Version 4: 3 clusters, 5 samples, 10 variants—linear

Simulate data

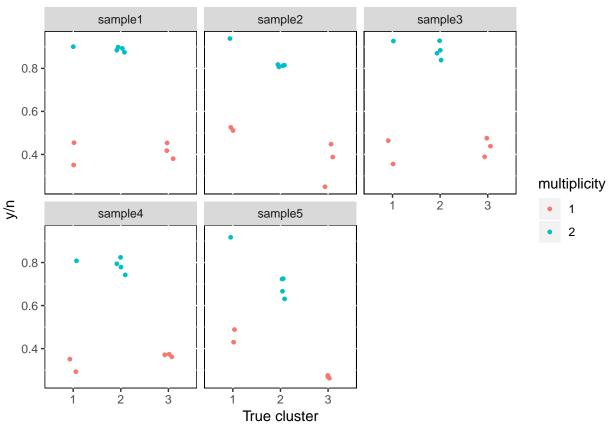
```
I <- 10
K <- 3
S <- 5
set.seed(123)
pi \leftarrow c(0.2, 0.5, 0.3)
z <- sample(1:K, size = I, replace = T, prob = pi)
w \leftarrow matrix(c(0.9, 0.95, 0.9, 0.8, 0.9,
               0.88, 0.8, 0.85, 0.78, 0.7,
               0.85, 0.7, 0.83, 0.76, 0.6),
             byrow=T,
             nrow=K, ncol=S)
colnames(w) <- paste0("sample", 1:S)</pre>
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)
for (i in 1:I) {
  for (s in 1:S) {
    y[i, s] <- rbinom(1, n[i, s], theta[i,s])
  }
test.data <- list("I" = I, "S" = S, "K" = K,
                   "y" = y, "n" = n,
                    "m" = m, "tcn" = tcn)
```

Visualize densities of simulated data

```
Clustering is by \omega
```

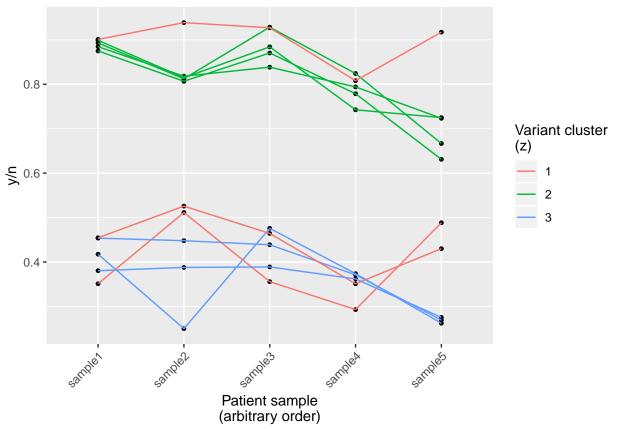
```
p <- test.data$y/test.data$n
colnames(w) <- colnames(p) <- paste0("sample", 1:S)
colnames(m) <- colnames(p)
m2 <- m %>%
    as_tibble() %>%
```

```
mutate(z=factor(z),
           variant_index=seq_len(nrow(.))) %>%
    gather("sample", "multiplicity", -c(z, variant_index)) %>%
    mutate(sample=factor(sample, levels=colnames(p)))
p2 <- p %>%
    as_tibble() %>%
    mutate(z=factor(z),
           variant_index=seq_len(nrow(.))) %>%
    gather("sample", "fraction", -c(z, variant_index)) %>%
    mutate(sample=factor(sample, levels=colnames(p))) %>%
    left_join(m2, by=c("z", "variant_index", "sample")) %>%
    mutate(multiplicity=factor(multiplicity))
## what the data looks like by sample
ggplot(p2, aes(z, fraction)) +
    geom_jitter(width=0.1, size=1, aes(color=multiplicity)) +
    facet_wrap(~sample) +
    ylab("y/n") +
    xlab("True cluster") +
    theme(panel.background=element_rect(fill="white", color="black"))
```



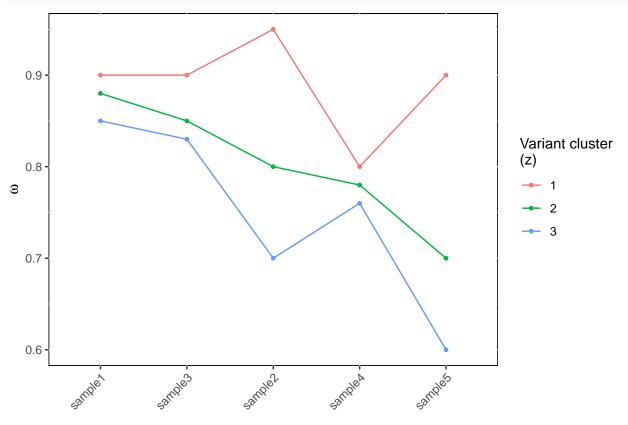
```
## by variant
ggplot(p2, aes(sample, fraction, group=variant_index)) +
    geom_point(size=1) +
    geom_line(aes(color=z)) +
    ylab("y/n") +
    xlab("Patient sample\n(arbitrary order)") +
    theme(axis.text.x=element_text(angle=45, hjust=1)) +
```

guides(color=guide_legend(title="Variant cluster\n(z)"))



```
##
## Cluster means and variances
##
       <- apply(W, 2, median)
slevels <- colnames(w)[order(meds, decreasing=TRUE)]</pre>
w2 <- w %>%
    as tibble() %>%
    mutate(z=factor(1:K)) %>%
             variant_index=seq_len(nrow(.))) %>%
    gather("sample", "omega", -z) %>%
    mutate(sample=factor(sample, levels=slevels))
##fig1 <- ggplot(w2, aes(z, omega)) +</pre>
      geom_jitter(width=0.1, size=1) +
##
##
      facet_wrap(~sample) +
##
      ylab(expression(omega)) +
##
      xlab("True cluster") +
      theme(panel.background=element_rect(fill="white", color="black"))
##
fig2 <- ggplot(w2, aes(sample, omega, group=z)) +</pre>
    geom_point(size=1, aes(color=z)) +
    geom_line(aes(color=z)) +
    ylab(expression(omega)) +
    xlab("") +
    theme(axis.text.x=element_text(angle=45, hjust=1),
          panel.background=element_rect(fill="white", color="black"),
          legend.key=element_rect(fill="white", color="white")) +
```

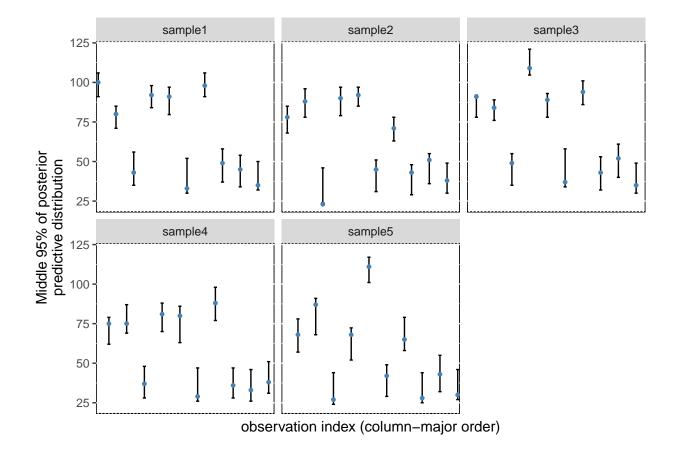
```
guides(color=guide_legend(title="Variant cluster\n(z)"))
fig2
```



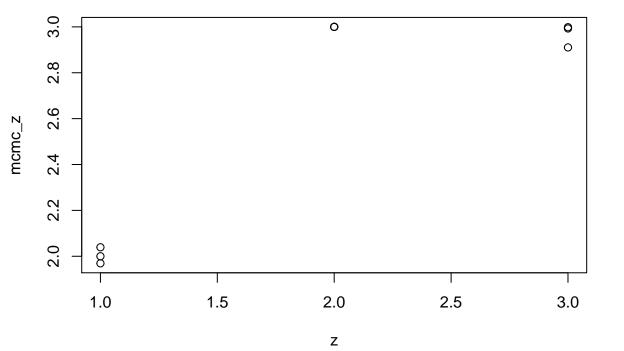
JAGS

```
jags.file <- file.path(models.dir, "w.jags")</pre>
inits <- list(".RNG.name" = "base::Wichmann-Hill",</pre>
               ".RNG.seed" = 123)
jags.m <- jags.model(jags.file, test.data,</pre>
                       n.chains = 1,
                       inits = inits,
                       n.adapt = 1000)
## Compiling model graph
##
      Resolving undeclared variables
      Allocating nodes
##
## Graph information:
      Observed stochastic nodes: 50
##
##
      Unobserved stochastic nodes: 76
##
      Total graph size: 808
##
## Initializing model
params <- c("z", "w", "ystar")</pre>
samps <- coda.samples(jags.m, params, n.iter=10000, thin=7)</pre>
jags_df <- ggs(samps)</pre>
\#ggs\_traceplot(jags\_df,\ family="w")
```

```
s <- summary(samps)</pre>
#effectiveSize(samps)
pdf(file.path(trace.dir, paste0(runName, "_trace.pdf")))
plot(samps)
dev.off()
## pdf
##
##
## 50 mutations x 10 samples
chains <- do.call(rbind, samps)</pre>
ystar <- chains[, grep("ystar", colnames(chains))]</pre>
## each row of MCMC is in column-major order
orig.order <- tibble(statistic=colnames(ystar))</pre>
ppd.summaries <- ystar %>%
    as_tibble() %>%
    gather("statistic", "value") %>%
    group_by(statistic) %>%
    summarize(mean=mean(value),
              q1=quantile(value, 0.025),
              q3=quantile(value, 0.975))
ppd.summaries2 <- left_join(orig.order,</pre>
                             ppd.summaries, by="statistic") %>%
    mutate(observed=as.numeric(test.data$y)) %>%
    mutate(sample=paste0("sample", rep(1:S, each=I)),
           variant=rep(1:I, S))
ggplot(ppd.summaries2, aes(x=statistic, y=mean,
                            ymin=q1,
                            ymax=q3)) +
    geom errorbar() +
    geom_point(aes(x=statistic, y=observed),
               size=1, color="steelblue") +
    theme(axis.text.x=element_blank(),
          axis.ticks.x=element_blank(),
          panel.background=element_rect(fill="white",
                                          color="black")) +
    ylab("Middle 95% of posterior\npredictive distribution") +
    xlab("observation index (column-major order)") +
    facet_wrap(~sample)
```



Plots



Z	mcmc_z
1	2
2	3
3	3

