

Cluster Analysis-Whiskey Data

Data Analytics and Visualizqation (Spring 2019)

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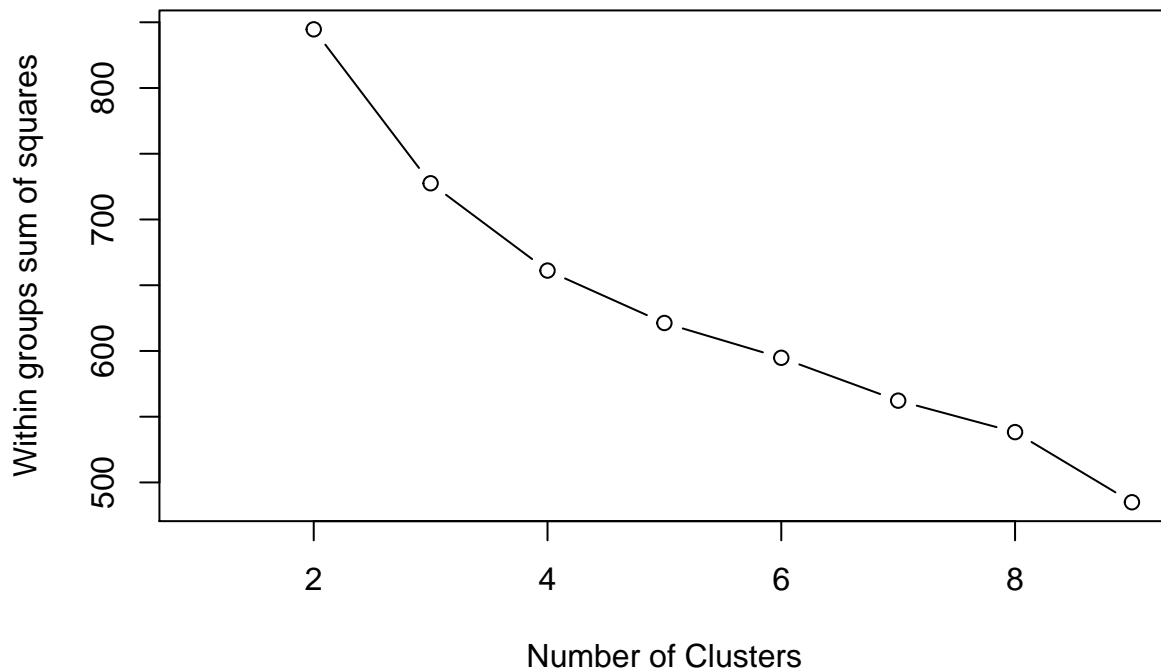
```
# Reading the data
whiskies = read.csv("C:/Users/zhuwe/Desktop/Visualization/Dataset/whiskies.txt")
whiskies = whiskies[,-1]
sum(is.na(whiskies)) # no missing observations
```

```
## [1] 0
```

```
# generating a subset of the data that included only the 12 flavor variables, rescaled for comparability
whiskies_k = scale(whiskies[,2:13]) # rescale selected vars for kmeans
head(whiskies_k)
```

```
##           Body Sweetness      Smoky Medicinal  Tobacco      Honey
## [1,] -0.07498567 -0.4052738  0.5385702 -0.5520139 -0.360623  0.8858842
## [2,]  0.99980888  0.9888682 -0.6193557 -0.5520139 -0.360623  3.2300701
## [3,] -1.14978021  0.9888682  0.5385702 -0.5520139 -0.360623  0.8858842
## [4,]  2.07460342 -1.7994159  2.8544220  3.4882579 -0.360623 -1.4583017
## [5,] -0.07498567 -0.4052738  0.5385702 -0.5520139 -0.360623 -0.2862087
## [6,] -0.07498567  0.9888682 -0.6193557  0.4580541 -0.360623 -0.2862087
##           Spicy      Winey      Nutty      Malty      Fruity      Floral
## [1,] -0.4890122  1.09701951  0.6509243  0.3142208  0.2536114  0.3535903
## [2,]  2.0597785  1.09701951  0.6509243  1.9038084  1.5365867  0.3535903
## [3,] -1.7634075 -1.04715499  0.6509243  0.3142208  1.5365867  0.3535903
## [4,]  0.7853832 -1.04715499 -0.5660211  0.3142208 -1.0293639 -1.9855456
## [5,] -0.4890122  0.02493226  0.6509243  1.9038084 -1.0293639 -0.8159776
## [6,] -0.4890122  0.02493226 -1.7829666 -1.2753668 -1.0293639  0.3535903
```

```
# applying k-means
ssPlot <- function(data, maxCluster = 9) {
  # Initialize within sum of squares
  SSw <- (nrow(data) - 1) * sum(apply(data, 2, var))
  SSw <- vector()
  for (i in 2:maxCluster) {
    SSw[i] <- sum(kmeans(data, centers = i)$withinss)
  }
  plot(1:maxCluster, SSw, type = "b", xlab = "Number of Clusters", ylab = "Within groups sum of squares")
}
ssPlot(whiskies_k)
```



Naturally, the within groups sum of squares decreases as we increase the number of clusters. However, there is a trend of diminishing marginal returns as we increase the number of clusters. Select the number of clusters based on the point at which the marginal return of adding one more cluster is less than was the marginal return for adding the clusters prior to that.

```
fit <- kmeans(whiskies_k, 4) # 4 cluster solution
```

append cluster assignment

```
whiskies <- data.frame(whiskies, fit$cluster)
whiskies$fit.cluster <- as.factor(whiskies$fit.cluster)
```

Cluster centers can inform on how taste profiles differ between clusters.

```
fit$centers
```

```
##          Body Sweetness      Smoky  Medicinal    Tobacco      Honey
## 1 -0.7292084 -0.6477333 -0.31728809 -0.33243389 -0.09093972  0.0705152
## 2 -0.3870228  0.7190342 -0.24583123 -0.06327132 -0.06049160 -0.2862087
## 3  1.1192305 -1.1797972  1.82515451  2.36596020  1.36235362 -1.1978366
## 4  0.8128881  0.1402600 -0.06556507 -0.50809788 -0.36062302  0.7839631
##          Spicy      Winey      Nutty      Malty      Fruity      Floral
## 1 -0.2673782 -0.3945801 -0.1427358  0.4524458  0.2536114  0.55699344
## 2 -0.1601360 -0.3209023 -0.3304833 -0.5062115 -0.3671831 -0.06141767
## 3  0.2189852 -0.5706718 -0.0251565 -0.5688834 -0.6017055 -1.46573763
## 4  0.3975237  1.0504070  0.5980136  0.4524458  0.4767375  0.09933641
```

Based on these centers, let us consider that David's choice for the full bodied, smoky and medicinal lies in cluster 4.

```
subset(whiskies, fit.cluster == 4)
```

##	Distillery	Body	Sweetness	Smoky	Medicinal	Tobacco	Honey	Spicy	Winey
## 1	Aberfeldy	2	2	2	0	0	2	1	2
## 2	Aberlour	3	3	1	0	0	4	3	2
## 8	Auchroisk	2	3	1	0	0	2	1	2
## 11	Balmenach	4	3	2	0	0	2	1	3
## 12	Belvenie	3	2	1	0	0	3	2	1
## 13	BenNevis	4	2	2	0	0	2	2	0
## 15	Benrinnies	3	2	2	0	0	3	1	1
## 16	Benromach	2	2	2	0	0	2	2	1
## 18	BlairAthol	2	2	2	0	0	1	2	2
## 27	Dailuaine	4	2	2	0	0	1	2	2
## 28	Dalmore	3	2	2	1	0	1	2	2
## 32	Edradour	2	3	1	0	0	2	1	1
## 39	GlenOrd	3	2	1	0	0	1	2	1
## 43	Glendronach	4	2	2	0	0	2	1	4
## 44	Glendullan	3	2	1	0	0	2	1	2
## 45	Glenfarclas	2	4	1	0	0	1	2	3
## 49	Glenlivet	2	3	1	0	0	2	2	2
## 53	Glenturret	2	3	1	0	0	2	2	2
## 62	Longmorn	3	2	1	0	0	1	1	1
## 63	Macallan	4	3	1	0	0	2	1	4
## 66	Mortlach	3	2	2	0	0	2	3	3
## 71	RoyalLochnagar	3	2	2	0	0	2	2	2
## 76	Strathisla	2	2	1	0	0	2	2	2
##	Nutty	Malty	Fruity	Floral	Postcode	Latitude	Longitude	fit.cluster	
## 1	2	2	2	2	\tPH15 2EB	286580	749680	4	
## 2	2	3	3	2	\tAB38 9PJ	326340	842570	4	
## 8	2	2	2	1	\tAB55 3XS	340754	848623	4	
## 11	3	0	1	2	\tPH26 3PF	307750	827170	4	
## 12	0	2	2	2	\tAB55 4DH	332680	840840	4	
## 13	2	2	2	2	\tPH33 6TJ	212600	775710	4	
## 15	2	3	2	2	\tAB38 9NN	325800	839920	4	
## 16	2	2	2	2	\tIV36 3EB	303330	859350	4	
## 18	2	2	2	2	\tPH16 5LY	294860	757580	4	
## 27	2	2	2	1	\tAB38 7RE	323520	841010	4	
## 28	1	2	3	1	\tIV17 0UT	266610	868730	4	
## 32	4	2	2	2	PH16 5JP	295960	757940	4	
## 39	1	2	2	2	IV6 7UJ	251810	850860	4	
## 43	2	2	2	0	AB54 6DA	361200	844930	4	
## 44	1	2	3	2	AB55 4DJ	333000	840300	4	
## 45	2	3	2	2	AB37 9BD	320950	838160	4	
## 49	1	2	2	3	AB37 9DB	319560	828780	4	
## 53	2	2	1	2	PH7 4HA	285630	723580	4	
## 62	3	3	2	3	IV30 3SJ	322640	861040	4	
## 63	2	2	3	1	AB38 9RX	327710	844480	4	
## 66	2	1	2	2	AB55 4AQ	332950	839850	4	
## 71	2	2	3	1	AB35 5TB	326140	794370	4	
## 76	3	3	3	2	AB55 3BS	340754	848623	4	

Identify the most representative whisky of each cluster by seeking out the observation closest to the center based on all 12 variables.

```
whiskies_r <- whiskies[c(2:13, 17)]
# extract just flavor variables & cluster
candidates <- by(whiskies_r[-13], whiskies_r[13], function(data) {
  # we apply this function to observations for each level of fit.cluster
  dists <- sapply(data, function(x) (x - mean(x))^2)
  # for each variable, calc each observation's deviation from average of the
  # variable across observations
  dists <- rowSums(dists)
  # for each observation, sum the deviations across variables
  rownames(data)[dists == min(dists)]
  # obtain the row number of the smallest sum
})

candidates <- as.numeric(unlist(candidates))

whiskies[candidates, ]
```

##	Distillery	Body	Sweetness	Smoky	Medicinal	Tobacco	Honey	Spicy	Winey
## 50	Glenlossie	1	2	1	0	0	1	2	0
## 42	Glenallachie	1	3	1	0	0	1	1	0
## 24	Clynelish	3	2	3	3	1	0	2	0
## 1	Aberfeldy	2	2	2	0	0	2	1	2

##	Nutty	Malty	Fruity	Floral	Postcode	Latitude	Longitude	fit.cluster
## 50	1	2	2	2	IV30 3SS	322640	861040	1
## 42	1	2	2	2	AB38 9LR	326490	841240	2
## 24	1	1	2	0	\tKW9 6LB	290250	904230	3
## 1	2	2	2	2	\tPH15 2EB	286580	749680	4