M1: Simple Linear Regression with Diagnostics

M1-Simple-Linear.Rmd | Compiled: 2026-01-26 09:32:28

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```r
# ============================================================================
# M1: SIMPLE LINEAR REGRESSION PARAMETERS
# Model: y = X  +   (no random effects)
# Only one variance component:   (residual precision)

# PARAMETERS
n <- 300  # Total observations
p <- 3    # Number of regression coefficients (intercept + 2 predictors)

# True parameter values
tau_e_true <- 0.5   # Residual precision (variance = 2)
beta_true  <- c(0.5, -2, 3)  # Regression coefficients

# Prior hyperparameters (flat priors)
alpha_e <- 0
gamma_e <- 0
alpha_u <- 0
gamma_u <- 0

# gibbs Sampler Settings
run_gibbs    <- TRUE   # Set FALSE for quick testing, TRUE for full run
gibbs_iter   <- 5000
gibbs_burnin <- 1000

# display Settings
RENDER_FUNCTIONS <- FALSE  # TRUE to show function code, FALSE to hide

# M1: Simple Linear Regression - no Q configurations needed


# ============================================================================
# Dr John Holmes' Gibbs sampler for hierarchical models
# EXACT original from Dr John - NO modifications
normalmm.Gibbs<-function(iter,Z,X,y,burnin,taue_0,tauu_0,Kinv,a.u,b.u,a.e,b.e){
  n   <-length(y) #no. observations
  p   <-dim(X)[2] #no of fixed effect predictors.
  q   <-dim(Z)[2] #no of random effect levels
  tauu<-tauu_0
  taue<-taue_0
  beta0<-rnorm(p)
  u0   <-rnorm(q,0,sd=1/sqrt(tauu))

  #Building combined predictor matrix.
  W<-cbind(X,Z)
  WTW <-crossprod(W)
  WTy <-crossprod(W,y)
  library(mvtnorm)

  #storing results.
  par <-matrix(0,iter,p+q+2)
  #Calculating log predictive densities
  lppd<-matrix(0,iter,n)

  #Create modified identity matrix for joint posterior.
  I0  <-diag(p+q)
  diag(I0)[1:p]<-0
  I0[-c(1:p),-c(1:p)]  <-Kinv

  for(i in 1:iter){
    #Conditional posteriors.
    uKinvu <- t(u0)%*%Kinv%*%u0
    uKinvu <-as.numeric(uKinvu)
    tauu <-rgamma(1,a.u+0.5*q,b.u+0.5*uKinvu)
    #Updating component of normal posterior for beta,u
    Prec <-WTW*taue + tauu*I0
    P.var <-solve(Prec)
    P.mean<- P.var%*%WTy*taue
    betau <-rmvnorm(1,mean=P.mean,sigma=P.var)
    betau <-as.numeric(betau)
    err   <- y-W%*%betau
    taue  <-rgamma(1,a.e+0.5*n,b.e+0.5*sum(err^2))
    #storing iterations.
    par[i,]<-c(betau,tauu,taue)
    beta0  <-betau[1:p]
    u0     <-betau[p+1:q]
    lppd[i,]= dnorm(y,mean=as.numeric(W%*%betau),sd=1/sqrt(taue))
  }

  lppd      = lppd[-c(1:burnin),]
  lppdest   = sum(log(colMeans(lppd)))        #Estimating lppd for whole dataset.
  pwaic2    = sum(apply(log(lppd),2,FUN=var)) #Estimating effective number of parameters.
  par <-par[-c(1:burnin),]
  colnames(par)<-c(paste('beta',1:p,sep=''),paste('u',1:q,sep=''),'tau_u','tau_e')
  mresult<-list(par,lppdest,pwaic2)
  names(mresult)<-c('par','lppd','pwaic')
  return(mresult)
}
```

```
# Dr John Holmes' VB algorithm for hierarchical models
# EXACT original from Dr John - NO modifications
VB.mm<-function(epsilon,iter,Kinv,Z,X,y,taue_0,tauu_0,u0,beta0,a.e,g.e,a.u,g.u){
  n<-dim(X)[1]
  p<-dim(X)[2]
  q<-dim(Z)[2]
  W <-cbind(X,Z)
  WTW<-crossprod(W)
  WTY<-crossprod(W,y)
  Kinvall<-matrix(0,p+q,p+q)
  Kinvall[-c(1:p),-c(1:p)]<-Kinv

  for(i in 1:iter){
    Vub <-solve(taue_0*WTW+tauu_0*Kinvall) #update Var(b,u)
    ub  <-taue_0*Vub%*%WTY                 #update E(b,u)
    TrKinvub <- sum(diag(Kinvall%*%Vub))
    uKinvub  <- t(ub)%*%Kinvall%*%ub
    tauu    <- (a.u+0.5*q)/(g.u+0.5*as.numeric(uKinvub)+0.5*TrKinvub)
    tauu    <- as.numeric(tauu)
    err     <- y - W%*%ub
    TrWTWub  <- sum(diag(WTW%*%Vub))
    taue    <- (a.e+0.5*n)/(g.e+0.5*sum(err^2)+0.5*TrWTWub)
    taue    <- as.numeric(taue)

    if(i > 1){
      diffub  <- sqrt((ub-ub0)^2)/(abs(ub)+0.01)
      diffte <- abs(taue_0-taue)/(taue+0.01)
      difftu <- abs(tauu_0-tauu)/(tauu+0.01)
      diffvub <- sqrt((diag(Vub0) - diag(Vub))^2)/(diag(Vub))
      diff.all<-c(diffub,diffte,difftu,diffvub)
      if(max(diff.all) < epsilon) break
    }
    Vub0 <- Vub;ub0<-ub;taue_0<-taue;tauu_0<-tauu
    #Calculate relative change.
  }

  taue.param<-c((a.e+0.5*n),(g.e+0.5*sum(err^2)+0.5*TrWTWub))
  tauu.param<-c((a.u+0.5*q),(g.u+0.5*uKinvub+0.5*TrKinvub))
  param<-list(ub,Vub,taue.param,tauu.param,i)
  names(param)<-c('betau_mean','betau_var','tau_e','tau_u','iter')
  return(param)
}
```

```
# Simple Linear Regression VB algorithm WITH history tracking
# Model: y = X  +   (no random effects)
# Tracks E[ ] and ELBO at each iteration
VB.linear_with_history <- function(epsilon, iter, X, y, taue_0, beta0, a.e, g.e){
  n <- dim(X)[1]
  p <- dim(X)[2]
  XTX <- crossprod(X)
```

```r
  XTY <- crossprod(X, y)

  # Initialize history storage
  E_tau_e_history <- numeric(iter)
  elbo_history <- numeric(iter)

  for(i in 1:iter){
    Vb  <- solve(taue_0 * XTX)        # Update Var( )
    b   <- taue_0 * Vb %*% XTY        # Update E[ ]
    err <- y - X %*% b
    TrXTXb <- sum(diag(XTX %*% Vb))
    taue   <- (a.e + 0.5*n) / (g.e + 0.5*sum(err^2) + 0.5*TrXTXb)
    taue   <- as.numeric(taue)

    # Store history
    E_tau_e_history[i] <- taue

    # Calculate ELBO (simplified version for monitoring convergence)
    elbo <- -0.5 * n * log(2*pi) + 0.5 * n * (digamma(a.e+0.5*n) - log(g.e+0.5*sum(err^2)+0.5*TrXTXb))
    elbo_history[i] <- elbo

    if(i > 1){
      diffb  <- sqrt((b - b0)^2) / (abs(b) + 0.01)
      diffte <- abs(taue_0 - taue) / (taue + 0.01)
      diffvb <- sqrt((diag(Vb0) - diag(Vb))^2) / diag(Vb)
      diff.all <- c(diffb, diffte, diffvb)
      if(max(diff.all) < epsilon) break
    }
    Vb0 <- Vb; b0 <- b; taue_0 <- taue
  }

  # Trim history to actual iterations
  E_tau_e_history <- E_tau_e_history[1:i]
  elbo_history <- elbo_history[1:i]

  taue.param <- c((a.e + 0.5*n), (g.e + 0.5*sum(err^2) + 0.5*TrXTXb))
  param <- list(b, Vb, taue.param, i, E_tau_e_history, elbo_history)
  names(param) <- c('beta_mean', 'beta_var', 'tau_e', 'iter', 'E_tau_e_history', 'elbo_history')
  return(param)
}
```

```r
# Simple Linear Regression Gibbs Sampler WITH history tracking
# Model: y = X  +   (no random effects)
# Full conditionals:  |  , y  and   |  , y
normalmm.linear.Gibbs_with_history <- function(iter, X, y, burnin, taue_0, a.e, b.e){
  n <- length(y)       # Number of observations
  p <- dim(X)[2]       # Number of predictors
  taue <- taue_0
  beta0 <- rnorm(p)

  XTX <- crossprod(X)
  XTy <- crossprod(X, y)
  library(mvtnorm)
  # Storage for results
  par <- matrix(0, iter, p+1)
  lppd <- matrix(0, iter, n)

  for(i in 1:iter){
    # Sample   |  , y from multivariate normal
    Prec <- XTX * taue
    P.var <- solve(Prec)
    P.mean <- P.var %*% XTy * taue
    beta <- rmvnorm(1, mean=P.mean, sigma=P.var)
    beta <- as.numeric(beta)

    # Sample   |  , y from Gamma
    err <- y - X %*% beta
    taue <- rgamma(1, a.e + 0.5*n, b.e + 0.5*sum(err^2))

    # Store iterations
    par[i,] <- c(beta, taue)
    beta0 <- beta
    lppd[i,] <- dnorm(y, mean=as.numeric(X %*% beta), sd=1/sqrt(taue))
  }

  lppd <- lppd[-c(1:burnin),]
  lppdest <- sum(log(colMeans(lppd)))           # Estimate lppd for whole dataset
  pwaic2 <- sum(apply(log(lppd), 2, FUN=var))   # Estimate effective number of parameters
  par <- par[-c(1:burnin),]
  colnames(par) <- c(paste0('beta', 0:(p-1)), 'tau_e')
  mresult <- list(par, lppdest, pwaic2)
  names(mresult) <- c('par', 'lppd', 'pwaic')
  return(mresult)
}
```

1 scenario 1: Conditional on Model Type

```
cat(glue("\n=== Scenario 1: Simple Linear Regression (n={n}, p={p}) ===\n"))
```

```
## === Scenario 1: Simple Linear Regression (n=300, p=3) ===
```

```
# Generate design matrix X (intercept + p-1 predictors)
X_s1 <- cbind(1, matrix(rnorm(n*(p-1)), nrow=n, ncol=p-1))

# Generate response y = X  +   (no random effects)
linear_predictor_s1 <- X_s1 %*% beta_true
residuals_true_s1 <- rnorm(n, 0, sqrt(1/tau_e_true))  # sd = sqrt(2) when tau_e_true = 0.5
y_s1 <- as.vector(linear_predictor_s1 + residuals_true_s1)
```

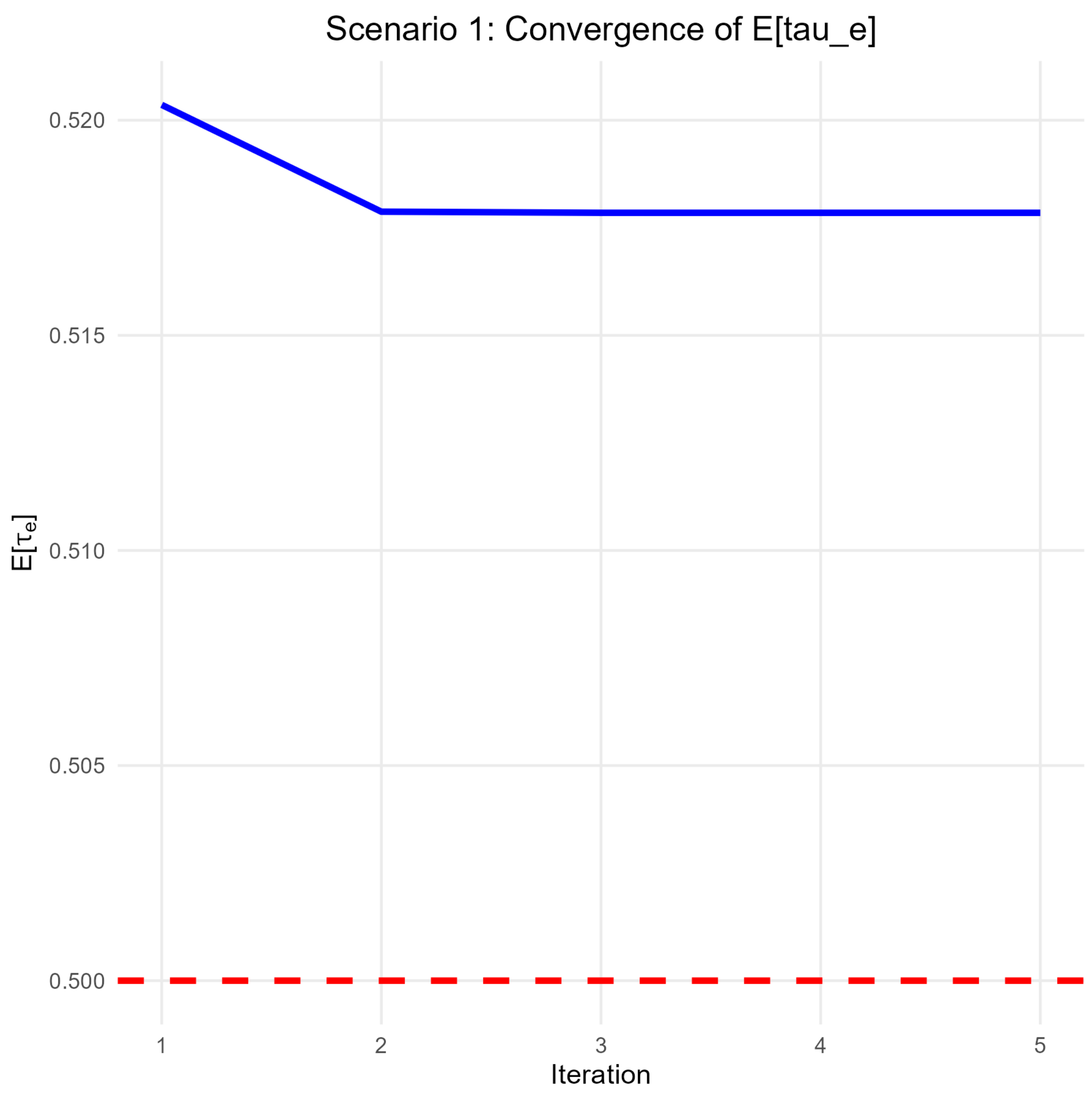
```
cat("\n=== SCENARIO 1: Simple Linear Regression ===\n")
```

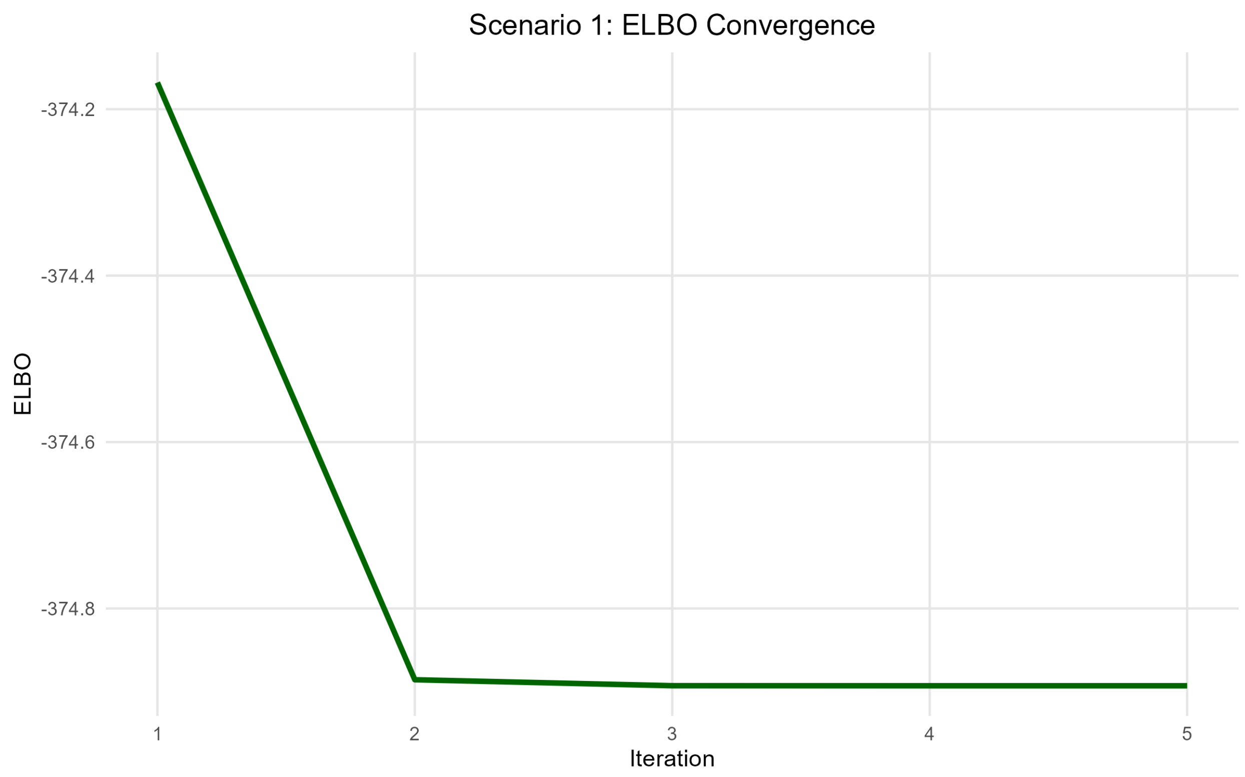
```
##
## === SCENARIO 1: Simple Linear Regression ===
```

```
results_s1 <- run_vb_algorithm(
  X          = X_s1,
  y          = y_s1,
  p          = p,
  n          = n,
  alpha_e    = alpha_e,
  gamma_e    = gamma_e
)
```

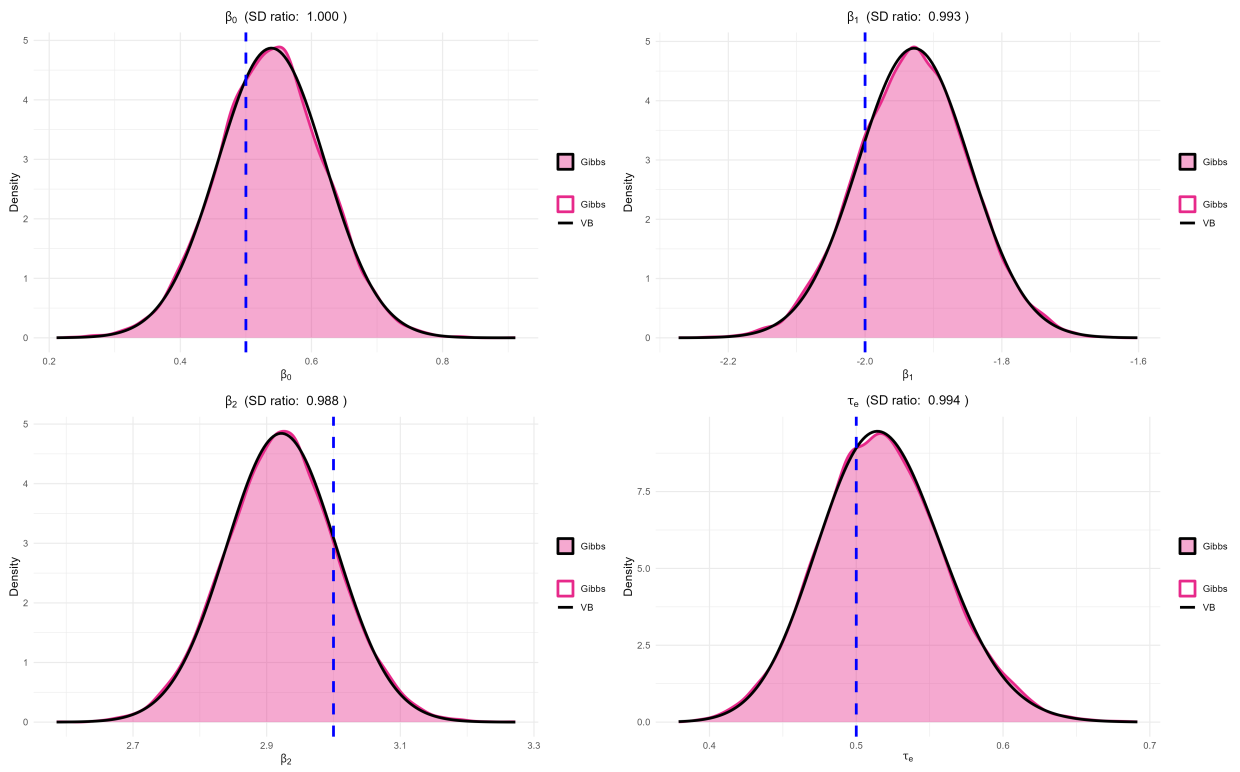
```
if (run_gibbs) {
  cat("\nRunning Gibbs sampler...\n")
  gibbs_s1 <- run_gibbs_sampler(
    X          = X_s1,
    y          = y_s1,
    p          = p,
    n          = n,
    alpha_e    = alpha_e,
    gamma_e    = gamma_e,
    n_iter     = gibbs_iter,
    n_burnin   = gibbs_burnin
  )

  cat("Gibbs posterior means:\n")
  cat("beta:", colMeans(gibbs_s1[, 1:p]), "\n")
  cat("tau_e:", mean(gibbs_s1[, "tau_e"]), "\n")

  gibbs_tau_e_s1 <- gibbs_s1[, "tau_e"]
} else {
  gibbs_s1 <- NULL
  gibbs_tau_e_s1 <- NULL
}
```

```
##
## Running Gibbs sampler...
## Gibbs posterior means:
## beta: 0.5378801 -1.929427 2.921659
## tau_e: 0.5177047
```


Scenario 1: Convergence of E[tau_e]
$E[\tau_e]$
0.520
0.515
0.510
0.505
0.500
1
2
3
4
5
Iteration



```
## M1: 4-panel posterior plot saved for Scenario 1
```



2 scenario 2: Conditional on Model Type (M3 only)

```r
if (model_type == "M3") {
  cat(glue("\n=== Scenario 2: Q={q_s2} groups (n={nq_s2} per group) ===\n"))

  # Dr John's method: generate then standardize
  u_true_s2 <- rnorm(q_s2, 0, 1)
  u_true_s2 <- scale(u_true_s2)

  X_s2 <- cbind(1, matrix(rnorm(n*(p-1)), nrow=n, ncol=p-1))
  Z_s2 <- table(1:n, rep(1:q_s2, n/q_s2))  # Dr John's method
  K_s2 <- diag(q_s2)

  linear_predictor_s2 <- X_s2 %*% beta_true + Z_s2 %*% u_true_s2
  residuals_true_s2   <- rnorm(n, 0, sqrt(2))  # Dr John's method: hardcoded
  y_s2 <- as.vector(linear_predictor_s2 + residuals_true_s2)
} else {
  cat("\nScenario 2 skipped (M3 only)\n")
}
```

```r
results_s2 <- run_vb_algorithm(
  X          = X_s2,
  Z          = Z_s2,
  y          = y_s2,
  K          = K_s2,
  p          = p,
  q          = q_s2,
  n          = n,
  alpha_e    = alpha_e,
  gamma_e    = gamma_e,
  alpha_u    = alpha_u,
  gamma_u    = gamma_u
)
```

```r
if (run_gibbs) {
  cat("\nRunning Gibbs sampler...\n")
  gibbs_s2 <- run_gibbs_sampler(
    X          = X_s2,
    Z          = Z_s2,
    y          = y_s2,
    p          = p,
    q          = q_s2,
    n          = n,
    alpha_e    = alpha_e,
    gamma_e    = gamma_e,
    alpha_u    = alpha_u,
    gamma_u    = gamma_u,
    n_iter     = gibbs_iter,
    n_burnin   = gibbs_burnin
  )

  cat("Gibbs posterior means:\n")
  cat("beta:", colMeans(gibbs_s2[, 1:p]), "\n")
  cat("tau_e:", mean(gibbs_s2[, "tau_e"]), "\n")
  cat("tau_u:", mean(gibbs_s2[, "tau_u"]), "\n")

  gibbs_tau_e_s2 <- gibbs_s2[, "tau_e"]
  gibbs_tau_u_s2 <- gibbs_s2[, "tau_u"]
} else {
  gibbs_s2 <- NULL
  gibbs_tau_e_s2 <- NULL
  gibbs_tau_u_s2 <- NULL
}
```

3 comparison Between Scenarios (M3 only)

```
# Simple linear regression: VB vs Gibbs comparison

if (!is.null(gibbs_s1)) {
  # Calculate statistics
  vb_beta_means <- results_s1$mu_beta
  vb_beta_sds <- sqrt(diag(results_s1$Sigma_beta))
  vb_tau_e_mean <- results_s1$E_tau_e
  vb_tau_e_sd <- sqrt(results_s1$a_e_new / (results_s1$b_e_new^2))

  gibbs_beta_means <- colMeans(gibbs_s1[, 1:p])
  gibbs_beta_sds <- apply(gibbs_s1[, 1:p], 2, sd)
  gibbs_tau_e_mean <- mean(gibbs_s1[, "tau_e"])
  gibbs_tau_e_sd <- sd(gibbs_s1[, "tau_e"])

  # Create comparison data frame
  comparison_df <- data.frame(
    Parameter = c(paste0("beta", 0:(p-1)), "tau_e"),
    True_Value = c(beta_true, tau_e_true),
    VB_Mean = c(vb_beta_means, vb_tau_e_mean),
    VB_SD = c(vb_beta_sds, vb_tau_e_sd),
    Gibbs_Mean = c(gibbs_beta_means, gibbs_tau_e_mean),
    Gibbs_SD = c(gibbs_beta_sds, gibbs_tau_e_sd),
    SD_Ratio = c(vb_beta_sds / gibbs_beta_sds, vb_tau_e_sd / gibbs_tau_e_sd)
  )

  # Format for display
  comparison_df_print <- comparison_df
  comparison_df_print[, 2:7] <- round(comparison_df_print[, 2:7], 4)

  cat("\n=== VB vs Gibbs Posterior Comparison ===\n\n")
  print(comparison_df_print, row.names = FALSE)

  cat("\n=== Under-dispersion Analysis ===\n")
  cat("SD Ratios (VB/Gibbs) < 1 indicate under-dispersion\n\n")
  for (i in 1:nrow(comparison_df)) {
    param <- comparison_df$Parameter[i]
    ratio <- comparison_df$SD_Ratio[i]
    pct <- (1 - ratio) * 100
    cat(sprintf("%s: SD ratio = %.3f (VB is %.1f%% narrower)\n", param, ratio, pct))
  }
```

```r
} else {
  cat("\nGibbs sampling disabled - comparison not available\n")
}
```

```
##
## === VB vs Gibbs Posterior Comparison ===
##
##  Parameter True_Value VB_Mean  VB_SD Gibbs_Mean Gibbs_SD SD_Ratio
##      beta0        0.5  0.5389 0.0819     0.5379   0.0819   0.9997
##      beta1       -2.0 -1.9284 0.0817    -1.9294   0.0822   0.9934
##      beta2        3.0  2.9219 0.0824     2.9217   0.0833   0.9884
##      tau_e        0.5  0.5178 0.0423     0.5177   0.0425   0.9938
##
## === Under-dispersion Analysis ===
## SD Ratios (VB/Gibbs) < 1 indicate under-dispersion
##
## beta0: SD ratio = 1.000 (VB is 0.0% narrower)
## beta1: SD ratio = 0.993 (VB is 0.7% narrower)
## beta2: SD ratio = 0.988 (VB is 1.2% narrower)
## tau_e: SD ratio = 0.994 (VB is 0.6% narrower)
```

4 sample Size Effects on _u (Multi-Configuration Analysis)

```r
# experimental design: Fix N=300, vary Q to show sample size per group effect
# Following Dr John's guidance (Meeting 16 Jan 2026)
# Q = 5 → 60 obs/group (rich data)
# Q = 10 → 30 obs/group
# Q = 20 → 15 obs/group
# Q = 50 → 6 obs/group (sparse data)

cat("\n========================================\n")
cat("Multi-Configuration _u Analysis\n")
cat("========================================\n")

group_configs <- list(
  list(q = 5,   nq = 60, label = "Q=5 (n=60 per group)"),
  list(q = 10,  nq = 30, label = "Q=10 (n=30 per group)"),
  list(q = 20,  nq = 15, label = "Q=20 (n=15 per group)"),
  list(q = 50,  nq = 6,  label = "Q=50 (n=6 per group)"),
  list(q = 100, nq = 3,  label = "Q=100 (n=3 per group)")
)

results_multi <- list()

for (i in seq_along(group_configs)) {
  config <- group_configs[[i]]
  cat("\n--- Running:", config$label, "---\n")

  # generate data using Dr John's exact method
  q_temp <- config$q
  nq_temp <- config$nq

  # Dr John's method: generate then standardize
```

```r
u_true_temp <- rnorm(q_temp, 0, 1)
u_true_temp <- scale(u_true_temp)

# Dr John's method: table() for incidence matrix
Z_temp <- table(1:n, rep(1:q_temp, n/q_temp))

# Dr John's method: simple X matrix (no correlation)
X_temp <- cbind(1, matrix(rnorm(n*(p-1)), n, p-1))

# Dr John's method: hardcoded residual sd = sqrt(2)
eta_temp <- X_temp %*% beta_true + Z_temp %*% u_true_temp
y_temp <- as.vector(eta_temp + rnorm(n, 0, sqrt(2)))

# Covariance matrix for random effects
K_temp <- diag(q_temp)

# Run VB
vb_result <- run_vb_algorithm(
  X       = X_temp,
  Z       = Z_temp,
  y       = y_temp,
  K       = K_temp,
  p       = p,
  q       = q_temp,
  n       = n,
  alpha_e = alpha_e,
  gamma_e = gamma_e,
  alpha_u = alpha_u,
  gamma_u = gamma_u,
  tol     = 1e-4,
  max_iter = 500
)

# Run Gibbs 3 times with different inits (Dr John's convergence check)
if (run_gibbs) {
  cat("Running Gibbs with 3 different initial values...\n")

  # Run 1: taue_0=3, tauu_0=0.5
  gibbs_run1 <- run_gibbs_sampler(
    X        = X_temp,
    Z        = Z_temp,
    y        = y_temp,
    p        = p,
    q        = q_temp,
    n        = n,
    alpha_e  = alpha_e,
    gamma_e  = gamma_e,
    alpha_u  = alpha_u,
    gamma_u  = gamma_u,
    n_iter   = gibbs_iter,
    n_burnin = gibbs_burnin,
    init_taue = 3,
    init_tauu = 0.5
  )

  # Run 2: taue_0=0.5, tauu_0=3
  gibbs_run2 <- run_gibbs_sampler(
    X        = X_temp,
    Z        = Z_temp,
    y        = y_temp,
    p        = p,
    q        = q_temp,
    n        = n,
    alpha_e  = alpha_e,
    gamma_e  = gamma_e,
    alpha_u  = alpha_u,
    gamma_u  = gamma_u,
    n_iter   = gibbs_iter,
    n_burnin = gibbs_burnin,
    init_taue = 0.5,
    init_tauu = 3
  )

  # Run 3: taue_0=5, tauu_0=5
  gibbs_run3 <- run_gibbs_sampler(
    X        = X_temp,
    Z        = Z_temp,
    y        = y_temp,
    p        = p,
    q        = q_temp,
    n        = n,
    alpha_e  = alpha_e,
    gamma_e  = gamma_e,
    alpha_u  = alpha_u,
    gamma_u  = gamma_u,
    n_iter   = gibbs_iter,
    n_burnin = gibbs_burnin,
    init_taue = 5,
    init_tauu = 5
  )

  # Combine all 3 runs (Dr John's method)
  gibbs_result <- rbind(gibbs_run1, gibbs_run2, gibbs_run3)
  cat("Combined", nrow(gibbs_result), "samples from 3 Gibbs runs\n")
} else {
  gibbs_result <- NULL
}

# Store results
results_multi[[i]] <- list(
  config = config,
  vb     = vb_result,
  gibbs  = gibbs_result
)

cat("VB E[tau_u]:", round(vb_result$E_tau_u, 4), "\n")
if (!is.null(gibbs_result)) {
  cat("HMC E[tau_u]:", round(mean(gibbs_result[, "tau_u"]), 4), "\n")
}
}

cat("\n========================================\n")
```

```
# Check if history data is available
if (!is.null(results_multi[[1]]$vb$E_tau_u_history) && length(results_multi[[1]]$vb$E_tau_u_history) > 
  par(mfrow = c(1, 2))

  # E[tau_u] convergence for all configurations
  max_len_tau <- max(sapply(results_multi, function(r) length(r$vb$E_tau_u_history)))

  plot(
    1:length(results_multi[[1]]$vb$E_tau_u_history),
    results_multi[[1]]$vb$E_tau_u_history,
    type = 'l',
    lwd  = 2,
    col  = '#1b9e77',
    xlab = 'Iteration',
    ylab = 'E[tau_u]',
    main = 'Comparison: E[tau_u] Convergence (varying Q, fixed N=300)',
    xlim = c(1, max_len_tau),
    ylim = range(c(sapply(results_multi, function(r) r$vb$E_tau_u_history), tau_u_true)))

  for (i in 2:length(results_multi)) {
    lines(1:length(results_multi[[i]]$vb$E_tau_u_history),
          results_multi[[i]]$vb$E_tau_u_history,
          col = c('#7570b3', '#e7298a', '#d95f02', '#66a61e')[i-1],
          lwd = 2)
  }

  abline(h = tau_u_true, col = 'red', lty = 2, lwd = 2)

  legend('topright',
         legend = c('Q=5', 'Q=10', 'Q=20', 'Q=50', 'Q=100', 'True value'),
         col    = c('#1b9e77', '#7570b3', '#e7298a', '#d95f02', '#66a61e', 'red'),
         lty    = c(rep(1, 5), 2),
         lwd    = 2,
         cex    = 0.8)

  # ELBO convergence for all configurations
  max_len_elbo <- max(sapply(results_multi, function(r) length(r$vb$elbo_history)))

  plot(
    1:length(results_multi[[1]]$vb$elbo_history),
    results_multi[[1]]$vb$elbo_history,
    type = 'l',
    lwd  = 2,
    col  = '#1b9e77',
    xlab = 'Iteration',
    ylab = 'ELBO',
    main = 'Comparison: ELBO Convergence (varying Q, fixed N=300)',
```

```r
    xlim = c(1, max_len_elbo),
    ylim = range(sapply(results_multi, function(r) r$vb$elbo_history)))

  for (i in 2:length(results_multi)) {
    lines(1:length(results_multi[[i]]$vb$elbo_history),
          results_multi[[i]]$vb$elbo_history,
          col = c('#7570b3', '#e7298a', '#d95f02', '#66a61e')[i-1],
          lwd = 2)
  }

  legend('bottomright',
         legend = c('Q=5', 'Q=10', 'Q=20', 'Q=50', 'Q=100'),
         col    = c('#1b9e77', '#7570b3', '#e7298a', '#d95f02', '#66a61e'),
         lty    = 1,
         lwd    = 2,
         cex    = 0.8)
  grid()
} else {
  plot.new()
  text(0.5, 0.5, "Convergence history not available\n(Using Dr John's original functions)",
       cex = 1.5, col = "gray50")
}
```

```r
# Create multi-panel comparison plot as requested by Dr John
# Focus on _u posterior distributions across different group sizes

plot_list <- list()

for (i in seq_along(results_multi)) {
  result <- results_multi[[i]]
  config <- result$config

  # VB posterior: Gamma(a_u_new, b_u_new)
  a_vb <- result$vb$a_u_new
  b_vb <- result$vb$b_u_new

  # Calculate VB range
  vb_mean <- a_vb / b_vb
  vb_sd <- sqrt(a_vb) / b_vb
  vb_min <- max(0, vb_mean - 4 * vb_sd)
  vb_max <- vb_mean + 4 * vb_sd

  # If Gibbs available, extend range to include both distributions
  if (!is.null(result$gibbs)) {
    gibbs_tau_u <- result$gibbs[, "tau_u"]
    gibbs_min <- quantile(gibbs_tau_u, 0.001)
    gibbs_max <- quantile(gibbs_tau_u, 0.999)

    x_min <- min(vb_min, gibbs_min, tau_u_true * 0.5)
    x_max <- max(vb_max, gibbs_max, tau_u_true * 3)
  } else {
    x_min <- min(vb_min, tau_u_true * 0.5)
    x_max <- max(vb_max, tau_u_true * 3)
  }
```

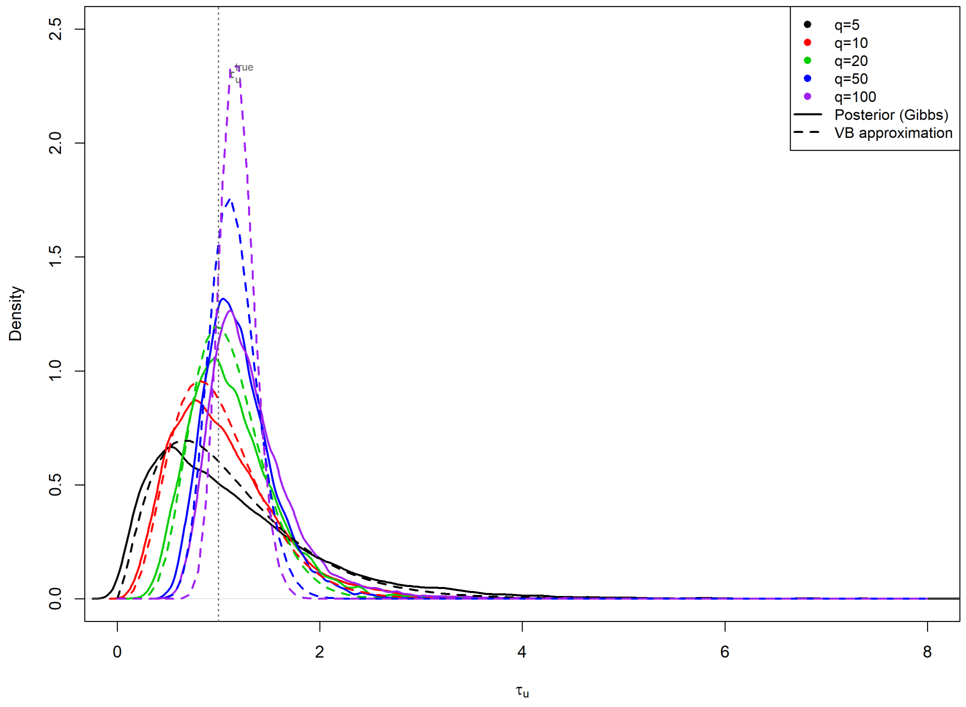
```r
x_range <- seq(x_min, x_max, length.out = 500)
vb_density <- dgamma(x_range, shape = a_vb, rate = b_vb)

df_plot <- data.frame(
  tau_u   = x_range,
  density = vb_density,
  method  = "VB",
  type    = "solid"
)

# Add Gibbs if available and calculate SD ratio
sd_ratio_text <- ""
if (!is.null(result$gibbs)) {
  dens_gibbs <- density(gibbs_tau_u, adjust = 1.5)

  df_gibbs <- data.frame(
    tau_u   = dens_gibbs$x,
    density = dens_gibbs$y,
    method  = "Gibbs",
    type    = "dashed"
  )

  df_plot <- rbind(df_plot, df_gibbs)

  # Calculate SD ratio
  vb_sd <- sqrt(a_vb) / b_vb
  gibbs_sd <- sd(gibbs_tau_u)
  sd_ratio <- vb_sd / gibbs_sd
  sd_ratio_text <- glue(" | SD ratio: {round(sd_ratio, 3)}")
}

# Create plot
p_tau <- ggplot(df_plot, aes(x = tau_u, y = density, color = method, linetype = method)) +
  geom_line(linewidth = 1.2) +
  geom_vline(xintercept = tau_u_true, color = "red", linetype = "dotted", linewidth = 0.8) +
  scale_color_manual(
    values = c("VB" = "black", "Gibbs" = "#E7298A")
  ) +
  scale_linetype_manual(
    values = c("VB" = "solid", "Gibbs" = "dashed")
  ) +
  labs(
    title = config$label,
    subtitle = glue("VB E[ _u] = {round(result$vb$E_tau_u, 3)}{sd_ratio_text}"),
    x = expression(tau[u]),
    y = "Density"
  ) +
  theme_minimal() +
  theme(
    legend.position = "top",
    plot.title = element_text(size = 12, face = "bold"),
    plot.subtitle = element_text(size = 10)
  )
  plot_list[[i]] <- p_tau
}

# Combine all 5 plots into a grid (2 rows, 3 columns)
combined_tau_u <- (plot_list[[1]] | plot_list[[2]] | plot_list[[3]]) /
                  (plot_list[[4]] | plot_list[[5]] | plot_spacer()) +
  plot_annotation(
    title = "Effect of Sample Size Per Group on  _u Posterior",
    subtitle = "VB approximation quality with sufficient groups for variance component estimation",
    theme = theme(
      plot.title = element_text(size = 16, face = "bold"),
      plot.subtitle = element_text(size = 12)
    )
  )

# Save plot
ggsave(
  filename = "../figs/M1_tau_u_sample_size_comparison.png",
  plot     = combined_tau_u,
  width    = 14,
  height   = 10,
  dpi      = 300
)

cat(" _u comparison plot saved to figs/M1_tau_u_sample_size_comparison.png\n")

# Display
img_tau_u <- readPNG("../figs/M1_tau_u_sample_size_comparison.png")
grid.newpage()
grid.raster(img_tau_u)
```

```
# Create 2-panel overlay plot: All Gibbs together, All VB together

# Prepare data for Gibbs panel
if (run_gibbs) {
  gibbs_combined <- data.frame()

  for (i in seq_along(results_multi)) {
    result <- results_multi[[i]]
    config <- result$config
    gibbs_tau_u <- result$gibbs[, "tau_u"]

    dens_gibbs <- density(gibbs_tau_u, adjust = 1.5)

    df_temp <- data.frame(
      tau_u   = dens_gibbs$x,
      density = dens_gibbs$y,
      config  = config$label
    )

    gibbs_combined <- rbind(gibbs_combined, df_temp)
  }
  # Gibbs panel
  p_gibbs <- ggplot(gibbs_combined, aes(x = tau_u, y = density, color = config)) +
    geom_line(linewidth = 1.2) +
    geom_vline(xintercept = tau_u_true, color = "red", linetype = "dotted", linewidth = 0.8) +
    scale_color_manual(
      values = c(
        "Q=5 (n=60 per group)"  = "gray50",
        "Q=10 (n=30 per group)" = "#d95f02",
        "Q=20 (n=15 per group)" = "#7570b3",
        "Q=50 (n=6 per group)"  = "#e7298a",
        "Q=100 (n=3 per group)" = "#1b9e77"
      )
    ) +
    coord_cartesian(xlim = c(0, 8)) +
    labs(
      title = "Gibbs Sampling Posteriors",
      subtitle = "All configurations show similar distributions",
      x = expression(tau[u]),
      y = "Density",
      color = "Configuration"
    ) +
    theme_minimal() +
    theme(
      legend.position = "right",
      legend.text = element_text(size = 9),
      legend.title = element_text(size = 10, face = "bold"),
      plot.title = element_text(size = 14, face = "bold"),
      plot.subtitle = element_text(size = 11)
    )
}

# Prepare data for VB panel
vb_combined <- data.frame()

for (i in seq_along(results_multi)) {
  result <- results_multi[[i]]
  config <- result$config

  a_vb <- result$vb$a_u_new
  b_vb <- result$vb$b_u_new

  # Use broad range to show all VB distributions
  x_range <- seq(0, 20, length.out = 500)
  vb_density <- dgamma(x_range, shape = a_vb, rate = b_vb)

  df_temp <- data.frame(
    tau_u   = x_range,
    density = vb_density,
    config  = config$label
  )

  vb_combined <- rbind(vb_combined, df_temp)
}
```

```r
# VB panel
p_vb <- ggplot(vb_combined, aes(x = tau_u, y = density, color = config)) +
  geom_line(linewidth = 1.2) +
  geom_vline(xintercept = tau_u_true, color = "red", linetype = "dotted", linewidth = 0.8) +
  scale_color_manual(
    values = c(
      "Q=5 (n=60 per group)"  = "gray50",
      "Q=10 (n=30 per group)" = "#d95f02",
      "Q=20 (n=15 per group)" = "#7570b3",
      "Q=50 (n=6 per group)"  = "#e7298a",
      "Q=100 (n=3 per group)" = "#1b9e77"
    )
  ) +
  coord_cartesian(xlim = c(0, 8)) +
  labs(
    title = "VB Posteriors",
    subtitle = "Consistent performance with sufficient groups",
    x = expression(tau[u]),
    y = "Density",
    color = "Configuration"
  ) +
  theme_minimal() +
  theme(
    legend.position = "right",
    legend.text = element_text(size = 9),
    legend.title = element_text(size = 10, face = "bold"),
    plot.title = element_text(size = 14, face = "bold"),
    plot.subtitle = element_text(size = 11)
  )

# Combine panels
if (run_gibbs) {
  combined_overlay <- p_gibbs | p_vb
  plot_title <- "Comparison: Gibbs vs VB Across All Configurations"
  plot_subtitle <- "Gibbs posteriors are consistent; VB posteriors vary dramatically with sample size p
  plot_width <- 14
} else {
  combined_overlay <- p_vb
  plot_title <- "VB Posteriors Across All Configurations"
  plot_subtitle <- "VB posterior quality varies dramatically with sample size per group"
  plot_width <- 8
}

combined_overlay <- combined_overlay +
  plot_annotation(
    title = plot_title,
    subtitle = plot_subtitle,
    theme = theme(
      plot.title = element_text(size = 16, face = "bold", margin = margin(b = 10)),
      plot.subtitle = element_text(size = 12, margin = margin(b = 20))
    )
  ) &
  theme(
    legend.position = "top",
    legend.box = "horizontal",
    legend.margin = margin(t = 10, b = 15),
    legend.spacing.x = unit(0.5, "cm"),
    plot.margin = margin(t = 15, r = 10, b = 10, l = 10)
  )

# Save plot
ggsave(
  filename = "../figs/M1_tau_u_overlay_comparison.png",
  plot     = combined_overlay,
  width    = plot_width,
  height   = 7,
  dpi      = 300
)

cat(" _u overlay comparison plot saved to figs/M1_tau_u_overlay_comparison.png\n")

# Display
img_overlay <- readPNG("../figs/M1_tau_u_overlay_comparison.png")
grid.newpage()
grid.raster(img_overlay)
```

```r
# Generate MY plot in Dr John's exact style
# Single panel with all Gibbs (solid) and VB (dashed) overlaid

cat("\n========================================\n")
cat("My  _u Comparison (Dr John's Style)\n")
cat("========================================\n\n")

# Prepare data: combine all Gibbs chains for each Q
gibbs_combined <- list()
vb_params <- list()

for (i in seq_along(results_multi)) {
  cfg <- group_configs[[i]]
  q_val <- cfg$q

  if (run_gibbs) {
    # results_multi[[i]]$gibbs is a matrix from run_gibbs_sampler
    # tau_u column name is "tau_u"
    gibbs_matrix <- results_multi[[i]]$gibbs
    gibbs_combined[[paste0("q", q_val)]] <- gibbs_matrix[, "tau_u"]
  }

  # VB gamma parameters from results_multi
  vb_result <- results_multi[[i]]$vb
  a_param <- vb_result$a_u_new
  b_param <- vb_result$b_u_new
  vb_params[[paste0("q", q_val)]] <- list(a = a_param, b = b_param)
}

# Create plot matching Dr John's style
png(filename = "../figs/M1_my_tau_u_comparison.png", width = 10, height = 8, units = "in", res = 300)
```

```r
# Colors for all 5 Q values
colors <- c("black", "red", "green3", "blue", "purple")
q_values <- c(5, 10, 20, 50, 100)

# Start with first Gibbs density
if (run_gibbs) {
  plot(density(gibbs_combined$q5),
       xlab = expression(tau['u']),
       main = '',
       ylim = c(0, 2.5),
       xlim = c(0, 8),
       lwd = 2,
       col = colors[1])

  # Add remaining Gibbs densities
  lines(density(gibbs_combined$q10), col = colors[2], lwd = 2)
  lines(density(gibbs_combined$q20), col = colors[3], lwd = 2)
  lines(density(gibbs_combined$q50), col = colors[4], lwd = 2)
  lines(density(gibbs_combined$q100), col = colors[5], lwd = 2)

  # Add VB approximations (dashed)
  curve(dgamma(x, vb_params$q5$a, vb_params$q5$b),
        add = TRUE, lty = 2, lwd = 2, col = colors[1])
  curve(dgamma(x, vb_params$q10$a, vb_params$q10$b),
        add = TRUE, lty = 2, lwd = 2, col = colors[2])
  curve(dgamma(x, vb_params$q20$a, vb_params$q20$b),
        add = TRUE, lty = 2, lwd = 2, col = colors[3])
  curve(dgamma(x, vb_params$q50$a, vb_params$q50$b),
        add = TRUE, lty = 2, lwd = 2, col = colors[4])
  curve(dgamma(x, vb_params$q100$a, vb_params$q100$b),
        add = TRUE, lty = 2, lwd = 2, col = colors[5])

  # Legend
  legend('topright',
         col = c(colors, "black", "black"),
         lty = c(0, 0, 0, 0, 0, 1, 2),
         lwd = c(NA, NA, NA, NA, NA, 2, 2),
         pch = c(19, 19, 19, 19, 19, NA, NA),
         legend = c('q=5', 'q=10', 'q=20', 'q=50', 'q=100', 'Posterior (Gibbs)', 'VB approximation'),
         cex = 0.9)
} else {
  # VB only version
  curve(dgamma(x, vb_params$q5$a, vb_params$q5$b),
        from = 0, to = 8,
        xlab = expression(tau['u']),
        ylab = "Density",
        main = '',
        ylim = c(0, 2.5),
        lwd = 2,
        col = colors[1])

  curve(dgamma(x, vb_params$q10$a, vb_params$q10$b),
        add = TRUE, lwd = 2, col = colors[2])
  curve(dgamma(x, vb_params$q20$a, vb_params$q20$b),
        add = TRUE, lwd = 2, col = colors[3])
  curve(dgamma(x, vb_params$q50$a, vb_params$q50$b),
        add = TRUE, lwd = 2, col = colors[4])
  curve(dgamma(x, vb_params$q100$a, vb_params$q100$b),
        add = TRUE, lwd = 2, col = colors[5])

  legend('topright',
         col = colors,
         lty = 1,
         lwd = 2,
         legend = c('q=5', 'q=10', 'q=20', 'q=50', 'q=100'),
         cex = 0.9)
}

# Add vertical line at true value
abline(v = tau_u_true, lty = 3, col = "gray40", lwd = 1.5)
text(tau_u_true, 2.3, labels = expression(tau[u]^true), pos = 4, cex = 0.9, col = "gray40")

dev.off()

cat("My plot saved to figs/M1_my_tau_u_comparison.png\n")
```

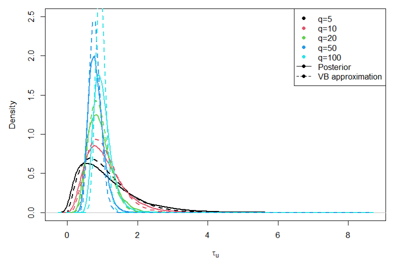


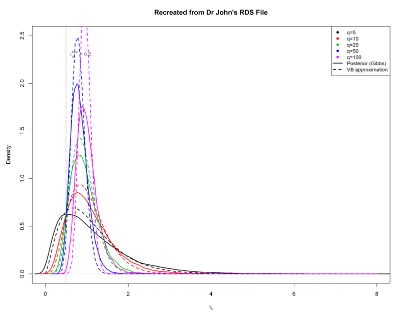
```
# Load Dr John's reference results from RDS
cat("\n========================================\n")
cat("Loading Dr John's Reference Data (RDS)\n")
cat("========================================\n\n")
```

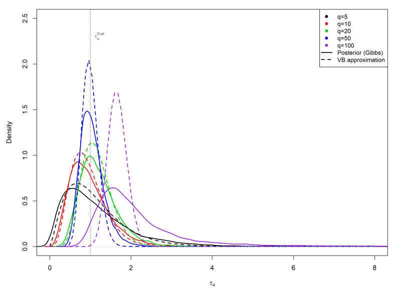
```r
# Use absolute path to ensure it works during knitting
project_root <- "d:/github/VI1"
rds_path <- file.path(project_root, "results", "dr_john_reference_tau_u.rds")

if (file.exists(rds_path)) {
  cat("Loading:", rds_path, "\n")
  dr_john_ref <- readRDS(rds_path)

  # Check structure
  cat("\nVB structure check:\n")
  cat("  q5 VB class:", class(dr_john_ref$vb$q5), "\n")
  if (is.list(dr_john_ref$vb$q5)) {
    cat("  q5 VB names:", names(dr_john_ref$vb$q5), "\n")
    cat("  q5$a =", dr_john_ref$vb$q5$a, "  q5$b =", dr_john_ref$vb$q5$b, "\n")
  } else {
    cat("  q5 VB values:", dr_john_ref$vb$q5, "\n")
  }

  cat("\nCreating plot from Dr John's saved RDS data...\n")

  colors_rds <- c("black", "red", "green3", "blue", "magenta")

  # Save plot to PNG file
  png(filename = file.path(project_root, "figs", "my_from_rds_tau_u_comparison.png"),
      width = 3500, height = 2800, res = 300)

  plot(density(dr_john_ref$gibbs$q5),
       xlab=expression(tau['u']),
       main='Recreated from Dr John\'s RDS File',
       ylim=c(0, 2.5),
       xlim=c(0, 8),
       lwd=2,
       col=colors_rds[1])

  lines(density(dr_john_ref$gibbs$q10), col=colors_rds[2], lwd=2)
  lines(density(dr_john_ref$gibbs$q20), col=colors_rds[3], lwd=2)
  lines(density(dr_john_ref$gibbs$q50), col=colors_rds[4], lwd=2)
  lines(density(dr_john_ref$gibbs$q100), col=colors_rds[5], lwd=2)

  # Add VB approximations - check if data is vector or list
  if (is.list(dr_john_ref$vb$q5)) {
    # VB stored as list(a=, b=)
    curve(dgamma(x, dr_john_ref$vb$q5$a, dr_john_ref$vb$q5$b),
          add = TRUE, lty = 2, lwd = 2, col = colors_rds[1])
    curve(dgamma(x, dr_john_ref$vb$q10$a, dr_john_ref$vb$q10$b),
          add = TRUE, lty = 2, lwd = 2, col = colors_rds[2])
    curve(dgamma(x, dr_john_ref$vb$q20$a, dr_john_ref$vb$q20$b),
          add = TRUE, lty = 2, lwd = 2, col = colors_rds[3])
    curve(dgamma(x, dr_john_ref$vb$q50$a, dr_john_ref$vb$q50$b),
          add = TRUE, lty = 2, lwd = 2, col = colors_rds[4])
    curve(dgamma(x, dr_john_ref$vb$q100$a, dr_john_ref$vb$q100$b),
          add = TRUE, lty = 2, lwd = 2, col = colors_rds[5])
  } else {
    # VB stored as vector c(a, b)
    curve(dgamma(x, dr_john_ref$vb$q5[1], dr_john_ref$vb$q5[2]),
          add = TRUE, lty = 2, lwd = 2, col = colors_rds[1])
    curve(dgamma(x, dr_john_ref$vb$q10[1], dr_john_ref$vb$q10[2]),
          add = TRUE, lty = 2, lwd = 2, col = colors_rds[2])
    curve(dgamma(x, dr_john_ref$vb$q20[1], dr_john_ref$vb$q20[2]),
          add = TRUE, lty = 2, lwd = 2, col = colors_rds[3])
    curve(dgamma(x, dr_john_ref$vb$q50[1], dr_john_ref$vb$q50[2]),
          add = TRUE, lty = 2, lwd = 2, col = colors_rds[4])
    curve(dgamma(x, dr_john_ref$vb$q100[1], dr_john_ref$vb$q100[2]),
          add = TRUE, lty = 2, lwd = 2, col = colors_rds[5])
  }

  legend('topright',
         col=c(colors_rds, "black", "black"),
         lty=c(0,0,0,0,0,1,2),
         lwd=c(NA,NA,NA,NA,NA,2,2),
         pch=c(19,19,19,19,19,NA,NA),
         legend=c('q=5', 'q=10', 'q=20', 'q=50', 'q=100', 'Posterior (Gibbs)', 'VB approximation'),
         cex=0.9)

  abline(v=0.5, lty=3, col="gray40", lwd=1.5)
  text(0.5, 2.3, labels=expression(tau[u]^true*" = 0.5"), pos=4, cex=0.9, col="gray40")

  dev.off()

  cat("Plot from RDS saved to figs/M1_my_from_rds_tau_u_comparison.png\n")

} else {
  cat("WARNING: RDS file not found at:", rds_path, "\n")
  cat("Run 'Code for David Ewing Random intercept example.R' to generate it.\n")
}
```

4.1 Three-Panel Validation Comparison

Panel status: - Dr John's baseline PNG: - My plot from RDS: - My new run with matched params:







Left: Dr John's baseline PNG (from his .R file)
Centre: My recreation from his RDS data
Right: My new run with matched parameters

```
# Diagnostic: Posterior variance / Prior variance ratio for u's
# As requested by Dr John [0:15:49]
# "When you do badly with tau_u, this ratio will be high. When you do well, this ratio will be low."
```

```r
cat("\nDiagnostic: Var_posterior(u) / Var_prior(u)\n")
cat("Diagnostic: Var_posterior(u) / Var_prior(u)\n")

# Prior variance: u_i ~ N(0, 1/tau_u_true)
var_prior_u <- 1 / tau_u_true

# Calculate ratio for each configuration
ratio_data <- data.frame()

for (i in seq_along(results_multi)) {
  result <- results_multi[[i]]
  config <- result$config
  q <- config$q

  # VB posterior variances: diagonal of Sigma_betau for u's
  Sigma_betau <- result$vb$Sigma_betau
  var_post_vb_u <- diag(Sigma_betau)[(p+1):(p+q)]
  mean_ratio_vb <- mean(var_post_vb_u / var_prior_u)

  # Gibbs posterior variances if available
  if (!is.null(result$gibbs)) {
    var_post_gibbs_u <- sapply(1:q, function(j) {
      var(result$gibbs[, paste0("u", j)])
    })
    mean_ratio_gibbs <- mean(var_post_gibbs_u / var_prior_u)
  } else {
    mean_ratio_gibbs <- NA
  }

  # Store results
  ratio_data <- rbind(ratio_data, data.frame(
    Q = q,
    n_per_group = config$nq,
    VB_ratio = mean_ratio_vb,
    Gibbs_ratio = mean_ratio_gibbs,
    label = config$label
  ))
}

print(ratio_data)

cat("\nInterpretation:\n")
cat("- Lower ratio = narrower posteriors = more information learnt\n")
cat("- Narrow posteriors for u → better tau_u estimation in VB\n")
cat("- As n_per_group increases, VB ratio decreases (posteriors concentrate)\n\n")

# Prepare data for plotting
plot_data <- data.frame(
  Q  = ratio_data$Q,
  VB = ratio_data$VB_ratio
)

if (run_gibbs) {
  plot_data$Gibbs <- ratio_data$Gibbs_ratio
  plot_data_long <- tidyr::pivot_longer(plot_data, cols = c(VB, Gibbs),
                                       names_to = "Method", values_to = "Ratio")
} else {
  plot_data_long <- data.frame(
    Q = plot_data$Q,
    Method = "VB",
    Ratio = plot_data$VB
  )
}

# Create diagnostic plot
p_diagnostic <- ggplot(plot_data_long, aes(x = factor(Q), y = Ratio, color = Method, group = Method)) +
  geom_point(size = 4) +
  geom_line(aes(linetype = Method), size = 1.2) +
  scale_color_manual(
    values = c("VB" = "black", "Gibbs" = "#E7298A")
  ) +
  scale_linetype_manual(
    values = c("VB" = "solid", "Gibbs" = "dashed")
  ) +
  labs(
    title = "Diagnostic: Posterior Variance / Prior Variance Ratio for Random Effects",
    subtitle = "Varying Q (fixed N=300): Lower ratio indicates concentrated posteriors and better  _u es
    x = "Number of Groups (Q) [n per group = 300/Q]",
    y = "Mean(Var_posterior(u) / Var_prior(u))",
    color = "Method"
  ) +
  theme_minimal() +
  theme(
    legend.position = "top",
    plot.title = element_text(size = 14, face = "bold"),
    plot.subtitle = element_text(size = 11)
  )

ggsave(
  filename = "../figs/M1_diagnostic_variance_ratio.png",
  plot = p_diagnostic,
  width = 10,
  height = 6,
  dpi = 300
)

img_diagnostic <- readPNG("../figs/M1_diagnostic_variance_ratio.png")
grid.newpage()
grid.raster(img_diagnostic)

cat("\n========================================\n")
cat("Key Finding (Dr John's insight):\n")
cat("As n per group increases (Q decreases from 50→5),\n")
cat("VB posteriors for u become narrower (ratio decreases),\n")
cat("leading to better tau_u estimation.\n")
cat("========================================\n")
```

```
##
## Saved M1 SD ratios to ../results/all_sd_ratios.rds
```