# MA8701 Advanced methods in statistical inference and learning

L10: Shrinkage methods for the GLM

# Mette Langaas

# 2/9/23

## Table of contents

1	Befo	e we begin	2
	1.1	Literature	2
2	Gen	ralized linear models	3
	2.1	The model	3
	2.2	Explaining $\beta$ in logistic regression	4
	2.3	Parameter estimation	5
		2.3.1 Logistic regression	6
		2.3.2 Algorithms	6
		2.3.3 Properties	6
		2.3.4 Penalized logistic regression	6
		2.3.5 Algorithms	7
		2.3.6 Ridge logistic regression IRWLS	7
		2.3.7 Lasso logistic regression fitting algoritm	7
		2.3.8 Criteria for choosing $\lambda$	7
3	Eval	ation metrics	8
	3.1	Confusion matrix, sensitivity, specificity	8
	3.2	ROC curves	9
	3.3	ROC-AUC	9
	3.4	ROC-PR	9
	3.5	Deviance	9
4	Exa	ple: South African heart disease	10
	4.1	Group discussion	10
	4.2	Data set	10

7	LXC	i Cises	29
	Evo	rcises	29
	6.9	The Bonferroni method controls the FWER	29
	6.8	Familywise error rate	28
	6.7	From single to multiple hypotheses	28
	6.6	p-value	27
	6.5	Single hypothesis test	26
	6.4	Bias corrected accelerated interval	26
	6.3	Percentile interval	
	6.2	Bootstrap confidence intervals	
•	6.1	Confidence interval	25
6	Prei	paring for inference for the lasso and ridge	25
	5.4	Lasso variants	25
		5.3.3 Additional modifications	25
		5.3.2 Penalties	24
		5.3.1 Family	
	5.3	cv.glmnet inputs	
	5.2	glmnet inputs	
•	5.1	Software links	
5	Con	nputational details for the glmnet	22
	4.7	Elastic net logistic regression	20
	4.6	Lasso logistic regression	17
	4.5	Ridge logistic regression	
	4.4	Logistic regression	14
	4.3	Data description	11

## 1 Before we begin

## 1.1 Literature

- [ELS] The Elements of Statistical Learning: Data Mining, Inference, and Prediction, Second Edition (Springer Series in Statistics, 2009) by Trevor Hastie, Robert Tibshirani, and Jerome Friedman. Ebook. Chapter 4.4.1-4.4.3 (4.4.4 is covered in 3.2 of HTW).
- [HTW] Hastie, Tibshirani, Wainwright: "Statistical Learning with Sparsity: The Lasso and Generalizations". CRC press. Ebook. Chapter 3.2,3.7, 5.4.3

and for the interested student

•	[WNvW]	Wessel N.	van \	Wieringen:	Lecture	notes	on ridg	ge regression	Chapter 5.

Supplemental sources useful for week 6 (see also the section on "Preparing for inference for the lasso and ridge")

- Bootstrap confidence intervals in the master thesis of Lene Tillerli Omdal Section 3.6.2 and teaching material from TMA4300 see the wikipage for that course.
- Short note on multiple hypothesis testing in TMA4267 Linear Statistical Models, Kari K. Halle, Øyvind Bakke and Mette Langaas, March 15, 2017.

## 2 Generalized linear models

(HTW 3.1, 3.2, and TMA4315 GLM background)

#### 2.1 The model

The GLM model has three ingredients:

- 1) Random component
- 2) Systematic component
- 3) Link function

We look into that for the binomial distribution - to get multiple linear regression and logistic regression.

• Write in class

pivec	l						l		
odds	0.11	0.25	0.43	0.67	1.0	1.5	2.33	4.0	9.0

## 2.2 Explaining $\beta$ in logistic regression

- The ratio  $\frac{P(Y_i=1)}{P(Y_i=0)} = \frac{\pi_i}{1-\pi_1}$  is called the *odds*.
- If  $\pi_i = \frac{1}{2}$  then the odds is 1, and if  $\pi_i = \frac{1}{4}$  then the odds is  $\frac{1}{3}$ . We may make a table for probability vs. odds in R:
- Odds may be seen to be a better scale than probability to represent chance, and is used in betting. In addition, odds are unbounded above.

We look at the link function (inverse of the response function). Let us assume that our linear predictor has k covariates present

$$\begin{split} \eta_i &= \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_k x_{ik} \\ \pi_i &= \frac{\exp(\eta_i)}{1 + \exp(\eta_i)} \\ \eta_i &= \ln(\frac{\pi_i}{1 - \pi_i}) \\ \ln(\frac{\pi_i}{1 - \pi_i}) &= \beta_0 + \beta_1 x_{i1} + \beta_2 x_{i2} + \dots + \beta_k x_{ik} \\ \frac{\pi_i}{1 - \pi_i} &= \frac{P(Y_i = 1)}{P(Y_i = 0)} = \exp(\beta_0) \cdot \exp(\beta_1 x_{i1}) \cdots \exp(\beta_k x_{ik}) \end{split}$$

We have a *multiplicative model* for the odds.

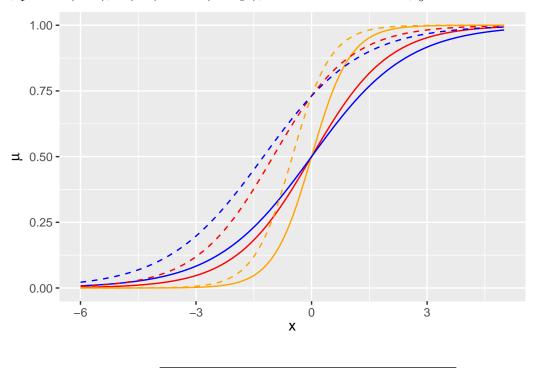
## So, what if we increase $x_{1i}$ to $x_{1i} + 1$ ?

If the covariate  $x_{1i}$  increases by one unit (while all other covariates are kept fixed) then the odds is multiplied by  $\exp(\beta_1)$ :

$$\begin{split} \frac{P(Y_i = 1 \mid x_{i1} + 1)}{P(Y_i = 0) \mid x_{i1} + 1)} &= \exp(\beta_0) \cdot \exp(\beta_1(x_{i1} + 1)) \cdots \exp(\beta_k x_{ik}) \\ &= \exp(\beta_0) \cdot \exp(\beta_1 x_{i1}) \exp(\beta_1) \cdots \exp(\beta_k x_{ik}) \\ &= \frac{P(Y_i = 1 \mid x_{i1})}{P(Y_i = 0 \mid x_{i1})} \cdot \exp(\beta_1) \end{split}$$

This means that if  $x_{i1}$  increases by 1 then: if  $\beta_1 < 0$  we get a decrease in the odds, if  $\beta_1 = 0$  no change, and if  $\beta_1 > 0$  we have an increase. In the logit model  $\exp(\beta_1)$  is easier to interpret than  $\beta_1$ .

The response function as a function of the covariate x and not of  $\eta$ . Solid lines:  $\beta_0=0$  and  $\beta_1$  is 0.8 (blue), 1 (red) and 2 (orange), and dashed lines with  $\beta_0=1$ .



## 2.3 Parameter estimation

First logistic regression, then ridge and lasso logistic regression - and (maybe) elastic net logistic regression.

## 2.3.1 Logistic regression

•	Maximum likelihood estimation = maximize the likelihood of the data.	We write for the
	loglikelihood $l(\beta_0, \beta; y, X)$ .	

•	We write out	the	loglikelihood	for	the	binomial	with	logit	link	=logistic	regression	n
---	--------------	-----	---------------	-----	-----	----------	------	-------	------	-----------	------------	---

## 2.3.2 Algorithms

To understand the ridge and lasso logistic regression we first look at the *iteratively reweighted* least squares (IRLS) - as a result of the Newton Raphson method for the logistic regression (unpenalized).

## 2.3.3 Properties

The parameter estimator is asymptotically normal. Unbiased with variance the inverse of the Fisher information matrix - as known TMA4315.

In class we now scroll down to the South African data set and look at the data and the logistic regression.

#### 2.3.4 Penalized logistic regression

- For penalized method we instead minimize the negative loglikelihood scaled with  $\frac{1}{N}$ .
- The ridge and lasso penalty is added to the scaled negative loglikelihood.
- Write in class

#### 2.3.5 Algorithms

- The likelihood for the GLM is differentiable, and the ridge and lasso objective functions are convex and can be solved with socalled "standard convex optimization methods".
- But, by popular demand also special algorithms are available building on the cyclic coordinate descent.

## 2.3.6 Ridge logistic regression IRWLS

## 2.3.7 Lasso logistic regression fitting algoritm

```
(HTW page 116)
```

```
OUTER LOOP: start with lambdamax and decrement

MIDDLE LOOP (with warm start)

compute quadratic approximation
for current beta-estimates

INNER LOOP: cyclic coordinate descent
to minimize quadratic approximation
added the lasso penalty
```

#### **2.3.8** Criteria for choosing $\lambda$

We use cross-validation to choose  $\lambda$ .

For regression we choose  $\lambda$  by minimizing the (mean) squared error.

For (ridge and) lasso logistic regression we may choose:

- misclassification error rate on the validation set
- ROC-AUC or PR-AUC
- binomial deviance

## 3 Evaluation metrics

## 3.1 Confusion matrix, sensitivity, specificity

(from TMA4268)

In a two class problem - assume the classes are labelled "-" (non disease,0) and "+" (disease,1). In a population setting we define the following event and associated number of observations.

	Predicted -	Predicted +	Total
True -	True Negative TN	False Positive FP	N
True +	False Negative FN	True Positive TP	P
Total	N*	P*	

(N in this context not to be confused with our sample size...)

**Specificity** is the proportion of correctly classified negative observations:  $\frac{\#\text{True Negative}}{\#\text{Condition Negative}} = \frac{\text{TN}}{N}$ .

We would like that a classification rule have both a high sensitivity and a high specificity.

#### Other useful quantities:

Name	Definition	Synonoms
False positive rate	FP/N	Type I error, 1-specificity
True positive rate	TP/P	1-Type II error, power, sensitivity, recall
Positive predictive value (PPV)	$TP/P^*$	Precision, 1-false discovery proportion
Negative predictive value (NPV)	$TN/N^*$	

Where the PPV can be used together with the sensitivity to make a precision-recall curve more suitable for low case rates.

#### 3.2 ROC curves

(also from TMA4268)

The receiver operating characteristics (ROC) curve gives a graphical display of the sensitivity against specificity, as the threshold value (cut-off on probability of success or disease) is moved over the range of all possible values. An ideal classifier will give a ROC curve which hugs the top left corner, while a straight line represents a classifier with a random guess of the outcome.

#### 3.3 ROC-AUC

- The **ROC-AUC** score is the area under the ROC curve. It ranges between the values 0 and 1, where a higher value indicates a better classifier.
- The AUC score is useful for comparing the performance of different classifiers, as all possible threshold values are taken into account.
- The ROC-AUC is closely connected to the robust U statistics.
- If the prevalence (case proportion) is very low (0.01ish), the ROC-AUC may be misleading, and the PR-AUC is more commonly used.

3.4 ROC-PR			
To be added.			

#### 3.5 Deviance

The deviance is based on the likelihood ratio test statistic.

The derivation assumes that data can be grouped into covariate patterns, with G groups (else interval solutions are used in practice).

**Saturated model:** If we were to provide a perfect fit to our data then we would estimate  $\pi_j$  by the observed frequency for the group,  $\hat{y}_j = y_j$ .

Candidate model: the model with the current choice of  $\lambda$ .

 $D_{\lambda} = 2(l(\text{saturated model}) - l(\text{candidate model}_{\lambda}))$ 

The **null deviance** is replacing the candidate model with a model where  $\hat{y}_i = \frac{1}{N} \sum_{i=1}^{N} y_i$  (the case proportion).

## 4 Example: South African heart disease

(ELS 4.4.2)

## 4.1 Group discussion

Comment on what is done and the results. Where are the CIs and p-values for the ridge and lasso version?

## 4.2 Data set

The data is presented in ELS Section 4.4.2, and downloaded from http://statweb.stanford.edu/~tibs/ElemStatLearn.1stEd/ with information in the file SAheat.info and data in SAheart.data.

- This is a retrospective sample of males in a heart-disease high-risk region in South Africa.
- It consists of 462 observations on the 10 variables. All subjects are male in the age range 15-64.
- There are 160 cases (individuals who have suffered from a conorary heart disease) and 302 controls (individuals who have not suffered from a conorary heart disease).
- The overall prevalence in the region was 5.1%.

The response value (chd) and covariates

- chd: conorary heart disease {yes, no} coded by the numbers {1, 0}
- sbp: systolic blood pressure

- tobacco: cumulative tobacco (kg)
- ldl: low density lipoprotein cholesterol
- adiposity: a numeric vector
- famhist: family history of heart disease. Categorical variable with two levels: {Absent, Present}.
- typea: type-A behaviorobesity: a numerical value
- alcohol: current alcohol consumption
- age : age at onset

The goal is to identify important risk factors.

## 4.3 Data description

4 170

7.50 6.41

We start by loading and looking at the data:

```
ds=read.csv("./SAheart.data",sep=",")[,-1]
  ds$chd=as.factor(ds$chd)
  ds$famhist=as.factor(ds$famhist)
  dim(ds)
[1] 462 10
  colnames(ds)
 [1] "sbp"
                              "ld1"
                                           "adiposity" "famhist"
                 "tobacco"
 [7] "obesity"
                 "alcohol"
                              "age"
                                           "chd"
  head(ds)
 sbp tobacco ldl adiposity famhist typea obesity alcohol age chd
1 160
        12.00 5.73
                       23.11 Present
                                         49
                                               25.30
                                                       97.20
                                                              52
                                                                    1
2 144
         0.01 4.41
                       28.61 Absent
                                         55
                                               28.87
                                                        2.06
                                                              63
                                                                    1
3 118
         0.08 3.48
                       32.28 Present
                                         52
                                                                    0
                                               29.14
                                                        3.81
                                                              46
```

51

31.99

24.26

58

1

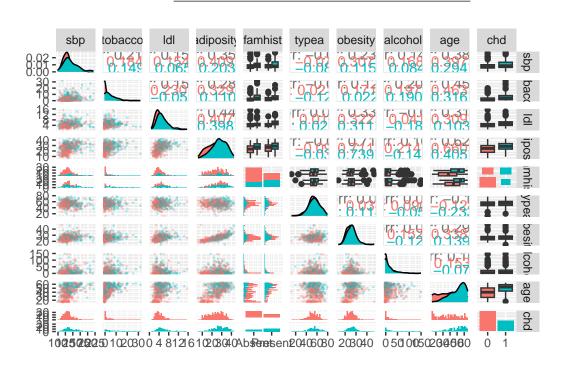
38.03 Present

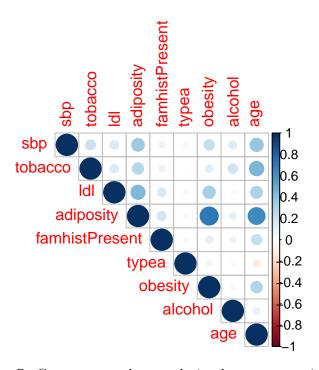
```
5 134
        13.60 3.50
                      27.78 Present
                                        60
                                             25.99
                                                     57.34 49
                                                                 1
6 132
        6.20 6.47
                      36.21 Present
                                             30.77
                                                     14.14 45
                                        62
                                                                 0
  # to be easier to compare with lasso and ridge, we standardize the xs
  xs=model.matrix(chd~.,data=ds)[,-1] # to take care of categorical variables, but not inclu
  xss=scale(xs)
  ys=as.numeric(ds[,10])-1 # not factor, must be numeric else errors...
  head(xss)
                               ldl adiposity famhistPresent
         sbp
                tobacco
                                                                  typea
1 1.0574173 1.8210988 0.4778941 -0.2951832
                                                   1.1845700 -0.4180170
2 0.2767892 -0.7893817 -0.1595071 0.4116942
                                                  -0.8423609 0.1931344
3 -0.9917313 -0.7741412 -0.6085852 0.8833742
                                                   1.1845700 -0.1124413
4 1.5453098 0.8413521 0.8062523 1.6223824
                                                   1.1845700 -0.2142999
5 -0.2111033 2.1694532 -0.5989276 0.3050200
                                                   1.1845700 0.7024273
6 -0.3086818  0.5583142  0.8352251  1.3884702
                                                   1.1845700 0.9061444
      obesity
                alcohol
                               age
1 -0.17659445 3.2741887 0.6286543
2 0.67064592 -0.6120811 1.3816170
3 0.73472292 -0.5405973 0.2179473
4 1.41109128 0.2947424 1.0393612
5 -0.01284211 1.6459912 0.4233008
6 1.12155816 -0.1186384 0.1494961
  table(ys)
уs
302 160
  dss=data.frame(ys,xss)
  colnames(dss)[1]="chd"
  apply(dss,2,sd)
                                                        ldl
                                                                 adiposity
           chd
                          sbp
                                     tobacco
                                                  1.0000000
                                                                 1.000000
     0.4763125
                    1.0000000
                                   1.0000000
famhistPresent
                        typea
                                     obesity
                                                    alcohol
                                                                       age
     1.0000000
                    1.0000000
                                   1.0000000
                                                                 1.0000000
                                                  1.0000000
```

## apply(dss,2,mean)

```
chd
                                                          ldl
                                                                   adiposity
                           sbp
                                      tobacco
                                                                1.557677e-15
  3.463203e-01
                 1.289252e-16
                                 5.166622e-16
                                               -3.961057e-15
famhistPresent
                        typea
                                      obesity
                                                     alcohol
                                                                         age
 -3.892990e-17
                -9.924721e-17
                                -5.292544e-15
                                               -6.411418e-16
                                                               -3.953067e-17
```

The coloring is done according to the response variable, where green represents a case Y = 1 and red represents a control Y = 0.





Q: Comment on the correlation between covariates, and what that may lead to?

## 4.4 Logistic regression

We now fit a (multiple) logistic regression model using the glm function and the full data set. In order to fit a logistic model, the family argument must be set equal to ="binomial". The summary function prints out the estimates of the coefficients, their standard errors and z-values. As for a linear regression model, the significant coefficients are indicated by stars where the significant codes are included in the R printout.

```
glm_heart = glm(chd~.,data=dss, family="binomial")
summary(glm_heart)

Call:
glm(formula = chd ~ ., family = "binomial", data = dss)

Deviance Residuals:
```

```
Min
              1Q
                   Median
                                 3Q
                                         Max
-1.7781
                 -0.4387
        -0.8213
                             0.8889
                                      2.5435
```

#### Coefficients:

```
Estimate Std. Error z value Pr(>|z|)
               -0.878545
                           0.123218 -7.130
                                            1.0e-12 ***
(Intercept)
sbp
                0.133308
                           0.117452
                                      1.135 0.256374
tobacco
                0.364578
                           0.122187
                                      2.984 0.002847 **
ldl
                           0.123554
                                      2.915 0.003555 **
                0.360181
adiposity
                0.144616
                           0.227892
                                      0.635 0.525700
famhistPresent 0.456538
                           0.112433
                                      4.061 4.9e-05 ***
                           0.120954
typea
                0.388726
                                      3.214 0.001310 **
               -0.265082
                           0.186446
                                     -1.422 0.155095
obesity
alcohol
                0.002978
                           0.109754
                                      0.027 0.978350
age
                0.660695
                           0.177203
                                      3.728 0.000193 ***
Signif. codes:
                0 '***' 0.001 '**' 0.01 '*' 0.05 '.' 0.1 ' ' 1
```

(Dispersion parameter for binomial family taken to be 1)

Null deviance: 596.11 degrees of freedom on 461 Residual deviance: 472.14 on 452 degrees of freedom

AIC: 492.14

Number of Fisher Scoring iterations: 5

```
exp(coef(glm_heart))
```

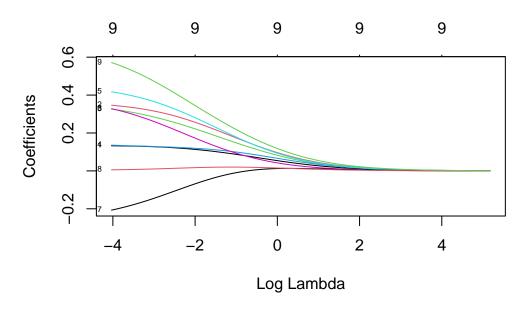
(Intercept)	sbp	tobacco	ldl	adiposity
0.4153868	1.1426023	1.4399061	1.4335883	1.1555963
famhistPresent	typea	obesity	alcohol	age
1.5785989	1.4750996	0.7671430	1.0029829	1.9361378

A very surprising result here is that sbp and obesity are NOT significant and obesity has negative sign. This is a result of the correlation between covariates. In separate models with only sbp or only obesity each is positive and significant.

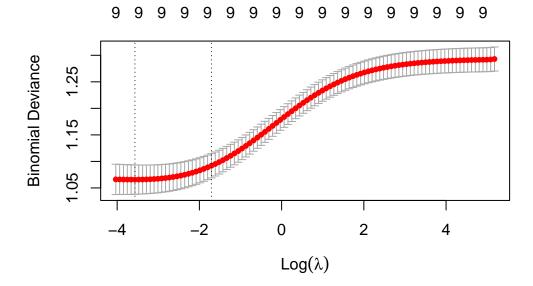
Q: How would you interpret the estimated coefficient for tobacco?

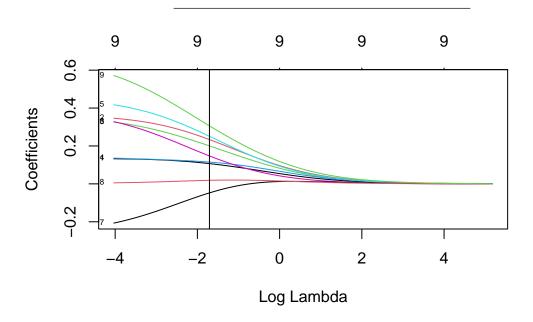
## 4.5 Ridge logistic regression

ridgefit=glmnet(x=xss,y=ys,alpha=0,standardize=FALSE,family="binomial") # already standard
plot(ridgefit,xvar="lambda",label=TRUE)



- [1] "The lamda giving the smallest CV error 0.0282259748786527"
- [1] "The 1sd err method lambda 0.18143863032661"





10 x 2 sparse Matrix of class "dgCMatrix" s1 (Intercept) -0.72240989 -0.878545196 sbp 0.10687796 0.133308398 tobacco 0.23373137 0.364577926 ldl 0.20036907 0.360180594 adiposity 0.11494180 0.144616485 famhistPresent 0.25104376 0.456537713 typea 0.14734996 0.388725509 obesity -0.04764114 -0.265082072 alcohol 0.01868168 0.002978424 0.30606849 0.660695163 age

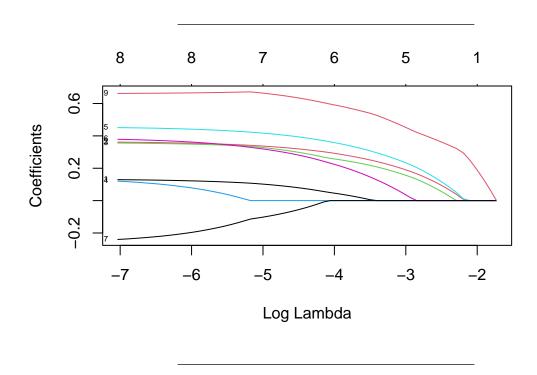
## 4.6 Lasso logistic regression

Numbering in plots is order of covariates, so:

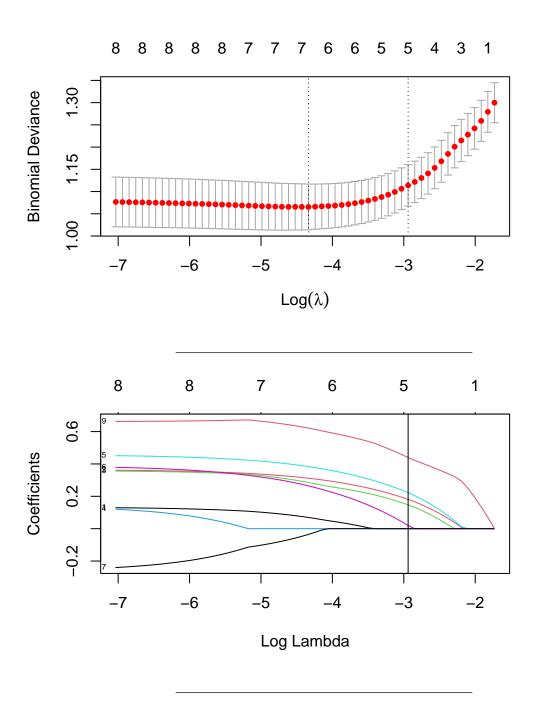
```
cbind(1:9,colnames(xss))
```

```
[,1] [,2]
[1,] "1"
          "sbp"
[2,] "2"
          "tobacco"
[3,] "3"
          "ldl"
[4,] "4"
          "adiposity"
[5,] "5"
          "famhistPresent"
[6,] "6"
          "typea"
[7,]
          "obesity"
     "7"
[8,] "8"
          "alcohol"
[9,] "9"
          "age"
```

lassofit=glmnet(x=xss,y=ys,alpha=1,standardize=FALSE,family="binomial") # already standard



- [1] "The lamda giving the smallest CV error 0.0131013369814589"
- [1] "The 1sd err method lambda 0.052890323504839"



10 x 3 sparse Matrix of class "dgCMatrix"

lasso ridge logistic

(Intercept) -0.70977228 -0.72240989 -0.878545196

sbp . 0.10687796 0.133308398

tobacco 0.18103811 0.23373137 0.364577926

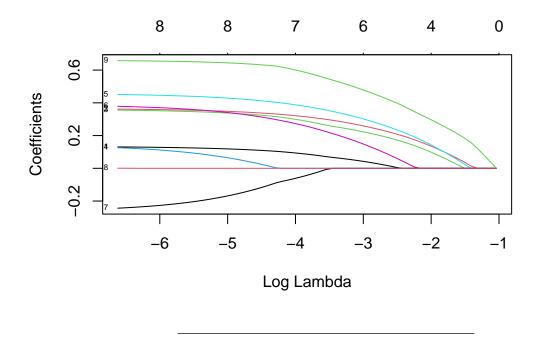
```
1d10.147268860.200369070.360180594adiposity.0.114941800.144616485famhistPresent0.222463850.251043760.456537713typea0.019547650.147349960.388725509obesity.-0.04764114-0.265082072alcohol.0.018681680.002978424age0.439901210.306068490.660695163
```

## 4.7 Elastic net logistic regression

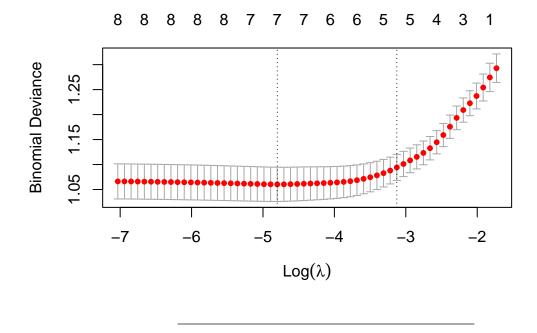
```
cbind(1:9,colnames(xss))
```

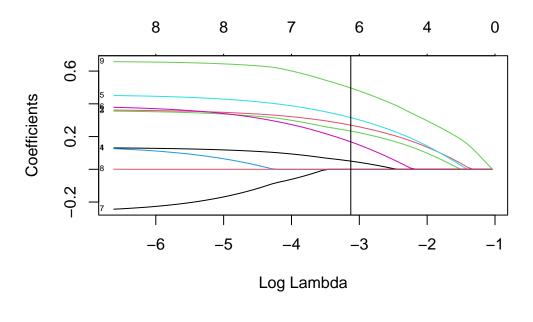
```
[,1] [,2]
[1,] "1" "sbp"
[2,] "2"
          "tobacco"
          "ld1"
[3,] "3"
         "adiposity"
[4,] "4"
[5,] "5"
          "famhistPresent"
[6,] "6"
          "typea"
[7,] "7"
          "obesity"
          "alcohol"
[8,] "8"
[9,] "9"
          "age"
```

 $\verb|elfit=glmnet(x=xss,y=ys,alpha=0.5,standardize=FALSE,family="binomial")| # already standardize=FALSE,family="binomial"| # already standardize=FALSE,family="binomia$ 



- [1] "The lamda giving the smallest CV error 0.00822802145212431"
- [1] "The 1sd err method lambda 0.0439104757579008"





10 x 4 sparse Matrix of class "dgCMatrix"

	elactic	lasso	ridge	logistic
(Intercept)	-0.76020589	-0.70977228	-0.72240989	-0.878545196
sbp	0.04999361		0.10687796	0.133308398
tobacco	0.26971690	0.18103811	0.23373137	0.364577926
ldl	0.23343256	0.14726886	0.20036907	0.360180594
adiposity		•	0.11494180	0.144616485
${\tt famhistPresent}$	0.31585816	0.22246385	0.25104376	0.456537713
typea	0.16769839	0.01954765	0.14734996	0.388725509
obesity		•	-0.04764114	-0.265082072
alcohol		•	0.01868168	0.002978424
age	0.49670298	0.43990121	0.30606849	0.660695163

## 5 Computational details for the glmnet

## (HTW 3.7)

glmnet is the implementation in R of the elastic net from HTW-book, and the package is maintained by Trevor Hastie.

The package fits generalized linear models using penalized maximum likelihood of elastic net type (lasso and ridge are special cases).

The logistic lasso is fitted using a quadratic approximation for the negative log-likelihood in a "proximal-Newton iterative approach".

#### 5.1 Software links

- R glmnet on CRAN with resources.
  - Getting started
  - GLM with glmnet

For Python there are different options.

- Python glmnet is recommended by Hastie et al.
- scikit-learn (seems to mostly be for regression? is there lasso for classification here?)

## 5.2 glmnet inputs

```
glmnet(x, y,
  family = c("gaussian", "binomial", "poisson", "multinomial","cox", "mgaussian"),
  weights = NULL, offset = NULL, alpha = 1, nlambda = 100,
  lambda.min.ratio = ifelse(nobs < nvars, 0.01, 1e-04),
  lambda = NULL, standardize = TRUE, intercept = TRUE,
  thresh = 1e-07, dfmax = nvars + 1,
  pmax = min(dfmax * 2 + 20, nvars),
  exclude = NULL, penalty.factor = rep(1, nvars),
  lower.limits = -Inf, upper.limits = Inf, maxit = 1e+05,
  type.gaussian = ifelse(nvars < 500, "covariance", "naive"),
  type.logistic = c("Newton", "modified.Newton"),
  standardize.response = FALSE,
  type.multinomial = c("ungrouped", "grouped"),
  relax = FALSE, trace.it = 0, ...)</pre>
```

## 5.3 cv.glmnet inputs

```
cv.glmnet(x, y, weights = NULL, offset = NULL, lambda = NULL,
  type.measure = c("default", "mse", "deviance", "class", "auc", "mae", "C"),
  nfolds = 10, foldid = NULL,
  alignment = c("lambda", "fraction"), grouped = TRUE,
  keep = FALSE, parallel = FALSE,
  gamma = c(0, 0.25, 0.5, 0.75, 1), relax = FALSE, trace.it = 0, ...)
```

type.measure defaults to deviance (according to help(cv.glmnet)). The last is for Cox models.

## **5.3.1 Family**

we have only covered gaussian (the default) and binomial.

Each family has implemented the deviance measure. Poisson regression and Cox proportional hazard (survival analysis) is also implemented in glmnet.

#### 5.3.2 Penalties

The elastic net is implemented, with three possible adjustment parameters.

$$\mathrm{minimize}_{\beta_0,\beta}\{-\frac{1}{N}l(y;\beta_0,\beta) + \lambda \sum_{i=1}^p \gamma_j((1-\alpha)\beta_j^2 + \alpha|\beta_j|)\}$$

- λ: the penalty, default a grid of 100 values is chosen, to cover the lasso path on the log scale.
- $\alpha$ : elastic net parameter  $\in [0,1]$ . This is usually manually selected by a grid search over 3-5 values. Default is  $\alpha = 1$  (lasso), and with  $\alpha = 0$  we get ridge.
- $\gamma_j$ : penalty modifier for each covariate to be able to always include ( $\gamma_j == 0$ ), or exclude ( $\gamma_j = \text{Inf}$ ), or give individual penalty modifications. Default  $\lambda_j = 1$ .

For the  $\lambda$  penalty the maximal value is for

- linear regression:  $\lambda_{\max} = \max_j |\hat{\beta}_{LS,j}|$  (standardized coefficients) or, should there also be a factor 1/N?
- logistic regression:  $\lambda_{\max} = \max_{j} |x_{j}^{T}(y-\bar{p})|$  where  $\bar{p}$  is the mean case rate.

#### 5.3.3 Additional modifications

- Coefficient bounds can be set (possible since coordinate descent is used)
- Some coefficients can be excluded from the penalization (than thus forced in).
- Offset can be added (popular if rate models for Poisson is used)
- For binary and multinomial data factors or matrices can be input.
- Sparse matrices with covariates can be supplied.

#### 5.4 Lasso variants

Elastic net is already in glmnet (alpha-parameter).

Other lasso variants have their own R packages:

- The group lasso https://cran.r-project.org/web/packages/grplasso/grplasso.pdf
- The fused lasso https://cran.r-project.org/web/packages/genlasso/genlasso.pdf
- The sparse group lasso https://arxiv.org/pdf/2208.02942 and https://cran.r-project.org/web/packages/sparsegl/vignettes/sparsegl.html
- Bayesian lasso blasso function for normal data in package monomvn https://rdrr.io/cran/monomvn/man/monomvn-package.html
- Elastic net for ordinal data: https://cran.r-project.org/web/packages/ordinalNet/ordinalNet.pdf

## 6 Preparing for inference for the lasso and ridge

#### 6.1 Confidence interval

#### Set-up

- We have a random sample  $Y_1, Y_2, \dots, Y_N$  from
- some distribution F with some (unknown) parameter  $\theta$ .
- Let  $y_1, y_2, \dots, y_N$  be the observed values for the random sample.

#### **Statistics**

- We have two statistics  $\hat{\theta}_L(Y_1,Y_2,\dots,Y_N)$  and  $\hat{\theta}_U(Y_1,Y_2,\dots,Y_N)$  so that

$$P(\hat{\theta}_L(Y_1,Y_2,\dots,Y_N) \leq \theta \leq \hat{\theta}_U(Y_1,Y_2,\dots,Y_N)) = 1 - \alpha$$

where  $\alpha \in [0, 1]$ 

## Confidence interval

The numerical interval

$$[\hat{\theta}_L(y_1,y_2,\dots,y_N),\hat{\theta}_U(y_1,y_2,\dots,y_N)]$$

is called a  $(1-\alpha)$  100% confidence interval.

- 6.2 Bootstrap confidence intervals
- 6.3 Percentile interval
- 6.4 Bias corrected accelerated interval

## 6.5 Single hypothesis test

$$H_0: \beta_j = 0$$
 vs.  $H_1: \beta_j \neq 0$ 

	Not reject $H_0$	Reject $H_0$
$\overline{H_0}$ true	Correct	Type I error
$H_0$ false	Type II error	Correct

- Two types of errors are possible, type I error and type II error.
- A type I error would be to reject  $H_0$  when  $H_0$  is true, that is concluding that there is a linear association between the response and the predictor where there is no such association. This is called a *false positive finding*.

• A type II error would be to fail to reject  $H_0$  when the alternative hypothesis  $H_1$  is true, that is not detecting that there is a linear association between the response and the covariate. This is called a *false negative finding*.

## **6.6** *p*-value

- A p-value p(X) is a test statistic satisfying  $0 \le p(Y) \le 1$  for every vector of observations Y.
- Small values give evidence that  $H_1$  is true.
- In single hypothesis testing, if the p-value is less than the chosen significance level (chosen upper limit for the probability of committing a type I error), then we reject the null hypothesis,  $H_0$ .
- The chosen significance level is often referred to as  $\alpha$ .

A p-value is valid if

$$P(p(Y) \le \alpha) \le \alpha$$

for all  $\alpha$ ,  $0 \le \alpha \le 1$ , whenever  $H_0$  is true, that is, if the *p*-value is valid, rejection on the basis of the *p*-value ensures that the probability of type I error does not exceed  $\alpha$ .

An exact p-value satisfies

$$P(p(Y) \le \alpha) = \alpha$$

for all  $\alpha$ ,  $0 \le \alpha \le 1$ .

- The exact p-value is uniformly distributed when the null hypothesis is true.
- This is a fact that is often misunderstood by users of p-values.
- The incorrect urban myth is that p-values from true null hypotheses are close to one, when the correct fact is that all values in intervals of the same length are equally probable (which is a property of the uniform distribution).

## 6.7 From single to multiple hypotheses

In many situations we are not interested in testing only one hypothesis, but instead m hypotheses.

	Not reject $H_0$	Reject $H_0$	Total
$H_0$ true	U	V	$m_0$
$H_0$ false	T	S	$m-m_0$
Total	m-R	R	m

- Out of the m hypotheses tested, the (unknown) number of true null hypotheses is  $m_0$ .
- V: the number of type I errors (false positive findings) and
- T: the number of type II errors (false negative findings).
- U: the number of true null hypotheses that are not rejected and
- S: the number of false null hypotheses that are rejected.
- R: the number of hypoteses rejected for a specific cut-off

Observe: only m and R is observed!

## 6.8 Familywise error rate

The familywise error rate (FWER) is defined as the probability of one or more false positive findings

$$FWER = P(V > 0)$$

The number of false positive findings V is not known in a real life situation, but still we may find a cut-off on the p-value, called  $\alpha_{loc}$ , that gives an upper limit to (controls) the FWER.

- Raw p-value,  $p_j$ , the lowest nominal level to reject the null hypothesis.
- Adjusted p-value,  $\tilde{p}_j$ , is the nominal level of the multiple (simultaneous) test procedure at which  $H_{0j}, j=1,\ldots,m$  is just rejected, given the values of all test statistics involved.

The adjusted p-values can be defined as

$$\tilde{p}_j = \inf\{\alpha \mid H_{0j} \text{ is rejected at FWER level } \alpha\}$$

In a multiple testing problem where all adjusted p-value below  $\alpha$  are rejected, the overall type I error rate (for example FWER) will be controlled at level  $\alpha$ .

## 6.9 The Bonferroni method controls the FWER

Single-step methods controls for multiple testing by estimating one local significance level,  $\alpha_{loc}$ , which is used as a cut-off to detect significance for each individual test.

The Bonferroni method is valid for all types of dependence structures between the test statistics.

The local significance level is

$$\alpha_{\mathrm loc} = \frac{\alpha}{m}$$

The adjusted p-value is

$$\tilde{p}_j = \min(1, mp_j)$$

## 7 Exercises

This week the best way to spend the time is to work on the Data Analysis Project 1.

But, also good to study the R-code for the South African heart disease example, and make some changes.

Smart: save this file as an .Rmd file and then run purl(file.Rmd) to produce a file with only the R-commands. (At the html-version you choose Code-Download Rmd on the top of the file).

• Change the CV criterion to auc and to class. Are there changes to what is the best choice for  $\lambda$ ?

## 8 References

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

Wieringen, Wessel N. van. 2021. "Lecture Notes on Ridge Regression." https://arxiv.org/pdf/1509.09169v7.pdf.