Model Selection and Validation

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Regression Analysis

Salary example

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Model annual salary (in $1000) as function of

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- education (years of post-high-school education), and
- political affiliation (pol = D for Democrat, pol = R for Republican, and pol = O for other).

```
> salary_data = read.table("path/to/salary.txt", header=FALSE)
> colnames(salary_data) = c('salary', 'age', 'educ', 'pol')
> head(salary_data)
  salary age educ pol
1     38  25    4   D
2     45  27    4   R
3     28  26    4   O
4     55  39    4   D
5     74  42    4   R
6     43  41    4   O
```

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```
Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  17.0313     7.3459   2.318  0.03735 *
age           0.8983     0.1968   4.565  0.00053 ***
educ          1.5039     1.1841   1.270  0.22632
polO        -16.5404     4.8807  -3.389  0.00484 **
polR          9.1587     4.8482   1.889  0.08139 .
---

Residual standard error: 8.209 on 13 degrees of freedom
Multiple R-squared:  0.8374,Adjusted R-squared:  0.7873
```

- We can also test quadratic effects and interactions.
- From the initial fit, `educ` is not needed with `age` and `pol` in the model. Let's refit:

Droc educ?

```
> m2 = update(m1, . ~ . - educ)
> anova(m1, m2)
Analysis of Variance Table

Model 1: salary ~ age + educ + pol
Model 2: salary ~ age + pol
  Res.Df    RSS Df Sum of Sq      F Pr(>F)
1     13 876.03
2     14 984.72 -1    -108.7 1.6131 0.2263

> summary(m2)
lm(formula = salary ~ age + pol, data = salary_data)

Coefficients:
            Estimate Std. Error t value Pr(>|t|)
(Intercept)  21.5172     6.5806   3.270  0.00559 **
age           1.0345     0.1686   6.136 2.58e-05 ***
polO        -16.7414     4.9838  -3.359  0.00468 **
polR          8.6379     4.9354   1.750  0.10196
Residual standard error: 8.387 on 14 degrees of freedom
Multiple R-squared:  0.8172,Adjusted R-squared:  0.778
```

Add 2nd order terms?

```
> salary_data$age2 = salary_data$age^2
> m3 = update(m2, . ~ . + age2 + age*pol)
> summary(m3)

Call:
lm(formula = salary ~ age + pol + age2 + age:pol, data = salary_data)

Coefficients:
             Estimate Std. Error t value Pr(>|t|)
(Intercept) -20.94355   20.34047  -1.030  0.32528
age           3.17751    0.93793   3.388  0.00606 **
polO        -16.90846   22.83050  -0.741  0.47444
polR         -1.18699   21.44129  -0.055  0.95684
age2         -0.02514    0.01255  -2.004  0.07037 .
age:polO      0.05101    0.65536   0.078  0.93936
age:polR      0.28944    0.61956   0.467  0.64950
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 7.434 on 11 degrees of freedom
Multiple R-squared:  0.8871,Adjusted R-squared:  0.8256
```

Drop 2nd order terms?

```
> anova(m3, m2)
Analysis of Variance Table

Model 1: salary ~ age + pol + age2 + age:pol
Model 2: salary ~ age + pol
  Res.Df    RSS Df Sum of Sq      F Pr(>F)
1     11 607.88
2     14 984.72 -3   -376.84 2.2731 0.1369
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We don't need *all* the 2nd order terms ($p = 0.137$), although theres some indication in the table of regression effects that age^2 might be needed.

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```
> anova(m4, m2)
Analysis of Variance Table

Model 1: salary ~ age + pol + age2
Model 2: salary ~ age + pol
  Res.Df    RSS Df Sum of Sq      F  Pr(>F)
1     13 645.09
2     14 984.72 -1   -339.64 6.8444 0.02134 *
```

Final model

Our final model is

$$\text{salary}_i = \beta_0 + \beta_1 \cdot \text{age} + \beta_2 \cdot \mathbb{I}[\text{pol} = \text{O}] + \beta_3 \cdot \mathbb{I}[\text{pol} = \text{R}] + \beta_4 \cdot \text{age}^2 + \epsilon_i$$

```
> summary(m4)

Call:
lm(formula = salary ~ age + pol + age2, data = salary_data)

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept) -24.751745  18.529243  -1.336  0.20452
age           3.272388   0.867049   3.774  0.00232 **
polO        -15.891696   4.198662  -3.785  0.00227 **
polR          9.260234   4.152253   2.230  0.04399 *
age2         -0.024576   0.009394  -2.616  0.02134 *
---

Residual standard error: 7.044 on 13 degrees of freedom
Multiple R-squared:  0.8802,Adjusted R-squared:  0.8434
```

Scatterplots

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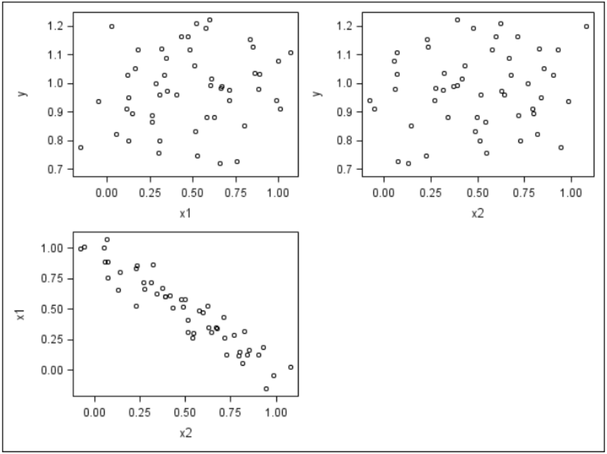
- Nonlinear relationship between Y and x_j ($j = 1, \ldots, k$) *marginally* may or may not be present in the joint relationship.
- Actually, any strong relationship between Y and x_j marginally doesn't mean that x_j will be needed in the presence of other variables.
- Seeing no marginal relationship between Y and x_j does not mean that x_j is not needed in a model including other predictors.

No relationship?

Here Y vs. x_1 and Y vs. x_2 shows nothing. There seems to be some multicollinearity though.



proc reg output

x_1 important marginally? $Y_i = \beta_0 + \beta_1 x_{i1} + \epsilon_i$

Variable	DF	Parameter Estimate	Standard Error	t Value	Pr > |t|
Intercept	1	0.94576	0.03602	26.26	<.0001
x1	1	0.06974	0.06311	1.11	0.2745

x_2 important marginally? $Y_i = \beta_0 + \beta_2 x_{i2} + \epsilon_i$

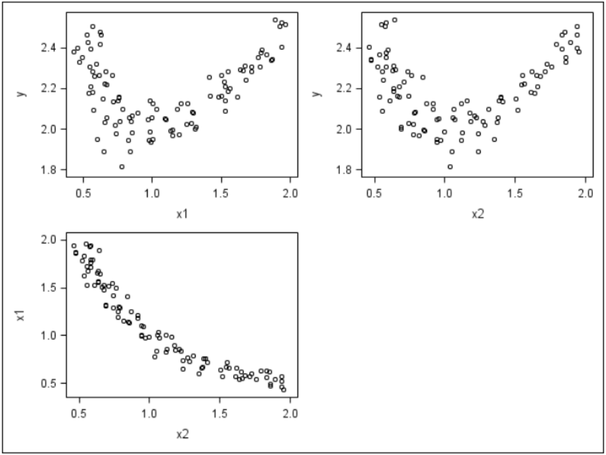
Variable	DF	Parameter Estimate	Standard Error	t Value	Pr > |t|
Intercept	1	0.95180	0.03730	25.52	<.0001
x2	1	0.05603	0.06458	0.87	0.3898

x_1, x_2 important jointly? $Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \epsilon_i$

Variable	DF	Parameter Estimate	Standard Error	t Value	Pr > |t|
Intercept	1	-0.08151	0.10876	-0.75	0.4572
x1	1	1.07327	0.11065	9.70	<.0001
x2	1	1.08548	0.11271	9.63	<.0001

Nonlinear relationship?

Marginally, x_1 and x_2 have highly nonlinear relationships with Y. Should we transform?



Regression output

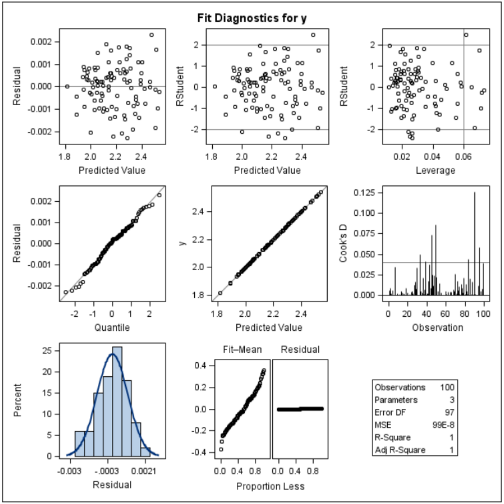
Let's try fitting a simple main effects model without any transformation.

$$Y_i = \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \epsilon_i$$

Variable	DF	Parameter Estimate	Standard Error	t Value	Pr > |t|
Intercept	1	-0.00036626	0.00130	-0.28	0.7791
x1	1	1.00022	0.00059936	1668.80	<.0001
x2	1	1.00009	0.00060998	1639.54	<.0001

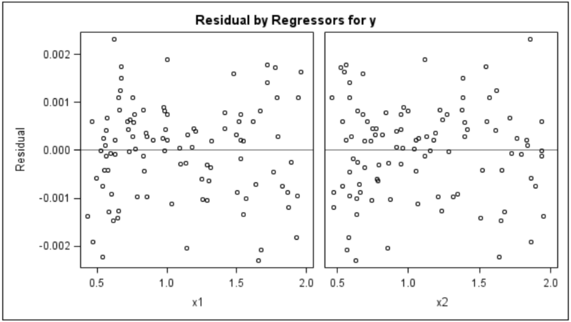
both x_1 and x_2 are important, but does the model fit okay?

Model fit is okay



Look at Y_i vs. $\hat{Y}_i$ and R^2!

No pattern here, either



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Model validation should not be confused with model diagnostics (residual analysis).

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  - **Exploratory studies**: it is hypothesized that some or all of potential predictors are associated with Y.

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  - Exploratory Studies: Often have many potential predictors (and polynomials and interactions). Want to fit parsimonious model that explains much of the variation in Y, while keeping model as basic as possible. Caution: one shall not make decisions based on single variable t-tests.

9.2 Surgical unit example

- First steps often involve plots:
  - Plots to indicate correct functional form of predictors and/or response.
  - Plots to indicate possible interaction.
  - Exploration of correlation among predictors (maybe).
  - Often a first-order model is a good starting point.
- Once a reasonable set of potential predictors is identified, formal model selection begins.
- If the number of predictors is large, say $k \geq 10$, we can use (automated) stepwise procedures to reduce the number of variables (and models) under consideration.

Surgical unit example: predictors

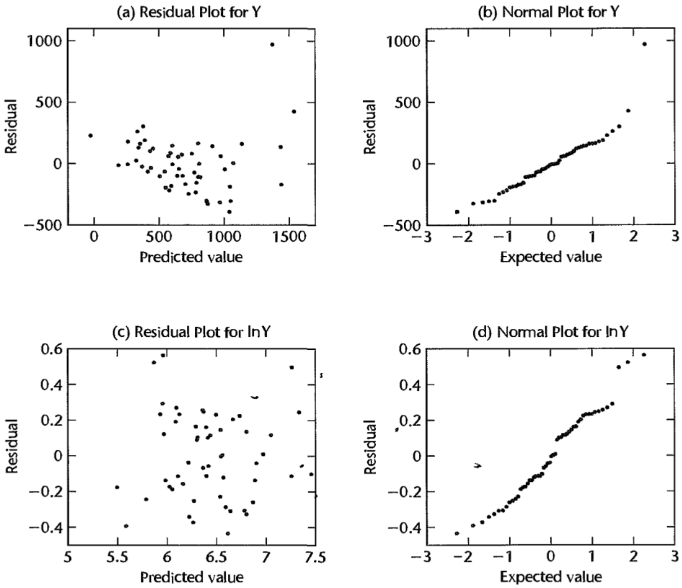
A hospital surgical unit was interested in predicting survival in patients undergoing a particular type of liver operation. A random selection of 108 patients was available for analysis.

X_1	blood clotting score
X_2	prognostic index
X_3	enzyme function test score
X_4	liver function test score

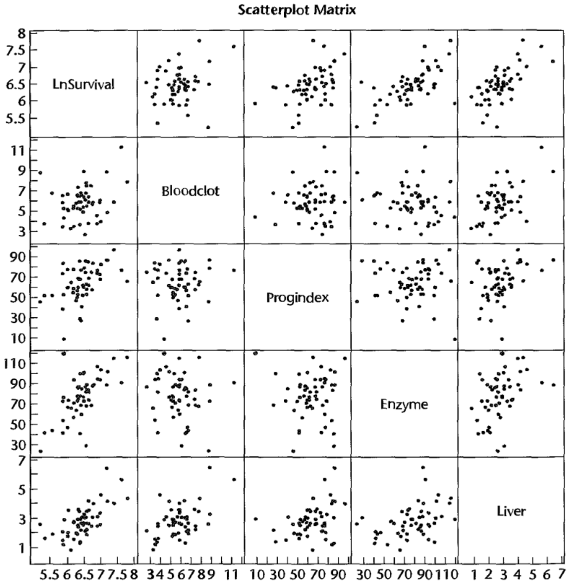
...

Case Number i	Blood-Clotting Score X_{i1}	Prognostic Index X_{i2}	Enzyme Test X_{i3}	Liver Test X_{i4}	Age X_{i5}	Gender X_{i6}	Alc. Use: Mod. X_{i7}	Alc. Use: Heavy X_{i8}	Survival Time Y_i	$Y_i' = \ln Y_i$
1	6.7	62	81	2.59	50	0	1	0	695	6.544
2	5.1	59	66	1.70	39	0	0	0	403	5.999
3	7.4	57	83	2.16	55	0	0	0	710	6.565
...	...	...	...	...	...	...	...	...	...	...
52	6.4	85	40	1.21	58	0	0	1	579	6.361
53	6.4	59	85	2.33	63	0	1	0	550	6.310
54	8.8	78	72	3.20	56	0	0	0	651	6.478

Surgical unit example: residual plots



Surgical unit example: scatterplot matrix



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Say we have k predictors $x_1, \ldots, x_k$ and we want to find a good subset of predictors that predict the data well. There are several useful criteria to help choose a subset of predictors.

Adjusted-R^2, R_a^2

The *adjusted* R^2, denoted R_a^2 “fixes” R^2 to provide a measure of how good the model will predict data not used to build the model. For a candidate model with $p-1$ predictors

$$R_a^2 = 1 - \frac{\text{SSE}/(n-p)}{\text{SSTO}/(n-1)}$$

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$$\mathrm{AIC} = -2 \ln L(\hat{\boldsymbol{\theta}}) + 2p$$

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- $2p$ is "penalty" term for adding predictors.

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- $2p$ is "penalty" term for adding predictors.
- Like R_a^2, AIC favors models with small SSE, but penalizes models with too many variables p.

Akaike Information Criterion

In general, **Akaike Information Criterion (AIC)** is

$$\mathrm{AIC} = -2 \ln L(\hat{\boldsymbol{\theta}}) + 2p$$

for a model with parameters $\boldsymbol{\theta} \in \mathbb{R}^p$ and likelihood function L.

Exercise. Show that for the MLR with normal errors,

$$\mathrm{AIC} = n \ln(\mathrm{SSE}) + 2p + C$$

where C is a constant that does not depend on SSE and p.

- $2p$ is "penalty" term for adding predictors.
- Like R_a^2, AIC favors models with small SSE, but penalizes models with too many variables p.
- $\Rightarrow$ Between two models, we prefer the one with lower AIC.

Bayesian Information Criterion

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- BIC is similar to AIC, but for $n \geq 8$, the BIC "penalty term" is more severe.

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Full model with k predictors and Reduced model with $p - 1$ predictors.

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$$C_p \approx \frac{(n-p)\sigma^2}{\sigma^2} - n + 2p = p$$

- The Full model always has $C_{k+1} = k + 1$.

Mallow's C_p

If $C_p \approx p$ then the reduced model predicts as well as the full model. If $C_p < p$ then the reduced model is estimated to be less *biased* than the full model.

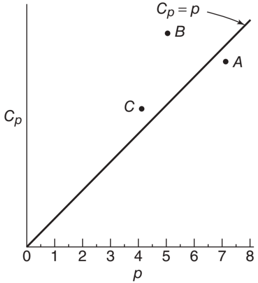

Figure: A C_p plot

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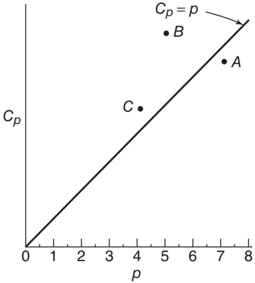

Figure: A C_p plot

In practice, just choose model with smallest C_p.

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R_a^2, AIC, BIC, and C_p may give different "best" models, or they may agree. Ultimate goal is to find model that balances:

- A good fit to the data.
- Low bias.
- Parsimony.

All else being equal, the simpler model is often easier to interpret and work with. Christensen (1996) recommends C_p and notes the similarity between C_p and AIC.

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- Automated procedures *cannot* assess a good functional form for a predictor, *cannot* think about which interactions might be important, etc.
- Anyway, automated procedures are widely used and *can* produce good models. But they can also produce models that are *substantially inferior* to other models built from the same predictors using scientific input and common sense.

Example: cruise ships

https://github.com/zh3nis/MATH440/blob/main/chp09/cruise.R

A cruise ship company wishes to model the `crew size` needed for a ship using predictors such as: `age`, `tonnage`, `passengers`, `length`, `cabins` and passenger density (`passdens`).

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```
> cruise <- read.fwf("http://www.stat.ufl.edu/~winner/data/cruise_ship.dat", ...)
> head(cruise)
         ship      cline age tonnage passengers length cabins passdens  crew
1 Journey        Azamara   6  30.277       6.94   5.94   3.55    42.64  3.55
2 Quest          Azamara   6  30.277       6.94   5.94   3.55    42.64  3.55
3 Celebration   Carnival  26  47.262      14.86   7.22   7.43    31.80  6.70
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5 Destiny       Carnival  17 101.353      26.42   8.92  13.21    38.36 10.00
6 Ecstasy       Carnival  22  70.367      20.52   8.55  10.20    34.29  9.20
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```

Without concerning ourselves with potential interactions we will look at simple additive models.

Cruise ships — Full model

```
> fit0 = lm(crew ~ age + tonnage + passengers + length + cabins + passdens, data=cruise)
> summary(fit0)

Call:
lm(formula = crew ~ age + tonnage + passengers + length + cabins +
    passdens, data = cruise)

Residuals:
    Min      1Q  Median      3Q     Max
-1.7700 -0.4881 -0.0938  0.4454  7.0077

Coefficients:
              Estimate Std. Error t value Pr(>|t|)
(Intercept) -0.5213400  1.0570350  -0.493  0.62258
age         -0.0125449  0.0141975  -0.884  0.37832
tonnage      0.0132410  0.0118928   1.113  0.26732
passengers  -0.1497640  0.0475886  -3.147  0.00199 **
length       0.4034785  0.1144548   3.525  0.00056 ***
cabins       0.8016337  0.0892227   8.985 9.84e-16 ***
passdens    -0.0006577  0.0158098  -0.042  0.96687
---
Signif. codes:  0 *** 0.001 ** 0.01 * 0.05 . 0.1   1

Residual standard error: 0.9819 on 151 degrees of freedom
Multiple R-squared:  0.9245,Adjusted R-squared:  0.9215
F-statistic:   308 on 6 and 151 DF,  p-value: < 2.2e-16
```

Best subsets

```
> library(leaps)
> allcruise <- regsubsets(crew ~ age + tonnage + passengers + length + cabins + passdens,
+                         nbest=4, data=cruise)
> all_output <- summary(allcruise)
> with(all_output, round(cbind(which, rsq, adjr2, cp, bic), 3))
  (Intercept) age tonnage passengers length cabins passdens   rsq adjr2      cp      bic
1           1   0       0          0      0      1        0 0.904 0.903  37.772 -360.238
1           1   0       1          0      0      0        0 0.860 0.859 125.086 -300.954
1           1   0       0          1      0      0        0 0.838 0.837 170.523 -277.122
1           1   0       0          0      1      0        0 0.803 0.801 240.675 -246.201
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2           1   0       0          0      0      1        1 0.912 0.911  24.261 -368.502
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4           1   1       0          1      1      1        0 0.923 0.921   5.084 -380.652
4           1   0       0          1      1      1        1 0.923 0.921   5.197 -380.534
4           1   0       1          0      1      1        1 0.919 0.917  13.056 -372.631
5           1   1       1          1      1      1        0 0.924 0.922   5.002 -377.752
5           1   0       1          1      1      1        1 0.924 0.922   5.781 -376.939
5           1   1       0          1      1      1        1 0.924 0.921   6.240 -376.462
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```

A good model choice might be the model with 4 predictors: tonnage, passengers, length, and cabins, whose $R_a^2 = 0.922$, $C_p = 3.847$, and BIC $= 381.933$.

AIC full vs reduced

```
> fit3 <- update(fit0, . ~ . - age - passdens)
> AIC(fit3)
[1] 448.3229
> AIC(fit0)
[1] 451.4394
```

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There are 3 automated procedures

- Backward Elimination (Top down approach)
- Forward Selection (Bottom up approach)
- Stepwise Regression (Combines Forward/Backward)

We will explore these procedures using two different elimination/selection criteria. One that uses t-test and p-value and another that uses the AIC value.

Backward elimination

1. Select a significance level to *stay* in the model (e.g. $\alpha_s = 0.20$, generally .05 is too low, causing too many variables to be removed).

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   - If p-value $> \alpha_s$, remove the predictor and fit model without this variable (must re-fit model here because partial regression coefficients change).

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4. Continue until all predictors have p-values $\leq \alpha_s$.

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4. Continue until no new predictors have p-values $\leq \alpha_e$.

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3. Re-test all "old variables" that have already been entered, must have p-value $\leq \alpha_s$ to stay in model.
4. Continue until no new variables can be entered and no old variables need to be removed.

Backward and Forward for cruise ships

```
> library(olsrr)
> ols_step_backward_p(fit0)

                              Elimination Summary
------------------------------------------------------------------------
        Variable                  Adj.
Step    Removed     R-Square    R-Square     C(p)        AIC        RMSE
------------------------------------------------------------------------
   1    passdens      0.9245       0.922    5.0017    449.4412    0.9786
   2    age            0.924      0.9221    3.8468    448.3229    0.9782
------------------------------------------------------------------------

> ols_step_forward_p(fit0)

                              Selection Summary
---------------------------------------------------------------------------
        Variable                  Adj.
Step     Entered      R-Square    R-Square     C(p)         AIC        RMSE
---------------------------------------------------------------------------
   1    cabins          0.9041      0.9034    37.7724    479.2060    1.0886
   2    length          0.9160      0.9149    15.9524    460.2507    1.0221
   3    passengers      0.9220      0.9205     5.8566    450.4411    0.9878
   4    tonnage         0.9240      0.9221     3.8468    448.3229    0.9782
---------------------------------------------------------------------------
```

Stepwise procedure for cruise ships

```
> ols_step_both_p(fit0)
```

Stepwise Selection Summary

Step	Variable	Added/ Removed	R-Square	Adj. R-Square	C(p)	AIC	RMSE
1	cabins	addition	0.904	0.903	37.7720	479.2060	1.0886
2	length	addition	0.916	0.915	15.9520	460.2507	1.0221
3	passengers	addition	0.922	0.921	5.8570	450.4411	0.9878
4	tonnage	addition	0.924	0.922	3.8470	448.3229	0.9782

PRESS_p criterion

$$\text{PRESS}_p = \sum_{i=1}^{n} (Y_i - \hat{Y}_{i(i)})^2 \quad \left(= \sum_{i=1}^{n} \left[\frac{e_i}{1 - h_{ii}} \right]^2 \right),$$

where $\hat{Y}_{i(i)}$ is the fitted value at $\mathbf{x}_i$ with the $(\mathbf{x}_i, Y_i)$ omitted.

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- This is leave-one-out prediction error. The smaller, the better.

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where $\hat{Y}_{i(i)}$ is the fitted value at $\mathbf{x}_i$ with the $(\mathbf{x}_i, Y_i)$ omitted.

- This is leave-one-out prediction error. The smaller, the better.
- Having $\text{PRESS}_p \approx \text{SSE}_p$ supports the *validity* of the model with p predictors (p. 374).

Caveats for automated procedures

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- There is no "best" way to search for good models.
- There may be *several* "good" models.
- If you use the same data to *estimate* the model and *choose* the model, the regression effects are *biased*! $This$ leads to the idea of data splitting; one portion of the data is the *training data* and the other portion is the *validation set* (Section 9.6, p. 372). PRESS_p can also be used.