

STK-IN4300
Statistical Learning Methods in Data
Science

OBLIG 2

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Problem 1

(a)

We consider two linear regression models:

Model 1 (raw counts): each count variable ($H050, nN, C040$) enters linearly.

Model 2 (dummy counts): counts are transformed to binary indicators $I(\text{count} > 0)$.

Both models were fitted on the training set and evaluated using test MSE. Model 1 yields:

$$\text{Train MSE} = 1.597, \quad \text{Test MSE} = 1.135.$$

Model 2 yields:

$$\text{Train MSE} = 1.662, \quad \text{Test MSE} = 1.159.$$

Model 1 performs slightly better on both sets. A scatterplot of observed vs. predicted LC50 for Model 1 is displayed in Figure 1.

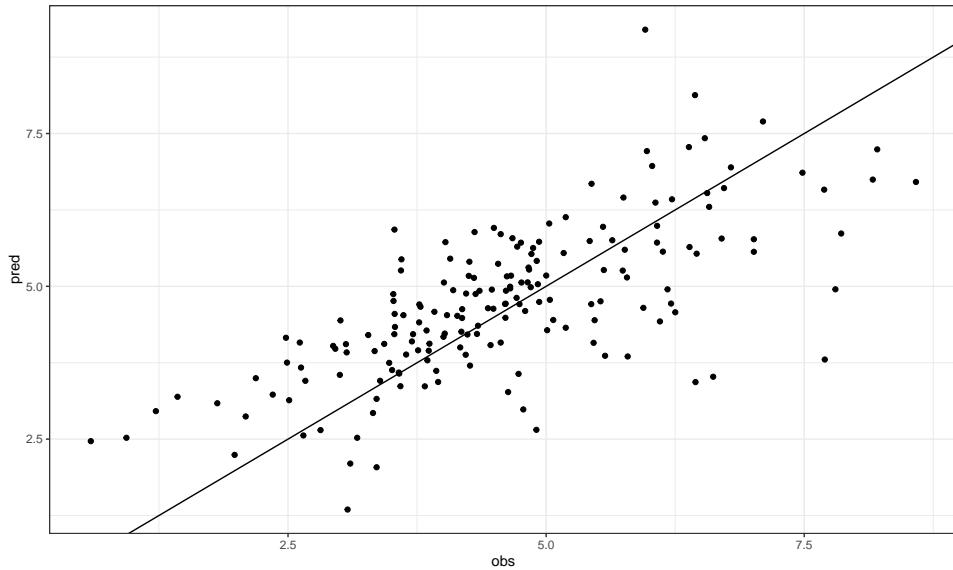


Figure 1: Observed vs. predicted LC50 on the test set for the full linear model.

Comment: The raw numeric encoding preserves more information than the binary transformation. Dummy-encoding destroys magnitude information (e.g., count 1 vs. count 6 both become 1), producing weaker predictive performance.

```
> cat("train_mse_m1", mean((tr$LC50 - p1)^2),
  "test_mse_m1", mean((te$LC50 - q1)^2), "\n")
```

```

train_mse_m1 1.596771 test_mse_m1 1.135048

> cat("train_mse_m2", mean((tr$LC50 - p2)^2),
"test_mse_m2", mean((te$LC50 - q2)^2), "\n")

train_mse_m2 1.661986 test_mse_m2 1.159321

```

(b)

We repeated the procedure in (a) 200 times, each time taking a new random split and refitting both models. The empirical distributions of the resulting test MSE values are shown in Figure 2.

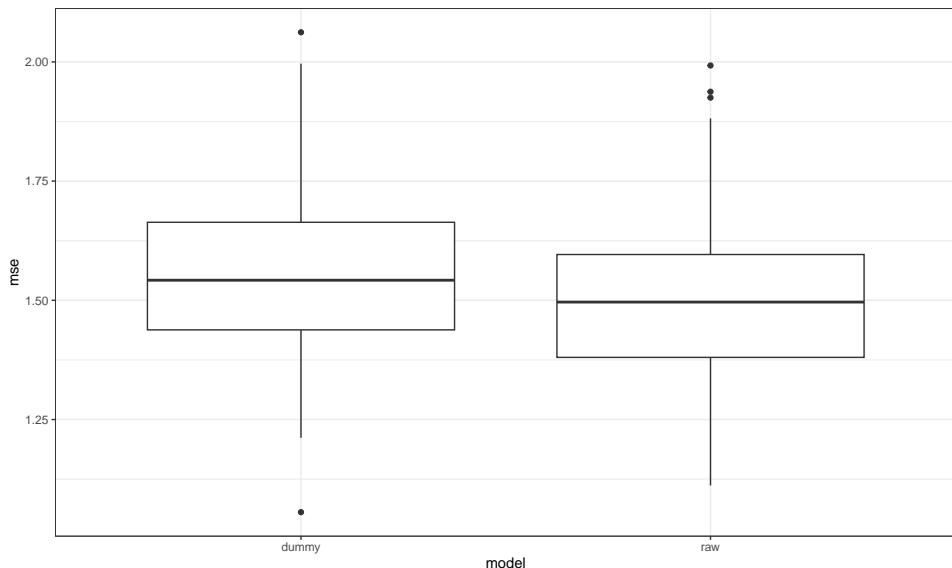


Figure 2: Empirical distribution of test MSE across 200 repetitions for raw count encoding vs. dummy encoding.

Average test error:

Raw counts mean MSE = 1.50, Dummy counts mean MSE = 1.55.

Comment: Repeating the experiment avoids conclusions based on a single lucky (or unlucky) split. Again, dummy-encoding performs worse on average because it removes valuable numerical information about the atomic counts.

```

> cat("mean_test_mse_raw", mean(e1), "\n")
mean_test_mse_raw 1.501142
> cat("mean_test_mse_dummy", mean(e2), "\n")
mean_test_mse_dummy 1.552159

```

(c)

Using the split from (a), we applied variable selection with AIC and BIC, using both forward and backward selection. The selected models were:

- Backward AIC: $LC50 \sim TPSA + SAacc + MLOGP + RDCHI + GATS1p + nN$
- Forward AIC: $LC50 \sim MLOGP + TPSA + SAacc + nN + GATS1p + RDCHI$
- Backward BIC: $LC50 \sim TPSA + SAacc + MLOGP + nN$
- Forward BIC: $LC50 \sim MLOGP + TPSA + SAacc + nN$

Both AIC procedures agree (six predictors). Both BIC procedures agree (four predictors). BIC is more conservative and penalises complexity more strongly.

```
backward_AIC: LC50 ~ TPSA + SAacc + MLOGP + RDCHI + GATS1p + nN
forward_AIC : LC50 ~ MLOGP + TPSA + SAacc + nN + GATS1p + RDCHI
backward_BIC: LC50 ~ TPSA + SAacc + MLOGP + nN
forward_BIC : LC50 ~ MLOGP + TPSA + SAacc + nN
```

(d)

We fit ridge regression over a grid $\lambda = 10^{-4}, \dots, 10^4$ and select λ using both 10-fold cross-validation and a bootstrap OOB estimate. The resulting MSE as a function of $\log \lambda$ is shown in Figure 3.

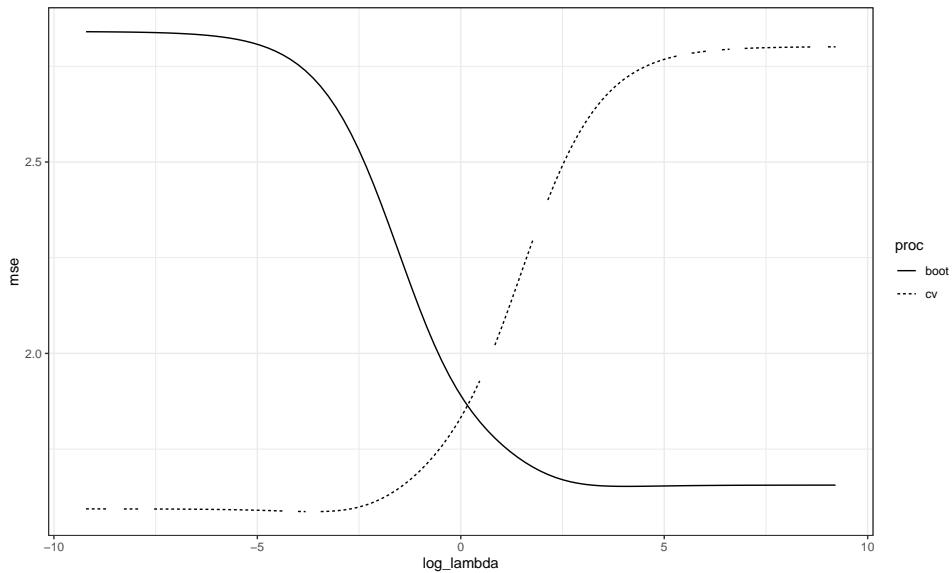


Figure 3: Ridge regression: bootstrap vs. cross-validation test error curves.

Cross-validation and bootstrap produce nearly identical minima. The ridge model achieves test MSE ≈ 1.33 , competitive with the best linear models.

(e)

To allow nonlinear effects, we fit GAM models with smoothing splines. We tried:

$$k = 4 \quad (\text{low complexity}), \quad k = 7 \quad (\text{higher complexity}).$$

$$\text{GAM}_{k=4} : \text{Test MSE} = 1.39, \quad \text{GAM}_{k=7} : \text{Test MSE} = 1.44.$$

The smoother model ($k = 7$) overfits slightly and generalises worse. The GAM with moderate flexibility improves over plain linear regression, but not over AIC-selected models or ridge.

(f)

We fitted a regression tree and pruned it using cost-complexity pruning. The optimal CP value was obtained from the minimum cross-validated error in the CP table. Figure 4 shows the CP curve, and the pruned tree is shown in Figure 5.

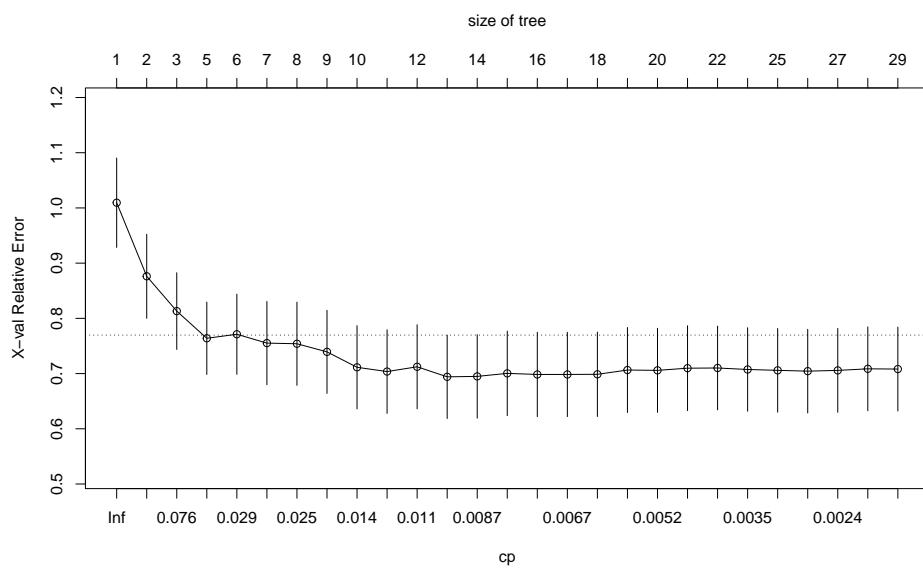


Figure 4: Cost-complexity pruning plot for the regression tree.

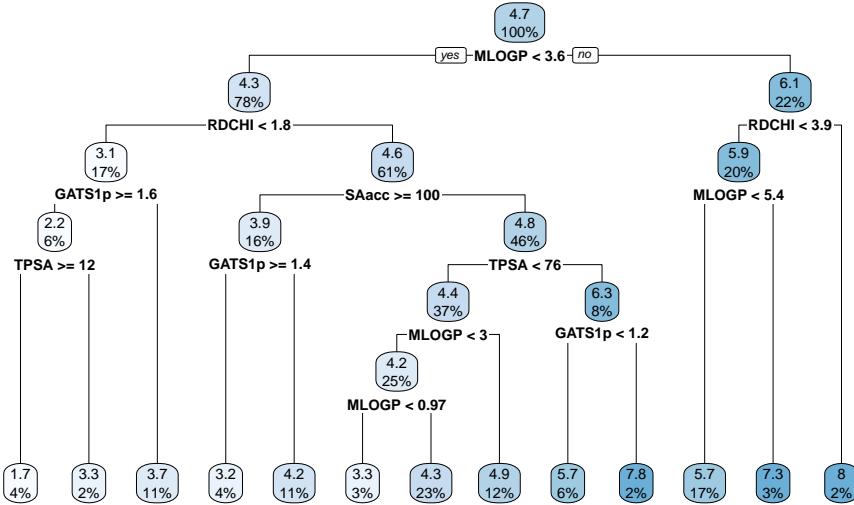


Figure 5: Pruned regression tree predicting LC50.

The final tree achieves

$$\text{Train MSE} = 1.16, \quad \text{Test MSE} = 1.79,$$

indicating substantial overfitting relative to linear and GAM models.

(g)

Table 1 summarises the training and test MSE of all methods.

Model	Train MSE	Test MSE
Stepwise AIC (forward/backward)	1.49	1.32
Ridge (CV)	1.49	1.33
GAM ($k = 4$)	1.40	1.39
Stepwise BIC	1.52	1.43
GAM ($k = 7$)	1.26	1.44
Full linear model	1.60	1.14
Tree	1.16	1.79

Table 1: Comparison of predictive performance across all models.

Conclusion: The lowest test error is obtained by the AIC-selected linear models and ridge regression. Tree-based models overfit heavily. GAMs help capture nonlinearities, but moderate smoothing works best. Overall, model selection + linear regression (or ridge) is the preferred choice.

Problem 2

(a)

We split the data into training and test sets while preserving class balance (two-thirds for training, one-third for testing). For $k = 1, \dots, 30$ we computed:

- 5-fold CV error
- LOOCV error
- Test error on the held-out set

Figure 6 shows the error curves.

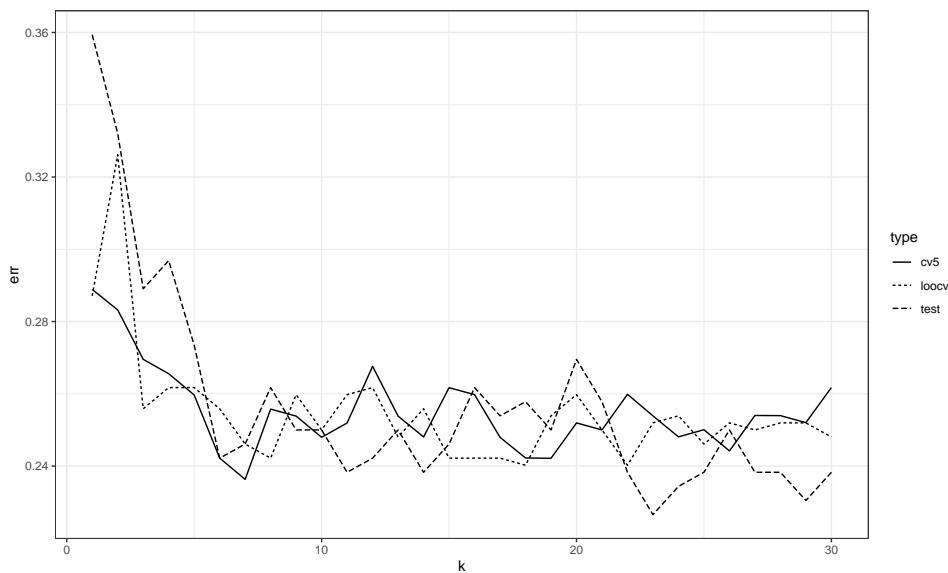


Figure 6: 5-fold CV, LOOCV and test error for k -NN.

Minimum 5-fold CV error:

$$\min(\text{CV}_5) = 0.236, \quad \text{Test error at this } k = 0.246.$$

5-fold CV and LOOCV give very similar minima, confirming stability in choice of k .

```
2a_cv5_min 0.2363125
2a_loocv_min 0.2402344
2a_test_at_k_cv5 0.2460938
```

(b)

We fit a GAM with separate smooth functions for each predictor:

$$\text{logit}(P(\text{pos})) = s(\text{pregnant}) + s(\text{glucose}) + s(\text{pressure}) + s(\text{triceps}) + s(\text{insulin}) + s(\text{mass}) + s(\text{pedigree}) + s(\text{age}).$$

Using the trained model on the test set:

$$\text{GAM test error} = 0.25.$$

The GAM performs similarly to the optimal k -NN, capturing smooth nonlinear effects without overfitting strongly.

```
> cat("2b_gam_test", te_gam, "\n")
2b_gam_test 0.25
```

(c)

We compare tree-based classifiers on the same split:

- Pruned CART tree (cp chosen by cross-validation) - Bagging (200 trees) - Random forest (500 trees)

The pruned tree is shown in Figure 7.

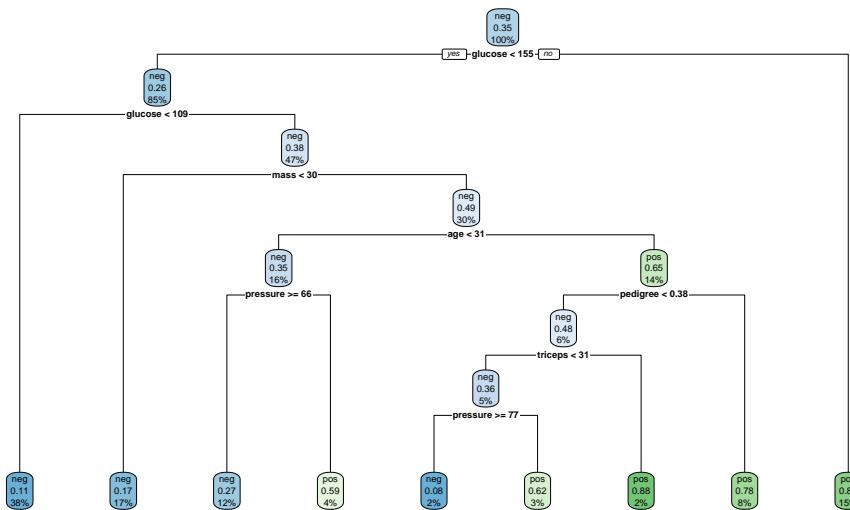


Figure 7: Pruned classification tree for diabetes prediction.

Training and test errors:

Tree: Train = 0.176, Test = 0.254

Bagging: Train = 0, Test = 0.227

Random forest: Train = 0, Test = 0.238

Bagging achieves the lowest test error among tree-based methods. The CART tree overfits less but is less accurate.

```
2c_tree 0.1757812 0.2539062
2c_bag 0 0.2265625
2c_rf 0 0.2382812
```

(d)

Comparing all methods so far:

Best test error = 0.227 (bagging).

Bagging improves substantially over a single CART tree. The unpruned tree has high variance, and even after pruning its performance remains worse. Bagging averages many trees trained on bootstrap samples, reducing variance and producing the best generalisation error among all methods we have tried so far.

```
2d_best_by_test 0.2265625
```

(e)

We repeat the entire analysis on PimaIndiansDiabetes2, removing missing values. Using the same best k from (a), and fitting GAM, tree, bagging, and random forest:

k -NN: Test error = 0.169

GAM: Test error = 0.208

Tree: Test error = 0.200

Bagging: Test error = 0.192

Random forest: Test error = 0.192

The cleaned dataset reduces overall error rates. The best performer is k -NN with test error 0.169, followed by bagging and random forest.

Summary

- Cross-validated k -NN and GAM perform similarly on the original data.
- Bagging and random forest reduce variance and outperform a single tree.
- After removing missing values, all models improve; k -NN becomes the clear winner.

```
2e_knn 0.1692308
2e_gam 0.2076923
2e_tree 0.2
2e_bag 0.1923077
2e_rf 0.1923077
```

R-code

Problem 1

```

1 library(tidyverse)
2 library(MASS)
3 library(rpart)
4 library(rpart.plot)
5 library(glmnet)
6 library(mgcv)
7 set.seed(4300)
8 theme_set(theme_bw())
9
10 # =====
11 # Problem 1: QSAR Aquatic Toxicity Regression
12 # =====
13
14 # -----
15 # Load and prepare data
16 # -----
17 df <- read.csv("data/qsar_aquatic_toxicity.csv", sep=";", header=
18   FALSE) %>%
19   as_tibble()
20
21 colnames(df) <- c("TPSA", "SAacc", "H050", "MLOGP", "RDCHI", "GATS1p", "nN",
22   "C040", "LC50")
23
24 # Train/test split ( 2/3 training, 1/3 test)
25 i <- sample(1:nrow(df), round(2 * nrow(df) / 3))
26 tr <- df[i, ]
27 te <- df[-i, ]
28
29 # -----
30 # (a) Linear models: raw counts vs. dummy-encoded counts
31 # -----
32
33 # Model with raw counts included as linear terms
34 m1 <- lm(LC50 ~ ., data = tr)
35
36 # Dummy model: use 0/1 indicators for count variables
37 m2 <- lm(LC50 ~ TPSA + SAacc + MLOGP + RDCHI + GATS1p +
38   I(H050 > 0) + I(nN > 0) + I(C040 > 0),
39   data = tr)
40
41 # Predictions and train/test MSE
42 p1 <- predict(m1, tr); q1 <- predict(m1, te)
43 p2 <- predict(m2, tr); q2 <- predict(m2, te)
44
45 cat("train_mse_m1", mean((tr$LC50 - p1)^2),
46     "test_mse_m1", mean((te$LC50 - q1)^2), "\n")

```

```

45 cat("train_mse_m2", mean((tr$LC50 - p2)^2),
46     "test_mse_m2", mean((te$LC50 - q2)^2), "\n")
47
48 # Scatterplot of observed vs predicted
49 p <- ggplot(tibble(obs = te$LC50, pred = q1),
50               aes(obs, pred)) +
51   geom_point() +
52   geom_abline()
53 ggsave("plots/plot1a.pdf", p, width=10, height=6)
54
55 # -----
56 # (b) Repeat experiment 200 times to estimate test error
57 # distribution
58 # -----
58 e1 <- numeric(200) # raw counts model
59 e2 <- numeric(200) # dummy model
60
61 for (k in 1:200) {
62   i <- sample(1:nrow(df), round(2 * nrow(df) / 3))
63   tr <- df[i, ]; te <- df[-i, ]
64
65   m1 <- lm(LC50 ~ ., data=tr)
66   m2 <- lm(LC50 ~ TPSA + SAacc + MLOGP + RDCHI + GATS1p +
67             I(H050 > 0) + I(nN > 0) + I(C040 > 0),
68             data=tr)
69
70   e1[k] <- mean((te$LC50 - predict(m1, te))^2)
71   e2[k] <- mean((te$LC50 - predict(m2, te))^2)
72 }
73
74 # Boxplot of empirical MSE distributions
75 t <- tibble(model = rep(c("raw", "dummy"), each=200),
76             mse = c(e1, e2))
77
78 p <- ggplot(t, aes(model, mse)) + geom_boxplot()
79 ggsave("plots/plot1b.pdf", p, width=10, height=6)
80
81 cat("mean_test_mse_raw", mean(e1), "\n")
82 cat("mean_test_mse_dummy", mean(e2), "\n")
83
84 # -----
85 # (c) Variable selection: forward/backward with AIC and BIC
86 # -----
87 full <- lm(LC50 ~ ., data=tr)
88 null <- lm(LC50 ~ 1, data=tr)
89
90 b_aic <- step(full, direction="backward", k=2, trace=0)
91 f_aic <- step(null, scope=formula(full), direction="forward", k=2,
92                 trace=0)
92 b_bic <- step(full, direction="backward", k=log(nrow(tr)), trace=0)

```

```

93 f_bic <- step(null, scope=formula(full), direction="forward", k=log(
94   nrow(tr)), trace=0)
95
95 cat("backward_AIC:", deparse(formula(b_aic)), "\n")
96 cat("forward_AIC :", deparse(formula(f_aic)), "\n")
97 cat("backward_BIC:", deparse(formula(b_bic)), "\n")
98 cat("forward_BIC :", deparse(formula(f_bic)), "\n")
99
100 # -----
101 # (d) Ridge regression: CV vs bootstrap OOB estimate
102 # -----
103 xtr <- as.matrix(dplyr::select(tr, -LC50))
104 ytr <- tr$LC50
105 xte <- as.matrix(dplyr::select(te, -LC50))
106 yte <- te$LC50
107
108 lambda_grid <- 10^seq(-4, 4, length=100)
109
110 # Cross-validation
111 cv <- cv.glmnet(xtr, ytr, alpha=0, lambda=lambda_grid, standardize=
112   TRUE)
113 lam_cv <- cv$lambda.min
114
114 tr_cv <- mean((ytr - predict(cv$glmnet.fit, s=lam_cv, newx=xtr))^2)
115 te_cv <- mean((yte - predict(cv$glmnet.fit, s=lam_cv, newx=xte))^2)
116
117 # Bootstrap OOB
118 B <- 200
119 oob_mse <- matrix(NA, B, length(lambda_grid))
120
121 for(b in 1:B){
122   idx <- sample(seq_len(nrow(tr)), replace=TRUE)
123   oob <- setdiff(seq_len(nrow(tr)), unique(idx))
124
125   fit <- glmnet(xtr[idx,], ytr[idx], alpha=0, lambda=lambda_grid,
126     standardize=TRUE)
127
127   if(length(oob) > 5){
128     pred_oob <- predict(fit, newx=xtr[oob,])
129     oob_mse[b,] <- colMeans((ytr[oob] - pred_oob)^2)
130   }
131 }
132
133 boot_curve <- colMeans(oob_mse, na.rm=TRUE)
134 lam_boot <- lambda_grid[which.min(boot_curve)]
135
136 # Save CV vs bootstrap plot
137 p <- tibble(log_lambda=log(lambda_grid),
138               cv=cv$cvm[match(lambda_grid, cv$lambda)],
139               boot=boot_curve) %>%
140   pivot_longer(-log_lambda, names_to="method", values_to="mse") %>%

```

```

141  ggplot(aes(log_lambda, mse, linetype=method)) +
142    geom_line()
143
144 ggsave("plots/plot1d.pdf", p, width=10, height=6)
145
146 # -----
147 # (e) GAM models with different smoothness
148 # -----
149 g1 <- gam(LC50 ~ s(TPSA,k=4) + s(SAacc,k=4) + s(H050,k=3) +
150   s(MLOGP,k=4) + s(RDCHI,k=4) + s(GATS1p,k=4) +
151   s(nN,k=3) + s(C040,k=3),
152   data=tr, method="REML")
153
154 g2 <- gam(LC50 ~ s(TPSA,k=7) + s(SAacc,k=7) + s(H050,k=3) +
155   s(MLOGP,k=7) + s(RDCHI,k=7) + s(GATS1p,k=7) +
156   s(nN,k=3) + s(C040,k=3),
157   data=tr, method="REML")
158
159 tr_g1 <- mean((tr$LC50 - predict(g1,tr))^2)
160 te_g1 <- mean((te$LC50 - predict(g1,te))^2)
161 tr_g2 <- mean((tr$LC50 - predict(g2,tr))^2)
162 te_g2 <- mean((te$LC50 - predict(g2,te))^2)
163
164 # -----
165 # (f) Regression tree + cost-complexity pruning
166 # -----
167 tree0 <- rpart(LC50 ~ ., data=tr, method="anova", cp=0.001)
168 cp_opt <- tree0$cptable[which.min(tree0$cptable[, "xerror"]), "CP"]
169
170 tree <- prune(tree0, cp=cp_opt)
171
172 tr_tree <- mean((tr$LC50 - predict(tree,tr))^2)
173 te_tree <- mean((te$LC50 - predict(tree,te))^2)
174
175 pdf("plots/plot1f_tree.pdf", width=10, height=6); rpart.plot(tree);
176   dev.off()
176 pdf("plots/plot1f_cp.pdf", width=10, height=6); plotcp(tree0); dev
177   .off()
178
179 # -----
180 # (g) Compare all models
181 # -----
181 res <- tibble(
182   model=c("lm_raw","lm_dummy","step_back_AIC","step_fwd_AIC",
183     "step_back_BIC","step_fwd_BIC","ridge_cv","ridge_boot",
184     "gam_k4","gam_k7","tree"),
185   train=c(mean((tr$LC50 - p1)^2), mean((tr$LC50 - p2)^2),
186     mean((tr$LC50 - predict(b_aic,tr))^2),
187     mean((tr$LC50 - predict(f_aic,tr))^2),
188     mean((tr$LC50 - predict(b_bic,tr))^2),
189     mean((tr$LC50 - predict(f_bic,tr))^2),

```

```
190     tr_cv, tr_boot, tr_g1, tr_g2, tr_tree),  
191 test=c(mean((te$LC50 - q1)^2), mean((te$LC50 - q2)^2),  
192     mean((te$LC50 - predict(b_aic,te))^2),  
193     mean((te$LC50 - predict(f_aic,te))^2),  
194     mean((te$LC50 - predict(b_bic,te))^2),  
195     mean((te$LC50 - predict(f_bic,te))^2),  
196     te_cv, te_boot, te_g1, te_g2, te_tree)  
197 ) %>% arrange(test)  
198  
199 print(res)
```

Problem 2

```
1 library(tidyverse)
2 library(mlbench)
3 library(class)
4 library(mgcv)
5 library(rpart)
6 library(rpart.plot)
7 library(ipred)
8 library(randomForest)
9 set.seed(4300)
10 theme_set(theme_bw())
11
12 # -----
13 # Problem 2 - Classification on PimaIndiansDiabetes
14 # -----
15
16 data("PimaIndiansDiabetes")
17 df <- as_tibble(PimaIndiansDiabetes)
18
19 # -----
20 # (a) Train/test split + kNN
21 # -----
22
23 # Stratified split: keep class balance
24 ix_pos <- which(df$diabetes == "pos")
25 ix_neg <- which(df$diabetes == "neg")
26
27 tr_ix <- c(
28   sample(ix_pos, round(2 * length(ix_pos) / 3)),
29   sample(ix_neg, round(2 * length(ix_neg) / 3))
30 )
31
32 tr <- df[tr_ix, ]
33 te <- df[-tr_ix, ]
34
35 # Standardize predictors using training mean/sd
36 Xtr <- scale(dplyr::select(tr, -diabetes))
37 ctr <- attr(Xtr, "scaled:center")
38 str <- attr(Xtr, "scaled:scale")
39
40 Xte <- scale(dplyr::select(te, -diabetes), center = ctr, scale = str)
41
42 ytr <- tr$diabetes
43 yte <- te$diabetes
44
45 kvals <- 1:30
46 cv5 <- rep(NA, length(kvals))
47 loocv <- rep(NA, length(kvals))
48 te_err <- rep(NA, length(kvals))
```

```

49
50 # Stratified 5-fold CV
51 folds <- 5
52 pos_f <- split(sample(which(ytr == "pos")), rep(1:folds, length.out
53   = sum(ytr == "pos")))
54 neg_f <- split(sample(which(ytr == "neg")), rep(1:folds, length.out
55   = sum(ytr == "neg")))
56
56
57
58 # 5-fold CV error
59 cv5[i] <- mean(sapply(1:folds, function(f){
60   tr_id <- c(unlist(pos_f[-f]), unlist(neg_f[-f]))
61   va_id <- c(unlist(pos_f[f]), unlist(neg_f[f]))
62   pr <- knn(train = Xtr[tr_id,], test = Xtr(va_id,], cl = ytr[tr_
63     id], k = k)
64   mean(pr != ytr(va_id))
65 }))
66
67 # LOOCV error
68 loocv[i] <- mean(knn.cv(Xtr, ytr, k = k) != ytr)
69
70 # Test error
71 te_err[i] <- mean(knn(train = Xtr, test = Xte, cl = ytr, k = k) !=
72   yte)
73
74 # Plot all three error curves
75 p <- tibble(k = kvals, cv5 = cv5, loocv = loocv, test = te_err) %>%
76   pivot_longer(-k, names_to = "type", values_to = "err") %>%
77   ggplot(aes(k, err, linetype = type)) + geom_line()
78
79 ggsave("plots/plot2a.pdf", p, width = 10, height = 6)
80
81 cat("2a_cv5_min", min(cv5),
82     "2a_loocv_min", min(loocv),
83     "2a_test_at_k_cv5", te_err[which.min(cv5)], "\n")
84
85 # -----
86 # (b) GAM model
87 # -----
88
89 g_full <- gam(
90   diabetes ~ s(pregnant) + s(glucose) + s(pressure) + s(triceps) +
91   s(insulin) + s(mass) + s(pedigree) + s(age),
92   family = binomial,
93   data = tr,
94   method = "REML",
95   select = TRUE

```

```

96 )
97
98 # Classify based on predicted probability > 0.5
99 pr_b <- ifelse(predict(g_full, te, type = "response") > 0.5, "pos",
100   "neg")
101 te_gam <- mean(pr_b != yte)
102 cat("2b_gam_test", te_gam, "\n")
103
104
105 # -----
106 # (c) Trees, Bagging, Random Forest
107 # -----
108
109 # CART tree + prune using optimal CP
110 tree <- rpart(diabetes ~ ., data = tr, method = "class", cp = 0.001)
111 cp_opt <- tree$cptable[which.min(tree$cptable[, "xerror"]), "CP"]
112 tree <- prune(tree, cp = cp_opt)
113
114 p_tr <- predict(tree, tr, type = "class")
115 p_te <- predict(tree, te, type = "class")
116
117 tr_tree <- mean(p_tr != ytr)
118 te_tree <- mean(p_te != yte)
119
120 # Save tree plot
121 pdf("plots/plot2c_tree.pdf", width = 10, height = 6)
122 rpart.plot(tree)
123 dev.off()
124
125 # Bagging
126 bag <- bagging(diabetes ~ ., data = tr, nbagg = 200)
127 tr_bag <- mean(predict(bag, tr, type = "class") != ytr)
128 te_bag <- mean(predict(bag, te, type = "class") != yte)
129
130 # Random Forest
131 rf <- randomForest(diabetes ~ ., data = tr, ntree = 500)
132 tr_rf <- mean(predict(rf, tr) != ytr)
133 te_rf <- mean(predict(rf, te) != yte)
134
135 cat("2c_tree", tr_tree, te_tree,
136   "2c_bag", tr_bag, te_bag,
137   "2c_rf", tr_rf, te_rf, "\n")
138
139
140 # -----
141 # (d) Best model by test error
142 # -----
143
144 cat("2d_best_by_test",
145   c("tree" = te_tree,

```

```

146     "bag" = te_bag,
147     "rf" = te_rf,
148     "gam" = te_gam)[ which.min(c(te_tree, te_bag, te_rf, te_gam))
149     ] ,
150
151
152 # -----
153 # (e) Repeat analysis on cleaned dataset
154 # -----
155
156 data("PimaIndiansDiabetes2")
157 df2 <- as_tibble(PimaIndiansDiabetes2) %>% drop_na()
158
159 # Stratified split again
160 ix_pos2 <- which(df2$diabetes == "pos")
161 ix_neg2 <- which(df2$diabetes == "neg")
162
163 tr_ix2 <- c(
164   sample(ix_pos2, round(2 * length(ix_pos2) / 3)),
165   sample(ix_neg2, round(2 * length(ix_neg2) / 3)))
166 )
167
168 tr2 <- df2[tr_ix2, ]
169 te2 <- df2[-tr_ix2, ]
170
171 # Standardize
172 Xtr2 <- scale(dplyr::select(tr2, -diabetes))
173 ctr2 <- attr(Xtr2, "scaled:center")
174 str2 <- attr(Xtr2, "scaled:scale")
175
176 Xte2 <- scale(dplyr::select(te2, -diabetes), center = ctr2, scale =
177   str2)
178
179 ytr2 <- tr2$diabetes
180 yte2 <- te2$diabetes
181
182 # Use best k from (a)
183 k <- kvals[which.min(cv5)]
184
185 te_knn2 <- mean(knn(train = Xtr2, test = Xte2, cl = ytr2, k = k) !=
186   yte2)
187
188 # GAM on cleaned data
189 g2 <- gam(
190   diabetes ~ s(pregnant) + s(glucose) + s(pressure) + s(triceps) +
191   s(insulin) + s(mass) + s(pedigree) + s(age),
192   family = binomial,
193   data = tr2,
194   method = "REML",
195   select = TRUE

```

```
194 )
195
196 te_gam2 <- mean(ifelse(predict(g2, te2, type = "response") > 0.5, "
197   pos", "neg") != yte2)
198
199 # Tree
200 tree2 <- rpart(diabetes ~ ., data = tr2, method = "class", cp =
201   0.001)
202 cp_opt2 <- tree2$cptable[which.min(tree2$cptable[, "xerror"]), "CP"]
203 tree2 <- prune(tree2, cp = cp_opt2)
204 te_tree2 <- mean(predict(tree2, te2, type = "class") != yte2)
205
206 # Bagging
207 bag2 <- bagging(diabetes ~ ., data = tr2, nbagg = 200)
208 te_bag2 <- mean(predict(bag2, te2, type = "class") != yte2)
209
210 # Random Forest
211 rf2 <- randomForest(diabetes ~ ., data = tr2, ntree = 500)
212 te_rf2 <- mean(predict(rf2, te2) != yte2)
213
214 cat("2e_knn", te_knn2,
215     "2e_gam", te_gam2,
216     "2e_tree", te_tree2,
217     "2e_bag", te_bag2,
218     "2e_rf", te_rf2, "\n")
```