Mandatory 1 - STK2100

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Problem 1

a) Given the regression models for the response Y and single covariate x, we can write the following as linear regression models
As is (i):

$$2. \quad Y = \beta_0 + \beta_1 \frac{1}{x} + \beta_2 x^2 + \varepsilon$$

If a parameter is kept fixed (ii):

$$\begin{aligned} 1. \quad Y &= \frac{\beta_0}{1+\beta_1 x} + \beta_2 x^{1/2} + \varepsilon \\ &\Downarrow \quad Z = \frac{1}{1+\beta_1 x} \quad | \ \beta_1 \text{ fixed} \\ Y &= \beta_0 Z + \beta_2 x^{1/2} + \varepsilon \end{aligned}$$

$$4. \quad Y = \beta_0 + \beta_1 x^{\beta_2} + \varepsilon \quad | \ \beta_2 \text{ fixed}$$

After a suitable transformation (iii):

$$\begin{aligned} 3. \quad Y &= \frac{1}{\beta_0 + \beta_1 x + \beta_2 x^2 + \varepsilon} \\ &\Downarrow \ Z = (Y^{-1}) \\ Z &= \beta_0 + \beta_1 x + \beta_2 x^2 + \varepsilon \end{aligned}$$

Both (ii) and (iii):

$$\begin{aligned} 5. \quad Y &= \beta_0 x^{\beta_1} \ \varepsilon \\ &\Downarrow \ Z = (\ln Y), \text{ and } \beta_0 \text{ fixed} \\ Z &= \ln(\beta_0) + \beta_1 \ln(x) + \ln(\varepsilon) \end{aligned}$$

b) For the models that can be used, their dimensions will be

- For 1. (after transformation) $\quad \mathbf{X}: \ (N \times 2)$ matric (without intercept), $\quad \beta: \ (2 \times 1)$ vector

- For 2. $\mathbf{X}:$ $(N \times 3)$ matrix (with intercept), $\beta:$ (3×1) vector
- For 4. $\mathbf{X}:$ $(N \times 2)$ matrix (with intercept), $\beta:$ (2×1) vector
- For 3. (after transformation) $\mathbf{X}:$ $(N \times 3)$ matrix (with intercept), $\beta:$ (3×1) vector
- For 5. (after transformation) $\mathbf{X}:$ $(N \times 2)$ matrix (with intercept), $\beta:$ (2×1) vector

Problem 2

a) Fit a linear regression model with $y = \log($ `cost` $)$ as the response, including all 10 covariates.

[1]:
```
options(warn = -1) # suppressing warnings
```

[2]:
```
nuclear.data <- read.table("https://www.uio.no/studier/emner/matnat/math/
↪STK2100/data/nuclear.dat", sep = "\t", header = FALSE)
```

[3]:
```
# Converting first row to column names, and then deleting it
colnames(nuclear.data) <- nuclear.data[1, ]
nuclear.data <- nuclear.data[-1, ]
head(nuclear.data) # Taking a look at the data

# Setting a seed for reproducibility
set.seed(1977)
```

A data.frame: 6×11

	cost <chr>	date <chr>	t1 <chr>	t2 <chr>	cap <chr>	pr <chr>	ne <chr>	ct <chr>	bw <chr>	cum <chr>
2	460.05	68.58	14	46	687	0	1	0	0	14
3	452.99	67.33	10	73	1065	0	0	1	0	1
4	443.22	67.33	10	85	1065	1	0	1	0	1
5	652.32	68	11	67	1065	0	1	1	0	12
6	642.23	68	11	78	1065	1	1	1	0	12
7	345.39	67.92	13	51	514	0	1	1	0	3

[4]:
```
nuclear.data <- data.frame(apply(nuclear.data, 2, as.numeric)) # converting the␣
↪chr's to numbers
nuclear.fit <- lm(log(cost) ~ . , data = nuclear.data) # fitting the model
summary(nuclear.fit) # taking a look at the summary
```

```
Call:
lm(formula = log(cost) ~ ., data = nuclear.data)

Residuals:
      Min        1Q    Median        3Q       Max
-0.284032 -0.081677  0.009502  0.090890  0.266548

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept) -1.063e+01  5.710e+00  -1.862  0.07662 .
```

```
date          2.276e-01  8.656e-02   2.629  0.01567 *
t1            5.252e-03  2.230e-02   0.236  0.81610
t2            5.606e-03  4.595e-03   1.220  0.23599
cap           8.837e-04  1.811e-04   4.878 7.99e-05 ***
pr           -1.081e-01  8.351e-02  -1.295  0.20943
ne            2.595e-01  7.925e-02   3.274  0.00362 **
ct            1.155e-01  7.027e-02   1.644  0.11503
bw            3.680e-02  1.063e-01   0.346  0.73261
cum.n        -1.203e-02  7.828e-03  -1.536  0.13944
pt           -2.220e-01  1.304e-01  -1.702  0.10352
---
Signif. codes:  0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1

Residual standard error: 0.1697 on 21 degrees of freedom
Multiple R-squared:  0.8635,        Adjusted R-squared:  0.7985
F-statistic: 13.28 on 10 and 21 DF,  p-value: 5.717e-07
```

To find the confidence interval for the coefficients β_j, we need to compute

$$\hat{\beta}_j \pm t_{\alpha/2;N-p-1} \cdot SE(\hat{\beta}_j),$$

where $\hat{beta}_j$ is the estimate for the coefficients, $t_{\alpha/2;N-p-1}$ is the quantile from the t-distrubution with $N-p-1$ degrees of freedom, and $SE(\hat{\beta}_j) = \hat{\sigma} \cdot \sqrt{v_{jj}}$ is the standard error of $\hat{\beta}_j$, where v_{jj} is the diagonal element $(X^T X)^{-1}$. The residual standard deviation is given by

$$\hat{\sigma} = \sqrt{\frac{\sum r_i^2}{N-p-1}},$$

where r_i are the residuals from the regression model.

[5]:
```r
N <- nrow(nuclear.data) # number of observations
p <- length(coef(nuclear.fit)) - 1 # number of coefficients (excluding␣
 ↪intercept)
alpha <- 0.05 # 95% CI

beta.hats <- coef(nuclear.fit)[c("t1", "t2", "bw")] # the actual coefficients

# computing the residual deviation
sigma.hat <- sqrt(sum(nuclear.fit$residuals ^ 2)/ (N - p - 1))

X <- model.matrix(nuclear.fit) # design matrix
v <- solve(t(X)%*%X) # computing covariance matrix
v_jj <- diag(v)[c("t1", "t2", "bw")] # getting the SE for the coefficints from␣
 ↪diagonal

# computing sigma hat
```

```
se.beta.hats <- sigma.hat * sqrt(v_jj)

t.value <- qt(1 - alpha/2, df = N - p - 1) #quantile from the t-distribution␣
 ↪(using qt) here

# constructing CI's for each of the residual
conf.ints <- cbind(
    beta.hats - t.value * se.beta.hats, # lower bound
    beta.hats + t.value * se.beta.hats # upper bound
    )
conf.ints

# comparing with R's confint()-function
confint(nuclear.fit, level=0.95)[c("t1", "t2", "bw"), ]
```

A matrix: 3 × 2 of type dbl

t1	-0.041123331	0.05162679
t2	-0.003949911	0.01516185
bw	-0.184211843	0.25780411

A matrix: 3 × 2 of type dbl

	2.5 %	97.5 %
t1	-0.041123331	0.05162679
t2	-0.003949911	0.01516185
bw	-0.184211843	0.25780411

b) From the theory, a $(1-\alpha)\cdot 100\%$ prediction interval for Y is given by:

$$\hat{y} \pm t_{1-\alpha/2;N-p-1}\hat{\sigma}\sqrt{1+\mathbf{x}^T(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}}$$

Since we have $Y = \log(Z)$, we transform using $Z = \exp(Y)$. Because the exponential function is monotonous, the probability content of the prediction interval remains unchanged under this transformation:

$$P(L < Y < U) = P(\exp(L) < Z < \exp(U)).$$

Applying the transformation to both bounds, the $(1-\alpha)\cdot 100\%$ prediction interval for Z is:

$$(\exp(L), \exp(U)) = \left(\exp\left(\hat{y} - t_{1-\alpha/2;N-p-1}\hat{\sigma}\sqrt{1+\mathbf{x}^T(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}}\right), \exp\left(\hat{y} + t_{1-\alpha/2;N-p-1}\hat{\sigma}\sqrt{1+\mathbf{x}^T(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{x}}\right)\right).$$

We have now shown that the $(1-\alpha)\cdot 100\%$ prediction interval for Z is given by $(\exp(L), \exp(U))$.

[6]:
```
# creating a data frame from the given x covariate vector
new.x <- data.frame(date = 70.0,
                    t1 = 13,
                    t2 = 50,
                    cap = 800,
                    pr = 1,
                    ne = 0,
```

```
                    ct = 0,
                    bw = 1,
                    cum.n = 8,
                    pt = 1)

pred.y <- predict(nuclear.fit, new.x, interval="predict")

# getting the cost z=(exp(y)) by transforming y
pred.z <- exp(pred.y)
pred.z
```

A matrix: 1 × 3 of type dbl

	fit	lwr	upr
1	389.2163	220.1366	688.1607

c) We will test, for `t1`, `t2`, `bw` that $H_0 : \beta_j = 0$ vs $H_A : \beta_j \neq 0$. For each coefficient β_j, we have that

$$t_j = \frac{\hat{\beta}_j}{SE(\hat{\beta}_j)},$$

with the coefficient estimates and standard errors that we computed in **2a)**.

[7]:
```
t_values <- beta.hats / se.beta.hats # computing t-values for coefficients
p_values <- 2 * pt(-abs(t_values), (N - p - 1)) # getting p-values from the␣
 ↪cumulative p-distribution

# printing in table form
results <- data.frame(
  Estimate = beta.hats,
  Std_Error = se.beta.hats,
  t_value = t_values,
  p_value = p_values
)
print(results)

# comparing with the coefficients in R's summary function
summary(nuclear.fit)$coefficients[c("t1", "t2", "bw"), ]
```

```
     Estimate   Std_Error   t_value   p_value
t1 0.005251730 0.022299843 0.2355053 0.8160981
t2 0.005605968 0.004595026 1.2200080 0.2359862
bw 0.036796131 0.106273564 0.3462397 0.7326075
```

A matrix: 3 × 4 of type dbl

	Estimate	Std. Error	t value	Pr(>|t|)
t1	0.005251730	0.022299843	0.2355053	0.8160981
t2	0.005605968	0.004595026	1.2200080	0.2359862
bw	0.036796131	0.106273564	0.3462397	0.7326075

- `t1`: $p(> |t|) = 0.816 \gg 0.05 \longrightarrow$ `t1` is not significant (H_0 can not be discarded)

- `t2`: $p(>|t|) = 0.236 \gg 0.05 \longrightarrow$ `t2` is not significant
- `bw`: $p(>|t|) = 0.733 \gg 0.05 \longrightarrow$ `bw` is not significant

We then find a **joint test** by computing the F-statistic and $p(>|F|)$ between the reduced set and the original set, by using the formula

$$F = \frac{(RSS_0 - RSS)/q}{RSS/(N-p-1)},$$

where RSS_0 is the residual sum of squares from the reduced model, RSS is from the full model, q is the amount of removed covariates, N is the total observations (rows), and p are the number of covariates in the full model (excluding intercept). Furthermore, we subtract 1, which is the df belonging to the intercept. In R we may obtain the same values with the `anova()` function.

[8]:
```r
# the full model rss
full_model <- nuclear.fit
rss_full <- sum(residuals(full_model)^2)

# getting the reduced model rss by subtracting t1, t2, bw
reduced_model <- lm(log(cost) ~ . -t1 -t2 -bw, data = nuclear.data)
rss_reduced <- sum(residuals(reduced_model)^2)

q <- 3 # number of covariates we want to remove
N <- nrow(nuclear.data) # number of observations
p <- length(coef(full_model)) - 1 # number of parameters in full model␣
 ↪(excluding intercept)

# computing F-statistic
F_stat <- ((rss_reduced - rss_full) / q) / (rss_full / (N - p - 1))
print(paste("F-stat:", F_stat))

p_value <- pf(F_stat, df1 = q, df2 = (N - p - 1), lower.tail = FALSE)
print(paste("p-value:", p_value))

# we can now use ANOVA for a comparison
anova(reduced_model, full_model)
```

```
[1] "F-stat: 0.781959483788322"
[1] "p-value: 0.517266415865109"
```

A anova: 2 × 6

	Res.Df <dbl>	RSS <dbl>	Df <dbl>	Sum of Sq <dbl>	F <dbl>	Pr(>F) <dbl>
1	24	0.6719537	NA	NA	NA	NA
2	21	0.6044333	3	0.06752034	0.7819595	0.5172664

The 95% confidence intervals for all three covariates include 0, suggesting that we cannot rule out that their true effects are zero. In the individual H_0-tests, their $Pr(>|t|)$-values are relatively high, indicating weak evidence against the null hypothesis $H_0 : \beta_j = 0$. This is also reflected in their low t-values. `t2` is the least likely to exclude here, with a significantly lower P-value and a higher t-value.

When comparing the full model with the reduced model (excluding `t1, t2, bw`), the residual sum of squares (RSS) slightly decreases, meaning that removing these variables, the model performs marginally better. Also, the F-test shows a relatively low F-value ($F = 0.7820$) and a high p-value ($p = 0.5173$). This confirms that there is no evidence that the full model is better than the reduced one.

Both individual and joint hypothesis tests show that `t1, t2, bw` do not provide a significant improvement to the model. This suggests that they can be removed without great loss of predictive performance.

d) Forward selection

[9]:
```
install.packages("leaps")
library(leaps)
```

```
The downloaded binary packages are in
/var/folders/dp/x5lf9lp142l0p7rp61v608h00000gn/T//RtmpGkv50V/downloaded_packages
```

[10]:
```
nvmax = ncol(nuclear.data) - 1
nuclear.fwd <- regsubsets(log(cost) ~ ., data=nuclear.data, nvmax=nvmax,␣
 ↪method="forward")
summary.nuclear.fwd <- summary(nuclear.fwd)
summary.nuclear.fwd
```

```
Subset selection object
Call: regsubsets.formula(log(cost) ~ ., data = nuclear.data, nvmax = nvmax,
    method = "forward")
10 Variables  (and intercept)
      Forced in Forced out
date      FALSE      FALSE
t1        FALSE      FALSE
t2        FALSE      FALSE
cap       FALSE      FALSE
pr        FALSE      FALSE
ne        FALSE      FALSE
ct        FALSE      FALSE
bw        FALSE      FALSE
cum.n     FALSE      FALSE
pt        FALSE      FALSE
1 subsets of each size up to 10
Selection Algorithm: forward
          date t1  t2  cap pr  ne  ct  bw  cum.n pt
1  ( 1 )  " "  " " " " " " " " " " " " " " " "   "*"
2  ( 1 )  " "  " " " " " "*" " " " " " " " " "   "*"
3  ( 1 )  "*"  " " " " " "*" " " " " " " " " "   "*"
4  ( 1 )  "*"  " " " " " "*" " " "*" " " " " "   "*"
5  ( 1 )  "*"  " " " " " "*" " " "*" "*" " " " "   "*"
6  ( 1 )  "*"  " " " " " "*" " " "*" "*" " " "*"   "*"
7  ( 1 )  "*"  " " " " " "*" " " "*" "*" "*" "*"   "*"
```

```
8  ( 1 )  "*"  " " " " " " "*" "*" "*" "*" "*" "*"   "*"
9  ( 1 )  "*"  " " "*" "*" "*" "*" "*" "*" "*"   "*"
10  ( 1 ) "*"  "*" "*" "*" "*" "*" "*" "*" "*"   "*"
```

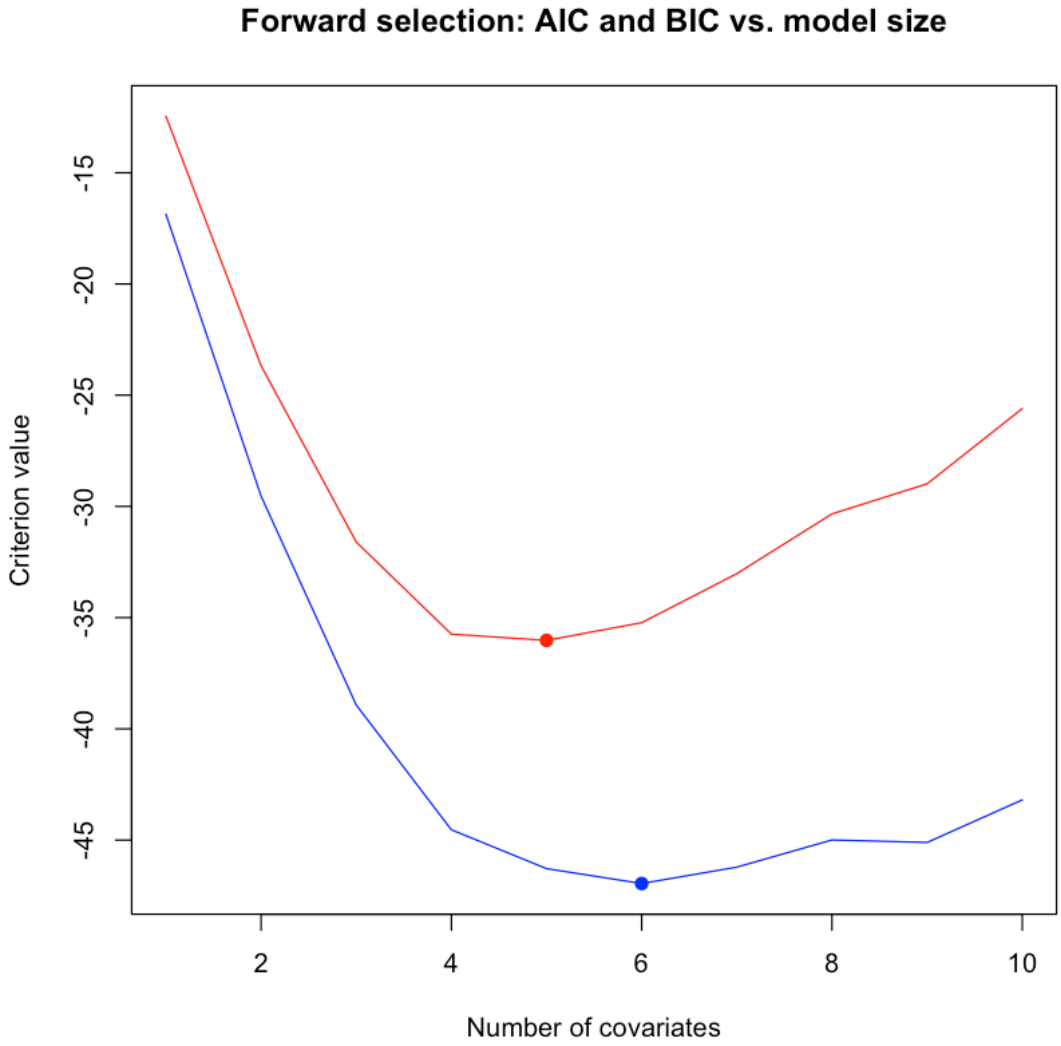
The lower table in the summary shows that the optimal forward selection was performed in this order: `pt, cap, date, ne, ct, cum.n, bw, pr, t2, t1`

We now want to use **Bayesian Information Criterion (BIC)** and **Akaike Information Criterion (AIC)** to determine the best models. BIC and AIC are obtained with the formulas

$$BIC = -2l(\hat{\theta}) + \log(N)d \qquad AIC = -2l(\hat{\theta}) + 2d$$

where $l(\hat{\theta})$ is the Maximum Likelihood Estimate of θ, N is the number of observations (rows) and d is the number of estimated parameters, including the intercept. BIC can be found in the `summary()`, and we can use this to determine AIC.

[11]:
```r
N <- nrow(nuclear.data) # number of observations

# estimating AIC from BIC, where AIC = BIC - log(N)d + 2d
d = (c(1 : nvmax) + 2)
summary.nuclear.fwd$aic = summary.nuclear.fwd$bic - log(N) * d + 2 * d

par(bg="white") # white background when using dark mode ;)
matplot(
  cbind(summary.nuclear.fwd$aic, summary.nuclear.fwd$bic),
  type = "l",
  lty = 1,
  col = c("blue", "red"),
  xlab = "Number of covariates",
  ylab = "Criterion value",
  main = "Forward selection: AIC and BIC vs. model size"
)

p.aic = which.min(summary.nuclear.fwd$aic)
p.bic = which.min(summary.nuclear.fwd$bic)

points(c(p.aic, p.bic),
       c(summary.nuclear.fwd$aic[p.aic], summary.nuclear.fwd$bic[p.bic]),
       col=c("blue", "red"), pch=19)
```



[12]:
```
# covariates chosen by AIC and BIC
best_model_fwd_aic <- which.min(summary.nuclear.fwd$aic)
best_model_fwd_bic <- which.min(summary.nuclear.fwd$bic)

# getting variable names
selected_vars_aic <- names(which(summary.nuclear.fwd$which[best_model_fwd_aic,␣
↪]))[-1] # no intercept
selected_vars_bic <- names(which(summary.nuclear.fwd$which[best_model_fwd_bic,␣
↪]))[-1]

cat("Best model in forward selection, AIC:", selected_vars_aic, "\n")
cat("Best model in forward selection, BIC:", selected_vars_bic, "\n")
```

```
Best model in forward selection, AIC: date cap ne ct cum.n pt
Best model in forward selection, BIC: date cap ne ct pt
```

We see here that both AIC and BIC have chosen the covariates `date, cap, ne, pt`, and AIC has furthermore included `cum.n` This is very much in line with the significance star codes in the original `summary()`. Since BIC tends to lean towards fewer covariates, it seems logical that it has omitted `cum.n`, which according to the mentioned summary is the least significant covariate now.

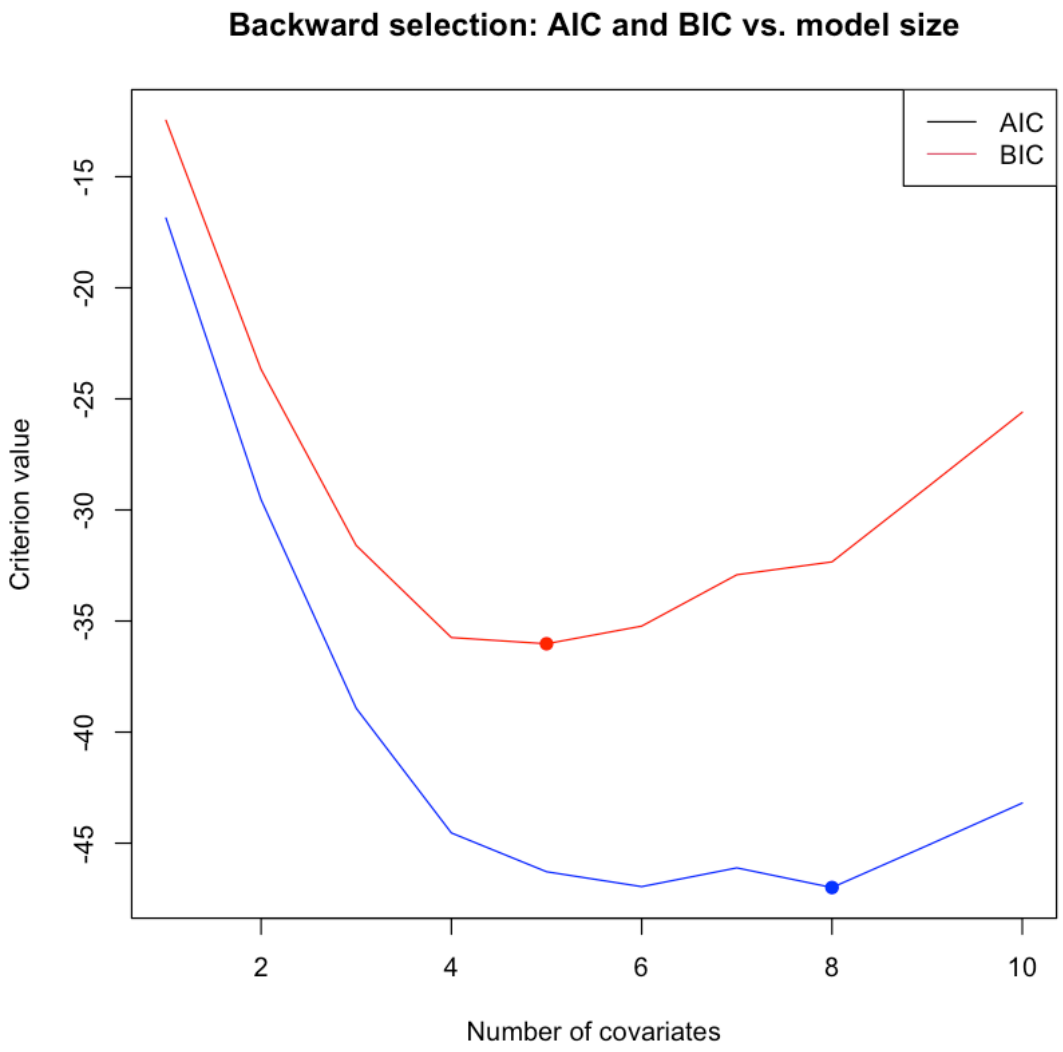
e) Backward selection

[13]:
```
nvmax = ncol(nuclear.data) - 1
nuclear.bwd <- regsubsets(log(cost) ~ ., data=nuclear.data, nvmax=nvmax,␣
 ↪method="backward")
summary.nuclear.bwd <- summary(nuclear.bwd)
summary.nuclear.bwd
```

```
Subset selection object
Call: regsubsets.formula(log(cost) ~ ., data = nuclear.data, nvmax = nvmax,
    method = "backward")
10 Variables  (and intercept)
      Forced in Forced out
date      FALSE      FALSE
t1        FALSE      FALSE
t2        FALSE      FALSE
cap       FALSE      FALSE
pr        FALSE      FALSE
ne        FALSE      FALSE
ct        FALSE      FALSE
bw        FALSE      FALSE
cum.n     FALSE      FALSE
pt        FALSE      FALSE
1 subsets of each size up to 10
Selection Algorithm: backward
          date t1  t2  cap pr  ne  ct  bw  cum.n pt
1  ( 1 )  " "  " " " " " " " " " " " " " " " "   "*"
2  ( 1 )  " "  " " " " " " "*" " " " " " " " " "   "*"
3  ( 1 )  "*"  " " " " " " "*" " " " " " " " " "   "*"
4  ( 1 )  "*"  " " " " " " "*" " " "*" " " " " "   "*"
5  ( 1 )  "*"  " " " " " " "*" " " "*" "*" " " "   "*"
6  ( 1 )  "*"  " " " " " " "*" " " "*" "*" " " "*"   "*"
7  ( 1 )  "*"  " " "*" "*" " " " " "*" "*" " " "*"   "*"
8  ( 1 )  "*"  " " "*" "*" "*" "*" "*" " " " " "*"   "*"
9  ( 1 )  "*"  " " "*" "*" "*" "*" "*" "*" "*" "*"   "*"
10  ( 1 ) "*"  "*" "*" "*" "*" "*" "*" "*" "*" "*"   "*"
```

Backward selection starts with all the covariates, then remove them one by one in the following order: `t1, bw, pr, t2, cum.n, ct, ne, date, cap, pt`

[14]:
```
summary.nuclear.bwd$aic = summary.nuclear.bwd$bic - log(N) * d + 2 * d

par(bg="white")

matplot(
  cbind(summary.nuclear.bwd$aic, summary.nuclear.bwd$bic),
  type = "l",
  lty = 1,
  col = c("blue", "red"),
  xlab = "Number of covariates",
  ylab = "Criterion value",
  main = "Backward selection: AIC and BIC vs. model size"
)

p.aic = which.min(summary.nuclear.bwd$aic)
p.bic = which.min(summary.nuclear.bwd$bic)

points(c(p.aic, p.bic),
       c(summary.nuclear.bwd$aic[p.aic], summary.nuclear.bwd$bic[p.bic]),
       col=c("blue", "red"), pch=19)

legend("topright",c("AIC","BIC"),lty=1,col=1:3,)
```



[15]:
```
best_model_bwd_aic <- which.min(summary.nuclear.bwd$aic)
best_model_bwd_bic <- which.min(summary.nuclear.bwd$bic)

selected_vars_aic <- names(which(summary.nuclear.bwd$which[best_model_bwd_aic,␣
↪]))[-1]
selected_vars_bic <- names(which(summary.nuclear.bwd$which[best_model_bwd_bic,␣
↪]))[-1]

cat("Best model in backward selection, AIC:", selected_vars_aic, "\n")
cat("Best model in backward selection, BIC:", selected_vars_bic, "\n")
```

```
Best model in backward selection, AIC: date t2 cap pr ne ct cum.n pt
Best model in backward selection, BIC: date cap ne ct pt
```

After both forward and backward selection has been performed, and since BIC rendered 5 covariates in both tests (see the summary after each test for covariates), we are left with three "best" models. Interestingly, AIC choose to include `t2` in the backward selection. As discussed in **c)** this *could* be logical, as `t2` has a higher significance than `t1` and `bw` according to the results from the hypothesis testing, and by visual inspection of the confidence intervals.

f) K-Fold Cross Validation

This algorithm splits up the data in 10 "folds", and for each iteration, fits the model to the data in 9 of them, and then performs evaluation on the last one, using MSE:

$$MSE = \frac{1}{N}\sum_{i=1}^{N}(y_i - \hat{y}_i)^2,$$

where y_i is the true log-scaled value, $\hat{y}_i$ is the predicted log-scaled value, and N are the total number of observations.

[16]:
```
Err.Kcv <- rep(0, 4) # number of models
K <- 10
N <- nrow(nuclear.data) # observations

# we need the covariates from our "best of" models
covariates_fwd_aic <- names(which(summary.nuclear.fwd$which[best_model_fwd_aic,␣
 ↪]))[-1]
covariates_fwd_bic <- names(which(summary.nuclear.fwd$which[best_model_fwd_bic,␣
 ↪]))[-1]
covariates_bwd_aic <- names(which(summary.nuclear.bwd$which[best_model_bwd_aic,␣
 ↪]))[-1]
covariates_bwd_bic <- names(which(summary.nuclear.bwd$which[best_model_bwd_bic,␣
 ↪]))[-1]

models <- list(
  "AIC (forward)" = covariates_fwd_aic,
  "BIC (forward)" = covariates_fwd_bic,
  "AIC (backward)" = covariates_bwd_aic,
  "BIC (backward)" = covariates_bwd_bic
)

# creating indices for the folds
index <- sample(rep(1:K, ceiling(N/K))[1:N])

for (p in 1:4) {
    # setting a formula-string
    formula.str <- paste("log(cost) ~", paste(models[[p]], collapse = " + "))

    SSE <- 0 # initializing SSE value

    for (k in 1:K) {
```

```
    # training the model on everything but the fold k
    nuclear.Kcv <- lm(
        as.formula(formula.str),
        data = nuclear.data,
        subset = (1:N)[-which(index == k)]
    )

    # testing for fold k
    test_inds <- which(index == k)

    for (i in test_inds) {
        # log scaling
        y_true_log <- log(nuclear.data$cost[i])
        y_pred_log <- predict(nuclear.Kcv, newdata = nuclear.data[i, , drop =␣
 ↪FALSE])
        SSE <- SSE + (y_true_log - y_pred_log)^2
    }
    }
    # finding total MSE over all folds
    Err.Kcv[p] <- SSE / N

}

names(Err.Kcv) <- c("AIC (forward)", "BIC (forward)", "AIC (backward)", "BIC␣
 ↪(backward)")
print(data.frame(Method = names(Err.Kcv), MSE = Err.Kcv))
```

```
                      Method        MSE
AIC (forward)   AIC (forward) 0.03822791
BIC (forward)   BIC (forward) 0.03821806
AIC (backward) AIC (backward) 0.03923557
BIC (backward) BIC (backward) 0.03821806
```

We see that MSE for `BIC (forward)` and `BIC (backward)` are the same, which is expected, since the models are identical.

g) Bootstrap 0.632-model

We now want to use a bootstrap 0.632-approach to compare the four models. For our training set, we draw a bootstrap selection of $B = 1000$ with replacement from `nuclear.data`. The observations that are not drawn, will be our test set. The in-sample error (`SSE_Train`) is computed from the training set, while the test error is computed from the test set. We then compute

$$MSE_{\text{train}} = \frac{SSE_{\text{train}}}{n_{\text{train}}}, \quad MSE_{\text{test}} = \frac{SSE_{\text{test}}}{n_{\text{test}}}.$$

Then, to get a less optimistic error than the in-sample error, we compute the $MSE_{0.632}$ as

$$MSE_{0.632} = 0.368 \cdot MSE_{\text{train}} + 0.632 \cdot MSE_{\text{test}}.$$

[17]:
```r
B <- 1000 # setting the bootstrap selection size
N <- nrow(nuclear.data) # making a list of indices

# initializing containers for the four models
SSE_Train <- rep(0, 4)
SSE_Test  <- rep(0, 4)
n_train    <- rep(0, 4)
n_test     <- rep(0, 4)

for (b in 1:B) {
    # creating samples based on the indices in N
    index <- sample(N, replace = TRUE) # sampling with replacement

    # splitting into training and test data
    temp.train.data <- nuclear.data[index, , drop = FALSE]
    temp.test.data  <- nuclear.data[-index, , drop = FALSE] # the data not␣
 ↪sampled

    # adding a log cost response variable in training and test sets
    temp.train.data$logCost <- log(temp.train.data$cost)
    temp.test.data$logCost  <- log(temp.test.data$cost)

    # iterating over the models
    for (m in 1:4) {
        # making a formula string for the model m
        formula.str <- paste("logCost ~", paste(models[[m]], collapse = " + "))

        # fitting model m on training data
        model.boot <- lm(as.formula(formula.str), data = temp.train.data)

        y_pred_train <- predict(model.boot, newdata = temp.train.data) #␣
 ↪in-sample prediction
        y_true_train <- temp.train.data$logCost
        SSE_Train[m] <- SSE_Train[m] + sum((y_true_train - y_pred_train)^2) #␣
 ↪in-sample error
        n_train[m]    <- n_train[m] + nrow(temp.train.data) # number of␣
 ↪observations

        if (nrow(temp.test.data) > 0) {
            y_pred_test <- predict(model.boot, newdata = temp.test.data)
            y_true_test <- temp.test.data$logCost
            SSE_Test[m] <- SSE_Test[m] + sum((y_true_test - y_pred_test)^2)
            n_test[m]    <- n_test[m] + nrow(temp.test.data)
        }
    }
}
```

```r
# getting MSE
MSE_Train <- SSE_Train / n_train
MSE_Test  <- SSE_Test  / n_test

# getting MSE_0.632
MSE_632 <- 0.368 * MSE_Train + 0.632 * MSE_Test

best.model <- which.min(MSE_632)

# printing results
results <- data.frame(
  Model    = names(models),
  MSE_632   = MSE_632
)

results
```

A data.frame: 4 × 2

Model <chr>	MSE_632 <dbl>
AIC (forward)	0.03659303
BIC (forward)	0.03529443
AIC (backward)	0.03972387
BIC (backward)	0.03529443

Also after bootstrap with $B = 1000$ and using the "0.632-estimator", the model with the best result is the BIC forward or backward models, namely the model with the least covariates. With this method we obtained a slightly lower $MSE = 0.0353$ than with K-Fold Cross Validation ($MSE = 0.0382$).

h) Shrinkage with Ridge

Ridge-regression is an Ordinary Least Squares regression with an added $L2$-penalty on the β-coefficients, in order to shrink the least contributing ones, with the added bonus of removing any rank deficiency from the design matrix X. In matrix form, the analytical expression of Ridge-regression is known as:

$$\hat{\beta}_{ridge} = (X^T X + \lambda I)^{-1} X^T y,$$

where λ is a hyper parameter to control the level of shrinkage. At $\lambda = 0$, $\hat{\beta}_{ridge}$ is in fact equivalent to $\hat{\beta}_{OLS}$.

In R, we can use the `glmnet`-package, which computes this, along with a built in `cv.glmnet()`-function for 10-fold cross validation to find the optimal value for the hyper parameter λ. Then, we use 10-fold cross validation again, to compute the MSE with this chosen hyper parameter in place.

[18]:
```r
# downloading packages
install.packages("glmnet")
library(glmnet)
```

```
The downloaded binary packages are in
/var/folders/dp/x5lf9lp142l0p7rp61v608h00000gn/T//RtmpGkv50V/downloaded_packages

Loading required package: Matrix

Loaded glmnet 4.1-8
```

[33]:
```r
# setting seed again, to be sure
set.seed(1977)

# getting the design matrix (without intercept) and response for glmnet function
X <- model.matrix(log(cost) ~ ., data = nuclear.data)[,-1]
y <- log(nuclear.data$cost)

K <- 10  # number of folds
N <- nrow(nuclear.data) # number of observations

index <- sample(rep(1:K, ceiling(N/K))[1:N])  # setting cross-validation indices

# using cross-validation to find the optimal lambda
lambda.grid <- 10^seq(5, -2, length = 100)
fit.ridge.cv <- cv.glmnet(X, y, lambda = lambda.grid, alpha = 0)

optimal_lambda_ridge <- fit.ridge.cv$lambda.min

cat("Optimal lambda chosen by 10-fold CV for Ridge:", optimal_lambda_ridge,␣
 ↪"\n")

# using cross-validation again to calculate MSE
SE_Ridge_Kcv <- 0

for (k in 1:K) {
    # training and test split
    train_inds <- which(index != k)
    test_inds  <- which(index == k)

    X_train <- X[train_inds, ]
    y_train <- y[train_inds]
    X_test  <- X[test_inds, ]
    y_test  <- y[test_inds]

    # fitting with optimal lambda
    fit.ridge <- glmnet(X_train, y_train, lambda = optimal_lambda_ridge, alpha␣
 ↪= 0)

    # predicting on test set
```

```
    y_pred_ridge <- predict(fit.ridge, newx = X_test, s = optimal_lambda_ridge)


    # storing the error
    SE_Ridge_Kcv <- SE_Ridge_Kcv + sum((y_test - y_pred_ridge)^2)
}

# Compute final MSE for Ridge
MSE_Ridge_Kcv <- SE_Ridge_Kcv / N

# Print results
cat("MSE for Ridge Regression (10-fold CV):", MSE_Ridge_Kcv, "\n")
```

```
Optimal lambda chosen by 10-fold CV for Ridge: 0.05994843
MSE for Ridge Regression (10-fold CV): 0.03991514
```

We note that Ridge regression with 10-fold Cross Validation renders a best $MSE = 0.0399$ (using $\lambda = 0.06$) which is higher than the result from the bootstrap 0.632-method ($MSE_{0.632} = 0.0353$). The model's choice of a low λ-value could indicate that there is not much to gain from shrinkage.

One reason for this may be that there is a low collinearity between our covariates, meaning that the model does not suffer from instability in estimating the coefficients.

Additionally, our initial testing showed that there was not that much to gain from removing the least contributing parameters. This further supports that shrinkage is not necessary, as the model is already performing well without regularization.

i) Shrinkage with Lasso

In a similar fashion as with Ridge Regression, we now want to perform Lasso Regression, which uses $L1$-regularization to optimize

$$\hat{\beta}_\lambda = \arg\min_\beta \sum_{i=1}^{N} (y_i - X_i\beta)^2 + \lambda \sum_{j=1}^{p} |\beta_j|,$$

where the first term is an OLS-regression, and the second term is the $L1$-regularization, penalizing large coefficients by setting them to zero. Also in lasso, $\lambda = 0$ is an OLS-regression, whilst a large λ set more coefficients to zero. Again, we can use R's `glmnet`, and we want to use KCV to find the best λ, and then again to compute the MSE_{lasso}.

[34]:
```
set.seed(1977)

index <- sample(rep(1:K, ceiling(N/K))[1:N])

lambda.grid <- 10^seq(5, -2, length = 100)
fit.lasso.cv <- cv.glmnet(X, y, lambda = lambda.grid, alpha = 1)

optimal_lambda_lasso <- fit.lasso.cv$lambda.min
```

```r
cat("Optimal lambda chosen by 10-fold CV for Lasso:", optimal_lambda_lasso,␣
 ↪"\n")

SE_Lasso_Kcv <- 0

for (k in 1:K) {
    train_inds <- which(index != k)
    test_inds  <- which(index == k)

    X_train <- X[train_inds, ]
    y_train <- y[train_inds]
    X_test  <- X[test_inds, ]
    y_test  <- y[test_inds]

    fit.lasso <- glmnet(X_train, y_train, lambda = optimal_lambda_lasso, alpha␣
 ↪= 1)
    y_pred_lasso <- predict(fit.lasso, newx = X_test, s = optimal_lambda_lasso)

    SE_Lasso_Kcv <- SE_Lasso_Kcv + sum((y_test - y_pred_lasso)^2)
}

MSE_Lasso_Kcv <- SE_Lasso_Kcv / N

# Print results
cat("MSE for Lasso Regression (10-fold CV evaluation):", MSE_Lasso_Kcv, "\n")
```

```
Optimal lambda chosen by 10-fold CV for Lasso: 0.03125716
MSE for Lasso Regression (10-fold CV evaluation): 0.04220735
```

Lasso regression with 10-fold Cross Validation leaves us with a best $MSE = 0.0422$ which is marginally higher than for Ridge, and also slightly higher than for with the bootstrap 0.632-method ($MSE = 0.0353$). Again, a very low optimal $\lambda = 0.0313$ tells us that there is not much to be gained from Lasso-regression, as the model is quite close to OLS.