# MA8701 Advanced methods in statistical inference and learning

## L3-4: Model selection and assessment

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## **Table of contents**

1	Model assessment and selection 1.1 Plan	<b>2</b> 3
2	Optimism of the training error rate	3
	2.1 In-sample error	4
	2.2 Optimism	4
	2.3 Average optimism	4
	2.4 Covariance result	5
	2.5 Group discussion	5
3	Expected in-sample prediction error	5
	3.1 Result for $\omega$	6
	3.2 Group discussion	6
4	Three ways to perform model selection	7
5	Estimates of (expected) in-sample prediction error	7
	$5.1  C_p \text{ statistics} \dots \dots$	8
	5.2 Akaike information criterion (AIC)	
	5.3 Expected in-sample prediction error for binary classification	9
	5.4 Group discussion	9
6	The effective number of parameters	10
7	Cross-validation (CV)	11
	7.1 Formal set-up for model assessment	11

	7.2 Formal set-up for model selection	11
	7.3 Choice of $K$	12
	7.4 Generalized cross-validation (GCV)	12
	7.5 What is estimated?	13
	7.6 The wrong and the right way to do cross-validation	13
8	Bootstrap methods	13
9	Conclusions: Model selection and assessment and future use	16
10	Exercises	16
	10.1 Expected training and test MSE for linear regression	16
	10.2 Establish the average optimism in the training error	16
	10.3 Relate the covariance to the trace of a linear smoother	16
	10.4 Derive the estimate of in-sample error	17
	10.5 Additive error model effective degrees of freedom	17
	10.6 UiO STK-IN4300/STK-IN9300 — Statistical learning methods in Data Science	17
	10.7 Comparing methods	18
11	Solutions to exercises	18
	11.0.1 UiO STK-IN4300/STK-IN9300 Solutions (from UiO)	18
12	Reference links	19
13	Bibliography	19
Со	urse homepage: https://wiki.math.ntnu.no/ma8701/2023v/start	

## 1 Model assessment and selection

(ESL Ch 7.1-7.6,7.10-7.12)

The generalization performance of  $\hat{f}$  can be evaluated from the EPE (expected prediction error) on an independent test set.

We use this for

- Model assessment: evaluate the performance of a selected model
- Model selection: select the best model for a specific task among a set of models

#### 1.1 Plan

- 1) Look at  $EPE(x_0)$  (now called  $Err(x_0)$ ) and how model complexity can be broken down into irreducible error, squared bias and variance (should be known from before)
- 2) Study EPE (Err) unconditional and conditional on the training set
- 3) Study optimism of the training error rate, and how in-sample error may shed light
- 4) Cross-validation and .632 bootstrap estimates of EPE
- 5) How will we build on this in the rest of the course?

We finished 1) and 2) in L2, now we continue!

## 2 Optimism of the training error rate

(again - focus is on regression)

First, nothing new, but new notation  $(X^0, Y^0)$  to specify that a new test observation is drawn from the joint distribution F (both over new X and new Y):

$$\operatorname{Err}_T = \operatorname{E}_{X^0, Y^0} [L(Y^0, \hat{f}(X^0)) \mid T]$$

and then the averaging over the training set (both Xs and Ys in the training set):

$$\mathrm{Err} = \mathrm{E}_T \mathrm{E}_{X^0,Y^0} [L(Y^0,\hat{f}(X^0)) \mid T]$$

This is also called *extra-sample error* (in contrast to what we now will define to be in-sample).

We saw before - from the ESL Figure 7.1, the training error err is (in general) less than (or equal to) the true test error, so not a good estimator for the test error.

$$\overline{\text{err}} = \frac{1}{N} \sum_{i=1}^{N} L(y_i, \hat{f}(x_i))$$

[In Exercise 2.9 we prove that the expected training error is smaller or equal the expected error of a testset - for MLR. Important to work on this exercise!]

Part of this is due to where the X values are "placed". The test input vectors need not be "in the same positions" as in the training X values (when the mean is taken over the full distribution of X).

To eliminate this "confusing fact", calculations can be made be assuming the X-values in the training data are kept fixed - and this is called the *in-sample error*. (We did the same in TMA4267 using the Fahrmeir et al book, Chapter 3.4.)

#### 2.1 In-sample error

$$\mathrm{Err}_{\mathrm{in}} = \frac{1}{N} \sum_{i=1}^{N} \mathrm{E}_{Y^0} [L(Y_i^0, \hat{f}(x_i)) \mid T]$$

Observe that we now take the expected value over distribution of the response - but that the (new) responses are found at the original training points. The training predictor positions  $x_i$ , i = 1, ..., N are fixed. In addition the responses in the training data are also kept fixed, so the only random quantity here is the new responses at the fixed predictors.

#### 2.2 Optimism

Optimism is defined as the difference between the in-sample error and the training error:

$$\mathrm{op} = \mathrm{Err}_{\mathrm{in}} - \overline{\mathrm{err}}$$

#### 2.3 Average optimism

is defined as the expected value of the optimism, where the expectation is taken over the distribution of the training responses - denoted y (training predictors still kept fixed):

$$\omega = \mathrm{E}_{\mathbf{y}}(op) = \mathrm{E}_{\mathbf{y}}(\mathrm{Err}_{\mathrm{in}}) - \mathrm{E}_{\mathbf{y}}(\overline{\mathrm{err}})$$

Observe that if we write T then the expectation is taken over the distribution of both the predictors and responses in the training set, and we here write  $\mathbf{y}$  for taking the distribution only over the reponses in the training set (not the predictors in the training set).

We will focus on "modelling"  $\omega$ , "instead of" Err.

#### 2.4 Covariance result

For squared error, 0-1 loss, and "other loss functions" it can be shown

$$\omega = \frac{2}{N} \sum_{i=1}^{N} \text{Cov}(\hat{y}_i, y_i)$$

#### 2.5 Group discussion

- 1) Give an interpretation of the result.
- 2) How do you think this result can be used?
- 3) Study the derivation of the covariance formula for squared loss. This is Exercise 7.4 and solutions are available here and in the ESL solutions to exercises.

Interpretation:

- how much the training error underestimates the true error depends on how strongly the observed response  $y_i$  affects its own prediction  $\hat{y}_i$ .
- the *harder* we fit the data the greater the covariance which increases the expected (averaged) optimism.

## 3 Expected in-sample prediction error

$$\mathbf{E}_{\mathbf{y}}(\mathrm{Err_{in}}) = \mathbf{E}_{\mathbf{y}}(\overline{\mathrm{err}}) + \frac{2}{N} \sum_{i=1}^{N} \mathrm{Cov}(\hat{y}_i, y_i)$$

This is the starting point for several methods to "penalize" fitting complex models!

#### 3.1 Result for $\omega$

Additive error model and squared loss:  $Y = f(X) + \varepsilon$ , with  $\hat{y}_i$  obtained by a linear fit with d inputs (or basis functions)

$$\omega = 2\frac{d}{N}\sigma_{\varepsilon}^2$$

Proof: ESL 7.1

For the proof: Remember that the trace of a square matrix is the sum of the diagonal elements, and trace is often denoted tr.

What is the trace (tr) for MLR?

 $\operatorname{tr}(\mathbf{H}) = \operatorname{tr}(\mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T) = \operatorname{tr}((\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T\mathbf{X}) = \operatorname{tr}(\mathbf{I})_{p+1} = (p+1) \text{ if intercept model with } p \text{ covariates.}$ 

#### 3.2 Group discussion

- Comment on the derivation of  $\omega$  anything unclear?
- How does d and N and  $\sigma_{\varepsilon}^2$  influence the average optimism?

Observe that the optimism increases with d and decreases with N.

Comment: versions of the formula hold approximately for other error models than linear with squared loss (ESL mention binary data and entropy loss), but not in general for 0-1 loss (page 231, bottom, with reference to Efron 1986 - consult the ESL book).

## 4 Three ways to perform model selection

- Estimate of expected in-sample prediction error (ESL Ch 7.5-7.6): We may develop the average optimism for a class of models that are linear in the parameters (Mallows Cp, AIC, BIC, ...) and compare models of different complexity using E<sub>y</sub>(Err<sub>in</sub>). Remark: in-sample error is not of interest, but used to choose between models effectively.
- Estimate Err (ESL Ch 7.10-7.11): We may instead use resampling methods (cross-validation and bootstrapping) to estimate Err directly (and use that for model selection and assessment).
- In the data rich approach: we have so much data that we use a separate validation set for model selection (and a separate test set for model assessment). That is not the focus of ESL Ch 7.

## 5 Estimates of (expected) in-sample prediction error

We have the following result:

$$\mathbf{E}_{\mathbf{y}}(\mathrm{Err}_{\mathrm{in}}) = \mathbf{E}_{\mathbf{y}}(\overline{\mathrm{err}}) + \frac{2}{N} \sum_{i=1}^{N} \mathrm{Cov}(\hat{y}_{i}, y_{i})$$

where now

$$\omega = \frac{2}{N} \sum_{i=1}^{N} \text{Cov}(\hat{y}_i, y_i)$$

We now want to get an estimate of the average optimism, to get an estimate of the in-sample prediction error:

$$\widehat{\mathrm{Err}_{\mathrm{in}}} = \overline{\mathrm{err}} + \widehat{\omega}$$

Comment: observe that  $\overline{\operatorname{err}}$  is now an estimate of  $E_{\mathbf{y}}(\overline{\operatorname{err}})$  and even though we write  $\widehat{\operatorname{Err}}_{\operatorname{in}}$  we are aiming to estimate  $E_{\mathbf{y}}(\operatorname{Err}_{\operatorname{in}})$ . Focus now is on  $\widehat{\omega}!$ 

## 5.1 $C_p$ statistics

for squared error loss (follows directly from the  $\omega$ -result for additive error model)

$$C_p = \overline{\operatorname{err}} + 2\frac{d}{N}\hat{\sigma}_{\varepsilon}^2$$

where  $\hat{\sigma}_{\varepsilon}^2$  is estimated from a "low-bias model" (in MLR we use a "full model").

(This method is presented both in TMA4267 and TMA4268, see also exam question Problem 3 in TMA4267 in 2015 and solutions.)

#### 5.2 Akaike information criterion (AIC)

Based on different asymptotic  $(N \to \infty)$  relationship for log-likelihood loss functions

$$-2\mathrm{E}[\log P_{\hat{\theta}}(Y)] \approx -\frac{2}{N}\mathrm{E}[\mathrm{loglik}] + 2\frac{d}{N}$$

- $P_{\hat{\theta}}(Y)$ : family of density for Y where the true density is included
- $\hat{\theta}$ : MLE of  $\theta$
- loglik: maximized log-likelihood  $\sum_{i=1}^N \log P_{\hat{\theta}}(y_i)$

Logistic regression with binomial loglikelihood

$$AIC = -\frac{2}{N}loglik + 2\frac{d}{N}$$

Multiple linear regression if variance  $\sigma_{\varepsilon}^2 = \hat{\sigma}_{\varepsilon}^2$  assumed known then AIC is equivalent to  $C_p$ .

For nonlinear or similar models then d is replaced by some measure of model complexity.

AIC as function of tuning parameter (back to squared error loss)

We have a set of models  $f_{\alpha}(x)$  indexed by some tuning parameter  $\alpha.$ 

$$AIC(\alpha) = \overline{err}(\alpha) + 2\frac{d(\alpha)}{N}\hat{\sigma}_{\varepsilon}^2$$

- $\overline{\operatorname{err}}(\alpha)$ : training error
- $d(\alpha)$  number of parameters
- $\hat{\sigma}_{\varepsilon}^2$  estimated variance of large model

The model complexity  $\alpha$  is chosen to minimize AIC( $\alpha$ ).

This is not true if the models are chosen adaptively (for example basis functions) this formula underestimates the optimism - and we may regard this as the *effective number of parameters* is larger than d.

#### 5.3 Expected in-sample prediction error for binary classification

(Efron and Hastie (2016) page 225)

Misclassification loss function:  $L(\hat{G}(X), G) = 1$  for incorrect classification and 0 for correct.

The training error is then  $\overline{\text{err}} = (\#(\hat{G}_i \neq G_i))/N$ .

The insample error is then  $\frac{1}{N} \sum_{i=1}^N P(G_{0i}(X_i) \neq \hat{G}(X_i)).$ 

The estimate of (expected) in-sample prediction error is then

$$\widehat{\mathrm{Err}_{\mathrm{i}n}} = \frac{\#(\hat{G}_i \neq G_i)}{N} + \frac{2}{N} \sum_{i=1}^{N} \mathrm{Cov}(\hat{G}(X_i), G(X_i))$$

where

$$\begin{split} &\operatorname{Cov}(\hat{G}(X_i), G(X_i)) = \operatorname{E}(\hat{G}(X_i) \cdot G(X_i)) - \operatorname{E}(\hat{G}(X_i)) \cdot \operatorname{E}(G(X_i)) \\ &= \mu_i (1 - \mu_i) [P(\hat{G}(X_i) = 1 \mid G(X_i) = 1) - P(\hat{G}(X_i) = 1 \mid G(X_i) = 0)] \end{split}$$

where  $\mu_i = P(G(X_i) = 1)$ .

#### 5.4 Group discussion

What is the take home message from this part on "Estimates of (expected) in-sample prediction error"?

## 6 The effective number of parameters

(ESL 7.6)

The number of parameters d can be generalized into an effective number of parameters. We will look at linear fitting method:

$$\hat{\mathbf{y}} = \mathbf{S}y$$

where **S** as a  $n \times n$  matrix depending on covariates  $x_i$  but not responses  $y_i$ .

- MLR  $\mathbf{H} = \mathbf{X}(\mathbf{X}^T\mathbf{X})^{-1}\mathbf{X}^T$
- cubic smoothing splines
- ridge regression

The effective number of parameters is

$$\mathrm{df}(\mathbf{S}) = \mathrm{trace}(\mathbf{S})$$

Additive error model and squared loss:  $Y = f(X) + \varepsilon$  with  $\mathrm{Var}(\varepsilon) = \sigma_\varepsilon^2$  then

$$\sum_{i=1}^{N} \text{Cov}(\hat{y}_i, y_i) = \text{trace}(\mathbf{S}) \sigma_{\varepsilon}^2$$

leading to a generalization

$$\mathrm{df}(\hat{\mathbf{y}}) = \frac{\sum_{i=1}^{N} \mathrm{Cov}(\hat{y}_i, y_i)}{\sigma_{\varepsilon}^2}$$

See exercise 7.5 to prove this.

## 7 Cross-validation (CV)

(ESL Ch 7.10, 7.12 - most should be known from TMA4268)

The aim is to estimate  $\mathrm{Err}_T$ , but from simulation analyses (ESL Ch 7.12) it turns out that cross-validation estimates  $\mathrm{Err}$  "the best".

The starting point for the method is that we only have one training set - and try to use that for either model selection or model assessment (not both).

What to do when both is needed, is not covered in this chapter. Nested cross-validations aka two-layers of cross-validation is one possibility. Another is to set aside data for a test set for model assessment, but use the training set in cross-validation for model selection.

#### 7.1 Formal set-up for model assessment

- The allocation of observation  $\{1, ..., N\}$  to folds  $\{1, ..., K\}$  is done using an indexing function  $\kappa : \{1, ..., N\} \to \{1, ..., K\}$ , that for each observation allocate the observation to one of K folds.
- Further,  $\hat{f}^{-k}(x)$  is the fitted function, computed on the observations except the kth fold (the observations from the kth fold is removed).
- The CV estimate of the expected prediction error  $\text{Err} = \mathbf{E}_T \mathbf{E}_{X^0,Y^0}[L(Y^0,\hat{f}(X^0)) \mid T]$  is then

$$\mathrm{CV}(\hat{f}) = \frac{1}{N} \sum_{i=1}^N L(y_i, \hat{f}^{-k(i)}(x_i))$$

#### 7.2 Formal set-up for model selection

- The indexing function  $\kappa$  is unchanged, and for the fitting function we add a tuning parameter  $\alpha$ :  $f(x,\alpha)$  such that  $\hat{f}^{-k}(x,\alpha)$  is the fitted function using tuning parameter  $\alpha$ , with the kth fold removed from the model fitting.
- The expected prediction error is estimated by

$$\mathrm{CV}(\hat{f},\alpha) = \frac{1}{N} \sum_{i=1}^N L(y_i,\hat{f}^{-k(i)}(x_i,\alpha))$$

- We find the best tuning parameter  $\hat{\alpha}$  that minimize the  $\mathrm{CV}(\hat{f}, \alpha)$ . Alternatively the one-standard error rule can be used: choose the most parsimonious ("smallest") model whose error is no more than one standard error above the error of the best model.
- This best chosen model is then fit to all the data. (ESL page 242).

#### 7.3 Choice of K

- Popular choices are 5 and 10 based on observations in simulation studies- and arguments similar to a bias-variance trace off.
- K = N is called *leave-one-out* cross-validation LOOCV, and gives the lowest bias for estimating the Err.

#### 7.4 Generalized cross-validation (GCV)

For LOOCV with squared loss and linear fitting. Remember

$$\hat{\mathbf{y}} = \mathbf{S}y$$

For many fitting methods (including MLR)

$$\frac{1}{N} \sum_{i=1}^{N} [y_i - \hat{f}^{-i}(x_i)]^2 = \frac{1}{N} \sum_{i=1}^{N} [\frac{y_i - \hat{f}(x_i)}{1 - S_{ii}}]^2$$

where  $S_{ii}$  is the ith diagonal element of S. This leads to the GCV approximation:

$$GCV(\hat{f}) = \frac{1}{N} \sum_{i=1}^{N} [\frac{y_i - \hat{f}(x_i)}{1 - \text{tr}(\mathbf{S})/N}]^2$$

where we recognise the effective number of parameters trace( $\mathbf{S}$ ). In some settings the trace( $\mathbf{S}$ ) is computed more easily than the individual elements  $S_{ii}$ .

#### 7.5 What is estimated?

Efron and Hastie (2016) page 218: "CV( $\hat{f}$ ) is estimating the average prediction error of the algorithm producing  $\hat{f}$ , not  $\hat{f}$  itself".

#### 7.6 The wrong and the right way to do cross-validation

In short: make sure that all part of the model fit process is "inside" the CV.

See learning material from TMA4268: Module 5: Resampling, and I also recommend to work on Problem 3 with solutions

#### 8 Bootstrap methods

(ESL Ch 7.11 - bootstrapping is known from TMA4268 and TMA4300, but not the special case of estimating Err). Bootstrap in TMA4268: Module 5

**Notation:**  $\mathbf{Z} = (z_1, \dots, z_N)$  is the training set with  $z_i = (x_i, y_i)$ .

**Aim:** Of interest is some quantity calculated from the data  $\mathbf{Z}$ , denoted  $S(\mathbf{Z})$ . We will have focus on the expected prediction error.

**Resampling:** We draw with replacement from **Z** a total of N observations into  $\mathbf{Z}^{*b}$ . We repeat this B times.

Estimator for expected predicted error Err:

$$\widehat{\text{Err}}_{\text{boot}} = \frac{1}{B} \frac{1}{N} \sum_{b=1}^{B} \sum_{i=1}^{N} L(y_i, \hat{f}^{*b}(x_i))$$

However -  $\widehat{\text{Err}}_{\text{boot}}$  is not a good estimator: bootstrap datasets are acting as training data and the original data as a test sample - and the two samples have observations in common.

This overlap can make predictions too good. Remember, in CV we have no overlap.

**Q:** What is the probability that observation i is included in bootstrap sample b?

The problem is given in TMA4268 Module 5 as Problem 1 with (handwritten) solutions.

The answer is  $1 - (1 - \frac{1}{N})^N \approx 1 - e^{-1} = 0.632$ .

Why is this relevant?

What if we try to change the bootstrap Err estimator - so that we for each observation i only keep predictions from bootstrap samples where this observation is not present? Then we would mimic the CV-estimator.

The leave-one-out bootstrap estimate:

$$\widehat{\text{Err}}^{(1)} = \frac{1}{N} \sum_{i=1}^{N} \frac{1}{|C^{-i}|} \sum_{b \in C^{-i}} L(y_i, \hat{f}^{*b}(x_i))$$

where  $C^{-i}$  are the indices in the bootstrap sample b that do not contain observation i, and  $|C^{-i}|$  is the number of samples. (B must be large enough that we do not get any  $C^{-i}$ s that are empty, or leave out these zero sets in the formula.)

Comment: this is also called out-of-bootstrap, and is closely connected to the popular out-of-bag estimate for random forests.

There is an addition fix to make the estimate even better.

Since the average number of distinct observations in each bootstrap sample is approximately 0.632N - and the bootstrap sample behaves like a training set - this gives a so called training-set-size bias (similar to C with K=2), meaning that the leave-one-out bootstrap estimator will be biased upwards. This can be fixed by weighing together the leave-one-out boostrap estimator with the training error.

The ".632" estimator:

$$\widehat{\mathrm{Err}}^{(.632)} = 0.368\overline{\mathrm{err}} + 0.632\widehat{\mathrm{Err}}^{(1)}$$

According to ESL (page 251): the derivation of the .632 estimator is complex, and the estimator is expected to work well in situation where the data is not overfitted, but may break down in overfit situations.

According to CASI (page 323) the .632 rule is less variable than the leave-one-out CV.

Example of this on page 251-252: two equal size classes where predictors independent of class, classification with 1NN gives  $\overline{\text{err}} = 0$  and  $\widehat{\text{Err}}^{(1)} = 0.5$  and thus  $\widehat{\text{Err}}^{(.632)} = 0.632 \cdot 0.5 = 0.316$ , where here the true error rate is 0.5.

There is an improved version of the estimator - taking into account the amount of overfitting, leading to an adjustment to the weight w=0.632 (and 1-w=0.368) dependent on a socalled no-information error rate= $\gamma$ =the error rate of the prediction rule when predictors and class labels are independent.

$$\hat{\gamma} = \frac{1}{N^2} \sum_{i=1}^{N} \sum_{i'=1}^{N} L(y_i, \hat{f}(x_{i'}))$$

Further the relative overfitting rate is defined to be

$$\hat{R} = \frac{\widehat{\text{Err}}^{(1)} - \overline{\text{err}}}{\hat{\gamma} - \overline{\text{err}}}$$

Finally, the ".632+"-estimator is

$$\widehat{\operatorname{Err}}^{(.632+)} = (1-\hat{w})\overline{\operatorname{err}} + \hat{w}\widehat{\operatorname{Err}}^{(1)}$$

where  $\hat{w} = \frac{0.632}{1-0.368\hat{R}}$ .

For details on this approach consult ESL page 252-253.

#### 9 Conclusions: Model selection and assessment and future use

**Group discussion:** Construct a "mind map" or "overview sheet" or "concept map" for the "Model assessment and selection" topics, and write down important take home messages!

#### 10 Exercises

#### 10.1 Expected training and test MSE for linear regression

Do exercise 2.9.

Important take home message: We have proven (for MLR) that the expected test MSE is always at least as large as the expected training MSE.

#### 10.2 Establish the average optimism in the training error

$$\omega = \frac{2}{N} \sum_{i=1}^{N} \text{Cov}(\hat{y}_i, y_i)$$

Exercise 7.4

#### 10.3 Relate the covariance to the trace of a linear smoother

Exercise 7.5

Need to know about covariance and variance of linear combinations. The reading list in TMA4267 included Härdle and Simar (2015): Applied Multivariate Statistical Analysis (fourth edition) - ebook from Springer available at NTNU. Alternatively classnotes from TMA4267 (page 58-59)

#### 10.4 Derive the estimate of in-sample error

for the additive error model

$$Y = f(X) + \varepsilon$$

of Eq (7.24):

$$\mathbf{E}_{y}(\mathbf{Err_{in}}) = \mathbf{E}_{y}(\bar{\mathbf{err}}) + 2 \cdot \frac{d}{N}\sigma_{\varepsilon}^{2}$$

Prove this for the MLR OLS solution.

#### 10.5 Additive error model effective degrees of freedom

Exercise 7.6

Show that for an additive-error model, the effective degrees-of freedom for the k-nearest-neighbors regression fit is N/k.

Hint: write this as a linear smoother.

## 10.6 UiO STK-IN4300/STK-IN9300 — Statistical learning methods in Data Science

Exam 2018, Problem 2: Bootstrapping for model evaluation

Consider the following procedure to estimate the prediction error:

- 1. generate B bootstrap samples  $z_1, z_2, ..., z_B$  where  $z_b = \{(y_1^*, x_1^*), ..., (y_N^*, x_N^*)\}, b = 1, ..., B$  and  $(y_i^*, x_i^*), i = 1, ..., N$ , is an observation sampled from the original dataset;
- 2. apply the prediction rule to each bootstrap sample to derive the preditions  $\hat{f}_b^*(x_i)$ ,  $b = 1, \dots, B$ .
- 3. compute the error for each point, and take the average,

$$\widehat{\mathrm{Err}}_{\mathrm{boot}} = \frac{1}{B} \sum_{b=1}^{B} \frac{1}{N} \sum_{i=1}^{N} L(y_i, \widehat{f}_b^*(x_i))$$

- a) Explain why this procedure is incorrect and suggest a different way to proceed which still uses a bootstrap approach.
- b) Describe the 0.632 bootstrap and the 0.632+ bootstrap procedures, explaining in particular the rationale behind their construction.

#### 10.7 Comparing methods

Exercise 7.9 (minus BIC).

For the prostate data of ESL Chapter 3, carry out a best-subset linear regression analysis, as in Table 3.3 (third column from left). Compute the AIC, five- and tenfold cross-validation, and bootstrap .632 estimates of prediction error. Discuss the results.

#### 11 Solutions to exercises

Please try yourself first, or take a small peek - and try some more - before fully reading the solutions. Report errors or improvements to Mette.Langaas@ntnu.no. (The solutions given here are very similar to the UiO STK-IN4300 solutions, see link under References.)

- 2.9
- 7.4
- 7.5
- 7.1
- 7.6
- Solution from Hastie: 7.9 also using utils.R

#### 11.0.1 UiO STK-IN4300/STK-IN9300 Solutions (from UiO)

a) The procedure is incorrect because the prediction error is computed on observations already used to train the prediction rule. This lead to underestimation of the error (writing "too optimistic" was acceptable).

A possible solution is to compute the prediction error only on those observations (in average 36.8% of the original sample) not included in the bootstrap sample. Since this approach leads to overestimating the prediction error, solutions like those described in the point (b) has been implemented.

b) The 0.632 bootstrap procedure addresses the problem of overestimation of the correct procedure described in point (a) by averaging it (with weight 0.632 and 0.368, respectively) with the training error (underestimated error). The result is a sort of compromise between overestimation and underestimation.

$$\widehat{\operatorname{Err}}^{(0.632)} = 0.632 \cdot \widehat{\operatorname{Err}}^{(1)} + 0.368 \cdot \overline{\operatorname{err}}$$

where  $\overline{\text{err}}$  is the training error and  $\widehat{\text{Err}}^{(1)}$  the corrected procedure decribed in (a). Since the 0.632 and 0.382 weights may not be the best choice (e.g., in case of complete overfitting in the training set), the 0.632+ bootstrap has been developed. In the latter procedure,

$$\widehat{\operatorname{Err}}^{(0.632+)} = \widehat{w} \cdot \widehat{\operatorname{Err}}^{(1)} + (1 - \widehat{w}) \cdot \overline{\operatorname{err}}$$

the weights depend on the relative overfitting rate, so the 0.632+ bootstrap can be seen as a better compromise between the overestimation and underestimation of the prediction error done by the corrected procedure described at point (a) and the training error, respectively.

#### 12 Reference links

- ESL official errata: and choose "Errata" in the left menu
- ESL solutions to exercises
- ESL solutions from UiO
- CASI Computer Age Statistical Inference, Efron and Hastie (2017). Chapter 12: Cross-Validation and  $C_p$  Estimates of Prediction Error
- Burnham and Andersen (2002): Model Selection and Multimodel Inference: A Practical Information-Theoretic Approach. Springer. Chapter 7: Statistical Theory and Numerical Results

## 13 Bibliography

Efron, Bradley, and Trevor Hastie. 2016. Computer Age Statistical Inference - Algorithms, Evidence, and Data Science. Cambridge University Press. https://hastie.su.domains/CASI/.