

lab10

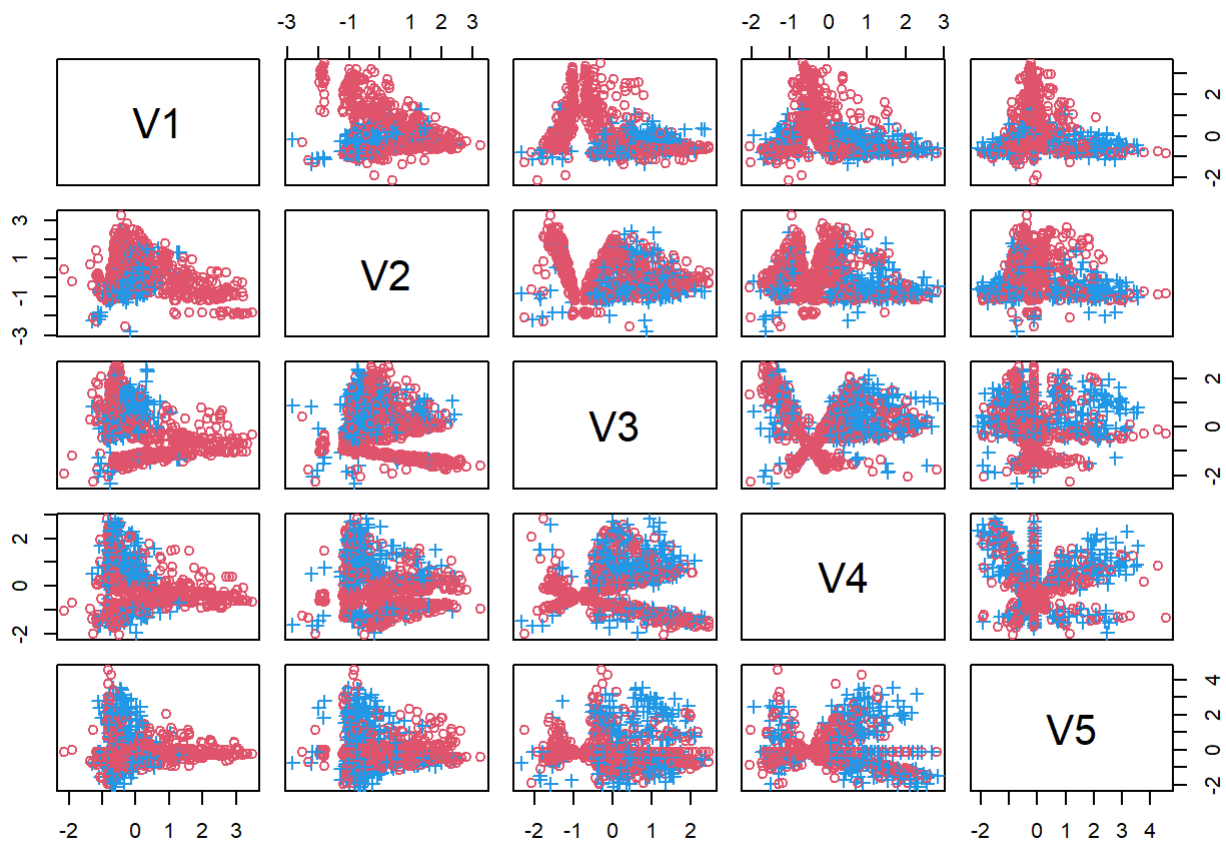
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17 October 2021

The Data: The source of the data we use in this lab is from Open ML, Phoneme data set.

Import data

```
phoneme = read.csv("phoneme.csv", stringsAsFactors=TRUE)
with(phoneme, pairs(phoneme[, -6], col=c(2,4)[Class], pch=c(1,3)[Class]))
```



```
library(mclust)
```

```
## Warning: package 'mclust' was built under R version 4.0.5
```

```
## Package 'mclust' version 5.4.7
```

```
## Type 'citation("mclust")' for citing this R package in publications.
```

```
knitr::opts_chunk$set(echo = TRUE)
```

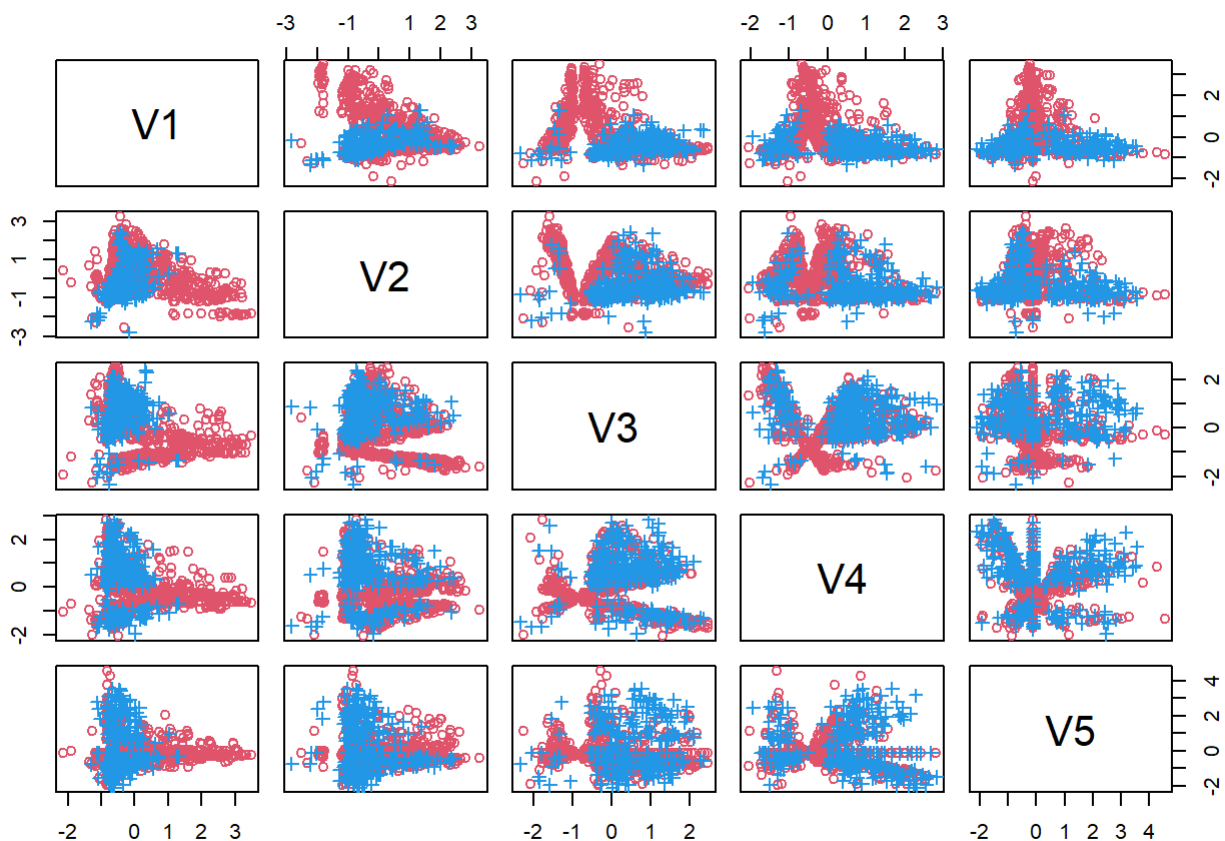
Visualisation

1, The data was sorted according to class label, the majority is in the front, thus is plotted firstly by pairs(), the minority class is plotted secondly, therefore on top.

```
table(as.numeric(factor(phoneme$Class))) ## majority is class 1 -Nasal
```

```
##
## 1 2
## 709 291
```

```
phoneme<- phoneme[order(as.numeric(factor(phoneme$Class))),] ## sort data with class number o
f column Class
with(phoneme, pairs(phoneme[, -6], col=c(2,4)[Class], pch=c(1,3)[Class]))
```



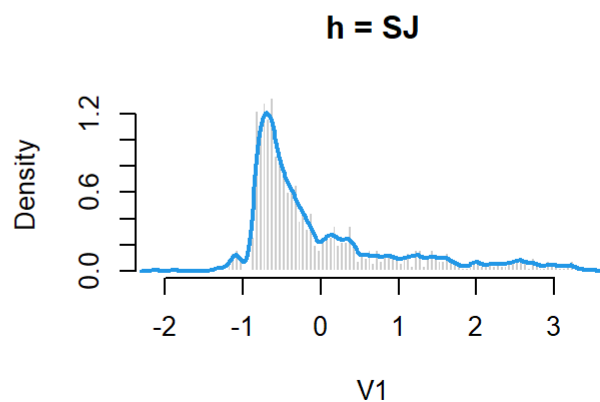
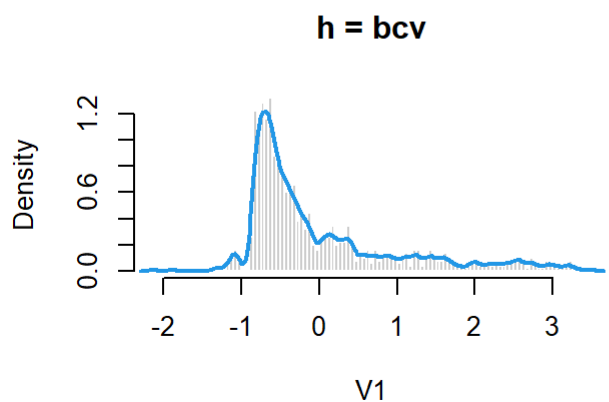
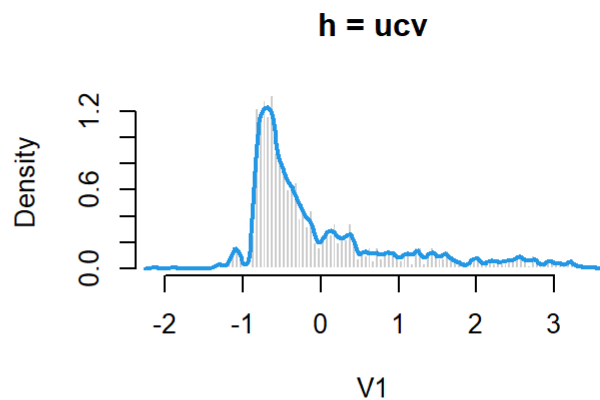
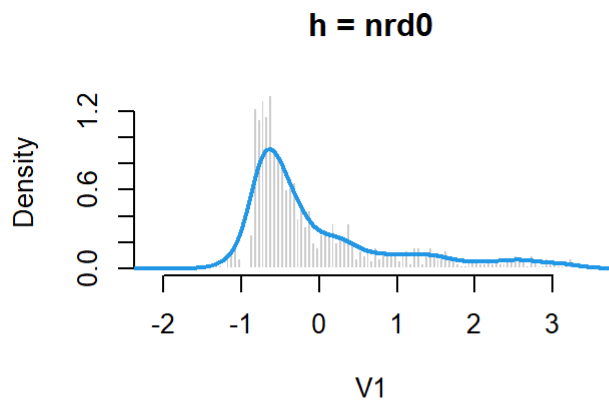
Univariate Density Estimation

2, Plot each of the kernel density estimate, by superimposing it on a histogram (with breaks=100), for V1, with the bandwidth values chosen by methods nrd0, ucv, bcv and SJ, respectively.

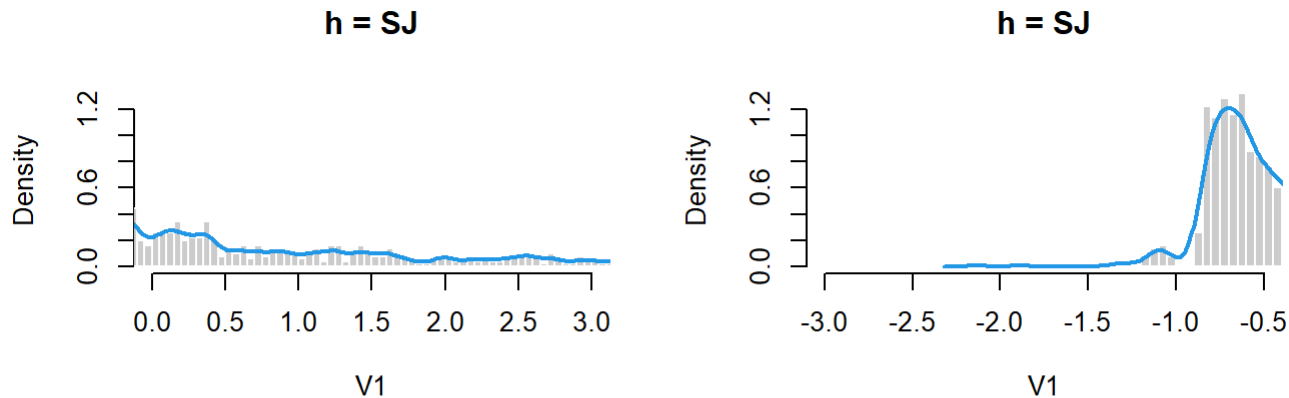
The nrd0 is underfitting and over-smoothing. Ucv, bcv and SJ methods are all somewhat overfitting, esp at high range.

from teacher -Overfitting and underfitting can occur in different regions. Let's take SJ as an example (which is usually considered as a good default bandwidth selector). It is underfitted/oversmoothed around $V1 = -1$, but at the same time is overfitted/undersmoothed for $V1 \geq 1$, as shown in the next two plots. The reason is that different regions require different bandwidth values for correct smoothing, but KDE uses a common one everywhere.

```
par(mfrow=c(2,2))
for(bw in c("nrd0", "ucv", "bcv", "SJ")) {
  hist(phoneme$V1, freq=FALSE, breaks=100,
       col="gray80", border="white",
       main=paste0("h = ", bw), xlab="V1")
  lines(density(phoneme$V1, bw=bw), col=4, lwd=2)
}
```



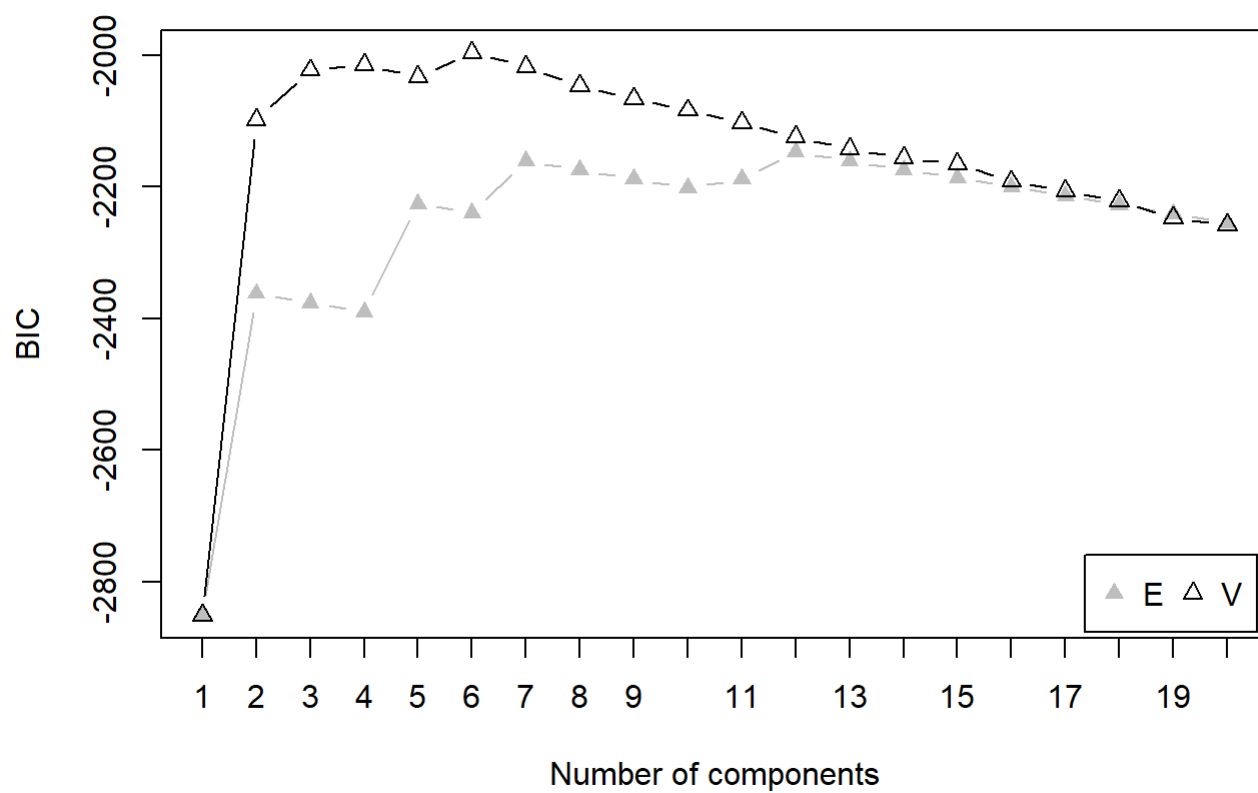
```
## Lower limit
hist(phoneme$V1, freq=FALSE, breaks=100,
     col="gray80", border="white",
     main=paste0("h = ", "SJ"),xlim=c(0,3), xlab="V1")
lines(density(phoneme$V1, bw="SJ"), col=4, lwd=2)
##upper limit
hist(phoneme$V1, freq=FALSE, breaks=100,
     col="gray80", border="white",
     main=paste0("h = ", "SJ"),xlim=c(-3,-0.5), xlab="V1")
lines(density(phoneme$V1, bw="SJ"), col=4, lwd=2)
```



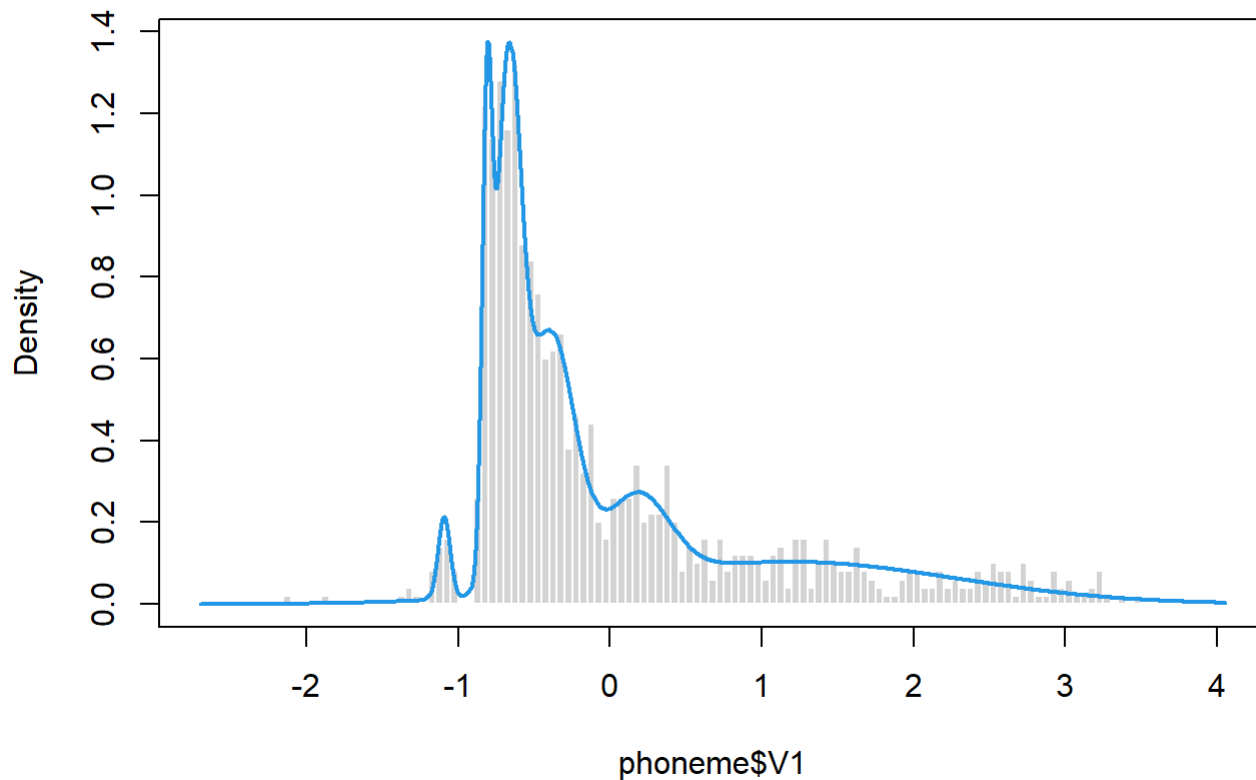
3, Find BIC selected the best normal mixture fit to V1 in both equal and varying variance subfamilies, with the number of components ranging from 1 to 20. Plot the fitted density, along with a histogram of the data.

BIC values of varying variance is bigger than that of equal variance density estimates, indicating varying variance fitting is better. The plot looks well-fitted, better than the results of KDEs. (teacher) It has much less underfitting or overfitting and is a better fit than any of the above KDEs, as can also be seen in the plots below. This is because a mixture with varying variances is more adaptive to the data everywhere.

```
r<-densityMclust(phoneme$V1,G=1:20)
#r$parameters
plot(r, what="BIC")
```



```
### the fitted density with 6 components - maximum BIC for model Varying variance
r6 = densityMclust(phoneme$V1, G=6, modelNames="V") # 6 components, varying variance
plot(r6, phoneme$V1, "density", breaks=100, lwd=2, col=4)
```



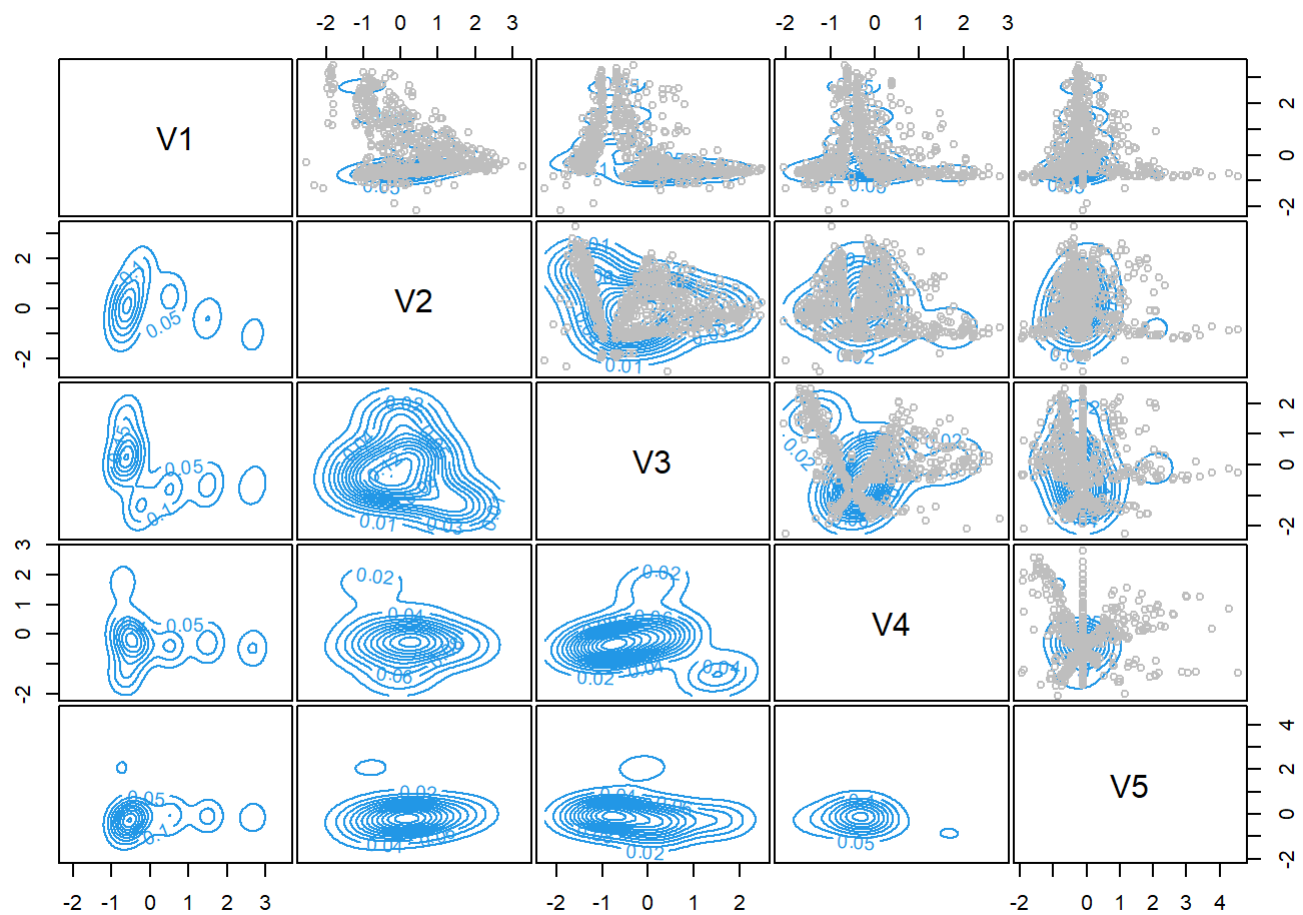
Multivariate density estimation

4, For each of the two classes, find a density estimate in the equal variance (EEE)subfamily of multivariate normal mixtures, with the number of components ranging from 1 to 9. Pairwise plot of estimated density with data are plotted.

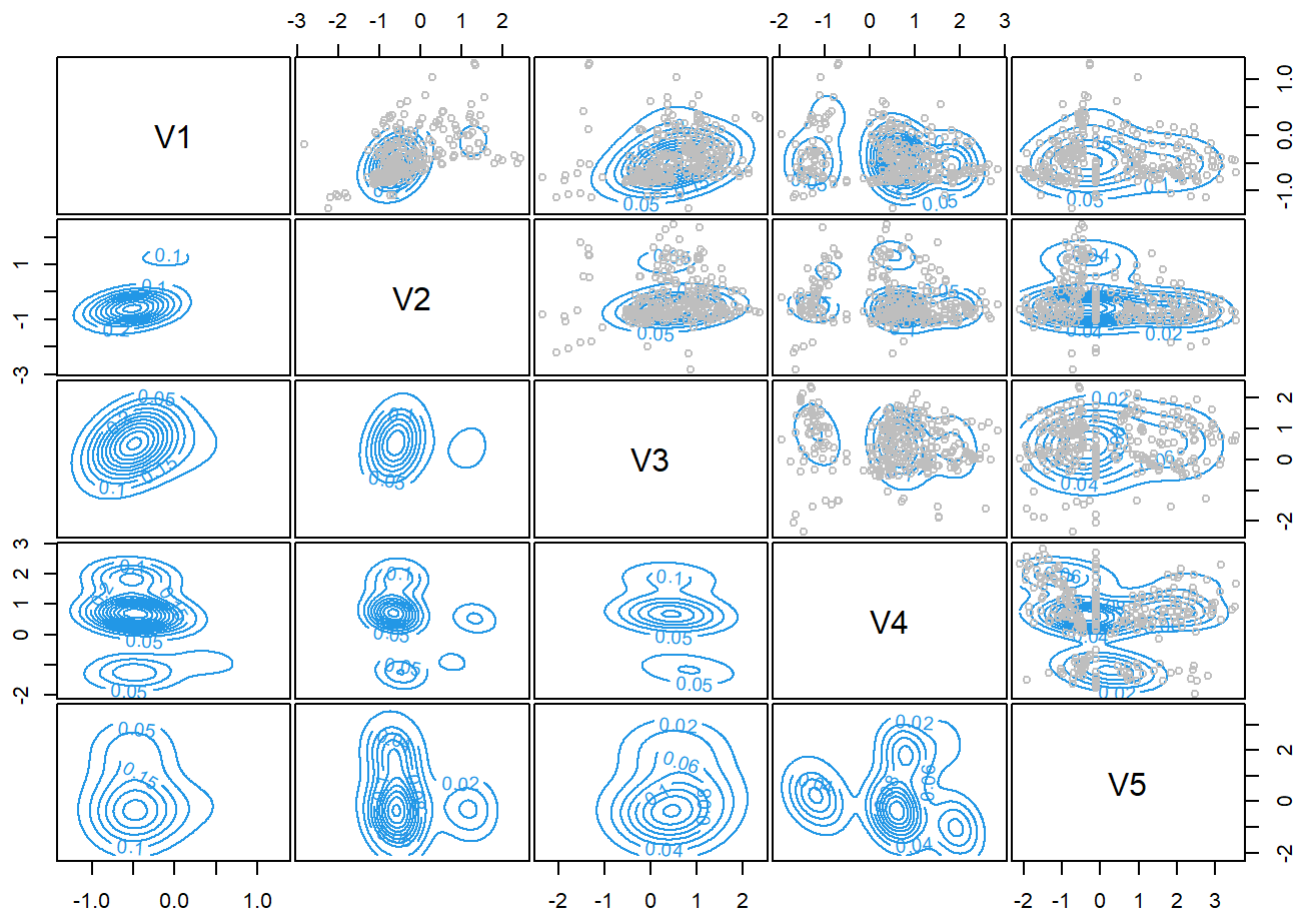
```
## subset data into oral and nasal
oral<- phoneme[phoneme$Class=="Oral",]
nasal<- phoneme[phoneme$Class=="Nasal",]

## estimated EEE density for oral and nasal
r.eoral<-densityMclust(oral[,-6],G=1:9 ,modelName="EEE")
r.enasal<-densityMclust(nasal[,-6],G=1:9 ,modelName="EEE")

## pairwise plot of estimated density of Nasal & Oral with method "EEE"
plot(r.enasal,nasal[,-6],what="density",col=4, points.col="grey")
```

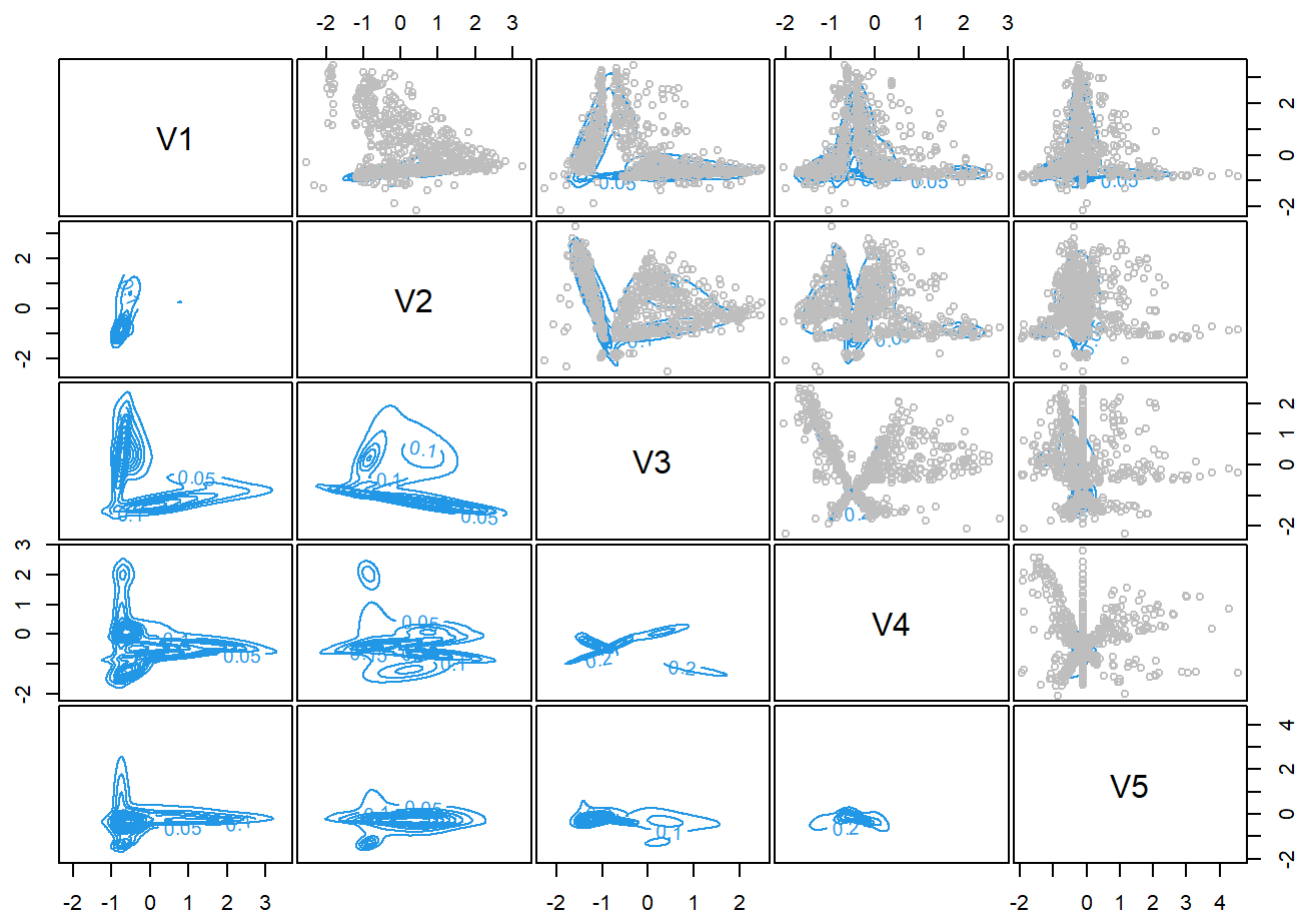


```
plot(r.eoral,oral[, -6], what="density", col=4, points.col="grey")
```

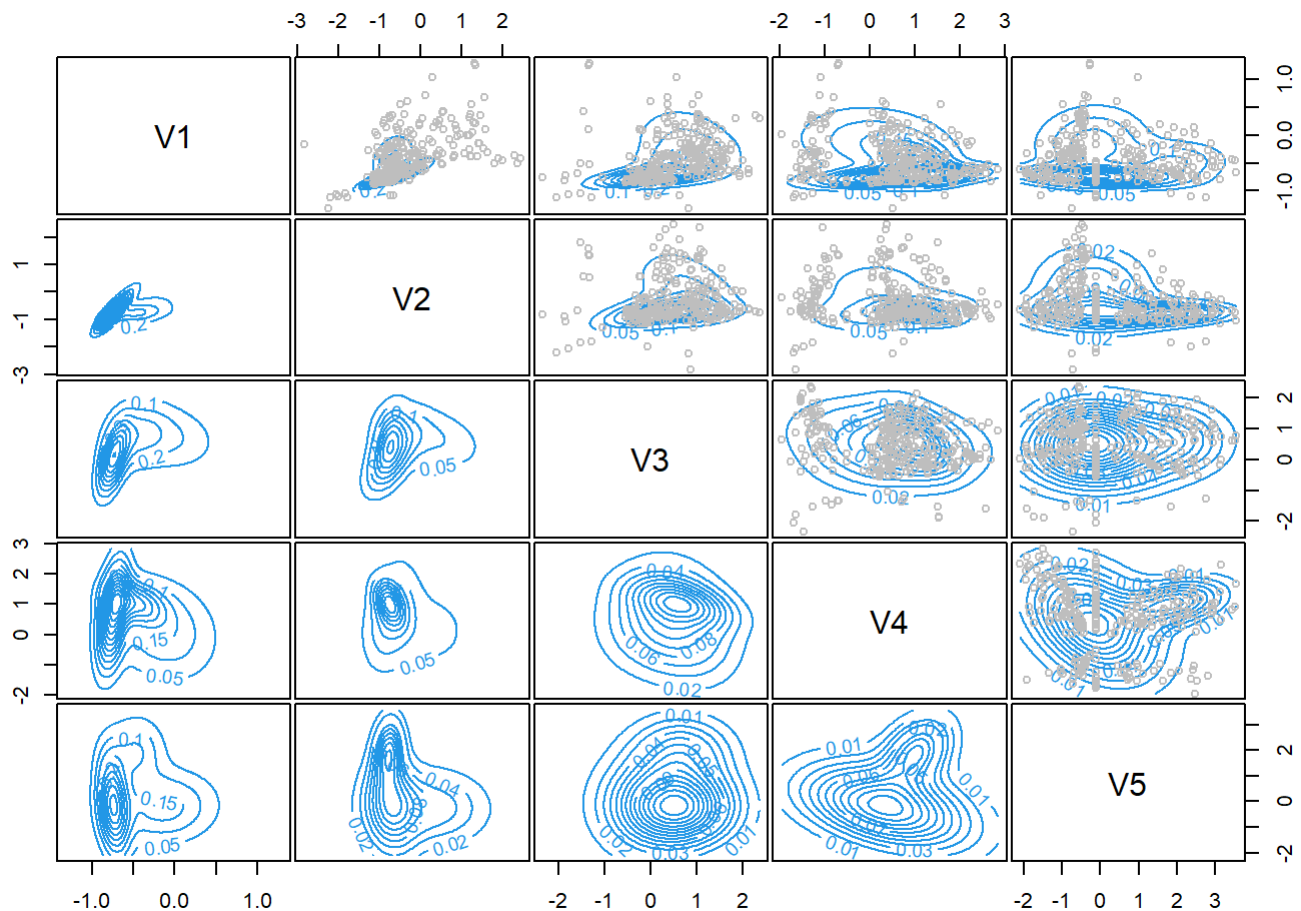


5, Repeat Task 4, but for the varying variance subfamily of normal mixtures.

```
## estimated VVV density for oral and nasal
r.voral<-densityMclust(oral[,-6],G=1:9 ,modelNames="VVV")
r.vnasal<-densityMclust(nasal[,-6],G=1:9 ,modelNames="VVV")
## pairwise plot of density of Nasal & Oral with method "VVV"
plot(r.vnasal,nasal[,-6],what="density",col=4, points.col="grey")
```

```
plot(r.voral,oral[, -6], what="density", col=4, points.col="grey")
```



6, By applying the fundamental rule of classification, we multiply the prior probability of each class with predicted posterior probability of each class, and compared them to get the number of classification. we compare this classification with the column "Class" in phoneme and calculate the misclassification rate for both model "EEE" & "VVV".

the misclassification rate for method "EEE" is 18%; 16.5 for method "VVV".

```
prior.p<-prop.table(table(phoneme$Class))          ## prior probability of oral & Nasal in phoneme
## EEE model
p.eoral<-predict(r.eoral,phoneme[,1:5])*prior.p[2]  ## posterior probability of Oral (EEE)
p.enasal<-predict(r.enasal,phoneme[,1:5])*prior.p[1] ## posterior probability of Nasal (EEE)
t.e<- ifelse(p.eoral>p.enasal,2,1)

## misclassification rate of model EEE
mean(t.e!=as.numeric(factor(phoneme[,6])))
```

```
## [1] 0.18
```

```
## VVV model
p.voral<-predict(r.voral,phoneme[,1:5])*prior.p[2]  ## posterior probability of Oral (VVV)
p.vnasal<-predict(r.vnasal,phoneme[,1:5])*prior.p[1]  ## posterior probability of Nasal (VVV)
t.v<- ifelse(p.voral>p.vnasal,2,1)

## misclassification rate of model VVV
mean(t.v!=as.numeric(factor(phoneme[,6])))
```

```
## [1] 0.165
```

all data estimation with both VVV & EEE

```
### test with whole data phoneme for both model "EEE" and "VVV"
r.all<-densityMclust(phoneme[, -6], G=1:9 ,modelNames=c("VVV","EEE"))
#(r.all$parameters), model with 9 components has highest BIC
p.all<-ifelse(predict(r.all,phoneme[, -6])>0.5,2,1)
#misclassification rate of whole dataset phoneme ~34%, Larger error
mean(p.all!=as.numeric(factor(phoneme[,6])))
```

```
## [1] 0.337
```

K-means

7, With the K-means method, find the clustering results with two clusters. Show the results in a pairwise plot of the data, using different colors and point types for observations of different clusters.

The majority of class (Nasal) was plotted firstly as red triangles, then the class (Oral) in blue crosses. The center of clusters is in either black (Nasal) or green (oral). Hardly any centers (black/green) can be seen, indicating poor clustering.

```
## with two clusters
set.seed(432)
(r0 = kmeans(phoneme[, -6], centers=2)) # K = 2
```

K-means clustering with 2 clusters of sizes 608, 392

##

Cluster means:

##	V1	V2	V3	V4	V5
## 1	-0.5356951	-0.2092974	0.5824347	0.2396484	0.07774704
## 2	0.8308753	0.3246247	-0.9033689	-0.3716992	-0.12057806

##

Clustering vector:

##	1	2	5	7	8	9	10	12	13	14	15	17	18	19	20	22
##	2	2	2	1	2	2	2	2	1	1	2	1	2	2	2	1
##	23	25	26	29	31	32	33	34	35	36	37	38	39	41	43	44
##	2	1	1	2	1	2	2	2	1	2	2	1	1	1	1	2
##	45	47	48	49	50	51	52	53	54	55	57	58	59	60	61	62
##	2	1	2	2	1	2	1	1	2	2	1	1	1	1	2	2
##	63	64	66	68	70	72	73	74	76	77	78	79	80	81	82	83
##	2	2	1	2	2	2	1	2	2	2	2	1	2	1	2	2
##	84	88	89	90	91	93	94	101	102	103	104	105	107	108	109	110
##	1	2	1	1	2	2	1	1	2	2	2	2	2	2	1	2
##	111	113	114	115	116	117	118	119	120	122	124	125	126	127	130	131
##	2	1	2	2	1	1	1	1	1	2	1	1	1	1	1	1
##	132	134	135	138	143	144	145	146	148	150	152	153	154	155	156	158
##	1	1	1	2	1	2	2	1	1	2	2	1	2	1	2	2
##	159	161	162	164	165	166	167	168	169	170	172	173	174	177	178	179
##	2	2	2	2	2	1	1	2	2	2	2	2	2	1	1	2
##	180	181	183	185	186	187	188	189	190	191	193	194	198	199	201	203
##	2	2	2	2	2	1	2	2	1	2	2	2	2	1	2	2
##	205	206	208	210	212	213	215	216	217	218	220	221	222	223	224	225
##	2	1	1	1	2	2	2	2	1	1	2	2	2	1	2	1
##	230	232	233	234	235	237	238	239	241	242	243	246	248	251	252	254
##	1	1	2	1	1	1	1	2	1	1	2	2	2	1	1	1
##	257	259	261	262	263	264	266	268	269	270	271	274	276	277	278	279
##	1	1	1	1	1	2	1	1	1	2	1	1	1	2	1	1
##	281	282	283	287	288	289	290	291	292	293	294	295	296	298	299	301
##	2	2	1	1	2	2	1	1	1	1	2	2	1	2	2	2
##	302	303	304	305	309	310	312	313	314	315	317	319	320	321	322	323
##	2	1	2	2	1	1	2	2	2	2	2	2	1	1	2	2
##	324	325	328	329	331	332	333	335	337	338	340	342	343	344	345	347
##	2	1	2	2	2	1	1	2	2	2	1	1	2	2	2	2
##	348	350	351	352	353	357	358	359	360	361	362	363	364	365	368	369
##	2	2	1	2	2	1	2	2	1	2	2	1	2	2	2	1
##	371	372	374	375	376	377	378	379	381	382	383	384	385	386	387	388
##	1	2	2	2	2	1	2	2	2	2	2	1	1	1	1	2
##	389	390	391	393	394	395	397	398	399	400	401	403	404	408	409	410
##	2	2	2	2	1	2	1	1	2	1	1	1	1	1	1	2
##	411	413	414	415	416	417	418	419	420	421	423	424	425	426	427	428
##	1	2	2	1	2	2	2	2	2	1	2	1	1	2	1	2
##	429	430	431	432	433	434	435	436	437	438	439	440	442	443	445	446
##	2	1	2	2	1	2	2	1	2	1	1	1	2	2	1	2
##	448	449	450	451	452	453	454	456	458	459	460	461	462	465	466	467
##	1	2	2	2	1	2	2	1	2	1	1	1	1	1	2	1
##	468	470	471	472	473	474	475	476	479	481	482	483	485	487	489	490
##	2	1	1	1	2	1	2	2	1	1	2	2	2	1	2	2

##	491	492	494	495	496	497	498	499	500	501	502	503	504	505	506	507
##	1	2	1	1	1	2	2	2	1	1	1	1	2	2	2	1
##	508	514	516	517	518	519	520	523	524	525	526	527	528	529	530	531
##	2	1	1	2	2	2	2	2	1	1	1	1	1	1	1	2
##	533	534	537	538	539	540	541	542	544	545	546	547	550	552	553	554
##	1	1	2	1	1	2	1	1	2	2	2	2	2	2	2	1
##	555	557	558	559	560	562	563	565	566	567	568	569	570	571	573	574
##	1	1	1	2	2	2	1	1	1	2	1	2	2	2	2	2
##	576	577	578	579	580	581	583	584	586	588	589	591	592	593	594	595
##	2	2	2	1	2	1	1	2	2	1	2	1	2	2	2	1
##	596	598	600	601	603	604	605	606	609	611	612	613	615	616	617	620
##	2	2	2	1	1	1	2	1	1	2	1	2	1	2	2	2
##	621	623	624	625	626	627	628	629	630	631	632	633	635	637	639	640
##	2	1	2	1	2	2	1	2	1	2	2	1	2	1	2	2
##	641	643	644	645	646	648	649	651	652	653	654	655	656	657	658	659
##	1	1	1	2	2	2	2	2	1	2	1	2	2	1	1	1
##	660	661	662	663	664	665	668	670	671	672	673	674	675	676	677	678
##	2	1	2	2	2	1	1	2	2	2	2	1	1	1	2	2
##	679	681	682	684	685	687	689	690	691	692	693	694	695	696	699	700
##	2	1	1	2	2	1	1	2	1	2	1	2	2	1	1	2
##	702	703	704	705	706	707	708	710	711	714	715	716	717	718	719	721
##	1	1	1	2	1	2	2	2	2	2	1	2	1	1	2	1
##	722	723	724	725	728	729	731	732	733	734	736	738	739	740	743	744
##	1	1	2	2	2	2	1	2	2	2	1	1	2	2	1	2
##	745	746	747	748	750	751	753	755	756	758	759	760	761	763	764	766
##	2	1	2	2	2	1	1	2	1	2	2	1	2	1	1	1
##	768	769	770	771	772	775	777	781	783	784	786	788	789	790	791	793
##	1	2	1	2	1	1	2	1	2	2	1	1	1	2	1	1
##	795	797	801	802	804	805	806	809	810	812	814	816	817	820	822	823
##	2	1	2	2	1	1	1	1	1	1	2	2	2	2	1	2
##	824	825	827	828	831	832	833	834	835	837	838	840	844	845	846	847
##	1	2	1	2	2	1	1	1	2	1	2	1	1	2	1	1
##	848	849	852	853	855	858	859	860	861	863	865	866	868	869	870	873
##	1	2	2	1	2	2	2									

```

## 204 207 209 211 214 219 226 227 228 229 231 236 240 244 245 247
## 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
## 249 250 253 255 256 258 260 265 267 272 273 275 280 284 285 286
## 1 1 1 1 1 2 1 1 1 1 1 1 1 1 2 1
## 297 300 306 307 308 311 316 318 326 327 330 334 336 339 341 346
## 1 2 1 1 2 1 1 1 2 1 1 1 1 1 1 1
## 349 354 355 356 366 367 370 373 380 392 396 402 405 406 407 412
## 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
## 422 441 444 447 455 457 463 464 469 477 478 480 484 486 488 493
## 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
## 509 510 511 512 513 515 521 522 532 535 536 543 548 549 551 556
## 1 2 1 1 1 1 1 1 1 1 2 1 1 1 1 1
## 561 564 572 575 582 585 587 590 597 599 602 607 608 610 614 618
## 1 1 1 1 1 1 1 2 1 1 1 1 1 1 1 1
## 619 622 634 636 638 642 647 650 666 667 669 680 683 686 688 697
## 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
## 698 701 709 712 713 720 726 727 730 735 737 741 742 749 752 754
## 1 1 1 1 1 1 1 1 1 1 1 2 1 2 1 1
## 757 762 765 767 773 774 776 778 779 780 782 785 787 792 794 796
## 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
## 798 799 800 803 807 808 811 813 815 818 819 821 826 829 830 836
## 1 2 1 1 1 1 1 1 1 1 1 1 1 1 1 1
## 839 841 842 843 850 851 854 856 857 862 864 867 871 872 876 877
## 1 1 2 2 1 1 1 1 1 1 1 1 1 1 1 1
## 879 881 882 884 885 886 889 894 898 899 900 902 913 919 920 921
## 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1 1
## 923 925 930 932 935 936 937 938 945 946 952 956 971 973 977 978
## 1 1 1 2 1 1 1 1 1 1 1 1 1 2 1 1
## 980 981 984 985 987 991 992 998
## 1 1 1 1 1 1 1 1
##
## Within cluster sum of squares by cluster:
## [1] 2519.854 1337.500
## (between_SS / total_SS = 22.8 %)
##
## Available components:
##
## [1] "cluster" "centers" "totss" "withinss" "tot.withinss"
## [6] "betweenss" "size" "iter" "ifault"

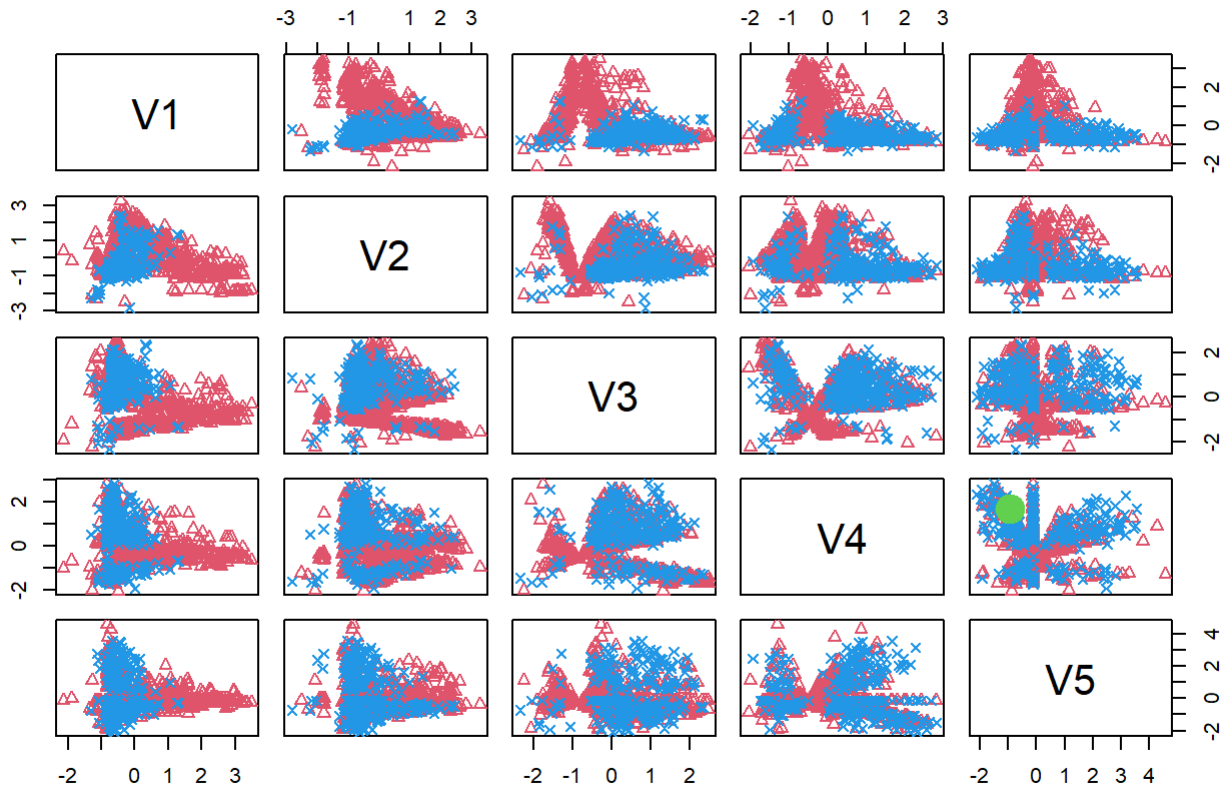
```

```

#o = order.majority(r0$cluster)
#(count1 = attr(o, "count.majority"))
with(phoneme, pairs(phoneme[, -6], col=c(2,4)[Class], pch=c(2,4)[Class], main="K = 2 (K-means EE
E)"))
points(r0$centers, col=c(1,3), pch=19, cex=2)

```

K = 2 (K-means EEE)



8, Compare the results obtained with K means clustering (unsupervised clustering) with the available class in phoneme dataset.

The classification accuracy is very low about 35% with 2 clustering centers, and reducing with the increasing of clustering centers.

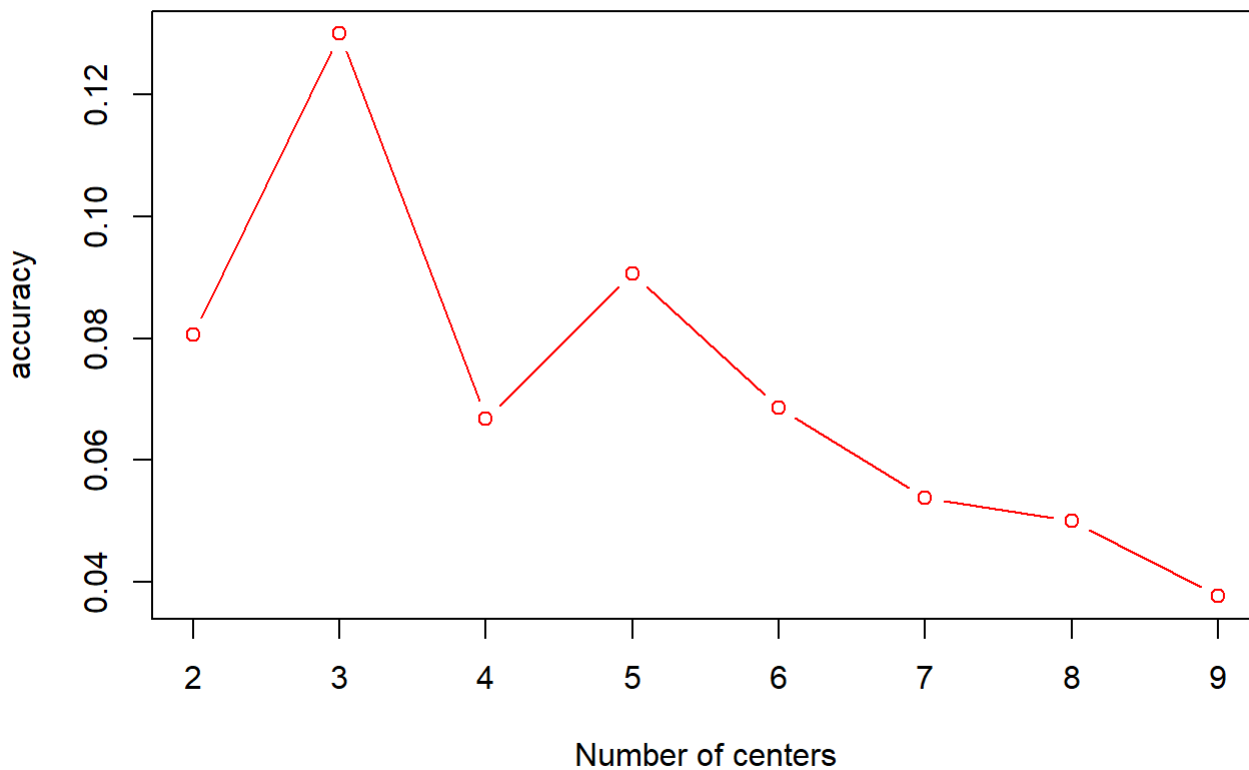
```
accuracy = double(8)

for(k in 2:9) {
  set.seed(432)
  r = kmeans(phoneme[, -6], centers=k)
  accuracy[k-1] <- adjustedRandIndex(r$cluster, as.numeric(factor(phoneme$Class)))
}
## clustering accuracy
accuracy
```

```
## [1] 0.08058490 0.12999026 0.06678252 0.09069357 0.06855240 0.05386771 0.04999859
## [8] 0.03767955
```

```
plot(2:9, accuracy, type="b", col="red", xlab="Number of centers", ylab="accuracy", main="K means methods")
```

K means methods



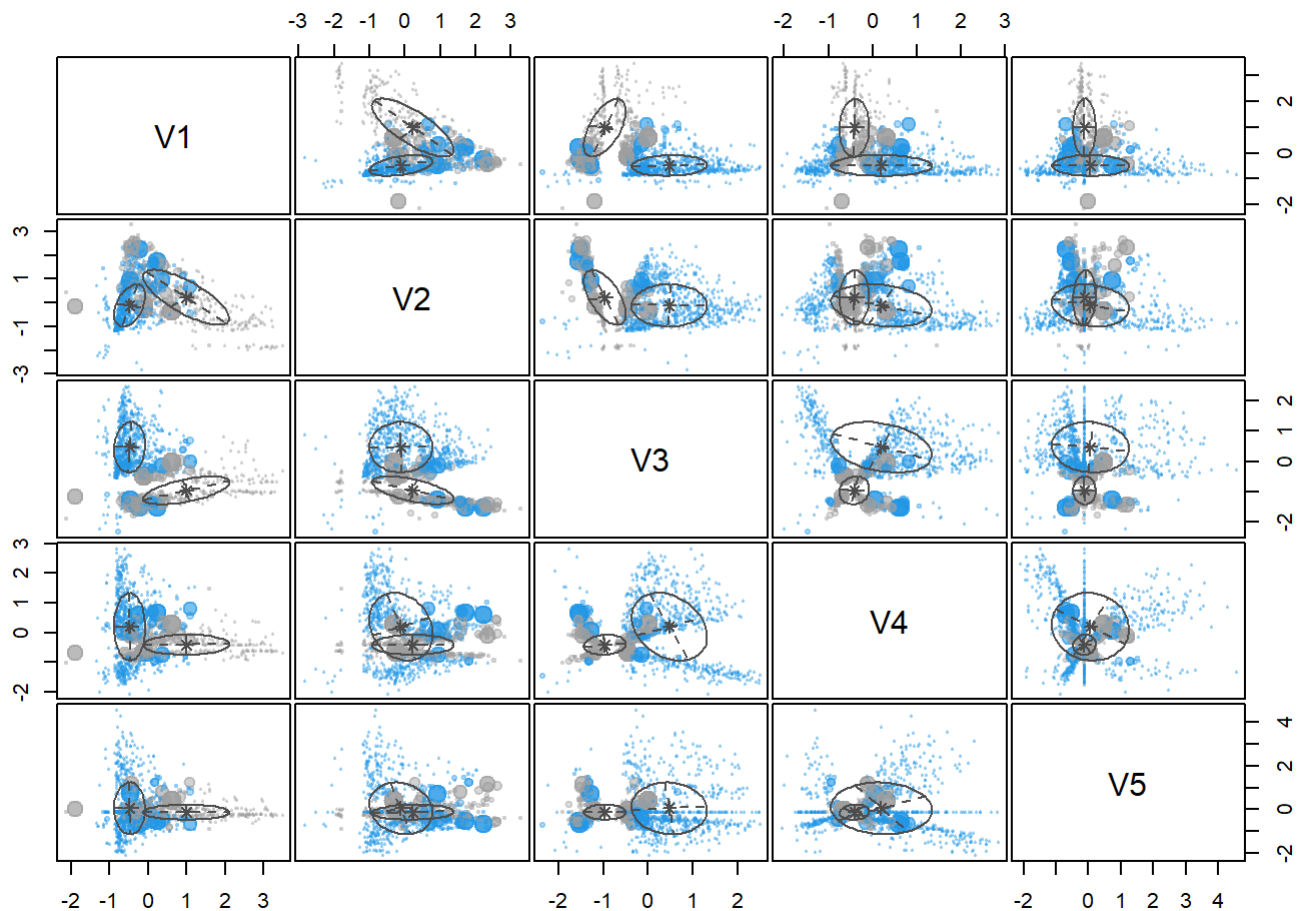
Mixture-based clustering

9, Use the varying variance subfamily of multivariate normal mixtures to find the clustering results with two clusters, and show the results in a pairwise plot, compute the adjusted Rand indices for K=2,...9 clusters.

The classification accuracy is almost 0, indicating no similarity of mixture based clustering comparing to original class.

```
set.seed(432)
r.mbc = Mclust(phoneme[,-6], G=2, modelNames="VVV")

plot(r.mbc,"uncertainty",col=c(8,4), main="K = 2 (k-means, VVV)") ## uncertainty plot of varying variance method with 2 centers
```

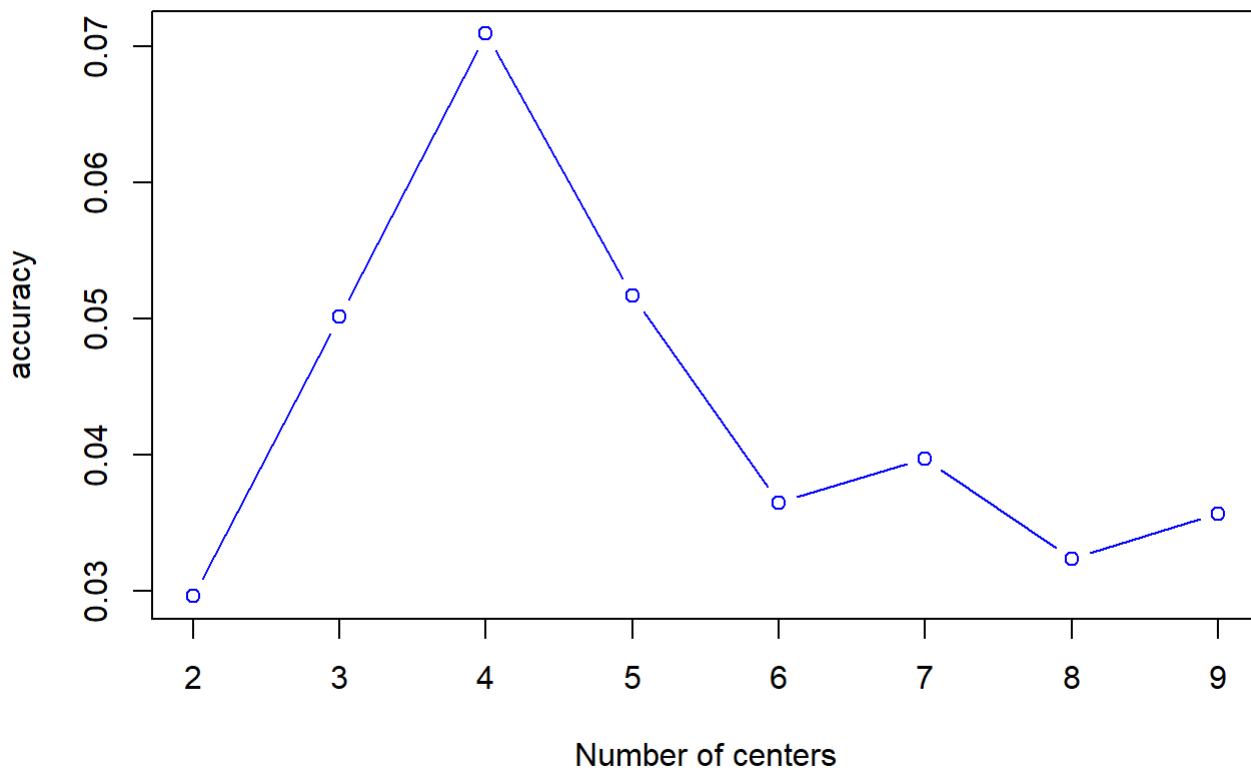
```
### compute clustering accuracy for k = 2~9
accuracy.v = double(8)
for(k in 2:9) {
  r.mbc = Mclust(phoneme[,-6], G=k, modelNames = "VVV")
  accuracy.v[k-1]<- adjustedRandIndex(r.mbc$classification, as.numeric(factor(phoneme$Class)))
}
```

```
## clustering accuracy
accuracy.v
```

```
## [1] 0.02963741 0.05014537 0.07091669 0.05169660 0.03648900 0.03973215 0.03236527
## [8] 0.03569147
```

```
plot(2:9,accuracy.v,type="b",col="blue", xlab="Number of centers",ylab="accuracy", main="Varying
variance mixture-based clustering method")
```

Varying variance mixture-based clustering method



Hierarchical Clustering

10, Produce a dendrogram of the hierarchical clustering results using the complete and the single linkage method, respectively.

Explain why they look very much different? Complete linkage clustering maximizes the pairwise observations' dissimilarity, while single linkage clustering minimizes the dissimilarity. For this dataset, there is no clear boundary between different clusters, thus by comparing euclidean distance of pairwised observations is not sufficient for clustering.

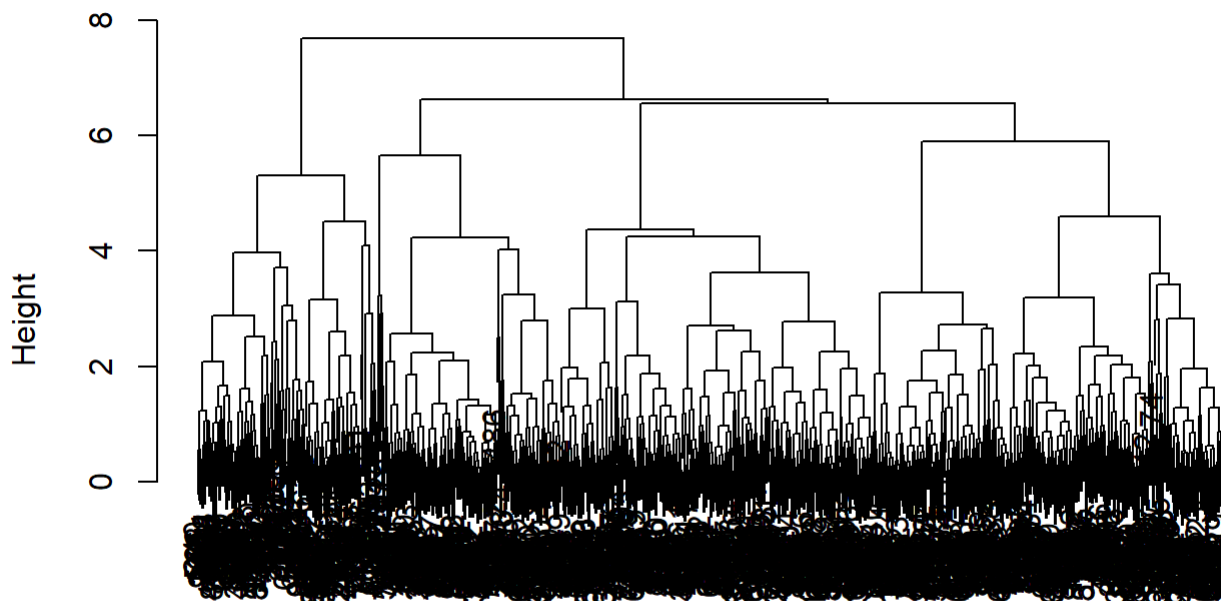
(from teacher) The complete-linkage method tends to produce more compact clusters and relatively large clusters near the top of the clustering tree. With the single-linkage method, clusters are linked purely based on two closest observations and may exhibit an extended, chain shape. It thus tends to produce clusters with very few observations even near the top of the clustering tree.

```
## standardize phoneme - euclidean distance matrix
phoneme3<-dist(phoneme[,-6])
## complete Linkage
r.cl = hclust(phoneme3)           # complete Linkage by default
names(r.cl)
```

```
## [1] "merge"      "height"     "order"      "labels"     "method"
## [6] "call"       "dist.method"
```

```
plot(r.cl)
```

Cluster Dendrogram

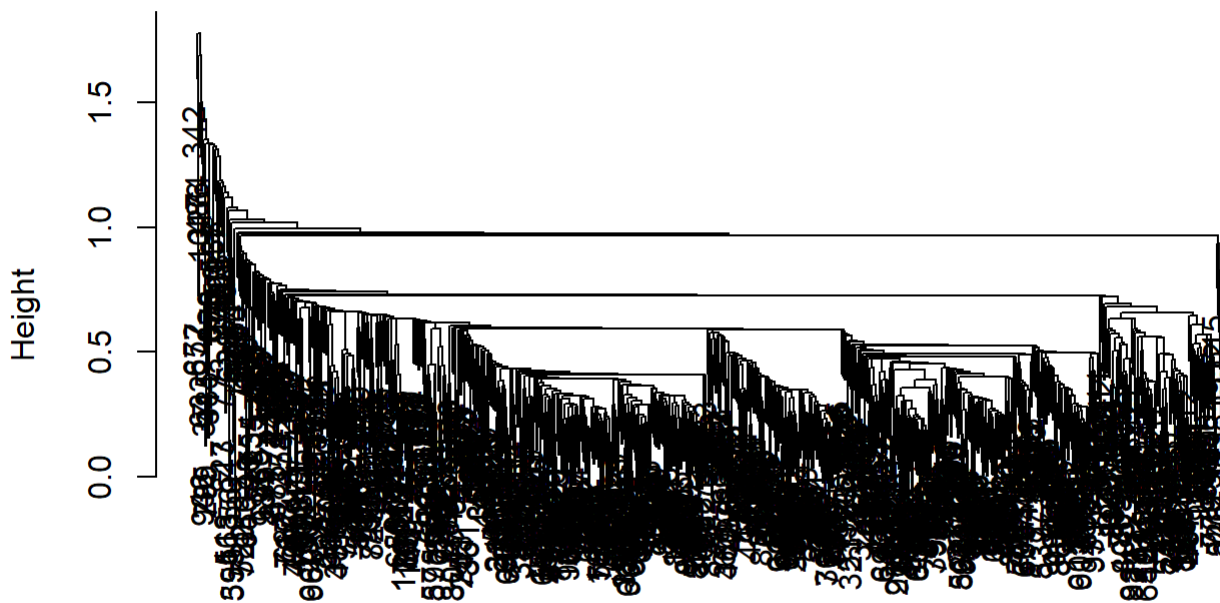


```
## single Linkage
r.sl= hclust(phoneme3,method="single")
names(r.sl)
```

```
## [1] "merge"      "height"     "order"      "labels"     "method"
## [6] "call"       "dist.method"
```

```
plot(r.sl)
```

Cluster Dendrogram



```
phoneme3
hclust (*, "single")
```

11, Compute the adjusted Rand indices for $K=2, \dots, 9$ clusters produced by the complete and the single linkage method, respectively.

The result shows very low ARI values, close to 0, which means both tree clustering methods of complete and single linkage methods are not consistent, indicating data can not be separable with pairwise euclidean distances dissimilarity.

```
### compute ari
ari = double(9)
for(k in 2:9) {
  r.cl = hclust(phoneme3)
  ari[k-1] = adjustedRandIndex(cutree(r.cl,k), cutree(r.sl,k))
}
ari
```

```
## [1] -0.0015711706  0.0033555333  0.0002705179  0.0006832815  0.0017865693
## [6]  0.0019591100  0.0051464297  0.0080570515  0.0000000000
```

For the complete-linkage method, the 2-cluster partition is a little bit similar to that according to class labels, as ARI = 0.152.

For the single-linkage method, all ARI-values are virtually 0, indicating no similarity between any of its clustering partitions and the one according to class labels.

```
round(sapply(1:8, function(j) adjustedRandIndex(phoneme[,6], cutree(r.cl,j+1))), 3)
```

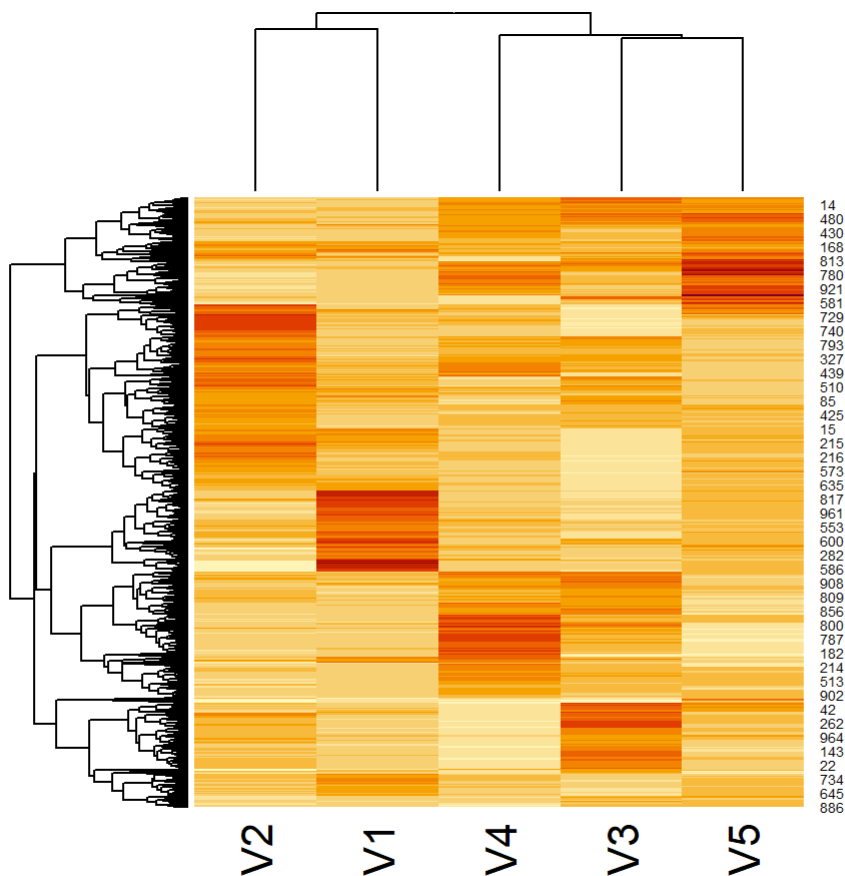
```
## [1] 0.152 0.087 0.048 0.069 0.070 0.075 0.081 0.082
```

```
round(sapply(1:8, function(j) adjustedRandIndex(phoneme[,6], cutree(r.s1,j+1))), 3)
```

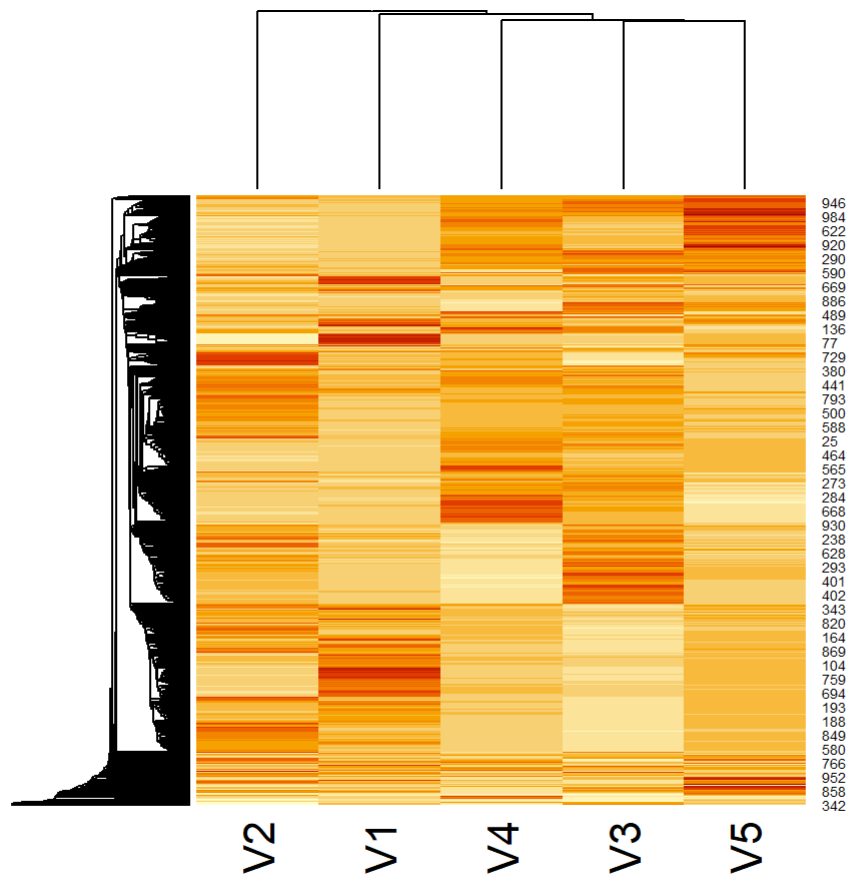
```
## [1] -0.001 0.001 -0.001 0.002 0.005 0.004 0.008 0.014
```

12, Produce the heatmaps for both the complete and single linkage methods. High values are in red, low values are in yellow.

```
## complete Linkage  
heatmap(as.matrix(phoneme[, -6]), scale="column", distfun=dist, hclustfun=hclust)
```



```
## single Linkage  
hclust.single<- function(x, ...) hclust(x, method="single", ...)  
heatmap(as.matrix(phoneme[, -6]), scale="none", distfun=dist, hclustfun=hclust.single)
```



Summary

In this lab we get to know density estimation and clustering methods. For density estimation we compared results of equal variance and varying variance density estimation, the result shows that nrd0 is underfitted, ucv, bcv and SJ methods are better fitted. Further we use BIC selected normal mixture estimate and choose 6 variables VVV model for density estimate, the result looks overfitting, especially at peak. Afterwards, we do the multivariate density estimate for both classes oral and nasal and for both “EEE”, “VVV” methods, the calculated misclassification rate for method “EEE” is 18%; for method “VVV” is 16.5%.

For clustering, k means method does not give good results, probably because of no clear boundary between the class, thus methods using Euclidean distances fail, including hierarchical clustering. The heatmaps generated from single and complete linkage do not have consistency (ARI ~0), indicating poor clustering. While K-means clustering with two components gives a bit better results for phoneme data.