

Supplemental Material S3. R code for cluster inspection and principal component analysis.

Screplot of within cluster distance for one to ten clusters

```
> wss <- (nrow(dataset)-1)*sum(apply(dataset,2,var))
> for (i in 2:10) wss[i] <- sum(kmeans(dataset, centers=i)$withinss)
> plot(1:10, wss, type="b", xlab="Number of Clusters", ylab="Within groups sum of squares")
```

Silhouette analysis to determine consistency of the two clusters

```
> dataset_dist_eu <- dist(dataset, method = "euclidean")
> library(cluster)
> plot(silhouette(dataset$Cluster, dataset_dist_eu))
```

Principal Component Analysis of the four input variables

```
> pc <- prcomp(dataset, center = TRUE, scale. = TRUE)
```

Plot percentage of variance explained

```
> library(factoextra)
> library(ggplot2)
> library(viridis)
> library(cowplot)
> theme_set(theme_cowplot())
> eigenvalues <- get_eigenvalue(pc)
> varexplained <- as.data.table(eigenvalues$variance.percent)
> varexplained $PC <- c("PC1", "PC2", "PC3", "PC4")
> ggplot(varexplained, aes(x=PC, y=V1, fill=PC)) +
  geom_bar(stat="identity", color="white") +
  scale_fill_viridis(discrete=TRUE, begin=0.1, end=0.9) +
  theme(axis.title.x=element_blank()) +
  theme(axis.text = element_text(face="bold", size=12)) +
  theme(strip.text.x = element_text(size = 15, face="bold")) +
  theme(plot.title = element_text(hjust = 0.5)) +
  theme(axis.text.x = element_text(angle = 90, vjust = 0.5, hjust=1)) +
  labs(title="% variance explained", y="% variance explained")
```

Plot eigenvectors of the first two principal components

```
> contribution <- as.data.table(pc$rotation)
> contribution$stut <- rownames(pc$rotation)
> contribution2 <- melt(contribution[,c(1:2,5)], id.vars = "stut", variable.name = "PC", value.name =
"association")
> ggplot(contribution2, aes(x=stut, y=association, fill=PC)) +
  geom_bar(stat="identity", position=position_dodge(), linewidth=1, color="white") +
  scale_fill_viridis(discrete=TRUE, begin=0.1, end=0.4) +
  theme(axis.title.x=element_blank()) +
  theme(axis.text = element_text(face="bold", size=12)) +
  theme(strip.text.x = element_text(size = 15, face="bold")) +
  theme(plot.title = element_text(hjust = 0.5)) +
  theme(axis.text.x = element_text(angle = 90, vjust = 0.5, hjust=1)) +
  labs(title="Eigenvectors", y="Loading")
```