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"
)</pre>
```

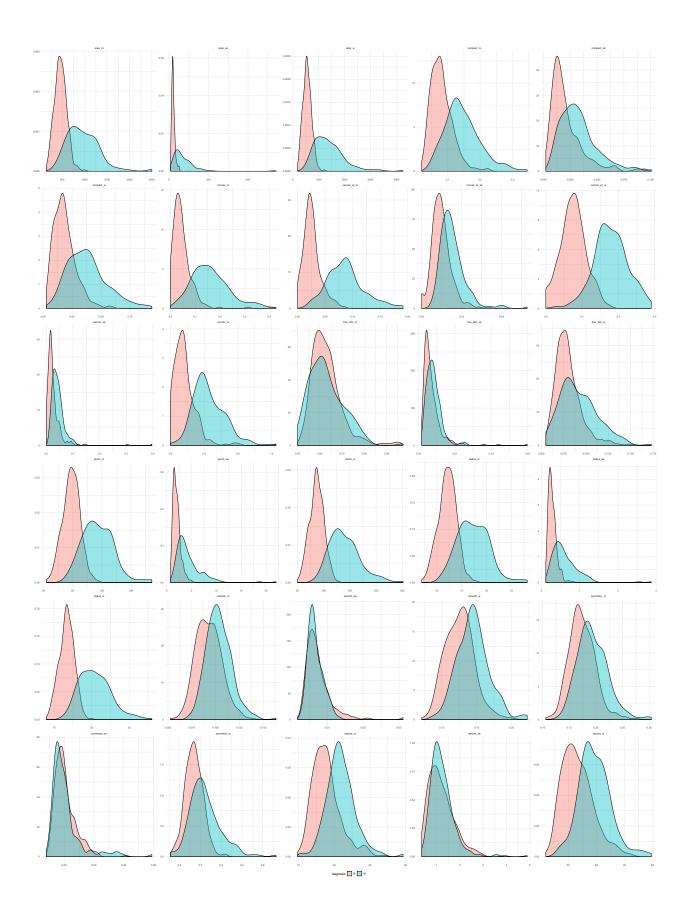
Check for missing values in every column.

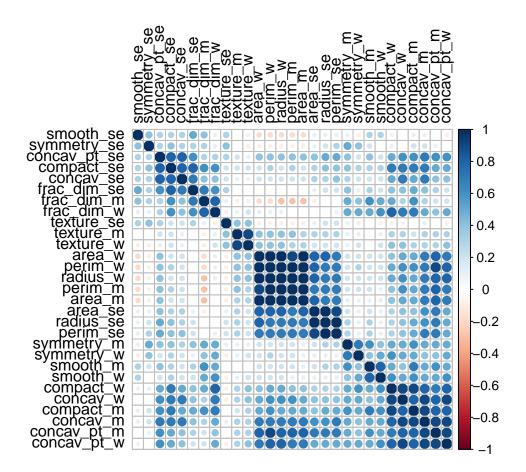
```
colSums(is.na(data))
```

```
##
              id
                     diagnosis
                                    radius_m
                                                  texture_m
                                                                   perim_m
                                                                                  area_m
##
                                            0
               0
                                                           0
                                                                                        0
##
       smooth m
                     compact m
                                     concav_m
                                                concav_pt_m
                                                               symmetry_m
                                                                              frac dim m
##
               0
                                            0
                                                           0
##
      radius_se
                    texture_se
                                    perim_se
                                                                smooth se
                                                                              compact_se
                                                    area_se
##
               0
##
                                               frac_dim_se
                                                                               texture_w
      concav_se concav_pt_se
                                 symmetry_se
                                                                 radius_w
##
               0
                              0
                                            0
##
        perim_w
                        area_w
                                     smooth_w
                                                  compact_w
                                                                  concav_w
                                                                             concav_pt_w
##
               0
                              0
                                            0
                                                                         0
##
                    frac_dim_w
                                          X33
     symmetry_w
```

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

```
train <- data %>% sample_frac(0.8)
test <- anti_join(data, train, by = "id")</pre>
# need ids for later
id_train <- train$id</pre>
id_test <- test$id</pre>
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]]</pre>
training_classes <- train[1]</pre>
test_data <- test[2:dim(test)[2]]</pre>
test_classes <- test[1]</pre>
                                                  0.6
0.6
                                                  0.4
0.4 -
                                                  0.2
0.2
0.0
                                                  0.0
               В
                                   M
                                                                 В
                                                                                     M
```



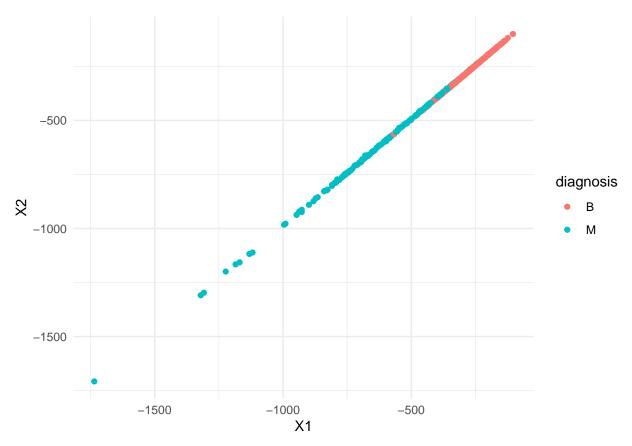


Dimensionality Reduction and Feature Selection

PCA

Code

```
normalise_z <- function(X) {</pre>
  mean_cols <- colMeans(X)</pre>
  sd_cols <- apply(X, 2, sd)</pre>
  mean_normalised_X <- t(apply(X, 1, function(x) {</pre>
    x - mean_cols
  }))
  normalised_X <- t(apply(mean_normalised_X, 1, function(x) {</pre>
    x / sd_cols
  }))
  return(normalised_X)
}
pca <- function(X, number_components_keep) {</pre>
  normalised_X <- normalise_z(X)</pre>
  corr_mat <- t(normalised_X) %*% normalised_X</pre>
  eigenvectors <- eigen(corr_mat, symmetric = TRUE)$vectors</pre>
  reduced_data <- X %*% eigenvectors[, 1:number_components_keep]</pre>
  relevant_eigs <- eigenvectors[, 1:number_components_keep]</pre>
  returnds <- list(reduced_data, relevant_eigs)</pre>
  names(returnds) <- c("reduced_data", "reduction_matrix")</pre>
  return(returnds)
Apply to dataset
pca_result <- pca(as.matrix(training_data), 2)</pre>
pca_reduced_training_data <- data.frame(cbind(pca_result$reduced_data, training_classes))</pre>
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:

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

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

where

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

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

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

A and b_0 require slightly more manipulation this time around with

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

and

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

where

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

and

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

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)</pre>
```

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

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

Which can be made as functions in R as so:

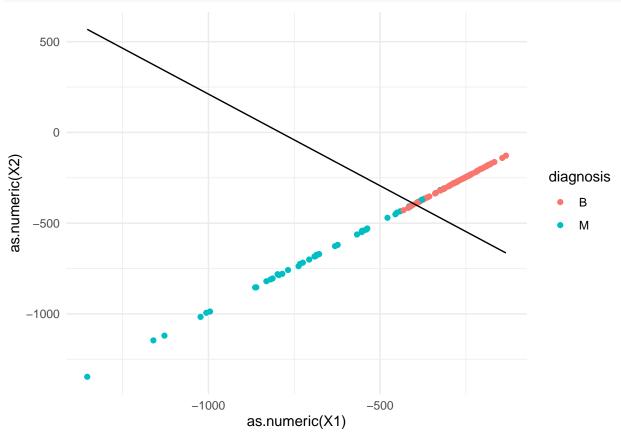
```
calculate_b <- function(w, X, y, a, C) {
    ks <- sapply(a, function(x) {
        return(x > 0 && x < C)
    })
    indices <- which(ks)
    sum_bs <- 0
    for (i in indices) {
        sum_bs <- sum_bs + (y[i] - w %*% X[i, ])
    }
    return(sum_bs / length(indices))
}

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

We can see the results of using the dual regression below

```
soft_margin_svm_plotter <- function(w, b) {</pre>
  plotter <- function(x) {</pre>
    return(1 / w[2] * -(b + (w[1] * as.numeric(x))))
  }
  return(plotter)
factor_to_label <- function(x) {</pre>
  if (as.character(x) == "M") {
    return(1)
  else {
    return(-1)
  }
label_to_factor <- function(x) {</pre>
  if (x == 1) {
    return(as.factor("M"))
  else {
    return(as.factor("B"))
  }
}
numeric_test_labels <- apply(test_classes, 1, factor_to_label)</pre>
numeric_training_labels <- apply(training_classes, 1, factor_to_label)</pre>
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</pre>
pca_reduced_prediction_fn <- function(x) {</pre>
  p <- x %*% pca_result$reduction_matrix</pre>
  reduced prediction fn(t(p))
pca_reduced_test_data <- t(apply(as.matrix(test_data), 1, function(x) x %*%
                                     pca_result$reduction_matrix))
pred_svm <- apply(as.matrix(test_data), 1, pca_reduced_prediction_fn)</pre>
accuracy_calc(numeric_test_labels, pred_svm)
## [1] 88.59649
svm_plotter <- soft_margin_svm_plotter(model$params$w, model$params$b)</pre>
embedded_test_data <- data.frame(cbind(as.matrix(test_data) %*%</pre>
                                  pca_result$reduction_matrix), test_classes)
```

```
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 $\mathbf{x} = (x_1, \dots x_d)$, where $x_1, \dots x_d$ are the features. The probability of an observation having label y is given by Bayes rule,

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

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 naive 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
}</pre>
```

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)
}</pre>
```

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)</pre>
```

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"</pre>
```

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</pre>
```

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

Fit the model to the PCA-reduced dataset.

```
model_naive_pca <- naive_bayes(pca_result$reduced_data, training_classes)</pre>
```

```
pred_naive_pca <- predict(model_naive_pca, pca_reduced_test_data)
acc_naive_pca <- calc_accuracy(test_classes, pred_naive_pca)
acc_naive</pre>
```

[1] 0.9210526

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

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

Maximum-A-Posteriori and Ridge Regularization

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

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

Gradient Ascent (MLE, No Regularization)

Updates take the form

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

Gradient Ascent (MAP, Ridge Regularization)

The update takes the form

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

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 $\alpha = 0.1$.

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

In practice we would solve the corresponding system for 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

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

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))</pre>
```

Maximum a Posteriori

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

Maximum Likelihood Estimation

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

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
),</pre>
```

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

## MLE MAP
## BFGS 0.9385965 0.9210526
## NM 0.9385965 0.9210526
## GA 0.9035088 0.9035088</pre>
```

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)</pre>
  # create vector deciding iterations where we record the samples
  store <- seq(from = (1 + burnin), to = niter, by = thinning)
  # n_samples <- (niter - burnin) %/% thinning</pre>
  # Generate matrix containing the samples. Initialize first sample with the starting value
  samples <- matrix(0, nrow = length(store), ncol = nrow(start))</pre>
  samples[1, ] <- start</pre>
  # Generate uniform random numbers in advance, to save computation. Take logarithm?
  log_u <- log(runif(niter))</pre>
  # Proposal is a multivariate standard normal distribution. Generate samples and
  # later on use linearity property of Gaussian distribution
  vcov <- diag(nrow(start)) %*% vcov</pre>
  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, ]</pre>
    # calculate log target of candidate and store it in case it gets accepted
    p_candidate <- logtarget(candidate)</pre>
    # use decision rule explained in blog posts
    if (log_u[i] <= p_candidate - pz) {</pre>
      # Accept!
      z <- candidate
      pz <- p_candidate
    # Finally add the sample to our matrix of samples
    if (i %in% store) samples[which(store == i), ] <- z</pre>
  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)]))</pre>
```

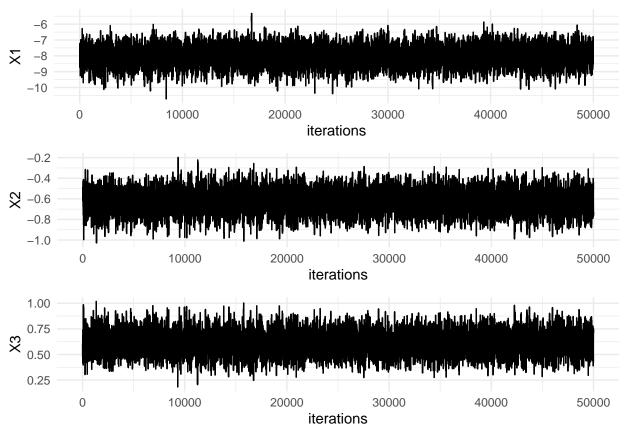
We run logistic regression using the BFGS optimization method on MAP. Since we need the Hessian matrix for

sampling later on, we simply use the optim function on the unnormalized version of the posterior distribution for logistic regression.

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.

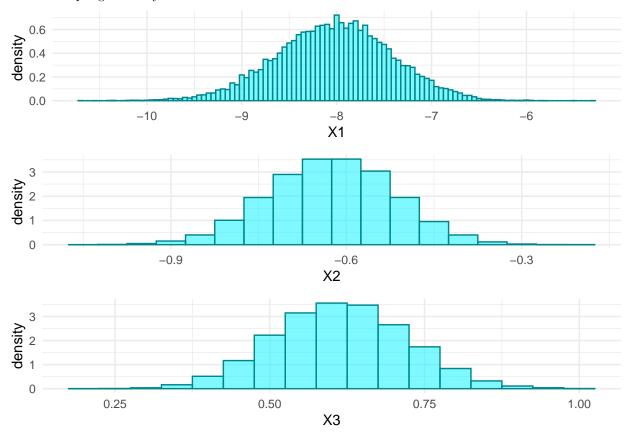
```
samples <- rwmh_multivariate_log(start,
  niter = 50000, log_posterior_unnormalized,
  vcov, thinning = 1, burnin = 0
)</pre>
```

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

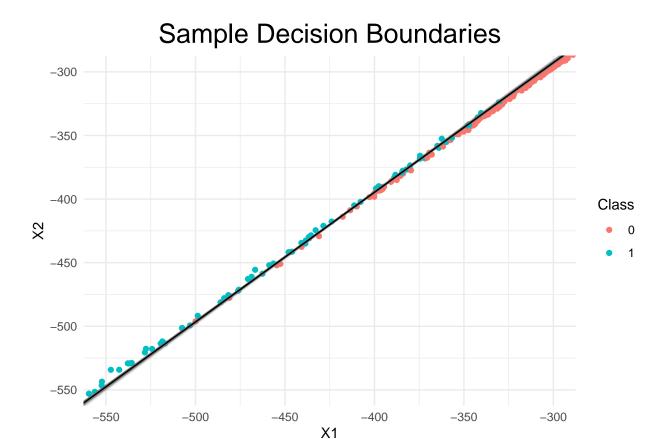


Plotting the histograms of the samples for each coordinate of the parameter vector shows that RWMH is

indeed sampling correctly.



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



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

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

[1] 0.9385965

Conclusion

Merge all predictions

```
id <- seq(length(id_test))</pre>
all_pred <- cbind(id, numeric_test_labels, pred_naive, pred_svm)
colnames(all_pred) <- c("id", "actual", "naive", "svm")</pre>
all_pred[all_pred == -1] <- 0
all_pred %<>% as.data.frame()
confusion_plot <- function(actual, predicted) {</pre>
  confusion_matrix <- as.data.frame(table(actual, predicted))</pre>
  g <- ggplot(confusion_matrix, aes(x = actual, y = predicted)) +</pre>
    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()
```

