## Optimization for Classification

```
library(MASS)
library(microbenchmark)
library(tidyverse)
```

## Utility functions

The kernel\_matrix function calculates the kernel matrix with squared exponential in a vectorized way. This function is borrowed from the profiling portfolio.

```
kernel_matrix <- function(X, sigmasq, Y=NULL){
   if (is.null(Y)){
        Y <- X
   }
   n <- nrow(X)
   m <- nrow(Y)
   # Find three matrices above
   Xnorm <- matrix(apply(X^2, 1, sum), n, m)
   Ynorm <- matrix(apply(Y^2, 1, sum), n, m, byrow=TRUE)
   XY <- tcrossprod(X, Y)
   return(exp(-(Xnorm - 2*XY + Ynorm) / (2*sigmasq)))
}</pre>
```

The function  $make_flags$  takes a y vector of length n and containing K class labels 0, 1, ..., K-1 and returns a matrix with n rows and K columns, where each row is a one-hot encoding for the class corresponding to that observation.

The function calc\_func\_per\_class generate flags from the vector y and then uses each column to perform an operation on X for every element in the corresponding class.

```
# Calculates a function (usually mean or sd) for all classes
calc_func_per_class <- function(X, y, func){
  flags <- make_flags(y)
  return(t(apply(flags, 2, function(f) apply(X[f, ], 2, func))))
}</pre>
```

This is a faster version of the classic dmvnorm leveraging cholesky decomposition and computations in the log scale.

```
# Calculates density of a gaussian
gaussian_density <- function(x, mu, sigma, log=FALSE, precision=FALSE){</pre>
  # If precision=TRUE, we're provided with precision matrix, which is the inverse
  # of the variance-covariance matrix
  if (!precision){
    # Cholesky, L is upper triangular
    L <- chol(sigma)
    kernel <- -0.5*crossprod(forwardsolve(t(L), x - mu))</pre>
    value \leftarrow -length(x)*log(2*pi)/2 -sum(log(diag(L))) + kernel
  } else {
    kernel <- -0.5* t(x- mu) %*% (sigma %*% (x - mu))
    value <- \operatorname{length}(x) * \log(2*pi)/2 - \log(\det(L)) + \ker(L)
  }
  if (!log){
    value <- exp(value)</pre>
  return(value[[1]])
```

Fastest known pure-R way to compute means across dimensions.

```
center_matrix <- function(A) {
  return(A - rep(1, nrow(A)) %*% t(colMeans(A)))
}</pre>
```

## **Binary Dataset Generation**

Generate data from two multivariate gaussian distributions with similar means and same variance-covariance. Decide the number of data points for each class, the mean and the variance-covariance matrix.

```
n1 <- 100; m1 <- c(6, 6); s1 <- matrix(c(1, 0, 0, 10), nrow=2, ncol=2)
n2 <- 100; m2 <- c(-1, 1); s2 <- matrix(c(1, 0, 0, 10), nrow=2, ncol=2)
```

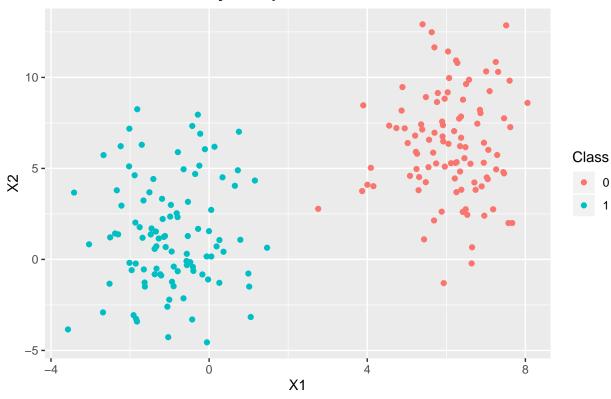
Then define the data-generating function.

Finally, we generate data with a random seed for reproducibility.

```
set.seed(123)
data <- generate_binary_data(n1, n2, m1, s1, m2, s2)
X <- data %>% dplyr::select(-y, -y2) %>% as.matrix
y <- data %>% dplyr::select(y) %>% as.matrix
```

## Data Appearance

# **Linearly Separable Dataset**



## Fisher Discriminant Analysis

## FDA Class

Define an S3 object performing FDA.

```
muks <- rep(0, ncol(flags)) # embedded center for class k</pre>
  swks <- rep(0, ncol(flags))</pre>
                                   # within class scatterness
  sbks <- rep(0, ncol(flags))</pre>
                                   # between class scatterness
  for (class in 1:ncol(flags)){
    Xk <- X[flags[, class], ]</pre>
    mk <- mean(Xk %*% w)
    muks[class] <- mk</pre>
    swks[class] \leftarrow sum(((Xk %*% w) - mk)^2)
    sbks[class] <- sum(flags[, class]) * (mk - mu)^2</pre>
  }
  # Calculate objective value
  value <- sum(sbks) / sum(swks)</pre>
  return(-value) # remember we want to maximize, but optim minimizes
# Optimize
w_start <- matrix(1, nrow=ncol(X), ncol=1)</pre>
sol <- optim(par=w_start, fn=fda_objective, method="BFGS")$par</pre>
# Return object
fda_object <- list(sol=sol, flags=flags, X=X, y=y)</pre>
class(fda_object) <- "FDA"</pre>
return(fda_object)
```

## FDA Plot Method

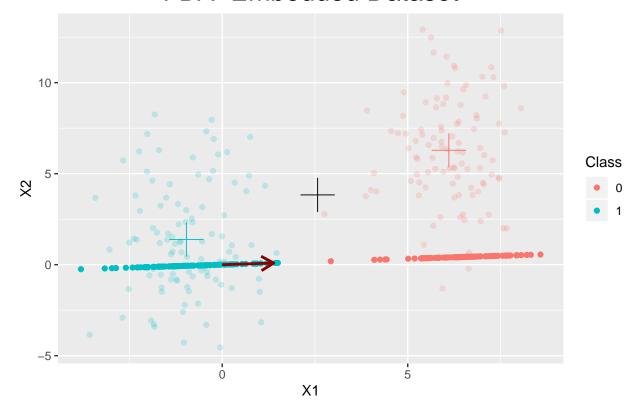
This method will plot the dataset, the embedded dataset, the embedding vector w, the mean of the whole dataset, and the mean for each class.

```
plot.FDA <- function(x, y=NULL, ...){
  # Find unit vector of w and take dot product
  sol_unit <- x$sol / sqrt(sum(x$sol^2))</pre>
  dot_products <- x$X %*% sol_unit</pre>
  if (ncol(x$X) > 2){
    # Plot on a simple horizontal line
  df <- data.frame(x1=dot_products, x2=rep(0, nrow(dot_products)), y=x$y)</pre>
  p <- ggplot(data=df) +</pre>
        geom_point(aes(x=x1, y=x2, color=as_factor(x$y)))
  } else {
    # Find embedded points in 2D
    x_emb <- dot_products %*% t(sol_unit)</pre>
    dfembed \leftarrow data.frame(x1=x_emb[, 1], x2=x_emb[, 2], y=x$y)
    # Find data mean, and mean per cluster
    datamean <- apply(x$X, 2, mean)</pre>
    datamean <- data.frame(x=datamean[1], y=datamean[2])</pre>
    meanmatrix <- calc_func_per_class(x$X, x$y, mean)</pre>
    dfclassmeans <- data.frame(meanmatrix, y=(1:nrow(meanmatrix) - 1))</pre>
    # Dataframe to plot w
    wdf \leftarrow data.frame(x=x$sol[1], y=x$sol[2], x0=c(0.0), y0=c(0.0))
    # Plot
    p <- ggplot() +</pre>
          geom_point(data=data.frame(x$X, x$y),
                       aes(x=X1, y=X2, color=as_factor(y)), alpha=0.2) +
           geom_point(data=dfclassmeans,
```

We can now look at the results of our optimization.

```
fda_object <- fda(X, y)
plot(fda_object)</pre>
```

## FDA-Embedded Dataset



## **Naive Bayes**

#### Mathematics

$$\widehat{y} = \arg\max_{k \in \{1, \dots, K\}} p(C_k) \prod_{i=1}^{N} p(x_i \mid C_k)$$

Let's assume each class is Gaussian distributed.

## Naive Bayes Class

```
naive_bayes <- function(X, y){
    # For every class, find mean and variance (one class per row)
    means <- calc_func_per_class(X, y, mean)
    vars <- calc_func_per_class(X, y, function(x) sd(x)^2)
    # Create a gaussian for each class
    nb <- list(means=means, vars=vars, X=X, y=y)
    class(nb) <- "naive_bayes"
    return(nb)
}</pre>
```

## **Predict Method**

```
predict.naive_bayes <- function(x, xtest){</pre>
  # for every test point (row of xtest), want to calculate the density value for
  # every class, and pick the highest one.
  # Instantiate matrix of correct dimensions.
  table <- matrix(0, nrow=nrow(xtest), ncol=nrow(x$means))
  # calculate priors from data
  priors <- log(apply(make_flags(x$y), 2, function(f) length(x$y[f, ]) / length(x$y)))</pre>
  # need two for loops unfortunately
  for (r ix in 1:nrow(xtest)){
    for (c_ix in 1:nrow(x$means)){
      # independence gives
      table[r_ix, c_ix] <- gaussian_density(
        x=matrix(as.double(xtest[r_ix, ])),
        mu=matrix(x$means[c_ix,]),
        sigma=diag(x$vars[c_ix, ]), log=TRUE)
    }
  table <- table + priors
  classes <- apply(table, 1, which.max)</pre>
  return(classes - 1)
```

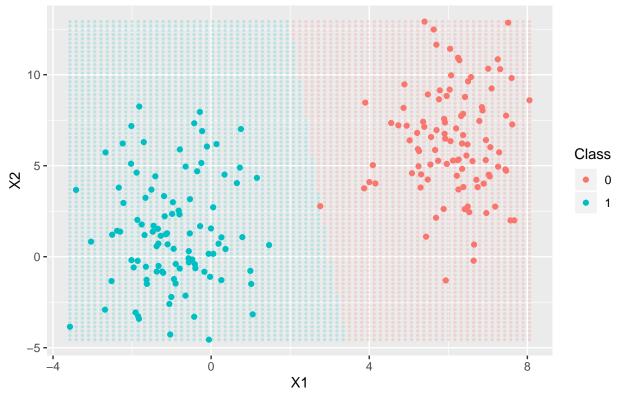
## Plot Method for Naive Bayes

This will plot the two classes and will predict points on a grid, to show the decision boundary.

```
plot.naive_bayes <- function(x, y=NULL, ngrid=75, ...){</pre>
  if (ncol(x$X) > 2) {
    print("Naive Bayes plotting for more than 2 dimensions, not implemented.")
    # Generate a grid of points on X
    coord_range <- apply(x$X, 2, range)</pre>
    grid <- expand.grid(</pre>
      X1=seq(from=coord_range[1, 1], to=coord_range[2, 1], length=ngrid),
      X2=seq(from=coord_range[1, 2], to=coord_range[2, 2], length=ngrid)
    # Use naive bayes to predict at each point of the grid
    cl <- predict(x, grid)</pre>
    dfgrid <- data.frame(grid, y=cl)</pre>
    # plot those points
    ggplot() +
      geom_point(data=dfgrid, aes(x=X1, y=X2, color=as_factor(y)), alpha=0.2, size=0.5) +
      geom_point(data=data.frame(x$X, y=x$y), aes(x=X1, y=X2, color=as_factor(y))) +
      labs(color="Class", title="Naive Bayes Decision Boundary") +
      theme(plot.title=element_text(hjust=0.5, size=20))
}
```

plot(naive\_bayes(X, y))

# Naive Bayes Decision Boundary



## 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

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

#### **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

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

Often we don't want to regularize the intercept. For this reason we place an isotropic Gaussian prior on  $\beta_{1:p-1} := (\beta_1, \dots, \beta_{p-1})$  and instead we place a uniform distribution on  $\beta_0$ , which doesn't depend on  $\beta_0$ . This leads to

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

## Laplace Approximation

A fully-Bayesian treatment is intractable. Instead we approximate the posterior with a multivariate Gaussian distribution centered at the mode

$$q(oldsymbol{eta}) = N\left(oldsymbol{eta}_{ ext{MAP}}, \left[-
abla^2 \ln p(oldsymbol{eta}_{ ext{MAP}} \mid \mathbf{y})\right]^{-1}
ight)$$

where one can show that the variance-covariance matrix

$$-\nabla_{\boldsymbol{\beta}}^{2} \ln p(\boldsymbol{\beta} \mid \mathbf{y}) = \boldsymbol{\Sigma}_{0}^{-1} + \sum_{i=1}^{n} \sigma(\mathbf{x}_{i}^{\top} \boldsymbol{\beta}) (1 - \sigma(\mathbf{x}_{i}^{\top} \boldsymbol{\beta})) \mathbf{x}_{i} \mathbf{x}_{i}^{\top} = \boldsymbol{\Sigma}_{0}^{-1} + \boldsymbol{X}^{\top} D \boldsymbol{X}$$

where

$$D = \begin{pmatrix} \sigma(\mathbf{x}_1^{\top}\boldsymbol{\beta})(1 - \sigma(\mathbf{x}_1^{\top}\boldsymbol{\beta})) & 0 & \dots & 0 \\ 0 & \sigma(\mathbf{x}_2^{\top}\boldsymbol{\beta})(1 - \sigma(\mathbf{x}_2^{\top}\boldsymbol{\beta})) & \dots & 0 \\ \vdots & & \ddots & \vdots \\ 0 & 0 & \dots & \sigma(\mathbf{x}_n^{\top}\boldsymbol{\beta})(1 - \sigma(\mathbf{x}_n^{\top}\boldsymbol{\beta})) \end{pmatrix}$$

## Gradient Ascent (MLE, No Regularization)

Updates take the form

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

where the step size  $\gamma$  can either be chosen small.

## Gradient Ascent (MAP, Ridge Regularization)

The update takes the form

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

#### Newton's Method (MLE, No Regularization)

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

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

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

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

## Implementations of the Optimization Methods

```
sigmoid <- function(x) 1.0 / (1.0 + exp(-x))
```

```
grad_ascent <- function(beta, niter=100, gamma=0.001, cost="MLE", sigmab=1.0){
  if (cost=="MLE"){
    for (i in 1:niter) beta <- beta + gamma * t(X) %*% (y - sigmoid(X %*% beta))
  } else if (cost=="MAP"){
    for (i in 1:niter) {
      beta <- beta + gamma*(sigmab^2*t(X) %*% (y - sigmoid(X %*% beta)) - beta)
    }
  }
  return(beta)
}</pre>
```

```
newton_method <- function(beta, niter=100, alpha=0.1, cost="MLE", sigmab=1.0){
# Learning rate is suggested at 0.1. For 1.0 standard Newton method is recovered
if (cost=="MLE"){
   for (i in 1:niter){
      D_k <- diag(drop(sigmoid(X%*%beta)*(1 - sigmoid(X%*%beta))))</pre>
```

```
d_k <- solve(t(X)%*%D_k %*% X, alpha*t(X) %*% (y - sigmoid(X %*% beta)))
    beta <- beta + d_k
}
} else if (cost=="MAP"){
    n <- ncol(X)
    for (i in 1:niter){
        D_k <- diag(drop(sigmoid(X%*%beta)*(1 - sigmoid(X%*%beta))))
        d_k <- solve(
            sigmab^2*t(X)%*%D_k%*%X + diag(n),
            alpha*(sigmab^2*t(X)%*%(y - sigmoid(X %*% beta)) - beta)
        )
        beta <- beta + d_k
}
return(beta)
}</pre>
```

## The Logistic Regression S3 Class and Its methods

```
logistic_regression <- function(X, y, cost="MLE", method="BFGS", sigmab=1.0, niter=100,</pre>
                                  alpha=0.1, gamma=0.001, laplace=FALSE){
  start <- matrix(0, nrow=ncol(X))</pre>
  # Define cost functions
  mle_cost <- function(beta) sum(log(1 + exp((1 - 2*y) * (X %*% beta))))
  map_cost <- function(beta) (sigmab^2)*mle_cost(beta) + 0.5*sum(beta^2)</pre>
  # Determine selected Cost Function
          (cost == "MLE") costfunc <- mle cost</pre>
  else if (cost == "MAP") costfunc <- map_cost</pre>
  # Use selected method for selected cost function
  if
          (method=="BFGS") sol <- optim(par=start, fn=costfunc, method=method)$par
  else if (method=="GA")
                             sol <- grad_ascent(start, niter, gamma, cost, sigmab)</pre>
  else if (method=="NEWTON") sol <- newton method(start, niter, alpha, cost, sigmab)
  # Laplace only works with MAP, not MLE
  # Can specify precision == TRUE in my builtin gaussian function
  first <- (sigmab^2)*diag(ncol(X))</pre>
  second <- t(X) %*% diag(drop(sigmoid(X %*% sol)*(1-sigmoid(X %*% sol)))) %*% X</pre>
  precision <- first + second</pre>
  # Build S3 object and return it
  lr <- list(X=X, y=y, beta=sol, cost=cost, method=method,</pre>
             prec=precision, costfunc=costfunc)
  class(lr) <- "logistic_regression"</pre>
  return(lr)
}
```

We provide a print method to compare results later.

The predict function will be useful for plotting. The sigmoid function gives the probability of being in class 1.

```
predict.logistic_regression <- function(x, xtest){
    # sigmoid gives probability of being in class 1. So will give (rounded) 1 to 1
    return(round(1.0 / (1.0 + exp(-xtest %*% x$beta))))
}</pre>
```

## Comparing Different Optimization Implementations

Let's run all the different algorithms with both the MLE cost function and the MAP with an isotropic gaussian as a prior. Before doing that, we need to append a column of 1s to the design matrix, for the intercept term.

```
X <- cbind(1, X)

lr_bfgs_mle <- logistic_regression(X, y, cost="MLE", method="BFGS")
lr_bfgs_map <- logistic_regression(X, y, cost="MAP", method="BFGS")
lr_ga_mle <- logistic_regression(X, y, cost="MLE", method="GA", niter = 1000)
lr_ga_map <- logistic_regression(X, y, cost="MAP", method="GA", niter = 1000)
lr_nm_mle <- logistic_regression(X, y, cost="MLE", method="NEWTON")
lr_nm_map <- logistic_regression(X, y, cost="MAP", method="NEWTON")</pre>
```

In particular we can see how in general Newton is closer to BFGS than gradient ascent is. However, we can see that gradient ascent on the regularized problem seems to achieve similar results as the Newton and Quasi-Newton methods!

```
print(lr_bfgs_mle)
## S3 Object of Class logistic_regression.
## Cost Function:
                         MLE
## Optimization Method:
## Solution:
                         20.67967 -9.520793 -0.5258984
print(lr_ga_mle)
## S3 Object of Class logistic_regression.
## Cost Function:
                         MLE
## Optimization Method:
## Solution:
                         3.950815 -1.976916 0.03972224
print(lr_nm_mle)
## S3 Object of Class logistic_regression.
## Cost Function:
                         MLE
## Optimization Method: NEWTON
## Solution:
                         14.93055 -6.723051 -0.2957674
```

```
print(lr_bfgs_map)
## S3 Object of Class logistic_regression.
## Cost Function:
                          MAP
## Optimization Method:
                          BFGS
## Solution:
                          2.823674 -1.5538 0.05431627
print(lr_ga_map)
## S3 Object of Class logistic_regression.
## Cost Function:
                          MAP
## Optimization Method:
## Solution:
                          2.782169 -1.545746 0.0572492
print(lr_nm_map)
## S3 Object of Class logistic regression.
## Cost Function:
                          MAP
## Optimization Method:
                          NEWTON
## Solution:
                          2.823061 -1.552847 0.0542555
```

## Plotting

We can also specify what happens when we plot an object of class logistic\_regression. In this case, we show the decision boundary and the confidence interval obtained from the Laplace Approximation to the posterior.

```
plot.logistic_regression <- function(x, y=NULL, ngrid=70, ...){</pre>
  # Grid to show decision boundary
  coord_range <- apply(x$X, 2, range)</pre>
  grid <- expand.grid(</pre>
      X1=seq(from=coord_range[1, 2], to=coord_range[2, 2], length=ngrid),
      X2=seq(from=coord_range[1, 3], to=coord_range[2, 3], length=ngrid)
  )
  # need to append 1 and transform to numeric, somehow it's losing it
  grid <- matrix(as.numeric(unlist(grid)), nrow=ngrid^2)</pre>
  # Predict at each point of the grid
  cl <- predict(x, cbind(1, grid))</pre>
  dfgrid <- data.frame(grid, y=cl)</pre>
  # plot those points
  p <- ggplot(data=dfgrid)</pre>
  if (!is.null(x$prec)) {
    # calculate confidence interval
    sd <- sqrt(diag(solve(x$prec)))</pre>
    beta_min <- x$beta - sd
    beta_max <- x$beta + sd
    # get range. Each column is one dimension
    ranges <- apply(x$X, 2, range)</pre>
    # understand what are the x_1 limits, from the limits of the second coordinate x_2
    x_lims <- sort((ranges[, 3] * x$beta[3] + x$beta[1]) / (-x$beta[2]))</pre>
    x1_vals <- seq(from=x_lims[1], to=x_lims[2], length.out = 200)</pre>
```

```
x2_{vals} \leftarrow -(x_{beta[2]}/x_{beta[3]})*x1_{vals} - (x_{beta[1]}/x_{beta[3]})
# define lines
min_line <- function(x) -beta_min[2] *x/beta_min[3] - beta_max[1]/beta_min[3]
max_line <- function(x) -beta_max[2]*x/beta_max[3] - beta_min[1]/beta_max[3]</pre>
# create a poly df
x_poly <- seq(from=ranges[1, 2], to=ranges[2, 2], length.out=500)</pre>
dfpoly <- data.frame(x=c(x_poly,x_poly), y=c(min_line(x_poly), max_line(x_poly)))</pre>
# same but for confidence interval
dflaplace <- data.frame(x1=x1_vals, x2=x2_vals)</pre>
p <- p +
  coord_cartesian(xlim=ranges[, 2], ylim=ranges[, 3]) +
  geom_polygon(data=dfpoly, aes(x=x, y=y), fill="grey80") +
  geom_line(data=dflaplace, aes(x=x1, y=x2))
geom_point(data=dfgrid, aes(x=X1, y=X2, color=as_factor(y)), alpha=0.2, size=0.5) +
geom_point(data=data.frame(x$X, y=x$y), aes(x=X1, y=X2, color=as_factor(y))) +
labs(color="Class", title="Logistic Regression Decision Boundary") +
theme(plot.title=element_text(hjust=0.5, size=20))
```

We can see indeed that the laplace approximation to the posterior is more uncertain when points from either side are closer together, as one would expect.

```
plot(logistic_regression(X, y, cost="MAP", method="BFGS", laplace = TRUE))
```

# Logistic Regression Decision Boundary

