Journal

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```
devtools::load_all()
library(WASABI)
library(BNPmix)
library(mcclust)
library(salso)
library(superheat)
library(ggplot2)
```

Test Binder.Rcpp function. Aug 01

1. Check the accuracy of the function.

```
cls1 <- matrix(sample(0:3,25,replace = TRUE), nrow = 1)
cls2 <- matrix(sample(0:6,25,replace = TRUE), nrow = 1)
salso_loss <- salso::binder(cls1,cls2)
print(salso_loss)
```

```
## [1] 0.2944
```

```
rcpp_loss <- Binder_compute_Rcpp(cls1,cls2, 4, 7)
print(rcpp_loss)
```

```
## [1] 0.2944
```

2. Compare the speed.

```
library(microbenchmark)
microbenchmark(
  salso = salso::binder(cls1,cls2),
  cpp = Binder_compute_Rcpp(cls1,cls2, 4, 7),
  times = 100L
)
```

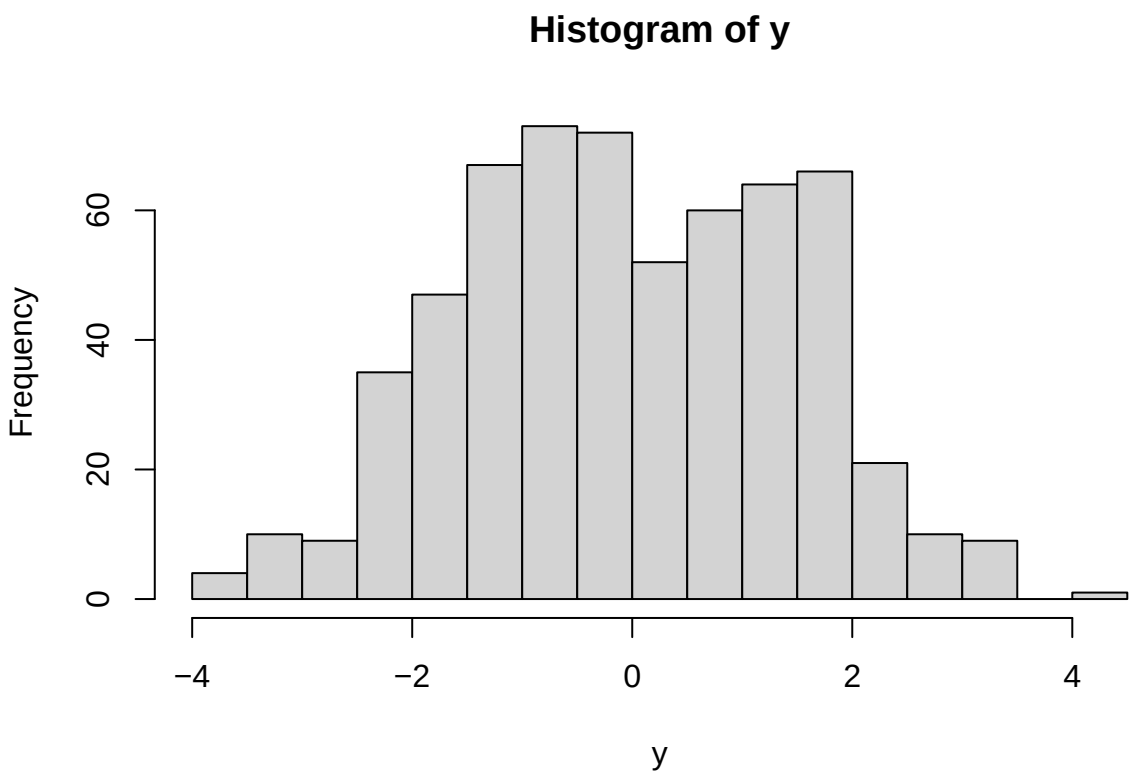
```
## Warning in microbenchmark(salso = salso::binder(cls1, cls2), cpp =
## Binder_compute_Rcpp(cls1, : less accurate nanosecond times to avoid potential
## integer overflows
```

```
## Unit: microseconds
##   expr   min    lq     mean median     uq    max neval
##  salso 9.102 9.471 10.53413  9.840 10.660 29.889   100
##    cpp 3.116 3.485  3.99709  3.854  4.346 13.407   100
```

Testing "loss = VI"

Let's first consider a simple bimodal (univariate) example:

```r
set.seed(12345)
mu <- c(-1.1, 1.1)
prop <- c(0.5, 0.5)
n <- 600
components <- sample(1:2, size = n, replace = TRUE, prob = prop)
y <- rnorm(n, mean = mu[components], sd = 1)
hist(y, breaks = 20)
```



We fit a Bayesian mixture model (you can use your own code, or a package such as BNPmix):

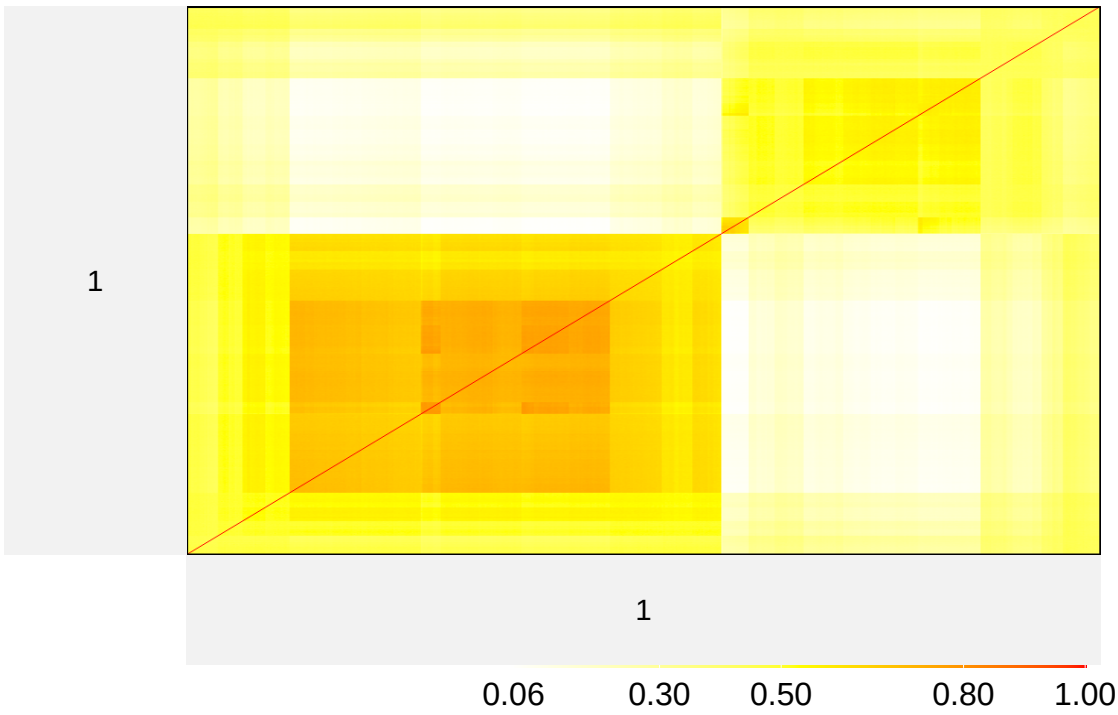
```r
est_model <- BNPmix::PYdensity(y = y,
                               mcmc = list(niter = 15000,
                                           nburn = 5000,
                                           model = "LS",
                                           print_message = FALSE),
                               output = list(out_type = "FULL",
                                             out_param = TRUE))
cls.draw = est_model$clust
z_minVI <- salso::salso(cls.draw)
table(z_minVI)
```

```
## z_minVI
##   1
## 600
```

The minVI estimator is the partition with one cluster.

```r
psm=mcclust::comp.psm(cls.draw+1)
superheat::superheat(psm,
                     heat.pal = c("white", "yellow", "red"),
                     heat.pal.values = c(0,.5,1),
```

```
                    pretty.order.cols = TRUE,
                    pretty.order.rows = TRUE,
                    membership.rows = z_minVI,
                    membership.cols = z_minVI,
                    bottom.label.text.size = 4,
                    left.label.text.size = 4)
```



However the posterior similarity matrix shows a potential two-cluster pattern, with moderate posterior uncertainty. Let's use WASABI to summarize the posterior with multiple point estimates:

```
out_WASABI <- WASABI.ext(cls.draw, psm = psm, L = 2,
                         method.init = "topvi", method = "salso", loss = "VI")
```

To explore multiple initializations, we can use `WASABI_multistart`. We can also use the `mini.batch` option, to run the algorithm on a subset of the mcmc draws (for example: 250). When using `mini.batch` it's advisable to reduce the number of `max.iter` (for example to 10) and allow a small number of `extra.iter` that are run with the full dataset after the mini-batch part. This allows to allocate each MCMC sample in `cls.draw` to one of the particles/regions of attractions, and for the algorithm to stabilize after using mini-batch.

Note, the multi-core option relies on `parallel::mclapply` which only works on MacOS and Linux. When running `WASABI_multistart` on Windows machines, set `ncores = 1` (which is also the default).

```
out_WASABI_ms <- WASABI_multistart.ext(cls.draw, psm = psm, L = 2,
                                       multi.start = 20, ncores = 4,
                                       mini.batch = 250,
                                       max.iter = 10, extra.iter = 5,
                                       method.init = "++", method = "salso",
                                       loss = "VI")
```

We should use the solution achieving the smallest Wasserstein distance (`wass.dist`):

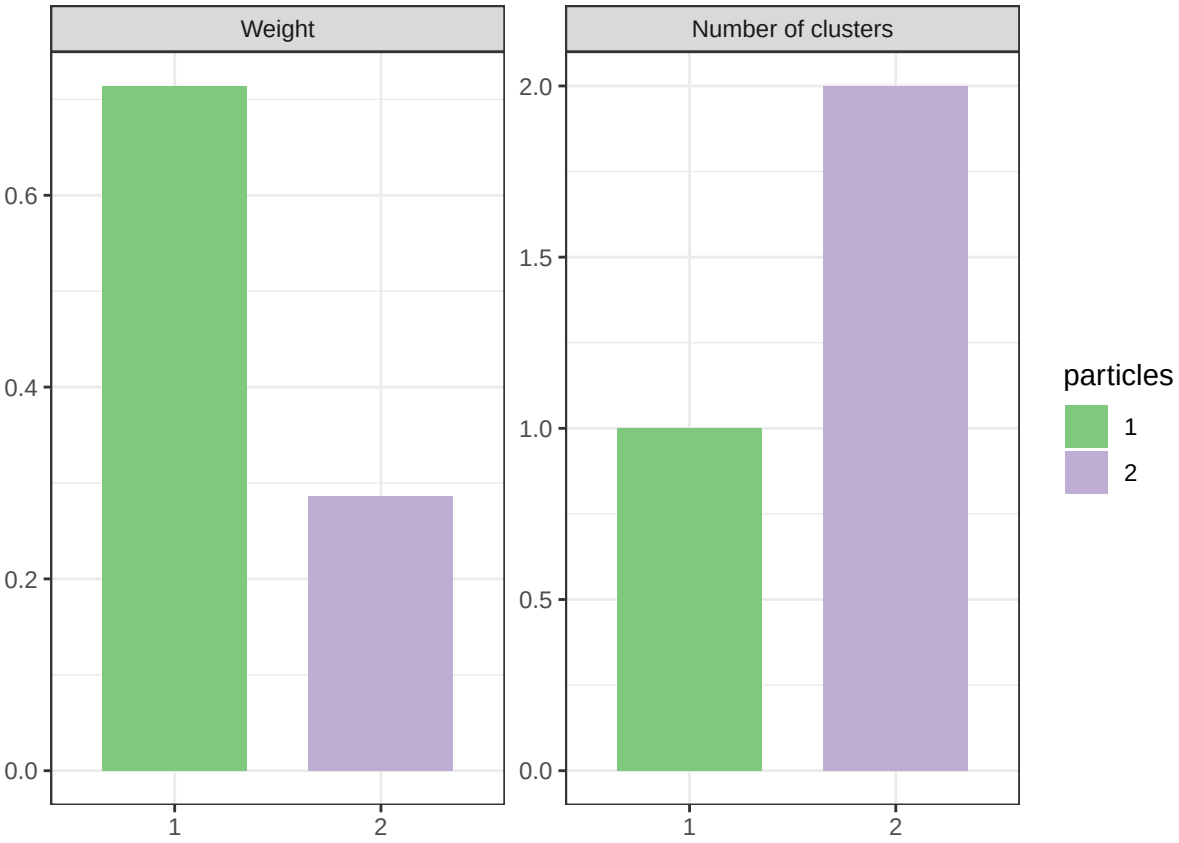
```
if(out_WASABI_ms$wass.dist < out_WASABI$wass.dist){
  out_WASABI <- out_WASABI_ms
```

```
}
```

We can now visualize the particles, and there are different options:

- visualize the weight for each particle and their number of clusters

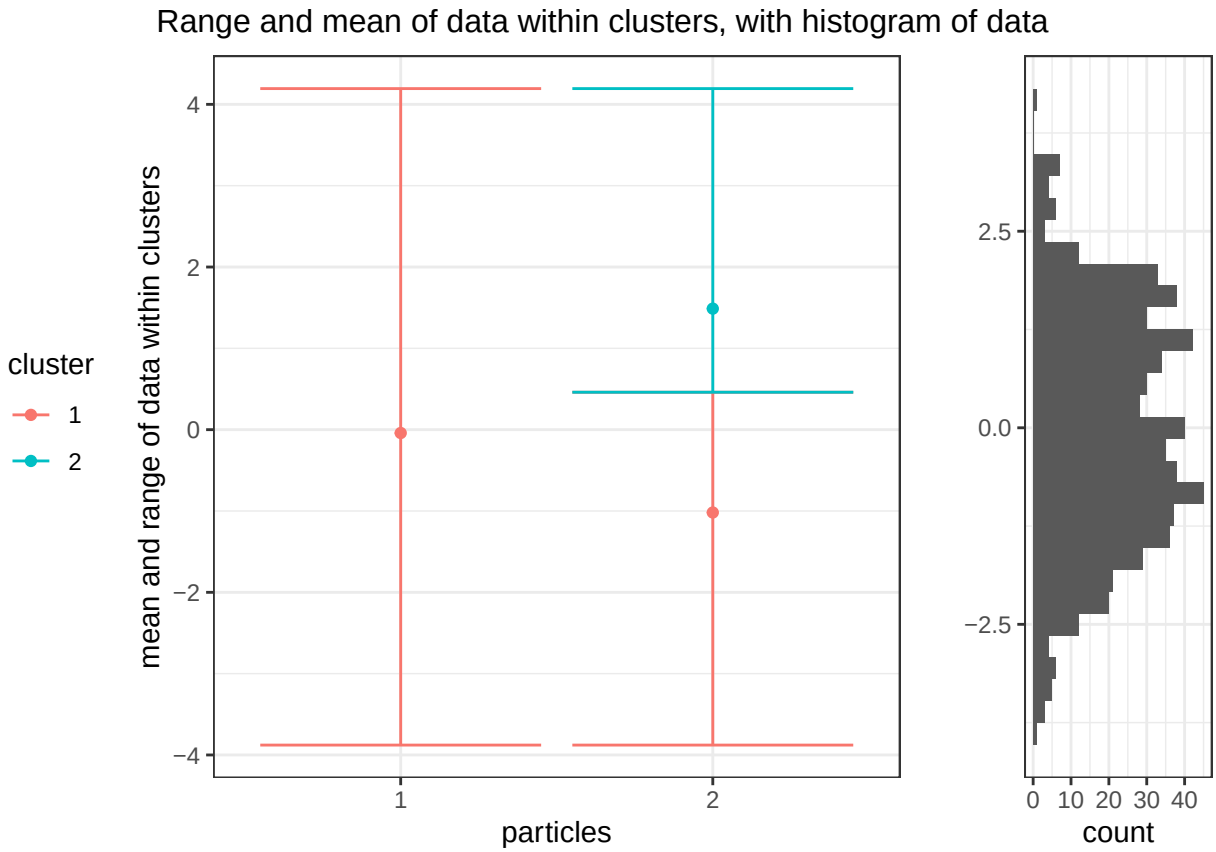
```
ggsummary(out_WASABI)
```



- visualize the the range for each particle's cluster, side by side with the histogram of the data:

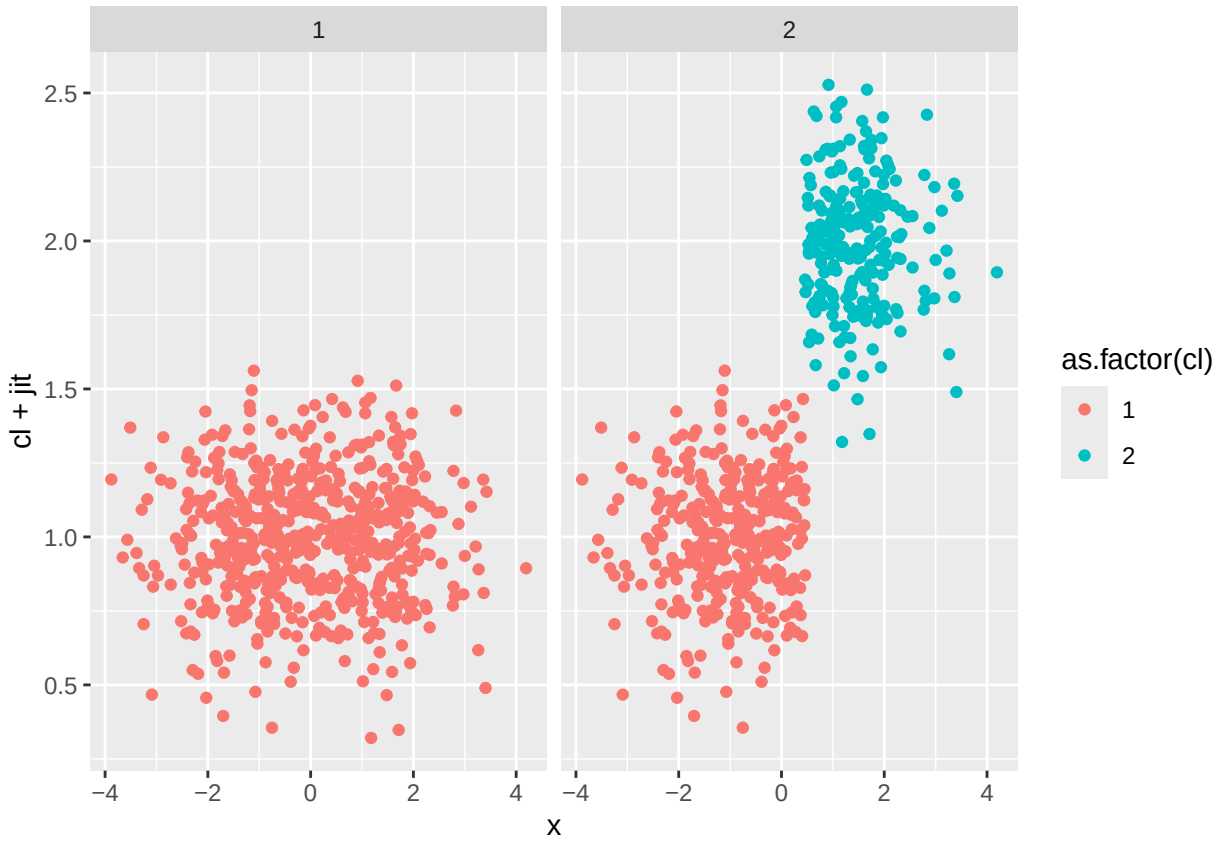
```
ggrange_hist(out_WASABI, y)
```

```
## `stat_bin()` using `bins = 30`. Pick better value with `binwidth`.
```



- visualize the data with the particles' cluster assignment, as a scatterplot (by adding some jitter in the y-axis):

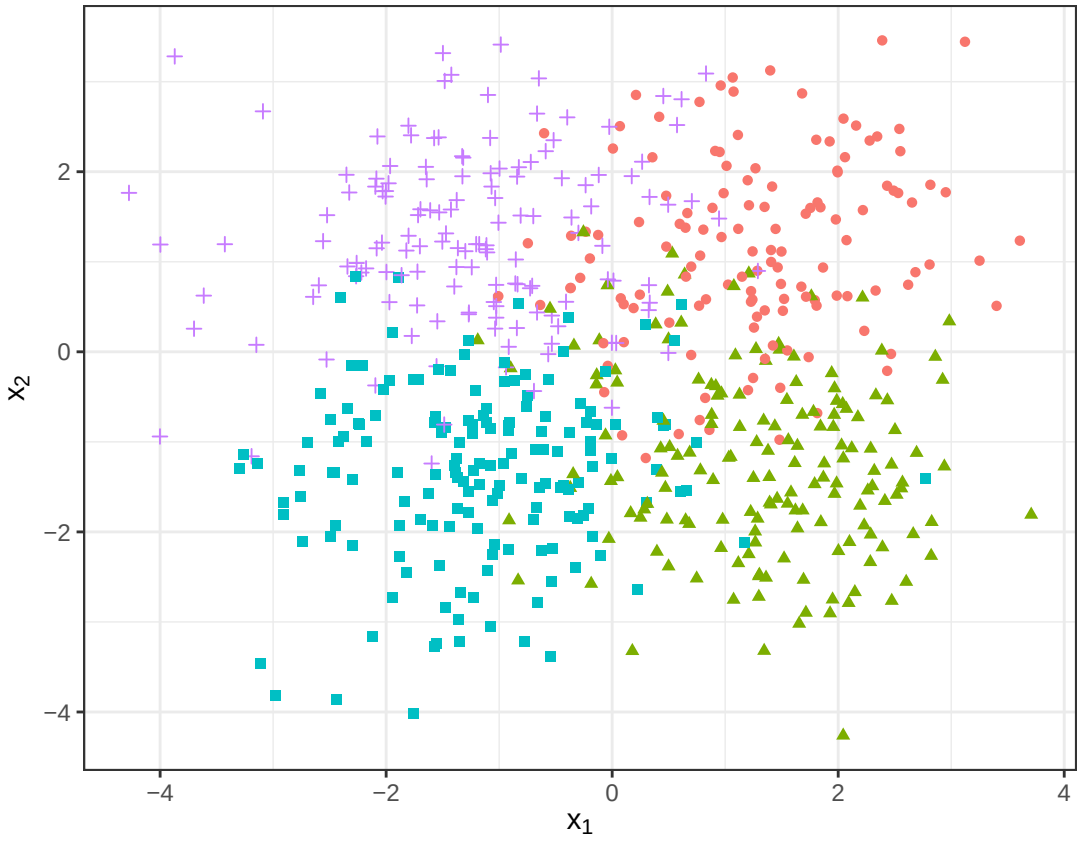
```
ggscatter_grid(out_WASABI, y)
```




```
m = 1.25
n = 600
p = 2
Kt = 4

set.seed(4321)

Y=matrix(rnorm(p*n),n,p)
usim=runif(n)
ind=ifelse(usim<1/4,1,ifelse(usim<1/2,2,ifelse(usim<3/4,3,4)))
Y[ind==1,] = Y[ind==1,] +m
Y[ind==2,1] = Y[ind==2,1] + m; Y[ind==2,2] = Y[ind==2,2] - m;
Y[ind==3,] = Y[ind==3,] -m
Y[ind==4,1] = Y[ind==4,1] - m; Y[ind==4,2] = Y[ind==4,2] + m;

cls.true = ind
```

```
library(ggplot2)
ggplot() +
  geom_point(aes(x = Y[,1],
                 y = Y[,2],
                 colour = as.factor(cls.true),
                 shape  = as.factor(cls.true))) +
  theme_bw() + guides(colour=guide_legend(title="Cluster"),
                      shape = guide_legend(title="Cluster")) +
```

```
  xlab(expression("x"[1])) + ylab(expression("x"[2]))
```



Two-dimensional data

Let's run the MCMC:

```
set.seed(4321)
### Parameters for DP mixture
alpha = 1
# using Fraley and Raftery recommendation
a_x=rep((p+2)/2,p)
khat = 4
b_x= rep(mean(apply(Y,2,var))/(khat^(2/p))/2,p)

### Parameters for MCMC function
S=10000
thin = 1
tot = S*thin
burnin=5000

est_model <- BNPmix::PYdensity(y = Y,
                        mcmc = list(niter = burnin + tot,
                                    nburn = burnin,
                                    model = "DLS",
                                    hyper = FALSE
                                    ),
                        prior = list(
                          k0 = 0.1*rep(1,p),
                          a0 = a_x,
```

```
                          b0 = b_x,
                          strength = alpha,
                          discount = 0),
                        output = list(out_type = "FULL", out_param = TRUE))
```

```
## Completed:   1500/15000 - in 0.522845 sec
## Completed:   3000/15000 - in 1.00934 sec
## Completed:   4500/15000 - in 1.48387 sec
## Completed:   6000/15000 - in 2.10978 sec
## Completed:   7500/15000 - in 2.72161 sec
## Completed:   9000/15000 - in 3.40499 sec
## Completed:   10500/15000 - in 4.10516 sec
## Completed:   12000/15000 - in 4.7655 sec
## Completed:   13500/15000 - in 5.40368 sec
## Completed:   15000/15000 - in 6.06662 sec
##
## Estimation done in 6.06666 seconds
```

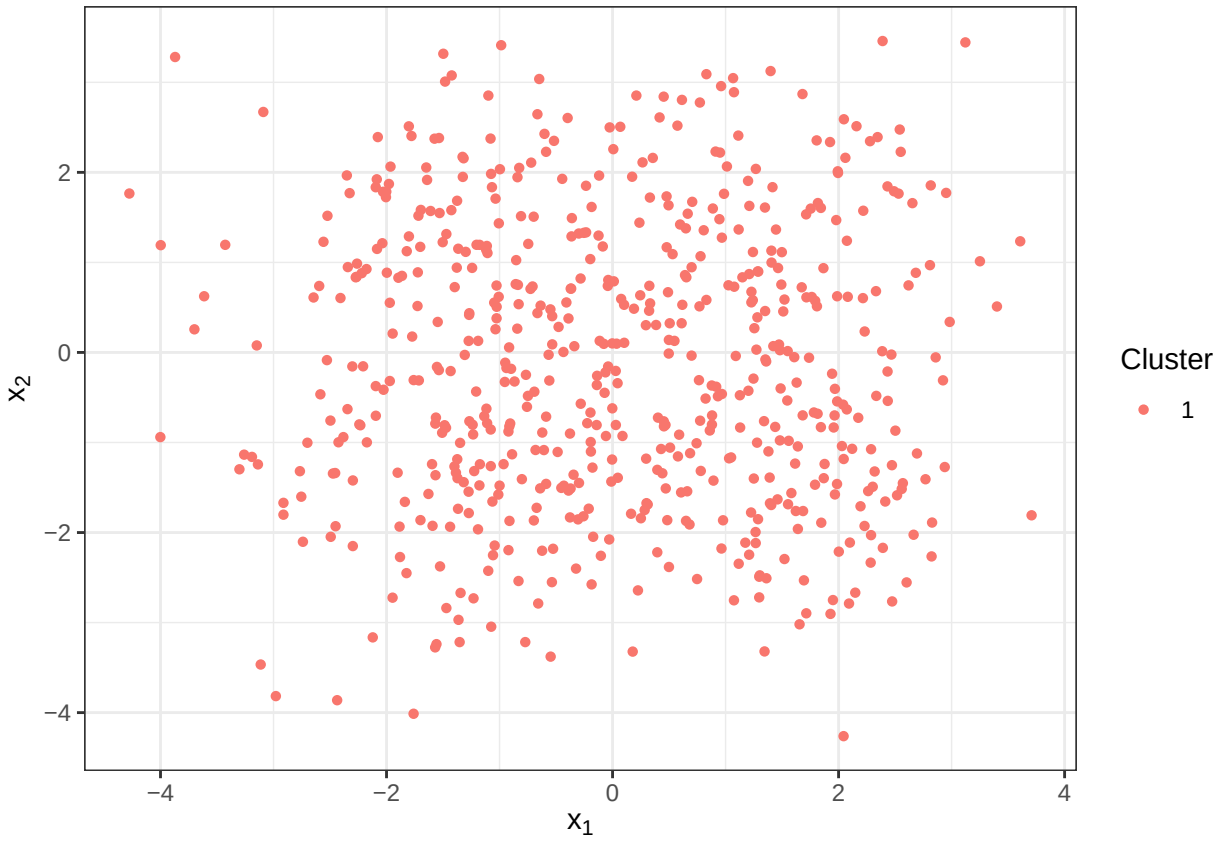
```
cls.draw = est_model$clust
psm=mcclust::comp.psm(cls.draw+1)
```

Let's inspect the minVI estimator:

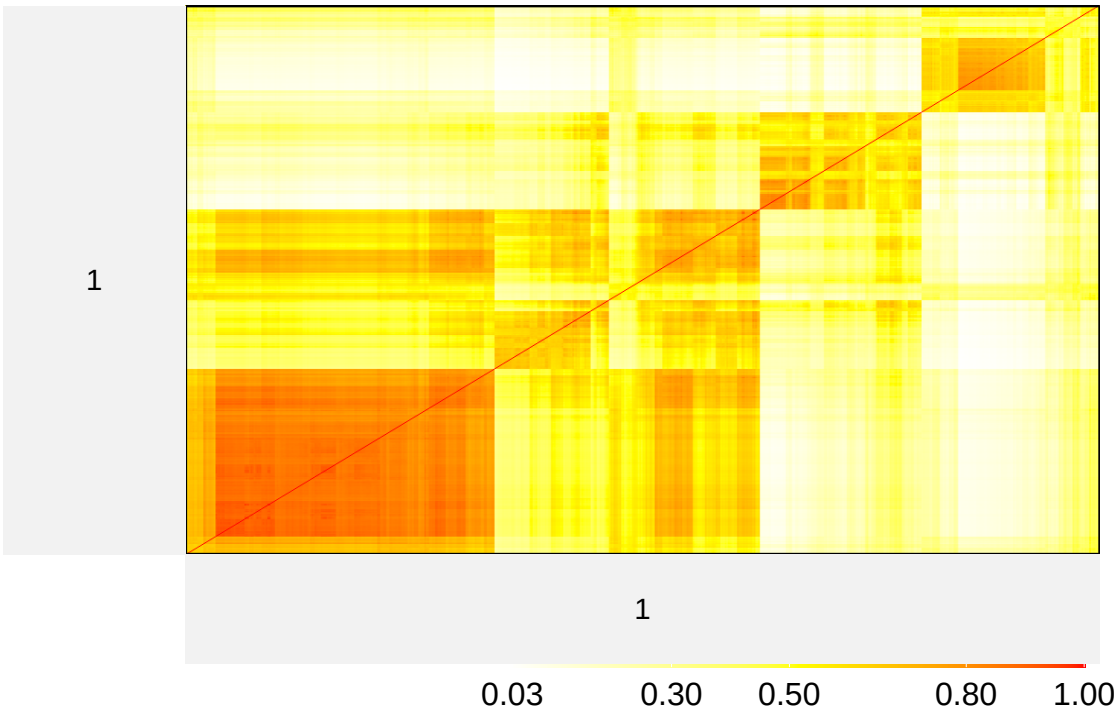
```
z_minVI <- salso::salso(cls.draw)
table(z_minVI)
```

```
## z_minVI
##   1
## 600
```

```
df = data.frame(x1 = Y[,1],
                x2 = Y[,2],
                Cluster = z_minVI)
df$Cluster = as.factor(df$Cluster)

ggplot(df)+
  geom_point(aes(x = x1, y = x2, color = Cluster, shape = Cluster)) +
  ylab(expression("x"[2]))+xlab(expression("x"[1]))+
  theme_bw()
```




```
superheat::superheat(psm,
                     heat.pal = c("white", "yellow", "red"),
                     heat.pal.values = c(0,.5,1),
                     pretty.order.cols = TRUE,
                     pretty.order.rows = TRUE,
                     membership.rows = z_minVI,
                     membership.cols = z_minVI,
                     bottom.label.text.size = 4,
                     left.label.text.size = 4)
```

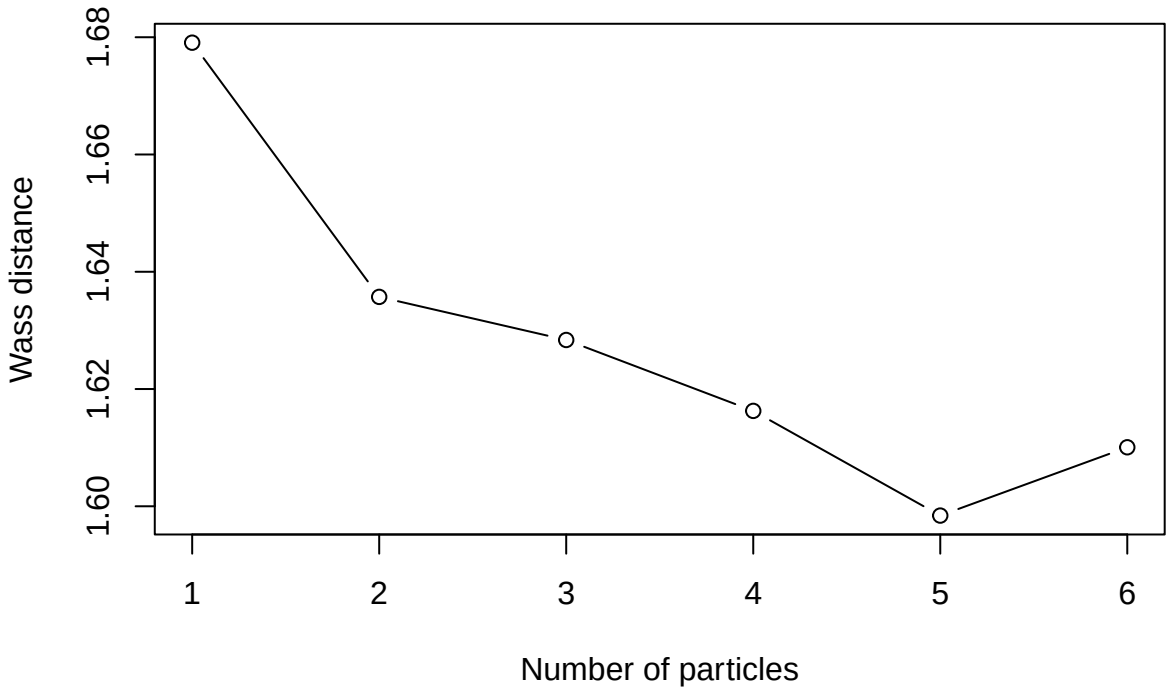


Let's use the `elbow` function to choose the number of particles L with the elbow method:

```
set.seed(123)
out_elbow <- elbow.ext(cls.draw, L_max = 6, psm = psm,
                   multi.start = 1,
                   method.init = "topvi", method = "salso",
                   loss = "VI")
```

```
## Completed  1 / 6
## Completed  2 / 6
## Completed  3 / 6
## Completed  4 / 6
## Completed  5 / 6
## Completed  6 / 6
```

```
plot(out_elbow$wass_vec, type = "b", ylab = "Wass distance", xlab = "Number of particles")
```



We can then choose $L = 3$.

```
L = 3
output_WASABI <- out_elbow$output_list[[L]]
```

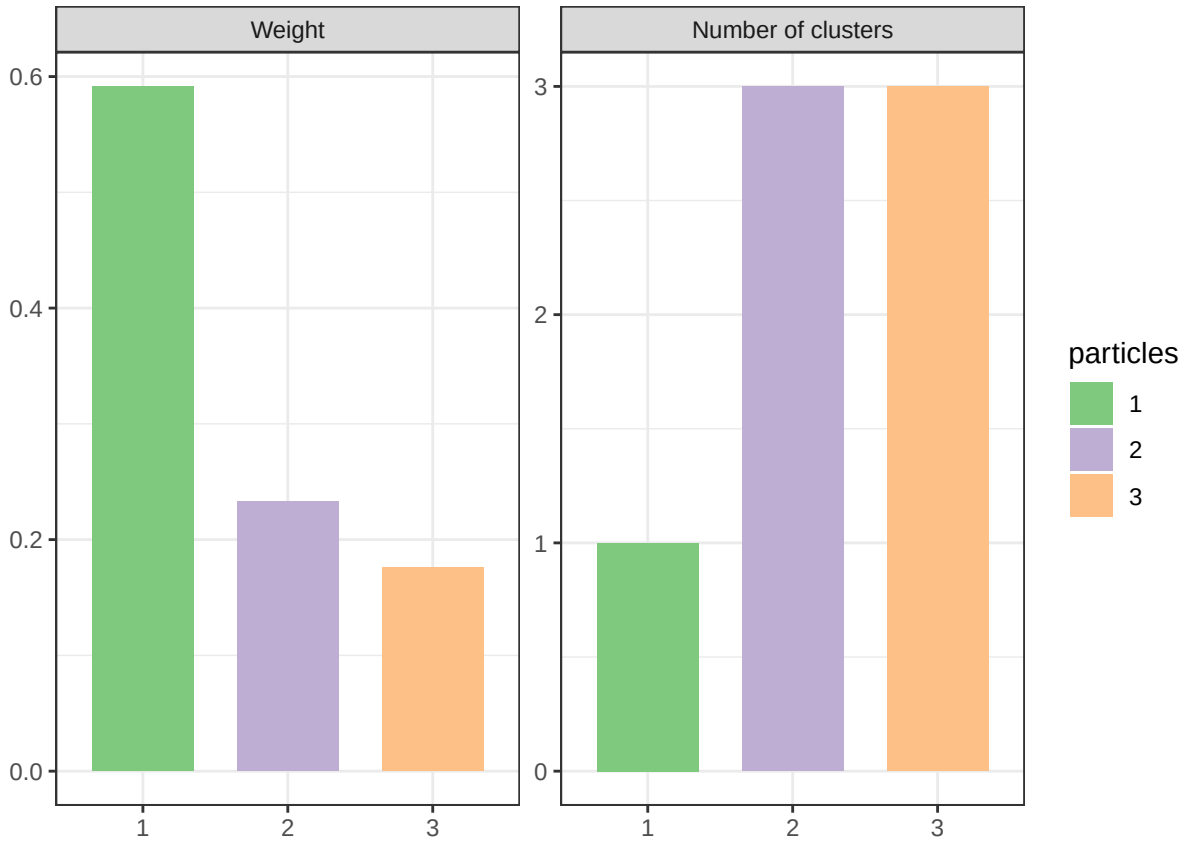
Once the value of L is chosen, we can run another set of initializations to see if we can find a better approximation:

```
output_WASABI_mb = WASABI_multistart.ext(cls.draw, psm,
                                         multi.start = 25, ncores = 4,
                                         method.init ="++", add_topvi = FALSE,
                                         method="salso", L=L,
                                         mini.batch = 500,
                                         max.iter= 10, extra.iter = 5,
                                         suppress.comment=FALSE,
                                         swap_countone = TRUE,
                                         seed = 54321, loss = "VI")
```

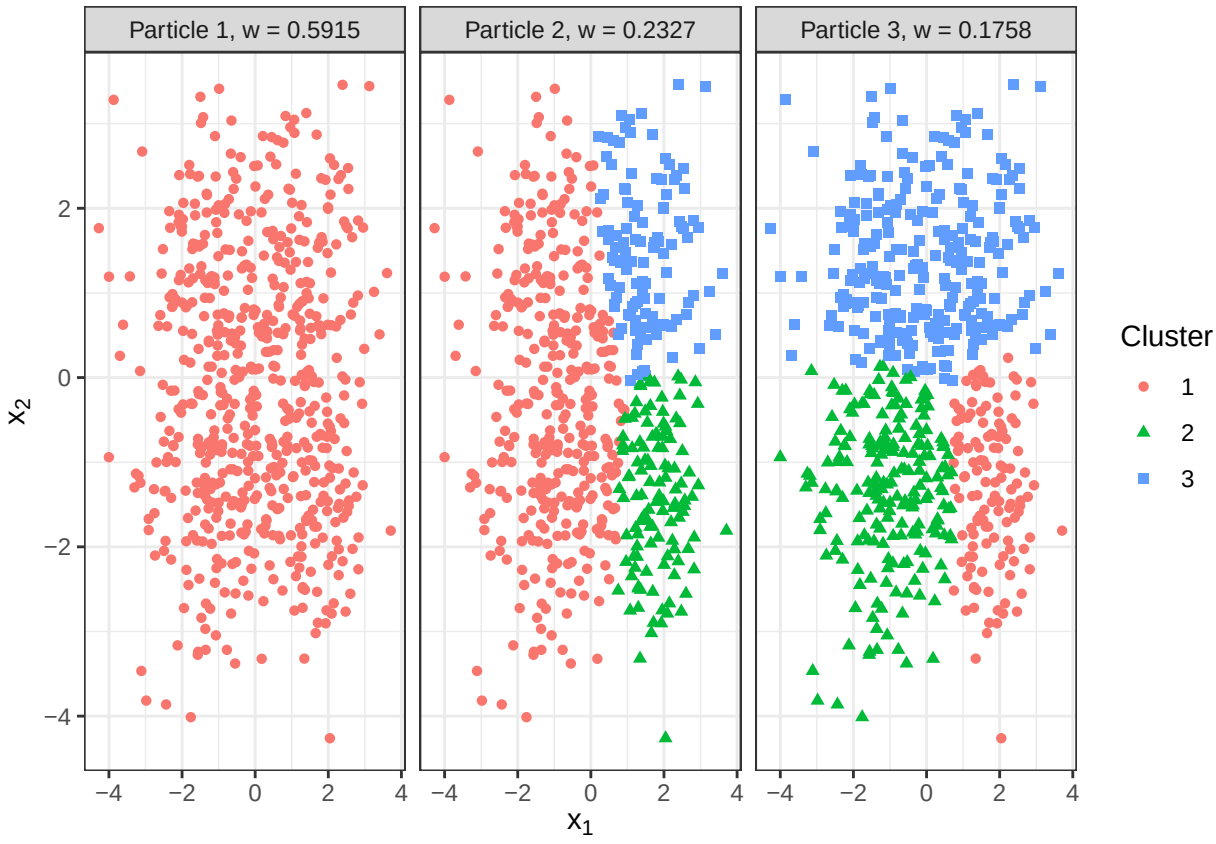
```
if(output_WASABI_mb$wass.dist < output_WASABI$wass.dist){
  output_WASABI <- output_WASABI_mb
}
print(output_WASABI$wass.dist)
```

```
## [1] 1.614746
```

```
ggsummary(output_WASABI)
```



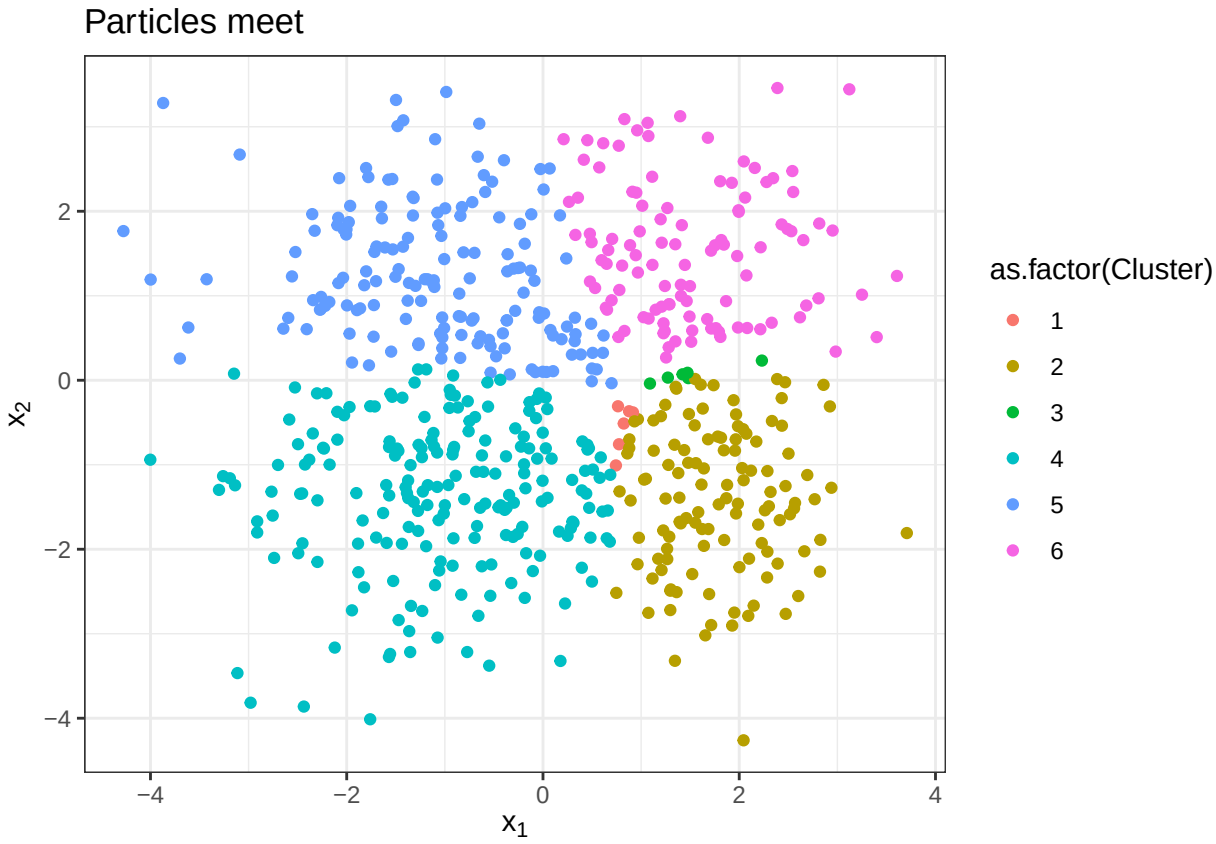

```
ggscatter_grid2d(output_WASABI, Y)
```



We can also find the meet of the particles:

```
output_meet = cls.meet(output_WASABI$particles)
z_meet = output_meet$cls.m
```

```
df_tmp <- data.frame(x1 = Y[,1],
           x2 = Y[,2],
           Cluster = z_meet)
ggplot(df_tmp) +
  geom_point(aes(x = x1,y = x2,
                 color = as.factor(Cluster))) +
  theme_bw() +
  xlab(expression("x"[1])) + ylab(expression("x"[2]))+
  ggtitle("Particles meet")+theme(legend.box = "horizotal")
```



Let's now look at the WASABI-approximation of the posterior similarity matrix, which is defined on the meet's clusters:

```
psm.m = psm.meet(z_meet, output_WASABI)
Km <- nrow(psm.m)
colnames(psm.m) <- 1:Km; rownames(psm.m) <- 1:Km
```

Let's plot it and simultaneously compare the meet with one of the particles (e.g. 2) We will now import `dplyr` to use the pipe, but equivalent base R code can be used:

```
library(dplyr)
```

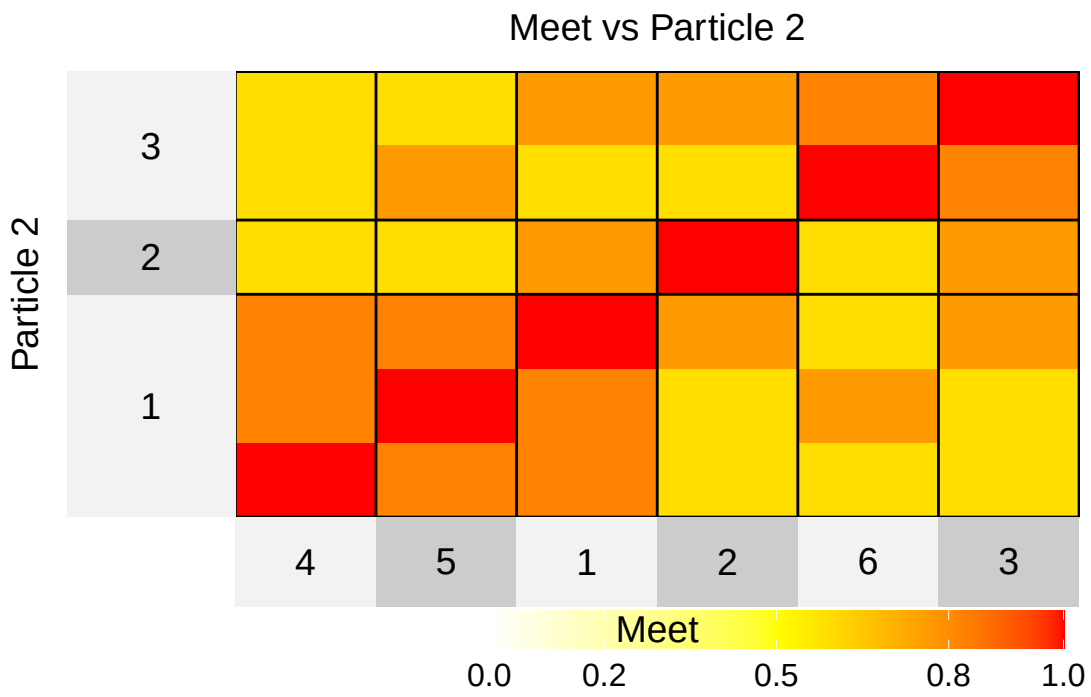
```
##
## Attaching package: 'dplyr'
```

```
## The following objects are masked from 'package:stats':
##
##     filter, lag
```

```
## The following objects are masked from 'package:base':
##
##     intersect, setdiff, setequal, union
```

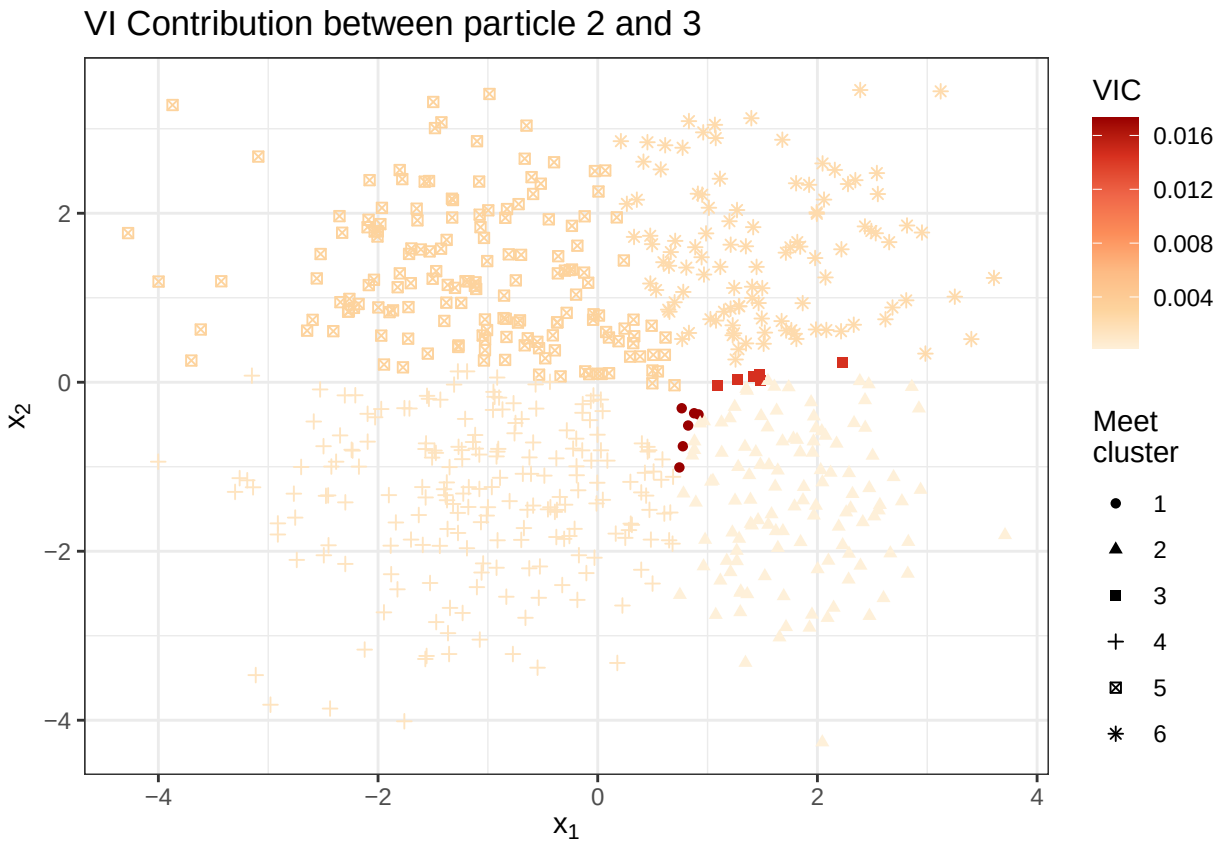
```
i = 2
part_cl = output_WASABI$particles[i,]
tb_meettop = table(part_cl,z_meet)
lbs_top = rownames(tb_meettop)[as.factor(apply(tb_meettop, 2, which.max))]

tmp = reshape2::melt(as.matrix(as.data.frame.matrix(tb_meettop))) %>%
  arrange(Var1,-value) %>% filter(value > 0) %>% pull(Var2)
```

```
superheat::superheat(psm.m,
                     title = paste('Meet vs Particle',i),
                     heat.pal = c("white", "yellow", "red"),
                     heat.pal.values = c(0,.5,1),
                     heat.lim = c(0,1), # this is important!!
                     row.title = paste('Particle',i),
                     column.title = paste('Meet'),
                     membership.rows = as.numeric(lbs_top),
                     order.cols = tmp,
                     order.rows = tmp)
```



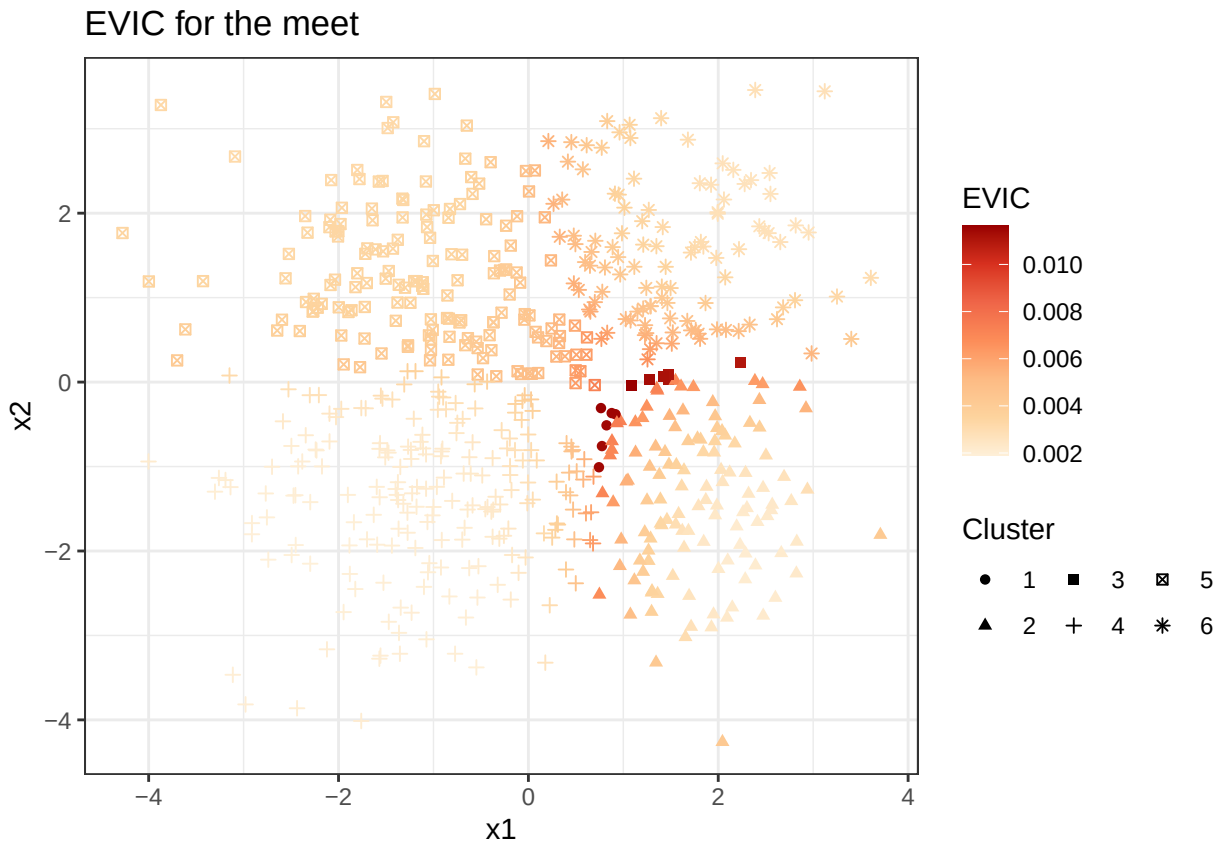
We can also look at the VI contribution of each point when comparing two partitions (e.g. particle 2 and particle 3):

```
VIC_23 = vi.contribution(output_WASABI$particles[2,],output_WASABI$particles[3,])

ggplot() +
  geom_point(aes(x = Y[,1],
                 y = Y[,2],
                 color = VIC_23,
                 shape = as.factor(z_meet))) +
  theme_bw() +
  scale_color_distiller(name = "VIC",palette = "OrRd",direction = 1)+
  guides(shape = guide_legend(title="Meet\ncluster")) +
  xlab(expression("x"[1])) + ylab(expression("x"[2])) +
  ggtitle("VI Contribution between particle 2 and 3")
```



Or we can inspect the Expected VI (EVI) for a given estimator, such as the meet of the particles

```
ec_full = evi.contribution(cls.draw, z_meet)

data.frame(x1 = Y[,1],
           x2 = Y[,2],
           VIC_full = ec_full,
           Cluster = as.factor(z_meet)) %>%
  ggplot() +
  geom_point(aes(x = x1,y = x2,
                 color = VIC_full,
                 shape = Cluster)) +
  scale_color_distiller("EVIC",palette = "OrRd",direction = 1)+
  # scale_shape_manual(values= c(18, 15,4, 8,19, 10,17))+
  theme_bw()+theme(legend.box = "horizotal") +
  guides(
    shape = guide_legend(title.position = "top", ncol = 3)
  )+ggtitle("EVIC for the meet")
```


EVIC for the meet
x2
x1
2
0
−2
−4
−4
−2
0
2
4
EVIC
0.010
0.008
0.006
0.004
0.002
Cluster
1
2
3
4
5
6