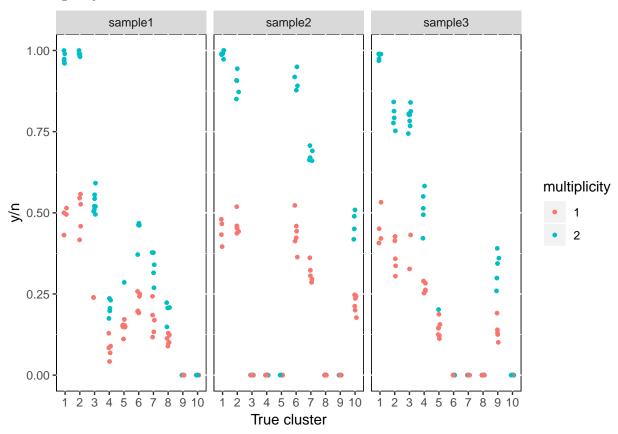
Version 6: Cluster first

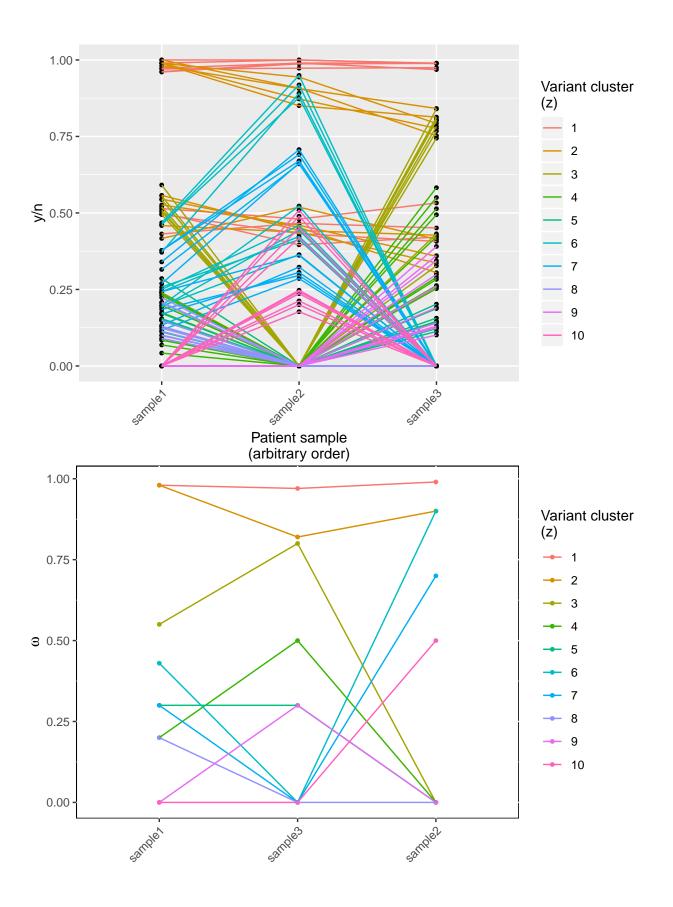
Simulate data

```
I <- 100
K <- 10
S <- 3
set.seed(123)
pi \leftarrow rep(0.1, 10)
\#z \leftarrow sample(1:K, size = I, replace = T, prob = pi)
z <- rep(1:10, each=10)
w \leftarrow matrix(c(0.98, 0.99, 0.97,
               0.98, 0.90, 0.82,
               0.55, 0.00, 0.80,
               0.20, 0.00, 0.50,
               0.30, 0.00, 0.30,
               0.43, 0.90, 0.00,
               0.30, 0.70, 0.00,
               0.20, 0.00, 0.00,
               0.00, 0.00, 0.30,
               0.00, 0.50, 0.00),
             byrow=T,
            nrow=K, ncol=S)
colnames(w) <- paste0("sample", 1:S)</pre>
##
         sample1 sample2 sample3
##
   [1,]
            0.98
                     0.99
                             0.97
                     0.90
                             0.82
## [2,]
            0.98
## [3,]
          0.55
                     0.00
                             0.80
## [4,]
                   0.00
          0.20
                             0.50
## [5,]
            0.30
                     0.00
                             0.30
## [6,]
                  0.90
                             0.00
          0.43
## [7,]
          0.30
                     0.70
                             0.00
## [8,]
            0.20
                     0.00
                             0.00
## [9,]
                     0.00
            0.00
                              0.30
## [10,]
            0.00
                     0.50
                             0.00
tcn <- matrix(2, nrow=I, ncol=S)</pre>
m <- matrix(rep(sample(1:2, size = I, replace = T), S),</pre>
            nrow=I, ncol=S)
W \leftarrow w[z,]
calcTheta <- function(m, tcn, w) {</pre>
  (m * w) / (tcn * w + 2*(1-w))
theta <- calcTheta(m, tcn, W)
n <- replicate(S, rpois(I, 100))</pre>
y <- matrix(NA, nrow=I, ncol=S)
```

Visualize densities of simulated data

Clustering is by ω





functions

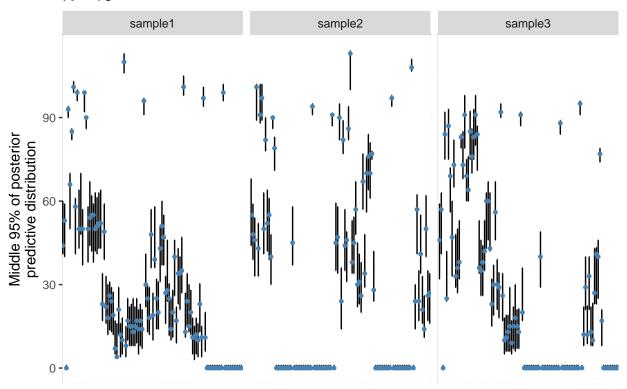
```
runMCMC <- function(data, K, jags.file, inits, params, n.iter, thin) {</pre>
  data$K <- K
  jags.m <- jags.model(jags.file, data,</pre>
                          n.chains = 1,
                          inits = inits,
                          n.adapt = 1000)
  samps <- coda.samples(jags.m, params, n.iter=n.iter, thin=thin)</pre>
  samps
}
getParamChain <- function(samps, param) {</pre>
  chains <- do.call(rbind, samps)</pre>
  chain <- chains[, grep(param, colnames(chains))]</pre>
}
reshapeW <- function(w, S, K) {</pre>
  w.mat <- matrix(w, nrow = K)</pre>
  colnames(w.mat) <- paste0("sample", 1:S)</pre>
  w.mat
}
calcLogLik <- function(z.iter, w.iter, data) {</pre>
  W <- w.iter[z.iter, ]</pre>
  theta <- calcTheta(data$m, data$tcn, W)
  sum(dbinom(data$y, data$n, theta, log=T))
}
calcChainLogLik <- function(samps, data, K) {</pre>
  z.chain <- getParamChain(samps, "z")</pre>
  w.chain <- getParamChain(samps, "w")</pre>
  lik \leftarrow c()
  for(iter in 1:nrow(z.chain)) {
    z.iter <- z.chain[iter,]</pre>
    w.iter <- reshapeW(w.chain[iter,], data$S, K)</pre>
    lik <- c(lik, calcLogLik(z.iter, w.iter, data))</pre>
  }
  mean(lik)
calcBIC <- function(n, k, ll) log(n)*k - 2*ll
```

Cluster - JAGS

```
n.iter = 10000
thin = 7
K <- 10
samps <- runMCMC(test.data, K, jags.file, inits, params, n.iter, thin)</pre>
## Compiling model graph
##
      Resolving undeclared variables
##
      Allocating nodes
##
  Graph information:
      Observed stochastic nodes: 300
##
      Unobserved stochastic nodes: 431
##
##
      Total graph size: 4196
##
## Initializing model
z.chain <- getParamChain(samps, "z")</pre>
w.chain <- getParamChain(samps, "w")</pre>
mcmc_vals <- summary(samps)$statistics</pre>
mcmc_w <- mcmc_vals[substr(rownames(mcmc_vals), 1, 1) == "w", "Mean"]</pre>
mcmc_w <- matrix(mcmc_w, nrow=K)</pre>
colnames(mcmc_w) <- paste0("sample", 1:S)</pre>
```

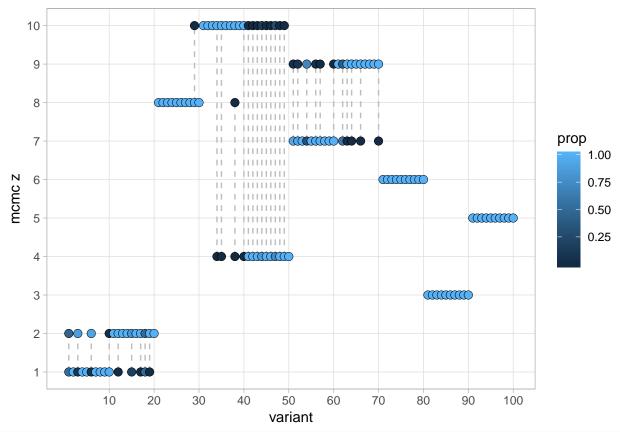
PPD

K = 10



observation index (column-major order)

```
plot.z <- function(samps, z) {</pre>
  mcmc vals <- summary(samps)$statistics</pre>
  mcmc_z <- as.vector(mcmc_vals[substr(rownames(mcmc_vals), 1, 1) == "z", "Mean"])</pre>
  plot(z, mcmc_z, type = "p")
  z_comp <- data.frame(z, mcmc_z)</pre>
z.chain.to.tb <- function(z.chain) {</pre>
  z.chain.tb <- z.chain %>%
    as_tibble() %>%
    mutate(iter=1:nrow(z.chain)) %>%
    gather(variant, mcmc_z, -c(iter))
  z.chain.tb <- z.chain.tb %>%
    mutate(variant = as.integer(gsub(".*\\[(.*)\\].*", "\\1", z.chain.tb$variant))) %>%
    mutate(true_z = rep(1:10, each=nrow(z.chain)*10)) %>%
    group_by(variant, mcmc_z) %>%
    mutate(count = n())
  z.chain.tb_simp <- distinct(select(z.chain.tb, -c(iter)))</pre>
  z.chain.tb_simp %>%
    group_by(variant) %>%
    mutate(prop = count/sum(count))
}
z.chain.tb <- z.chain.to.tb(z.chain)</pre>
z.chain.tb
## # A tibble: 135 x 5
## # Groups:
              variant [100]
##
      variant mcmc_z true_z count
                                     prop
##
        <int> <dbl> <int> <int> <dbl>
## 1
            1
                    2
                          1
                               657 0.460
## 2
                               771 0.540
            1
                    1
                           1
## 3
            2
                    1
                           1 1428 1
                           1 1260 0.882
## 4
            3
                   2
## 5
            3
                    1
                           1
                              168 0.118
                           1 1428 1
## 6
            4
                    1
                           1 1428 1
## 7
            5
                    1
            6
                    2
                           1 1315 0.921
## 8
## 9
                           1 113 0.0791
            6
                    1
            7
                           1 1428 1
## 10
                    1
## # ... with 125 more rows
z.seg.tb <- tibble(variant = numeric(),</pre>
                     mcmc z 1 = numeric(),
                     mcmc_z_2 = numeric())
for (i in 1:ncol(z.chain)) {
  z.vals <- as.integer(names(table(z.chain[,i])))</pre>
  if (length(z.vals) > 1) {
    z.seg.tb[i, ] \leftarrow c(i, z.vals[1], z.vals[2])
  } else {
    z.seg.tb[i, ] \leftarrow c(i, z.vals, z.vals)
  }
}
```

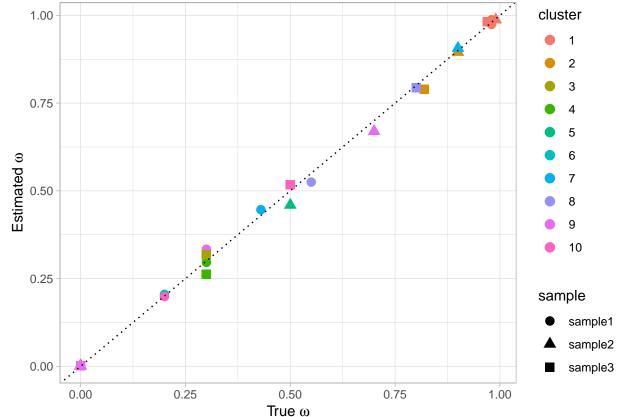


#gsave(file.path(figs.dir, "z_plot.pdf"), z.plot, width=14, height=6)

```
z.map.tb <- z.chain.tb %>%
  group_by(variant) %>%
  filter(prop == max(prop))
z.map.tb
## # A tibble: 100 x 5
```

```
## # A tibble: 100 x 5
## # Groups: variant [100]
## variant mcmc_z true_z count prop
## <int> <dbl> <int> <dbl>
```

```
771 0.540
##
##
    2
             2
                    1
                              1428 1
                            1
                              1260 0.882
##
    3
            3
                    2
   4
             4
                              1428 1
##
                    1
                            1
##
    5
            5
                    1
                           1
                              1428 1
##
   6
            6
                    2
                              1315 0.921
                           1
##
   7
            7
                    1
                           1
                              1428 1
                              1428 1
            8
##
   8
                    1
                            1
##
   9
            9
                    1
                            1
                              1428 1
## 10
           10
                              1381 0.967
                    1
                            1
## # ... with 90 more rows
z.map <- z.map.tb$mcmc_z</pre>
z.map
##
                                             2 2 2 2 2 2
                                                                 2
                                                                    2
                                                                       2
                                                                          8
                                                                             8
                                                                                8
     [1]
                 2
                          2
                            1 1 1 1
                                          2
                   1
                       1
    [24]
                   8
                       8
                          8 8 10 10 10 10 10 10 10 10 10 10
##
    [47]
          4
             4
                 4
                   4
                       7
                          7
                             7
                                9
                                   7
                                       7
                                          7
                                              7
                                                 7
                                                    7
                                                       9
                                                          7
                                                             9
                                                                 9
                                                                    9
                                                                       9
                                                                          9
                                                                              9
    [70]
          9
             6
                 6
                    6
                       6
                          6
                             6
                                6
                                    6
                                       6
                                          6
                                              3
                                                 3
                                                    3
                                                       3
                                                          3
                                                             3
                                                                 3
                                                                    3
                                                                       3
                                                                          3
                                                                             5
    [93]
          5
             5
                5
                   5 5 5 5
z.map.ind <- which(apply(z.chain, 1, function(x) all(x == z.map)))</pre>
\omega
mcmc_vals <- summary(samps)$statistics</pre>
mcmc_w <- mcmc_vals[substr(rownames(mcmc_vals), 1, 1) == "w", "Mean"]</pre>
mcmc_w <- matrix(mcmc_w, nrow=K)</pre>
colnames(mcmc_w) <- paste0("sample", 1:S)</pre>
round(mcmc_w, 2)
##
         sample1 sample2 sample3
                     0.99
                              0.98
##
   [1,]
            0.97
   [2,]
            0.99
                     0.89
                              0.79
##
                     0.00
   [3,]
            0.00
                              0.32
##
##
  [4,]
            0.30
                     0.00
                              0.26
## [5,]
            0.00
                     0.46
                              0.00
## [6,]
            0.21
                     0.00
                              0.00
##
   [7,]
            0.45
                     0.91
                              0.00
##
   [8,]
            0.52
                     0.00
                              0.79
                              0.00
##
  [9,]
            0.33
                     0.67
## [10,]
            0.20
                     0.00
                              0.52
mcmc_w_sd <- mcmc_vals[substr(rownames(mcmc_vals), 1, 1) == "w", "SD"]</pre>
mcmc_w_sd <- matrix(mcmc_w_sd, nrow=K)</pre>
colnames(mcmc_w_sd) <- paste0("sample", 1:S)</pre>
# order true w based on mcmc cluster numbering
w_{ordered} \leftarrow w[c(1,2,9,5,10,8,6,3,7,4),]
# scatter
mcmc_w_tb <- mcmc_w %>%
  as_tibble() %>%
  mutate(cluster=1:K) %>%
  gather("sample", "mcmc_w", -c(cluster))
```



#ggsave(file.path(figs.dir, "w_plot.pdf"))

Admat functions

```
rand.admat <- function(admat) {
  for(col in 1:ncol(admat)) {
    ind.0 <- which(admat[,col] == 0) # possible positions (0's)
    rand.ind <- sample(ind.0, size=1)
    admat[rand.ind,col] <- 1
}
while (sum(admat[1, ]) == 0) {</pre>
```

```
admat <- mutate.admat(admat)</pre>
 }
 admat
}
base.admat <- function(w, zero.thresh=0.01) {</pre>
  cluster.sample.presence <- apply(w, 1, function(x) which(x>zero.thresh))
 K <- nrow(w)</pre>
 S \leftarrow ncol(w)
  all.samples <- 1:S
  admat <- matrix(data=0, nrow=(1+K), ncol=K) # rows=from is root + 1:K, cols=to is 1:K
  # fill in restraints
  # can go from root to anyone, skip and start at nrow=2 (cluster 1)
  for (from in 2:(K+1)) {
    for (to in 1:K) {
      # can't go to self
      if ((from-1) == to) {
        admat[from, to] <- NA
        #print(c(from, to, "self"))
        next
      }
      # hierarchy restraints
      from.samples <- cluster.sample.presence[[from-1]]</pre>
      to.samples <- cluster.sample.presence[[to]]</pre>
      ## no restraints if same sample presence
      if (setequal(from.samples, to.samples)) {
        #print(c(from, to, "same"))
        next
      }
      ## restraint if # from.samples < # to.samples
      if(length(from.samples) < length(to.samples)) {</pre>
        #print(c(from, to, "from set is smaller than to set"))
        admat[from, to] <- NA
        next
      }
      ## no restraints if to.samples is subset of from.samples
      if (all(to.samples %in% from.samples)) {
        #print(c(from, to, "subset"))
        next
      } else {
        #print(c(from, to, "not subset"))
        admat[from, to] <- NA
      }
    }
 }
  admat
```

```
init.admat <- function(w, zero.thresh) {</pre>
  base <- base.admat(w, zero.thresh)</pre>
  rand.admat(base)
mutate.admat <- function(admat, ncol.to.mutate) {</pre>
  # choose a column(s) to mutate
  K <- ncol(admat)</pre>
  rand.ks <- sample(1:K, size=ncol.to.mutate)</pre>
  # mutate columns
  new.admat <- admat
  for (rand.k in rand.ks) {
    ## possible positions (0's)
    possiblePos <- which(!is.na(admat[, rand.k]) & admat[, rand.k] != 1)</pre>
    ## current position with 1
    ind.1 <- which(admat[, rand.k] == 1)</pre>
    ## select new position
    if (length(possiblePos) == 1) {
      new.1 <- possiblePos</pre>
    } else {
      new.1 <- sample(possiblePos, size=1)</pre>
    new.admat[ind.1, rand.k] <- 0</pre>
    new.admat[new.1, rand.k] <- 1</pre>
  while (sum(new.admat[1, ]) == 0) {
    new.admat <- mutate.admat(admat)</pre>
  }
  new.admat
```

SCHISM tree scoring

```
decide.ht <- function(pval, alpha=0.05) {
    # 1 signals rejection event for null of i -> j
    if (pval <= alpha) return(1)
    else return(0)
}

create.cpov <- function(mcmc_w, mcmc_w_sd, alpha=0.05) {
    cpov <- base.admat(mcmc_w, zero.thresh = 0.01)
    S <- ncol(mcmc_w) # number of samples

# root can go to anyone -- all 0's (default base admat value)

for (r in 2:nrow(cpov)) {</pre>
```

```
for (c in 1:ncol(cpov)) {
      if (is.na(cpov[r,c])) next # skip restricted position
      from <- r-1 # 'from' cluster node</pre>
      to <- c # 'to' cluster node
      statistic <- 0
      pval <- 0</pre>
      for(s in 1:S) {
        d <- mcmc_w[from,s] - mcmc_w[to,s]</pre>
        d_sd <- sqrt((mcmc_w_sd[from,s])^2 + (mcmc_w_sd[to,s])^2)</pre>
        I \leftarrow sum(d < 0)
        statistic <- statistic + (d / d_sd)^2 * I
        for (k in 0:S) {
        pval <- pval + ((1 - pchisq(statistic, k)) * choose(S, k) / (2^S))</pre>
      }
      cpov[r,c] <- decide.ht(pval, alpha)</pre>
    }
  }
  cpov
}
calc.topology.cost <- function(admat, cpov) {</pre>
  TC <- 0
  edges <- which(admat == 1, arr.ind=T)</pre>
 for (i in 1:nrow(edges)) {
    TC <- TC + cpov[edges[i,1], edges[i,2]]</pre>
  TC
calc.mass.cost <- function(admat, mcmc_w) {</pre>
  numChildren <- rowSums(admat, na.rm = T)</pre>
  nodes <- which(numChildren > 0, arr.ind = T) # not leaves
  mc.node <- rep(0, length(nodes))</pre>
  for (i in 1:length(nodes)) {
    node <- nodes[i]</pre>
    # root node: MCF = 1
    parent.w <- rep(1, ncol(mcmc_w))</pre>
    # not root node: look up MCF in mcmc_w
    if (node != 1) {
      parent.w <- mcmc_w[node-1,]</pre>
```

```
kids <- which(admat[node,] == 1, arr.ind = T)
if (numChildren[node] > 1) {
    children.w <- colSums(mcmc_w[kids,])
} else {
    children.w <- mcmc_w[kids,]
}

mc.s <- ifelse(parent.w >= children.w, 0, children.w - parent.w)
mc.node[i] <- sqrt(sum(mc.s^2))
}

sum(mc.node)
}

calc.tree.fitness <- function(admat, cpov, mcmc_w, scaling.coeff=5) {
    TC <- calc.topology.cost(admat, cpov)
    MC <- calc.mass.cost(admat, mcmc_w)
    Z <- TC + MC
    fitness <- exp(-scaling.coeff * Z)
    fitness
}</pre>
```

Tree MCMC

```
set.seed(1234)
answer <- base.admat(mcmc w)</pre>
answer[1,1] \leftarrow answer[2,2] \leftarrow answer[3,7] \leftarrow answer[3,8] \leftarrow
  answer[5,3] \leftarrow answer[8,9] \leftarrow answer[9,4] \leftarrow answer[9,10] \leftarrow
  answer[10,5] \leftarrow answer[11,6] \leftarrow 1
answer
##
          [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10]
   [1,]
                        0
                                         0
##
            1
                  0
                              0
                                   0
                                               0
                                                    0
                                                          0
## [2,]
          NA
                  1
                        0
                              0
                                   0
                                         0
                                               0
                                                    0
                                                          0
                                                                 0
## [3,]
                        0
            0
                NA
                              0
                                   0
                                         0
                                              1
                                                    1
                                                          0
                                                                 0
## [4,]
          NA
                NA
                       NΑ
                             NA
                                  NA
                                        NA
                                             NA
                                                   NA
                                                         NA
                                                               NA
## [5,]
           NA
                 NA
                       1
                             NA
                                  NA
                                        0
                                             NA
                                                    0
                                                         NA
                                                                0
                                        NA
## [6,]
           NA
                NA
                       NA
                            NA
                                  NA
                                             NA
                                                   NA
                                                         NA
                                                               NA
## [7,]
            NA
                NA
                       NA
                            NA
                                  NA
                                        NA
                                             NA
                                                   NA
                                                         NA
                                                               NA
## [8,]
            NA
                NA
                       NA
                            NA
                                         0
                                            NA
                                                   NA
                                                         1
                                                               NA
                                   0
                NA
## [9,]
            NA
                        0
                             1
                                  NA
                                         0
                                             NA
                                                   NA
                                                         NA
                                                                1
## [10,]
            NA
                 NA
                       NA
                            NA
                                         0
                                              0
                                                   NA
                                                         NA
                                                               NA
                                   1
## [11,]
                        0
                              0
                                  NA
                                              NA
                                                         NA
cpov <- create.cpov(mcmc_w, mcmc_w_sd)</pre>
calc.tree.fitness(answer, cpov, mcmc_w)
```

[1] 0.6366176

```
calc.tree.fitness(answer, cpov, w[c(1,2,9,5,10,8,6,3,7,4),])
## [1] 1
#admat.chain <- list(init.admat(mcmc_w, zero.thresh=0.01))</pre>
# start at best
best.admat.mcmc <- base.admat(mcmc_w)</pre>
best.admat.mcmc[1,1] \leftarrow best.admat.mcmc[2,2] \leftarrow best.admat.mcmc[3,7] \leftarrow
  best.admat.mcmc[3,8] <- best.admat.mcmc[5,6] <- best.admat.mcmc[8,9] <-
  best.admat.mcmc[9,4] \leftarrow best.admat.mcmc[9,10] \leftarrow best.admat.mcmc[10,5] \leftarrow
  best.admat.mcmc[11,3] <- 1
admat.chain <- list(best.admat.mcmc)</pre>
score.chain <- c()</pre>
numAccept = 0
ncol.to.mutate <- 1</pre>
numIter <- 1000
for (i in 1:numIter) {
  fit.prev <- calc.tree.fitness(admat.chain[[i]], cpov, mcmc_w)</pre>
  score.chain[i] <- fit.prev</pre>
  admat.star <- mutate.admat(admat.chain[[i]], ncol.to.mutate)</pre>
  fit.star <- calc.tree.fitness(admat.star, cpov, mcmc_w)</pre>
  r <- fit.star / fit.prev
  u <- runif(1,0,1)
  if(u <= r) {
    admat.chain[[i+1]] <- admat.star</pre>
    numAccept <- numAccept + 1</pre>
  } else {
    admat.chain[[i+1]] <- admat.chain[[i]]</pre>
  }
score.chain[i+1] <- calc.tree.fitness(admat.chain[[i+1]], cpov, mcmc_w)</pre>
acceptRate <- numAccept/(numIter)</pre>
acceptRate
## [1] 0.315
max(score.chain)
## [1] 0.8652116
max.score.ind <- which(score.chain == max(score.chain))</pre>
if(length(max.score.ind) > 1) max.score.ind <- max.score.ind[1]</pre>
max.admat <- admat.chain[[max.score.ind]]</pre>
max.admat
          [,1] [,2] [,3] [,4] [,5] [,6] [,7] [,8] [,9] [,10]
##
  [1,]
                        0
                                         0
                                              0
                                                    0
                                                          0
##
            1
                  0
                              0
                                   0
## [2,]
          NA
                  1
                        0
                              0
                                   0
                                         0
                                              0
                                                    0
                                                          0
                                                                0
## [3,]
            0
                 NA
                        0
                              0
                                   0
                                         0
                                              1
                                                    1
                                                          0
                                                                0
## [4,]
                 NA
                                                        NA
                                                               NA
          NA
                       NA
                            NA
                                  NA
                                        NA
                                             NA
                                                   NA
## [5,]
           NA
                 NA
                        0
                            NA
                                  NA
                                        1
                                             NA
                                                    0
                                                        NA
                                                                0
```

```
## [6,]
          NA
               NA
                    NA
                         NA
                              NA
                                   NA
                                       NA
                                             NA
                                                  NA
                                                       NA
## [7,]
         NA NA
                    NA
                         NA
                              NA
                                   NA
                                      NA
                                            NA
                                                 NA
                                                       NΑ
## [8,]
          NA
             NA
                    NA
                         NA
                              0
                                   0
                                      NA
                                             NA
                                                 1
                                                       NA
## [9,]
                                                        1
          NA
              NA
                     0
                              NA
                                    0
                                       NA
                                             NA
                                                 NA
                         1
## [10,]
          NA
               NA
                    NA
                         NA
                               1
                                    0
                                        0
                                             NA
                                                 NA
                                                       NA
## [11,]
          NA
               NA
                          0
                              NA
                                    0
                                        NA
                                             0
                                                 NA
                                                       NA
                     1
score_chain_master <- tibble(fitness = score.chain,</pre>
                            iter = 1:length(score.chain),
                            label = paste0("col mutated = ",
                                           ncol.to.mutate,
                                           "; acceptance rate = ",
                                           acceptRate))
```

Mutate 2 columns

```
admat.chain <- list(best.admat.mcmc)</pre>
score.chain <- c()</pre>
numAccept = 0
ncol.to.mutate <- 2</pre>
numIter <- 1000
for (i in 1:numIter) {
  fit.prev <- calc.tree.fitness(admat.chain[[i]], cpov, mcmc_w)</pre>
  score.chain[i] <- fit.prev</pre>
    admat.star <- mutate.admat(admat.chain[[i]], ncol.to.mutate)</pre>
    fit.star <- calc.tree.fitness(admat.star, cpov, mcmc_w)</pre>
  r <- fit.star / fit.prev
  u \leftarrow runif(1,0,1)
  if(u <= r) {
    admat.chain[[i+1]] <- admat.star</pre>
    numAccept <- numAccept + 1</pre>
  } else {
    admat.chain[[i+1]] <- admat.chain[[i]]</pre>
}
score.chain[i+1] <- calc.tree.fitness(admat.chain[[i+1]], cpov, mcmc_w)</pre>
acceptRate <- numAccept/(numIter)</pre>
acceptRate
```

```
## [1] 0.152
```

Mutate 3 columns

```
admat.chain <- list(best.admat.mcmc)</pre>
score.chain <- c()</pre>
numAccept = 0
ncol.to.mutate <- 3</pre>
numIter <- 1000
for (i in 1:numIter) {
  fit.prev <- calc.tree.fitness(admat.chain[[i]], cpov, mcmc_w)</pre>
  score.chain[i] <- fit.prev</pre>
    admat.star <- mutate.admat(admat.chain[[i]], ncol.to.mutate)</pre>
    fit.star <- calc.tree.fitness(admat.star, cpov, mcmc_w)</pre>
  r <- fit.star / fit.prev
  u <- runif(1,0,1)
  if(u <= r) {
    admat.chain[[i+1]] <- admat.star</pre>
    numAccept <- numAccept + 1</pre>
  } else {
    admat.chain[[i+1]] <- admat.chain[[i]]</pre>
  }
score.chain[i+1] <- calc.tree.fitness(admat.chain[[i+1]], cpov, mcmc_w)</pre>
acceptRate <- numAccept/(numIter)</pre>
acceptRate
## [1] 0.075
score_chain_master <- rbind(score_chain_master,</pre>
                               tibble(fitness = score.chain,
                                       iter = 1:length(score.chain),
                                       label = paste0("col mutated = ",
                                                       ncol.to.mutate,
                                                        "; acceptance rate = ",
                                                       acceptRate)))
```

Mutate 4 columns

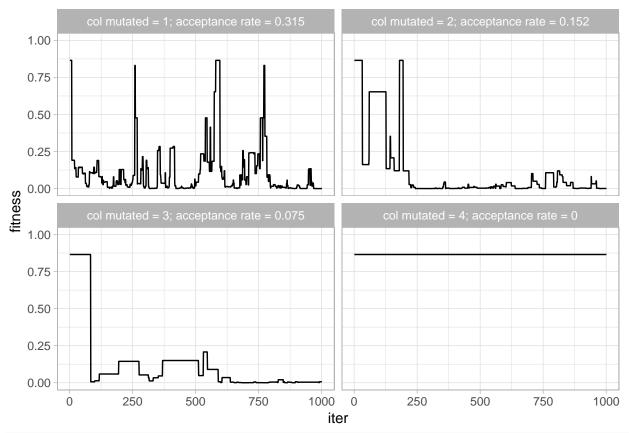
```
admat.chain <- list(best.admat.mcmc)
score.chain <- c()
numAccept = 0
ncol.to.mutate <- 4
numIter <- 1000
for (i in 1:numIter) {
   fit.prev <- calc.tree.fitness(admat.chain[[i]], cpov, mcmc_w)
   score.chain[i] <- fit.prev

   admat.star <- mutate.admat(admat.chain[[i]], ncol.to.mutate)
   fit.star <- calc.tree.fitness(admat.star, cpov, mcmc_w)

r <- fit.star / fit.prev
   u <- runif(1,0,1)
   if(u <= r) {</pre>
```

```
admat.chain[[i+1]] <- admat.star
numAccept <- numAccept + 1
} else {
   admat.chain[[i+1]] <- admat.chain[[i]]
}
score.chain[i+1] <- calc.tree.fitness(admat.chain[[i+1]], cpov, mcmc_w)
acceptRate <- numAccept/(numIter)
acceptRate</pre>
```

[1] 0



ggsave(file.path(figs.dir, "schism_scoring_mutate_cols_1-4.pdf"))

Saving 6.5×4.5 in image