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 involes 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)
```

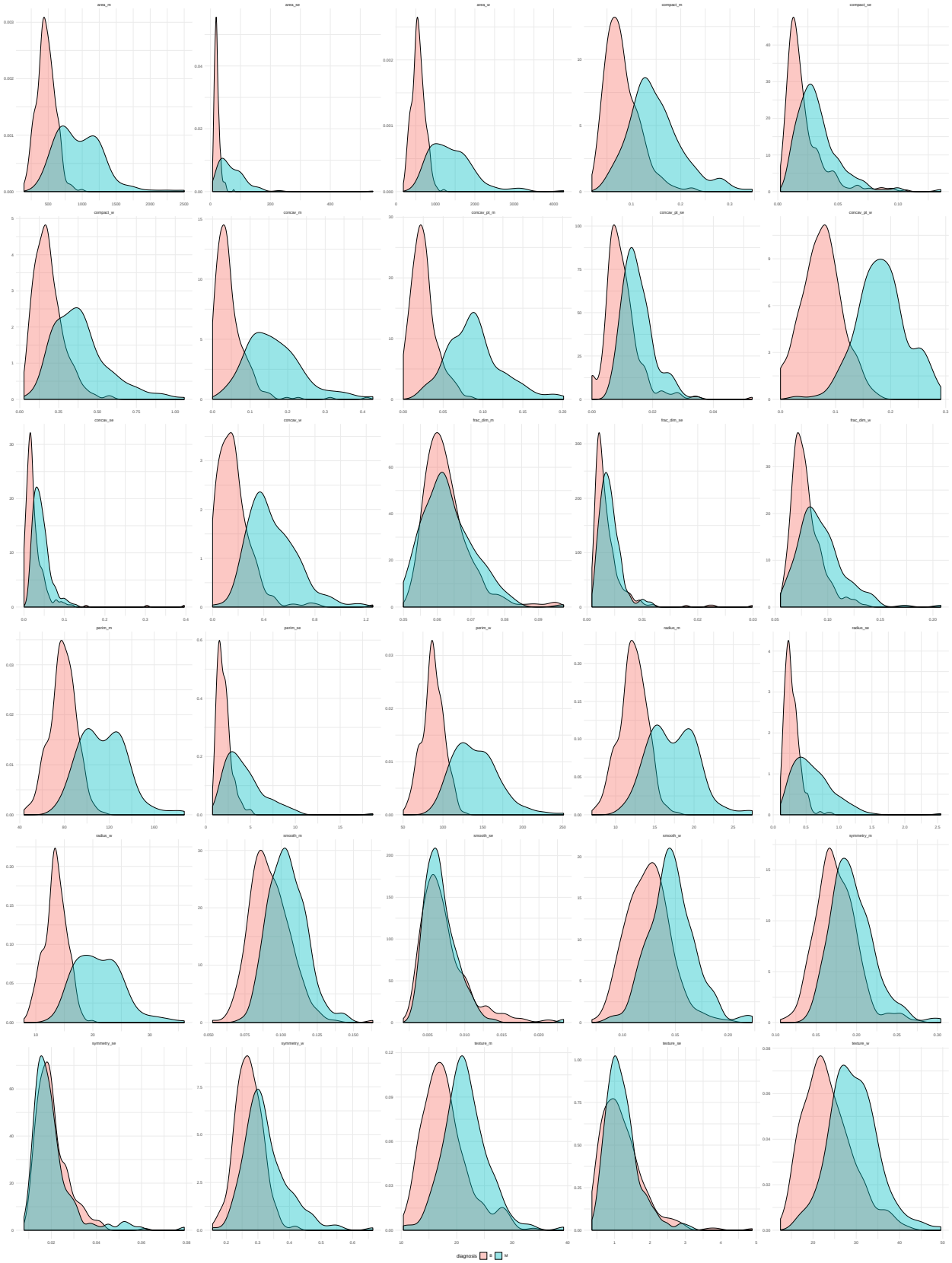
```
train <- data %>% sample_frac(0.8)
test <- anti_join(data,train, by='id')

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

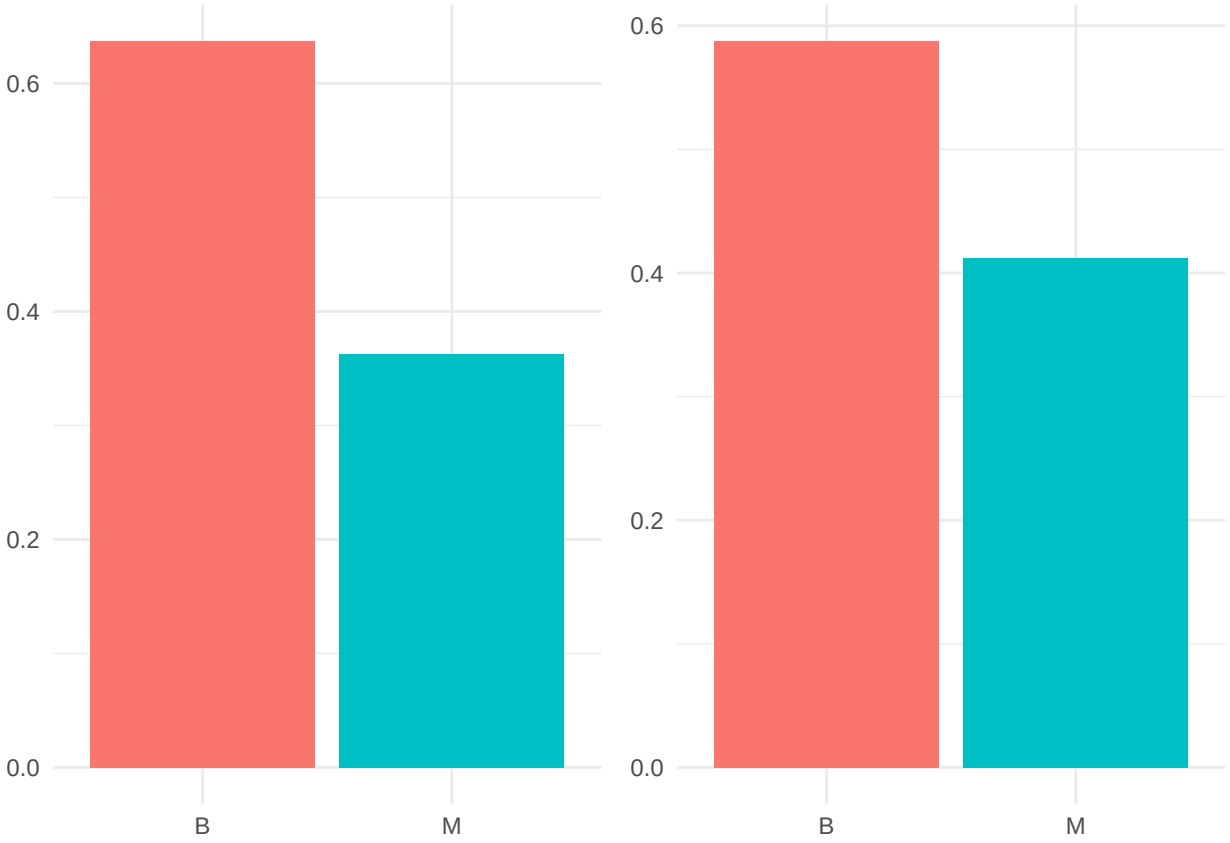
```
data %<>%
  dplyr::select(-c(id, X33))
train %<>%
  dplyr::select(-c(id, X33))
test %<>%
  dplyr::select(-c(id, X33))
```

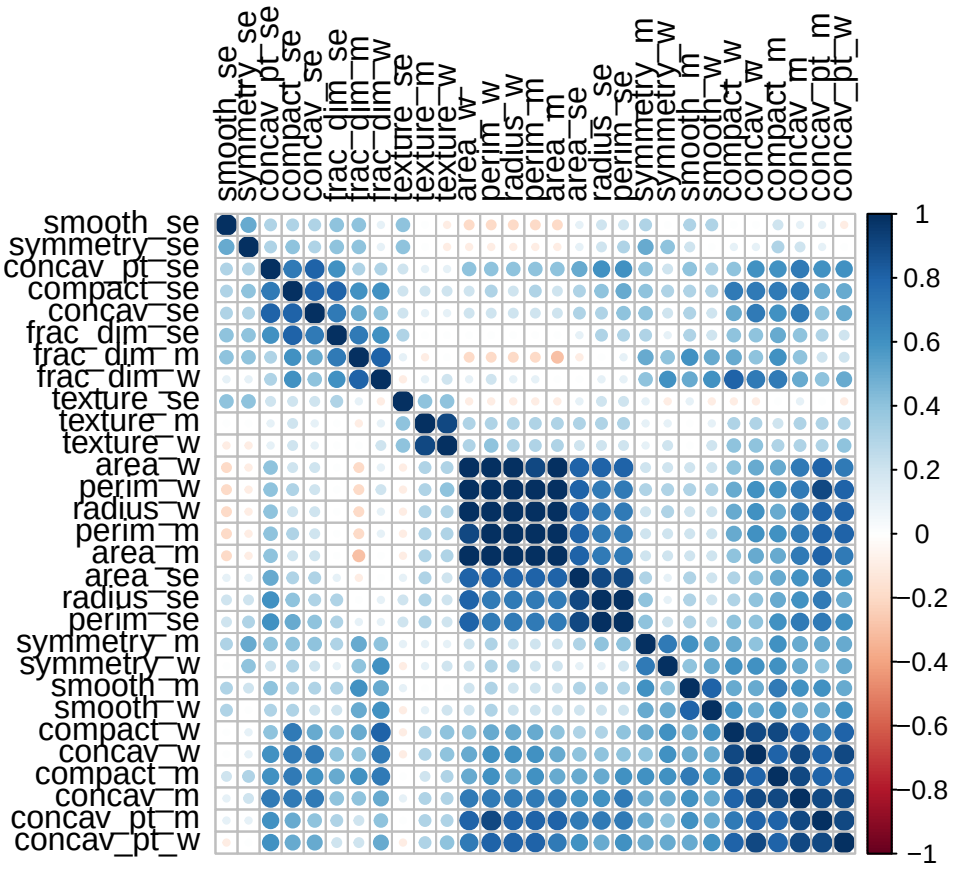
```
sum(is.na(data))
```

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

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


area_m
area_se
area_w
compact_m
compact_se
compact_w
concav_m
concav_pt_m
concav_pt_se
concav_pt_w
concav_se
concav_w
frac_dim_m
frac_dim_se
frac_dim_w
perim_m
perim_se
perim_w
radius_m
radius_se
radius_w
smooth_m
smooth_se
smooth_w
symmetry_m
symmetry_se
symmetry_w
texture_m
texture_se
texture_w
diagnosis B M


0.6
0.4
0.2
0.0
B
M
0.6
0.4
0.2
0.0
B
M


smooth_se
symmetry_se
concav_pt_se
compact_se
concav_se
frac_dim_se
frac_dim_m
frac_dim_w
texture_se
texture_m
texture_w
area_w
perim_w
radius_w
perim_m
area_m
area_se
radius_se
perim_se
symmetry_m
symmetry_w
smooth_m
smooth_w
compact_w
concav_w
compact_m
concav_m
concav_pt_m
concav_pt_w
1
0.8
0.6
0.4
0.2
0
−0.2
−0.4
−0.6
−0.8
−1

Dimensionality Reduction and Feature Selection

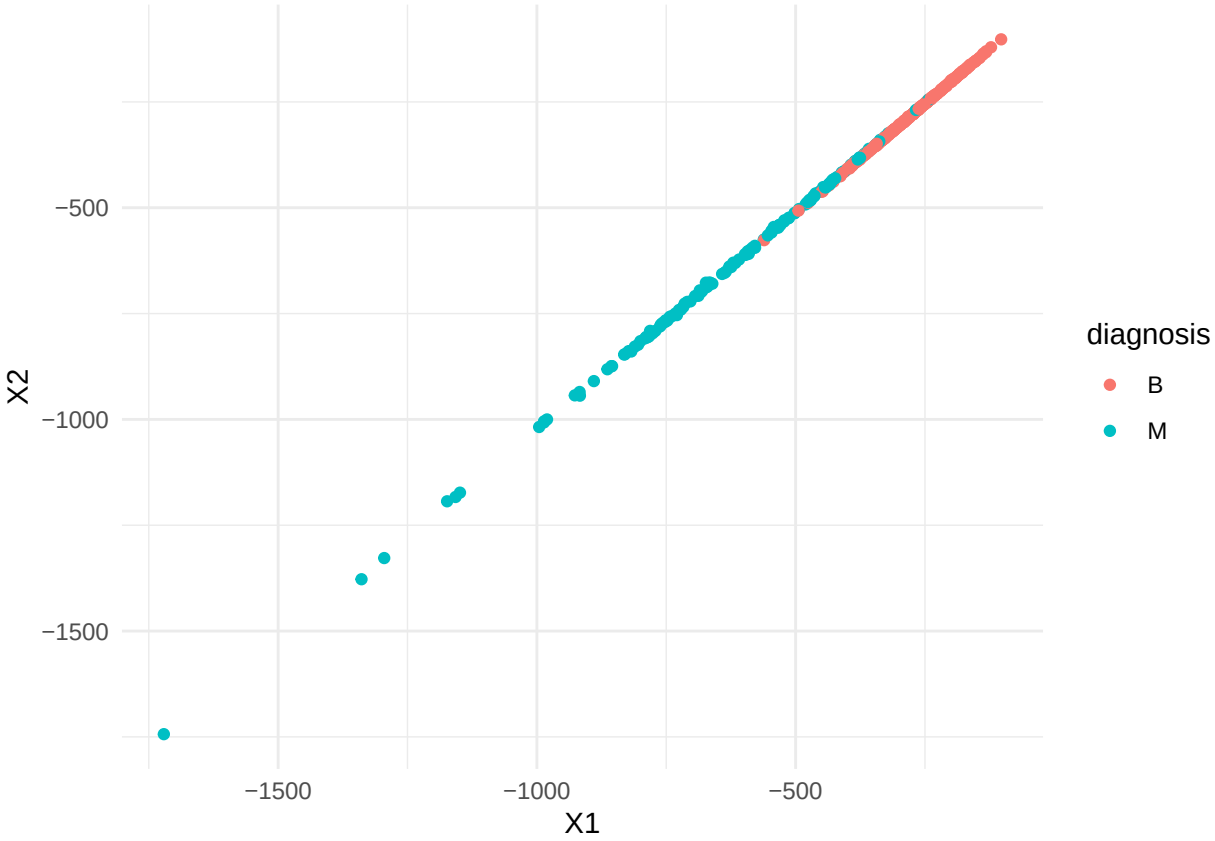
PCA

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))
```



- Correlation Feature Selection
- LDA

Classification

add list of methods+measure

SVM

To solve the problem of finding a SVM like classifier for non-separable data we must permit a certain number of points to violate the boundaries set however this number and the amount they violate the constraints by must be as small as possible. To formulate this we introduce a variable ϵ_i for each data point into the objective functions and the constraints leading to the optimisation problem:

$$\min_{w,\epsilon_i} \frac{1}{2} w^T w + C \sum_{i=0}^{n} \epsilon_i$$
$$\text{such that } w \cdot x_i + b + \epsilon_i > 1 \text{ if } y_i = 1$$
$$\text{and } w \cdot x_i + b + \epsilon_i < -1 \text{ if } y_i = -1$$

Note that we have swapped the sign of the b term in the equation for the hyperplane because I implemented it this way before realising they were different and am lazy.

As the above problem is convex (as it is quadratic) and Slater's condition holds then strong duality holds and we can take the Lagrangian of the optimisation problem and consider the result of the KKT conditions. By doing so we can reformulate the optimisation problem as the dual problem:

$$\min_{\lambda} \frac{\overline{\lambda} X X^T \overline{\lambda^T}}{4} + \lambda^T \mathbf{1}$$
$$\text{such that } 0 \leq \lambda_i \leq C$$
$$\text{and } \sum_{i}^{n} \lambda_i y_i = 0$$

where

$$X = \begin{pmatrix} x_1 \\ \vdots \\ x_n \end{pmatrix} \text{ and } \overline{\lambda} = [\lambda_1 \cdot y_i, ..., \lambda_n \cdot y_n] \text{ and } \mathbf{1} = [1, ..., 1] \in \mathbb{R}^{\ltimes}$$

As before we have to massage this optimisation problem into one that can be solved using `solve.QP`. In this formulation

$$d = \mathbf{1}$$

and

$$D = \begin{pmatrix} y_1 & 0 & ... & 0 \\ 0 & y_2 & ... & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & ... & y_n \end{pmatrix} X X^T \begin{pmatrix} y_1 & 0 & ... & 0 \\ 0 & y_2 & ... & 0 \\ \vdots & \vdots & \ddots & \vdots \\ 0 & 0 & ... & y_n \end{pmatrix}$$

A and b_0 require slightly more manipulation this time around with

$$A = \begin{pmatrix} y_1 & y_2 & ... & y_n \\ & I & & \\ & -I & & \end{pmatrix}$$

and

$$b_0 = \begin{pmatrix} 0 \\ \mathbf{0} \\ -\boldsymbol{C} \end{pmatrix}$$

where

$$\mathbf{0} = [0, ..., 0]^T \in \mathbb{R}^n$$

and

$$\boldsymbol{C} = [C, ..., C]^T \in \mathbb{R}^n$$

The code for this applied to the non-separable data can be found below.

```
C <- 1

X <- as.matrix(combined_class)[,1:2]
y <- as.matrix(combined_class)[,3]
Dmat2 <- diag(y) * X %*% t(X) %*% diag(y)
diag(Dmat2) <- diag(Dmat2) + 1e-11
dv2 <- rep(1, 30)

A2 <- rbind( y,diag(30))
A2 <- rbind(A2, -1*diag(30))

bv2 <- c(c(0), rep(0, 30), rep(-C, 30) )
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

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

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)
}
```

We can see the results of using the dual regression below

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

```
factor_to_label <- function(x)  {
  if(as.character(x) == "M")  {
    return(1)
  }
  else {
    return(-1)
  }
}
```

```
label_to_factor <- function(x) {
  if(x == 1) {
    return(as.factor("M"))
  }
  else{
    return(as.factor("B"))
  }
}
numeric_test_labels <- apply(test_classes, 1, factor_to_label)
numeric_training_labels <- apply(training_classes, 1, factor_to_label)
```

Use PCA then do SVM

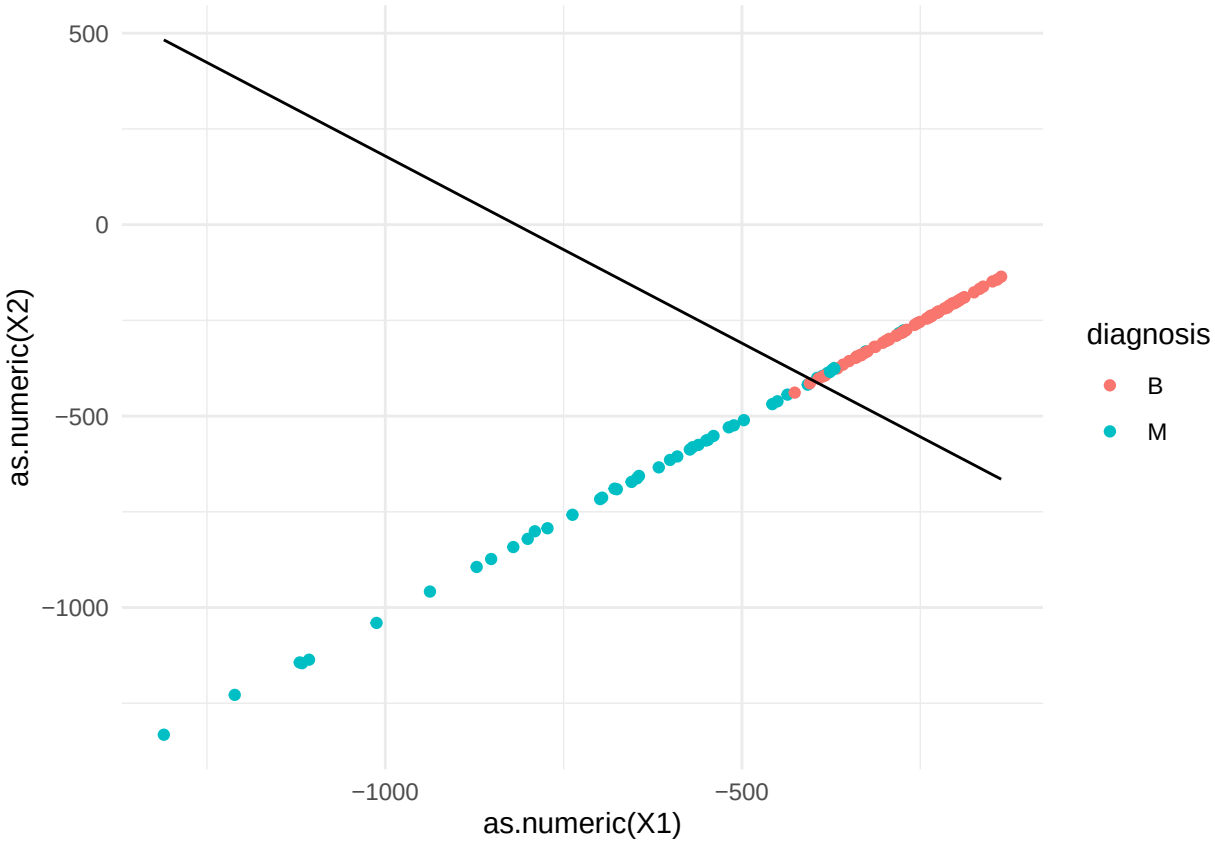
```
model <- svm(X=pca_result$reduced_data,
             classes=numeric_training_labels,
             C=100000, margin_type='soft',
             kernel_function = linear_kernel,
             feature_map = linear_basis_function)


reduced_prediction_fn <- model$prediction_function

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

```
pred_svm <- apply(as.matrix(test_data),1, pca_reduced_prediction_fn)
accuracy_calc(numeric_test_labels, pred_svm)
```

```
## [1] 89.47368
```

```
svm_plotter <- soft_margin_svm_plotter(model$params$w, model$params$b)
embedded_test_data <- data.frame(cbind(as.matrix(test_data) %*% pca_result$reduction_matrix), test_class
```

```
ggplot(embedded_test_data, aes(x=as.numeric(X1), y=as.numeric(X2))) +
  geom_point(aes(colour=diagnosis)) +
  stat_function(fun=svm_plotter)
```



Naive Bayes

Mathematical setting

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

$$\begin{aligned} P(y|x_1, \cdots, x_d) &= \frac{P(x_1, \cdots, x_d|y_k)P(y)}{P(x_1, \cdots, x_d)} \\ &\propto P(x_1, \cdots, x_d|y_k)P(y). \end{aligned}$$

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 *naive* is that very often this assumption is not actually realistic.

This assumption simplifies the posterior to

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

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

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

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 clasess 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

```
levels(training_classes$diagnosis) <- c(0,1)
training_classes %<>% as.matrix
mode(training_classes) <- 'numeric'

levels(test_classes$diagnosis) <-c(0,1)
test_classes %<>% as.matrix
mode(test_classes) <- 'numeric'
```

Fit the Naive Bayes model to the data, calculate predictions and check the accuracy using.

```
model_naive <- naive_bayes(training_data,training_classes)

pred_naive <- predict(model_naive,as.matrix(test_data))

# confusion_plot(test_classes,pred_naive)

calc_accuracy <- function(ytest, yhat) sum(drop(yhat) == drop(ytest)) / length(drop(ytest))

acc_naive <- calc_accuracy(test_classes,pred_naive)
acc_naive
```

```
## [1] 0.9385965
```

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

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

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

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

Maximum-A-Posteriori and Ridge Regularization

We can introduce an isotropic Gaussian prior on **all** the coefficients $p(\boldsymbol{\beta}) = N(\mathbf{0}, \sigma_{\boldsymbol{\beta}}^2 I)$. 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

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

Often we don't want to regularize the intercept, future work could look into placing an isotropic Gaussian prior on $\boldsymbol{\beta}_{1:p-1} := (\beta_1, \ldots, \beta_{p-1})$ and instead we place a uniform distribution on β_0, which doesn't depend on β_0. This would leads to

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

Gradient Ascent (MLE, No Regularization)

Updates take the form

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

Gradient Ascent (MAP, Ridge Regularization)

The update takes the form

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

Newton's Method (MLE, No Regularization)

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 $\mathbf{d}$

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

and then perform the update

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

Newton's Method (MAP, Ridge Regularization)

The update takes the form

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

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
lr_map_bfgs <- logistic_regression(Xtrain, training_classes, cost="MAP", method="BFGS")
yhat_map_bfgs <- predict(lr_map_bfgs, Xtest)
acc_map_bfgs <- calc_accuracy(test_classes, yhat_map_bfgs)
# MAP, NEWTON
lr_map_nm <- logistic_regression(Xtrain, training_classes, cost="MAP", method="NEWTON", niter=250)
yhat_map_nm <- predict(lr_map_nm, Xtest)
acc_map_nm <- calc_accuracy(test_classes, yhat_map_nm)
# MAP, GRADIENT ASCENT
lr_map_ga <- logistic_regression(Xtrain, training_classes, cost="MAP", method="GA", niter=1000)
yhat_map_ga <- predict(lr_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
lr_mle_bfgs <- logistic_regression(Xtrain, training_classes, cost="MLE", method="BFGS")
yhat_mle_bfgs <- predict(lr_mle_bfgs, Xtest)
acc_mle_bfgs <- calc_accuracy(test_classes, yhat_mle_bfgs)
```

```
# MLE, NEWTON
lr_mle_nm <- logistic_regression(Xtrain, training_classes, cost="MLE", method="NEWTON", niter=250)
yhat_mle_nm <- predict(lr_mle_nm, Xtest)
acc_mle_nm <- calc_accuracy(test_classes, yhat_mle_nm)
# MLE, GRADIENT ASCENT
lr_mle_ga <- logistic_regression(Xtrain, training_classes, cost="MLE", method="GA", niter=1000)
yhat_mle_ga <- predict(lr_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)
results
```

```
##            MLE       MAP
## BFGS 0.9649123 0.9385965
## NM   0.9561404 0.9385965
## GA   0.9122807 0.9210526
```

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 the samples. Initialize first sample 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. Take logarithm?
    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
    }
    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.

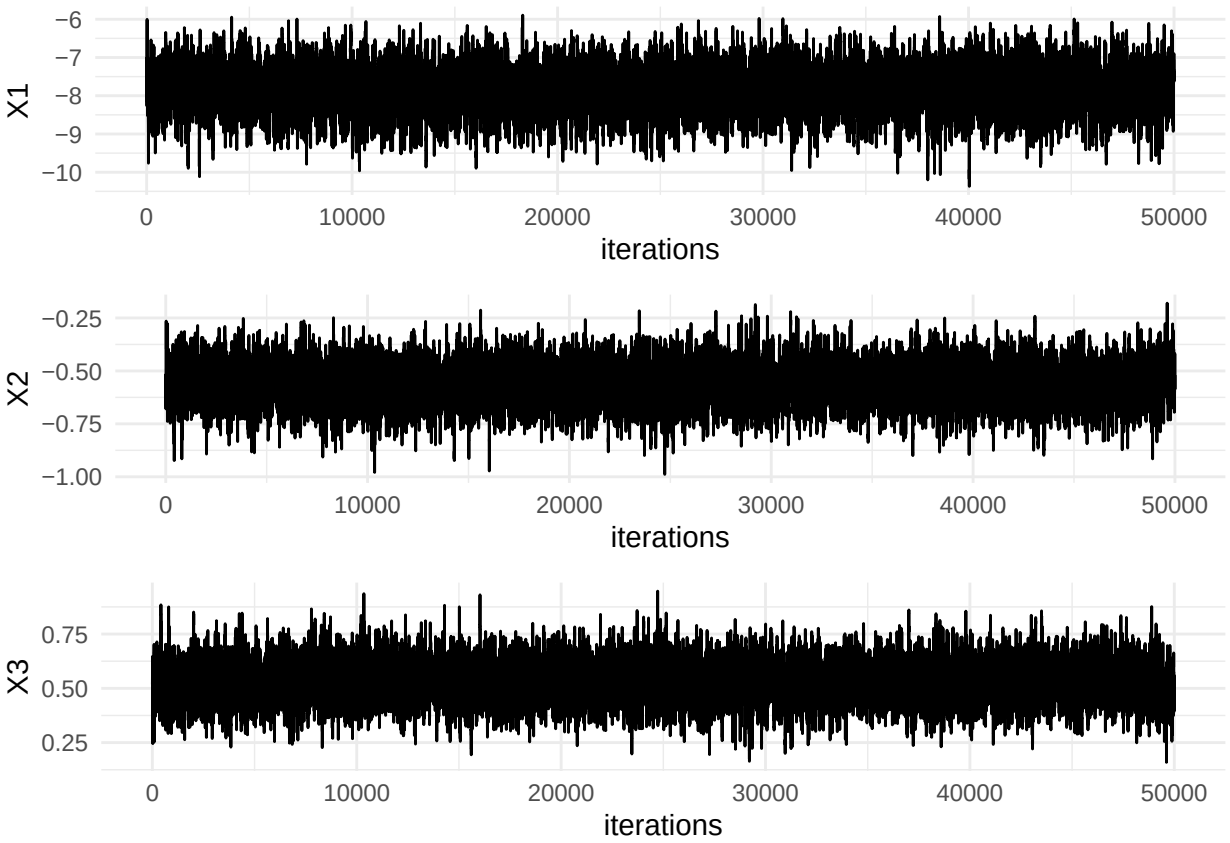
```
# up to normalizing constant
log_posterior_unnormalized <- function(beta){
    log_prior      <- -0.5*sum(beta^2)
    log_likelihood <- -sum(log(1 + exp((1 - 2*training_classes) * (Xrwmh %*% beta))))
    return(log_prior + log_likelihood)
}
# To start the algorithm more efficiently, start from MAP estimate
optim_results <- optim(c(0,0,0), function(x) - log_posterior_unnormalized(x), method="BFGS", hessian=TRU
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.

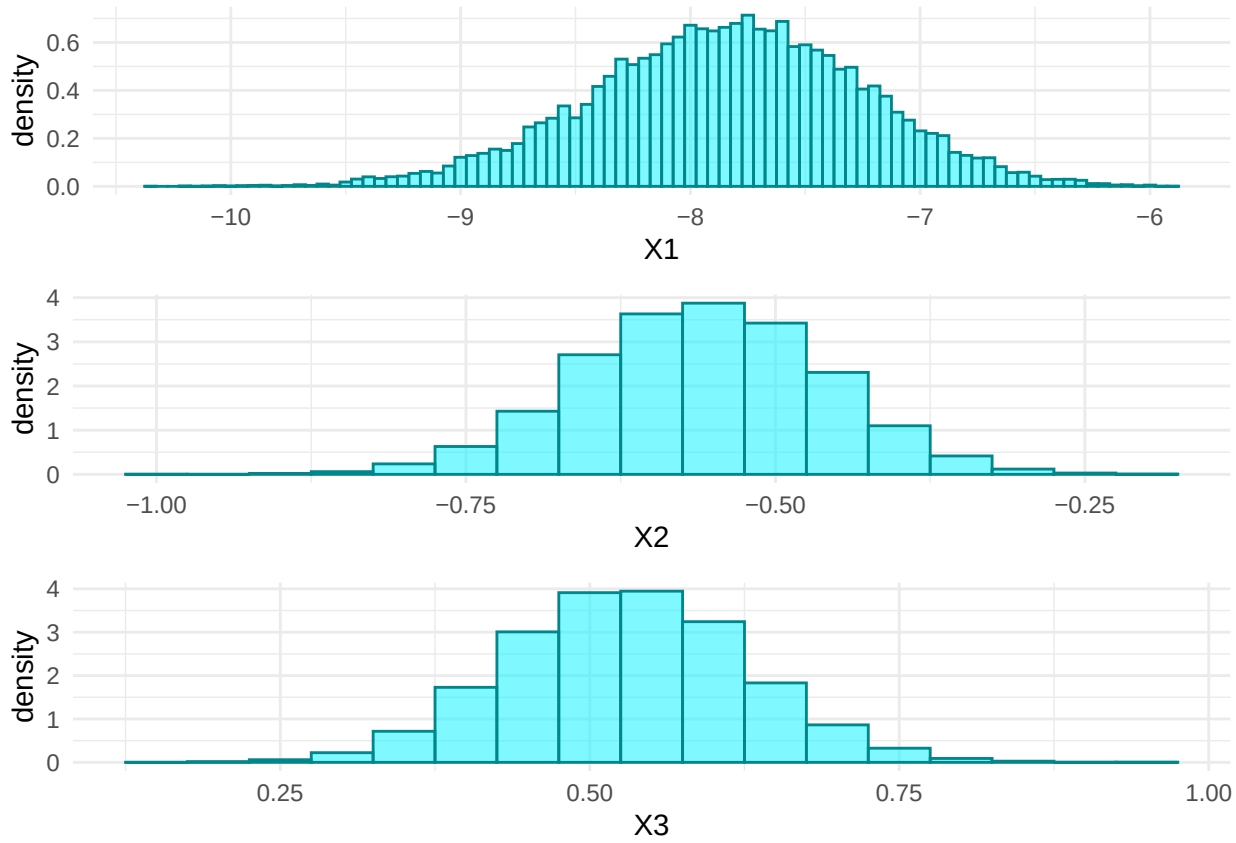
```
samples <- rwmh_multivariate_log(start, niter=50000, log_posterior_unnormalized,
                                 vcov, thinning=1, burnin=0)
```

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

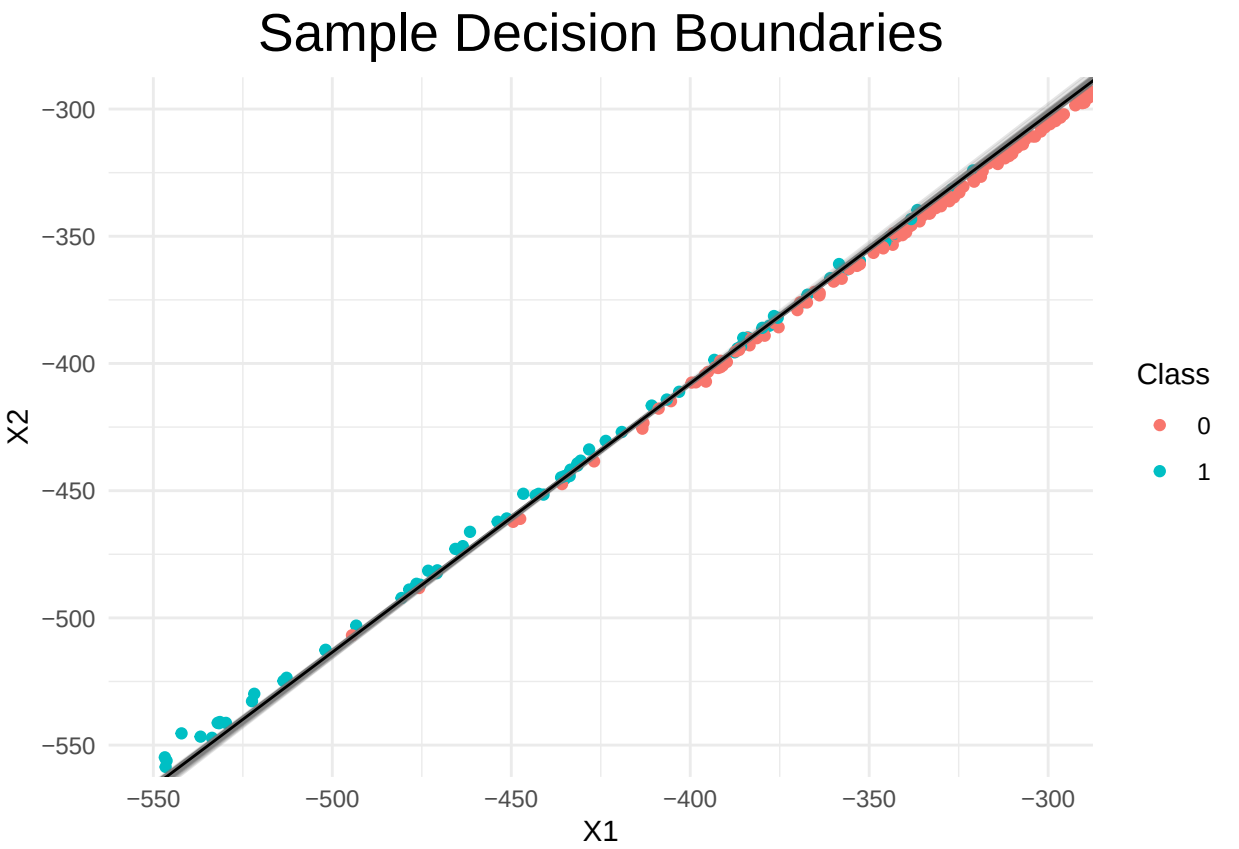
```
samplesdf <- data.frame(samples) %>% mutate(iterations=row_number())
trace1 <- ggplot(data=samplesdf, aes(x=iterations, y=X1)) + geom_line()
trace2 <- ggplot(data=samplesdf, aes(x=iterations, y=X2)) + geom_line()
trace3 <- ggplot(data=samplesdf, aes(x=iterations, y=X3)) + geom_line()
grid.arrange(trace1, trace2, trace3, ncol=1)
```



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.



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

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

```
## [1] 0.9210526
```

Conclusion

Merge all predictions

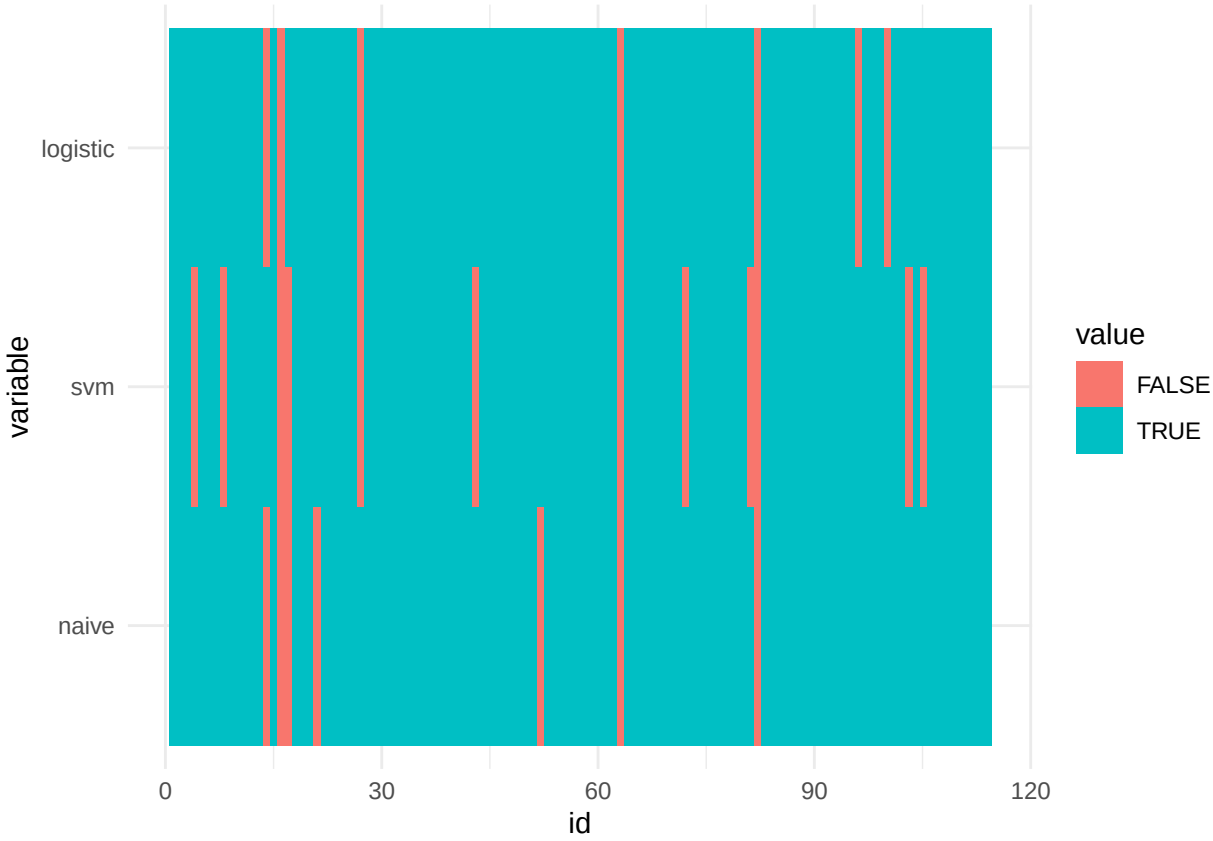
```
id <- seq(length(id_test))
all_pred <- cbind(id,numeric_test_labels,pred_naive,pred_svm)
colnames(all_pred) <- c('id','actual','naive','svm')
all_pred[all_pred==-1] <-0
all_pred %<>% as.data.frame()
```

```
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)
}
```

```
errors <- all_pred %>%
  mutate(naive=naive==actual,
         svm=svm==actual,
         logistic=yhat_map_bfgs==actual) %>%
  dplyr::select(-'actual') %>%
  melt(id='id')
```

Visualize which are the observations that the models missclassify.

```
ggplot(errors,aes(x=id,y=variable,fill=value))+
  geom_raster()+
  theme_minimal()
```


logistic
svm
naive
variable
0
30
60
90
120
id
value
FALSE
TRUE