# 732A91 - Bayesian learning

Lab2 - "Bayesian Regression and Classification"

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#### Question 1 - Linear and polynomial regression

The dataset TempLinkoping.txt contains daily temperatures (in Celcius degrees) at Malmslätt, Linköping over the course of the year 2016 (366 days since 2016 was a leap year). The response variable is *temp* and the covariate is:

```
time = \frac{the \ number \ of \ days \ since \ beginning \ of \ year}{366}.
```

The task is to perform a Bayesian analysis of a quadratic regression:

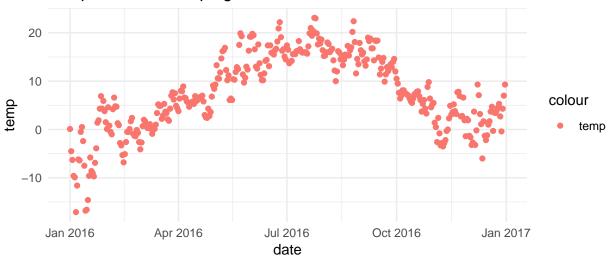
```
temp = \beta_0 + \beta_1 \cdot time + \beta_2 \cdot time^2 + \epsilon, \quad \epsilon \stackrel{iid}{\sim} N(0, \sigma^2).
```

#### 1a) - Determining prior distribution of model parameters

Determining the prior distribution of the model parameters. Use the conjugate prior for the linear regression model. Your task is to set the prior hyperparameters  $\mu_0$ ,  $\Omega_0$ ,  $\nu_0$ ,  $\sigma_0^2$  to sensible values. Start with  $\mu_0 = [-10, 100, -100]^T$ ,  $\Omega_0 = 0.01 \cdot I_3$ ,  $\nu_0 = 4$  and  $\sigma_0^2 = 1$ . Check if this prior agrees with your prior opinions by simulating draws from the joint prior of all parameters and for every draw compute the regression curve. This gives a collection of regression curves, one for each draw from the prior. Do the collection of curves look reasonable? If not, change the prior hyperparameters until the collection of prior regression curves do agree with your prior beliefs about the regression curve. [Hint: the R package mvtnorm will be handy. And use your  $Inv-\chi^2$  simulator from Lab 1.]

```
set.seed(12345)
temperatures <- read.delim("TempLinkoping.txt")
temperatures$date <- as_date(x = round(temperatures$time*366), origin="2015-12-31")
plot_temperatures <- ggplot(temperatures, aes(x = date, y = temp, col="temp")) + geom_point() +
    ggtitle("Temperatures Linkoping over time")
plot_temperatures</pre>
```

#### Temperatures Linkoping over time



The conjugate priors for the linear regression model can be seen below:

$$\beta | \sigma^2 \sim N(\mu_0, \ \sigma^2 \Omega_0^{-1})$$
  
 $\sigma^2 \sim Inv - \chi^2(\nu_0, \ \sigma_0^2)$ 

These priors are neat because the posterior distribution(s) can be written as:

$$\beta, \sigma^2 | \mathbf{y} \sim N(\mu_n, \ \sigma^2 \Omega_n^{-1})$$
  
 $\sigma^2 | \mathbf{y} \sim Inv \cdot \chi^2(\nu_n, \ \sigma_n^2)$ 

where the terms are calculated as:

$$\mu_{n} = (\mathbf{X}'\mathbf{X})^{-1}(\mathbf{X}'\mathbf{X}\hat{\beta} + \Omega_{0}\mu_{0})$$

$$\Omega_{n} = \mathbf{X}'\mathbf{X} + \Omega_{0}$$

$$\nu_{n} = \nu_{0} + n$$

$$\nu_{n}\sigma_{n}^{2} = \nu_{0}\sigma_{0}^{2} + (\mathbf{y}'\mathbf{y} + \mu_{0}'\Omega_{0}\mu_{0} - \mu_{n}'\Omega_{n}\mu_{n}) \Rightarrow$$

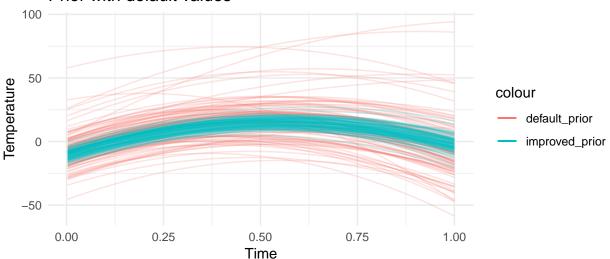
$$\Rightarrow \sigma_{n}^{2} = \frac{\nu_{0}\sigma_{0}^{2} + (\mathbf{y}'\mathbf{y} + \mu_{0}'\Omega_{0}\mu_{0} - \mu_{n}'\Omega_{n}\mu_{n})}{\nu_{n}}$$

The term  $\mu_n$  can with a little imagination (and cheating mathematics) be seen as the weighted mean of the prior beliefs and the actual data.

By sampling the sigma prior first, we can then later sample the beta according to this prior. The estimates for y are then computed by multiplying the prior betas with the X matrix (the data).

```
X_matrix <- as.matrix(cbind(1, temperatures$time, (temperatures$time)^2))</pre>
mu_0 \leftarrow matrix(c(-10, 100, -100), nrow = 3, ncol = 1)
identity <- matrix(0, nrow = 3, ncol = 3)</pre>
diag(identity) <- 1</pre>
omega_0 \leftarrow 0.01 * identity
v_0 <- 4
sigma_0_2 <- 1
prior_default <- data.frame("time" = seq(1/366, 1, by = 1/366), "default_prior" = 0)
chi_squared <- rchisq(1, df = v_0)</pre>
sigma 2 prior <- (sigma 0 2 * v 0) / chi squared
beta_prior <- rmvnorm(1, mean = mu_0, sigma = solve(omega_0)*sigma_2_prior)
prior_default$default_prior <- X_matrix%*%t(beta_prior)</pre>
plot <- ggplot(data = prior default, aes(x = time, y = default prior,</pre>
                                            col="default_prior")) + geom_line(alpha=0.2) +
  ggtitle("Prior with default values") + ylab("Temperature") + xlab("Time")
for (i in 1:100){
  chi_squared <- rchisq(1, df = v_0)</pre>
  sigma_2_prior <- (sigma_0_2 * v_0) / chi_squared
  beta_prior <- rmvnorm(1, mean = mu_0, sigma = solve(omega_0)*sigma_2_prior)
  df \leftarrow data.frame("time" = seq(1/366, 1, by = 1/366), "prior" = 0)
  df$prior <- X_matrix%*%t(beta_prior)</pre>
  plot <- plot + geom_line(data = df, aes(x = time, y = prior,</pre>
                                             col="default_prior"), alpha =0.2)
}
for (i in 1:100){
  mu 0 <- lm(temp ~ time + I(time^2), data = temperatures) $coefficients
  omega_0 <- identity
  v 0 <- 5
  sigma_0_2 <- 10
```

#### Prior with default values



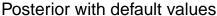
With the selected priors, we seem to catch the general trend swedish seasonal weather. However, some lines appear to be way of what can be seen as reasonable. We can check what parameters a frequentist polynomial model of order 2 would generate and use those parameters as a prior for  $\mu_0$ . In addition, the parameter  $\nu_0$  is increased, as this gives more weight to the prior beliefs.

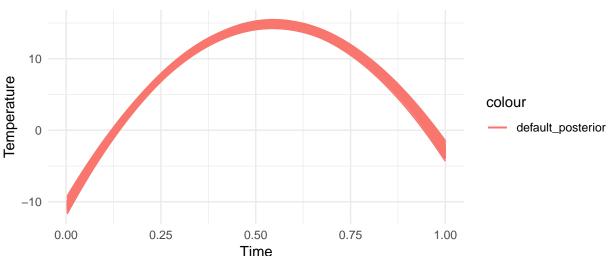
The curves seem to follow what resembles a normal year in sweden. It is not clear exactly what kind of measurements these temperatures are (average, at a specific time, or similar...) but it seems as the predicted temperatures for july are at least a little bit low. Obviously, these temperatures differ, but we don't want a model that overfits.

#### 1b) - Simulation from joint posterior distribution of $\beta_0$

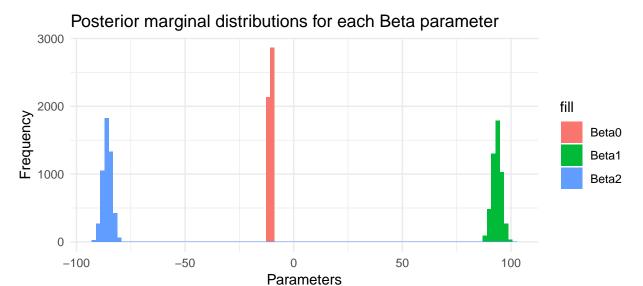
Write a program that simulates from the posterior distribution of  $\beta_0$ ,  $\beta_1$ ,  $\beta_2$  and  $\sigma^2$ . Plot the marginal posteriors for each parameter as a histogram. Also produce another figure with a scatter plot of the temperature data and overlay a curve for the posterior median of the regression function  $f(time) = \beta_0 + \beta_1 \cdot time + \beta_2 \cdot time^2$ , computed for every value of time. Also overlay curves for the lower 2.5 % and upper 97.5 % posterior credible interval for f(time). That is, compute the 95 % equal tail posterior probability intervals for every value of time and then connect the lower and upper limits of the interval by curves. Does the interval bands contain most of the data points? Should they?

```
n <- nrow(temperatures)</pre>
y <- temperatures$temp
XtX <- t(X_matrix)%*%X_matrix</pre>
mu_n <- solve(XtX + omega_0) %*% (XtX%*%mu_0 + omega_0 %*% mu_0)</pre>
omega_n <- XtX + omega_0</pre>
v_n < -v_0 + n
sigma n 2 <- ((v \ 0*sigma \ 0 \ 2) + t(v)%*%v +
                 t(mu_0)%*%omega_0%*%mu_0 -
                 t(mu_n)%*%omega_n%*%mu_n) / v_n
# posterior draws
chi_squared <- rchisq(1, df = v_n)</pre>
sigma_2_posterior <- as.numeric(sigma_n_2 * v_n) / chi_squared</pre>
beta_posterior <- rmvnorm(1, mean = mu_n,</pre>
                            sigma = sigma_2_posterior*solve(omega_n))
posterior_default <- data.frame(</pre>
  "time" = seq(1/366, 1, by = 1/366), "default_posterior" = 0)
posterior_default$default_posterior <- X_matrix%*%t(beta_posterior)</pre>
plot_posterior <- ggplot(data = posterior_default,</pre>
                           aes(x = time, y = default_posterior, col="default_posterior")) +
  geom_line() + ggtitle("Posterior with default values") + ylab("Temperature") + xlab("Time")
for (i in 1:100){
  chi_squared <- rchisq(1, df = v_n)</pre>
  sigma_2_posterior <- as.numeric(sigma_n_2 * v_n) / chi_squared</pre>
  beta_posterior <- rmvnorm(1, mean = mu_n,</pre>
                              sigma = sigma_2_posterior*solve(omega_n))
  df \leftarrow data.frame("time" = seq(1/366, 1, by = 1/366), "posterior" = 0)
  df$posterior <- X_matrix%*%t(beta_posterior)</pre>
  plot_posterior <- plot_posterior + geom_line(data = df,</pre>
                                                   aes(x = time, y = posterior, col="default_posterior"))
}
plot_posterior
```

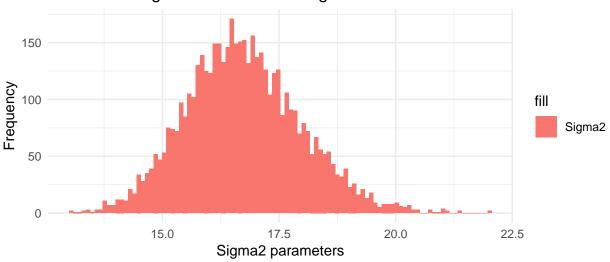




The posterior distribution seems a bit unsymmetric, probably this is caused by the data. The temperatures at the end of the year are slightly higher than at the beginning of the year, expected is that this raises the posterior curve at the end of the year.



#### Posterior marginal distribution for sigma2



Calculations for the posterior parameters are done according to the formulas presented in 1a and the lecture slides.

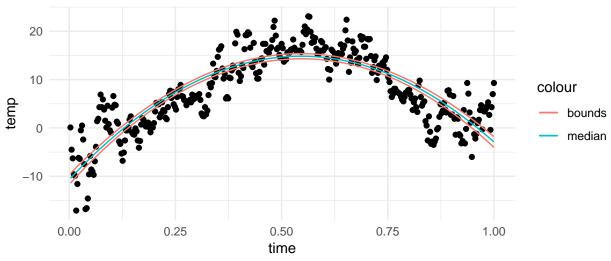
```
for (i in 1:nrow(temperatures)){
   temperatures2$median[i] <- median(temperatures_esimate[i,])
}

for (i in 1:nrow(temperatures)){
   temperatures2$bounds[i] <- quantile(temperatures_esimate[i,], probs = 0.025)
}

for (i in 1:nrow(temperatures)){
   temperatures2$high[i] <- quantile(temperatures_esimate[i,], probs = 0.975)
}

plot_temperatures2 <- ggplot(temperatures2, aes(x = time, y = temp)) + geom_point() +
   ggtitle("Temperatures Linkoping over time")
plot_temperatures2 <- plot_temperatures2 + geom_line(aes(x = time, y = median, col="median"))
plot_temperatures2 <- plot_temperatures2 + geom_line(aes(x = time, y = bounds, col="bounds"))
plot_temperatures2 <- plot_temperatures2 + geom_line(aes(x = time, y = high, col="bounds"))
plot_temperatures2</pre>
```

#### Temperatures Linkoping over time



The intervals are very tight around the median for each day. This is not strange since these intervals tell us with 95% certainty where the posterior regression line lies, not the actual points.

#### 1c) - Simulation from posterior distribution of $\bar{x}$

It is of interest to locate the *time* with the highest expected temperature (that is, the *time* where f(time) is maximal). Let's call this value  $\tilde{x}$ . Use the simulations in b) to simulate from the *posterior distribution* of  $\tilde{x}$ . [Hint: the regression curve is a quadratic. You can find a simple formula for  $\tilde{x}$  given  $\beta_0$ ,  $\beta_1$  and  $\beta_2$ .]

The expression for a polynomial model of order 2 can be written as  $f(x) = \beta_0 + \beta_1 \cdot x + \beta_2 \cdot x^2$ , where x is the time variable in oour data. All densities plotted are based on this function. Thus, if this function is maximized, so is the mode. The first order derivative is shown below:

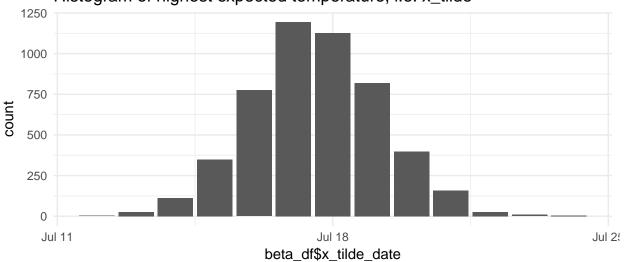
$$f(x) = \beta_0 + \beta_1 \cdot x + \beta_2 \cdot x^2 \quad \Rightarrow \quad f'(x) = \frac{\partial f}{\partial x} = \beta_1 + 2 \cdot \beta_2 \cdot x$$

Maximizing this concave function yields the maximum  $\tilde{x}$ :

$$f'(x) = 0 \Leftrightarrow \beta_1 + 2 \cdot \beta_2 \cdot x = 0 \Leftrightarrow \tilde{x} = -\frac{\beta_1}{2 \cdot \beta_2}$$

This is relatively easy to program, all that is needed is the matrix with our beta coefficients from 1b. To make sense of this density, we transform the  $\tilde{x}$  into dates from 2016.

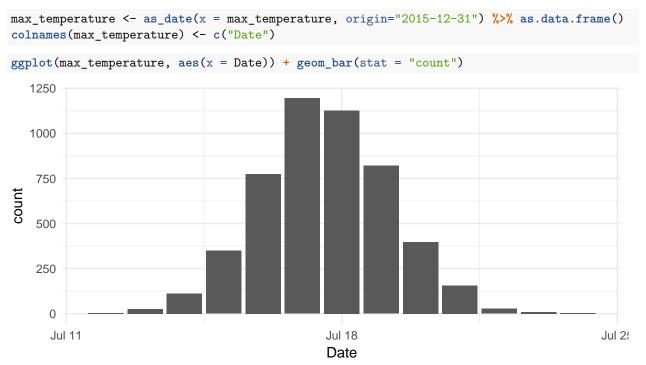




We observe that the highest temperatues occur in July.

```
# Simulation (bayesian) approach:
beta_df <- beta_df[, 1:3]
maximum_df <- as.data.frame(X_matrix%*%t(beta_df))

max_temperature <- apply(maximum_df, 2, which.max)</pre>
```



In answering this question we first did it analytically, however in the scope of this course the Bayesian way seems more appropriate. The highest expected temperatures center around the 18th of July, each year, when logically reasoning it, makes sense that the temperatures are generally the highest in summer.

#### 1d) - Polynomial model of order 7

Say now that you want to estimate a polynomial model of order 7, but you suspect that higher order terms may not be needed, and you worry about overfitting. Suggest a suitable prior that mitigates this potential problem. You do not need to compute the posterior, just write down your prior. [Hint: the task is to specify  $\mu_0$  and  $\Omega_0$  in a smart way.]

By combining the beta parameters in  $\mu_0$  to be close to 0 combined with a large  $\lambda_0$  we would obtain a tight conditional prior distribution:

$$\beta | \sigma^2 \stackrel{iid}{\sim} N(0, \sigma^2 [\lambda_0 \cdot \mathbf{I}]^{-1})$$

The idea is to use a bayesian approach to regularization. When doing so, the 'unimportant' beta coefficients will remain close to 0 and those that have a higher impact will 'stretch away' from 0.

Note: a large value of  $\lambda_0$  yields a tight distribution because we take the inverse of  $\lambda_0 \cdot \mathbf{I}$ .

# Question 2 - Posterior approximation for classification with logistic regression

The dataset WomenWork.dat contains $n = 200$ observations	(i.e. women	) on the following nine variables:
---	-------------	------------------------------------

Variable	Data type	Meaning	Role
Work	Binary	Whether or not the woman works	Response
Constant	1	Constant to the intercept	Feature
HusbandInc	Numeric	Husband's income	Feature
EducYears	Counts	Years of education	Feature
ExpYears	Counts	Years of experience	Feature
ExpYears2	Numeric	(Years of experience/10) <sup>2</sup>	Feature
Age	Counts	Age	Feature
NSmallChild	Counts	Number of child leq 6 years in household	Feature
NBigChild	Counts	Number of child >6 years in household	Feature

#### 2a) - Fit logistic regression model

Consider the logistic regression

$$Pr(y = 1|\mathbf{x}) = \frac{exp(\mathbf{x}^T \beta)}{1 + exp(\mathbf{x}^T \beta)}$$

where y is the binary variable with y=1 if the woman works and y=0 if she does not.  $\mathbf x$  is a 8-dimensional vector containing the eight features (including a one for the constant term that models the intercept). Fit the logistic regression using maximum likelihood estimation by the command:  $glmModel < -glm(Work \sim 0 + ., data = WomenWork, family = binomial)$ . Note how I added a zero in the model formula so that R doesn't add an extra intercept (we already have an intercept term from the Constant feature). Note also that a dot (.) in the model formula means to add all other variables in the dataset as features. family = binomial tells R that we want to fit a logistic regression.

```
women <- read.csv("womenWork.dat", sep = "")
glmModel <- glm(Work ~ 0 + ., data = women, family = binomial)
summary(glmModel)</pre>
```

```
##
  glm(formula = Work ~ 0 + ., family = binomial, data = women)
##
## Deviance Residuals:
##
       Min
                 1Q
                      Median
                                   3Q
                                           Max
                      0.4391
## -2.1662 -0.9299
                               0.9494
                                         2.0582
##
## Coefficients:
##
               Estimate Std. Error z value Pr(>|z|)
## Constant
                0.64430
                           1.52307
                                     0.423 0.672274
## HusbandInc -0.01977
                           0.01590 -1.243 0.213752
## EducYears
                0.17988
                           0.07914
                                     2.273 0.023024 *
## ExpYears
                0.16751
                           0.06600
                                     2.538 0.011144 *
## ExpYears2
               -0.14436
                           0.23585
                                    -0.612 0.540489
## Age
               -0.08234
                           0.02699
                                    -3.050 0.002285 **
## NSmallChild -1.36250
                           0.38996
                                    -3.494 0.000476 ***
                           0.14172 -0.179 0.857592
## NBigChild
              -0.02543
```

```
## ---
## Signif. codes: 0 '***' 0.001 '**' 0.05 '.' 0.1 ' ' 1
##
## (Dispersion parameter for binomial family taken to be 1)
##
## Null deviance: 277.26 on 200 degrees of freedom
## Residual deviance: 222.73 on 192 degrees of freedom
## AIC: 238.73
##
## Number of Fisher Scoring iterations: 4
```

The approach above is a frequentist appraach to a model estimation. HusbandInc, ExpYears2, Age, NSmall-Child and NBigChild have a negative effect on the probability that the mother is working or not, although not all of them have significant p-values.

#### 2b) - Approximate posterior distribution

Now the fun begins. Our goal is to approximate the posterior distribution of the 8-dim parameter vector  $\beta$  with a multivariate normal distribution

$$\beta|\mathbf{y},\mathbf{X} \sim N\Big(\tilde{\beta},J_{\mathbf{y}}^{-1}(\tilde{\beta})\Big), \qquad \quad J(\tilde{\beta}) = -\frac{\partial^2 ln[p(\beta|\mathbf{y})]}{\partial \beta \partial \beta^T}\Big|_{\beta = \tilde{\beta}}$$

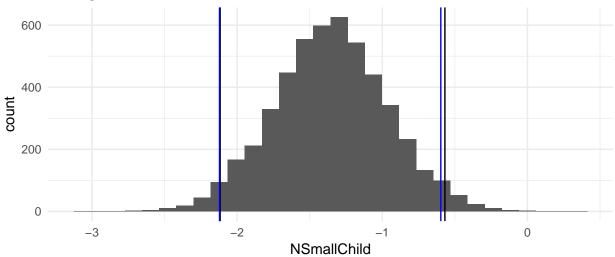
where  $\tilde{\beta}$  is the posterior mode and  $J(\tilde{\beta})$  is the observed Hessian evaluated at the posterior mode. Note that  $\frac{\partial^2 ln[p(\beta|\mathbf{y})]}{\partial\beta\beta\beta^T}$  is an 8×8 matrix with second derivatives on the diagonal and cross-derivatives  $\frac{\partial^2 ln[p(\beta|\mathbf{y})]}{\partial\beta_i\partial\beta_j}$  on the offdiagonal. It is actually not hard to compute this derivative by hand, but don't worry, we will let the computer do it numerically for you. Now, both  $\tilde{\beta}$  and  $J(\tilde{\beta})$  are computed by the optim function in R. See my code https://github.com/mattiasvillani/BayesLearnCourse/raw/master/Code/MainOptimizeSpam.zip where I have coded everything up for the spam prediction example (it also does probit regression, but that is not needed here). I want you to implement your own version of this. You can use my code as a template, but I want you to write your own file so that you understand every line of your code. Don't just copy my code. Use the prior  $\beta \sim N(0, \tau^2 I)$ , with  $\tau = 10$ .

Your report should include your code as well as numerical values for  $\tilde{\beta}$  and  $J_{\mathbf{y}}^{-1}(\tilde{\beta})$  for the WomenWork data. Compute an approximate 95 % credible interval for the variable NSmallChild. Would you say that this feature is an important determinant of the probability that a women works?

```
y <- as.vector(women[,1])
X <- as.matrix(women[, 2:ncol(women)])</pre>
covNames <- names(women) [2:ncol(women)]</pre>
nPara \leftarrow dim(X)[2]
# Prior:
tau <- 10
mu <- rep(0, nPara)
Sigma <- tau^2 * diag(nPara) # diag(nPara) creates the identity matrix
LogPostLogistic <- function(betaVect, y, X, mu, Sigma){</pre>
  nPara <- length(betaVect)
  linPred <- X%*%betaVect</pre>
  logLik <- sum(linPred*y - log(1+exp(linPred)))</pre>
  if (abs(logLik) == Inf) logLik = -20000
  logPrior <- dmvnorm(betaVect, matrix(0, nPara, 1), Sigma, log = TRUE)</pre>
  return(logLik + logPrior)
}
initVal <- as.vector(rep(0, dim(X)[2]))</pre>
logPost <- LogPostLogistic</pre>
OptimResults <- optim(initVal, logPost, gr = NULL, y, X, mu, Sigma, method = c("BFGS"),
                        control = list(fnscale=-1), hessian = TRUE)
PostMode <- OptimResults$par
postCov <- -solve(OptimResults$hessian)</pre>
names(PostMode) <- covNames</pre>
approxPostStd <- sqrt(diag(postCov))</pre>
names(approxPostStd) <- covNames</pre>
```

```
NSmallChild <- data.frame("NSmallChild" = rnorm(5000,
                                                 mean = PostMode["NSmallChild"],
                                                 sd = approxPostStd["NSmallChild"]))
confidence_intervals <- c(PostMode["NSmallChild"] - 1.96*approxPostStd["NSmallChild"],</pre>
                           PostMode["NSmallChild"] + 1.96*approxPostStd["NSmallChild"])
NSmallChild histogram <- ggplot(data = NSmallChild, aes(x = NSmallChild)) +
  geom_histogram() + ggtitle("Histogram of NSmallChild coefficient")
quantiles <- quantile(NSmallChild$NSmallChild, probs = c(0.025, 0.975))
#Simulated approach
NSmallChild_histogram <- NSmallChild_histogram + geom_vline(xintercept = quantiles[1])
NSmallChild_histogram <- NSmallChild_histogram + geom_vline(xintercept = quantiles[2])</pre>
# Theoretical approach
NSmallChild_histogram <- NSmallChild_histogram +</pre>
  geom_vline(xintercept = confidence_intervals[1], color="Blue")
NSmallChild_histogram <- NSmallChild_histogram +</pre>
  geom_vline(xintercept = confidence_intervals[2], color="Blue")
NSmallChild_histogram
```

### Histogram of NSmallChild coefficient

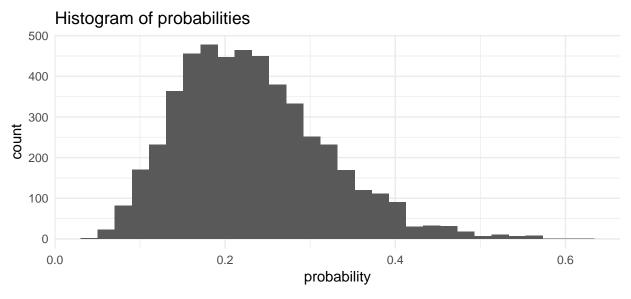


#### 2c) - Simulate from predictive distribution of the response variable

Write a function that simulates from the predictive distribution of the response variable in a logistic regression. Use your normal approximation from 2(b). Use that function to simulate and plot the predictive distribution for the Work variable for a 40 year old woman, with two children (3 and 9 years old), 8 years of education, 10 years of experience. and a husband with an income of 10.

[Hint: the R package mvtnorm will again be handy. And remember my discussion on how Bayesian prediction can be done by simulation.]

```
n <- nrow(women)</pre>
predictive_y <- function(x_data){</pre>
  betas <- rmvnorm(1, mean = PostMode, sigma = postCov)</pre>
  betas <- matrix(betas, ncol = 1)</pre>
  numerator <- exp(t(example_c)%*%betas)</pre>
  denominator <- 1 + numerator</pre>
  probability <- numerator/denominator</pre>
  return(probability)
example_c <- matrix(c("Constant" = 1, "HusbandInc" = 10,</pre>
                         "EducYears"=8, "ExpYears"=10,
                "ExpYears2"=1, "Age"=40, "NSmallChild"=1,
                 "NBigChild"=1), nrow=8, ncol = 1)
predictive_y(example_c)
##
              [,1]
## [1,] 0.1474939
probability <- c()</pre>
for (i in 1:5000){
  probability[i] <- predictive_y(example_c)</pre>
probability <- as.data.frame(probability)</pre>
ggplot(data = probability, aes(x=probability))+
  geom_histogram() + ggtitle("Histogram of probabilities")
```



If we now say that if probability is smaller than 0.5, we predict she will not work, and if probability is greater than 0.5 means she will work we get the following predictions:

```
probability[probability > 0.5] <- 1
probability[probability <= 0.5] <- 0
colnames(probability) <- c("work")

ggplot(data = probability, aes(work)) + geom_bar() +
    ggtitle("Expected outcomes according to p<0.5 is not working")</pre>
```

