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# PCA clusters based on a percentage of the variance explained in each
# component. The algorithm calculates the variance explained in each component
# and then calculates the number of possible divisions that hold the amount of
# variance defined. Example: component when explains 70% of the total variance,
# and the user defines 10% of explained variance for each cluster/component,
# then the component has 7 clusters.
#
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#           diversity and conservation of the terrestrial reptiles of Oman
#           (Sauropsida, Squamata). Submitted.

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```

cluster.pca <- function(pca, percent, comp = 1:2) {
  ### Function to compute pca clusters based on total variance
  ### pca - a pca object from 'princomp' or 'prcomp'
  ### percent - a percentage of explanation for each cluster
  ### comp - number of components to calculate clusters
  ###
  ### Outputs a list with clusters per sample and per component,
  ### a list of centroids (position in each component) for each
  ### cluster, and a list of breaks of each cluster in each component.

  var.expl <- pca$sdev**2 / sum(pca$sdev**2) * 100
  cluster.n <- var.expl / percent
  scores <- predict(pca)
  n <- length(comp)
  clusters <- matrix(NA, nrow(scores), n+1)
  centroids <- breaks <- list()

  for (i in 1:n) {
    size <- diff(range(scores[,comp[i]]))/cluster.n[comp[i]]
    brk <- c(min(scores[,comp[i]]),
             rev(seq(0, min(scores[,comp[i]]), -size)[-1]),
             seq(0, max(scores[,comp[i]]), size),
             max(scores[,comp[i]]))
    breaks[[i]] <- brk
    clusters[,i] <- .bincode(scores[,comp[i]], brk, F, T)
    centroids[[i]] <- brk[1:(length(brk)-1)] + diff(brk)/2
  }

  combined <- as.integer(apply(clusters[,1:n], 1, paste, collapse=""))
  clusters[,n+1] <- as.integer(as.factor(combined))
  colnames(clusters) <- c(paste("comp", comp, "cluster", sep="_"), "combined")

  return(list(clusters=clusters, centroids=centroids, breaks=breaks))
}

```

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#####
## Example usage ##
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pca <- princomp(iris[1:4])
cluster <- cluster.pca(pca, 100)

```

```
# plot the comp.1 and 2 from pca
plot(pca$scores[,1:2], asp=1)

# add to plot the cluster breaks of each component
abline(v=cluster$breaks[[1]], lty=2, col='red')
abline(h=cluster$breaks[[2]], lty=2, col='red')

# Get the centroids of each component cluster
x <- cluster$centroids[[1]][cluster$clusters[,1]]
y <- cluster$centroids[[2]][cluster$clusters[,2]]

# merge and get only as list of unique centroids/clusters
centroids <- data.frame(x, y, cluster$clusters[,3])
centroids <- unique(centroids)

## add the cluster unique ID to plot
text(centroids[,1], centroids[,2], centroids[,3], cex=2)
```