*

June 3, 2022

The results below are generated from an R script.

```
## Install a package manager and packages
if (!require("pacman")) {
  install.packages("pacman")
}
pacman::p_load(Rfast, foreach, doParallel, mvnfast, rstudioapi)
current_path = rstudioapi::getActiveDocumentContext()$path
setwd(dirname(current_path))

pacman::p_load_gh("pkimes/sigclust2")
shc = get("shc", env = environment(shc))

source("sequential_function.R")

# k = 3 # number of clusters (3 or 10)
# uneven = FALSE #whether or not to have uneven weights
# distribution = 't' # t distribution or normal distribution?
# iterations = 50 # number of iterations


n = 500 # total number of samples
alpha = 0.05


if (distribution=='t'){
  distribution_name = 'True distribution components: t-distrbution (df=3) mixture distribution'
  samplefunc <- function(n, mu, sigma, w){
    rmixt(n = n,mu = mus,sigma = sigmas,w = w,df = 3)
  }
}else{
  distribution_name = 'True distribution: Normal mixture distribution'
  samplefunc <- function(n, mu, sigma, w){
  rmixn(n=n, mu=mus, sigma=sigmas, w=w)
}
}


# formulating d, delta (dimension and distance between clusters)
if (k == 10){
  a = c(2, 1, 2, 2, 2, 3, 2, 4, 2, 5, 2, 6, 2, 7, 2, 8, 2, 9) # dim2
  b = c(8, 1, 8, 2, 8, 3, 8, 4, 8, 5, 8, 6, 8, 7, 8, 8, 8, 9) # dim8
  d_delta = matrix(c(a, b) , ncol = 2, byrow = T)
} else if (k == 3){
```

*This report is automatically generated with the R package **knitr** (version 1.37).

```
  a = c(2, 1, 2, 2, 2, 3, 2, 4, 2, 5, 2, 6, 2, 7, 2, 8, 2, 9) # dim2
  b = c(8, 1, 8, 2, 8, 3, 8, 4, 8, 5, 8, 6, 8, 7, 8, 8, 8, 9) # dim8
  d_delta = matrix(c(a, b) , ncol = 2, byrow = T)
} else {
  stop("k != 3 or 10")
}


#weights
w = rep.int(1, k)
if (uneven){
  w[1] = 1 / 4
  w[2] = 1 / 2
}
w = w / sum(w)


K = floor(sqrt(n / 2)) #num clusters to test
K = min(K, 14L) # to ensure not estimating too many clusters

coresToUse = floor(detectCores() / 2) # cores to use

# function which creates data and performs one iteration
simulation <- function(iteration) {
  # simulate data
  set.seed(18 + iteration)
  data = samplefunc(n=n, mu=mus, sigma=sigmas, w=w)


  D1 = data[1:floor(n / 2), ]
  D2 = data[(floor(n / 2) + 1):n, ]

  # Estimate no.clusters
  Cluster_numbers = estimate.cluster.all(D1, D2, alpha, K)
  sigclust_splits = sum(shc(data, alpha = alpha)$nd_type == "sig")
  return(c(unlist(Cluster_numbers, use.names = F), sigclust_splits + 1L))
}


meanEstimate = matrix(nrow = nrow(d_delta), ncol = iterations)
medianEstimate = meanEstimate
meanEstimatel2 = meanEstimate
medianEstimatel2 = meanEstimate
AICEstimate = meanEstimate
BICEstimate = meanEstimate
sigclustEstimate = meanEstimate
RIFThierEstimate = meanEstimate

# For parallel computing
cl <- makeCluster(coresToUse) #not to overload computer
registerDoParallel(cl)
```

```r
for (j in 1:nrow(d_delta)) {
  d = d_delta[j, 1]
  delta = d_delta[j, 2]



  #sigmas = lapply(c(3,1,1), function(x) diag(x, nrow=d))
  sigmas = lapply(rep.int(1, k), function(x)
    diag(x, nrow = d))


  #mus = zeros(k, d)
  #mus[1,1] = delta
  #mus[2,2] = -delta
  #mus[3,2] = delta
  mus = outer(rep.int(1L, k), seq.int(d)) + delta * seq.int(0, k - 1L)

  estimates <-
    foreach(
      i = 1:iterations,
      .combine = cbind,
      .inorder = F,
      .packages = c("mclust", "Rfast", "mvnfast", "MASS"),
      .verbose = F
    ) %dopar% {
      simulation(i)
    }

  # format data into table
  meanEstimate[j, ] = estimates[1, ]
  medianEstimate[j, ] = estimates[2, ]
  meanEstimatel2[j, ] = estimates[3, ]
  medianEstimatel2[j, ] = estimates[4, ]
  BICEstimate[j, ] = estimates[5, ]
  AICEstimate[j, ] = estimates[6, ]
  RIFThierEstimate[j, ] = estimates[7, ]
  sigclustEstimate[j, ] = estimates[8, ]
  df = stack(data.frame(
    cbind(
      "Mean" = meanEstimate[j, ],
      "Meanl2" = meanEstimatel2[j, ],
      "Median" = medianEstimate[j, ],
      "Medianl2" = medianEstimatel2[j, ],
      "AIC" = AICEstimate[j, ],
      "BIC" = BICEstimate[j, ],
      "RIFT.hc" = RIFThierEstimate[j, ],
      "shc" = sigclustEstimate[j, ]
    )
  ))
  print(paste0("(dimension, delta) = (", d, ",", delta, ")"))
  colnames(df) = c("ESTIMATE" , "METHOD")
  tableEstimates = with(df, table(METHOD, ESTIMATE))
  print(tableEstimates)
```

```
}
```

```
## [1] "(dimension, delta) = (2,1)"
##           ESTIMATE
## METHOD       1   2   3   4   5   7   8  11
##   Mean      53  40   6   1   0   0   0   0
##   Meanl2    59  35   5   1   0   0   0   0
##   Median     2  66  23   5   0   2   1   1
##   Medianl2   2  67  22   5   0   2   1   1
##   AIC        1  51  38   7   3   0   0   0
##   BIC        5  75  18   2   0   0   0   0
##   RIFT.hc    8  74  14   4   0   0   0   0
##   shc      100   0   0   0   0   0   0   0
## [1] "(dimension, delta) = (2,2)"
##           ESTIMATE
## METHOD       1  2  3  4  5  6  8
##   Mean      48 31 16  5  0  0  0
##   Meanl2    53 28 15  4  0  0  0
##   Median     6 24 45 19  2  3  1
##   Medianl2   8 24 43 19  2  3  1
##   AIC        1 12 40 32 13  2  0
##   BIC       11 29 40 17  3  0  0
##   RIFT.hc   41 22 29  7  1  0  0
##   shc       27 54 13  2  2  1  1
## [1] "(dimension, delta) = (2,3)"
##           ESTIMATE
## METHOD       1  2  3  4  5  6  7  9 10 11
##   Mean      14 46 19 16  5  0  0  0  0  0
##   Meanl2    16 45 18 16  5  0  0  0  0  0
##   Median     0 32 32 26  5  3  1  0  0  1
##   Medianl2   0 35 33 24  5  2  1  0  0  0
##   AIC        0  7 10 56 19  7  0  1  0  0
##   BIC        1 23 11 55  9  1  0  0  0  0
##   RIFT.hc   75 18  1  5  1  0  0  0  0  0
##   shc        1 11 74  8  4  0  1  0  1  0
## [1] "(dimension, delta) = (2,4)"
##           ESTIMATE
## METHOD       1  2  3  4  5  6  7  8  9 10 12
##   Mean       4 40 11 38  7  0  0  0  0  0  0
##   Meanl2     4 40 13 36  7  0  0  0  0  0  0
##   Median     0 20 24 41 10  1  1  0  1  1  1
##   Medianl2   0 22 25 41  7  1  1  0  1  1  1
##   AIC        0  1  4 58 34  0  2  1  0  0  0
##   BIC        0  6  5 75 13  0  1  0  0  0  0
##   RIFT.hc   47 37  8  6  1  1  0  0  0  0  0
##   shc        0  4 90  6  0  0  0  0  0  0  0
## [1] "(dimension, delta) = (2,5)"
##           ESTIMATE
## METHOD       1  2  3  4  5  6  7  8 10 13
##   Mean       4 20 23 48  4  1  0  0  0  0
##   Meanl2     4 20 24 47  4  1  0  0  0  0
##   Median     0 10 25 50  8  2  1  2  1  1
##   Medianl2   0 13 24 48  8  2  1  2  1  1
##   AIC        0  1  0 63 29  4  3  0  0  0
```

```
##   BIC       0  2  2 79 14  2  1  0  0  0
##   RIFT.hc  18 63  4  6  8  1  0  0  0  0
##   shc       0  0 93  7  0  0  0  0  0  0
## [1] "(dimension, delta) = (2,6)"
##           ESTIMATE
## METHOD      1  2  3  4  5  6  7  8  9 11 12
##   Mean      3  8 32 48  7  2  0  0  0  0  0
##   Meanl2    3  8 34 46  7  2  0  0  0  0  0
##   Median    0  1 27 50 15  4  0  1  1  0  1
##   Medianl2  0  3 27 50 14  3  0  1  1  1  0
##   AIC       0  0  1 50 41  6  1  0  1  0  0
##   BIC       0  1  4 76 14  5  0  0  0  0  0
##   RIFT.hc   6 71  4 11  7  0  1  0  0  0  0
##   shc       0  0 94  6  0  0  0  0  0  0  0
## [1] "(dimension, delta) = (2,7)"
##           ESTIMATE
## METHOD      1  2  3  4  5  6  7  8
##   Mean      3  5 36 47  7  2  0  0
##   Meanl2    3  5 39 46  5  2  0  0
##   Median    0  1 17 59 17  4  1  1
##   Medianl2  0  1 20 59 15  3  1  1
##   AIC       0  0  0 53 35  9  2  1
##   BIC       0  0  1 79 17  3  0  0
##   RIFT.hc   3 73  7  9  6  2  0  0
##   shc       0  0 95  5  0  0  0  0
## [1] "(dimension, delta) = (2,8)"
##           ESTIMATE
## METHOD      1  2  3  4  5  6  7  8
##   Mean      2  4 35 50  7  2  0  0
##   Meanl2    3  3 38 48  7  1  0  0
##   Median    0  1  8 57 27  6  0  1
##   Medianl2  0  1  8 64 23  3  0  1
##   AIC       0  0  1 51 41  5  2  0
##   BIC       0  0  4 77 17  2  0  0
##   RIFT.hc   2 71  5 15  7  0  0  0
##   shc       0  0 96  4  0  0  0  0
## [1] "(dimension, delta) = (2,9)"
##           ESTIMATE
## METHOD      1  2  3  4  5  6  7  8 10 12
##   Mean      1  5 33 54  6  1  0  0  0  0
##   Meanl2    2  4 35 52  6  1  0  0  0  0
##   Median    0  1  4 56 26  7  2  2  1  1
##   Medianl2  0  1  6 58 25  6  1  1  1  1
##   AIC       0  0  1 45 46  6  2  0  0  0
##   BIC       0  0  5 70 23  2  0  0  0  0
##   RIFT.hc   0 72  7 18  3  0  0  0  0  0
##   shc       0  0 96  4  0  0  0  0  0  0
## [1] "(dimension, delta) = (8,1)"
##           ESTIMATE
## METHOD      1  2  3  4  5  6  7  8  9 10 11 12 13 14 15 16 17 18 19 22 24
##   Mean     20 19 23 19 15  4  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
##   Meanl2   20 19 23 19 15  4  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
##   Median    0 17 63 18  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
##   Medianl2  0 17 63 18  2  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
```

```
##   AIC       0  1 12 29 43 12  2  1  0  0  0  0  0  0  0  0  0  0  0  0  0
##   BIC       0  1 39 46 11  3  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
##   RIFT.hc   2  5 76 16  1  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0  0
##   shc       0  4  7 11  6  4 11  5  6 10  9  6  3  1  4  4  3  2  2  1  1
## [1] "(dimension, delta) = (8,2)"
##           ESTIMATE
## METHOD      1  2  3  4  5  6  7  8  9 10 11 12
##   Mean     15  0 12 29 36  8  0  0  0  0  0  0
##   Meanl2   15  0 12 29 36  8  0  0  0  0  0  0
##   Median    0  0  9 55 33  3  0  0  0  0  0  0
##   Medianl2  0  0  9 55 33  3  0  0  0  0  0  0
##   AIC       0  1  0  8 53 31  3  3  0  1  0  0
##   BIC       0  1  0 29 55 11  1  3  0  0  0  0
##   RIFT.hc   2 44  6 37  9  1  1  0  0  0  0  0
##   shc       0  0  1  7 16 21 17 17  9  6  4  2
## [1] "(dimension, delta) = (8,3)"
##           ESTIMATE
## METHOD      1  2  3  4  5  6  7  8  9 10 11
##   Mean     12  0  8 26 44 10  0  0  0  0  0
##   Meanl2   12  0  8 26 44 10  0  0  0  0  0
##   Median    0  1  3 80 16  0  0  0  0  0  0
##   Medianl2  0  1  3 80 16  0  0  0  0  0  0
##   AIC       0  0  0  8 48 35  8  1  0  0  0
##   BIC       0  0  0 27 57 11  5  0  0  0  0
##   RIFT.hc  12 15 14 31 23  5  0  0  0  0  0
##   shc       0  0  3 12 23 24 14 11  8  3  2
## [1] "(dimension, delta) = (8,4)"
##           ESTIMATE
## METHOD      1  2  3  4  5  6  7  8  9 10
##   Mean     11  0  6 22 46 11  3  0  0  1
##   Meanl2   11  0  6 22 46 11  3  0  0  1
##   Median    0  0  2 73 24  1  0  0  0  0
##   Medianl2  0  0  2 73 24  1  0  0  0  0
##   AIC       0  0  0  3 51 30 11  2  2  1
##   BIC       0  0  0 19 67 13  1  0  0  0
##   RIFT.hc  30  5  3 22 28 12  0  0  0  0
##   shc       0  0  4 10 19 24 17 14  7  5
## [1] "(dimension, delta) = (8,5)"
##           ESTIMATE
## METHOD      1  2  3  4  5  6  7  8  9 10
##   Mean     10  1  4 12 52 12  6  1  2  0
##   Meanl2   10  1  4 12 52 12  6  1  2  0
##   Median    0  0  5 51 41  3  0  0  0  0
##   Medianl2  0  0  5 52 40  3  0  0  0  0
##   AIC       0  0  0  2 40 27 19  8  2  2
##   BIC       0  0  0 11 69 15  4  1  0  0
##   RIFT.hc  53 10  0 13 13 10  1  0  0  0
##   shc       0  0  3 12 18 28 14 13  9  3
## [1] "(dimension, delta) = (8,6)"
##           ESTIMATE
## METHOD      1  2  3  4  5  6  7  8  9 10 11
##   Mean     10  1  5 10 49 18  5  2  0  0  0
##   Meanl2   10  1  5 10 49 18  5  2  0  0  0
##   Median    0  0  6 39 53  2  0  0  0  0  0
```

```
##   Medianl2  0  0  6 44 48  2  0  0  0  0  0
##   AIC       0  0  0  2 23 43 22  6  3  0  1
##   BIC       0  0  0 11 67 17  4  0  1  0  0
##   RIFT.hc  51 17  1 12 11  6  2  0  0  0  0
##   shc       0  0  4 15 17 22 17 13  9  2  1
## [1] "(dimension, delta) = (8,7)"
##           ESTIMATE
## METHOD     -1  1  2  3  4  5  6  7  8  9 10
##   Mean      0 10  1  3  9 45 21  7  3  1  0
##   Meanl2    0 10  1  3  9 45 21  7  3  1  0
##   Median    0  0  0  1 32 60  6  1  0  0  0
##   Medianl2  0  0  0  1 45 48  5  1  0  0  0
##   AIC       0  0  0  0  4 23 32 25 12  4  0
##   BIC       0  0  0  0  8 63 21  8  0  0  0
##   RIFT.hc   1 53 20  2 15  4  5  0  0  0  0
##   shc       0  0  0  4 16 18 25 13 14  8  2
## [1] "(dimension, delta) = (8,8)"
##           ESTIMATE
## METHOD      1  2  3  4  5  6  7  8  9 10 11 12
##   Mean     10  2  5  6 43 16  9  6  2  0  0  1
##   Meanl2   10  2  5  6 43 16  9  6  2  0  0  1
##   Median    0  0  2 29 63  3  3  0  0  0  0  0
##   Medianl2  0  0  2 45 48  3  2  0  0  0  0  0
##   AIC       0  0  0  2 21 35 20 18  4  0  0  0
##   BIC       0  0  0  5 60 25  7  3  0  0  0  0
##   RIFT.hc  55 21  2 16  4  2  0  0  0  0  0  0
##   shc       0  0  5 13 22 22 15 13  6  3  1  0
## [1] "(dimension, delta) = (8,9)"
##           ESTIMATE
## METHOD      1  2  3  4  5  6  7  8  9 10 11
##   Mean     10  2  4  8 37 22 10  6  1  0  0
##   Meanl2   10  2  4  8 37 22 10  6  1  0  0
##   Median    0  0  1 28 61  9  1  0  0  0  0
##   Medianl2  0  0  1 51 38  9  1  0  0  0  0
##   AIC       0  0  0  4 19 32 26 11  7  1  0
##   BIC       0  0  0  7 54 26 12  1  0  0  0
##   RIFT.hc  51 28  3 12  5  1  0  0  0  0  0
##   shc       0  0  5 12 23 27 15  5  6  4  3
```

```
#stop cluster (parallel computing)
stopCluster(cl)
```

```
print(distribution_name )
```

```
## [1] "True distribution components: t-distrbution (df=3) mixture distribution"
```

```
print(paste(k, 'true clusters:'))
```

```
## [1] "3 true clusters:"
```

```
print('Cluster weights:')
```

```
## [1] "Cluster weights:"
```

```
print(w)
```

```
## [1] 0.1428571 0.2857143 0.5714286
```

The R session information (including the OS info, R version and all packages used):

```
sessionInfo()
```

```
## R version 4.1.2 (2021-11-01)
## Platform: x86_64-apple-darwin17.0 (64-bit)
## Running under: macOS Monterey 12.0.1
##
## Matrix products: default
## LAPACK: /Library/Frameworks/R.framework/Versions/4.1/Resources/lib/libRlapack.dylib
##
## locale:
## [1] en_GB.UTF-8/en_GB.UTF-8/en_GB.UTF-8/C/en_GB.UTF-8/en_GB.UTF-8
##
## attached base packages:
## [1] grid      parallel  stats     graphics  grDevices utils     datasets  methods
## [9] base
##
## other attached packages:
##  [1] arm_1.12-2         lme4_1.1-27.1      Matrix_1.3-4       knitr_1.37
##  [5] sigclust_1.1.0     mixtools_1.2.0     gridExtra_2.3      ggplot2_3.3.5
##  [9] MASS_7.3-54        pracma_2.3.6       mclust_5.4.9       sigclust2_1.2.4
## [13] rstudioapi_0.13    mvnfast_0.2.7      doParallel_1.0.16  iterators_1.0.13
## [17] foreach_1.5.1      Rfast_2.0.6        RcppZiggurat_0.1.6 Rcpp_1.0.8
## [21] pacman_0.5.1
##
## loaded via a namespace (and not attached):
##  [1] minqa_1.2.4            colorspace_2.0-2       ellipsis_0.3.2
##  [4] dynamicTreeCut_1.63-1  htmlTable_2.4.0        XVector_0.34.0
##  [7] base64enc_0.1-3        ggdendro_0.1.23        bit64_4.0.5
## [10] AnnotationDbi_1.56.2   fansi_0.5.0            codetools_0.2-18
## [13] splines_4.1.2          cachem_1.0.6           impute_1.68.0
## [16] Formula_1.2-4          nloptr_1.2.2.3         broom_0.7.12
## [19] WGCNA_1.70-3           cluster_2.1.2          kernlab_0.9-29
## [22] GO.db_3.14.0           png_0.1-7              compiler_4.1.2
## [25] httr_1.4.2             backports_1.4.1        fastmap_1.1.0
## [28] htmltools_0.5.2        tools_4.1.2            coda_0.19-4
## [31] gtable_0.3.0           glue_1.6.1             GenomeInfoDbData_1.2.7
## [34] dplyr_1.0.7            ggthemes_4.2.4         Biobase_2.54.0
## [37] vctrs_0.4.1            Biostrings_2.62.0      preprocessCore_1.56.0
## [40] nlme_3.1-153           xfun_0.30              fastcluster_1.2.3
## [43] stringr_1.4.0          lifecycle_1.0.1        zlibbioc_1.40.0
## [46] scales_1.1.1           RColorBrewer_1.1-2     yaml_2.3.4
## [49] memoise_2.0.1          rpart_4.1-15           segmented_1.3-4
## [52] latticeExtra_0.6-29    stringi_1.7.6          RSQLite_2.2.10
## [55] highr_0.9              S4Vectors_0.32.3       blme_1.0-5
## [58] checkmate_2.0.0        BiocGenerics_0.40.0    boot_1.3-28
## [61] GenomeInfoDb_1.30.1    rlang_1.0.2            pkgconfig_2.0.3
## [64] matrixStats_0.61.0     bitops_1.0-7           evaluate_0.15
## [67] lattice_0.20-45        purrr_0.3.4            htmlwidgets_1.5.4
## [70] bit_4.0.4              tidyselect_1.1.1       magrittr_2.0.2
## [73] R6_2.5.1               IRanges_2.28.0         generics_0.1.1
## [76] Hmisc_4.6-0            DBI_1.1.2              pillar_1.6.4
## [79] foreign_0.8-81         withr_2.4.3            survival_3.2-13
## [82] KEGGREST_1.34.0        abind_1.4-5            RCurl_1.98-1.6
```

```
## [85] nnet_7.3-16            tibble_3.1.6           crayon_1.4.2
## [88] utf8_1.2.2             rmarkdown_2.13         jpeg_0.1-9
## [91] data.table_1.14.2      blob_1.2.2             forcats_0.5.1
## [94] digest_0.6.29          tidyr_1.1.4            stats4_4.1.2
## [97] munsell_0.5.0

Sys.time()

## [1] "2022-06-03 01:47:02 BST"
```