P8160 Simulation Project - Hierarchical Logistic Model for Mulit-Center Clinical Trial

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Introduction and Background

Statistical Methods

overall description of what we did, the code in this section specifies functions

1. Initialization and Function Definitions

We specified the clinic random effect (b) as b ~ t_5 and the patient-level covariates (X) as X ~ Gamma(2, 1).

```
# logistic function
logistic <- function(z) {
  1 / (1 + exp(-z))
}

# Set model parameters
alpha <- 0        # Intercept
beta  <- 1        # Covariate coefficient

# Define random generators for non-normal distributions
#                   of random effect b and covariate x
# Example: b ~ t_5 (heavy-tailed distribution)
r_b <- function(n) {
  rt(n, df = 5)
}

# Example: x ~ Gamma(shape=2, rate=1)
r_x <- function(n) {
  rgamma(n, shape = 2, rate = 1)
}
```

2. Sampling from Simple Monte Carlo (MC)

```
simpleMC <- function(N) {
  # Sample b from f(b)
  b_samp <- r_b(N)
  # Sample x from f(x)
  x_samp <- r_x(N)

  # Compute p_i = logistic(alpha + b_i + beta*x_i)
  p_values <- logistic(alpha + b_samp + beta * x_samp)
```

```r
  # Simple MC estimate is the average of p_values
  est <- mean(p_values)

  return(list(est = est))
}
```

3. Designing Control Variate (CV)

```r
# 3.1 Define a control variate g(b, x)
#     It should be correlated with the target function but have a known or easily
#     approximated expectation. As an example, we use a probit-based function.

g_function <- function(b, x) {
  # Example: replace logistic with pnorm (probit)
  z <- alpha + 0.8 * b + 0.8 * x  # 0.8 is a heuristic factor here
  return(pnorm(z))
}

# 3.2 Approximate E[g] using a large-scale MC, since we might not have a closed-form
approx_Eg <- function(N = 5e5) {
  b_samp <- r_b(N)
  x_samp <- r_x(N)
  mean(g_function(b_samp, x_samp))
}

# 3.3 Control variate MC estimate
cvMC <- function(N, Eg_true = NULL) {
  if(is.null(Eg_true)) {
    # If not provided, approximate E[g] with a bigger MC sample
    Eg_true <- approx_Eg(N = 5e5)
  }
  # Sample from original distributions
  b_samp <- r_b(N)
  x_samp <- r_x(N)

  # Target function p(b,x)
  p_vals <- logistic(alpha + b_samp + beta * x_samp)
  # Control variate g(b,x)
  g_vals <- g_function(b_samp, x_samp)

  # (1) Simple estimates of p and g
  p_mean <- mean(p_vals)
  g_mean <- mean(g_vals)

  # (2) Optimal gamma via covariance
  cov_pg <- cov(p_vals, g_vals)
  var_g  <- var(g_vals)
  gamma_opt <- cov_pg / var_g

  # (3) Construct CV estimator
  p_cv <- p_mean - gamma_opt * (g_mean - Eg_true)

  # This returns the CV estimate, gamma, and other useful metrics
```

```r
  return(list(est = p_cv))
}
```

4. Importance Sampling (IS)

```r
# 4.1 Define the auxiliary distribution h(b,x)
#     Here we show an example of independent sampling from h(b)*h(x).
#     We'll pick t_3 for b (heavier tail) and tweak Gamma parameters for x.

# b ~ t_3
r_b_IS <- function(n) {
  rt(n, df = 3)
}
# PDF of b for t_3
d_b_IS <- function(b) {
  dt(b, df = 3)
}

# x ~ Gamma(shape=2, rate=0.5)
r_x_IS <- function(n) {
  rgamma(n, shape = 2, rate = 0.5)
}
# PDF of x for Gamma(shape=2, rate=0.5)
d_x_IS <- function(x) {
  dgamma(x, shape = 2, rate = 0.5)
}

# 4.2 Implement Importance Sampling
IS_MC <- function(N) {
  # Sample from h(b,x)
  b_samp <- r_b_IS(N)
  x_samp <- r_x_IS(N)

  # Compute original PDF values f(b), f(x)
  fb_vals <- dt(b_samp, df = 5)              # original t_5 for b
  fx_vals <- dgamma(x_samp, shape = 2, rate = 1)  # original Gamma for x

  # Compute auxiliary PDF values h(b), h(x)
  hb_vals <- d_b_IS(b_samp)
  hx_vals <- d_x_IS(x_samp)

  # Weights w_i = [f(b_i)*f(x_i)] / [h(b_i)*h(x_i)]
  w <- (fb_vals * fx_vals) / (hb_vals * hx_vals)

  # Target function p(b,x)
  p_vals <- logistic(alpha + b_samp + beta * x_samp)

  # IS estimate (unbiased if we average p*w)
  est <- mean(p_vals * w)

  # Rough variance estimate
  #p_var <- mean((p_vals * w)^2) - p_hat^2
  #se  <- sqrt(p_var / N)
```

```r
  #return(list(est = est, se = se, w_mean = mean(w)))
  return(list(est = est))
}
```

Results

5. Comparing Bias, Variance, and CPU Time for Simple MC, CV, and Importance Sampling

```
## Approx. True Value = 0.7859166
```

Table 1: Estimated model mean, bias, and variance for each method

Method	Estimated Mean	Bias	Variance
MC	0.7857719	-0.0001447	4e-07
CV	0.7857767	-0.0001399	0e+00
IS	0.7855314	-0.0003852	3e-06

expr	time
CV	15583075
IS	32919679
IS	32920294
MC	12911884
CV	15529037
CV	15399026
MC	12619841
MC	12768384
CV	15546585
CV	15387423
MC	12730664
CV	15371023
MC	12820003
MC	12865390
CV	15498574
CV	15385701
IS	38740900
IS	32983475
MC	12698069
IS	33160144
MC	12764817
MC	12686425
IS	32967649
IS	35326420
CV	15911649
IS	34617161
CV	17085684
IS	34819660
IS	36570647
MC	12726605

Monte Carlo (MC) is the fastest because it only generates random samples and computes the mean, with O(N) complexity and no additional calculations.

Control Variates (CV) is slightly slower due to the extra step of computing a regression coefficient to reduce variance, but it improves estimation accuracy.

Importance Sampling (IS) is the slowest because it requires computing importance weights, normalizing them, and handling probability density functions, making it computationally more expensive (O(N log N) or higher).

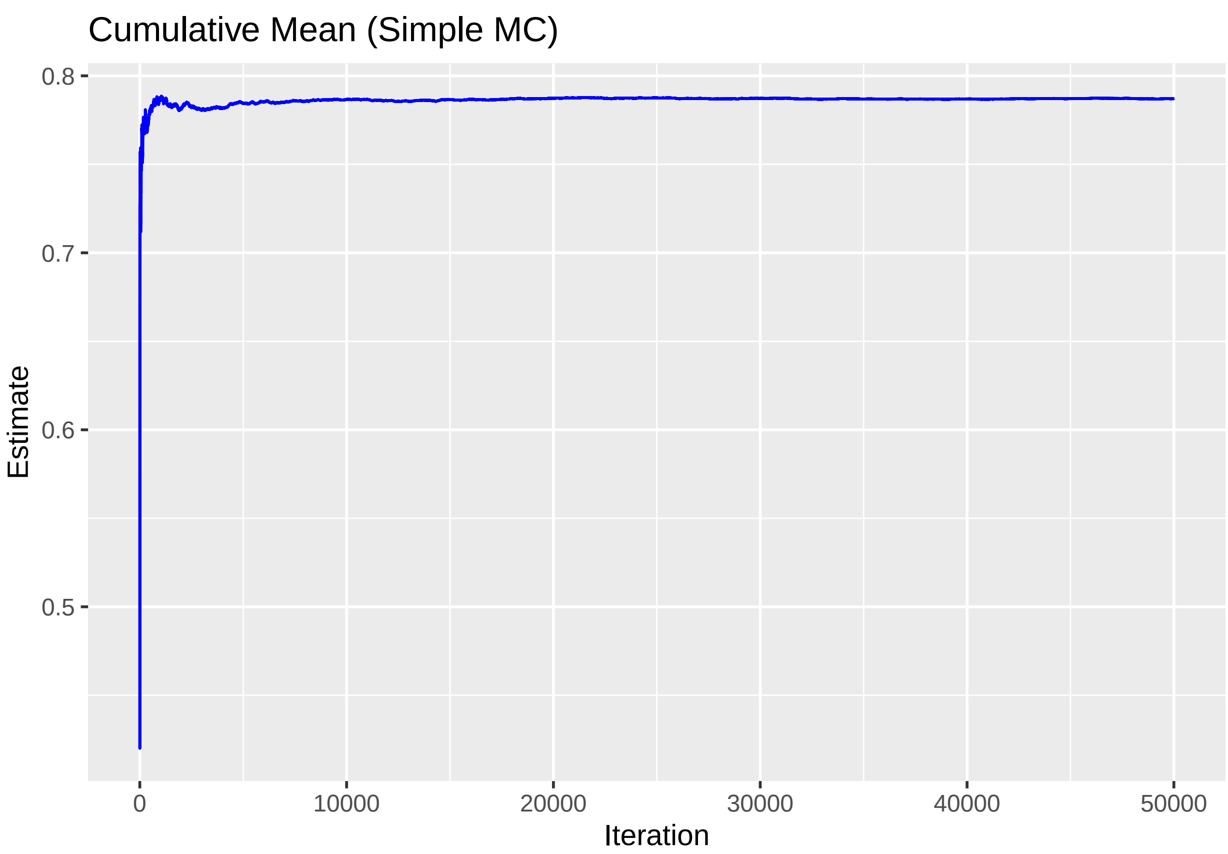
```r
# 5.1. Obtain a "true value" via a large-scale Simple MC
set.seed(9999)
N_large <- 5e6

res_truth <- simpleMC(N_large)
true_value <- res_truth$est
# cat("Approx. True Value =", true_value, "\n")


# 5.2. Repeat simulations for smaller N and compare bias, variance
simulate_three_methods <- function(N, Eg_true) {
  # Simple MC
  res_mc <- simpleMC(N)
  # CV
  res_cv <- cvMC(N, Eg_true = Eg_true)
  # IS
  res_is <- IS_MC(N)

  c(mc = res_mc$est, cv = res_cv$est, is = res_is$est)
}

set.seed(1234)
N_reps <- 50        # number of repeated simulations
N_small <- 1e5      # sample size for each repeated run


# Pre-calculate Eg_true for CV (to avoid doing it multiple times)
Eg_val <- approx_Eg(N=5e5)

results_matrix <- replicate(N_reps, simulate_three_methods(N_small, Eg_true = Eg_val))
# results_matrix is now 3 x N_reps, each column is one replicate

mc_est <- results_matrix["mc", ]
cv_est <- results_matrix["cv", ]
is_est <- results_matrix["is", ]

# Compute mean estimate, bias, variance
mc_mean <- mean(mc_est)
cv_mean <- mean(cv_est)
is_mean <- mean(is_est)

mc_bias <- mc_mean - true_value
cv_bias <- cv_mean - true_value
is_bias <- is_mean - true_value

mc_var <- var(mc_est)
cv_var <- var(cv_est)
is_var <- var(is_est)
```

```r
df_comparison <- data.frame(
  method   = c("MC", "CV", "IS"),
  mean_est = c(mc_mean, cv_mean, is_mean),
  bias     = c(mc_bias, cv_bias, is_bias),
  variance = c(mc_var, cv_var, is_var)
)

# df_comparison


# 5.3 Compare CPU time
test_time <- microbenchmark(
  MC = { simpleMC(N_small) },
  CV = { cvMC(N_small, Eg_true = Eg_val) },
  IS = { IS_MC(N_small) },
  times = 10  # repeat each method 10 times
)

# test_time
```

6. Cumulative Convergence Plots (Extra Credit)

Simple MC

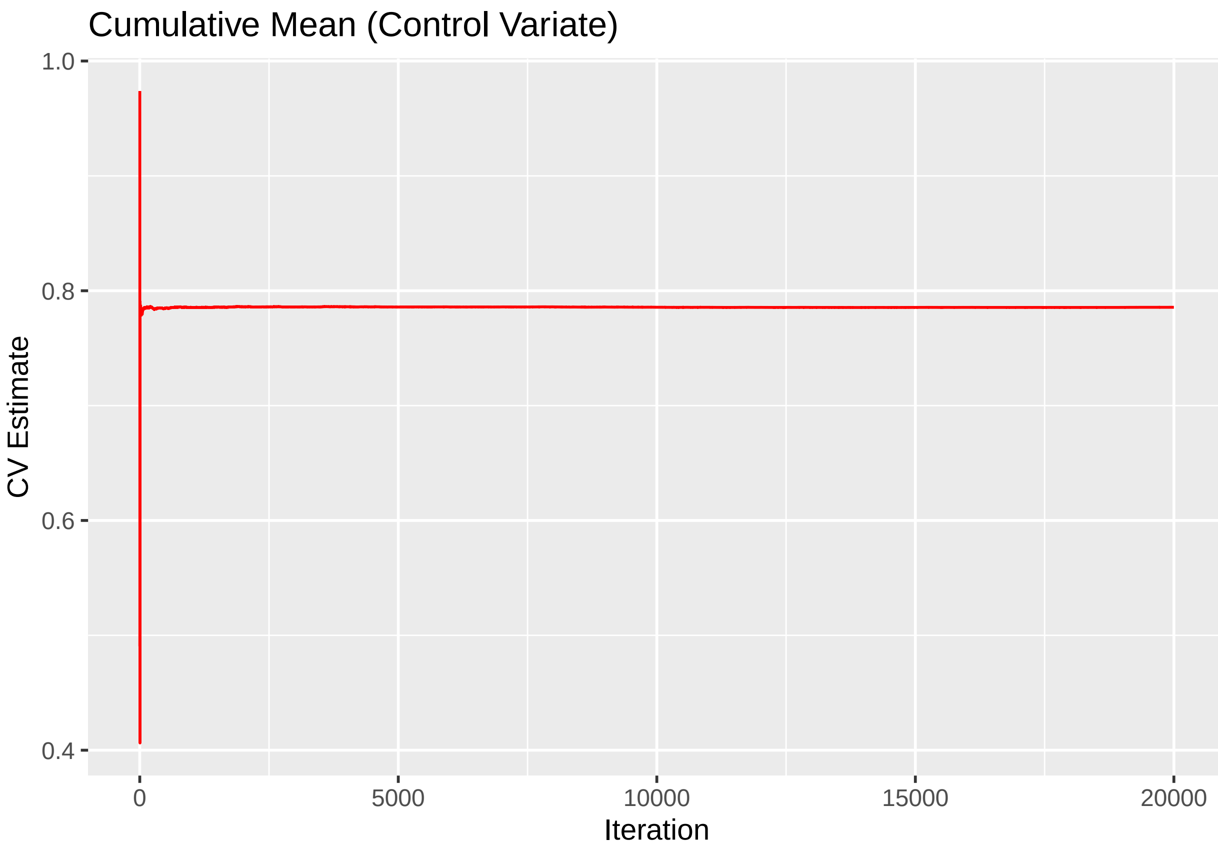
```r
# 6.1 Example of cumulative mean for Simple MC
cumulative_MC <- function(N) {
  b_samp <- r_b(N)
  x_samp <- r_x(N)
  p_vals <- logistic(alpha + b_samp + beta * x_samp)
  cum_mean <- cumsum(p_vals) / seq_len(N)
  return(cum_mean)
}

# 6.2 Plot cumulative mean
set.seed(999)
N <- 5e4
cm_mc <- cumulative_MC(N)

df_mc <- data.frame(
  iter = 1:N,
  mean_est = cm_mc
)

ggplot(df_mc, aes(x = iter, y = mean_est)) +
  geom_line(color = "blue") +
  labs(title = "Cumulative Mean (Simple MC)",
       x = "Iteration",
       y = "Estimate")
```



Control Variate Cumulative Mean

```
# This function returns a vector of CV estimates for i from 1 to N.
cumulative_CV <- function(N, Eg_true = NULL, largeN_approx = 5e5) {
  if (is.null(Eg_true)) {
    # If E[g] is not provided, approximate with a larger MC
    Eg_true <- approx_Eg(N = largeN_approx)
  }

  # Sample from original distributions
  b_samp <- r_b(N)
  x_samp <- r_x(N)

  # Compute p(b,x) and g(b,x)
  p_vals <- logistic(alpha + b_samp + beta * x_samp)
  g_vals <- g_function(b_samp, x_samp)

  # We will keep track of partial sums to compute means, covariance, etc.
  cum_p  <- cumsum(p_vals)
  cum_g  <- cumsum(g_vals)
  cum_pg <- cumsum(p_vals * g_vals)   # needed for Cov(p,g)
  cum_g2 <- cumsum(g_vals^2)         # needed for Var(g)

  # Vector to store CV estimates at each iteration
  pCV_cum <- numeric(N)
```

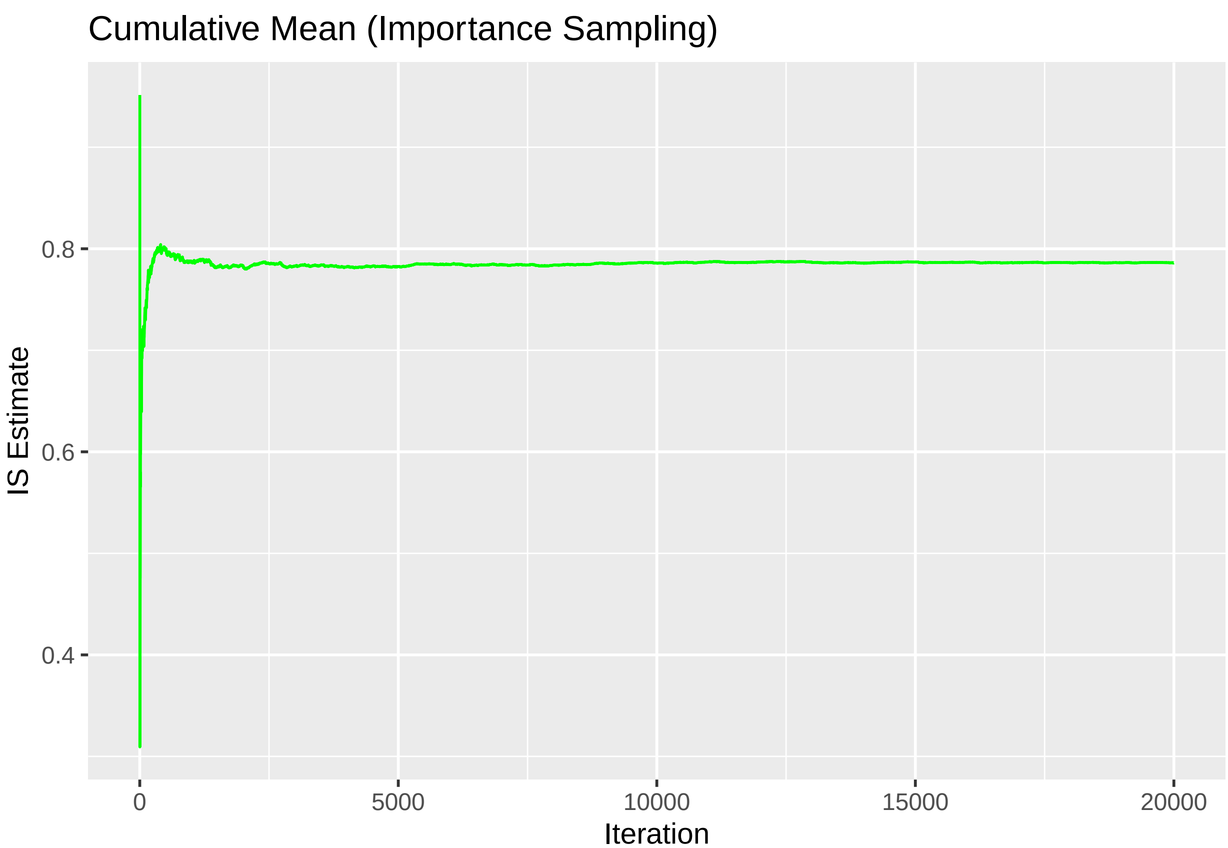
```r
  # The first data point (i=1) does not allow us to compute a covariance
  # We can simply set pCV_cum[1] to p_vals[1], or NA, etc.
  pCV_cum[1] <- p_vals[1]

  # Loop over i = 2 to N
  for (i in 2:N) {
    # partial means
    p_bar_i <- cum_p[i] / i
    g_bar_i <- cum_g[i] / i

    # Cov(p,g) = E[ p*g ] - E[p]*E[g ]
    # partial estimate of E[p*g] = cum_pg[i] / i
    pg_bar_i <- cum_pg[i] / i
    cov_pg_i <- pg_bar_i - (p_bar_i * g_bar_i)

    # Var(g) = E[g^2] - (E[g])^2
    g2_bar_i <- cum_g2[i] / i
    var_g_i  <- g2_bar_i - (g_bar_i^2)

    # Optimal gamma
    gamma_i <- cov_pg_i / var_g_i

    # CV estimate at iteration i
    pCV_cum[i] <- p_bar_i - gamma_i * (g_bar_i - Eg_true)
  }

  return(pCV_cum)
}

# Example usage and plotting:
set.seed(1234)
N <- 20000
cv_cum_values <- cumulative_CV(N)

df_cv <- data.frame(
  iter = 1:N,
  cv_est = cv_cum_values
)

library(ggplot2)
ggplot(df_cv, aes(x = iter, y = cv_est)) +
  geom_line(color = "red") +
  labs(title = "Cumulative Mean (Control Variate)",
       x = "Iteration",
       y = "CV Estimate")
```



Importance Sampling Cumulative Mean

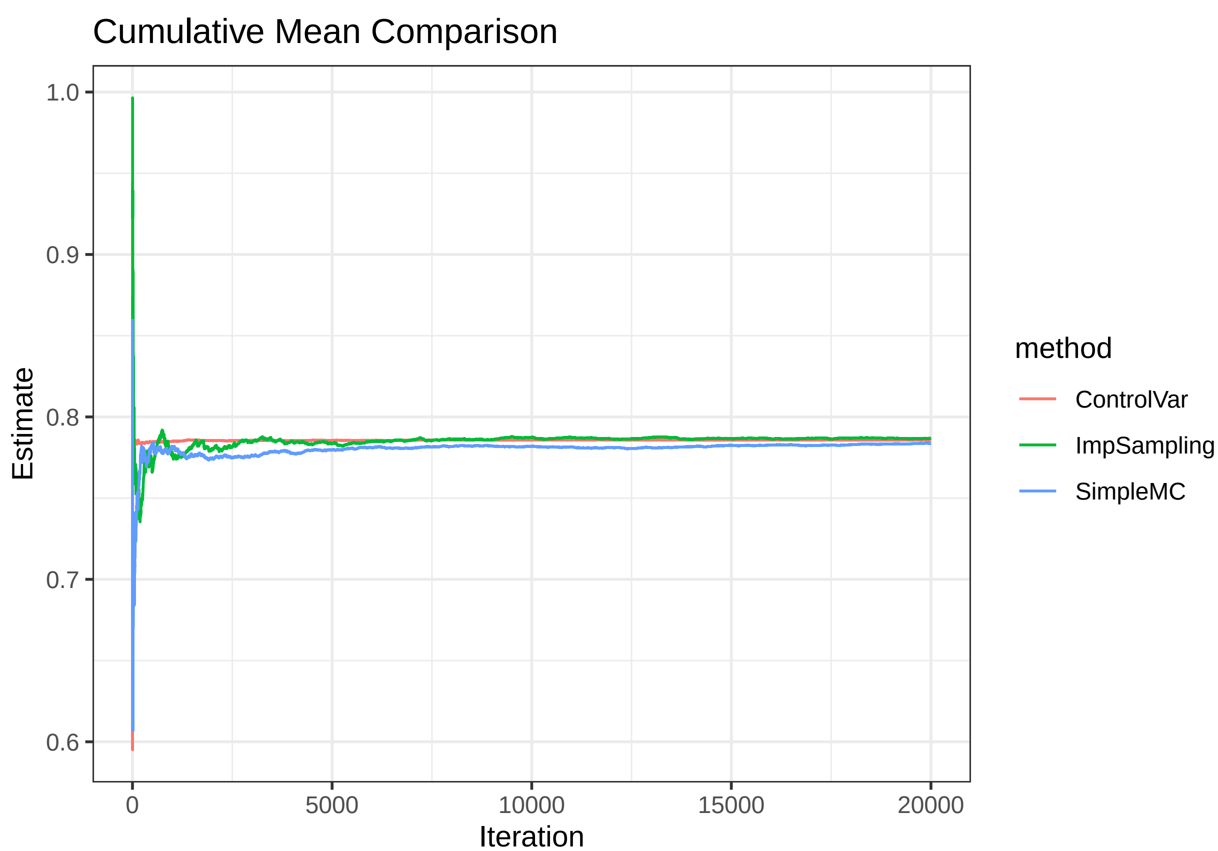
```
cumulative_IS <- function(N) {
  # Sample from auxiliary distribution h(b,x)
  b_samp <- r_b_IS(N)
  x_samp <- r_x_IS(N)

  # Compute original PDF f(b), f(x)
  fb_vals <- dt(b_samp, df = 5)           # original b ~ t_5
  fx_vals <- dgamma(x_samp, shape=2, rate=1)    # original x ~ Gamma(2,1)

  # Compute auxiliary PDF h(b), h(x)
  hb_vals <- d_b_IS(b_samp)
  hx_vals <- d_x_IS(x_samp)

  # Weights
  w <- (fb_vals * fx_vals) / (hb_vals * hx_vals)

  # Target function p(b,x)
  p_vals <- logistic(alpha + b_samp + beta * x_samp)

  # Build cumulative sums
  cum_w  <- cumsum(w)
  cum_pw <- cumsum(p_vals * w)

  # IS estimate at iteration i: cum_pw[i] / cum_w[i]
```

```r
  pIS_cum <- cum_pw / cum_w

  return(pIS_cum)
}

## Example usage and plotting:
set.seed(5678)
N <- 20000
is_cum_values <- cumulative_IS(N)

df_is <- data.frame(
  iter = 1:N,
  is_est = is_cum_values
)

ggplot(df_is, aes(x = iter, y = is_est)) +
  geom_line(color = "green") +
  labs(title = "Cumulative Mean (Importance Sampling)",
       x = "Iteration",
       y = "IS Estimate")
```




```r
N <- 20000
set.seed(999)

# 1. Simple MC
cm_mc <- cumulative_MC(N)
df_mc <- data.frame(iter = 1:N, method = "SimpleMC", estimate = cm_mc)
```

```r
# 2. CV
cm_cv <- cumulative_CV(N)
df_cv <- data.frame(iter = 1:N, method = "ControlVar", estimate = cm_cv)

# 3. IS
cm_is <- cumulative_IS(N)
df_is <- data.frame(iter = 1:N, method = "ImpSampling", estimate = cm_is)

# Combine
df_all <- rbind(df_mc, df_cv, df_is)

ggplot(df_all, aes(x = iter, y = estimate, color = method)) +
  geom_line() +
  labs(title = "Cumulative Mean Comparison",
       x = "Iteration",
       y = "Estimate") +
  theme_bw()
```



Discussion and Practical Implications

Conclusion