000   1st Qu.: 0.000
##  Median : 10.00   Median : 1.000   Median :0.500   Median : 0.000
##  Mean   : 31.95   Mean   : 3.639   Mean   :2.228   Mean   : 1.206
##  3rd Qu.: 70.00   3rd Qu.: 8.000   3rd Qu.:5.000   3rd Qu.: 0.000
##  Max.   :110.00   Max.   :13.000   Max.   :8.000   Max.   :10.000
##  NA's   :127      NA's   :127      NA's   :127     NA's   :127
##    sodium_mg       total_carb_g   dietary_fiber_g     sugars_g
##  Min.   :  0.00   Min.   : 6.00   Min.   :0.0000   Min.   : 6.00
##  1st Qu.: 10.00   1st Qu.:26.00   1st Qu.:0.0000   1st Qu.:21.00
##  Median : 20.00   Median :32.00   Median :0.0000   Median :24.00
##  Mean   : 34.19   Mean   :30.59   Mean   :0.3427   Mean   :23.83
##  3rd Qu.: 45.00   3rd Qu.:34.00   3rd Qu.:1.0000   3rd Qu.:27.00
##  Max.   :180.00   Max.   :38.00   Max.   :2.0000   Max.   :35.00
##  NA's   :127      NA's   :127     NA's   :127      NA's   :127
##    protein_g     primary_ingredient total_fat_per_serv
##  Min.   :0.000   chocolate:193      Min.   :0.00000
##  1st Qu.:0.000   dextrose :  9      1st Qu.:0.00000
##  Median :1.000   peanuts  :  6      Median :0.02703
##  Mean   :1.407   sugar    :484      Mean   :0.09263
##  3rd Qu.:3.000   syrup    :160      3rd Qu.:0.20455
##  Max.   :5.000   NA's     :127      Max.   :0.32353
##  NA's   :127                        NA's   :127
##  saturated_fat_per_serv cholesterol_per_serv sodium_per_serv
##  Min.   :0.00000        Min.   :0.00000      Min.   :0.0000
##  1st Qu.:0.00000        1st Qu.:0.00000      1st Qu.:0.2500
##  Median :0.01351        Median :0.00000      Median :0.4881
##  Mean   :0.05664        Mean   :0.03108      Mean   :0.8735
##  3rd Qu.:0.11905        3rd Qu.:0.00000      3rd Qu.:1.1250
##  Max.   :0.20000        Max.   :0.32051      Max.   :4.5000
##  NA's   :127            NA's   :127          NA's   :127
##  total_carb_per_serv dietary_fiber_per_serv sugars_per_serv
##  Min.   :0.5294      Min.   :0.00000        Min.   :0.4186
##  1st Qu.:0.7059      1st Qu.:0.00000        1st Qu.:0.5250
##  Median :0.8250      Median :0.00000        Median :0.6000
```

```
##  Mean   :0.7800      Mean   :0.00838        Mean   :0.6097
##  3rd Qu.:0.8580      3rd Qu.:0.02273        3rd Qu.:0.6750
##  Max.   :1.0000      Max.   :0.04651        Max.   :0.9211
##  NA's   :127         NA's   :127            NA's   :127
##  protein_per_serv
##  Min.   :0.00000
##  1st Qu.:0.00000
##  Median :0.02500
##  Mean   :0.03574
##  3rd Qu.:0.06977
##  Max.   :0.11765
##  NA's   :127
```

Using summary, it seems that our merge was successful. However, you will notice that there are some NAs. It is important we deal with these for subsequent analyses, because some methods, like PCA, can't handle missing data this way. Let's get rid of the NAs using na.omit

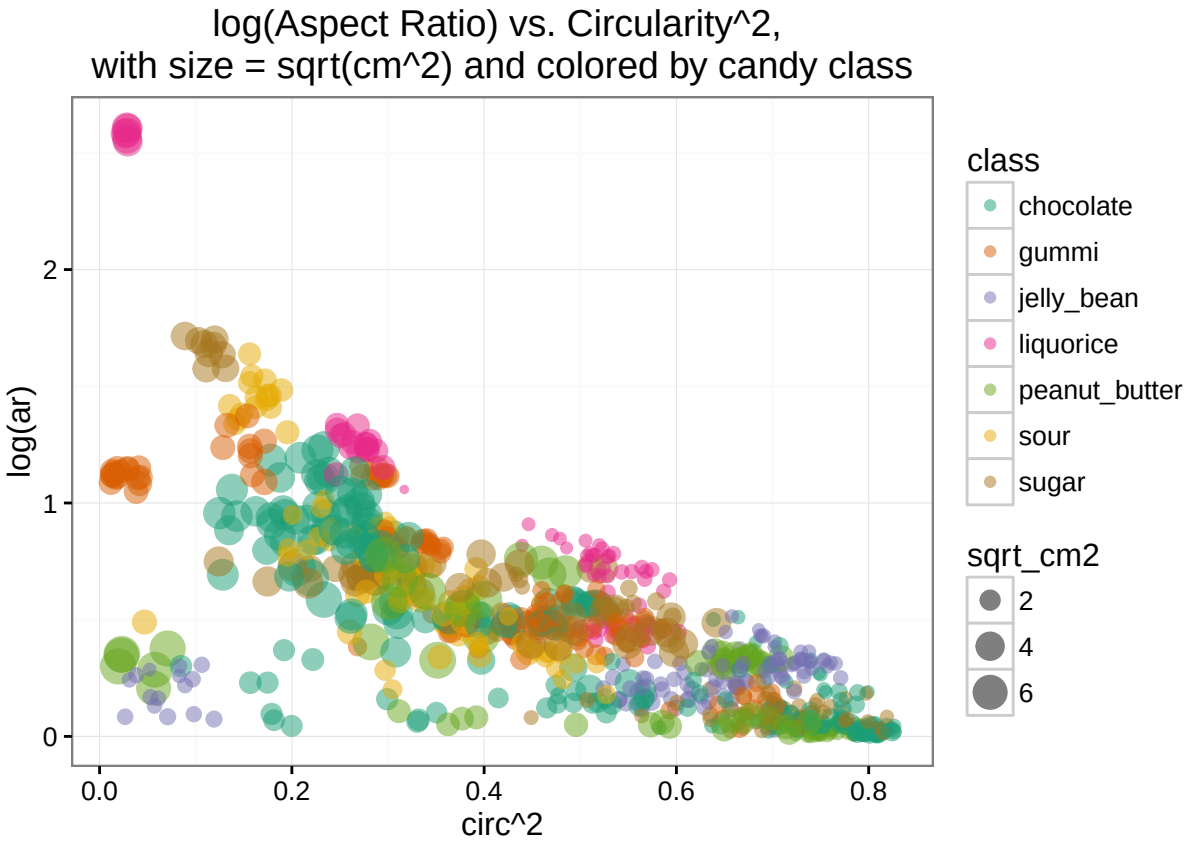
```
nonas_mdata <- na.omit(mdata)
summary(nonas_mdata)
```

```
##        id               label        candy_no          area
##  id_16  : 50   ID_10_01.jpg:  1   Min.   : 1.00   Min.   :  5721
##  id_14  : 30   ID_10_02.jpg:  1   1st Qu.: 5.00   1st Qu.: 10328
##  id_52  : 30   ID_10_03.jpg:  1   Median : 9.00   Median : 19701
##  id_64  : 28   ID_10_04.jpg:  1   Mean   :10.88   Mean   : 46853
##  id_20  : 25   ID_10_05.jpg:  1   3rd Qu.:15.00   3rd Qu.: 56382
##  id_61  : 25   ID_10_06.jpg:  1   Max.   :50.00   Max.   :356531
##  (Other):664   (Other)     :846
##       cm2              circ             ar             round
##  Min.   : 0.8363   Min.   :0.1090   Min.   : 1.003   Min.   :0.0740
##  1st Qu.: 1.5098   1st Qu.:0.5490   1st Qu.: 1.160   1st Qu.:0.4925
##  Median : 2.8799   Median :0.7170   Median : 1.528   Median :0.6540
##  Mean   : 6.8489   Mean   :0.6725   Mean   : 1.819   Mean   :0.6614
##  3rd Qu.: 8.2418   3rd Qu.:0.8293   3rd Qu.: 2.030   3rd Qu.:0.8618
##  Max.   :52.1172   Max.   :0.9090   Max.   :13.587   Max.   :0.9970
##
##      solid           sqrt_cm2                                name
##  Min.   :0.7120   Min.   :0.9145   reeses_pieces                : 50
##  1st Qu.:0.9210   1st Qu.:1.2287   good_and_plenty              : 30
##  Median :0.9570   Median :1.6970   original_skittles            : 30
##  Mean   :0.9388   Mean   :2.2666   tropical_wild_berry_skittles: 28
##  3rd Qu.:0.9720   3rd Qu.:2.8709   mms_original                 : 25
##  Max.   :0.9880   Max.   :7.2192   sweet_and_sour_starburst     : 25
##                                    (Other)                      :664
##       company              class     serving_size_g     calories
##  hershey  :215   chocolate    :217   Min.   : 7.00   Min.   : 25.0
##  wrigley  :167   gummi        :123   1st Qu.:40.00   1st Qu.:140.0
##  mars     : 99   jelly_bean   :109   Median :40.00   Median :150.0
##  haribo   : 62   liquorice    : 83   Mean   :39.22   Mean   :158.7
##  just_born: 60   peanut_butter:101   3rd Qu.:41.00   3rd Qu.:190.0
##  nestle   : 42   sour         : 84   Max.   :45.00   Max.   :220.0
##  (Other)  :207   sugar        :135
##   calories_fat     total_fat_g     saturated_fat_g cholesterol_mg
```

```
##  Min.   :  0.00   Min.   : 0.000   Min.   :0.000   Min.   : 0.000
##  1st Qu.:  0.00   1st Qu.: 0.000   1st Qu.:0.000   1st Qu.: 0.000
##  Median : 10.00   Median : 1.000   Median :0.500   Median : 0.000
##  Mean   : 31.95   Mean   : 3.639   Mean   :2.228   Mean   : 1.206
##  3rd Qu.: 70.00   3rd Qu.: 8.000   3rd Qu.:5.000   3rd Qu.: 0.000
##  Max.   :110.00   Max.   :13.000   Max.   :8.000   Max.   :10.000
##
##    sodium_mg       total_carb_g   dietary_fiber_g     sugars_g
##  Min.   :  0.00   Min.   : 6.00   Min.   :0.0000   Min.   : 6.00
##  1st Qu.: 10.00   1st Qu.:26.00   1st Qu.:0.0000   1st Qu.:21.00
##  Median : 20.00   Median :32.00   Median :0.0000   Median :24.00
##  Mean   : 34.19   Mean   :30.59   Mean   :0.3427   Mean   :23.83
##  3rd Qu.: 45.00   3rd Qu.:34.00   3rd Qu.:1.0000   3rd Qu.:27.00
##  Max.   :180.00   Max.   :38.00   Max.   :2.0000   Max.   :35.00
##
##    protein_g     primary_ingredient total_fat_per_serv
##  Min.   :0.000   chocolate:193      Min.   :0.00000
##  1st Qu.:0.000   dextrose :  9      1st Qu.:0.00000
##  Median :1.000   peanuts  :  6      Median :0.02703
##  Mean   :1.407   sugar    :484      Mean   :0.09263
##  3rd Qu.:3.000   syrup    :160      3rd Qu.:0.20455
##  Max.   :5.000                      Max.   :0.32353
##
##  saturated_fat_per_serv cholesterol_per_serv sodium_per_serv
##  Min.   :0.00000        Min.   :0.00000      Min.   :0.0000
##  1st Qu.:0.00000        1st Qu.:0.00000      1st Qu.:0.2500
##  Median :0.01351        Median :0.00000      Median :0.4881
##  Mean   :0.05664        Mean   :0.03108      Mean   :0.8735
##  3rd Qu.:0.11905        3rd Qu.:0.00000      3rd Qu.:1.1250
##  Max.   :0.20000        Max.   :0.32051      Max.   :4.5000
##
##  total_carb_per_serv dietary_fiber_per_serv sugars_per_serv
##  Min.   :0.5294      Min.   :0.000000       Min.   :0.4186
##  1st Qu.:0.7059      1st Qu.:0.000000       1st Qu.:0.5250
##  Median :0.8250      Median :0.000000       Median :0.6000
##  Mean   :0.7800      Mean   :0.008381       Mean   :0.6097
##  3rd Qu.:0.8580      3rd Qu.:0.022727       3rd Qu.:0.6750
##  Max.   :1.0000      Max.   :0.046512       Max.   :0.9211
##
##  protein_per_serv
##  Min.   :0.00000
##  1st Qu.:0.00000
##  Median :0.02500
##  Mean   :0.03574
##  3rd Qu.:0.06977
##  Max.   :0.11765
##
```

Great! All the NAs are gone. Let's look at our graph of aspect ratio, circularity, and sqrt_cm2 again, this time by candy class

```
p <- ggplot(nonas_mdata, aes(x=circ^2, y=log(ar), size=sqrt_cm2, colour=class))
p + geom_point(alpha=0.5) + scale_colour_brewer(type="qual", palette=2) + theme_bw() + ggtitle(label="l
```



If you want to save your graph, then `ggsave("all_candies.jpg")`

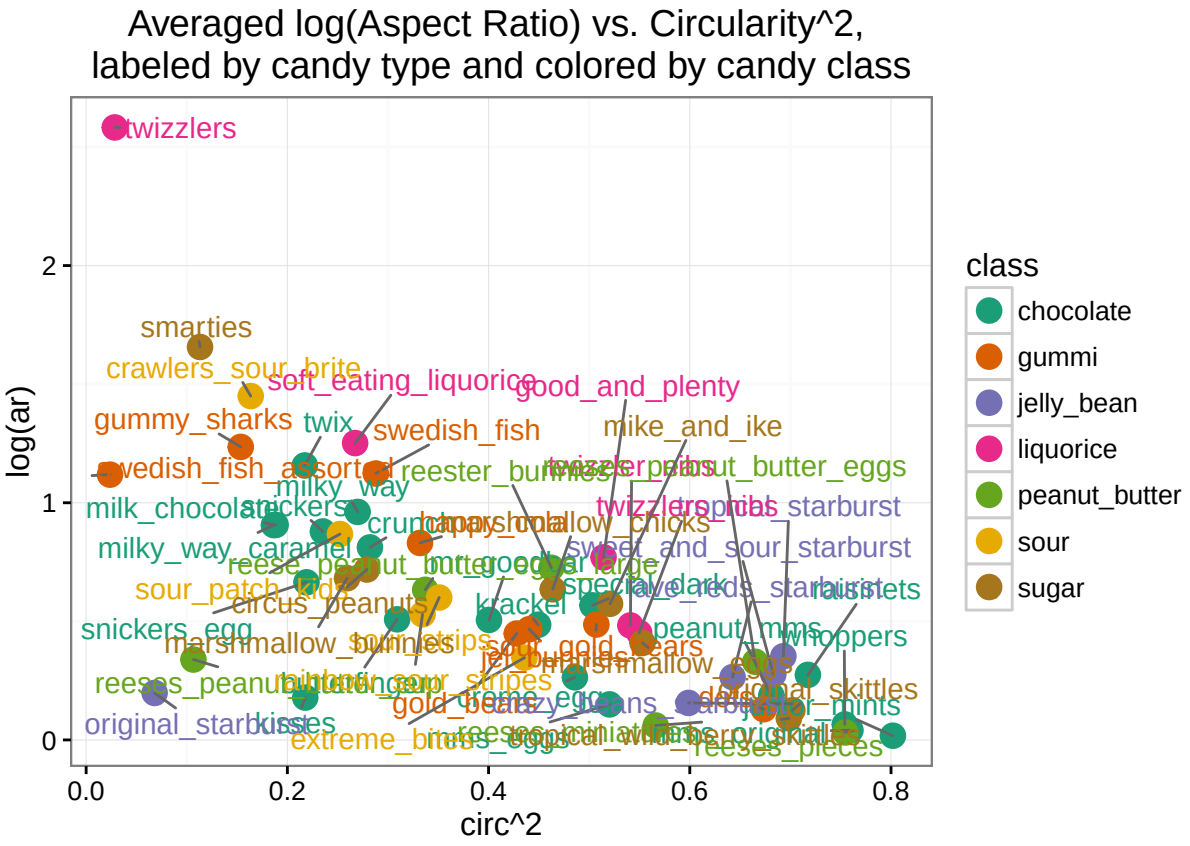
To get a feel for the shapes of the candies, let's take averages by candy type and replot this graph with labels

```
averaged <- aggregate(nonas_mdata[c(4:10,11,13,14:33)], by=list(nonas_mdata$name, nonas_mdata$class), FU
```

Now let's plot the averaged shape descriptor values and label by candy type and class

```
p <- ggplot(averaged, aes(x=circ^2, y=log(ar), colour=Group.2))
p + geom_point(alpha=1, size=4) + scale_colour_brewer(type="qual", palette=2) + geom_text_repel(data=ave
```

```
## Scale for 'colour' is already present. Adding another scale for
## 'colour', which will replace the existing scale.
```



If you want to save your graph, then `ggsave("averaged_candies.jpg")`

Final project

Previously, you should have isolated the RGB values per each candy piece. Your final project is to consider all the candy data as a whole. The three main datasets are:

1. Nutrition label information and candy class for each of the 75 candy types
2. Shape descriptor information and area for each of ~980 individual candy pieces
3. RGB color information for ~980 individual candy pieces (you should be in possession of this data)

You should first merge the three datasets together.

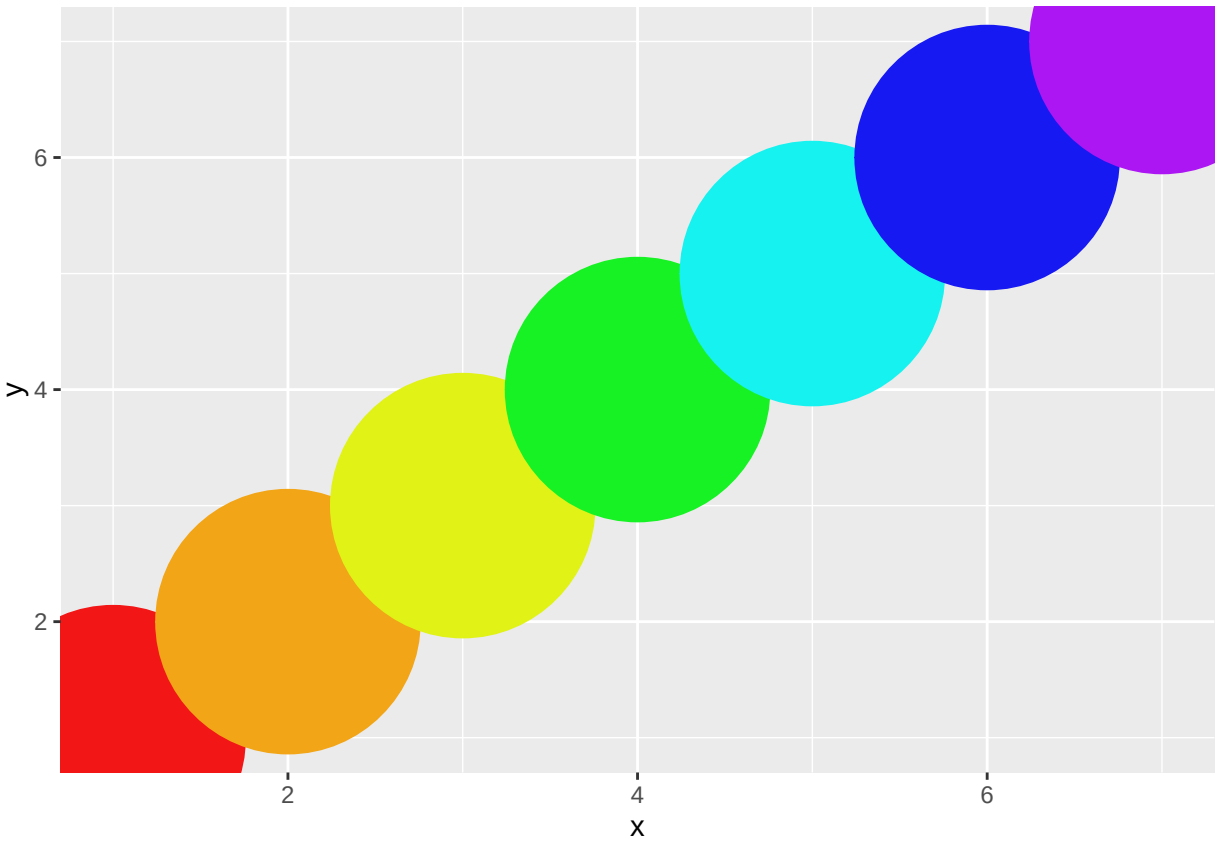
Then, considering data formating (NAs!) and scaling and centering of data as we discussed, use PCA and hierarchical clustering and provide commentary and notes on the results to discern patterns of relatedness of the candies. Please save both your code and commentary for the final project.

Provide ample data visualization to convey your results and make them understandable to others. Be sure to title and label your graphs too.

Additionally: because you have color information, in all your graphs (PCAs, scatterplots of individual variables) consider coloring your datapoints by the actual color of the individual candies. To do this, consider the following example data:

```
sample_colors <- read.table("./sample_colors.txt", header=TRUE)

p <- ggplot(sample_colors, aes(x,y, colour=rgb(r,g,b, maxColorValue=255)))
p + geom_point(size=46) + scale_colour_identity()
```



Coloring your data by actual candy piece rgb values should make for a striking graph!

Have fun, apply what you've learned, and analyze the multivariate data you worked so hard to collect!!! Email Dan your scripts, including commentary, no later than 5pm pon Thursday. Provide lots of analyses and data visualization, as well as explanation, for what you think is going on with your data!!!