

Cluster for whole data via Gower distance

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```
load("data/DiGiulio.RData")
otu_data = as.data.frame(DiGiulio$OTU) # 927 samples, 1271 OTU
taxonomy = DiGiulio$Taxonomy # 1271
sampledata = DiGiulio$SampleData # 927 samples, other covariates

otu_data_all=
  cbind(sampledata, otu_data) %>%
  mutate(
    Preg = as.factor(Preg),
    Subject = as.factor(Subject)
  ) %>%
  na.omit()
```

Term data

```
term =
  otu_data_all %>%
  filter(preterm == "Term")

term_data =
  term %>%
  dplyr::select(-SampleID, -Subject)
```

Gower distance for mixed variables

```
gower_dist <- daisy(term_data, metric = "gower")
gower_mat <- as.matrix(gower_dist)
```

```
#' Print most similar
term[which(gower_mat == min(gower_mat[gower_mat != min(gower_mat)]), arr.ind = TRUE)[1, ], 1:10]
```

```
##      SampleID Subject weeks  Race NumReads Preg preterm CST 4330849 4400869
## 27 1000601208   10006    20 White    2193 TRUE   Term    0         0         0
## 26 1000601198   10006    19 White    2385 TRUE   Term    0         0         0
```

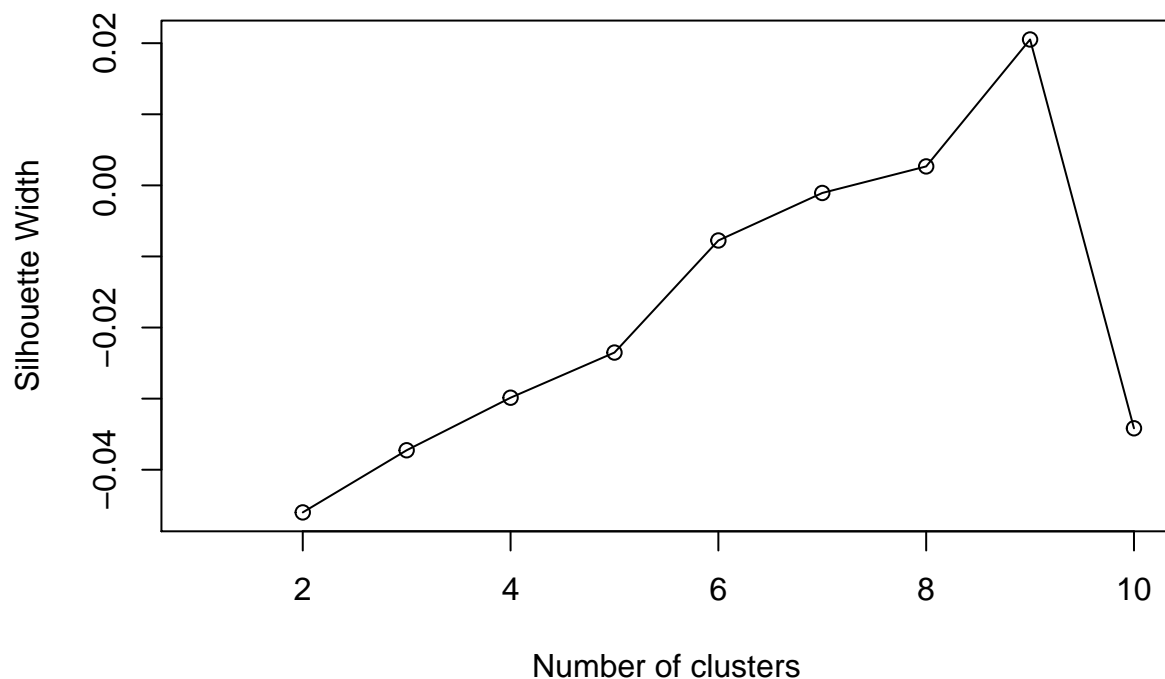
```
#' Print most dissimilar
term[which(gower_mat == max(gower_mat[gower_mat != max(gower_mat)]), arr.ind = TRUE)[1, ], 1:10]
```

```
##      SampleID Subject weeks  Race NumReads  Preg preterm CST 4330849
## 458 1004301328.rs   10043    32 White    5708 TRUE   Term    1         0
## 51   1000601718   10006    71 White   10165 FALSE   Term    0         0
##      4400869
```

```
## 458      0
## 51       0
```

Calculate silhouette width for many k using PAM

```
## Cluster
sil_width <- c(NA)
for(i in 2:10){
  pam_fit <- pam(gower_dist, diss = TRUE, k = i)
  sil_width[i] <- pam_fit$silinfo$avg.width
}
plot(1:10, sil_width,
     xlab = "Number of clusters",
     ylab = "Silhouette Width")
lines(1:10, sil_width)
```

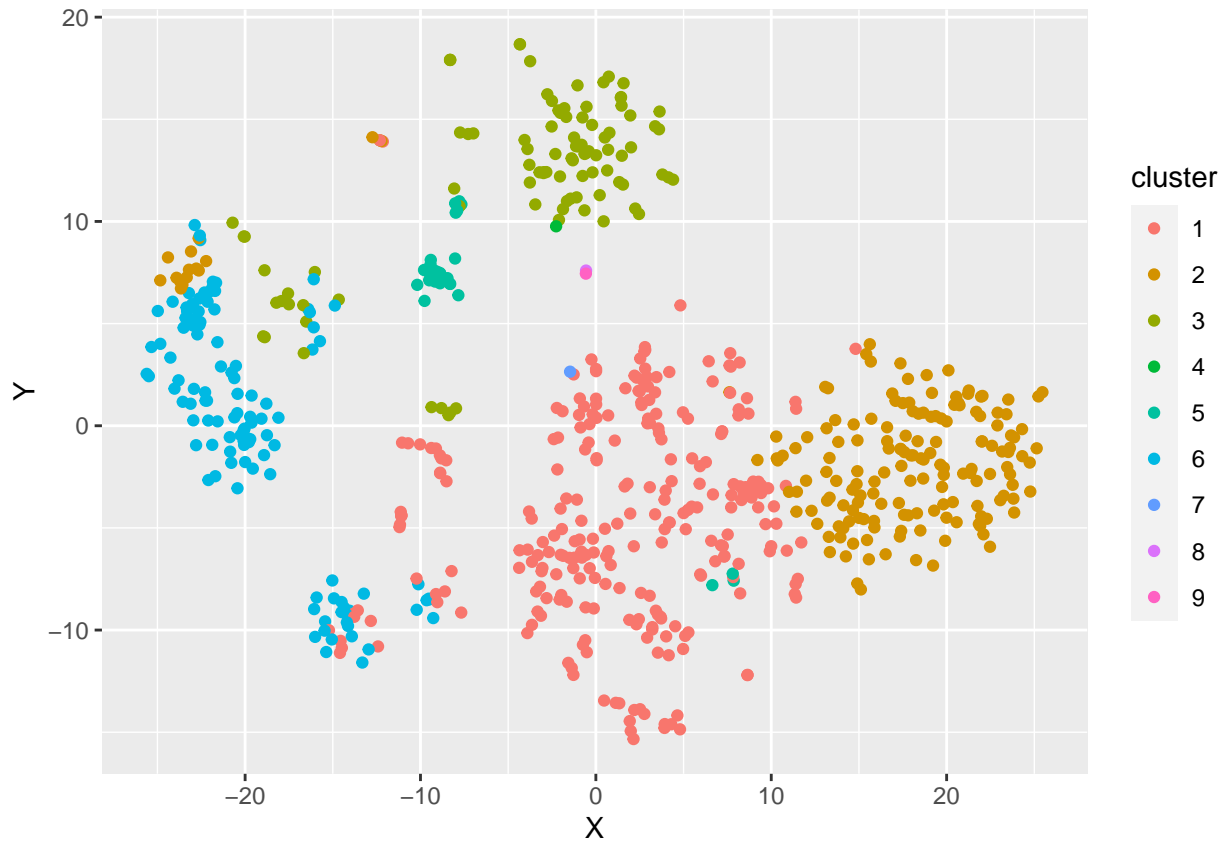


```
k <- 9
pam_fit <- pam(gower_dist, diss = TRUE, k)
pam_results <- term_data %>%
  mutate(cluster = pam_fit$clustering) %>%
  group_by(cluster) %>%
  do(the_summary = summary(.))
result = pam_results$the_summary
term[pam_fit$medoids, 1:10]
```

##	SampleID	Subject	weeks	Race	NumReads	Preg	preterm	CST
## 137	1002101308	10021	30	White	3408	TRUE	Term	0
## 159	1002201268	10022	27	White	5668	TRUE	Term	0
## 534	1004501618	10045	61	White	3820	FALSE	Term	0
## 51	1000601718	10006	71	White	10165	FALSE	Term	0
## 424	1004001338	10040	33	Indian	4335	TRUE	Term	0
## 630	1900501178	19005	18	Other (Specify below)	6134	TRUE	Term	0
## 389	1003901258	10039	26	White	8045	TRUE	Term	0

```
## 404 1003901458 10039 46 White 2218 FALSE Term 0
## 408 1003901608 10039 61 White 5415 FALSE Term 0
## 4330849 4400869
## 137 0 0
## 159 0 0
## 534 0 0
## 51 0 0
## 424 0 0
## 630 0 0
## 389 0 0
## 404 0 0
## 408 0 0
```

```
tsne_obj <- Rtsne(gower_dist, is_distance = TRUE)
tsne_data <- tsne_obj$Y %>%
  data.frame() %>%
  setNames(c("X", "Y")) %>%
  mutate(cluster = factor(pam_fit$clustering))
ggplot(aes(x = X, y = Y), data = tsne_data) +
  geom_point(aes(color = cluster))
```



Preterm data

```
preterm =
  otu_data_all %>%
  filter(preterm != "Term")
```

```
preterm_data =
  preterm %>%
  dplyr::select(-SampleID,-Subject)
```

Gower distance for mixed variables

```
gower_dist <- daisy(preterm_data, metric = "gower")
gower_mat <- as.matrix(gower_dist)
```

Print most similar

```
preterm[which(gower_mat == min(gower_mat[gower_mat != min(gower_mat)]), arr.ind = TRUE)[1, ], 1:10]
```

```
##      SampleID Subject weeks  Race NumReads Preg  preterm CST 4330849 4400869
## 195 1010101248   10101    14 White      8382 TRUE Marginal    0         0         0
## 194 1010101238   10101    14 White      8348 TRUE Marginal    0         0         0
```

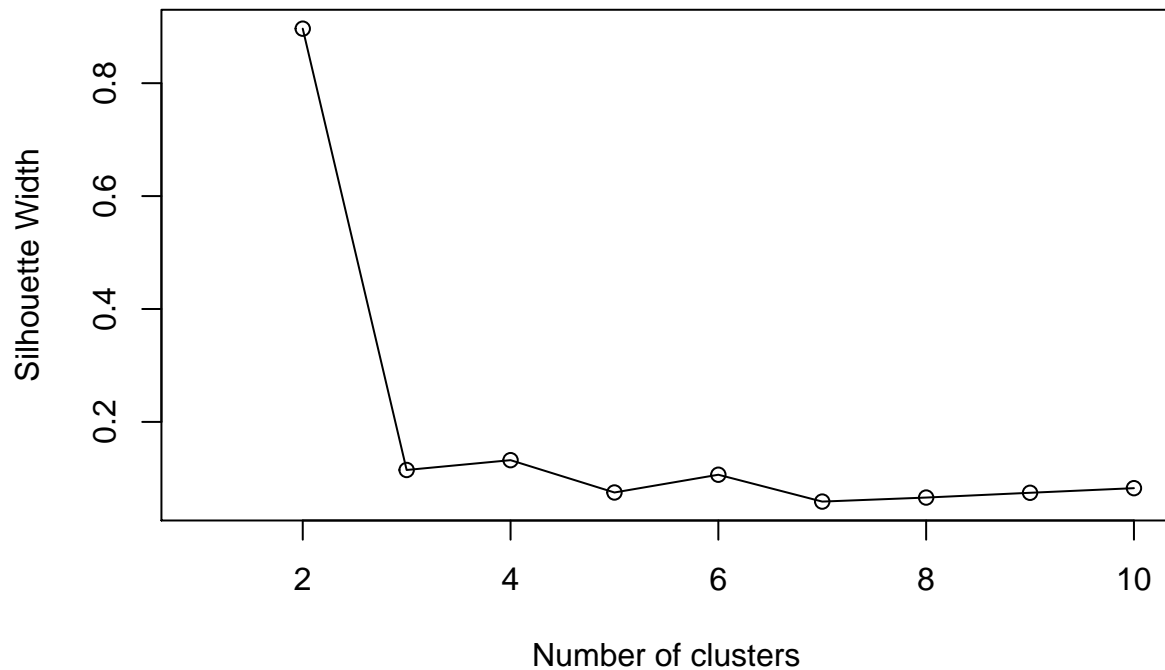
Print most dissimilar

```
preterm[which(gower_mat == max(gower_mat[gower_mat != max(gower_mat)]), arr.ind = TRUE)[1, ], 1:10]
```

```
##      SampleID Subject weeks      Race NumReads  Preg  preterm CST
## 220 1010101618   10101    58      White     9103 FALSE Marginal    0
## 45  1001801118   10018    12 American Indian    3599 TRUE  Preterm    1
##      4330849 4400869
## 220         0         0
## 45         0         0
```

Calculate silhouette width for many k using PAM

```
## Cluster
sil_width <- c(NA)
for(i in 2:10){
  pam_fit <- pam(gower_dist, diss = TRUE, k = i)
  sil_width[i] <- pam_fit$silinfo$avg.width
}
plot(1:10, sil_width,
     xlab = "Number of clusters",
     ylab = "Silhouette Width")
lines(1:10, sil_width)
```



```
k <- 2
pam_fit <- pam(gower_dist, diss = TRUE, k)
pam_results <- preterm_data %>%
  mutate(cluster = pam_fit$clustering) %>%
  group_by(cluster) %>%
  do(the_summary = summary(.))
result = pam_results$the_summary
term[pam_fit$medoids, 1:10]
```

```
##      SampleID Subject weeks  Race NumReads  Preg preterm CST 4330849 4400869
## 212 1002301618  10023    62 White    7341 FALSE   Term    0         0         0
## 220 1002401138  10024    14 White    5934  TRUE   Term    0         0         0
```

```
tsne_obj <- Rtsne(gower_dist, is_distance = TRUE)
tsne_data <- tsne_obj$Y %>%
  data.frame() %>%
  setNames(c("X", "Y")) %>%
  mutate(cluster = factor(pam_fit$clustering))
ggplot(aes(x = X, y = Y), data = tsne_data) +
  geom_point(aes(color = cluster))
```

