Printed Script: Qian et al. (2020)

## **Script: Generative Model**

```
# 2018.10.22 Tianchen Qian
# generative model:
# Y_t+1 = alpha_0 + alpha_1 X_t + b_0i + b_1i X_t + A_t (beta_0 + beta_1 X_t + b_2i + b_3i X_t) +
# epsilon_it
dgm_with_treatment <- function(sample_size, total_T, dgm_type) {</pre>
    # dgm_type is in c(1,2,3,4)
    stopifnot(dgm_type \%in\% c(1,2,3,4))
    \# dgm_type = 1 or 3
    alpha_0 <- - 1
    alpha_1 <- - 0.3
    beta_0 <- 0.5
    beta_1 <- 0.1
    sigma_b0 <- 2
    sigma_b1 <- 0
    sigma_b2 <- 1
    sigma_b3 <- 0
    sigma_eps <- 1
    if (dgm_type == 2) {
        sigma_b1 <- sigma_b3 <- 0.5
    }
    if (dgm_type == 4) {
        sigma_b2 <- 0
    }
    prob_a <- 0.5
    df_names <- c("userid", "day", "X", "prob_A", "A", "Y", "b0", "b1", "b2", "b3", "eps", "delta")
    dta <- data.frame(matrix(NA, nrow = sample_size * total_T, ncol = length(df_names)))</pre>
    names(dta) <- df_names
    dta$userid <- rep(1:sample_size, each = total_T)</pre>
    dta$day <- rep(1:total_T, times = sample_size)</pre>
    # uncorrelated random effects
    b_0i <- rnorm(sample_size, mean = 0, sd = sigma_b0)
    b_1i <- rnorm(sample_size, mean = 0, sd = sigma_b1)
    b_2i <- rnorm(sample_size, mean = 0, sd = sigma_b2)
    b_3i <- rnorm(sample_size, mean = 0, sd = sigma_b3)
    # b_1i[b_1i > 2] <- 2
    # b_1i[b_1i < -2] <- -2
    # b_3i[b_3i > 2] <- 2
    # b_3i[b_3i < -2] <- -2
    for (t in 1:total_T) {
```

```
# row index for the rows corresponding to day t for every subject
        row index <- seq(from = t, by = total T, length = sample size)
        if (dgm_type == 1) {
            if (t == 1) {
                dta$X[row_index] <- rnorm(sample_size)</pre>
            } else {
                dta$X[row_index] <- dta$Y[row_index_lag1] + rnorm(sample_size)</pre>
            }
            dta$prob_A[row_index] <- rep(prob_a, sample_size)</pre>
        } else if (dgm_type == 2) {
            if (t == 1) {
                dta$X[row_index] <- rnorm(sample_size)</pre>
            } else {
                dta$X[row_index] <- dta$Y[row_index_lag1] + rnorm(sample_size)</pre>
            dta$prob_A[row_index] <- ifelse(dta$X[row_index] > - 1.27, 0.7, 0.3)
        } else if (dgm_type \%in\% c(3,4)) {
            if (t == 1) {
                dta$X[row_index] <- rnorm(sample_size, mean = b_0i) # X involves b_i!!
            } else {
                dta$X[row_index] <- dta$Y[row_index_lag1] + rnorm(sample_size, mean = b_0i)
                # X involves b_i!!
            dta$prob_A[row_index] <- rep(prob_a, sample_size)</pre>
        }
        dta$A[row_index] <- rbinom(sample_size, 1, dta$prob_A[row_index])</pre>
        dta$eps[row_index] <- rnorm(sample size, mean = 0, sd = sigma_eps)
        dta$delta[row_index] <- beta_0 + beta_1 * dta$X[row_index] + b_2i + b_3i * dta$X[row_index]
        dta$Y[row_index] <- alpha_0 + alpha_1 * dta$X[row_index] + b_0i + b_1i * dta$X[row_index] +
            dta$A[row_index] * dta$delta[row_index] + dta$eps[row_index]
        dta$b0[row_index] <- b_0i
        dta$b1[row_index] <- b_1i
        dta$b2[row_index] <- b_2i
        dta$b3[row_index] <- b_3i
        row_index_lag1 <- row_index</pre>
    return(dta)
##### example: use of lmer() #####
if( 0 ){
    sample_size <- 1000</pre>
    total_T <- 20
    dta <- dgm_with_treatment(sample_size, total_T, dgm_type = 1)</pre>
    summary(dta)
    # dta$A <- dta$A - dta$prob_A # action centering doesn't matter when prob_A is constant
```

}

}

```
fit <- lmer(Y ~ X * A + (1 + A | userid), data = dta)
fit <- lmer(Y ~ X * A + (X * A | userid), data = dta)
fit
summary(fit)$coefficients
attr(summary(fit)$varcor$userid, "stddev") # estimated standard deviation of random effect
}</pre>
```

## **Script: Simulation**

```
# 2018.10.22 Tianchen Qian
# simulation study for the random effects model paper (Statistical Science)
# generative model:
# Y_t+1 = alpha_0 + alpha_1 X_t + b_0i + b_1i X_t + A_t (beta_0 + beta_1 X_t + b_2i + b_3i X_t) +
# epsilon_it
rm(list = ls())
set.seed(123)
library(rootSolve)
library(geepack)
library(lme4)
library(mvtnorm)
library(foreach)
library(doMC)
library(doRNG)
source("generative_model.R")
# simulation: using lmer() packag -----
# if(0) {
max_cores <- 16</pre>
registerDoMC(min(detectCores() - 1, max_cores))
set.seed(120)
nsim <- 1000
# full simulation in Appendix B
design <- expand.grid(sample_size = c(30, 50, 100, 200), total_T = c(10, 20, 30), dgm_type = 1:3)
# simulation in Section 4
design \leftarrow expand.grid(sample_size = c(30, 100, 200), total_T = c(10, 30), dgm_type = 1:3)
design <- design[order(design$dgm_type), ]</pre>
for (idesign in 1:nrow(design)) {
    sample_size <- design$sample_size[idesign]</pre>
    total_T <- design$total_T[idesign]</pre>
    dgm_type <- design$dgm_type[idesign]</pre>
    # create template output structure for simulated trials with estimation error
```

```
dta <- dgm_with_treatment(sample_size, total_T, dgm_type = dgm_type)</pre>
if (dgm_type \%in\% c(1,3,4)) {
    fit \leftarrow lmer(Y \sim X * A + (1 + A | userid), data = dta)
} else if (dgm_type == 2) {
    fit \leftarrow lmer(Y \sim X * A + (X * A | userid), data = dta)
}
coef <- summary(fit)$coefficients</pre>
varcor <- summary(fit)$varcor</pre>
for (irow in 1:nrow(coef)) {
    for (icol in 1:ncol(coef)) {
        coef[irow, icol] <- NA</pre>
    }
}
for (irow in 1:nrow(varcor$userid)) {
    for (icol in 1:ncol(varcor$userid)) {
        varcor$userid[irow, icol] <- NA</pre>
}
attr(varcor, "sc") <- NA
coef_NA_fill <- coef</pre>
varcor_NA_fill <- varcor</pre>
# start parallel jobs
writeLines(c(""), "log.txt")
sink("log.txt", append=FALSE)
set.seed(123)
result <- foreach(isim = 1:nsim, .combine = "c") %dorng% {</pre>
    if (isim \% 10 == 0) {
        cat(paste("Starting iteration",isim,"\n"))
    }
    dta <- dgm_with_treatment(sample_size, total_T, dgm_type = dgm_type)</pre>
    solution <- tryCatch(</pre>
        {
             if (dgm_type == 1 | dgm_type == 3) {
                 fit <- lmer(Y \sim X * A + (1 + A | userid), data = dta)
             } else if (dgm_type == 2) {
                 fit \leftarrow lmer(Y \sim X * A + (X * A | userid), data = dta)
             list(coef = summary(fit)$coefficients, varcor = summary(fit)$varcor)
        },
        error = function(cond) {
             message("\nCatched error in lmer():")
            message(cond)
            return(list(coef = coef_NA_fill, varcor = varcor_NA_fill))
        })
    output <- list(solution)</pre>
}
sink()
dir.create("simulation_result", showWarnings = FALSE)
saveRDS(result, file = paste0("simulation_result/", idesign, ".RDS"))
```

}

```
# collect results ---
varcomp_result <- design</pre>
varcomp_result$sigma_b0_bias <- varcomp_result$sigma_b0_sd <-</pre>
    varcomp_result$sigma_b1_bias <- varcomp_result$sigma_b1_sd <-</pre>
    varcomp_result$sigma_b2_bias <- varcomp_result$sigma_b2_sd <-</pre>
    varcomp_result$sigma_b3_bias <- varcomp_result$sigma_b3_sd <-</pre>
    varcomp_result$sigma_eps_bias <- varcomp_result$sigma_eps_sd <- NA
design$alpha_0_bias <- design$alpha_0_sd <- design$alpha_0_cp <-
    design$alpha_1_bias <- design$alpha_1_sd <- design$alpha_1_cp <-
    design$beta_0_bias <- design$beta_0_sd <- design$beta_0_cp <-</pre>
    design$beta_1_bias <- design$beta_1_sd <- design$beta_1_cp <- NA
for (idesign in 1:nrow(design)) {
    result <- readRDS(paste0("20181025_simulation for paper_result/", idesign, ".RDS"))
    dgm_type <- design$dgm_type[idesign]</pre>
    \# dgm_type = 1 or 3
    alpha_0_true <- - 1
    alpha_1_true <- - 0.3
    beta_0_true <- 0.5
    beta_1_true <- 0.1
    sigma_b0_true <- 2
    sigma_b1_true <- 0
    sigma b2 true <- 1
    sigma_b3_true <- 0
    sigma_eps_true <- 1
    if (dgm_type == 2) {
        sigma_b1_true <- sigma_b3_true <- 0.5
    }
    if (dgm_type == 4) {
        sigma_b2_true <- 0
    }
    alpha_0 <- sapply(result, function(1) 1$coef["(Intercept)", "Estimate"])
    alpha_0_sd <- sapply(result, function(1) 1$coef["(Intercept)", "Std. Error"])
    alpha 0 df <- sapply(result, function(1) 1$coef["(Intercept)", "df"])
    alpha_1 <- sapply(result, function(1) l$coef["X", "Estimate"])</pre>
    alpha 1 sd <- sapply(result, function(1) 1$coef["X", "Std. Error"])
    alpha_1_df <- sapply(result, function(1) l$coef["X", "df"])</pre>
    beta_0 <- sapply(result, function(1) 1$coef["A", "Estimate"])</pre>
    beta_0_sd <- sapply(result, function(1) 1$coef["A", "Std. Error"])</pre>
    beta_0_df <- sapply(result, function(1) 1$coef["A", "df"])</pre>
    beta_1 <- sapply(result, function(1) 1$coef["X:A", "Estimate"])</pre>
    beta_1_sd <- sapply(result, function(1) 1$coef["X:A", "Std. Error"])</pre>
    beta_1_df <- sapply(result, function(1) 1$coef["X:A", "df"])</pre>
```

```
varcor <- lapply(result, function(1) 1$varcor$userid) # variance matrix for random effects;</pre>
# this is "G"
sigma_eps <- sapply(result, function(1) attr(1$varcor, "sc"))</pre>
quantiles <- qt(0.975, alpha_0_df)
design$alpha_0_bias[idesign] <- mean(alpha_0) - alpha_0_true
design$alpha_0_sd[idesign] <- sd(alpha_0)</pre>
design$alpha_0_cp[idesign] <- mean((alpha_0_true < alpha_0 + quantiles * alpha_0_sd) &
                                       (alpha_0_true > alpha_0 - quantiles * alpha_0_sd))
# design$alpha_0_cp[idesign] <- mean((alpha_0_true < alpha_0 + 1.96 *
# design$alpha_0_sd[idesign]) & (alpha_0_true > alpha_0 - 1.96 * design$alpha_0_sd[idesign]))
quantiles <- qt(0.975, alpha_1_df)
design$alpha_1_bias[idesign] <- mean(alpha_1) - alpha_1_true
design$alpha_1_sd[idesign] <- sd(alpha_1)</pre>
design$alpha_1_cp[idesign] <- mean((alpha_1_true < alpha_1 + quantiles * alpha_1_sd) &
                                       (alpha_1_true > alpha_1 - quantiles * alpha_1_sd))
# design$alpha_1_cp[idesign] <- mean((alpha_1_true < alpha_1 + 1.96 *
# design$alpha_1_sd[idesign]) & (alpha_1_true > alpha_1 - 1.96 * design$alpha_1_sd[idesign]))
quantiles \leftarrow qt(0.975, beta_0_df)
design$beta_0_bias[idesign] <- mean(beta_0) - beta_0_true</pre>
design$beta_0_sd[idesign] <- sd(beta_0)</pre>
design$beta_0_cp[idesign] <- mean((beta_0_true < beta_0 + quantiles * beta_0_sd) &
                                      (beta_0_true > beta_0 - quantiles * beta_0_sd))
# design$beta_0_cp[idesign] <- mean((beta_0_true < beta_0 + 1.96 *
# design$beta 0_sd[idesign]) & (beta_0_true > beta_0 - 1.96 * design$beta_0_sd[idesign]))
quantiles \leftarrow qt(0.975, beta_1_df)
design$beta_1_bias[idesign] <- mean(beta_1) - beta_1_true</pre>
design$beta_1_sd[idesign] <- sd(beta_1)</pre>
design$beta_1_cp[idesign] <- mean((beta_1_true < beta_1 + quantiles * beta_1_sd) &
                                      (beta_1_true > beta_1 - quantiles * beta_1_sd))
# design$beta_1_cp[idesign] <- mean((beta_1_true < beta_1 + 1.96 *
# design$beta_1_sd[idesign]) & (beta_1_true > beta_1 - 1.96 * design$beta_1_sd[idesign]))
varcor_mean <- apply(simplify2array(varcor), 1:2, mean)</pre>
varcor_sd <- apply(simplify2array(varcor), 1:2, sd)</pre>
if (dgm_type == 1 | dgm_type == 3) {
    varcomp result$sigma b0 bias[idesign] <- varcor mean[1,1] - sigma b0 true^2</pre>
    varcomp_result$sigma_b0_sd[idesign] <- varcor_sd[1,1]</pre>
    varcomp result$sigma b2 bias[idesign] <- varcor mean[2,2] - sigma b2 true^2</pre>
    varcomp_result$sigma_b2_sd[idesign] <- varcor_sd[2,2]</pre>
} else if (dgm_type == 2) {
    varcomp_result$sigma_b0_bias[idesign] <- varcor_mean[1,1] - sigma_b0_true^2</pre>
    varcomp_result$sigma_b0_sd[idesign] <- varcor_sd[1,1]</pre>
    varcomp_result$sigma_b1_bias[idesign] <- varcor_mean[2,2] - sigma_b1_true^2</pre>
    varcomp_result$sigma_b1_sd[idesign] <- varcor_sd[2,2]</pre>
    varcomp_result$sigma_b2_bias[idesign] <- varcor_mean[3,3] - sigma_b2_true^2</pre>
    varcomp_result$sigma_b2_sd[idesign] <- varcor_sd[3,3]</pre>
    varcomp_result$sigma_b3_bias[idesign] <- varcor_mean[4,4] - sigma_b3_true^2</pre>
    varcomp_result$sigma_b3_sd[idesign] <- varcor_sd[4,4]</pre>
}
varcomp_result$sigma_eps_bias[idesign] <- mean(sigma_eps) - sigma_eps_true^2</pre>
```

```
varcomp_result$sigma_eps_sd[idesign] <- sd(sigma_eps)</pre>
design <- design[order(design$dgm_type, design$total_T, design$sample_size), ]</pre>
varcomp_result <- varcomp_result[order(varcomp_result$dgm_type, varcomp_result$total_T,</pre>
                                      varcomp_result$sample_size), ]
# make LaTeX tables -------
library(xtable)
reorder_col <- c(1:3, 9:7, 6:4, 15:13, 12:10)
design_reorder <- design[, reorder_col]</pre>
print(xtable(design\_reorder, digits = c(0, 0, 0, 0, rep(3, 12))),
     include.rownames = FALSE, hline.after = c(-1, 0, seq(from = 4,
                                                          to = nrow(design_reorder), by = 4)))
reorder_col <- c(1:3, 9:8, 7:6, 13:12, 11:10, 5:4)
varcomp_result_reorder <- varcomp_result[, reorder_col]</pre>
print(xtable(varcomp_result_reorder, digits = c(0, 0, 0, 0, rep(3, 10))),
     include.rownames = FALSE, hline.after = c(-1, 0, seq(from = 4,
                                                          to = nrow(varcomp_result_reorder), by = 4)))
```