BIOS 731 HW 2: Simulation Studies

```
source(here::here("source", "01_simulate_data.R"))
source(here::here("source", "02_apply_methods.R"))
source(here::here("source", "03_extract_estimates.R"))

# Define simulation function to parallelize
run_sim_scenario <- function(index){

  # Define row from parameters in global environment
  p <<- index

  # Load functions
  source(here::here("source", "01_simulate_data.R"))
  source(here::here("source", "02_apply_methods.R"))
  source(here::here("source", "03_extract_estimates.R"))

  # Run simulation process
  source(here::here("simulations", "run_simulations.R"))

  # Save results
  return(list("results" = results_df,
              "timing_log" = timing))
}
```

Problem 1.1: ADEMP Structure

- *A*: The goal of this simulation study is to evaluate the accuracy of a linear regression to estimate a binary treatment effect. We also want to compare the coverage and computational efficiency of three methods of estimating a 95% confidence interval around the treatment effect estimates: a Wald confidence interval, a bootstrap percentile interval, and a bootstrap t interval. All of these methods should generate intervals that cover the true treatment effect in at least 95% of simulations.

- *D*: We generate data under the assumption

$$Y_i = \beta_0 + \beta_{treat} X_i + \epsilon_i$$

for $i = 1, \ldots, n$.

In all scenarios, X_i is a binary variable that we randomly generate with $P(X_i = 1) = 0.5$, and we set $\beta_0 = 1$.

We set up a full factorial simulation design with the alternatives:

$n = 10,\ 50,$ or 500;

$\beta_{treat} = 0,\ 0.5,$ or 2;

$\epsilon_i \overset{iid}{\sim} N(0, 2)$ or $\epsilon_i = u * \sqrt{2 * \frac{\nu - 2}{\nu}},$ where $u \overset{iid}{\sim} t_\nu$ and $\nu = 3$.

Therefore, we include **18** total scenarios.

- *E*: We are trying to learn about one estimand through this study: $\hat{\beta}_{treat}$ from a linear regression.
- *M*: We are evaluating one method for a point estimate $\hat{\beta}_{treat}$, which is linear regression. We are then comparing three methods for a confidence interval around this estimand: a Wald confidence interval, a bootstrap percentile confidence interval, and a bootstrap t confidence interval.
- *P*: We will evaluate $\hat{\beta}_{treat}$ using its bias. We will compare the three methods for the confidence interval based on coverage and computation speed.

Problem 1.2: nSim

```
# Define desired coverage and max Monte Carlo error
ci_pct <- 0.95
mcse_max <- 0.01

# Calculate necessary simulations
nSim <- ci_pct * (1 - ci_pct) / (mcse_max)^2
```

Based on desired coverage of 95% with a maximum Monte Carlo standard error of 1%, we should perform 475 simulations for each scenario.

Problem 1.3: Implementation

Parameters

First, we set up the full factorial design, defining all of the parameters that change between scenarios and expanding them into a data frame of all combinations. We also define the number of outer and inner bootstrap resamples we will run. We use the recommended numbers from the homework: 500 outer bootstrap resamples and 100 inner bootstrap resamples.

```
# Define sample size, treatment effect, error distribution
data_n <- c(10, 50, 100)
beta_true <- c(0, 0.5, 2)
error_dist <- c("gauss", "t")

# Combine these into table
params <- expand_grid(data_n, beta_true, error_dist)

# Set bootstrap numbers
boot_outer <- 500
boot_inner <- 100
```

Setting seeds

Next, we define the seeds we will use for these simulations. We use a different seed for each simulation and for each outer bootstrap resample in each scenario. We generate these seeds by setting one seed arbitrarily, then randomly generating numbers from 1 to the total number of seeds we need. Then, we organize these into a nested list by scenario and by simulation number.

```
### Define seeds

# Count number of randomization steps we will perform
# -> For each scenario: n simulations, 1 data set,
#                       B_outer bootstrap samples per data set,
#                       B_inner resamples per outer sample
num_sims <- nrow(params) * nSim * (1 + boot_outer * boot_inner)

# -> We will use 1 seed per bootstrap
num_seeds <- nrow(params) * nSim * (1 + boot_outer)

# Set initial seed, outside of next range
set.seed(num_seeds + 413)
```

```r
# Randomize order of other seeds
seeds <- sample(1:num_seeds, num_seeds)

# Organize these by simulation step
seed_list <- split(
  seeds,
  cut(1:num_seeds, breaks = nrow(params))
) %>%
  map(~split(.x, cut(1:length(.x), breaks = nSim)))
```

Comparing possible regression functions

Then, before running these simulations, we try to improve the computational efficiency of our process. For both bootstrap methods of generating a confidence interval, we do not need the estimated standard error of our estimated β_{treat}; we only need the coefficient itself. While this is most easily generated by the function `lm`, it can also be calculated using the function `lm.fit`. We check that these two methods return the same coefficient, and also use `benchmark` to test their computation speeds against each other. We find that `lm.fit` is significantly quicker, so we use it in both of our bootstrap functions.

```r
set.seed(num_seeds + 978)

test_df <- get_simdata(n = max(data_n),
                       beta_treat = max(beta_true),
                       variance = 2,
                       error_dist = "gauss")

tibble(
  lm = coef(fit_model_lm(test_df)),
  lm.fit = coef(fit_model_lm_fit(x_mat = matrix(cbind(1, test_df$x),
                                                nrow = nrow(test_df)),
                                 y_vec = test_df$y))
)
```

lm	lm.fit
0.8763628	0.8763628
1.7465801	1.7465801

```r
bench <- microbenchmark::microbenchmark(
  "coef_lm" = coef(fit_model_lm(test_df))[2],
  "coef_lm.fit" =  coef(fit_model_lm_fit(x_mat = matrix(cbind(1, test_df$x),
                                                        nrow = nrow(test_df)),
                                         y_vec = test_df$y))[2]
  )

print(bench)
```

```
Unit: microseconds
        expr     min       lq     mean   median       uq     max neval cld
     coef_lm 120.212 125.3780 136.8851 131.4460 136.4685 616.312   100  a
 coef_lm.fit  15.006  16.1335  22.1359  16.8305  17.5890 534.271   100   b
```

Running simulation scenarios

Finally, we run simulations for all 18 scenarios listed. Results are saved in a nested list: for each scenario, we save one dataset of results for each simulation and one dataset of timing logs.

This process takes about 30 minutes total, so we set up a switch to load the output from these simulations if we are not running this code for the first time.

```r
# Determine number of cores available
num_cores <- detectCores() - 2

if(DO_SIMULATIONS){

  # Make cluster for parallelization
  cl <- makeCluster(num_cores)

  registerDoParallel(cl)

  # Combine results and timing from all scenarios
  simulation_output <- foreach(
    i = 1:nrow(params),
    .packages = c("tidyverse", "magrittr", "tictoc", "broom"),
    .inorder = F
  ) %dopar% {

    # Move all necessary variables to global environment
    .GlobalEnv$params <- params
```

```
    .GlobalEnv$nSim <- nSim
    .GlobalEnv$seed_list <- seed_list
    .GlobalEnv$boot_outer <- boot_outer
    .GlobalEnv$boot_inner <- boot_inner

    run_sim_scenario(index = i)
  }

  stopCluster(cl)

  # Save combined output
  save(simulation_output,
       file = here::here("data", "combined_scenario_output.rda"))

} else {

  # Load output
  load(file = here::here("data", "combined_scenario_output.rda"))
}
```

Problem 1.4: Results summary

We combine the results and timing datasets across all 18 scenarios to summarize the results. We also calculate coverage and bias at this stage.

```
# Collect results and timing into two separate datasets
results_all <- map(simulation_output, ~.[["results"]]) %>% bind_rows()
timing_all <- map(simulation_output, ~.[["timing_log"]]) %>% bind_rows()

# Merge information from parameters
params_merge <- params %>%
  mutate(scenario = 1:n())

# Merge parameters and calculate coverage
results_all %<>%
  left_join(params_merge) %>%
  mutate(coverage = as.numeric(beta_true >= conf.low & beta_true <= conf.high),
         bias = beta_hat - beta_true)
```

Next, we summarize the timing, average $\hat{\beta}$, coverage percent, confidence interval width, and standard error across all simulations by scenario and interval estimation method. The standard error under the

Wald method is taken from the output of `lm`; for the two bootstrap methods, we take the standard error of all bootstrap estimates $\hat{\beta}_1, \ldots, \hat{\beta}_B$. Therefore, the standard error estimates for both bootstrap methods are the same.

```
# Summarize time
scenario_timing <- timing_all %>%
  group_by(scenario, step) %>%
  summarize(time_total = sum(time)) %>%
  ungroup() %>%
  arrange(scenario, desc(time_total)) %>%
  group_by(scenario) %>%
  mutate(scenario_pct = time_total / first(time_total)) %>%
  ungroup()

# Trim down to only the methods we are summarizing
method_timing <- scenario_timing %>%
  filter(str_detect(step, "Boot|Wald")) %>%
  select(scenario, method = step, time_total) %>%
  mutate(method = case_match(method,
                             "Bootstrap t" ~ "Boot t",
                             "Bootstrap percentile" ~ "Boot Pct",
                             "Wald" ~ "Wald"))

# Summarize bias, coverage, SD
scenario_results <- results_all %>%
  group_by(scenario, data_n, beta_true, error_dist, method) %>%
  summarize(beta_hat_avg = mean(beta_hat, na.rm = T),
            coverage_pct = mean(coverage, na.rm = T),
            std_error = mean(std.error, na.rm = T),
            ci_width = mean(conf.high - conf.low, na.rm = T)) %>%
  ungroup() %>%
  mutate(bias = beta_hat_avg - beta_true) %>%
  left_join(method_timing) %>%
  mutate(method = factor(method,
                         levels = c("Wald", "Boot Pct", "Boot t")),
         error_dist = case_match(error_dist,
                                 "gauss" ~ "Gaussian",
                                 "t" ~ "t-Dist."))
```

Bias

The first performance measure we tracked was the bias of the linear regression estimate. This measure is compared across scenarios in the table below.

```
# Summarize bias
bias_table <- scenario_results %>%
  distinct(data_n, beta_true, error_dist,
           bias, beta_hat_avg) %>%
  arrange(error_dist, beta_true, data_n) %>%
  select("Error Dist." = error_dist,,
         "Beta" = beta_true,
         "N" = data_n,
         "Mean Est." = beta_hat_avg,
         "Bias" = bias)

# Print this table
kbl(bias_table,
    booktabs = T,
    caption = "Beta Estimation",
    digits = 3) %>%
  kable_classic(full_width = F) %>%
  column_spec(1:2, bold = T) %>%
  column_spec(3, italic = T) %>%
  collapse_rows(columns = 1:2,
                valign = "top",
                row_group_label_position = "first",
                latex_hline = "full") %>%
  add_header_above(c("Parameters" = 3,
                     "Performance Measures" = 2))
```

To see more details about the bias across simulations and scenarios, we also plot empirical density functions of the bias across scenarios.

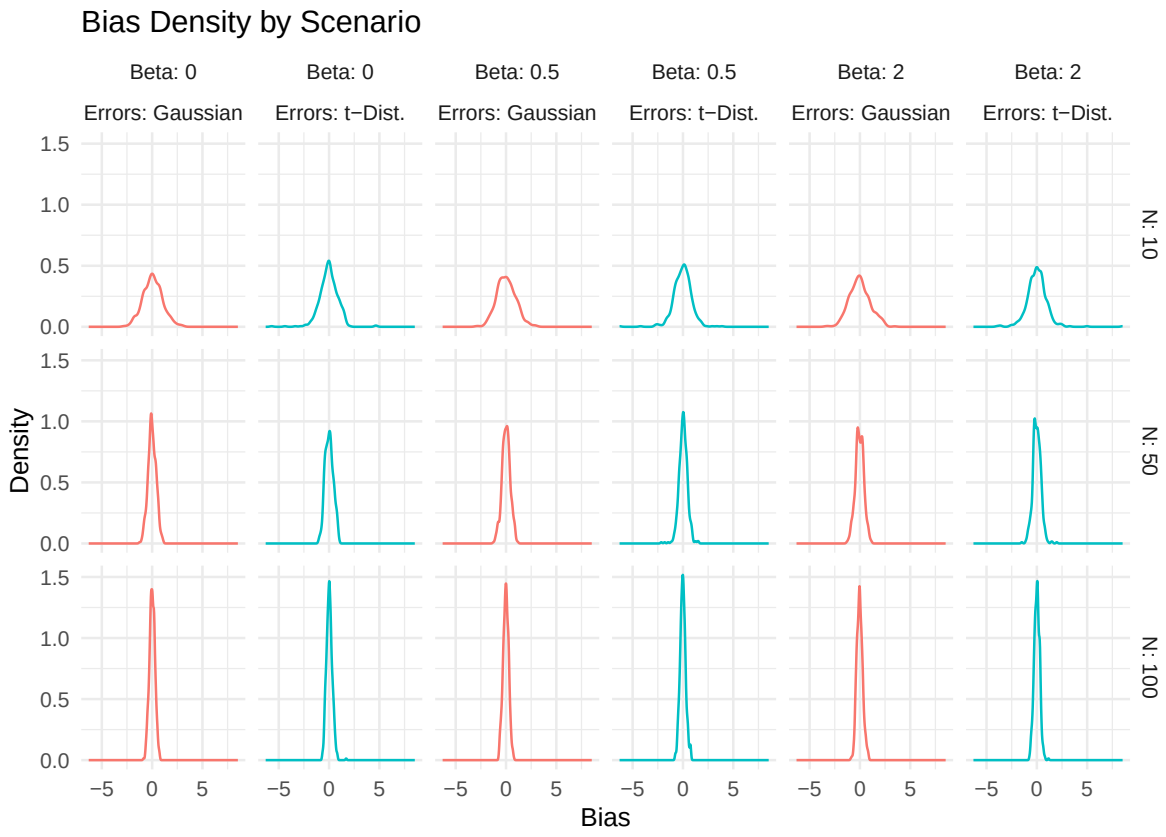
```
bias_plot <- ggplot(results_all %>%
                      mutate(error_dist = case_match(error_dist,
                                "gauss" ~ "Gaussian",
                                "t" ~ "t-Dist.")) %>%
                      rename("N" = data_n,
                             "Beta" = beta_true,
                             "Errors" = error_dist),
                    aes(x = bias,
```

Table 2: Beta Estimation

Parameters			Performance Measures	
Error Dist.	Beta	N	Mean Est.	Bias
Gaussian	**0.0**	*10*	0.066	0.066
		50	-0.006	-0.006
		100	0.006	0.006
	0.5	*10*	0.525	0.025
		50	0.508	0.008
		100	0.485	-0.015
	2.0	*10*	1.982	-0.018
		50	1.966	-0.034
		100	1.980	-0.020
t-Dist.	**0.0**	*10*	-0.040	-0.040
		50	0.012	0.012
		100	0.028	0.028
	0.5	*10*	0.455	-0.045
		50	0.524	0.024
		100	0.490	-0.010
	2.0	*10*	2.009	0.009
		50	2.002	0.002
		100	2.006	0.006

```
                          color = Errors)) +
  geom_density() +
  facet_grid(N ~ Beta + Errors, labeller = label_both) +
  labs(x = "Bias", y = "Density", color = "Error Distribution",
       title = "Bias Density by Scenario") +
  theme_minimal() +
  theme(legend.position = "none")

bias_plot
```



Coverage

Next, we compare the three methods of estimating a 95% confidence interval for $\hat{\beta}$. We compare three measures to understand the differences between these methods: average standard error, coverage percentage of the confidence interval, and total computation time over all simulations. These are presented in the table below.

```r
# Summarize coverage and standard error
covg_table <- scenario_results %>%
  select(data_n, beta_true, error_dist,
         method,
         std_error, coverage_pct, time_total) %>%
  arrange(error_dist, beta_true, data_n, method) %>%
  select("Error Dist." = error_dist,
         "Beta" = beta_true,
         "N" = data_n,
         se = std_error,
         cvg = coverage_pct,
         tms = time_total,
         method) %>%
  pivot_wider(names_from = method,
              values_from = c(se, cvg, tms)) %>%
  mutate(across(matches("se"),
                ~scales::label_number(accuracy = 0.01)(.)),
         across(matches("cvg"),
                ~scales::label_percent(accuracy = 0.1)(.)),
         across(matches("tms"),
                ~scales::label_number(accuracy = 0.1)(.)))


# Print this table
kbl(covg_table,
    booktabs = T,
    caption = "Coverage Estimation",
    col.names = str_remove_all(names(covg_table), "(.*_)?")) %>%
  kable_classic(full_width = F) %>%
  column_spec(1:2, bold = T) %>%
  column_spec(3, italic = T) %>%
  collapse_rows(columns = 1:2,
                valign = "top",
                row_group_label_position = "first",
                latex_hline = "full") %>%
  add_header_above(c("Parameters" = 3,
                     "Avg. Std. Error" = 3,
                     "Coverage" = 3,
                     "Time (Secs.)" = 3))
```

To make these results easier to view and interpret, we plot a comparison of coverage percentage. We also plot a comparison of the average width of the confidence intervals across the three interval calculation

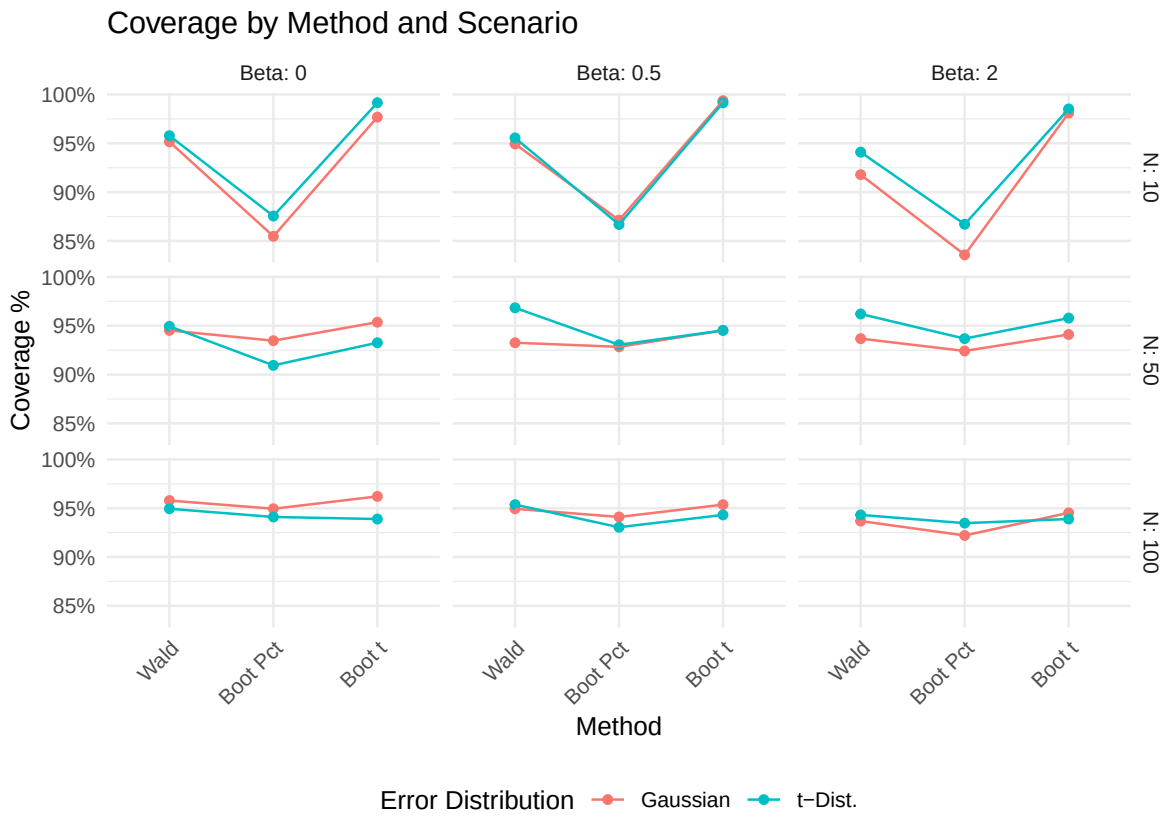
Table 3: Coverage Estimation

Parameters			Avg. Std. Error			Coverage			Time (Secs.)		
Error Dist.	Beta	N	Wald	Boot Pct	Boot t	Wald	Boot Pct	Boot t	Wald	Boot Pct	Boot t
Gaussian	**0.0**	*10*	0.92	0.81	0.81	95.2%	85.5%	97.7%	2.3	6.2	494.2
		50	0.40	0.40	0.40	94.5%	93.5%	95.4%	2.4	7.2	601.1
		100	0.28	0.28	0.28	95.8%	94.9%	96.2%	2.4	7.9	680.3
	0.5	*10*	0.91	0.83	0.83	94.9%	87.1%	99.4%	2.4	6.2	497.5
		50	0.40	0.40	0.40	93.3%	92.8%	94.5%	2.4	7.1	606.6
		100	0.28	0.28	0.28	94.9%	94.1%	95.4%	2.3	7.5	648.7
	2.0	*10*	0.92	0.81	0.81	91.8%	83.6%	98.1%	2.4	6.3	500.3
		50	0.40	0.40	0.40	93.7%	92.4%	94.1%	2.3	7.0	608.2
		100	0.28	0.28	0.28	93.7%	92.2%	94.5%	1.6	5.5	506.8
t-Dist.	**0.0**	*10*	0.81	0.73	0.73	95.8%	87.6%	99.2%	2.4	6.5	498.9
		50	0.38	0.37	0.37	94.9%	90.9%	93.3%	2.4	7.2	600.9
		100	0.27	0.27	0.27	94.9%	94.1%	93.9%	2.5	7.8	679.4
	0.5	*10*	0.81	0.73	0.73	95.6%	86.7%	99.2%	2.3	6.3	497.8
		50	0.38	0.38	0.38	96.8%	93.1%	94.5%	2.5	7.1	606.8
		100	0.27	0.27	0.27	95.4%	93.1%	94.3%	2.3	7.6	651.2
	2.0	*10*	0.82	0.73	0.73	94.1%	86.7%	98.5%	2.3	6.2	498.5
		50	0.38	0.38	0.38	96.2%	93.7%	95.8%	2.4	7.2	608.0
		100	0.26	0.26	0.26	94.3%	93.5%	93.9%	1.6	5.6	506.3

methods for each scenario.

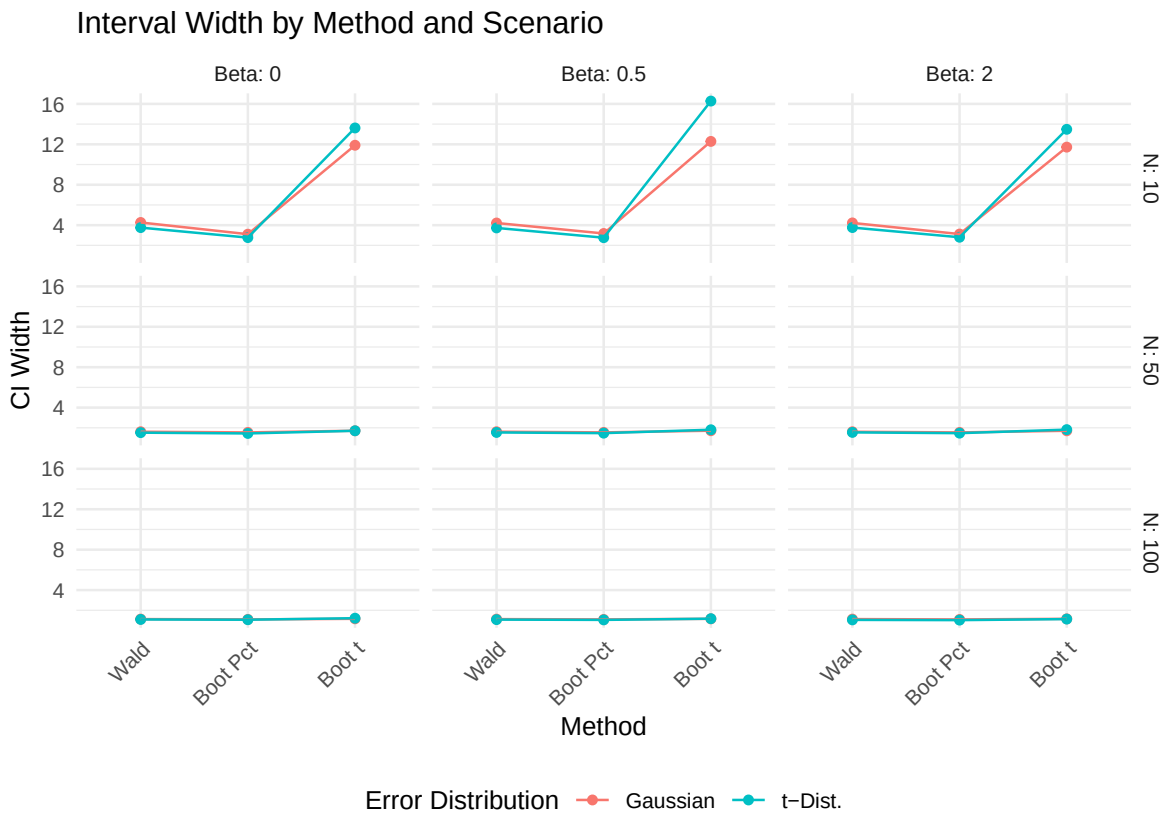
```
covg_plot <- ggplot(scenario_results %>%
                      rename("N" = data_n, "Beta" = beta_true),
                    aes(x = method, y = coverage_pct,
                        color = error_dist, group = error_dist)) +
  geom_point() +
  geom_line() +
  facet_grid(N ~ Beta, labeller = label_both) +
  labs(x = "Method", y = "Coverage %", color = "Error Distribution",
       title = "Coverage by Method and Scenario") +
  theme_minimal() +
  scale_y_continuous(labels = scales::label_percent()) +
  theme(axis.text.x = element_text(angle = 45, hjust = 1),
        legend.position = "bottom")

covg_plot
```



```r
width_plot <- ggplot(scenario_results %>%
                       rename("N" = data_n, "Beta" = beta_true),
                     aes(x = method, y = ci_width,
                         color = error_dist, group = error_dist)) +
  geom_point() +
  geom_line() +
  facet_grid(N ~ Beta, labeller = label_both) +
  labs(x = "Method", y = "CI Width", color = "Error Distribution",
       title = "Interval Width by Method and Scenario") +
  theme_minimal() +
  theme(axis.text.x = element_text(angle = 45, hjust = 1),
        legend.position = "bottom")

width_plot
```



Problem 1.5: Discussion