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Chair of Statistics
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Program leave-one-out posterior predictive checking in R

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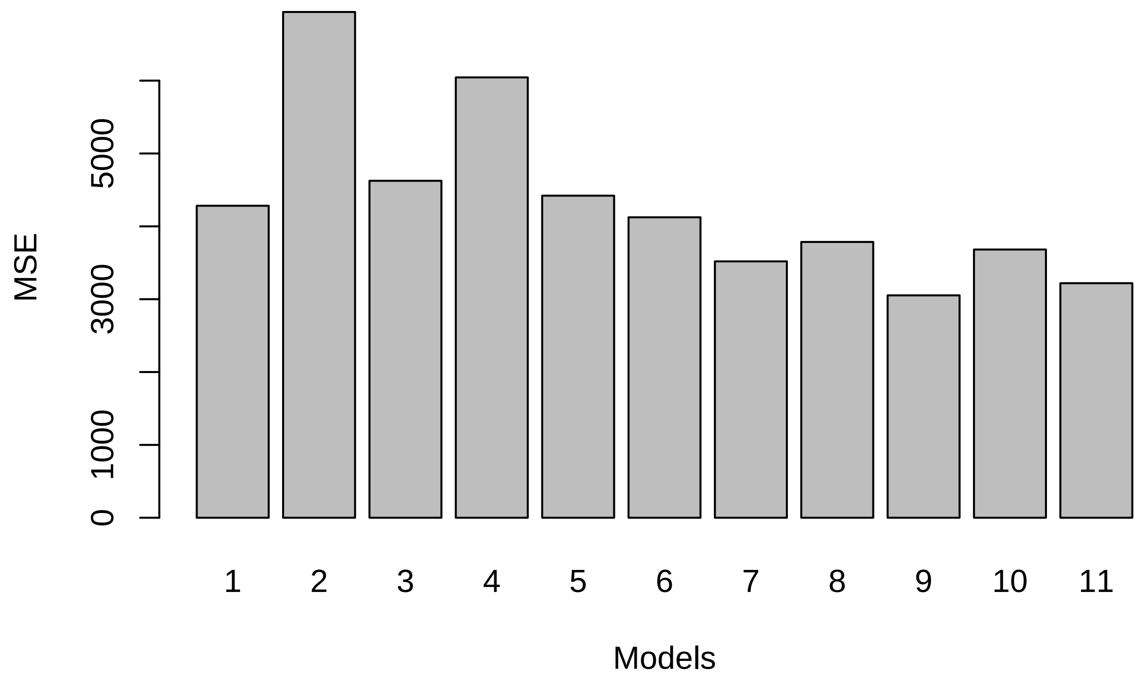
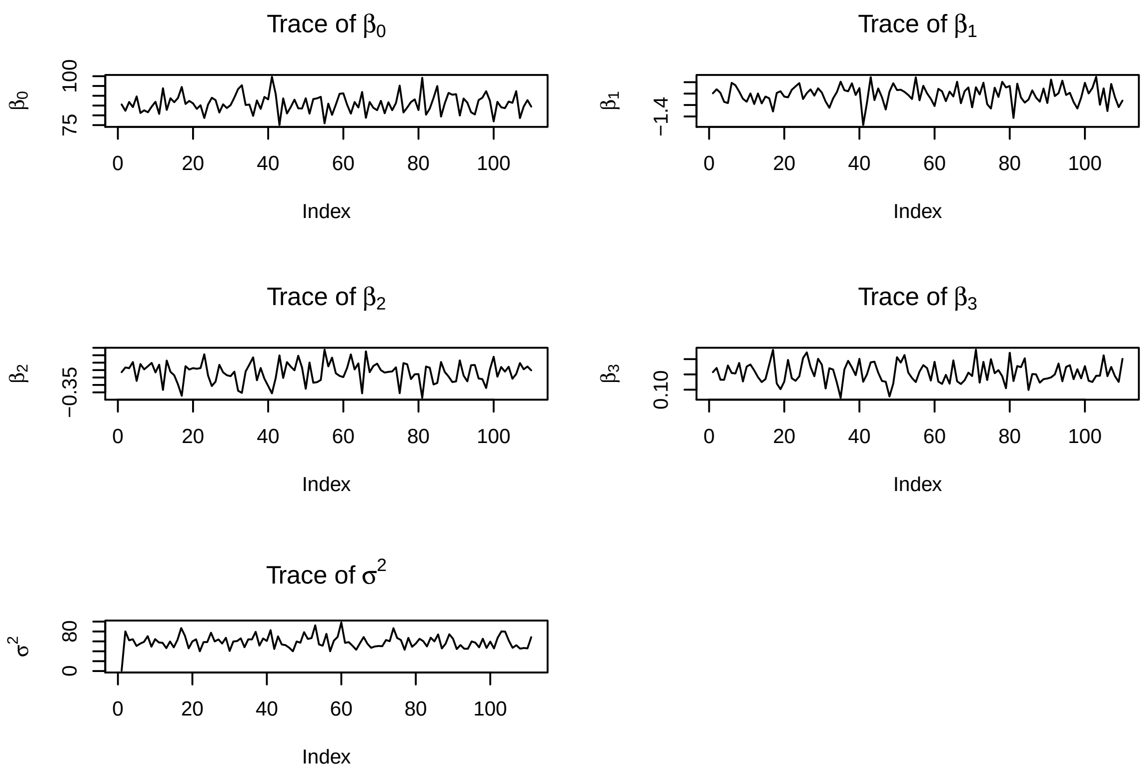
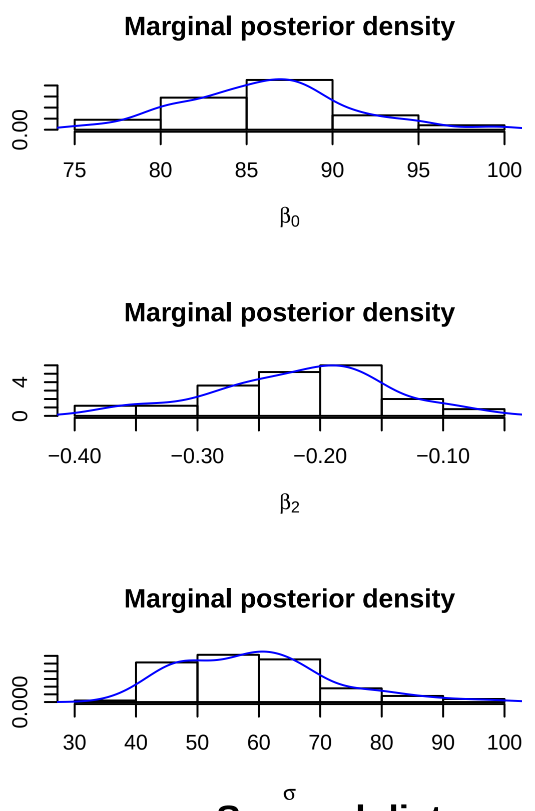
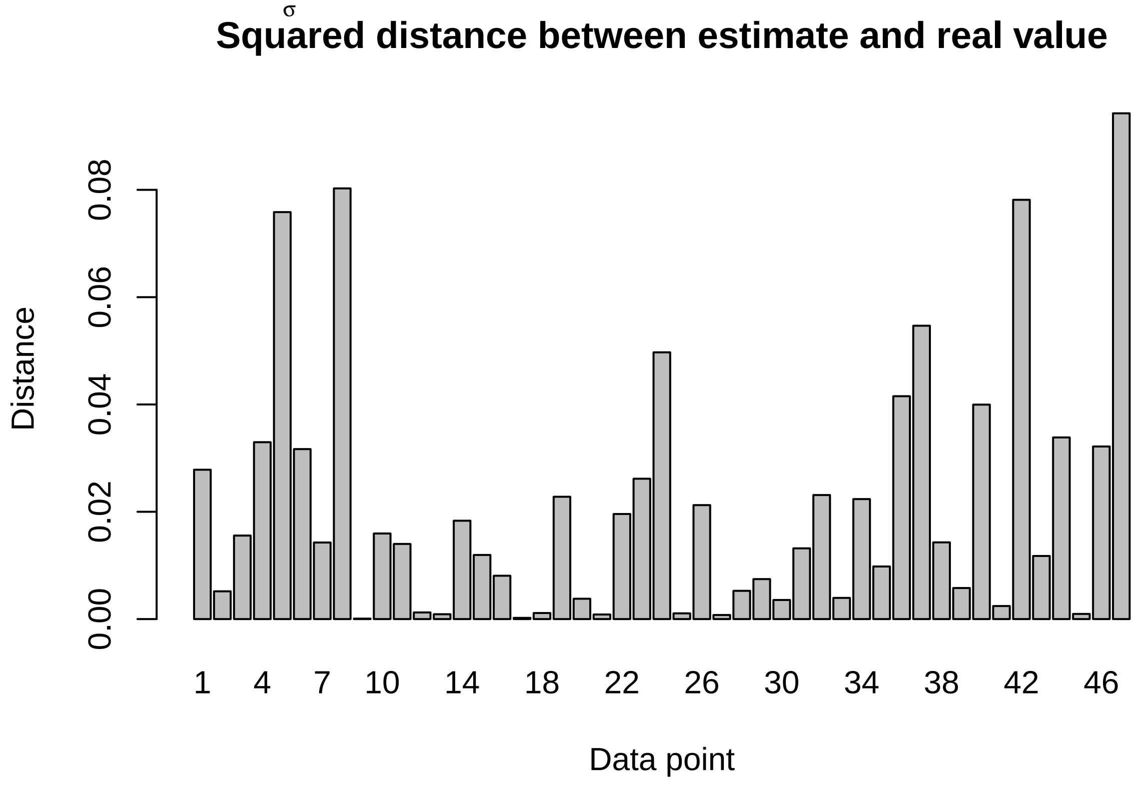
```r
plotSampling <- function(betas, sigma) {
  # Get number of parameters and adjust plot frame height
  q <- ncol(betas) + 1
  frameRows <- round(q/2+0.1)

  # Traces
  par(mfrow = c(frameRows,2))
  for(i in 1:ncol(betas)) {
    plot(betas[,i], type='l', ylab=bquote(beta[.(i-1)]), main=bquote("Trace of" ~ beta[.(i-1)]))
  }
  plot(sigma, type='l', ylab=bquote(sigma^2), main=bquote("Trace of" ~ sigma^2))

  # Marginal posterior densities (remove burn in)

  # Function to draw plot
  drawHistDensity <- function(para, para_name) {
    # para     : Parameter (e.b. Beta, Sigma)
    # para_name: Title of plot

    # Estimate density for parameter values
    density <- density(para)

    # Draw histogram and add estimated density line
    hist(para, freq = FALSE, ylim = c(0,max(density$y)), xlab = para_name,
         ylab=NULL, main = "Marginal posterior density")
    lines(density, col="blue")
  }

  # Adjust frame and plot all parameters
  par(mfrow = c(frameRows,2))
  for(i in 1:ncol(betas)) {
    drawHistDensity(betas[-(1:b),i], bquote(beta[.(i-1)]))
  }
  drawHistDensity(sigma[-(1:b)], bquote(sigma))
}

# The Gibbs Sampler
gibbsSampler <- function(X, Y, B) {
  # Size of design matrix
  n <- nrow(X)
  p <- ncol(X)

  # Variables to store the samples in
  betas <- matrix(NA, nrow = B, ncol = p)
  sigma <- c(1, rep(NA, B))

  # Sampling
  for(i in 1:B){
    # OLS of beta
    V <- solve(t(X)%*%X)     # (X^T X)^-1
    beta_hat <- V%*%t(X)%*%Y # (X^T X)^-1 X^T Y
    # OLS of sigma
    sigma_hat <- t(Y-X%*%beta_hat)%*%(Y-X%*%beta_hat)/(n-p)

    # Sample beta from the full conditional
    betas[i,] <- rmvnorm(1,beta_hat,sigma[i]*V)

    # Sample sigma from the full conditional
    sigma[i+1] <- 1/rgamma(1,(n-p)/2,(n-p)*sigma_hat/2)
  }

  return(list(betas = betas, sigma = sigma))
}

crossValidation <- function(X, Y, B, plotting = FALSE) {
  # Size of design matrix
  n <- nrow(X)
  p <- ncol(X)

  Yhat <- rep(NA, n)
  betas <- matrix(NA, nrow = n, ncol = p)

  for(i in 1:n) {
    # Remove i-th row from data
    Xi <- X[-i,]
    Yi <- Y[-i]

    # Run gibbs sampler to get sampled parameters
    res <- gibbsSampler(Xi, Yi, B)

    # Plot results from last run if plotting is set to TRUE
    if(i == n && plotting == TRUE) {
      plotSampling(res$betas, res$sigma)
    }

    # Calculate posterior mean from sampled betas
    betas[i,] <- apply(res$betas, 2, mean)

    # Predict value with posterior mean
    Yhat[i] <- X[i,]%*%betas[i,]
  }

  # Calculate beta estimate
  beta_cv <- colMeans(betas)

  # Return betas and distances
  return(list(betas = betas, dist = (Y-Yhat)^2))
}

bayesModelEvaluation <- function(models, Y, B, plotting = FALSE) {
  # Evaluate multiple models and return results from all models
  n <- length(Y)
  k <- length(models)
  results <- list()
  for(i in 1:k) {
    if(i == k && plotting == TRUE) {
      # Plot results for last model
      res <- crossValidation(models[[i]], Y, B, plotting = TRUE)
      par(mfrow = c(1,1))
      barplot(res$dist/sum(res$dist), xlab = "Data point", ylab = "Distance", names.arg = seq(1,n)
              main="Squared distance between estimate and real value")
    } else {
      # Just calculate
      res <- crossValidation(models[[i]], Y, B)
    }
    # Calculate beta estimates & MSE and add to results
    results[[i]] <- list(beta_est = colMeans(res$betas),
                         mse = sum(res$dist))
  }
  return(results)
}

# Swiss data
dat <- swiss

# Response variable
Y <- dat$Fertility

# Design matrix
n <- nrow(dat)
X <- matrix(c(rep(1,n), dat$Education, dat$Agriculture), nrow=n)

models <- list(
  matrix(c(rep(1,n), dat$Education), nrow=n),
  matrix(c(rep(1,n), dat$Agriculture), nrow=n),
  matrix(c(rep(1,n), dat$Examination), nrow=n),
  matrix(c(rep(1,n), dat$Catholic), nrow=n),
  matrix(c(rep(1,n), dat$Education, dat$Agriculture), nrow=n),
  matrix(c(rep(1,n), dat$Education, dat$Examination), nrow=n),
  matrix(c(rep(1,n), dat$Education, dat$Catholic), nrow=n),
  matrix(c(rep(1,n), dat$Education, dat$Agriculture, dat$Examination), nrow=n),
  matrix(c(rep(1,n), dat$Education, dat$Agriculture, dat$Catholic), nrow=n),
  matrix(c(rep(1,n), dat$Education, dat$Examination, dat$Catholic), nrow=n),
  matrix(c(rep(1,n), dat$Education, dat$Agriculture, dat$Examination ,dat$Catholic), nrow=n)
)

# Number of samples
b <- 10  # Burn in
R <- 100 # Random draws to evaluate
B <- R + b

res <- bayesModelEvaluation(models, Y, B)

# Plot Mean Squared Errors
MSEs <- sapply(res, function(el) { return(el$mse) })
par(mfrow = c(1,1))
barplot(MSEs, xlab = "Models", ylab = "MSE", names.arg = seq(1,length(models)))
```



```r
# Plot results from best model
best <- bayesModelEvaluation(models[which.min(MSEs)], Y, B, plotting = TRUE)
```







3 References