STAT 447 Assignment 8

Bayesian Workflow

Caden Hewlett

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Question 1: Calibration Analysis via Cross-Validation

One way to approximate the outcome of an experiment is via cross-validation. In particular, this exercise will teach you how to use leave-one-out cross-validation to assess the calibration of the model for the Hubble dataset.

Let's begin by loading and formatting the data again.

```r
df = read.csv("data/hubble.csv")[1:24, c(3:4)]
colnames(df) = c("distance", "velocity")
velocity = df$velocity/1000
distance = df$distance

# get the data frame size
N_obs = nrow(df)
```

Part 1

Now, we can build our modified Stan file, called `hubble_predict`.

```stan
// The input data are the distances 'd' of length 'N'.
data {
  int<lower=0> N;
  vector<lower = 0>[N] d;
  vector[N] v;
  real x_pred; // held-out point
}

// The parameters accepted by the model. Our model
// accepts two parameters 'beta' which is the slope
// and 'sigma', which is the variance (heteroskedastic)
parameters {
  real beta;
  real<lower=0> sigma;
}

// The model to be estimated.
// We model the velocity 'v' to be normally distributed
// with mean 'beta * d_i'and standard deviation 'sigma'.

model {
  beta ~ student_t(3, 0, 100);
  sigma ~ exponential(0.001);
  for (i in 1:N){
    v ~ normal(beta * d[i], sigma);
  }
}


// Values Produced by the model
generated quantities {
   real y_pred = normal_rng(beta*x_pred, sigma);
}
```

Part 2

Then, we can run `sampling()` with this object, using MCMC methodology to find $\mathbb{E}\big(y_n \mid x_n, \{(x_i, y_i)\}_{i=1}^{n-1}\big)$.

```
fit = sampling(
  hubble_predict,
  seed = 1990, # launch year of the Hubble
  data = list(
    N  = N_obs-1,
    d = df$distance[-N_obs],
    v = df$velocity[-N_obs],
    x_pred = df$distance[N_obs]
  )
)

q1_info = rstan::extract(fit)
```

Note that the true value y_n was $1,090$km/s. The reported value of $\mathrm{C}(y_{\neg n}, \alpha = 0.80)$ is given below:

```
ci_1 = round(c(quantile( q1_info$y_pred, 0.10 ),
          quantile( q1_info$y_pred, 0.90 )), 3)

kable(ci_1, caption = "80% Credible Interval")
```

Table 1: 80% Credible Interval

	x
10%	1.049
90%	1028.611

Part 3

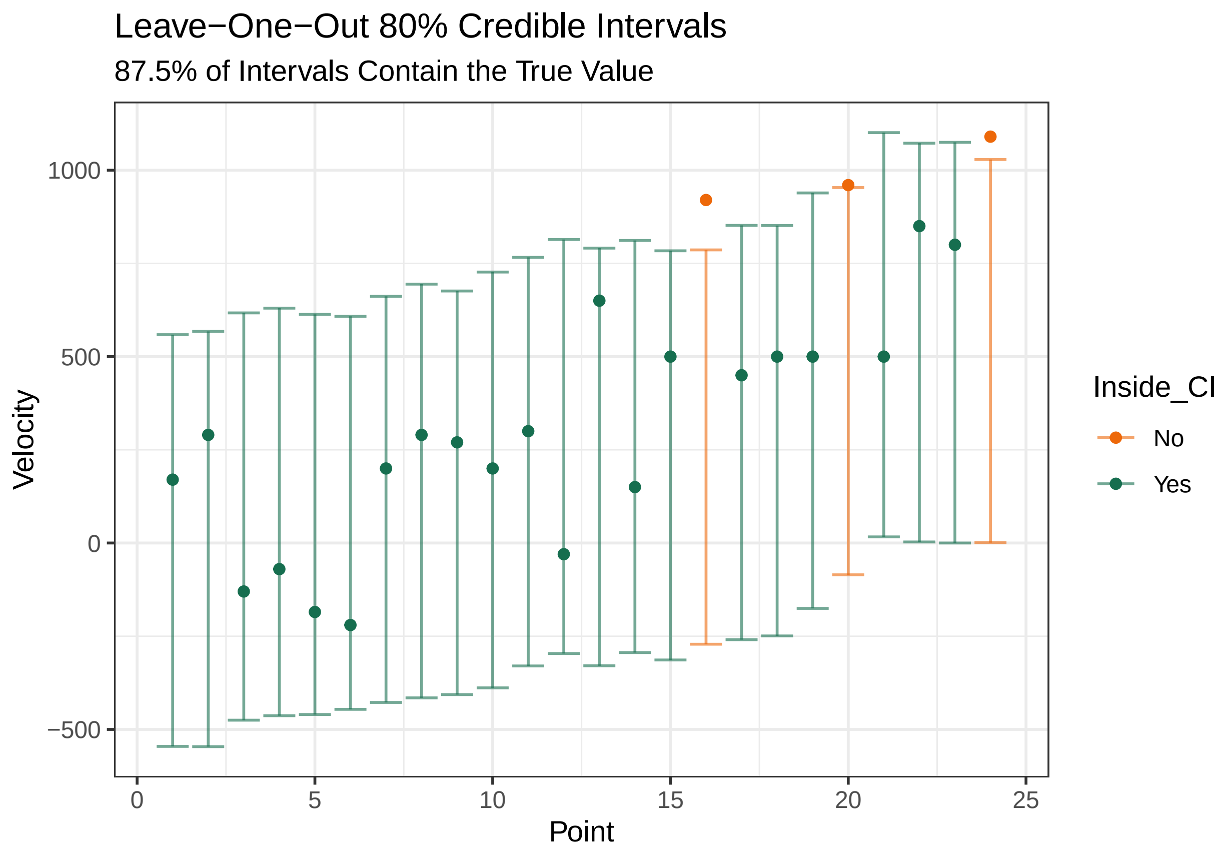
Now, we repeat this leave-one-out process for all observations. We will construct a matrix of `nrow(df)` rows and 2 columns called `ci_limits`, where the i-th row contains an 80% credible interval for the i-th observation left out.

To do this, we define a function called `CrI` which takes in an index and repeats the previous question's process:

```r
CrI <- function(index){
  # compute LOO MCMC
  one_out = sampling(
    hubble_predict,
    seed = 1990,
    data = list(
      N  = N_obs-1,
      d = df$distance[-index],
      v = df$velocity[-index],
      x_pred = df$distance[index]
    ))
  # extract and compute interval
  info = rstan::extract(one_out)
  return(c(
    quantile(info$y_pred, 0.10),
    quantile(info$y_pred, 0.90)
  ))
}

## use this to make the matrix
all_loo = sapply(1:N_obs, function(n){CrI(n)})
# populate matrix
ci_limits = matrix(all_loo, nrow = nrow(df), ncol = 2, byrow = T)
```

Then the plot is below:

```r
merged_df = df %>%
  bind_cols(data.frame(CI_L = ci_limits[, 1], CI_R = ci_limits[, 2])) %>%
  mutate(Inside_CI = (velocity >= CI_L & velocity <= CI_R))
plot = merged_df %>%
  ggplot(aes(
    x = 1:N_obs,
    y = velocity,
    ymin = CI_L,
    ymax = CI_R,
    color = Inside_CI
  )) +
  geom_point() +
  geom_errorbar(alpha = 0.6) +
  scale_color_manual(values = c("#ed6809", "#166e4f"),
                     labels = c("No", "Yes")) +
  theme_bw() +
  labs(
    x = "Point",
    y = "Velocity",
    title = "Leave-One-Out 80% Credible Intervals",
    subtitle = paste((sum(merged_df$Inside_CI)/N_obs)*100,
                     "% of Intervals Contain the True Value", sep = "")
  )
print(plot)
```



As the above plot shows, roughly 87.5% of the credible intervals contain the true value.

By the properties of well-specified confidence intervals, we know that:

$$\text{Well Specified Model} \implies \mathbb{P}\big(Y_n \in \mathrm{C}(Y_{\neg n})\big) = 1 - \alpha$$

Where in our case, $(1 - \alpha) = 0.80$.

Our observed proportion of intervals $\mathrm{C}(y_{\neg n})$ containing the true y_n value was 0.875. Since $0.875 \approx 0.80$, we don't currently have significant evidence to suggest the model is not well-specified. Using the language of hypothesis testing, we would fail to reject "H_0: The model is well-specified."

Question 2: Prior Predictive Checks

In this exercise we will investigate the effect of having fixed independent priors on the coefficients $\{\beta_i\}_{i=1}^{n_{\text{pred}}}$ as n_{pred} grows.

Part 1

To properly design this function, we will introduce some nomenclature. Let $\mathbf{X}$ be defined as follows:

$$\mathbf{X} = \begin{bmatrix} x_{1,1} & x_{1,2} & \dots & x_{1,n_{\text{pred}}} \\ x_{2,1} & x_{2,2} & \dots & x_{2,n_{\text{pred}}} \\ \vdots & \vdots & \ddots & \vdots \\ x_{n_{\text{obs}},1} & x_{n_{\text{obs}},2} & \dots & x_{n_{\text{obs}},n_{\text{pred}}} \end{bmatrix}_{n_{\text{obs}} \times n_{\text{pred}}}$$

Then, the vector of random normal pulls is denoted $\vec{\beta}$, where:

$$\vec{\beta} = \left\{ \beta_i \mid \beta_i \overset{\text{iid}}{\sim} N(0,1),\ \text{for } i \in [1, n_{\text{pred}}] \right\}$$

Finally, the likelihood is given by:

$$\vec{\mathbf{y}} \mid \vec{\beta} \sim \text{bern}\Big(\text{logistic}\big(\mathbf{X}\vec{\beta}\,\big)\Big)$$

Then, letting $\vec{\mathbf{1}}$ be the vector of 1s, we let the mean of $\vec{y}$ be

$$\bar{\mathbf{y}} := n_{\text{obs}}^{-1}(\vec{\mathbf{1}} \cdot \vec{\mathbf{y}}) = \frac{1}{n_{\text{obs}}} \sum_{\{y\,:\,y \in \vec{\mathbf{y}}\}} y$$

Now that we've clarified the model, let's proceed with the design of the `logistic_regression` function.

Given $\mathbf{X}$, the function will sample $\vec{\beta}$ first before computing $\text{logistic}\big(\mathbf{X}\vec{\beta}$ and then conducting n_{obs} Bernoulli trials to create $\vec{\mathbf{y}}$ and then computing the mean of $\vec{\mathbf{y}}$. (NOTE: we know there are n_{obs} trials due to the fact that $\mathbf{X}_{n_{\text{obs}} \times n_{\text{pred}}} \times \vec{\beta}_{n_{\text{pred}} \times 1} = \vec{\mathbf{y}}_{1 \times n_{\text{obs}}}$.)

We will denote this function as follows:

$$\text{Logistic Regression} : f : \mathbb{R}^{n_{\text{obs}} \times n_{\text{pred}}} \to \mathbb{R},\ \text{ where } f\left(\mathbf{X}\right) = \bar{\mathbf{y}}$$

We attempt to inherit the terminology and process described above.

```r
logistic_regression <- function(X){
  # get the matrix sizes
  n_pred = ncol(X)
  n_obs = nrow(X)

  # simulate beta values
  beta = rnorm(n_pred)

  # compute the p parameter of the bernoulli distribution
  p = plogis(X%*%beta) # 1 / (1 + exp(-X%*%beta))

  # then the y values
  y = rbinom(n_obs, size = 1, prob = p)

  # then take the mean
  ybar = mean(y)

  # and return it
  return(ybar)
}
```

Part 2

Now, we let $n_{\text{obs}} = 100$ and consider $n_{\text{pred}} \in \{2, 4, 15\}$.

We will create a set of data matrices $\mathcal{X}$ defined by the following, letting $x_{i,j}$ be the (i, j) cell of $\mathbf{X}$

$$\mathcal{X} = \Big\{ \mathbf{X}_{100 \times n},\ \text{where } x_{i,j} \overset{\text{iid}}{\sim} \text{bern}(0.9),\ \text{for } i \in [1, 100], j \in [1, n] \text{ and } n \in \{2, 4, 15\} \Big\} \tag{1}$$

Then, for $M = 100,000$, we complete the simulation process, letting $\mathbf{X}_k \subset \mathcal{X}$ be the matrix in $\mathcal{X}$ with k columns. We can think of the resulting process creating a $M \times K$ matrix, where $K = |\mathcal{X}|$ denoted as follows:

$$\overline{\mathbf{Y}}_{M,K} = \begin{bmatrix} \bar{\mathbf{y}}_{1,1} & \bar{\mathbf{y}}_{1,2} & \cdots & \bar{\mathbf{y}}_{1,K} \\ \bar{\mathbf{y}}_{2,1} & \bar{\mathbf{y}}_{2,2} & \cdots & \bar{\mathbf{y}}_{2,K} \\ \vdots & \vdots & \ddots & \vdots \\ \bar{\mathbf{y}}_{M,1} & \bar{\mathbf{y}}_{M,2} & \cdots & \bar{\mathbf{y}}_{M,K} \end{bmatrix}_{M \times K} \tag{2}$$

$$\text{Where } \bar{\mathbf{y}}_{m,k} = f(\mathbf{X}_k) \text{ for } \mathbf{X}_k \in \mathcal{X}, k \in [1, K],\ \text{and } m \in [1, M] \tag{3}$$

Then we plot a histogram for each column of $\overline{\mathbf{Y}}_{M,K}$. In our example there are only three columns, but the language here is designed to be extended upon if desired. The tags on the above equations have been added to direct the reader through the code.

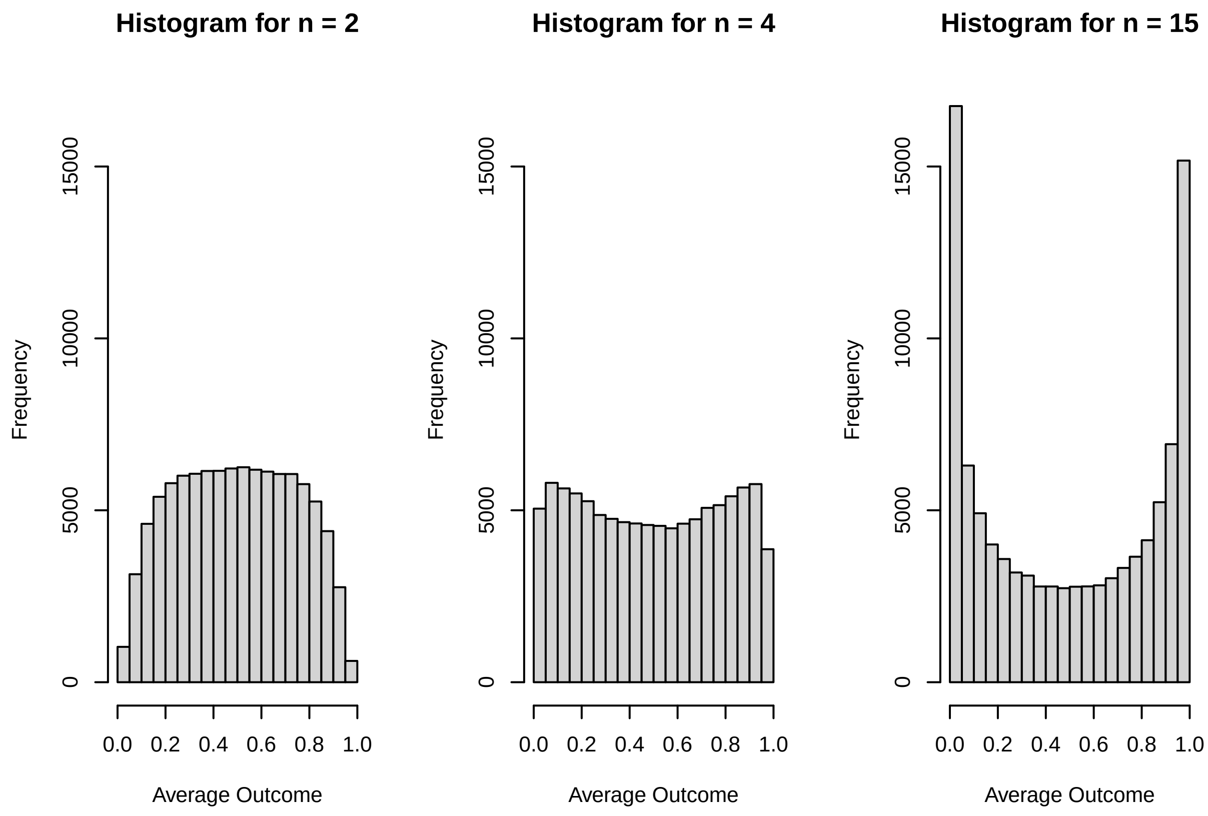
The entire simulation study is conducted below, with the $\overline{\mathbf{Y}}_{M,K}$ matrix previewed at the end.

```r
set.seed(1928)
# declare parameters
M = 100000
p = 0.9
m = 100
n_pred = c(2, 4, 15)
K = length(n_pred)
# rename the logistic_regression to match the terminology provided
f <- logistic_regression
remove(logistic_regression)

# create the set of matrices described earlier: (1)
X <- sapply(n_pred, function(n){
  matrix(data = rbinom(n*m, size = 1, prob = p),
         nrow = m, ncol = n)
})

# then, create Y: k in [1, K], m in [1, M] : (2)
Y = matrix(rep(1:K, each = M), nrow = M, ncol = K, byrow = F)
# finally, populate this matrix: (3)
Ybar = apply(Y,  MARGIN = c(1,2), function(k){ f(X[[k]]) })
head(Ybar)
```

```
##      [,1] [,2] [,3]
## [1,] 0.17 0.28 0.43
## [2,] 0.74 0.84 0.12
## [3,] 0.80 0.83 0.03
## [4,] 0.42 0.24 0.99
## [5,] 0.24 0.77 0.40
## [6,] 0.43 0.06 1.00
```

Then, we can make the plots as follows (note, I added $n = 1$):

```
par(mfrow=c(1, K))
for (k in 1:K) {
  hist(Ybar[, k],  breaks=20, ylim=c(0,17000),
       main=paste("Histogram for n =", n_pred[k]), xlab="Average Outcome", ylab="Frequency")
}
```



Part 3

Do you observe any change in the distributions obtained in step 2?

Yes, we see that as n_{pred} increases, the plot of average outcomes becomes increasingly concave. In this sense, there is higher frequency for the $[0.00, 0.05]$ and $[0.95, 1.00]$ as $n_{\text{pred}} \uparrow$. In running repeated tests for different n_{pred}, I found that the concavity becomes evident for $n_{\text{pred}} \geq 4$

Do you think this is desirable in a model?

No. The prior is becoming increasingly opinionated as n_{pred} increases. Potentially, as $n_{\text{pred}} \to \infty$, we could start to see densities of zero on values in the prior. Under Cromwell's Rule, this is undesirable. I would hypothesize that this increasing preference of the prior is due to the "bloat" in predictors, and hence over-fitting.

If yes, why? If not, how would you fix this?

There are many fixes to this issue, such as using LOO-CV with the leave-one-out methods discussed in this section. Alternatively, we could take a "spike-and-slab" approach as we have done with previous models, selecting only those predictors which are relevant.

Q.3: Hierarchical Models Revisited

In this original question, we had $\mu_p \sim \text{betaMP}(0.1, 10)$ among other distributions.

Noting that $\mu = 0.1$ and $s = 10$ in this case, we can remodel this in "standard" beta parameters as follows:

$$\alpha = \mu s = 0.1(10) = 1, \text{ and } \beta = (1-\mu)s = (0.9)(10) = 9$$

So, now, $\mu_p \sim \text{beta}(1, 9)$.

Similarly, we also have

$$(p \mid \{\mu_p, \lambda_p\}) \sim \text{betaMP}(\mu_p, \lambda_p) \equiv \text{beta}\big(\mu_p\lambda_p, (1-\mu_p)\lambda_p\big)$$

Now, let's load in and pre-process our data using nice `tidybayes` logic. We also preview the names of the object.

```r
data = read.csv("data/vaccines_full.csv")
data$is_vaccinated = ifelse(data$arms == "vaccinated", 1, 0)
stan_converted = compose_data(data)
kable(t(names(stan_converted)))
```

trial	n_trial	arms	n_arms	groupSizes	numbersOfCases	is_vaccinated	n

With this nice list in mind, we replicate the model with the following Stan structure:

```stan
//** ************* **//
//** VACCINE MODEL **//
//** ************* **//

data {
  // maintaining the same formatting as in the tutorial
  int n;
  int n_trial;
  array[n] int<lower=1,upper=n_trial> trial;
  array[n] int arms;
  int n_arms;
  array[n] int groupSizes;
  array[n] int numbersOfCases;
  array[n] int is_vaccinated;
}
```

```
parameters {
    // priors on effectiveness
  real mu_e;
  real <lower=0> lambda_e;
  // priors on incidence
  real mu_p;
  real <lower=0> lambda_p;
  // effectiveness and prevalence
  vector<lower=0,upper=1>[n_trial] efficiencies;
  vector<lower=0,upper=1>[n_trial] prevalences;
}

model {
   // generate prior values
  mu_e ~ uniform(0, 1);
  lambda_e ~ exponential(0.001);
  // using conversion from beta
  mu_p ~ beta(1, 9);
  lambda_p ~ exponential(0.001);
  // now, trial aren't just beta (1,1)
  for (t in 1:n_trial) {
    efficiencies[t] ~ beta( lambda_e * mu_e,
                            lambda_e * (1 - mu_e)) ;
    prevalences[t] ~  beta( lambda_p * mu_p,
                            lambda_p * (1 - mu_p)) ;
  }
  // full model, I think
  for (i in 1:n) {
    numbersOfCases[i] ~ binomial(groupSizes[i], (prevalences[trial[i]] *
    (is_vaccinated[i] == 1 ? 1.0 - efficiencies[trial[i]] : 1.0)));
  }
}

// indicator of if Moderna is better than Pfizer, as done previously
generated quantities {
  // pfizer = 3, moderna = 2
  real is_moderna_better = efficiencies[2] > efficiencies[3] ? 1 : 0;
}
```

Now, we can run the MCMC and get info from it.

```
v_fit = sampling(
  vaccine_h_model,
  seed = 1990,
  data = stan_converted
)
v_fit  %<>% recover_types(data)
```

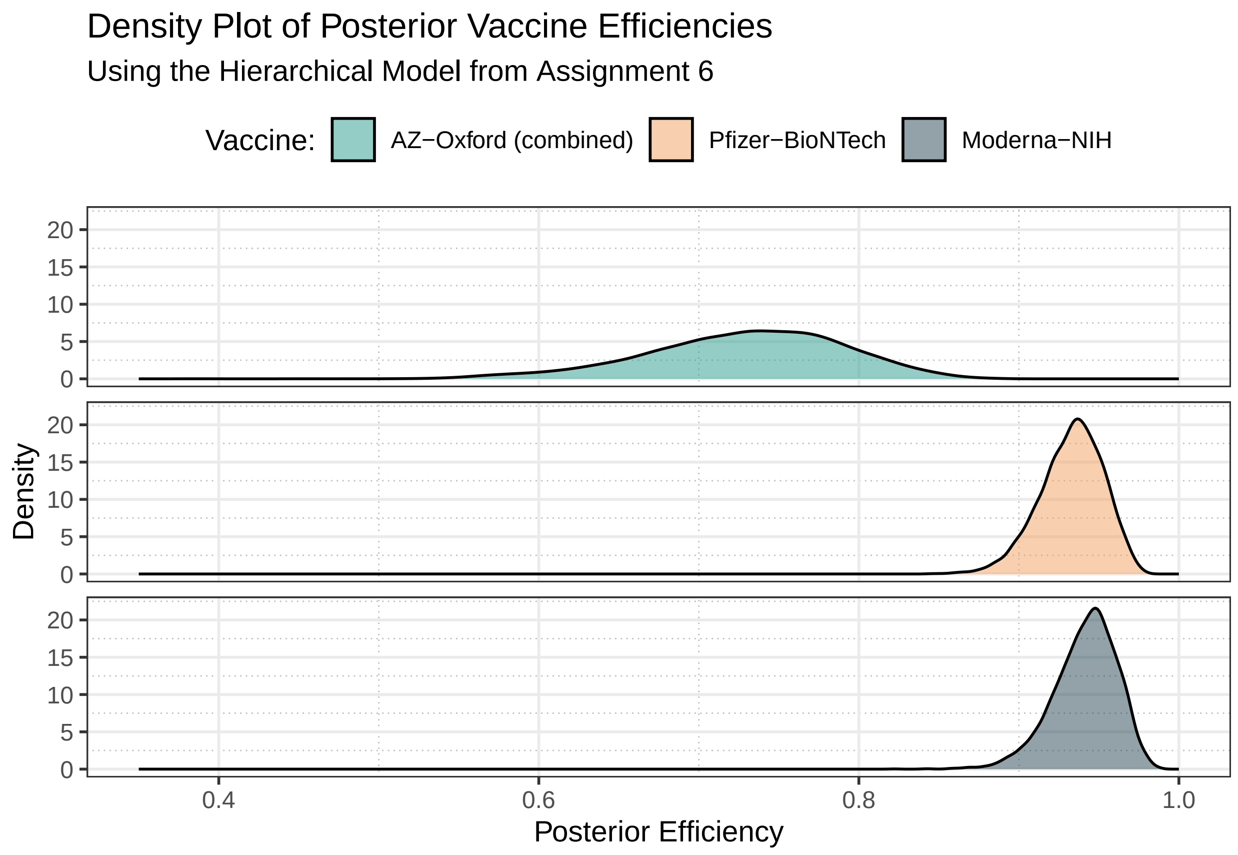
Which we preview below:

```
kable(v_fit %>% spread_draws(efficiencies[trials], prevalences[trials]) %>% head(5))
```

trials	efficiencies	.chain	.iteration	.draw	prevalences
1	0.7454787	1	1	1	0.0159489
1	0.6564084	1	2	2	0.0160991
1	0.7861252	1	3	3	0.0187622
1	0.7605333	1	4	4	0.0179109
1	0.7524374	1	5	5	0.0182773

Now, to confirm that everything has gone according to plan, we will produce a density plot and compare the `is_moderna_better` to the simPPLe results found in Assignment 6.

```r
# use spread_draws to get relevant values
df = v_fit %>% spread_draws(efficiencies[trials], prevalences[trials])
# melt the values into a data frame
plotDF = melt(data.frame(
  A =  df$efficiencies[df$trials == 1],
  P =  df$efficiencies[df$trials == 2],
  M =  df$efficiencies[df$trials == 3]
))
# greate density plots
plo  = ggplot(plotDF, aes(x = value, fill = variable)) +
  geom_density(alpha = 0.5) +
  xlim(0.35, 1) +  ylim(0, 22) +
  labs(
    title = "Density Plot of Posterior Vaccine Efficiencies",
    x = "Posterior Efficiency",
    y = "Density",
    subtitle = "Using the Hierarchical Model from Assignment 6"
  ) +
  theme_bw() +
  scale_fill_manual(
    name = "Vaccine:",
    values  =  c(
      "A" = "#2a9d8f",
      "P" = "#f4a261",
      "M" = "#264653"
    ),
    # get original names
    labels = unique(data$trial)
  ) +
  theme(
    legend.position = "top",
    panel.grid.minor = element_line(color = "grey", linetype = "dotted"),
    strip.background = element_blank(),
    strip.text = element_blank()
  ) +
  facet_wrap( ~ variable, scales = "free_y", ncol = 1)
print(plo)
```



Now, getting the indicator of Moderna outperforming Pfizer:

```r
samples = rstan::extract(v_fit)
results = data.frame(
  vaccine = unique(data$trial)[-1],
  prop_better = as.numeric(table(samples$is_moderna_better) /
                             length(samples$is_moderna_better)))

colnames(results)=c("Vaccine", "Proportion Better")
kable(results)
```

Vaccine	Proportion Better
Pfizer-BioNTech	0.63175
Moderna-NIH	0.36825

The above value for Moderna of 0.36825 closely matches those found on Assignment 6. It seems like the hierarchical implementation has gone according to plan.