# hw2\_coding

#### Muhammad Ahmed Chaudhry, Isaac Kleisle-Murphy, Kai Okada

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Public GitHub link here: https://github.com/isaackleislemurphy/Stanford-STATS-315B/tree/main/PS1

## Problem 2 - Stepwise Linear Regression

#### Part (a)

The fitted intercept if **X** is mean-centered is  $\frac{1}{N} \sum_{i=1}^{N} y_i$ . When we mean-center the columns of X, this intercept will change, but the other coefficients will not. As proof, we can see that we originally obtain predictions based on  $\hat{y}_i = \hat{\beta}_0 + \sum_{j=1}^p x_i j \hat{\beta}_j$ . With centering, we can rearrange this as:  $\hat{y}_i = (\hat{\beta}_0 + \sum_{i=1}^p \mu_j \hat{\beta}_j) + \sum_{j=1}^p (x_{ij} - \mu_j) \hat{\beta}_j$ . Note that any values of  $\hat{\beta}$  that could reduce the error further for the centered case would also reduce the error in the non-centered case. Therefore, the coefficient vector  $\hat{\beta}$  remains consistent and the intercept shifts by the sum of the average for each feature multiplied by its coefficient.

## Part (b) Determining Next Feature

If we take the product  $Z^T r_s \in \mathbb{R}^{p-q}$ , the elements of larger magnitude will correspond to features that are more highly correlated with the residuals, so adding them to the model will contribute most to fitting the model in the direction of the residuals, i.e. reducing error.

#### Part (c) Overall Strategy

At a high-level, our plan to perform forward stepwise regression breaks down as follows:

- 0.) Mean-center the features. This saves us intercept recalculations down the road, as no matter how many (mean-centered) features we add, this will remain the intercept.
- 1.) Initialise the "null" model to be the mean of the y. This mean, by the centering in 0.), will remain the intercept hereafter.
- 2.) Scan the remaining p features; for each, compute a univariate regression, and the univariate regression that maximizes  $||(y \bar{y})||_2^2 RSS_{uv}$  most is the first feature included.
- 3.) Once this feature has been selected, and it's (univariate) coefficient saved, initialise a QR factorization process (i.e. a running Graham-Schmidt algorithm) with this first feature as the "jumping off point". 4.) Scan the remaining p-1 features. For each feature, temporarily add it to the running Graham-Schmidt/QR decomposition. Then use the triangular structure of the QR decomposition to efficiently solve for the temporary/proposed coefficients of the next step.
- 5.) Evaluate the drops in RSS's of all the "temporary" Graham-Schmidt advancements (these are cheap they just build off of the previous "permanent" results); retain that which results in the largest drop permanently. 6.) Repeat 4-5 until all features have been used up.
- 7.) Now, Q is an  $n \times p$  orthogonal matrix, and R is a  $p \times p$  upper triangular matrix. If we wish to retrieve

coefficients retroactive to a particular step number, we need only to backsolve via Q[1:step], R[1:step], R[1:step]. In this way, the QR/G-S decomposition allows us to preserve previous iterations of the model, for ease of comparison.

#### Part (d) Forward Stepwise Regression in R

```
lm_step_construct <- function(X, y){</pre>
  #' Constructor function for lm step object
  #' @param X: matrix. A matrix of features to train on.
  #' Oparam y: numeric. A vector of targets to train on
  #' @return : lm_step. a constructed lm_step object.
  Z = matrix(rep(0, nrow(X) * (ncol(X)+1)), ncol=ncol(X)+1)
  Z[, 1] = 1
  lm_init = list(
   n=nrow(X), # number of samples
   p=ncol(X), # max no. predictors
   k=0, # no features chosen yet
   X=X, # the data
   x \text{ sel idx=c()},
   X_sel=matrix(rep(NA, nrow(X)*ncol(X)), ncol=ncol(X)), # actual columns selected
   X_nonsel_idx=1:ncol(X), # indices of columns in X not selected
   y=y, # targets
   beta_step=matrix(rep(0, ncol(X)^2), ncol=ncol(X)), # log of betas
   r2 step=c(), # r-squared at each step
   rss_step=c(), # rss at each step
   tss =sum(sapply(y, function(y_i) (y_i - mean(y))^2)),
    \# is_fit=F, \# for checks
    j=1 # current predictor number
  lm_init$Q = matrix(rep(0, (lm_init$p) * lm_init$n), ncol=lm_init$p)
  lm_init$R = matrix(rep(0, (lm_init$p)^2), ncol=lm_init$p)
  attr(lm_init, "class") = "lm_step"
  lm_init
}
advance qr <- function(lm step, new col idx){
  \#' Performs G-S decomposition for one new column of X
  #' Oparam lm_step: lm_step. An lm_step object, partially fitted
  #' @param new_col_idx: integer. The index of the new column to add to the decomposition.
  #' @return : lm_step.
  # GRAM SCHMIDT STEP
  ai = lm_step$X[, new_col_idx]
  if (lm_step$j == 1 & is.null(lm_step$X_sel)){
   vi = ai
  }else{
   vi = ai + lapply(1:(lm_step$j - 1), function(ll)
      - as.numeric(t(ai) %*% lm_step$Q[, 11]) * lm_step$Q[, 11]
    ) %>%
     do.call("cbind", .) %>%
```

```
rowSums()
  }
  ei = vi/as.numeric(sqrt(t(vi) %*% vi))
  lm_step$Q[, lm_step$j] = ei
  lm_step$x_sel_idx = append(lm_step$x_sel_idx, new_col_idx)
  lm_step$X_nonsel_idx = setdiff(lm_step$X_nonsel_idx, new_col_idx)
  lm step$X sel[, lm step$j] = lm step$X[, new col idx]
  lm_step$R[1:(lm_step$j), lm_step$j] = sapply(1:lm_step$j, function(11) t(ai)
                                                %*% lm step$Q[, 11])
 lm_step_j = lm_step_j + 1
 lm_step
}
get_beta <- function(lm_step, k=NULL){</pre>
 #' Gets the coefficients (not the intercept) from an lm_step object,
  #' retroactive to a step number
  #' @param lm_step: lm_step. A (at least partially) fitted lm_step object
  #' @param k: integer. The stepnumber to get beta retroactive to.
  #'
               If null, uses entirety of fit
  #' Oreturn : numeric[k]. A vector of OLS coefficients
  y = lm_step$y
  k = ifelse(is.null(k), lm_step$j-1, k)
  Q = lm_step$Q[, 1:k]; R = lm_step$R[1:k, 1:k]
 backsolve(R, crossprod(Q, y)) %>%
   as.numeric()
}
advance_selection <- function(lm_step){</pre>
 #' Identifies which "next feature" to add, and adds that feature to a
  #' copied version of the input
  #' @param lm_step: An partially fit lm_step object
  #' @return : lm_step. The lm_step, having been advanced to include the
             next available feature that most reduces RSS
  beta_current = get_beta(lm_step);
  \#beta\_compare = coef(lm(lm\_step\$y \sim lm\_step\$X\_sel[, 1:(lm\_step\$j-1)])) compare results to lm\_step\$y
  lm_step$beta_step[lm_step$j-1,lm_step$x_sel_idx] = beta_current;
  if (length(beta current) == 1){
   rss_current = sum((lm_step$y - mean(lm_step$y) -
                         lm_step$X_sel[, 1:(lm_step$j-1)] * beta_current)^2)
   rss current = sum((lm step$y - mean(lm step$y) -
                         lm_step$X_sel[, 1:(lm_step$j-1)] %*% beta_current)^2)
  lm_step$rss_step = append(lm_step$rss_step, rss_current)
  lm_step$r2_step = append(lm_step$r2_step, 1 - rss_current / lm_step$tss)
  candidates = lapply(lm_step$X_nonsel_idx, function(l1){
   lm_step_cand = advance_qr(lm_step, 11);
   beta_cand = get_beta(lm_step_cand);
   rss_delta = rss_current - sum((lm_step_cand$y - mean(lm_step_cand$y) -
```

```
lm_step_cand$X_sel[, 1:(lm_step_cand$j-1)] %*% beta_cand)^2);
   list(lm_step_cand, rss_delta);
 })
  candidates[[which.max(sapply(candidates, function(x) x[[2]]))]][[1]]
}
stepwise.fit <- function(X, y, k=NULL){</pre>
 #' Fits OLS stepwise.
 #' @param X: numeric[n, p]. A matrix of features, mean centered
  #' @param y: numeric[n]. A vector of OLS targets
  #' Cparam k: integer. The optional number of steps to take. If NULL, takes p steps
  #' @return : lm_step. A fitted lm_step object.
  k = ifelse(is.null(k), ncol(X), k)
  lm_step = lm_step_construct(unname(as.matrix(X)), y)
  init_beta = which.min(sapply(1:ncol(lm_step$X), function(ll)
    sum((lm_step$y - mean(lm_step$y) -
           as.numeric((t(lm_step$X[, l1]) %*%
                         lm_step$y))/as.numeric(t(lm_step$X[, ll]) %*%
                                                   lm_step$X[, 11]) * lm_step$X[, 11])^2)
  ))
  lm_step = advance_qr(lm_step, init_beta)
  for (iter in 2:k){
   lm_step = advance_selection(lm_step)
 lm_step
```

### Part (e) Prediction on new Matrix

```
stepwise.predict <- function(X, lm_step, k=NULL){</pre>
  #' Predicts from a fitted lm_step.
  #' @param X: numeric[n1, p]. A matrix of features to predict.
           Note columns must be ordered identical to original input.
  #' @param lm_step: lm_step. A fitted lm_step object
  #' Oparam k: integer. Number of features to retroactively predict.
  #'
            If null, uses entirety of fit.
  #' @return : numeric[n1]. A vector of predictions.
  k = ifelse(is.null(k), lm_step$j-1, k)
  beta_hat = get_beta(lm_step, k=k)
  if(length(beta_hat) - 1){
   return(as.numeric(mean(lm_step$y) +
                        unname(as.matrix(X))[, lm_step$x_sel_idx[1:k]] %*% beta_hat))
 }else{
   return(as.numeric(mean(lm_step$y) +
                        unname(as.matrix(X))[, lm_step$x_sel_idx[1:k]] * beta_hat))
 }
}
allsteps.predict <- function(model, X_eval) {</pre>
 #' Predicts target based on each step of the forward stepwise model
 #' @param model: lm_step. An lm_step containing the model parameters
```

```
#' Oparam X_eval: numeric[n1, p]. A matrix of features to predict.
  #' @return : Matrix of predictions based on each coefficient set
  as.matrix(lapply(1:length(model$x_sel_idx), function(z){
      yhat = stepwise.predict(X_eval, model, k=z);
 }))
}
coef.matrix <- function(model, k) {</pre>
  #' Returns formatted coefficient matrix for fitted model, with step
  \#' and R^2 (for k steps)
  #' Oparam model: lm_step. An lm_step containing the model parameters
  #' Oparam k: integer number of steps to view
  \#' Oreturn : data.frame[k, k+2] of coefficient sets for model
  betas_df <- data.frame(model$beta_step)</pre>
  betas_df <- betas_df[1:(k-1), colSums(betas_df, dims = 1L) != 0]</pre>
  betas_df$step <- 1:(k-1)</pre>
  betas_df$r2 <- overall_results$r2_step
  betas_df
prediction.score <- function(model, X_eval, y_eval) {</pre>
    #' Outputs the rss, mse, and misclassification error of a prediction
    #' @param model: Im step. An lm step containing the model parameters
    #' Oparam X_eval: numeric[n1, p]. A matrix of features to predict.
    #' Oparam y_eval: numeric[n1]. The target to evaluate against
    #' Creturn : data.frame. The RSS, MSE, and Misclassification error for each partial model
    scoring = lapply(1:length(model$x_sel_idx), function(z){
    yhat = stepwise.predict(X_eval, model, k=z);
    yhat_binary = sapply(yhat, function(y) ifelse(y >= .5, 1, 0));
    rss = sum((y_eval - yhat)^2);
    mse = mean((y_eval - yhat)^2);
    misclass = mean(y_eval != yhat_binary);
    c(rss, mse, misclass)
  }) %>%
    do.call("rbind", .) %>%
    data.frame() %>%
    `colnames<-`(c("RSS", "MSE", "MISCLASS"))</pre>
  scoring$nfeat = 1:length(model$x_sel_idx)
  scoring
}
```

#### Part (f) Application to Spam Data

```
spam_data = read.csv("spamdata_indicated.csv")
spam_data[, 55:57] = log(spam_data[, 55:57])

train_x_unscaled = spam_data[spam_data[, 59] == 0, 1:57];
train_y = spam_data[spam_data[, 59] == 0, 58];
test_x_unscaled = spam_data[spam_data[, 59] == 1, 1:57];
```

```
test_y = spam_data[spam_data[, 59] == 1, 58];
# centering
centers = train_x_unscaled %>%
  colMeans() %>%
  as.numeric()
train x scaled = lapply(1:nrow(train x unscaled), function(i)
  as.numeric(train_x_unscaled[i, 1:57]) - centers
) %>%
 do.call("rbind", .)
test_x_scaled = lapply(1:nrow(test_x_unscaled), function(i)
  as.numeric(test_x_unscaled[i, 1:57]) - centers
) %>%
 do.call("rbind", .)
# fit the full model
k = ncol(train_x_scaled)
full_model = stepwise.fit(train_x_scaled, train_y, k = k)
```

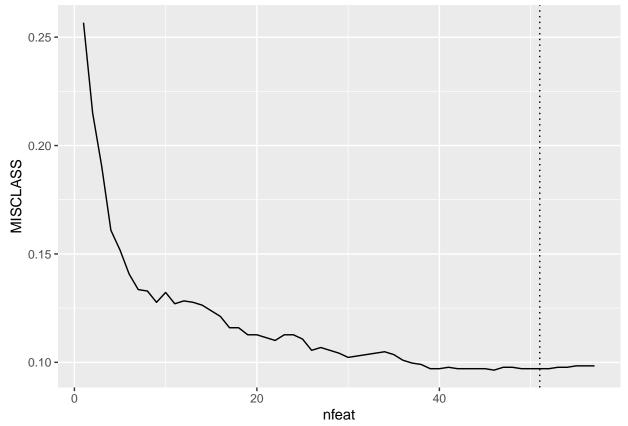
## Part (g) Cross Validation

```
stepwise.cv.fit <- function(X, y, nfolds=10, k=NULL, S=2020){
  #' Runs cross-validation on forward stepwise linear regression
  #' Oparam X: numeric[n1, p]. A matrix of features to predict.
           Note columns must be ordered identical to original input.
  #' @param y: numeric[n1]. The target
  #' Oparam nfolds: integer. The number of cross-validation folds
  #' Oparam k: integer. Number of features to retroactivelly predict.
          If null, uses entirety of fit.
  #' @param S: integer. The seed for CV sampling
  #' @return : numeric[n1]. A vector of predictions.
  set.seed(S)
  # cv preprocessing step
  fold_idx = sample(1:nrow(X), nrow(X), replace=F)
  folds = split(fold_idx, ceiling(seq_along(fold_idx) / ceiling(length(fold_idx)/nfolds)))
  cv_result = lapply(folds, function(fold){
   cat('-')
   X_train = X[setdiff(fold_idx, fold), ]; y_train = y[setdiff(fold_idx, fold)];
   X_dev = X[fold, ]; y_dev = y[fold];
   # center data
   centers = X_train %>% colMeans()
    # apply centers to training
   X_train = lapply(1:nrow(X_train), function(i)
     as.numeric(X_train[i, ]) - centers
   ) %>%
     do.call("rbind", .)
   X_dev = lapply(1:nrow(X_dev), function(i)
     as.numeric(X_dev[i, ]) - centers
   ) %>%
```

```
do.call("rbind", .)
    model = stepwise.fit(X_train, y_train, k=k)
    scoring = prediction.score(model, X_dev, y_dev)
    scoring
  })
  cv_agg = do.call("rbind", cv_result) %>%
    group_by(nfeat) %>%
    summarise_all(., mean)
# note that CV automatically centers, so use unscaled here
cv_results = stepwise.cv.fit(train_x_unscaled, train_y, nfolds=10, S=2020)
# Minimum misclassification error achieved at 51 featues
k_cv= which.min(cv_results$MISCLASS)
k_cv
## [1] 51
# plot misclassification error as a function of step in CV.
ggplot(cv_results, aes(x = nfeat, y = MISCLASS)) + geom_point()
  0.25 -
WISCLASS
  0.15 -
  0.10 -
                                   20
                                                              40
         Ö
                                              nfeat
```

#### Part (h) Predictions on Test Data

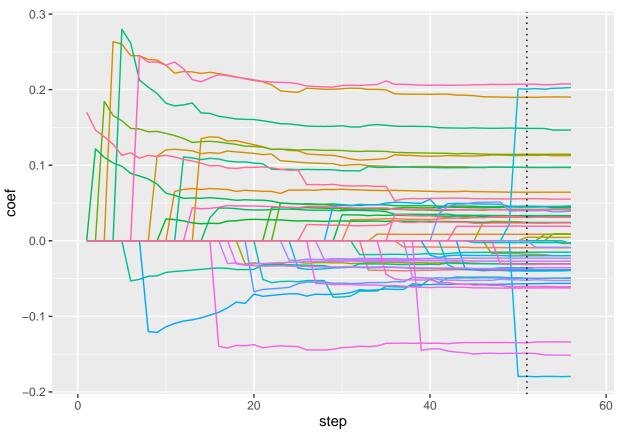
```
# predict results on test
full_model = stepwise.fit(train_x_scaled, train_y)
test_results <- prediction.score(full_model, test_x_scaled, test_y)
ggplot(test_results, aes(x = nfeat, y = MISCLASS)) +
    geom_line() +
    geom_vline(xintercept=k_cv, linetype="dotted")</pre>
```



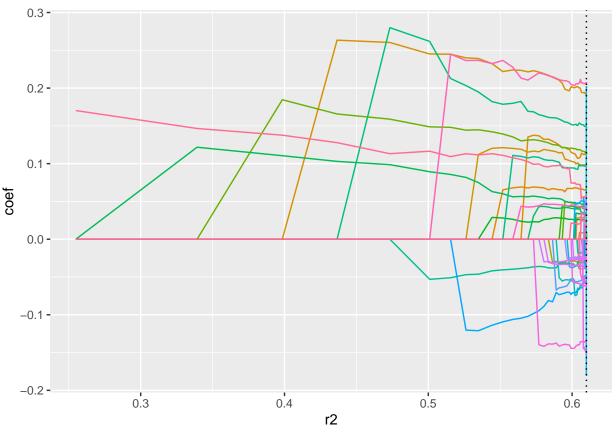
The vertical line corresponds the number of steps selected by CV.

### Part (i) Plots of fit per step

```
# plot coefficient path as a function of step and R~2
ggplot(betas_dfStep, aes(x = step, y = coef, group_by(beta))) +
  geom_path(aes(colour = beta), show.legend=FALSE) +
  xlim(c(0,k+1)) +
  geom_vline(xintercept=k_cv, linetype="dotted")
```



```
ggplot(betas_dfR2, aes(x = r2, y = coef, group_by(beta))) +
geom_path(aes(colour = beta), show.legend=FALSE) +
geom_vline(xintercept=betas_df$r2[k_cv], linetype="dotted")
```



```
# first 10 features selected
first_ten.feats <- colnames(spam_data)[overall_results$x_sel_idx[1:10]]
first_ten.coefs <- sapply(1:10, function(i) {
   overall_results$beta_step[i,overall_results$x_sel_idx[i]]
})
# show table for clarity
data.frame(feature = first_ten.feats, coef1 = first_ten.coefs)</pre>
```

```
##
      feature
                   coef1
## 1
         X61 0.17026498
## 2
       X0.96 0.12171339
## 3 X0.32.1 0.18454562
## 4
        X0.3 0.26341833
## 5
       X0.14 0.27993126
       X0.16 -0.05306591
## 6
## 7
       X0.44 0.24494795
## 8
       X0.28 -0.12030062
## 9
        X0.4 0.11209760
       X1.93 0.02885550
## 10
```

## Problem 7

Preprocessing

```
# Read in and preprocess data

zz_train = gzfile('zip.train.gz', 'rt')
```

#### Part (i)

```
# Compare results of linear regression, LDA, and
# multiclass linear logistic regression
# helper function to obtain class prediction from regression outputs
lr_to_pred <- function(y) {round(min(max(y,0), 9))}</pre>
# helper function to obtain error rate based on predicted vs. actual
err_rate <- function(pred.y, test.y) {mean(pred.y != test.y)}</pre>
# Linear Regression
model.lr <- lm(digit ~ ., data = dataset.train)</pre>
output.lr <- lapply(predict(model.lr, newdata = dataset.test[-1]), lr_to_pred)</pre>
err_rate.lr <- err_rate(output.lr, dataset.test$digit)</pre>
err_rate.lr # 74.5% test error
## [1] 0.7453911
# LDA
model.lda <- lda(digit ~ ., data = dataset.train)</pre>
output.lda <- predict(model.lda, newdata = dataset.test)$class</pre>
err_rate.lda <- err_rate(output.lda, dataset.test$digit)</pre>
err rate.lda # 11.5% test error
## [1] 0.1145989
# Multiclass Logistic Regression
model.mlr <- multinom(digit ~ ., data = dataset.train, MaxNWts = 4000, maxit=500)</pre>
## # weights: 2580 (2313 variable)
## initial value 16788.147913
## iter 10 value 2598.959017
## iter 20 value 1494.978090
## iter 30 value 903.291402
## iter 40 value 443.785686
## iter 50 value 260.626756
## iter 60 value 190.835491
## iter 70 value 160.773160
## iter 80 value 114.048146
## iter 90 value 88.746976
## iter 100 value 76.302570
## iter 110 value 63.400188
```

```
## iter 120 value 54.375215
## iter 130 value 46.291174
## iter 140 value 38.303473
## iter 150 value 28.822812
## iter 160 value 17.888650
## iter 170 value 9.531259
## iter 180 value 2.985635
## iter 190 value 0.715017
## iter 200 value 0.209663
## iter 210 value 0.066709
## iter 220 value 0.030412
## iter 230 value 0.014034
## iter 240 value 0.006701
## iter 250 value 0.004145
## iter 260 value 0.001842
## iter 270 value 0.001125
## iter 280 value 0.000743
## iter 290 value 0.000464
## iter 300 value 0.000307
## iter 310 value 0.000265
## iter 320 value 0.000214
## final value 0.000083
## converged
output.mlr <- predict(model.mlr, newdata = dataset.test[-1])</pre>
err_rate.mlr <- err_rate(output.mlr, dataset.test$digit)</pre>
err_rate.mlr # 16.6% test error
```

#### ## [1] 0.1664175

Linear Regression fares much worse than LDA and Logistic Regression, likely due to masking effects. LDA is ultimately the best classifier in the absence of shrinkage.

#### Part (ii)

```
# Helper function for obtaining predicted class from logistic regression
f.extract_mlm <- function(x) { which.max(x) - 1}</pre>
#' Get data frame of % deviance vs. test error from qlmnet model
#' @param train.x the training inputs as a matrix
#' Oparam train.y the training outputs (list or matrix)
#' @param test.x the test inputs as a matrix
#' Oparam test.y the test outputs (list or matrix)
#' @param alpha hyperparameter for L1 vs. L2 penalty
#' Oparam family the (GLM) model family to fit
#' @param f.extract a function to extract predictions from the model
#' Creturn a data frame of the % deviance vs. test error for each lambda
glm_dev_vs_err <- function(train.x, train.y, test.x, test.y,</pre>
                           alpha, family, f.extract) {
  train_coded.y <- model.matrix(~ as.factor(train.y) + 0)</pre>
 fit <- glmnet(train.x, train_coded.y, alpha = alpha, family = family)</pre>
  # apply model to the test data
  result <- lapply(fit$lambda,
                   function(s) predict(fit, type = "response",
```

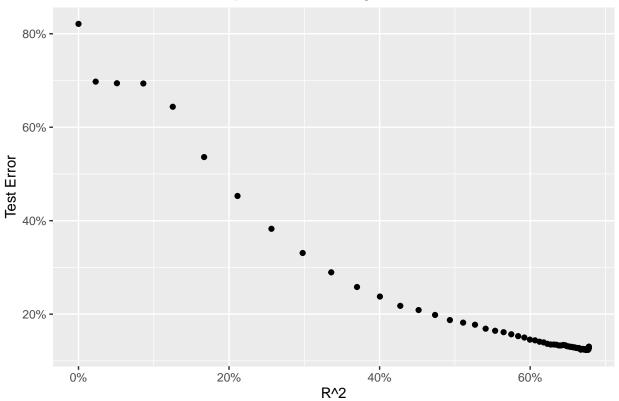
```
newx = test.x, s = s))
# obtain predicted classes from results
ghats <- lapply(result, function(t) apply(t, MARGIN = 1, FUN = f.extract))

# obtain error rates for each lambda
err_rates <- lapply(ghats, err_rate, test.y = test.y)
data.frame(dev = fit$dev.ratio, test_error = unlist(err_rates))
}

# adapt train and test data to glmnet
train.y <- dataset.train[[1]]
train.x <- as.matrix(dplyr::select(dataset.train, -c("digit")))
test.y <- dataset.test[[1]]
test.x <- as.matrix(dplyr::select(dataset.test, -c("digit")))</pre>
```

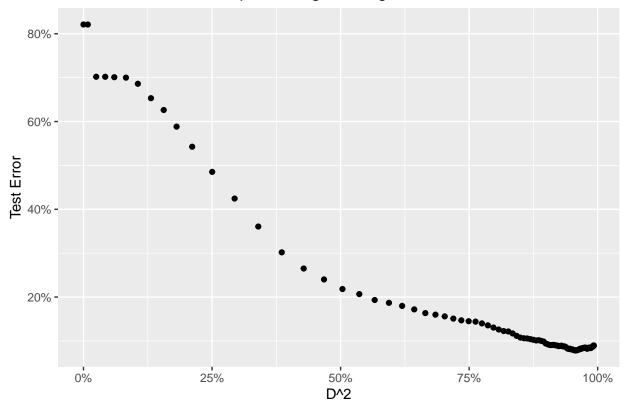
Plot for Linear Regression

## Test Error for Multi–Response Linear Regression



Plot for Multi-class Logistic Regression

## Test Error for Multi-Response Logistic Regression



## Part (iii)

The optimization problem being solved in Linear Regression is:  $\hat{\beta} = \operatorname{argmin}_{(\beta,\beta_0)} \left[ \frac{1}{2N} \sum_{i=1}^{N} ||y_i - \beta_0 - x_i^T \beta||_F^2 + \lambda \left[ (1-\alpha) \frac{1}{2} ||\beta||_F^2 + \alpha \sum_{j=1}^{p} ||\beta_j||_2 \right] \right]$ 

In the multiresponse case,  $\beta$  is a matrix composed of coefficient vectors per response, so the operation that corresponds to the L2-norm in the vector case is the Frobenius Norm  $||.||_F$ , which takes the the sum of squares for each element in the matrix. Meanwhile, the operation that corresponds to the L1-norm is the sum of the magnitudes of the feature vectors (this is L1 in the feature dimension, while the Frobenius norm is L2 in the feature dimension.)

The optimization problem being solved in Multinomial Logistic Regression is:  $\hat{\beta} = \operatorname{argmin}_{(\beta,\beta_0)}[-l(\beta) - \lambda[(1-\alpha)\frac{1}{2}||\beta||_F^2 + \alpha\sum_{j=1}^p ||\beta_j||_2]]$ , where  $l(\beta)$  is the likelihood function:

$$l(\beta) = \frac{1}{N} \sum_{i=1}^{N} (\sum_{l=1}^{K} I(g_i = l) \log \mathbb{P}(G = k | X = x_i)) = \frac{1}{N} \sum_{i=1}^{N} [\sum_{l=1}^{K} I(g_i = l) (\beta_{0k} + \beta_k^T x_i) - \log(\sum_{l=1}^{K} \exp(\beta_{0k} + x_i^T \beta_k))]$$