EM

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Contents

1 Example of model based clustering with two groups

We will use a toy example to explain the EM algorithm for model based clustering.

- Two groups $k = 1, 2$
- Univariate observations are observed x_i with $i = 1, \ldots, n$
- The data of group j follows a normal distribution $N(u_j, 1)$ with a variance $\sigma^2 = 1$ and a mean μ_j that depends on the group $j = 1, 2$.

The data follows the following mixture distribution:

$$f(x) = \pi_1 f_1(x) + (1 - \pi_1) f_2(x)$$

With

- π_1 the probability that a random sample from the population belongs to group 1
- $f_1(x)$ the density of the data in group 1, i.e. $N(\mu_1, 1)$
- $f_2(x)$ the density of the data in group 2, i.e. $N(\mu_2, 1)$.
- Unknowns? Group membership z_i, the group means μ_j and the proportion of subjects in the population of group 1 π_1 are unknown.

We can estimate the model parameters $\boldsymbol{\theta} = [\mu_1, \mu_2, \pi_1]^T$ using maximum likelihood.

$$L\left(\mu_1, \mu_2, \pi_1 | \mathbf{X}\right) = \prod_{i=1}^{n} \left[\pi_1 f_1(x_i) + (1 - \pi_1) f_2(x_i)\right]$$

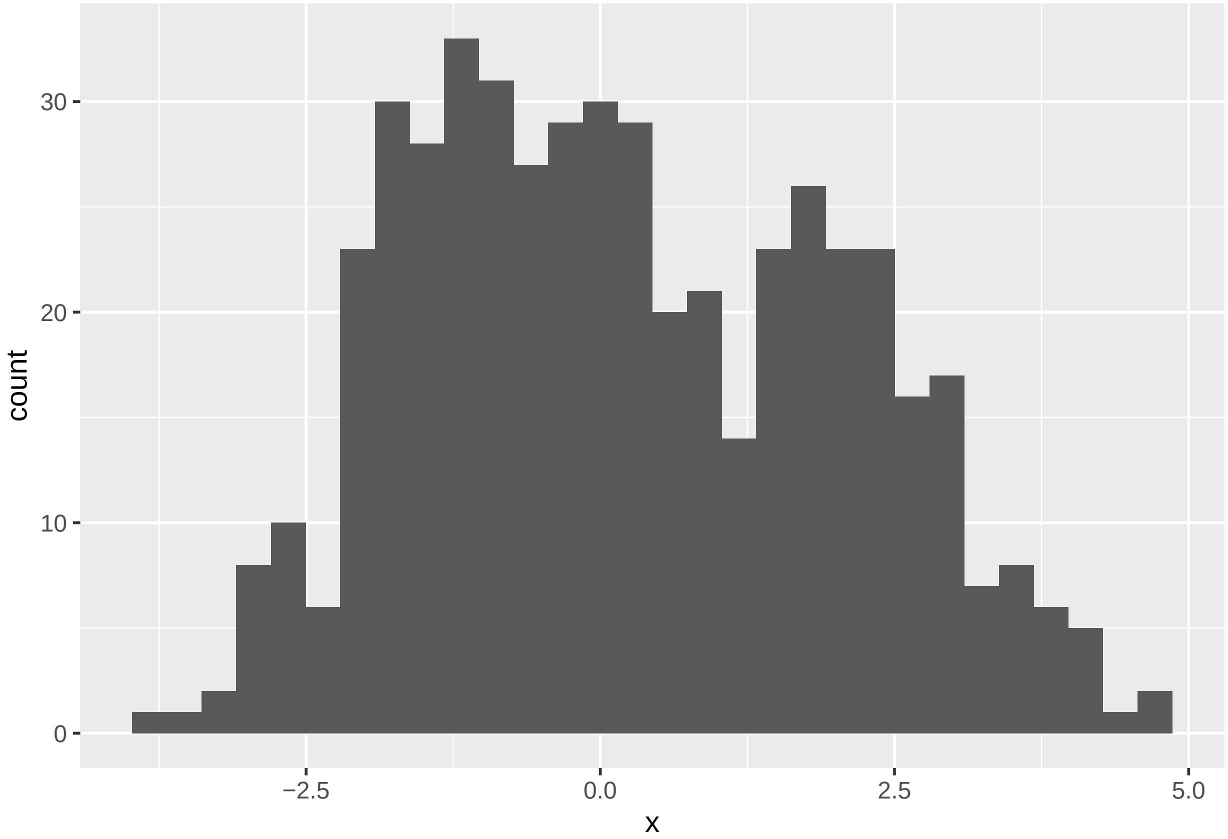
It is easier to maximise the log-likelihood:

$$l\left(\mu_1,\mu_2,\pi_1|\mathbf{X}\right) = \sum_{i=1}^{n} \log\left[\pi_1 f_1(x_i) + (1-\pi_1) f_2(x_i)\right]$$

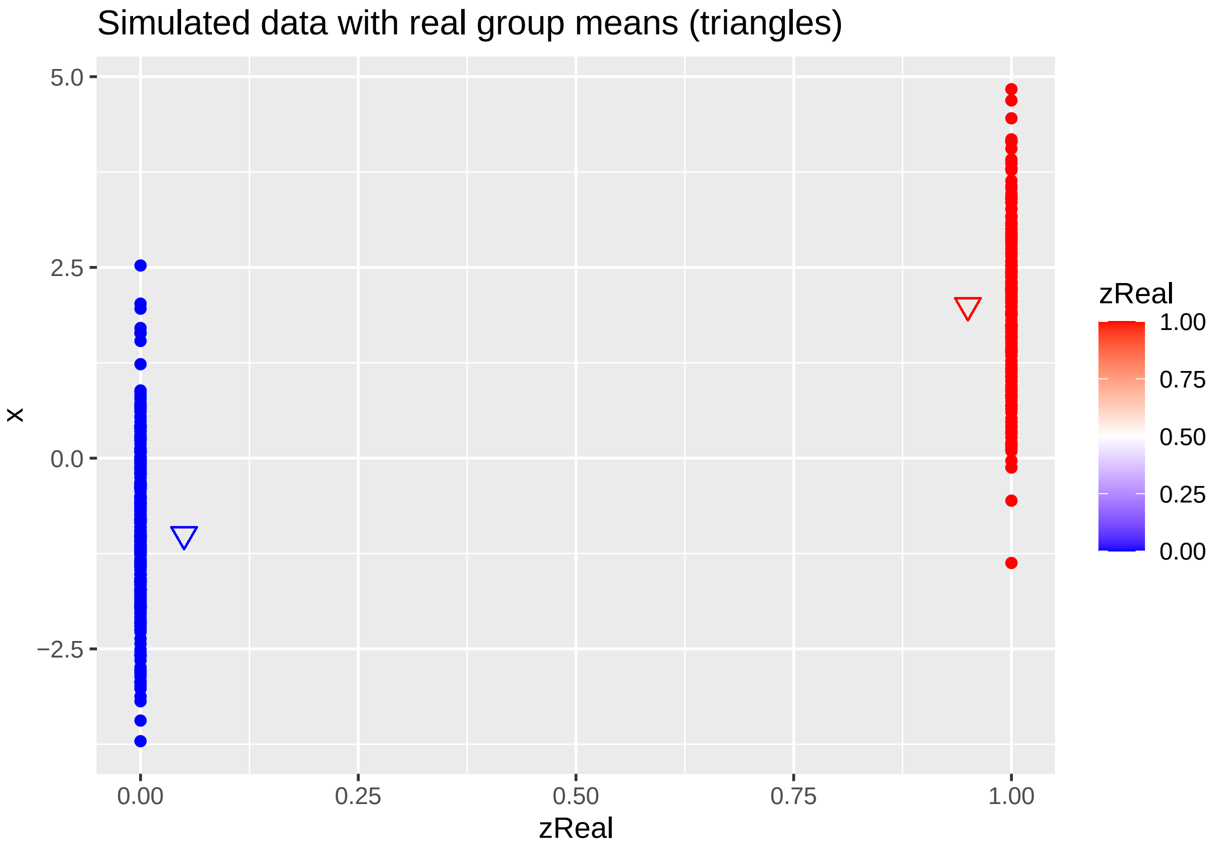
The optimisation is difficult because we have to take the log of a sum and the likelihood does not factorise further.

2 Simulate toy Data

```
library(tidyverse)
mu1Real <- 2
mu2Real <- -1
pi1Real = .4
set.seed(114)
zReal <- rbinom(500, size = 1, prob = pi1Real)
x <- ifelse(zReal==1, rnorm(500,mean=mu1Real), rnorm(500, mean=mu2Real))
data.frame(x) %>%
  ggplot(aes(x = x)) +
  geom_histogram()
```



```
data.frame(x,zReal) %>%
    ggplot(aes(zReal,x,color=zReal)) +
    geom_point() +
    scale_colour_gradient2(
      low = "blue",
      mid="white",
      high="red",
      midpoint = 0.5) +
      geom_point(x=.95,y=mu1Real, shape=25, col="red", size=3) +
      geom_point(x=0.05,y=mu2Real, shape=25, col="blue", size=3) +
      ggtitle("Simulated data with real group means (triangles)")
```



3 Parameter estimation

If we would know the cluster membership z_{i1}

$$z_{i1} = \begin{cases} 1 & \text{if } x_i \text{ belongs to group 1} \\ 0 & \text{if } x_i \text{ belongs to group 2} \end{cases}$$

with z_{i1} follows a Bernoulli distribution

$$B(\pi_1) = \pi_1^{z_{i1}}(1-\pi_1)^{(1-z_{i1})}$$

Then the density of x_i given z_{i1} becomes

$$f(x_i|z_{i1}) = f_1(x_i)^{z_{i1}} f_2(x_i)^{1-z_{i1}}$$

and the joint distribution of z_{i1} and x_i then becomes

$$\begin{aligned} f(x_i, z_{i1}) &= f(x_i|z_{i1})f(z_{i1}) && (1) \\ &= f_1(x_i)^{z_{i1}} f_2(x_i)^{1-z_{i1}} \pi_1^{z_{i1}}(1-\pi_1)^{(1-z_{ik})} && (2) \end{aligned}$$

and the log likelihood of the complete data becomes

$$l\left(\mu_1, \mu_2, \pi_1 | \mathbf{X}, \mathbf{Z}\right) = \sum_{i=1}^{n} z_{i1} \log\left[\pi_1 f_1(x_i)\right] + (1 - z_{i1}) \log\left[(1 - \pi_1) f_2(x_i)\right]$$

- Note, that in the notation of the Frayley and Raftery (1998) $z_2 = 1 - z_1$ and $\pi_2 = 1 - \pi_1$

3.1 EM algorithm

If we would know the cluster membership, we could estimate all model parameters based on the complete likelihood.

Note, that the complete likelihood also factorises nicely!

However, the cluster membership is unknown.

The EM algorithm has been developed for missing data problems.

It is an iterative algorithm that consists of two steps:

1. E-step: calculate the expected log likelihood given the data and the current model parameter estimates
2. M-step: maximise the expected log-likelihood
3. Iterate between 1 and 2 until convergence.

3.1.1 E-step

In iteration m+1

$$\begin{aligned} Q\left(\mu_1, \mu_2, \pi_1 | \mathbf{X}, \mathbf{Z}\right) &= E\left[l\left(\mu_1, \mu_2, \pi_1 | \mathbf{X}, \mathbf{Z}\right) | \mathbf{X}, \mu_1 = \mu_1^m, \mu_2 = \mu_2^m, \pi_1 = \pi_1^m\right] \\ &= E\left[\sum_{i=1}^{n} z_{i1} \log\left[\pi_1 f_1(x_i)\right] + (1 - z_{i1}) \log\left[(1 - \pi_1) f_2(x_i)\right] | \mathbf{X}, \mu_1 = \mu_1^m, \mu_2 = \mu_2^m, \pi_1 = \pi_1^m\right] \\ &= \sum_{i=1}^{n} E\left[z_{i1} | x_i, \mu_1 = \mu_1^m, \mu_2 = \mu_2^m, \pi_1 = \pi_1^m\right] \log\left[\pi_1 f_1(x_i)\right] + \sum_{i=1}^{n} (1 - E\left[z_{i1} | x_i, \mu_1 = \mu_1^m, \mu_2 = \mu_2^m, \pi_1 = \right.\end{aligned}$$

Note, that the expected log likelihood simplifies to replacing the unknown class memberships in the complete likelihood by their expected values.

$$\begin{aligned} E\left[z_{i1} | \mathbf{X}, \mu_1 = \mu_1^m, \mu_2 = \mu_2^m, \pi_1 = \pi_1^m\right] &= 1 \times f(z_{i1} = 1 | x_i, \mu_1 = \mu_1^m, \mu_2 = \mu_2^m, \pi_1 = \pi_1^m) + 0 \times f(z_{i1} = 0 | x_i, \mu_1 = \mu_1^m, \mu_2 = \\ &= f(z_{i1} = 1 | x_i, \mu_1 = \mu_1^m, \mu_2 = \mu_2^m, \pi_1 = \pi_1^m) \\ &= \frac{f(z = 1, x_i)}{f(x_i)} \\ &= \frac{\pi_1^m f_1(x_i)}{\pi_1^m f_1(x_i) + (1 - \pi_1^m) f_2(x_i)} \end{aligned}$$

We will refer to the expected class membership as $\hat{z}_{i1}^{m+1}$

3.1.2 M-step

Maximise the expected log-likelihood to obtain the unknown model parameters:

$$Q\left(\mu_1, \mu_2, \pi_1 | \mathbf{X}, \mathbf{Z}\right) = \sum_{i=1}^{n} \hat{z}_{i1}^{m} \log \pi_1 + \sum_{i=1}^{n} \hat{z}_{i1}^{m} \log f_1(x_i) + \sum_{i=1}^{n} (1 - \hat{z}_{i1}) \log(1 - \pi_1) + \sum_{i=1}^{n} (1 - \hat{z}_{i1}) \log f_2(x_i)$$

So we observe that the expected log likelihood implies an estimation orthogonality between the normal distributions and the Bernoulli distribution.

So the parameter estimates that maximise the expected log-likelihood become:

$$\hat{\pi}_1^{m+1} = \frac{\sum_{i=1}^{n} \hat{z}_{i1}^{m+1}}{n}$$

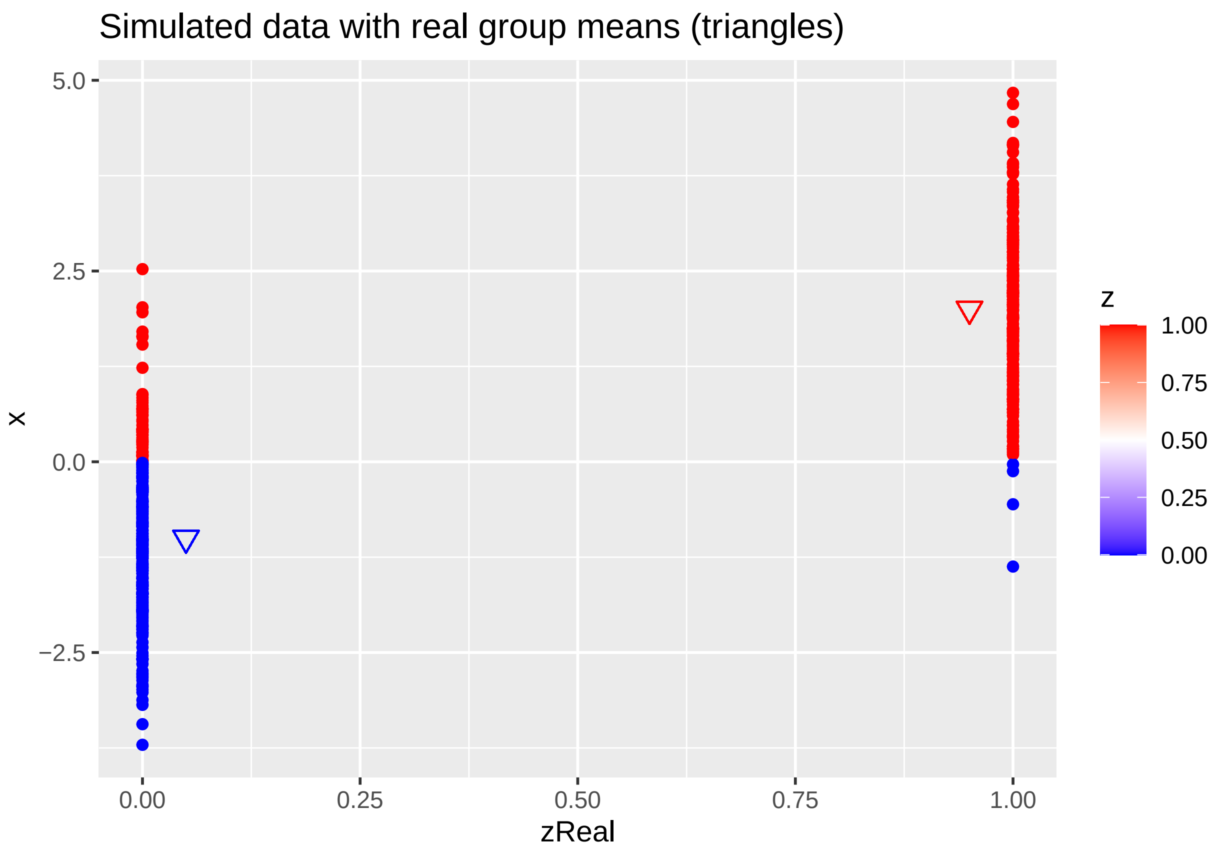
$$\hat{\mu}_1^{m+1} = \frac{\sum_{i=1}^{n} \hat{z}_{i1}^{m+1} x_i}{\sum_{i=1}^{n} \hat{z}_{i1}^{m+1}}$$

$$\hat{\mu}_2^{m+1} = \frac{\sum_{i=1}^{n} (1 - \hat{z}_{i1}^{m+1}) x_i}{\sum_{i=1}^{n} (1 - \hat{z}_{i1}^{m+1})}$$

4 Example

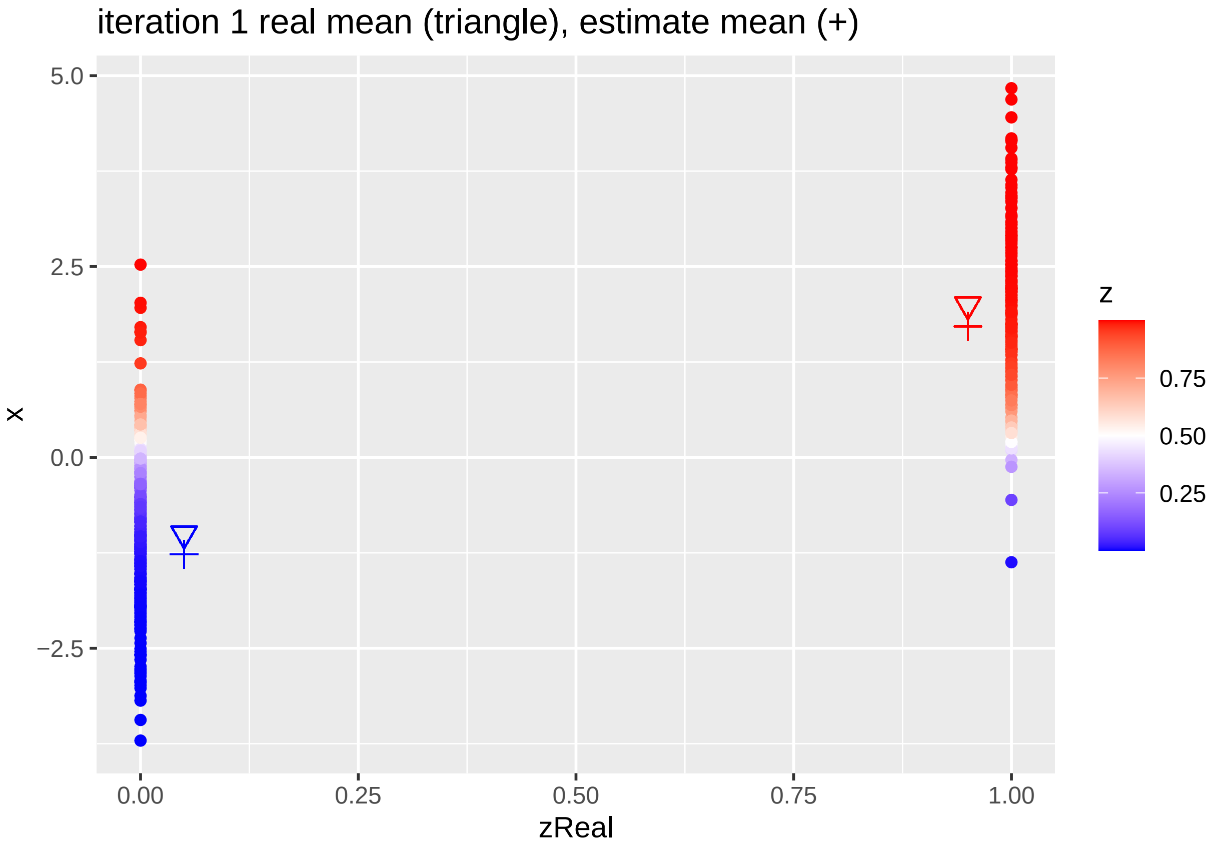
4.1 Initialize

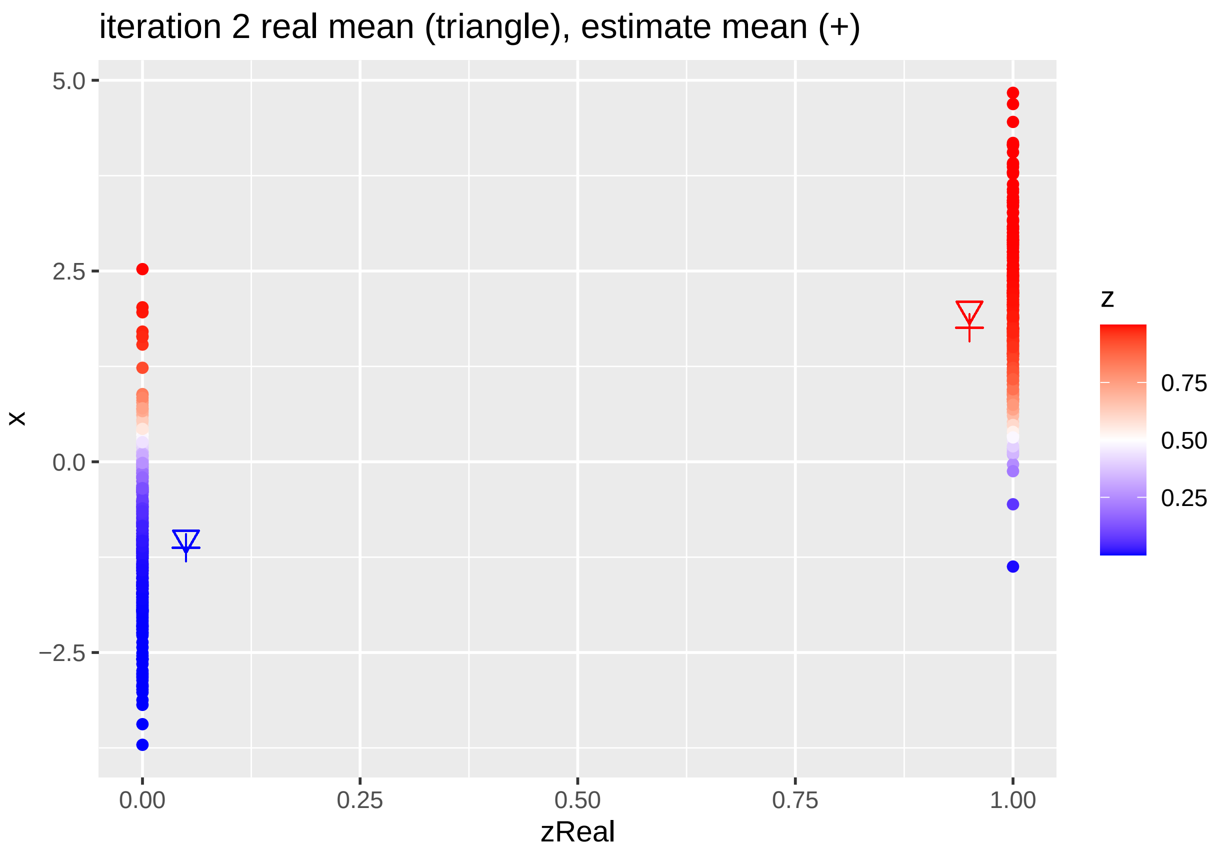
```r
z <- as.double(x > 0)
n <- length(z)

p <- data.frame(x,zReal,z) %>%
  ggplot(aes(zReal,x,color=z)) +
  geom_point() +
  scale_colour_gradient2(
    low = "blue",
    mid="white",
    high="red",
    midpoint = 0.5) +
  geom_point(x=.95,y=mu1Real, shape=25, col="red", size=3) +
  geom_point(x=0.05,y=mu2Real, shape=25, col="blue", size=3) +
  ggtitle("Simulated data with real group means (triangles)")


p
```

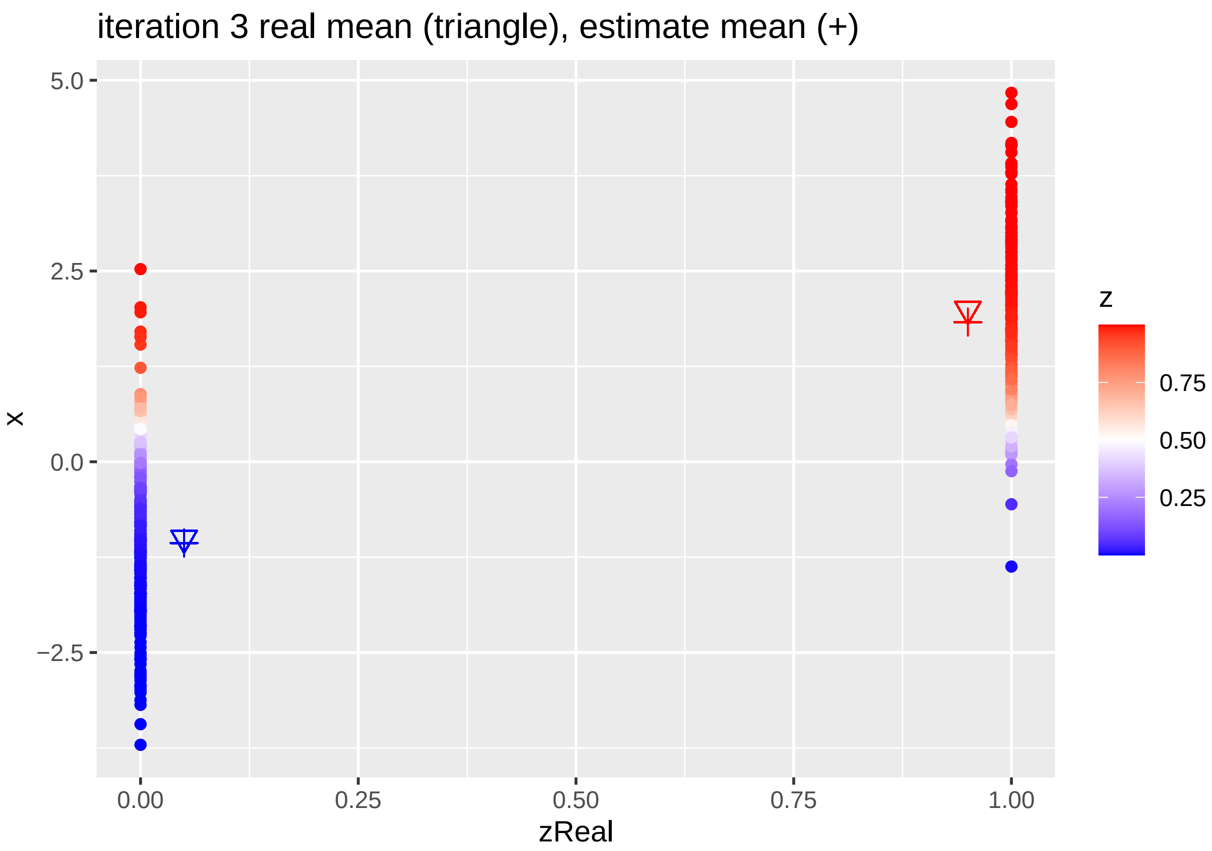


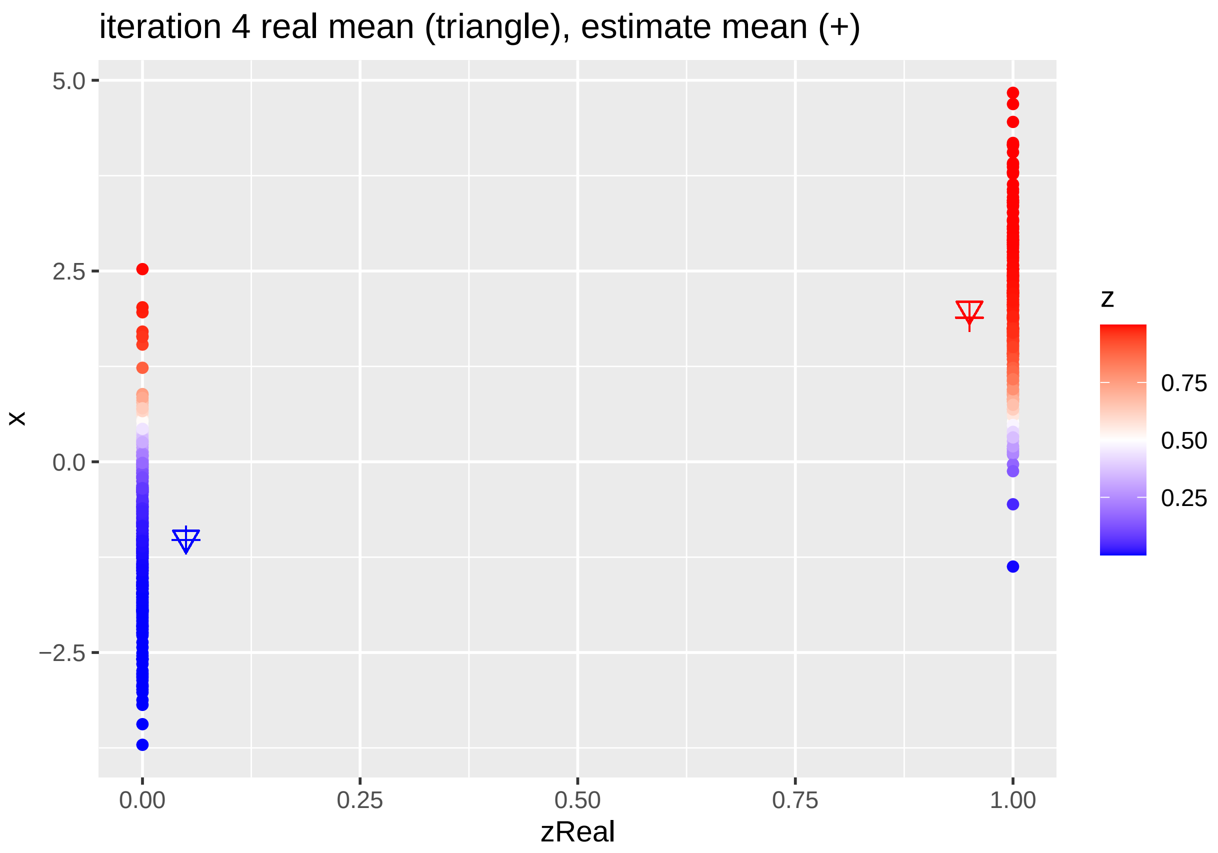
4.2 EM algorithm

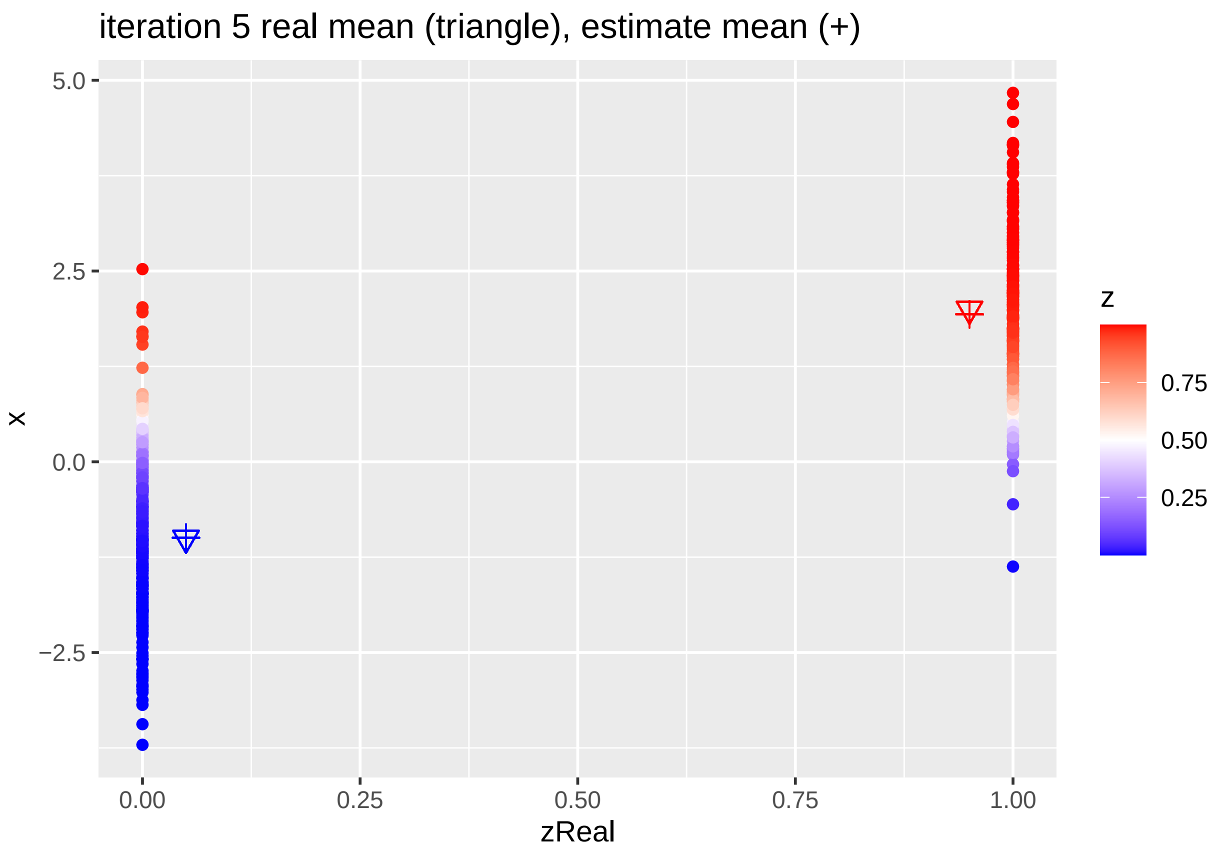
```
for (k in 1:10)
{
  ## M-step
  pi1 <- sum(z)/n
  mu1 <- sum(z * x)/sum(z)
  mu2 <- sum((1-z) * x)/sum(1-z)

  ## E-step
  d1 <- dnorm(x,mean=mu1)
  d2 <- dnorm(x,mean=mu2)
  d <- pi1 * d1 + (1-pi1)*d2
  z <- pi1*d1/d
  p <- data.frame(x,zReal,z) %>%
    ggplot(aes(zReal,x,color=z)) +
    geom_point() +
    scale_colour_gradient2(
      low = "blue",
      mid="white",
      high="red",
      midpoint = 0.5) +
      geom_point(x=.95,y=mu1Real, shape=25, col="red", size=3) +
      geom_point(x=0.05,y=mu2Real, shape=25, col="blue", size=3) +
      geom_point(x=.95,y=mu1, shape=3, col="red", size=3) +
      geom_point(x=.05,y=mu2, shape=3, col="blue", size=3) +
      ggtitle(paste0("iteration ",k, " real mean (triangle), estimate mean (+)"))

  print(p)
}
```

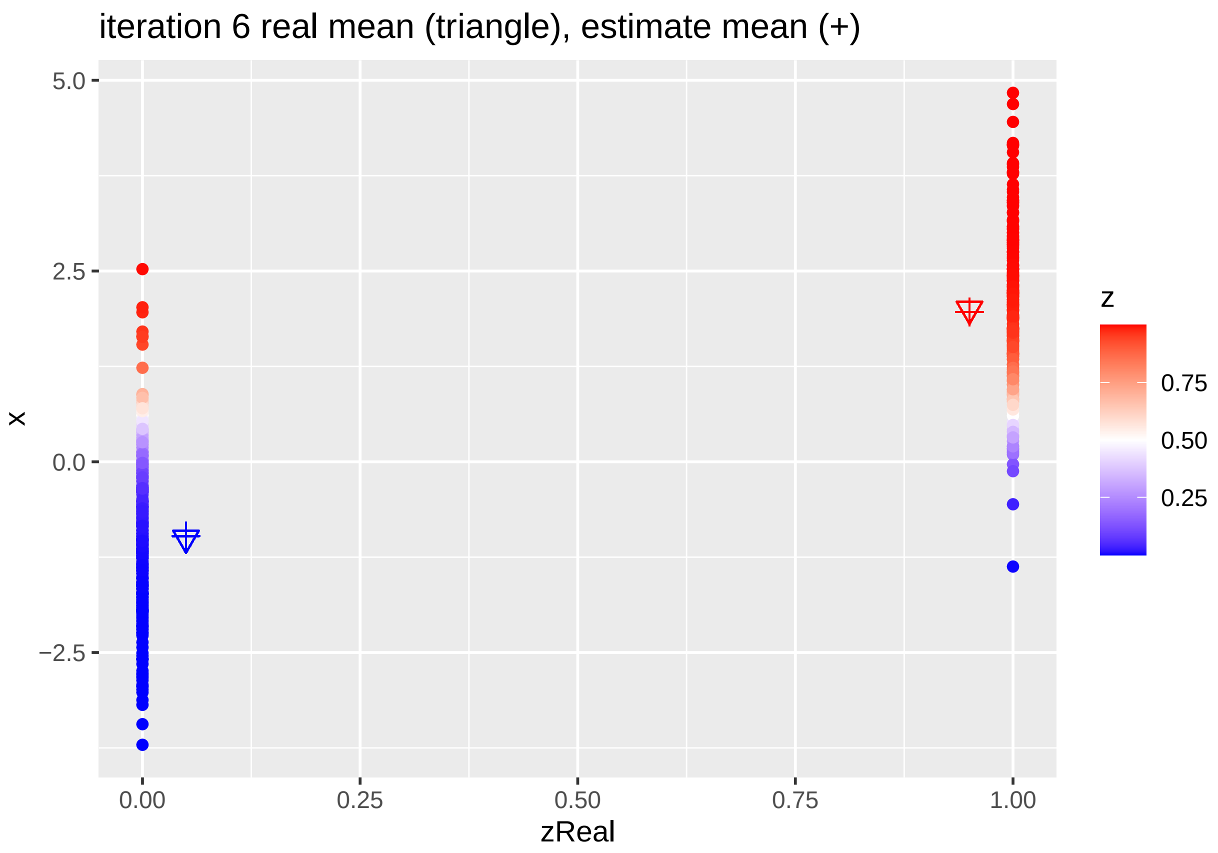


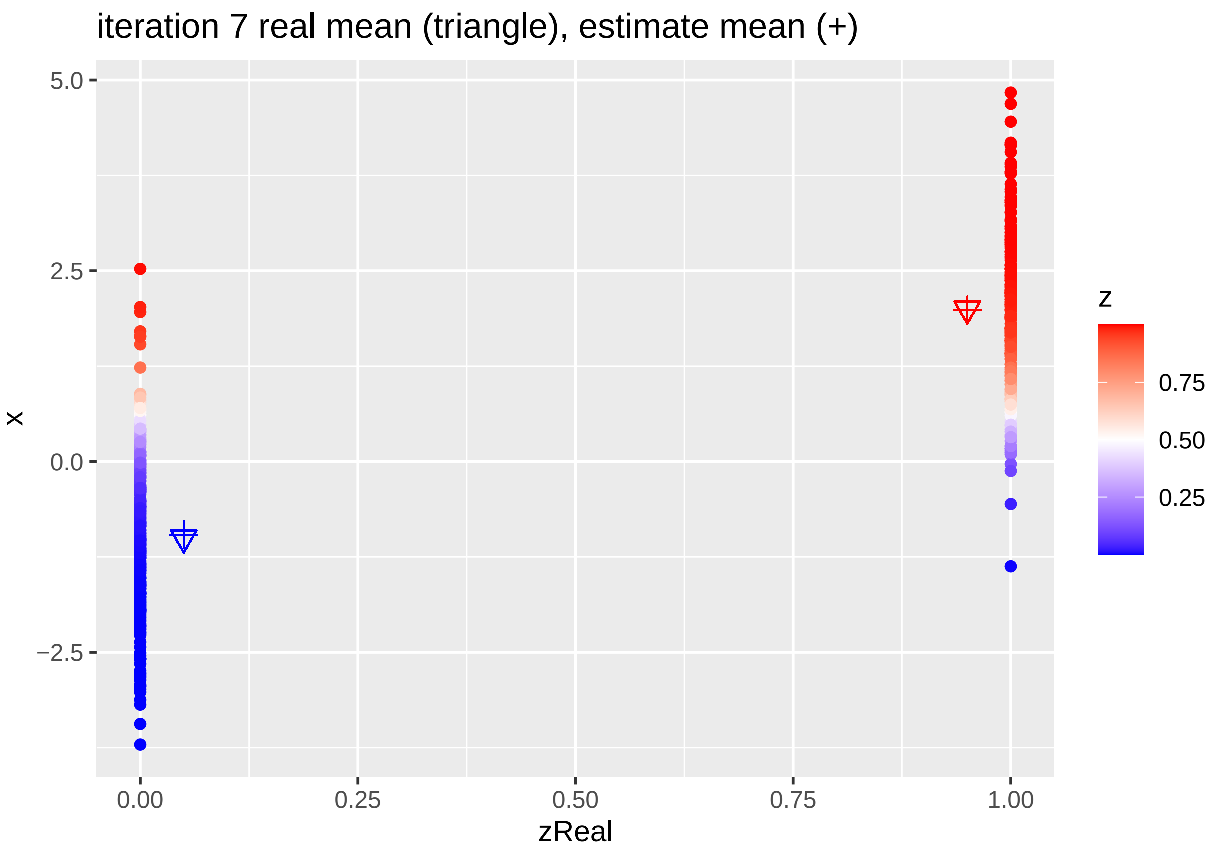

iteration 2 real mean (triangle), estimate mean (+)
x
5.0
2.5
0.0
−2.5
zReal
0.00
0.25
0.50
0.75
1.00
z
0.75
0.50
0.25

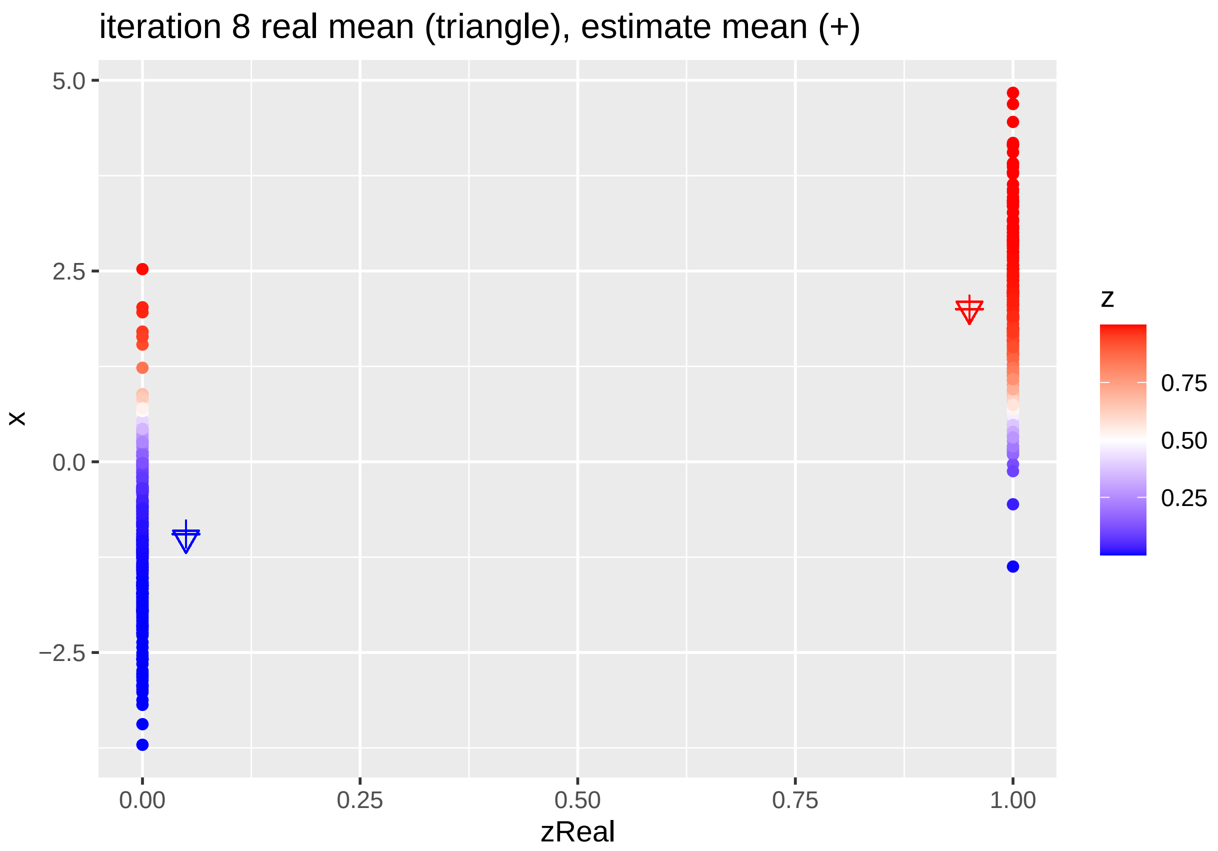

iteration 3 real mean (triangle), estimate mean (+)
5.0
2.5
0.0
−2.5
x
0.00
0.25
0.50
0.75
1.00
zReal
z
0.75
0.50
0.25

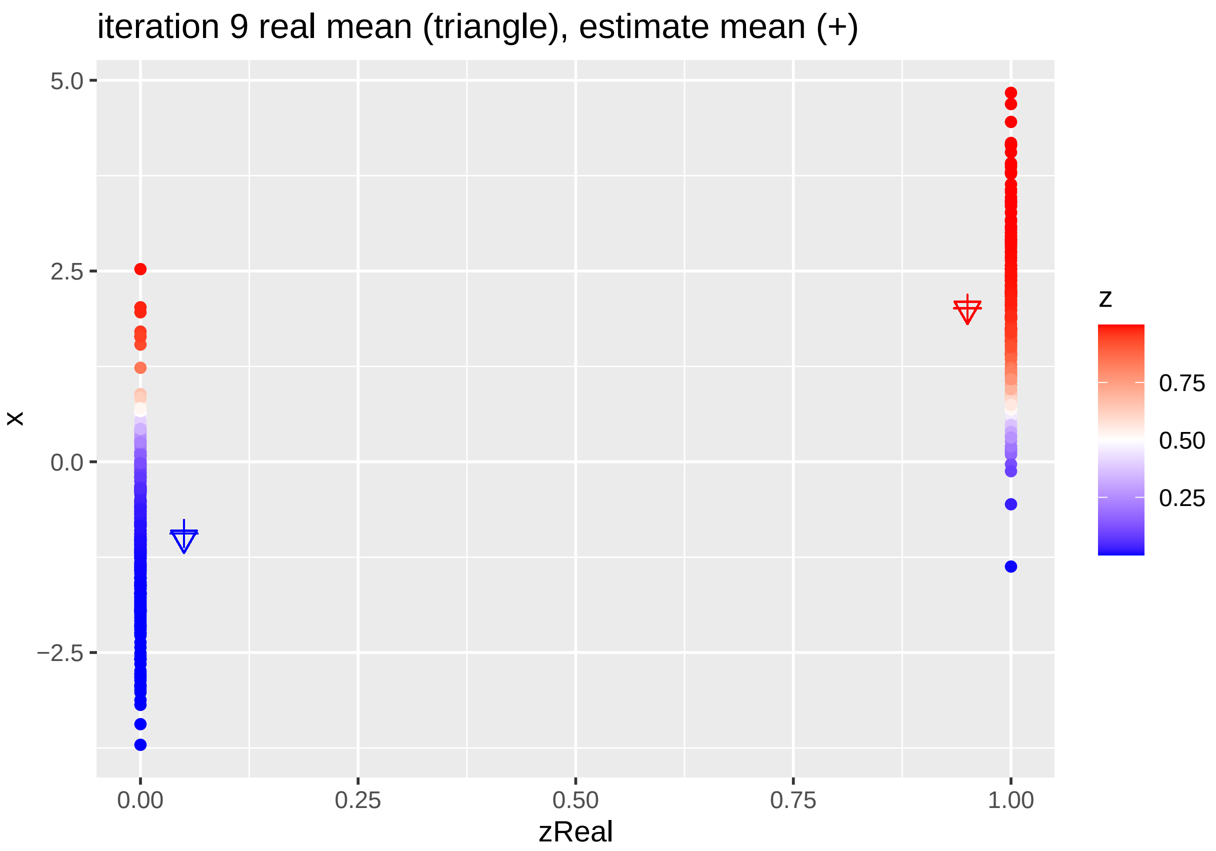

iteration 4 real mean (triangle), estimate mean (+)
5.0
2.5
0.0
−2.5
x
0.00
0.25
0.50
0.75
1.00
zReal
z
0.75
0.50
0.25

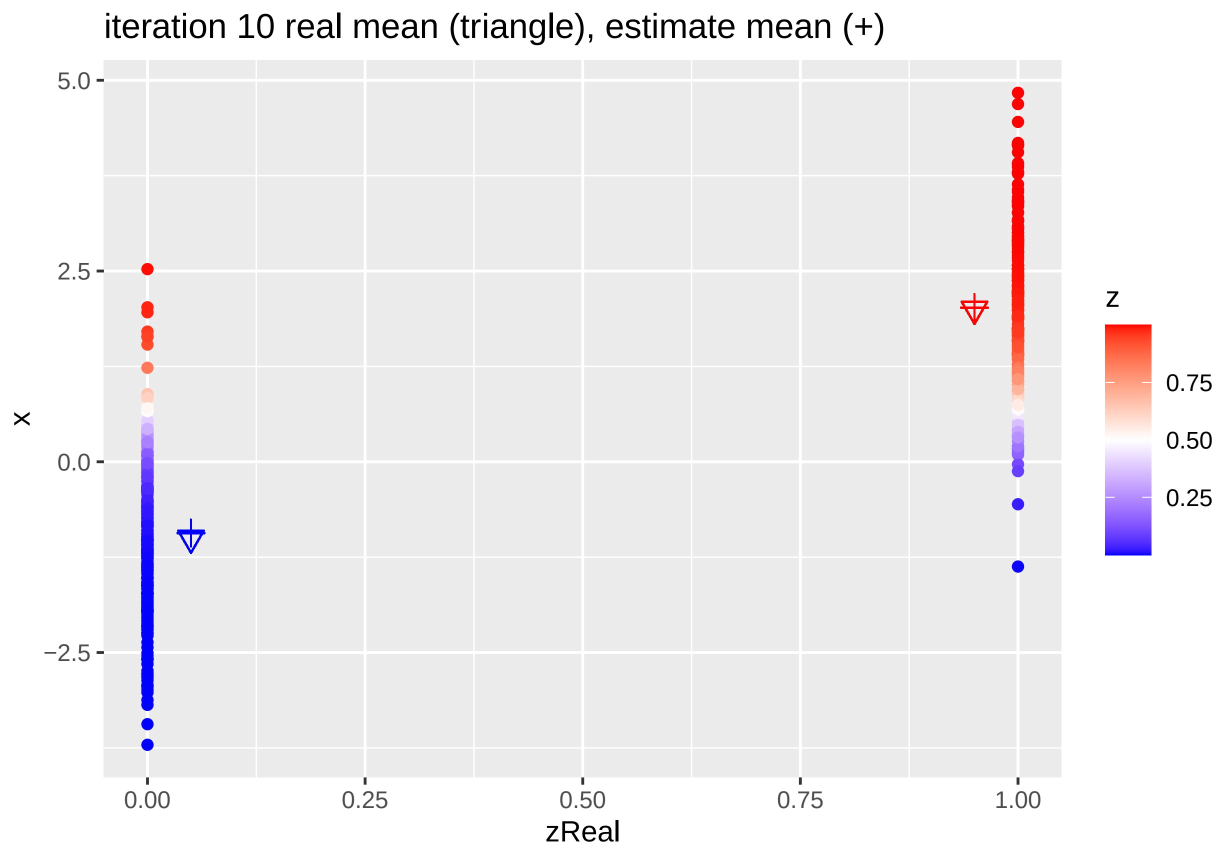

iteration 5 real mean (triangle), estimate mean (+)
5.0
2.5
0.0
−2.5
x
0.00
0.25
0.50
0.75
1.00
zReal
z
0.75
0.50
0.25


iteration 6 real mean (triangle), estimate mean (+)
5.0
2.5
0.0
−2.5
x
0.00
0.25
0.50
0.75
1.00
zReal
z
0.75
0.50
0.25


iteration 7 real mean (triangle), estimate mean (+)
5.0
2.5
0.0
−2.5
x
0.00
0.25
0.50
0.75
1.00
zReal
z
0.75
0.50
0.25


iteration 8 real mean (triangle), estimate mean (+)
5.0
2.5
0.0
−2.5
x
0.00
0.25
0.50
0.75
1.00
zReal
z
0.75
0.50
0.25


iteration 9 real mean (triangle), estimate mean (+)
5.0
2.5
0.0
−2.5
x
0.00
0.25
0.50
0.75
1.00
zReal
z
0.75
0.50
0.25



4.2.1 Estimates

parameter	population	initial	estimate
mu1	2.0	1.715	2.020
mu2	-1.0	-1.270	-0.935
pi1	0.4	0.512	0.404

Session info

Session info

```
#> [1] "2024-10-07 12:40:59 CEST"
```

```
#> - Session info ---------------------------------------------------------------
#>  setting  value
#>  version  R version 4.4.0 RC (2024-04-16 r86468)
#>  os       macOS Big Sur 11.6
#>  system   aarch64, darwin20
#>  ui       X11
#>  language (EN)
#>  collate  en_US.UTF-8
#>  ctype    en_US.UTF-8
#>  tz       Europe/Brussels
#>  date     2024-10-07
#>  pandoc   3.1.1 @ /Applications/RStudio.app/Contents/Resources/app/quarto/bin/tools/ (via rmarkdown)
```

```
#>
#> - Packages -------------------------------------------------------------------
#>  package     * version date (UTC) lib source
#>  bookdown      0.40    2024-07-02 [1] CRAN (R 4.4.0)
#>  bslib         0.8.0   2024-07-29 [1] CRAN (R 4.4.0)
#>  cachem        1.1.0   2024-05-16 [1] CRAN (R 4.4.0)
#>  cli           3.6.3   2024-06-21 [1] CRAN (R 4.4.0)
#>  colorspace    2.1-1   2024-07-26 [1] CRAN (R 4.4.0)
#>  digest        0.6.37  2024-08-19 [1] CRAN (R 4.4.1)
#>  dplyr       * 1.1.4   2023-11-17 [1] CRAN (R 4.4.0)
#>  evaluate      1.0.0   2024-09-17 [1] CRAN (R 4.4.1)
#>  fansi         1.0.6   2023-12-08 [1] CRAN (R 4.4.0)
#>  farver        2.1.2   2024-05-13 [1] CRAN (R 4.4.0)
#>  fastmap       1.2.0   2024-05-15 [1] CRAN (R 4.4.0)
#>  fontawesome   0.5.2   2023-08-19 [1] CRAN (R 4.4.0)
#>  forcats     * 1.0.0   2023-01-29 [1] CRAN (R 4.4.0)
#>  generics      0.1.3   2022-07-05 [1] CRAN (R 4.4.0)
#>  ggplot2     * 3.5.1   2024-04-23 [1] CRAN (R 4.4.0)
#>  glue          1.8.0   2024-09-30 [1] CRAN (R 4.4.1)
#>  gtable        0.3.5   2024-04-22 [1] CRAN (R 4.4.0)
#>  highr         0.11    2024-05-26 [1] CRAN (R 4.4.0)
#>  hms           1.1.3   2023-03-21 [1] CRAN (R 4.4.0)
#>  htmltools     0.5.8.1 2024-04-04 [1] CRAN (R 4.4.0)
#>  jquerylib     0.1.4   2021-04-26 [1] CRAN (R 4.4.0)
#>  jsonlite      1.8.9   2024-09-20 [1] CRAN (R 4.4.1)
#>  knitr         1.48    2024-07-07 [1] CRAN (R 4.4.0)
#>  labeling      0.4.3   2023-08-29 [1] CRAN (R 4.4.0)
#>  lifecycle     1.0.4   2023-11-07 [1] CRAN (R 4.4.0)
#>  lubridate   * 1.9.3   2023-09-27 [1] CRAN (R 4.4.0)
#>  magrittr      2.0.3   2022-03-30 [1] CRAN (R 4.4.0)
#>  munsell       0.5.1   2024-04-01 [1] CRAN (R 4.4.0)
#>  pillar        1.9.0   2023-03-22 [1] CRAN (R 4.4.0)
#>  pkgconfig     2.0.3   2019-09-22 [1] CRAN (R 4.4.0)
#>  purrr       * 1.0.2   2023-08-10 [1] CRAN (R 4.4.0)
#>  R6            2.5.1   2021-08-19 [1] CRAN (R 4.4.0)
#>  readr       * 2.1.5   2024-01-10 [1] CRAN (R 4.4.0)
#>  rlang         1.1.4   2024-06-04 [1] CRAN (R 4.4.0)
#>  rmarkdown     2.28    2024-08-17 [1] CRAN (R 4.4.0)
#>  rstudioapi    0.16.0  2024-03-24 [1] CRAN (R 4.4.0)
#>  sass          0.4.9   2024-03-15 [1] CRAN (R 4.4.0)
#>  scales        1.3.0   2023-11-28 [1] CRAN (R 4.4.0)
#>  sessioninfo   1.2.2   2021-12-06 [1] CRAN (R 4.4.0)
#>  stringi       1.8.4   2024-05-06 [1] CRAN (R 4.4.0)
#>  stringr     * 1.5.1   2023-11-14 [1] CRAN (R 4.4.0)
#>  tibble      * 3.2.1   2023-03-20 [1] CRAN (R 4.4.0)
#>  tidyr       * 1.3.1   2024-01-24 [1] CRAN (R 4.4.0)
#>  tidyselect    1.2.1   2024-03-11 [1] CRAN (R 4.4.0)
#>  tidyverse   * 2.0.0   2023-02-22 [1] CRAN (R 4.4.0)
#>  timechange    0.3.0   2024-01-18 [1] CRAN (R 4.4.0)
#>  tzdb          0.4.0   2023-05-12 [1] CRAN (R 4.4.0)
#>  utf8          1.2.4   2023-10-22 [1] CRAN (R 4.4.0)
#>  vctrs         0.6.5   2023-12-01 [1] CRAN (R 4.4.0)
#>  withr         3.0.1   2024-07-31 [1] CRAN (R 4.4.0)
#>  xfun          0.47    2024-08-17 [1] CRAN (R 4.4.0)
#>  yaml          2.3.10  2024-07-26 [1] CRAN (R 4.4.0)
#>
#>  [1] /Library/Frameworks/R.framework/Versions/4.4-arm64/Resources/library
#>
#> ------------------------------------------------------------------------------
```