

SC1_Proj

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Introduction

One of the most common types of cancer diagnosed in women is breast cancer. There are multiple tests that people are subjected to, but one of the most indicative ones is fine needle aspiration which involves extracting a sample of cells to be examined under a microscope. Multiple numerical metrics are computed from the obtained images. The aim is to use the extracted metrics to make accurate diagnoses.

The dataset consists of 569 images which have been processed as described and a total of 30 variables have been computed for each observation.

The aim of this report is to implement a number of classification algorithms, use them to obtain predictions, and compare their performances.

Exploratory analysis

```
data <- read_csv("../data/data.csv")
colnames(data)[3:32] <- c(
  "radius_m", "texture_m", "perim_m", "area_m", "smooth_m", "compact_m",
  "concav_m", "concav_pt_m", "symmetry_m", "frac_dim_m", "radius_se",
  "texture_se", "perim_se", "area_se", "smooth_se", "compact_se",
  "concav_se", "concav_pt_se", "symmetry_se", "frac_dim_se", "radius_w",
  "texture_w", "perim_w", "area_w", "smooth_w", "compact_w", "concav_w",
  "concav_pt_w", "symmetry_w", "frac_dim_w"
)
```

Check for missing values in every column.

```
colSums(is.na(data))
```

```
##      id      diagnosis      radius_m      texture_m      perim_m      area_m
##      0          0          0          0          0          0
##      smooth_m      compact_m      concav_m      concav_pt_m      symmetry_m      frac_dim_m
##      0          0          0          0          0          0
##      radius_se      texture_se      perim_se      area_se      smooth_se      compact_se
##      0          0          0          0          0          0
##      concav_se      concav_pt_se      symmetry_se      frac_dim_se      radius_w      texture_w
##      0          0          0          0          0          0
##      perim_w      area_w      smooth_w      compact_w      concav_w      concav_pt_w
##      0          0          0          0          0          0
##      symmetry_w      frac_dim_w      X33
##      0          0          569
```

```
data %<>% mutate_at(vars(diagnosis), factor)
```

```
train <- data %>% sample_frac(0.8)
test <- anti_join(data, train, by = "id")
```

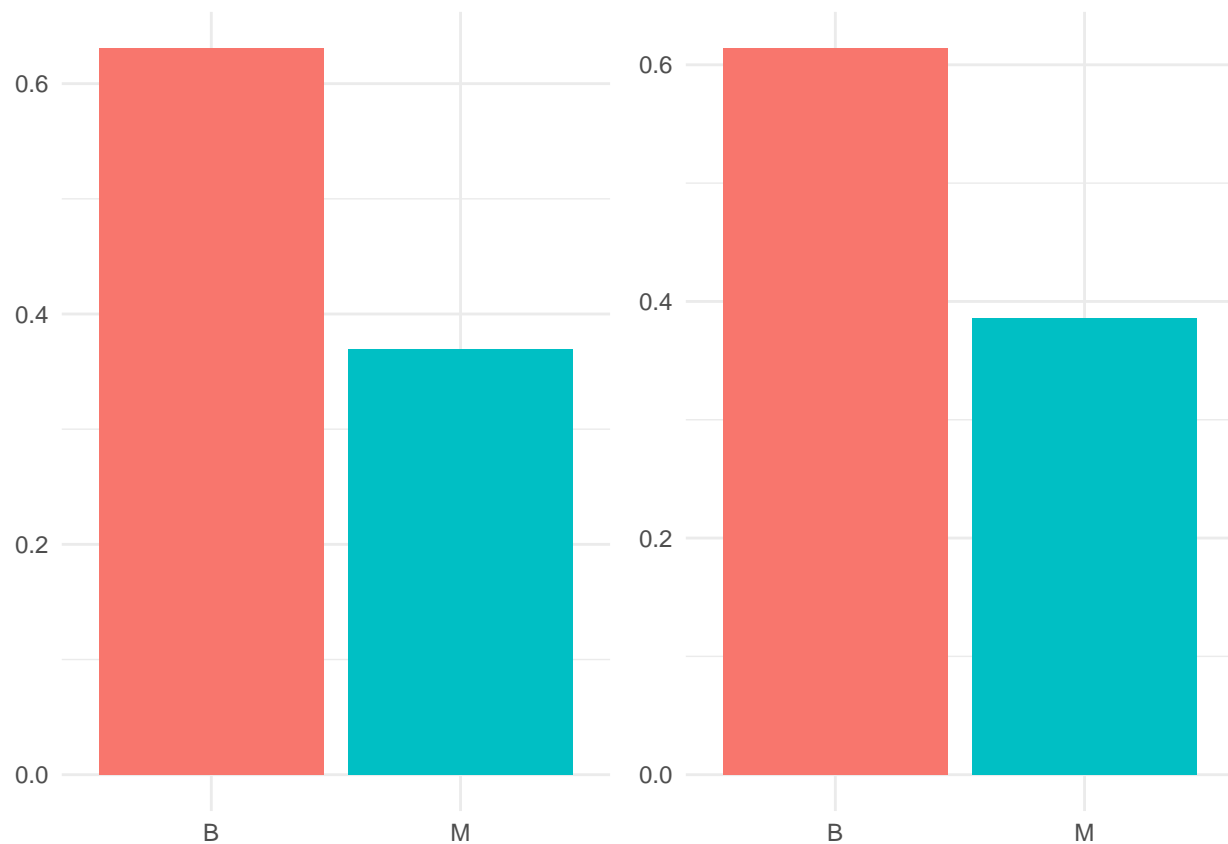
```
# need ids for later
id_train <- train$id
id_test <- test$id
```

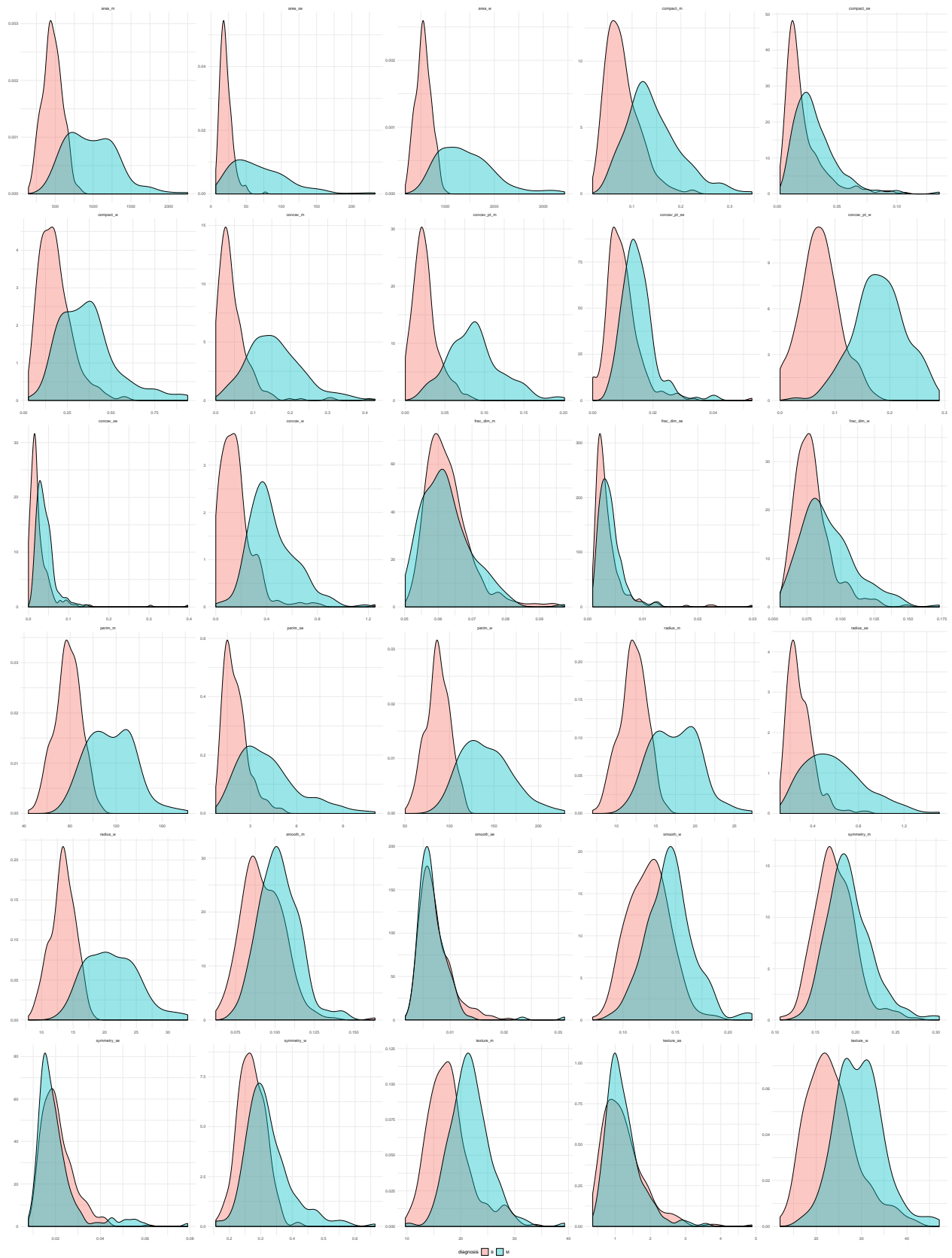
```
data %<>%
  dplyr::select(-c(id, X33))
train %<>%
  dplyr::select(-c(id, X33))
test %<>%
  dplyr::select(-c(id, X33))
```

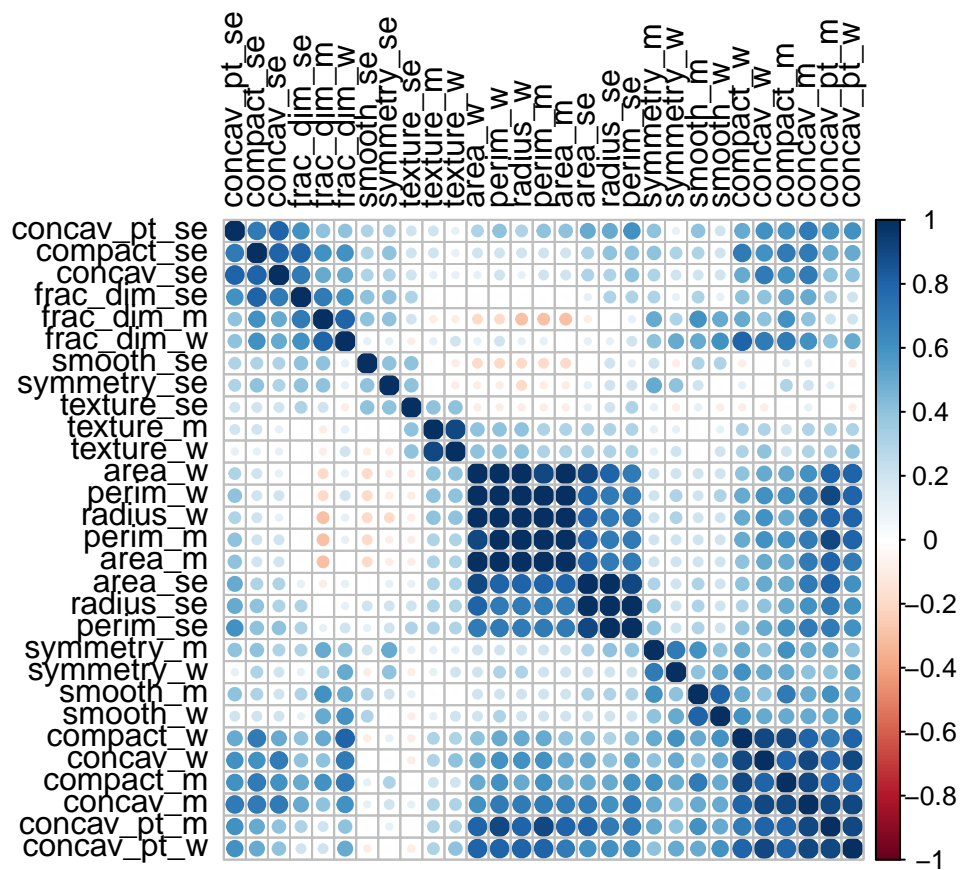
```
sum(is.na(data))
```

```
## [1] 0
```

```
training_data <- train[2:dim(train)[2]]
training_classes <- train[1]
test_data <- test[2:dim(test)[2]]
test_classes <- test[1]
```







Dimensionality Reduction and Feature Selection

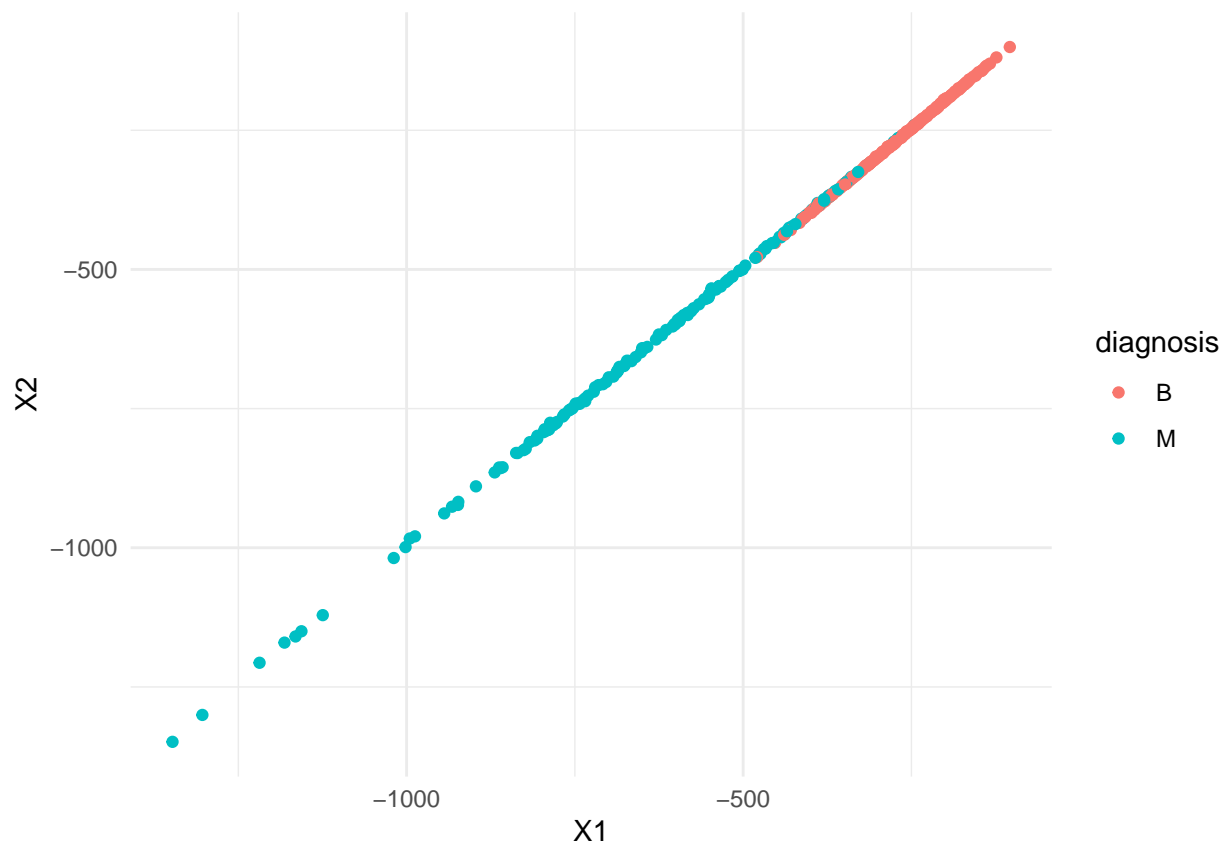
PCA

Code

```
normalise_z <- function(X) {  
  mean_cols <- colMeans(X)  
  sd_cols <- apply(X, 2, sd)  
  mean_normalised_X <- t(apply(X, 1, function(x) {  
    x - mean_cols  
  }))  
  normalised_X <- t(apply(mean_normalised_X, 1, function(x) {  
    x / sd_cols  
  }))  
  return(normalised_X)  
}  
  
pca <- function(X, number_components_keep) {  
  normalised_X <- normalise_z(X)  
  
  corr_mat <- t(normalised_X) %*% normalised_X  
  
  eigenvectors <- eigen(corr_mat, symmetric = TRUE)$vectors  
  
  reduced_data <- X %*% eigenvectors[, 1:number_components_keep]  
  relevant_eigs <- eigenvectors[, 1:number_components_keep]  
  returnds <- list(reduced_data, relevant_eigs)  
  names(returnds) <- c("reduced_data", "reduction_matrix")  
  return(returnds)  
}
```

Apply to dataset

```
pca_result <- pca(as.matrix(training_data), 2)  
pca_reduced_training_data <- data.frame(cbind(pca_result$reduced_data, training_classes))  
  
ggplot(data = pca_reduced_training_data, aes(x = X1, y = X2)) +  
  geom_point(aes(colour = diagnosis))
```



Classification

add list of methods+measure

SVM

From the application of PCA to the dataset we can see that, after reducing to 2 dimensions, the data appears to be almost linearly separable. Given this, an appropriate method of classifying the data would be to apply a soft-margin SVM to the reduced dimension data. Soft-margin SVMs solve the problem of classifying non-separable data by permitting a certain number of points to be incorrectly classified however the number and the amount they violate the constraints by must be as small as possible. After manipulating the reformulated optimisation problem we end up with the optimisation problem

$$\begin{aligned} \min_{\lambda} \quad & \frac{\bar{\lambda} X X^T \bar{\lambda}^T}{4} + \lambda^T \mathbf{1} \\ \text{such that} \quad & 0 \leq \lambda_i \leq C \\ \text{and} \quad & \sum_i^n \lambda_i y_i = 0 \end{aligned}$$

where

$$X = \begin{pmatrix} x_1^T \\ \vdots \\ x_n^T \end{pmatrix} \text{ and } \bar{\lambda} = [\lambda_1 \cdot y_1, \dots, \lambda_n \cdot y_n] \text{ and } \mathbf{1} = [1, \dots, 1] \in \mathbb{R}^n$$

For some predefined C . This is a quadratic programming problem with linear constraints which can be solved using the R package `quadprog` with the function `solve.QP`. From its documentation, this function can solve (for b) problems in the form $\min_b (-d^T b + \frac{1}{2} b^T D b)$ with the constraints that $A^T b \geq b_0$. By transforming the above problem into this format we can implement soft-margin SVM using the following code

```
train_soft_svm <- function(X, y, C) {  
  
  num_observation <- nrow(X)  
  dim_num <- ncol(X)  
  
  Dmat2 <- diag(y) * X %*% t(X) %*% diag(y)  
  diag(Dmat2) <- diag(Dmat2) + 1e-6  
  dv2 <- rep(1, num_observation)  
  
  A2 <- rbind( y, diag(num_observation))  
  A2 <- rbind(A2, -1*diag(num_observation))  
  
  bv2 <- c(c(0), rep(0, num_observation), rep(-C, num_observation) )  
  model <- solve.QP(Dmat2, dv2, t(A2), bv2, meq = 1)  
}
```

In order to recover w and b from λ we use the relationship

$$w = \sum_{i=0}^{n-1} \lambda_i x_i^T y_i$$

and

$$b = \text{mean}\left(\sum_{i=0}^k y_i - w \cdot x_i\right) \cdot \forall i. 0 < \lambda_i < C$$

Which can be made as functions in R as so:

```

calculate_b <- function(w, X, y, a, C) {
  ks <- sapply(a, function(x) {
    return(x > 0 && x < C)
  })
  indices <- which(ks)
  sum_bs <- 0
  for (i in indices) {
    sum_bs <- sum_bs + (y[i] - w %*% X[i, ])
  }
  return(sum_bs / length(indices))
}

recover_w <- function(a, y, X) {
  colSums(diag(a) %*% diag(y) %*% X)
}

```

From the parameters we can recover the equation of the line corresponding to the decision boundary which can later be used for plotting

```

soft_margin_svm_plotter <- function(w, b) {
  plotter <- function(x) {
    return(1 / w[2] * -(b + (w[1] * as.numeric(x))))
  }
  return(plotter)
}

```

TODO: prediction function

We are now able to define a function which first embeds the vector in the reduced space and then predicts the class based upon the prediction function produced by the parameters found by the SVM. Below is code that will do the following based upon a package written for this assignment found [here](#)

```

model <- svm(
  X = pca_result$reduced_data,
  classes = numeric_training_labels,
  C = 100000, margin_type = "soft",
  kernel_function = linear_kernel,
  feature_map = linear_basis_function
)

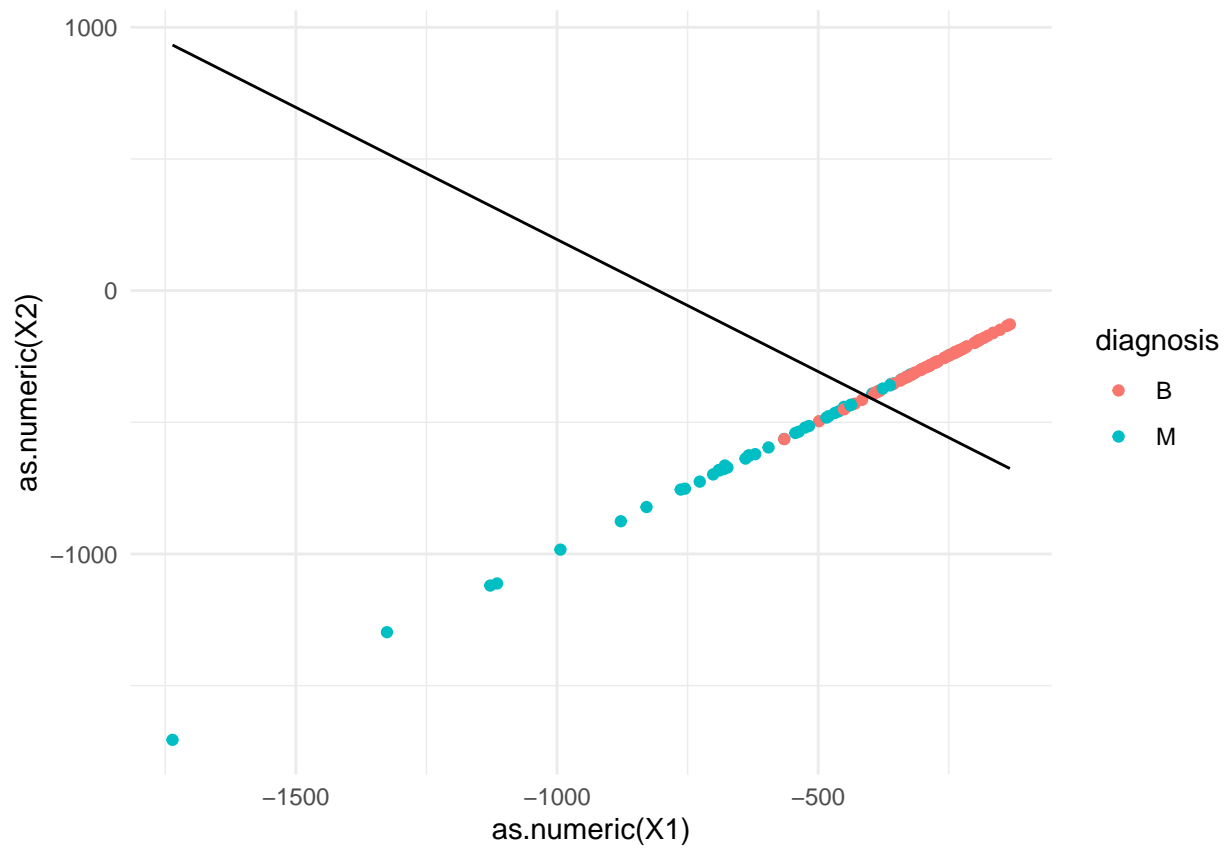
reduced_prediction_fn <- model$prediction_function

pca_reduced_prediction_fn <- function(x) {
  p <- x %*% pca_result$reduction_matrix
  reduced_prediction_fn(t(p))
}

pca_reduced_test_data <- t(apply(as.matrix(test_data), 1, function(x) x %*%
                                pca_result$reduction_matrix))

```

When running the trained SVM prediction function on the test set we achieve 86.8421053 %. We can plot this code as below



Naive Bayes

Mathematical setting

Let y be the class label that we want to assign to an observation $\mathbf{x} = (x_1, \dots, x_d)$, where x_1, \dots, x_d are the features. The probability of an observation having label y is given by Bayes rule,

$$P(y|x_1, \dots, x_d) = \frac{P(x_1, \dots, x_d|y)P(y)}{P(x_1, \dots, x_d)} \\ \propto P(x_1, \dots, x_d|y)P(y).$$

The prior class probability $P(y)$ can be easily obtained by the proportion of observation that are in the given class.

The main assumption is that every feature is conditionally independent given the class label y . The reason why this classifier is called *naïve* is that very often this assumption is not actually realistic.

This assumption simplifies the posterior to

$$P(y|x_1, \dots, x_d) \propto P(y) \prod_{i=1}^d P(x_i|y).$$

There are various types of Naive Bayes classifiers based on the type of features. In our case, since we have continuous variables we assume that all features are normally distributed. Therefore, the conditional probabilities can be calculated as

$$P(x_i|y) = \frac{1}{\sqrt{2\pi\sigma_y^2}} \exp\left(-\frac{(x_i - \mu_y)^2}{2\sigma_y^2}\right)$$

Finally, to assign the class to an observation we use the Maximum A Posteriori decision rule. For every observation, we pick the class the has the highest probability

$$y = \underset{y}{\operatorname{argmax}} P(y) \prod_{i=1}^d P(x_i|y).$$

Implementation

Here are some code snippets just to illustrate how these theoretical aspects are implemented. The full code can be found in the package.

The observations are stored as rows in X and the corresponding class labels are entires in the column matrix y .

First we calculate the prior class probabilities based on the number of observations in each class.

```
n <- dim(X)[1]
d <- dim(X)[2]
classes <- sort(unique(y)[, 1])
k <- length(classes)

prior <- rep(0, k)
for (i in 1:k) {
  prior[i] <- sum(y == classes[i]) / n
}
```

Then we create an array of the mean and sd of the data split by classes and features.

```
summaries <- array(rep(1, d * k * 2), dim = c(k, d, 2))
for (i in 1:k) {
  X_k <- X[which(y == (i - 1)), ]
  summaries[i, , 1] <- apply(X_k, 2, mean)
  summaries[i, , 2] <- apply(X_k, 2, sd)
}
```

Finally, the predictions are obtained by taking the largest posterior class probability. Note that in order to avoid underflow, we take the maximum of the *log* posterior class probabilities.

```
probs <- matrix(rep(0, n * k), nrow = n)
for (obs in 1:n) {
  for (class in 1:k) {
    class_prob <- log(prior[class])
    for (feat in 1:d) {
      mu <- summaries[class, feat, 1]
      sd <- summaries[class, feat, 2]
      cond <- dnorm(x_new[obs, feat], mu, sd, log = TRUE)
      class_prob <- class_prob + cond
    }
    probs[obs, class] <- class_prob
  }
}

pred <- apply(probs, 1, which.max)
```

Fit model to dataset

Fitting the model to the full dataset and the reduced dataset we obtain the following accuracies.

full	0.9386
reduced	0.8684

Logistic Regression

Mathematical Setting

Let $Y_i \mid \mathbf{x}_i \sim \text{Bernoulli}(p_i)$ with $p_i = \sigma(\mathbf{x}_i^\top \boldsymbol{\beta})$ where $\sigma(\cdot)$ is the **sigmoid function**. The joint log-likelihood is given by

$$\ln p(\mathbf{y} \mid \boldsymbol{\beta}) = \sum_{i=1}^n y_i \ln(p_i) + (1 - y_i) \ln(1 - p_i) = - \sum_{i=1}^n \ln(1 + \exp((1 - 2y_i)\mathbf{x}_i^\top \boldsymbol{\beta}))$$

Maximum Likelihood Estimation

Maximizing the likelihood is equivalent to minimizing the negative log-likelihood. Minimizing the negative log likelihood is equivalent to solving the following optimization problem

$$\min_{\boldsymbol{\beta}} \sum_{i=1}^n \ln(1 + \exp((1 - 2y_i)\mathbf{x}_i^\top \boldsymbol{\beta}))$$

Maximum-A-Posteriori and Ridge Regularization

We can introduce an isotropic Gaussian prior on **all** the coefficients $p(\boldsymbol{\beta}) = N(\mathbf{0}, \sigma_\beta^2 I)$. Maximizing the posterior $p(\boldsymbol{\beta} \mid \mathbf{y})$ is equivalent to minimizing the negative log posterior $-\ln p(\boldsymbol{\beta} \mid \mathbf{y})$ giving

$$\min_{\boldsymbol{\beta}} \sigma_\beta^2 \sum_{i=1}^n \ln(1 + \exp((1 - 2y_i)\mathbf{x}_i^\top \boldsymbol{\beta})) + \frac{1}{2} \boldsymbol{\beta}^\top \boldsymbol{\beta}$$

Gradient Ascent

Maximum Likelihood updates take the form

$$\boldsymbol{\beta}_{k+1} \leftarrow \boldsymbol{\beta}_k + \gamma X^\top (\mathbf{y} - \sigma(X\boldsymbol{\beta}_k))$$

whereas for MAP we have

$$\boldsymbol{\beta}_{k+1} \leftarrow \boldsymbol{\beta}_k + \gamma_k [\sigma_\beta^2 X^\top (\mathbf{y} - \sigma(X\boldsymbol{\beta}_k)) - \boldsymbol{\beta}_k]$$

Newton's Method for Maximum Likelihood Estimation

The iterations are as follows, where for stability one can add a learning rate α , which is in practice often set to $\alpha = 0.1$.

$$\boldsymbol{\beta}_{k+1} \leftarrow \boldsymbol{\beta}_k + \alpha (X^\top DX)^{-1} X^\top (\mathbf{y} - \sigma(X\boldsymbol{\beta}_k))$$

In practice we would solve the corresponding system for \mathbf{d}_k

$$(X^\top DX)\mathbf{d}_k = \alpha X^\top (\mathbf{y} - \sigma(X\boldsymbol{\beta}_k))$$

and then perform the update

$$\boldsymbol{\beta}_{k+1} \leftarrow \boldsymbol{\beta}_k + \mathbf{d}_k$$

Newton's Method for Maximum-A-Posteriori

The update takes the form

$$\boldsymbol{\beta}_{k+1} \leftarrow \boldsymbol{\beta}_k + \alpha [\sigma_\beta^2 X^\top DX + I]^{-1} (\sigma_\beta^2 X^\top (\mathbf{y} - \sigma(X\boldsymbol{\beta}_k)) - \boldsymbol{\beta}_k)$$

Implementation

First, we need to add a column of 1s to the design matrix so that we can fit the bias coefficient.

```
Xtrain <- as.matrix(cbind(1, training_data))
Xtest  <- as.matrix(cbind(1, test_data))
```

Maximum a Posteriori

We implement BFGS, Newton's Method and Gradient Ascent.

```
# MAP, BFGS
map_bfgs <- logistic_regression(Xtrain, training_classes, cost = "MAP",
                               method = "BFGS")
yhat_map_bfgs <- predict(map_bfgs, Xtest)
acc_map_bfgs <- calc_accuracy(test_classes, yhat_map_bfgs)
# MAP, NEWTON
map_nm <- logistic_regression(Xtrain, training_classes, cost = "MAP",
                             method = "NEWTON", niter = 250)
yhat_map_nm <- predict(map_nm, Xtest)
acc_map_nm <- calc_accuracy(test_classes, yhat_map_nm)
# MAP, GRADIENT ASCENT
map_ga <- logistic_regression(Xtrain, training_classes, cost = "MAP",
                             method = "GA", niter = 1000)
yhat_map_ga <- predict(map_ga, Xtest)
acc_map_ga <- calc_accuracy(test_classes, yhat_map_ga)
```

Maximum Likelihood Estimation

Similarly, we also implement the same algorithms for Maximum Likelihood Estimation.

```
# MLE, BFGS
mle_bfgs <- logistic_regression(Xtrain, training_classes, cost = "MLE",
                               method = "BFGS")
yhat_mle_bfgs <- predict(mle_bfgs, Xtest)
acc_mle_bfgs <- calc_accuracy(test_classes, yhat_mle_bfgs)
# MLE, NEWTON
mle_nm <- logistic_regression(Xtrain, training_classes, cost = "MLE",
                             method = "NEWTON", niter = 250)
yhat_mle_nm <- predict(mle_nm, Xtest)
acc_mle_nm <- calc_accuracy(test_classes, yhat_mle_nm)
# MLE, GRADIENT ASCENT
mle_ga <- logistic_regression(Xtrain, training_classes, cost = "MLE",
                             method = "GA", niter = 1000)
yhat_mle_ga <- predict(mle_ga, Xtest)
acc_mle_ga <- calc_accuracy(test_classes, yhat_mle_ga)
```

Comparing Cost Functions and Optimization Methods

Below we can see the accuracy of the different optimization methods (BFGS, Newton's method and Gradient Ascent) on the different cost functions (MAP or MLE).

```
# put everything together into a nice table
results_matrix <- matrix(c(
  acc_mle_bfgs, acc_mle_nm, acc_mle_ga,
  acc_map_bfgs, acc_map_nm, acc_map_ga
),
```

```
dimnames = list(c("BFGS", "NM", "GA"), c("MLE", "MAP")),
nrow = 3, ncol = 2
)
results <- data.frame(results_matrix)
kable(results)
```

	MLE	MAP
BFGS	0.9736842	0.9473684
NM	0.9385965	0.9473684
GA	0.8859649	0.9122807

Random-Walk Metropolis-Hastings Implementation on Reduced Data

Next, we can define a function that performs Random Walk Metropolis Hastings with a normal proposal distribution. To make it more efficient we can work with the log posterior and change the decision rule. In addition, we can pre-calculate all the normal and uniform samples and just access them later.

```
rwmh_multivariate_log <- function(start, niter, logtarget, vcov, thinning, burnin){
  # Set current z to the initial point and calculate its log target to save computations
  z <- start      # It's a column vector
  pz <- logtarget(start)
  # create vector deciding iterations where we record the samples
  store <- seq(from=(1+burnin), to=niter, by=thinning)
  #n_samples <- (niter - burnin) %% thinning
  # Generate matrix containing samples. Initialize with the starting value
  samples <- matrix(0, nrow=length(store), ncol=nrow(start))
  samples[1, ] <- start
  # Generate uniform random numbers in advance, to save computation. Log them.
  log_u <- log(runif(niter))
  # Proposal is a multivariate standard normal distribution. Generate samples and
  # later on use linearity property of Gaussian distribution
  vcov <- diag(nrow(start)) %*% vcov
  normal_shift <- mvrnorm(n=niter, mu=c(0,0,0), Sigma=vcov)
  for (i in 2:niter){
    # Sample a candidate
    candidate <- z + normal_shift[i, ]
    # calculate log target of candidate and store it in case it gets accepted
    p_candidate <- logtarget(candidate)
    # use decision rule explained in blog posts
    if (log_u[i] <= p_candidate - pz){
      # Accept!
      z <- candidate
      pz <- p_candidate
    }
    # Finally add the sample to our matrix of samples
    if (i %in% store) samples[which(store==i), ] <- z
  }
  # Finally add the sample to our matrix of samples
  if (i %in% store) samples[which(store == i), ] <- z
  return(samples)
}
```

Now we can add a column of 1s to the reduced dataset created by PCA so that we can run Logistic Regression

on the reduced data.

```
Xrwmh <- cbind(1, as.matrix(pca_reduced_training_data[, c(1, 2)]))
```

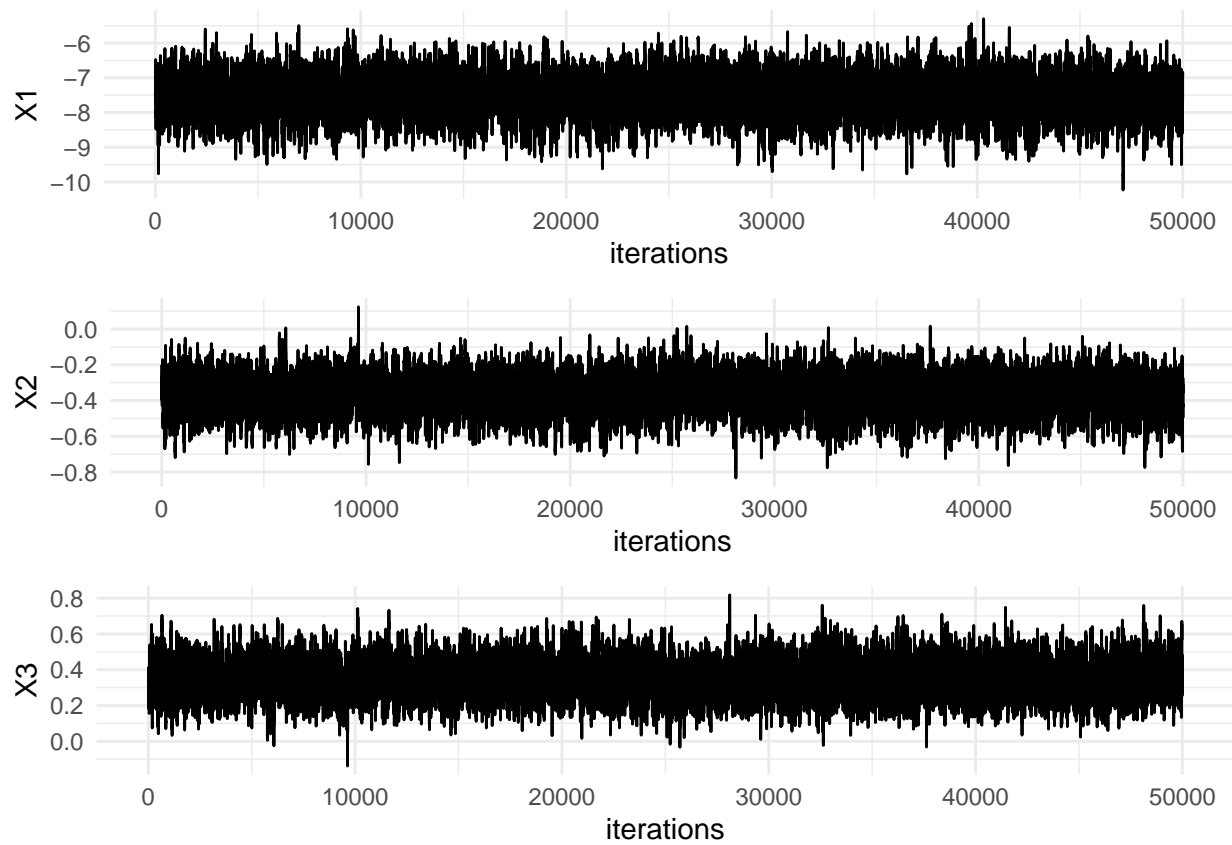
We run logistic regression using the BFGS optimization method on MAP. Since we need the Hessian matrix for sampling later on, we simply use the `optim` function on the unnormalized version of the posterior distribution for logistic regression.

```
# up to normalizing constant
log_posterior_unnormalized <- function(beta) {
  log_prior <- -0.5 * sum(beta^2)
  log_likelihood <- -sum(log(1 + exp((1 - 2 * training_classes) * (Xrwmh %*% beta))))
  return(log_prior + log_likelihood)
}
# To start the algorithm more efficiently, start from MAP estimate
optim_results <- optim(c(0, 0, 0), function(x) -log_posterior_unnormalized(x),
  method = "BFGS", hessian = TRUE)
start <- matrix(optim_results$par)
# Use inverse of approximate hessian matrix as vcov of normal proposal
vcov <- solve(optim_results$hessian)
```

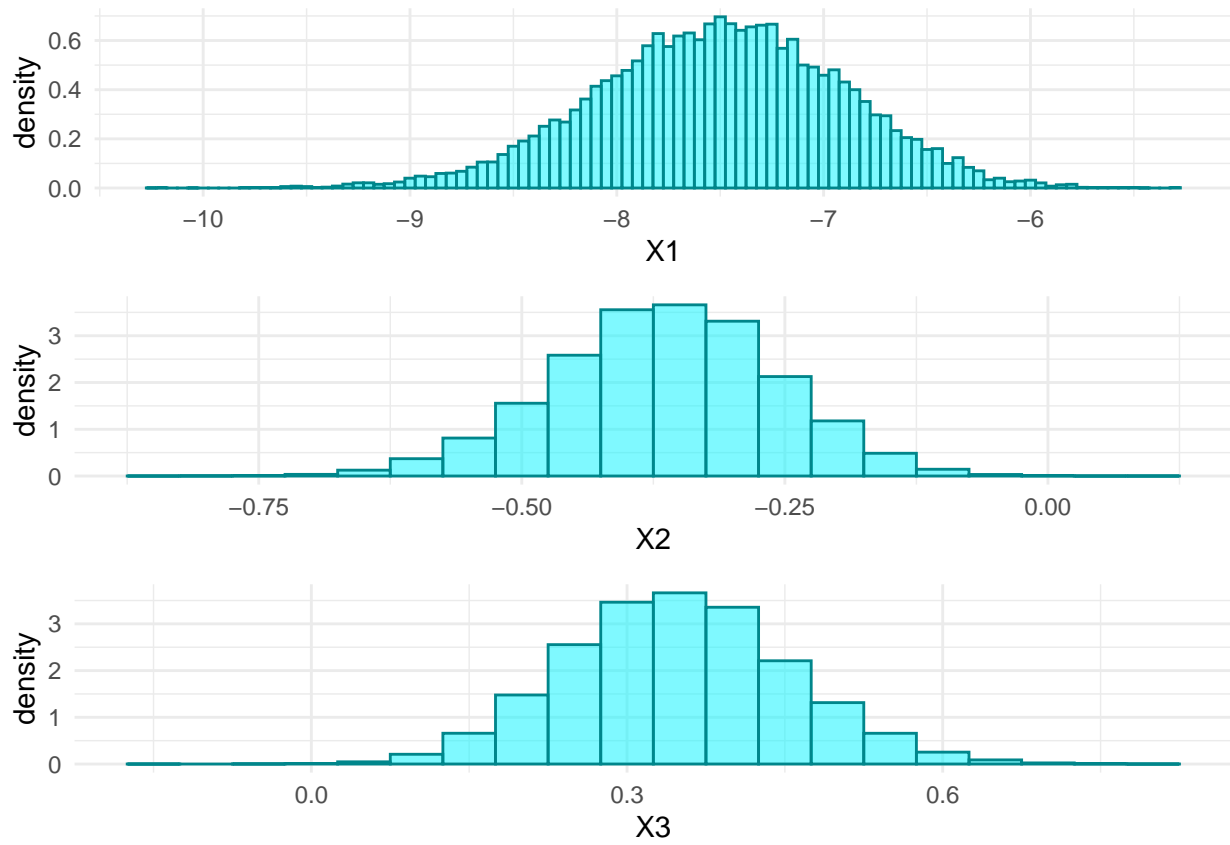
We're now ready to start sampling starting at the MAP estimate and using, as a proposal, the normal distribution with variance-covariance matrix given by the inverse of the approximated hessian matrix coming from the optimization routine.

```
samples <- rwmh_multivariate_log(start, niter=50000, log_posterior_unnormalized,
  vcov, thinning=1, burnin=0)
```

We can look at the trace plots and notice how the chain is mixing quickly, signalling a good exploratory behavior.

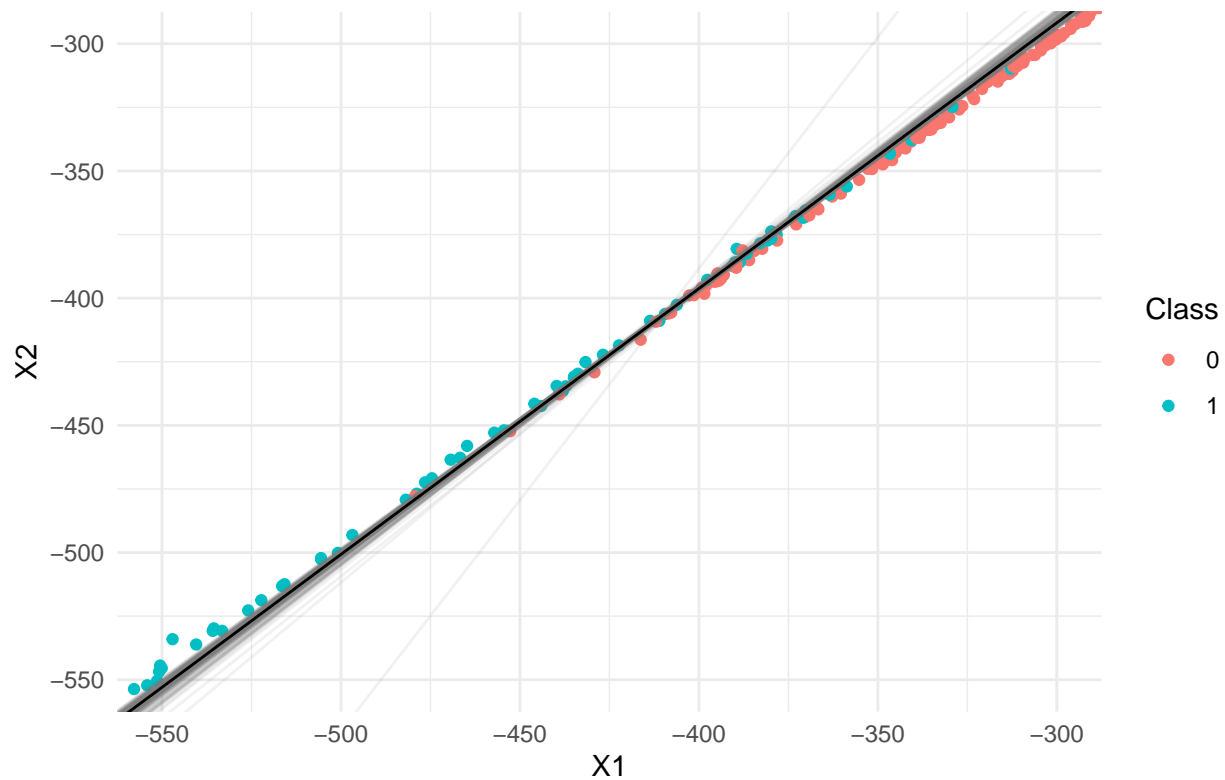


Plotting the histograms of the samples for each coordinate of the parameter vector shows that RWMH is indeed sampling correctly.



The next thing to do is to plot the decision boundary found by BFGS together with the sampled lines.

Sample Decision Boundaries



Finally, we can look at the performance of logistic regression on this reduced dataset. As a decision rule we just use a threshold.

```
Xtest_embedded <- cbind(1, as.matrix(embedded_test_data[, c(1, 2)]))
lr_embedded_preds <- round(1.0 / (1.0 + exp(-Xtest_embedded %*% start)))
calc_accuracy(test_classes, lr_embedded_preds)
```

```
## [1] 0.9122807
```

Conclusion

```
# merge all predictions
id <- seq(length(id_test))
all_pred <- cbind(id, numeric_test_labels, pred_naive, pred_naive_pca, pred_svm, yhat_map_bfgs, yhat_map_ga, yhat_map_nm, yhat_mle_bfgs, yhat_mle_ga, yhat_mle_nm)
all_pred[all_pred == -1] <- 0
all_pred %<>% as.data.frame()
colnames(all_pred) <- c('id', 'actual', 'naive', 'naive_red', 'SVM', 'map_bfgs', 'map_ga', 'map_nm', 'mle_bfgs', 'mle_ga', 'mle_nm')

confusion_plot <- function(actual, predicted) {
  confusion_matrix <- as.data.frame(table(actual, predicted))
  g <- ggplot(confusion_matrix, aes(x = actual, y = predicted)) +
    geom_tile(aes(fill = Freq)) +
    geom_text(aes(label = sprintf("%1.0f", Freq)), color = "white", fontface = "bold") +
    labs(x = "Actual class", y = "Predicted class") +
    theme_minimal()
  return(g)
}
```

Visualize which are the observations that the models missclassify.

```
all_pred %>%
  mutate_at(vars(-c(id, actual)), funs(==actual)) %>%
  dplyr::select(-'actual') %>%
  melt(id='id') %>%
  ggplot(aes(x = id, y = variable, fill = value)) +
  geom_raster() +
  theme_minimal()
```

