Code for slide deck on penalised regression and cross-validation

Benjamin Skov Kaas-Hansen

11/02/2020

Contents

Setup	2
Cross-validation Pima	2
Homegrown	2
Using packages	3
Lasso regression example: biopsies from breast cancer patients	4
Lasso regression	4
Ridge and elastic net models	6
Over-fitting biopsy	9
Delassoing	11
Cross-validation	13
Test out-of-sample performance of the CV model	14
Cross-validation to pick best combination of λ and α	14
Resampling methods: jackknife and bootstrap	15
Sampling distribution	15
Jacknife	18
Exercise: cross-validation	19
1. LOO-CV error rate	20
2. Use proper cost function	20
3. Difference between error rates, and their interpretation	20
4 10 fold CV	91

```
Exercise: penalised regression
     22
     22
22
22
22
22
22
```

Setup

```
packages <- c("plyr", "tidyr", "broom", "boot", "glmnet", "selectiveInference", "MASS", "tidyverse")
for (p in packages)
    library(p, character.only = TRUE)
knitr::opts_chunk$set(fig.align = "center")

theme_set(theme_minimal())

# Little helper to get the glmnet coefficients in nice tidy format
pretty_coefs <- function(coefs) { # coefs: the output from coef(fit_object, s = [value])
    enframe(coefs[, 1], "predictor", "coefficient") %>%
        filter(coefficient != 0) %>%
        arrange(desc(abs(coefficient)))
}
```

Cross-validation Pima

Homegrown

summary(PimaIndiansDiabetes2)

```
##
      pregnant
                       glucose
                                       pressure
                                                       triceps
   Min.
         : 0.000
                                    Min. : 24.00
##
                    Min. : 44.0
                                                    Min. : 7.00
   1st Qu.: 1.000
                    1st Qu.: 99.0
                                    1st Qu.: 64.00
                                                    1st Qu.:22.00
## Median : 3.000
                                    Median : 72.00
                    Median :117.0
                                                    Median :29.00
## Mean : 3.845
                    Mean :121.7
                                    Mean : 72.41
                                                    Mean
                                                          :29.15
## 3rd Qu.: 6.000
                    3rd Qu.:141.0
                                    3rd Qu.: 80.00
                                                    3rd Qu.:36.00
## Max.
          :17.000
                    Max.
                           :199.0
                                    Max.
                                          :122.00
                                                    Max.
                                                           :99.00
##
                    NA's
                                    NA's
                                           :35
                                                    NA's
                                                            :227
                          :5
      insulin
##
                         mass
                                    pedigree
                                                         age
                                                                    diabetes
## Min. : 14.00
                    Min.
                          :18.20
                                   Min.
                                         :0.0780
                                                    Min.
                                                           :21.00
                                                                    neg:500
## 1st Qu.: 76.25
                    1st Qu.:27.50
                                   1st Qu.:0.2437
                                                    1st Qu.:24.00
                                                                    pos:268
## Median :125.00
                    Median :32.30
                                    Median :0.3725
                                                    Median :29.00
## Mean
         :155.55
                    Mean :32.46
                                    Mean :0.4719
                                                    Mean :33.24
## 3rd Qu.:190.00
                    3rd Qu.:36.60
                                    3rd Qu.:0.6262
                                                    3rd Qu.:41.00
          :846.00
                    Max.
## Max.
                           :67.10
                                    Max. :2.4200
                                                    Max. :81.00
## NA's
          :374
                    NA's
                           :11
set.seed(42)
pima <- na.exclude(PimaIndiansDiabetes2) %>%
   mutate(cv_fold = sample(1:10, n(), replace = TRUE))
table(pima$cv_fold) # fairly equal distribution
##
## 1 2 3 4 5 6 7 8 9 10
## 44 40 29 39 39 47 29 26 46 53
err_cv <- c()
for (i in unique(pima$cv_fold)) {
   train <- filter(pima, cv_fold != i)</pre>
   mod <- glm(diabetes ~ age + mass + insulin + pregnant, data = train, family = binomial)</pre>
   val <- filter(pima, cv_fold == i)</pre>
   y_pred <- predict(mod, newdata = val, type = "response")</pre>
   y_true <- as.numeric(val$diabetes) - 1 # bring binary factor to 0/1 scale
   err <- mean(abs(y_true - y_pred) > 0.5)
   err_cv <- c(err_cv, err)</pre>
}
err_cv
## [1] 0.2500000 0.2564103 0.2608696 0.2641509 0.3333333 0.2500000 0.3076923
  [8] 0.3103448 0.3448276 0.2978723
mean(err_cv)
## [1] 0.2875501
Using packages
binary_pred_cost <- function(y_true, y_pred) {</pre>
   mean(abs(y_true - y_pred) > 0.5)
```

```
library(boot)
pima_glm <- glm(diabetes ~ age + mass + insulin + pregnant, data = pima, family = binomial)
pima_loo <- cv.glm(pima, pima_glm, cost = binary_pred_cost)
pima_loo$delta # 1st is raw estimate, 2nd is bias-corrected

## [1] 0.2857143 0.2844908

pima_cv1 <- cv.glm(pima, pima_glm, cost = binary_pred_cost, K = 10)
pima_cv1$delta # 1st is raw estimate, 2nd is bias-corrected

## [1] 0.2806122 0.2801112

# This model doesn't really overfit</pre>
```

The modelr-package has some powerful functionalities for CV, LOOCV and bootstrapping.

Lasso regression example: biopsies from breast cancer patients

Lasso regression

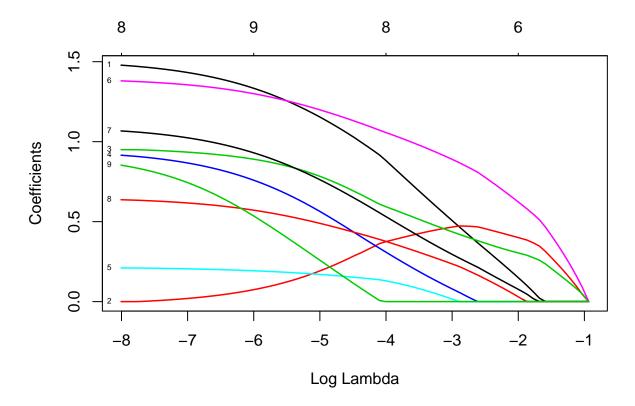
Let's look at the data

```
data(biopsy)
```

summary(biopsy) # NA's in V6; mean varies across variables but anyway somewhere around 2 and 4

```
##
         ID
                                               ٧2
                                                                 VЗ
                              V1
##
   Length:699
                               : 1.000
                                                : 1.000
                                                                  : 1.000
                       Min.
                                         Min.
                                                           Min.
  Class : character
                        1st Qu.: 2.000
                                         1st Qu.: 1.000
                                                           1st Qu.: 1.000
   Mode : character
                       Median : 4.000
                                         Median : 1.000
                                                           Median : 1.000
                                               : 3.134
##
                               : 4.418
                                                                  : 3.207
                        Mean
                                         Mean
                                                           Mean
##
                        3rd Qu.: 6.000
                                         3rd Qu.: 5.000
                                                           3rd Qu.: 5.000
##
                       Max.
                               :10.000
                                                :10.000
                                                           Max.
                                         Max.
                                                                  :10.000
##
##
          ۷4
                            ۷5
                                             ۷6
                                                               ۷7
##
    Min.
          : 1.000
                            : 1.000
                                              : 1.000
                                                                : 1.000
                     Min.
                                       Min.
                                                         Min.
   1st Qu.: 1.000
                     1st Qu.: 2.000
                                       1st Qu.: 1.000
                                                         1st Qu.: 2.000
  Median : 1.000
                     Median : 2.000
                                       Median : 1.000
                                                         Median : 3.000
                                              : 3.545
          : 2.807
##
   Mean
                     Mean
                             : 3.216
                                       Mean
                                                         Mean
                                                                : 3.438
##
    3rd Qu.: 4.000
                     3rd Qu.: 4.000
                                       3rd Qu.: 6.000
                                                         3rd Qu.: 5.000
##
   Max.
          :10.000
                     Max.
                             :10.000
                                       Max.
                                              :10.000
                                                         Max.
                                                                :10.000
##
                                       NA's
                                              :16
##
          ٧8
                            ۷9
                                             class
##
           : 1.000
                     Min.
                            : 1.000
                                                :458
  Min.
                                       benign
   1st Qu.: 1.000
                     1st Qu.: 1.000
                                       malignant:241
## Median : 1.000
                     Median : 1.000
##
   Mean
          : 2.867
                     Mean
                           : 1.589
## 3rd Qu.: 4.000
                     3rd Qu.: 1.000
           :10.000
                            :10.000
  {\tt Max.}
                     Max.
##
```

```
biopsy_complete <- na.exclude(biopsy) # remove rows with any missing value
biopsy_predictors <- select(biopsy_complete, -ID, -class) %>%
    scale() # note attributes "remember" normlisation factors; useful for transforming test set
bind_rows(gather(as_tibble(biopsy_predictors), var, value) %>%
            mutate(scale = "normalised"),
          gather(select(biopsy_complete, -ID, -class), var, value) %>%
            mutate(scale = "original")) %>%
    ggplot(aes(x = value, colour = scale)) +
        geom_density(position = "identity") +
        scale_x_continuous(breaks = -2:10) +
        facet_wrap(~ var, scales = "free_y") +
        theme(axis.text.y = element_blank())
              V1
                                      V2
                                                              V3
              V4
                                      V5
                                                              V6
                                                                              scale
 density
                                                                                  normalised
                                                                                  original
              V7
                                      V8
     -10 1 2 3 4 5 6 7 8 9 10
                            -10 1 2 3 4 5 6 7 8 9 10 -10 1 2 3 4 5 6 7 8 9 10
                                     value
lasso_logreg <- glmnet(biopsy_predictors, biopsy_complete$class, family = "binomial")</pre>
# Coefficient profile plot (built-in: ugly but easy)
plot(lasso_logreg, xvar = "lambda", label = TRUE, lwd = 1.5)
```

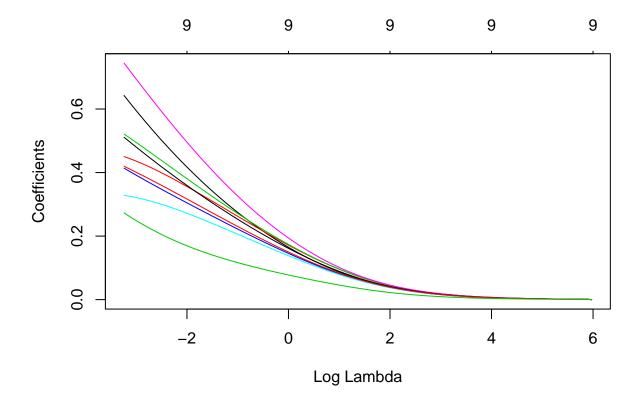


```
pretty_coefs(coef(lasso_logreg, s = exp(-1.2)))
```

BACK TO PRESENTATION

Ridge and elastic net models

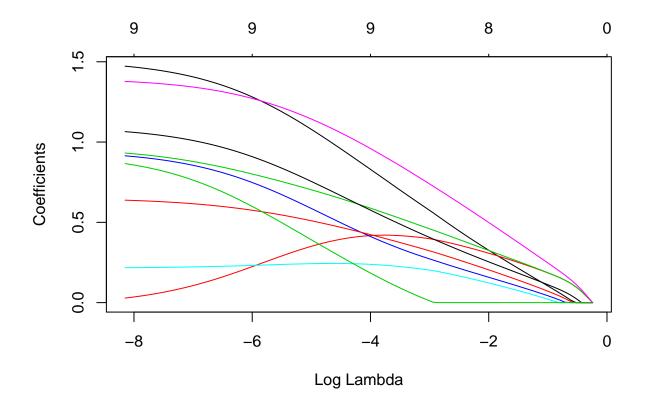
```
ridge_logreg <- update(lasso_logreg, alpha = 0)
plot(ridge_logreg, xvar = "lambda")</pre>
```



 $pretty_coefs(coef(ridge_logreg, s = exp(2)))$ # all shrunk but no real ranking or anything

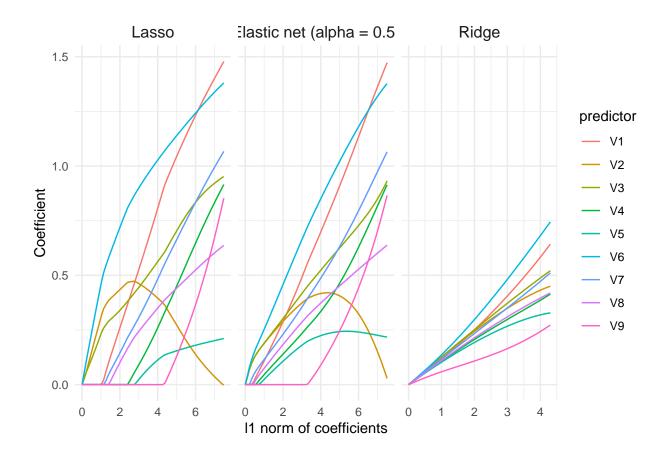
```
## # A tibble: 10 x 2
##
      predictor coefficient
      <chr>
##
                         <dbl>
##
    1 (Intercept)
                       -0.630
                        0.0457
    2 V6
##
##
    3 V3
                        0.0448
##
    4 V2
                        0.0447
##
    5 V7
                        0.0414
    6 V1
                        0.0395
##
                        0.0391
##
    7 V8
                        0.0383
##
    8 V4
                        0.0373
## 9 V5
## 10 V9
                        0.0224
```

```
elastic_logreg <- update(lasso_logreg, alpha = 0.5)
plot(elastic_logreg, xvar = "lambda")</pre>
```



pretty_coefs(coef(elastic_logreg, s = exp(-1.2))) # all shrunk AND "ranking"

```
## # A tibble: 9 x 2
##
     predictor
                 coefficient
     <chr>>
                        <dbl>
                      -0.719
## 1 (Intercept)
                       0.298
## 2 V6
## 3 V3
                       0.215
## 4 V2
                       0.213
## 5 V1
                       0.148
## 6 V7
                       0.141
                       0.0996
## 7 V8
## 8 V4
                       0.0675
## 9 V5
                       0.0435
```



Over-fitting biopsy

It's a little data set but let's try and split into training and test sets. There is quite some over-fitting on the relative scale, but the absolute prediction error difference is minor.

```
set.seed(42) # reproducible stochastic code
train_idx <- runif(nrow(biopsy_complete)) <= 0.8 # not exactly indices
mean(train_idx) # fraction in training set

## [1] 0.806735

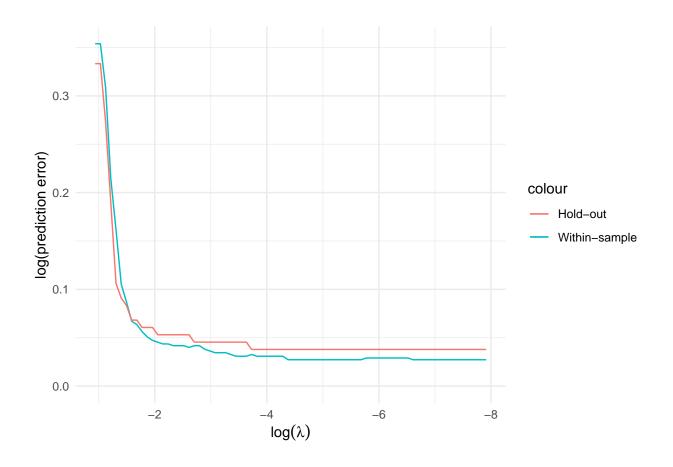
biopsy_train <- filter(biopsy_complete, train_idx)
biopsy_test <- filter(biopsy_complete, !train_idx)
all_equal(biopsy_complete, bind_rows(biopsy_train, biopsy_test)) # sanity check

## [1] TRUE

# Alternative with actual indices (mostly a matter of taste)
set.seed(42)
train_idx <- which(runif(nrow(biopsy_complete)) <= 0.8)
length(train_idx) / nrow(biopsy_complete)

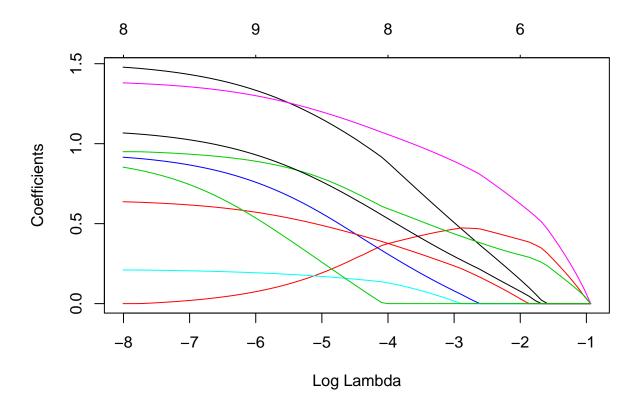
## [1] 0.806735</pre>
```

```
biopsy_train <- slice(biopsy_complete, train_idx)</pre>
biopsy_test <- slice(biopsy_complete, -train_idx)</pre>
all_equal(biopsy_complete, bind_rows(biopsy_train, biopsy_test)) # sanity check
## [1] TRUE
# Normalise predictors and put them in matrix format
predictors_train <- select(biopsy_train, -ID, -class) %>%
    scale()
predictors_test <- select(biopsy_test, -ID, -class) %>%
    scale()
# Train model
lasso_biopsy_train <- glmnet(predictors_train, biopsy_train$class, family = "binomial")</pre>
D_train <- predict(lasso_biopsy_train, predictors_train, type = "class") %>%
    apply(2, function(.) mean(. != biopsy_train$class)) # s39 is the best-performing
D_test <- predict(lasso_biopsy_train, predictors_test, type = "class") %>%
    apply(2, function(.) mean(. != biopsy_test$class))
tibble(D_test = D_test[which.min(D_train)],
       D_train = D_train[which.min(D_train)],
       D_diff_abs = scales::percent(D_test - D_train),
       D_diff_rel = scales::percent((D_test - D_train) / D_train, big.mark = ","))
## # A tibble: 1 x 4
    D_test D_train D_diff_abs D_diff_rel
      <dbl> <dbl> <chr>
                               <chr>>
## 1 0.0379 0.0272 1%
                               39%
ggplot(mapping = aes(x = log(lasso_biopsy_train$lambda))) +
    coord_cartesian(ylim = c(0, NA)) +
    geom_line(aes(y = D_train, colour = "Within-sample")) +
    geom_line(aes(y = D_test, colour = "Hold-out")) +
   labs(y = "log(prediction error)", x = expression(log(lambda))) +
    scale_x_reverse()
```



Delassoing

plot(lasso_logreg, xvar = "lambda")



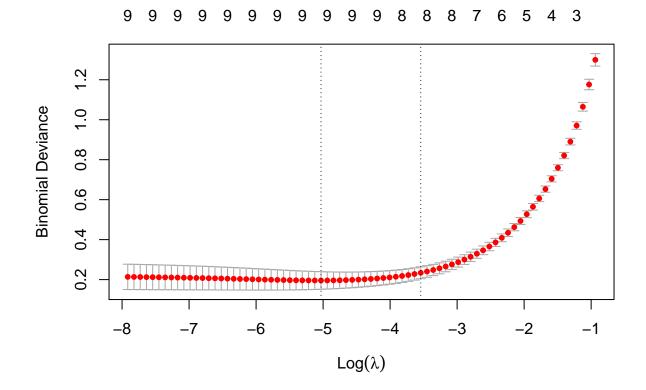
```
lambda \leftarrow \exp(-4.5)
beta <- coef(lasso_logreg, x = biopsy_predictors, y = biopsy_complete$class,
             s = lambda/nrow(biopsy_complete), exact = TRUE)
delasso_fit <- fixedLassoInf(biopsy_predictors, as.numeric(biopsy_complete$class)-1, beta, lambda, "bin
                              alpha = 0.05)
## Warning in fixedLogitLassoInf(x, y, beta, lambda, alpha = alpha, type =
## type, : Solution beta does not satisfy the KKT conditions (to within specified
## tolerances)
delasso_fit
##
## Call:
## fixedLassoInf(x = biopsy_predictors, y = as.numeric(biopsy_complete$class) -
##
       1, beta = beta, lambda = lambda, family = "binomial", alpha = 0.05)
##
   Testing results at lambda = 0.011, with alpha = 0.050
##
##
          Coef Z-score P-value LowConfPt UpConfPt LowTailArea UpTailArea
##
    Var
                                              2.005
##
         1.509
                 3.770
                          0.596
                                   -9.749
                                                          0.025
                                                                      0.024
##
      2 -0.019
                -0.030
                          0.989
                                    0.857
                                                Inf
                                                          0.025
                                                                      0.000
        0.964
                          0.962
                                              0.570
                                                          0.000
                                                                      0.025
##
                 1.399
                                     -Inf
##
        0.947
                 2.680
                          0.808
                                  -17.165
                                              1.237
                                                          0.025
                                                                      0.024
                                  -10.079
##
      5 0.215
                 0.617
                          0.863
                                              0.635
                                                          0.025
                                                                      0.024
##
      6
        1.396
                 4.084
                          0.000
                                    0.743
                                              3.114
                                                          0.025
                                                                      0.025
                          0.749
##
      7
        1.095
                 2.611
                                  -14.329
                                              1.537
                                                          0.025
                                                                      0.025
##
        0.650
                 1.889
                          0.805
                                  -12.461
                                              1.008
                                                          0.025
                                                                      0.025
        0.927
                          0.705
                                  -10.952
                                              1.724
                                                                      0.025
##
                 1.629
                                                          0.025
```

```
##
## Note: coefficients shown are full regression coefficients
```

Cross-validation

Use cross-validation to find best λ value. We found quite clear over-fitting above. Let's try to remedy this with cross-validation.

```
lasso_logreg_cv <- cv.glmnet(predictors_train, biopsy_train$class, family = "binomial")
plot(lasso_logreg_cv)</pre>
```

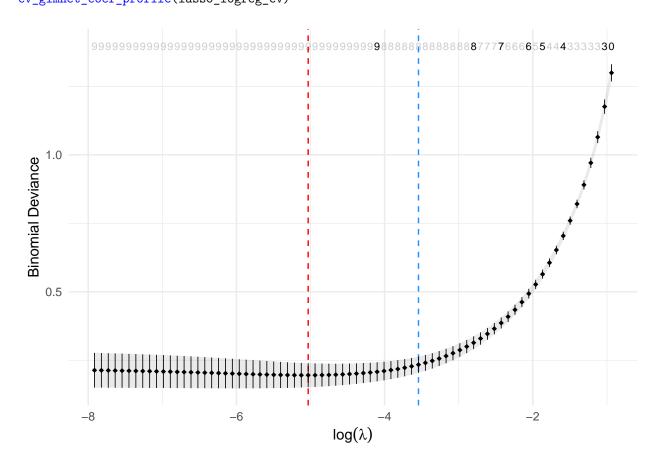


```
with(lasso_logreg_cv, data.frame(lambda.min, lambda.1se))

## lambda.min lambda.1se
## 1 0.006531203 0.02893729

# With ggplot2 (more control and prettier)
cv_glmnet_coef_profile <- function(fit) {
    fade_text <- function(x, alpha = 0.2) {
        ifelse(paste(x) == lag(paste(x), default = ""), alpha, 1)
    }
    every_n <- function(x, n = 5) {
        seq_along(x) %% n == 0
    }
    with(fit, tibble(log_lambda = log(lambda), cvm, cvup, cvlo, nzero)) %>%
        ggplot(aes(x = log_lambda)) +
        geom_vline(xintercept = log(fit$lambda.min), linetype = 2, size = 0.5, colour = "red") +
```

```
geom_vline(xintercept = log(fit$lambda.1se), linetype = 2, size = 0.5, colour = "dodgerblue
geom_linerange(aes(ymin = cvlo, ymax = cvup), size = 0.3) +
geom_ribbon(aes(ymin = cvlo, ymax = cvup), alpha = 0.1) +
geom_point(aes(y = cvm), shape = 18, size = 1.5) +
geom_text(aes(y = max(cvup) * 1.05, label = nzero, alpha = fade_text(nzero)), size = 8 / gg
scale_alpha_identity() +
labs(x = expression(log(lambda)), y = fit$name) +
theme_minimal()
}
cv_glmnet_coef_profile(lasso_logreg_cv)
```



Test out-of-sample performance of the CV model

```
pred_min <- predict(lasso_logreg_cv, predictors_test, s = "lambda.min", type = "class")
pred_1se <- predict(lasso_logreg_cv, predictors_test, s = "lambda.1se", type = "class")</pre>
```

Cross-validation to pick best combination of λ and α

• grid search over alpha and lambda

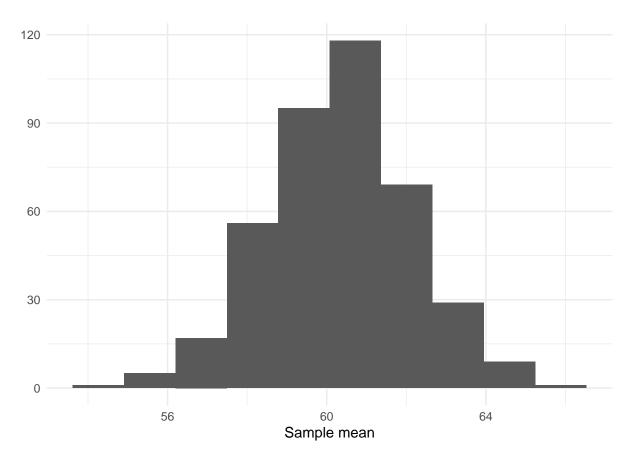
Resampling methods: jackknife and bootstrap

Sampling distribution

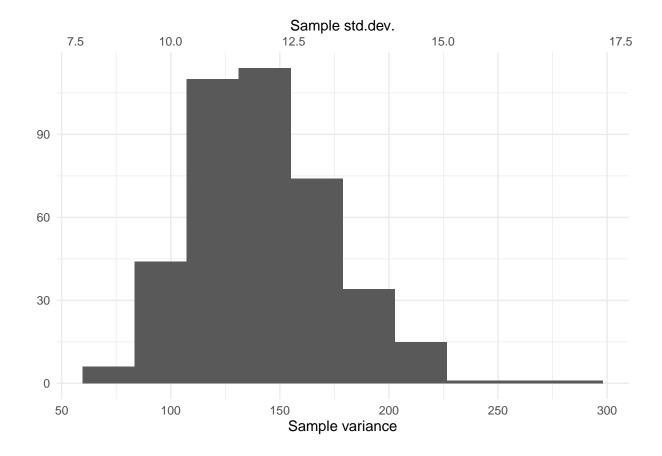
```
age <- rnorm(1000, 60, 12)
age <- age + 2 * (age < 30)
age_samples <- ldply(setNames(1:400, 1:400), function(i) {</pre>
        set.seed(42 + i)
        enframe(sample(age, 40, replace = FALSE))
    }, .id = "sample") %>%
    group_by(sample) %>%
    mutate(facet_title = sprintf("%s: Mean = %.1f", sample, mean(value)))
ggplot(filter(age_samples, sample %in% 1:20), aes(value)) +
    geom_histogram(bins = 10) +
    facet wrap(~ facet title, ncol = 5) +
    labs(x = "Age", y = "N")
         1: Mean = 57.0
                          10: Mean = 59.9
                                             11: Mean = 59.4
                                                               12: Mean = 61.7
                                                                                 13: Mean = 60.8
   15
   10
    5
    0
        14: Mean = 60.1
                          15: Mean = 60.4
                                             16: Mean = 61.0
                                                               17: Mean = 61.3
                                                                                 18: Mean = 58.9
   15
   10
    5
    0
Z
        19: Mean = 60.9
                           2: Mean = 61.9
                                             20: Mean = 61.1
                                                               3: Mean = 63.6
                                                                                 4: Mean = 60.3
   15
   10
    5
    0
         5: Mean = 61.0
                           6: Mean = 60.6
                                             7: Mean = 62.2
                                                               8: Mean = 60.0
                                                                                 9: Mean = 57.6
   15
   10
    5
    0
      20 40 60 80 100 20 40 60 80 100 20 40 60 80 100 20 40 60 80 100 20 40 60 80 100 20 40 60 80 100
                                                 Age
aggregate_stats_age <- group_by(age_samples, sample) %>%
    summarise("Sample mean" = mean(value),
               "Sample variance" = var(value),
               "Sample 90-percentile" = quantile(value, 0.9))
## 'summarise()' ungrouping output (override with '.groups' argument)
```

```
sample_plot <- llply(paste("Sample", c("mean", "variance", "90-percentile")),
     function(.) qplot(x = !!sym(.), data = aggregate_stats_age, geom = "histogram", bins = 10))</pre>
```

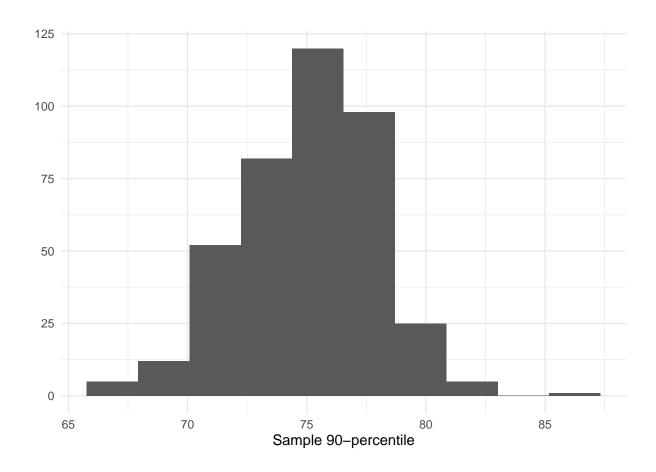
sample_plot[[1]]



sample_plot[[2]] + scale_x_continuous(sec.axis = sec_axis(sqrt, "Sample std.dev."))



sample_plot[[3]]



Jacknife

```
x < -c(8.26, 6.33, 10.4, 5.27, 5.35, 5.61, 6.12, 6.19, 5.2, 7.01, 8.74, 7.78, 7.02, 6, 6.5, 5.8, 5.12, 7.01, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.12, 6.1
coef_var <- function(x) sqrt(var(x))/mean(x) # coefficient of variation</pre>
coef_var(x)
## [1] 0.2524712
library(bootstrap)
##
## Attaching package: 'bootstrap'
## The following object is masked from 'package:broom':
##
##
                                       bootstrap
jackknife(x, coef_var)
## $jack.se
## [1] 0.05389943
##
## $jack.bias
## [1] -0.009266436
```

```
##
## $jack.values
## [1] 0.2563873 0.2565586 0.2384298 0.2507329 0.2513200 0.2530603 0.2557374
## [8] 0.2560293 0.2501992 0.2580969 0.2541045 0.2577524 0.2581067 0.2551946
## [15] 0.2571038 0.2541711 0.2495662 0.2581975 0.2571609 0.2561093 0.2020978
## [22] 0.2529980 0.2515338 0.2573745 0.2541045
##
## $call
## jackknife(x = x, theta = coef_var)
```

Exercise: cross-validation

```
library(MASS)
data(biopsy)
biopsy_complete <- na.exclude(biopsy)</pre>
summary(biopsy complete)
                                                                VЗ
##
         ID
                             V1
                                               ٧2
                             : 1.000
                                               : 1.000
                                                                : 1.000
##
   Length:683
                       Min.
                                        Min.
                                                          Min.
                       1st Qu.: 2.000
                                        1st Qu.: 1.000
   Class :character
                                                          1st Qu.: 1.000
##
  Mode :character
                       Median : 4.000
                                        Median : 1.000
                                                          Median : 1.000
##
                       Mean
                             : 4.442
                                        Mean : 3.151
                                                          Mean
                                                                 : 3.215
                       3rd Qu.: 6.000
                                        3rd Qu.: 5.000
##
                                                          3rd Qu.: 5.000
##
                       Max.
                              :10.000
                                        Max.
                                               :10.000
                                                          Max.
                                                                 :10.000
##
          ۷4
                          V5
                                           ۷6
                                                             ۷7
         : 1.00
                    Min. : 1.000
                                           : 1.000
                                                             : 1.000
##
  Min.
                                     Min.
                                                       Min.
   1st Qu.: 1.00
                    1st Qu.: 2.000
                                     1st Qu.: 1.000
                                                       1st Qu.: 2.000
##
  Median: 1.00
                    Median : 2.000
                                     Median : 1.000
                                                       Median : 3.000
## Mean
         : 2.83
                    Mean : 3.234
                                     Mean
                                           : 3.545
                                                       Mean : 3.445
  3rd Qu.: 4.00
                                     3rd Qu.: 6.000
                                                       3rd Qu.: 5.000
##
                    3rd Qu.: 4.000
##
   Max.
          :10.00
                    Max.
                           :10.000
                                             :10.000
                                                       Max.
                                                              :10.000
                                     Max.
##
          ٧8
                          V9
                                            class
  Min.
          : 1.00
                    Min.
                           : 1.000
                                     benign
                                               :444
  1st Qu.: 1.00
                    1st Qu.: 1.000
                                     malignant:239
##
## Median : 1.00
                    Median : 1.000
## Mean
          : 2.87
                          : 1.603
                    Mean
## 3rd Qu.: 4.00
                    3rd Qu.: 1.000
## Max.
           :10.00
                    Max.
                           :10.000
predictors <- biopsy_complete %>%
    select(-ID, -class)
pca_fit <- prcomp(predictors, scale = TRUE)</pre>
df_pca <- data.frame(pca_fit$x[, 1:4], outcome = biopsy_complete$class)</pre>
glm_fit <- glm(outcome ~ PC1 + PC2 + PC3 + PC4, data = df_pca, family = binomial)</pre>
summary(glm_fit)
##
## Call:
## glm(formula = outcome ~ PC1 + PC2 + PC3 + PC4, family = binomial,
##
       data = df_pca)
##
## Deviance Residuals:
```

```
Median
                1Q
                                  3Q
                              0.0228
## -3.1791 -0.1304 -0.0619
                                       2.4799
##
## Coefficients:
              Estimate Std. Error z value Pr(>|z|)
                           0.3035 -3.539 0.000402 ***
## (Intercept) -1.0739
                           0.2556 -9.445 < 2e-16 ***
## PC1
               -2.4140
                           0.5050 -0.315 0.752540
## PC2
               -0.1592
## PC3
                0.7191
                           0.3273
                                   2.197 0.028032 *
## PC4
               -0.9151
                           0.3691 -2.479 0.013159 *
## Signif. codes: 0 '*** 0.001 '** 0.01 '* 0.05 '.' 0.1 ' 1
## (Dispersion parameter for binomial family taken to be 1)
##
##
      Null deviance: 884.35 on 682 degrees of freedom
## Residual deviance: 106.12 on 678 degrees of freedom
## AIC: 116.12
## Number of Fisher Scoring iterations: 8
tidy(glm_fit)
## # A tibble: 5 x 5
              estimate std.error statistic p.value
   term
                  <dbl>
    <chr>
                           <dbl>
                                      <dbl>
                                                <dbl>
                  -1.07
                             0.303
                                      -3.54 4.02e- 4
## 1 (Intercept)
## 2 PC1
                  -2.41
                             0.256
                                      -9.44 3.56e-21
                                      -0.315 7.53e- 1
## 3 PC2
                  -0.159
                             0.505
## 4 PC3
                  0.719
                             0.327
                                      2.20 2.80e- 2
                                      -2.48 1.32e- 2
## 5 PC4
                  -0.915
                             0.369
```

1. LOO-CV error rate

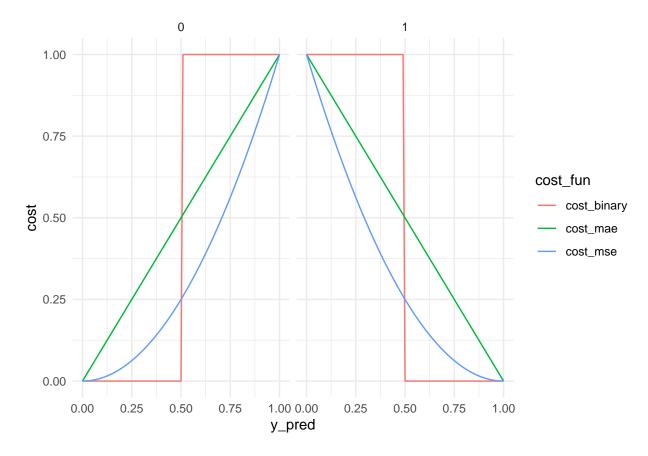
```
library(boot)
glm_fit_loocv <- cv.glm(df_pca, glm_fit)
glm_fit_loocv$delta
## [1] 0.02301890 0.02301788</pre>
```

2. Use proper cost function

```
glm_fit_loocv2 <- cv.glm(df_pca, glm_fit, cost = function(r, pi = 0) mean(abs(r-pi) > 0.5))
glm_fit_loocv2$delta
## [1] 0.02781845 0.02785918
```

3. Difference between error rates, and their interpretation

The binary cost function forces the predictions into a binary class assignment (w.r.t. the 0.5 thresh



4. 10-fold CV

```
# The error rates change quite a bit, which makes sense because 10-fold CV has a lot fewer folds than L glm_fit_10cv <- update(glm_fit_loocv, K = 10) glm_fit_10cv$delta

## [1] 0.02412049 0.02399288

# glm_fit_10cv2 <- cv.glm(df_pca, glm_fit, cost = function(r, pi = 0) mean(abs(r-pi) > 0.5), K = 10) glm_fit_10cv2 <- update(glm_fit_loocv2, K = 10) glm_fit_10cv2$delta

## [1] 0.03074671 0.03118830
```

Exercise: penalised regression

- 1. + 2. Lasso regression
- 3. Why does it normally make sense to normalise predictors
- 4. Using CV to get reasonable estimate of λ
- 5. Obtain coefficients for "best" λ
- 6. Re-fit with correct family

Quite some difference between the sets of predictors kept:

- 7. As ridge regression
- 8. Get idea about sparse solution using ridge results?
- 9. Elastic net ($\alpha = 0.5$)

Ideally, one should do CV over α as well.

- 10. Delasso the results
- 11. Selective inference